



Welcome to the 62nd ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Baltimore Convention Center. Corporate Member hospitality suites are located in the Hilton Hotel.

**SPONSORS**

ASMS gratefully acknowledges the support of these companies.



**CONFERENCE SPONSORS**



**CONTRIBUTORS**

- Fluid Management Systems
- IDEX Health & Science
- New Objective, Inc
- Prosolia, Inc
- Silicon Kinetics
- Tandem Labs
- Thermo Scientific
- Zef Scientific

**TABLE OF CONTENTS**

**GENERAL INFORMATION**..... 2  
**HOTELS AND TRANSPORTATION** ..... 5  
**ASMS BOARD OF DIRECTORS** ..... 6  
**INTEREST GROUPS AND COMMITTEES** ..... 7  
**AWARDS**..... 8  
**CONVENTION CENTER FLOOR PLANS** ..... 10  
**POSTER / EXHIBIT HALL FLOOR PLAN** .....11  
**CORPORATE HOSPITALITY SUITES** ..... 12  
**ASMS CORPORATE MEMBERS** ..... 13  
**PROGRAM ACKNOWLEDGEMENTS** ..... 17  
**PROGRAM OVERVIEW** ..... 18  
**WORKSHOPS** ..... 23

*Titles in the following sections are provided by authors. The complete abstracts are available online: [www.asms.org](http://www.asms.org)*

*The PDF document of proceedings submissions for orals and posters may be viewed online one day after presentation at the conference.*

**SUNDAY** ..... 28  
**MONDAY ORAL SESSIONS** ..... 28  
**TUESDAY ORAL SESSIONS**..... 34  
**WEDNESDAY ORAL SESSIONS**..... 41  
**THURSDAY ORAL SESSIONS** ..... 47  
**MONDAY POSTERS** ..... 54  
**TUESDAY POSTERS**..... 88  
**WEDNESDAY POSTERS**..... 122  
**THURSDAY POSTERS** ..... 156  
**INDEX OF AUTHORS** ..... 190

## GENERAL INFORMATION

**REGISTRATION** is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm on Monday through Thursday.

### SUNDAY TUTORIAL SESSION, 5:00 - 6:30 PM

Exhibit Hall AB, level 1



**5:00 - 5:45 pm**  
**Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know but Were Afraid to Ask**

**Lucinda Cohen**  
Merck Research Laboratories



**5:45 - 6:30 pm**  
**Imaging Mass Spectrometry**

**Ron M.A. Heeren**  
FOM-AMOLF

### SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM

Exhibit Hall AB, level 1



**Welcome, Jenny Brodbelt,**  
University of Texas, Austin  
ASMS Vice President for Programs



**The James Webb Space Telescope: From First Light to the Search for Earth 2.0**

**Jason Kalirai**  
Telescope Science Institute

### SUNDAY WELCOME RECEPTION, 7:45 - 9:00 PM

Exhibit Hall C-G. Conference name badge is required.

## PLENARY SESSIONS

### MONDAY, 4:45 - 5:30 PM

#### AWARD LECTURE

Exhibit Hall AB, level 1



**Award for a Distinguished Contribution in Mass Spectrometry**

**Richard M. Caprioli**  
Vanderbilt University

### TUESDAY, 4:45 - 5:30 PM

#### AWARD LECTURE

Exhibit Hall AB, level 1



**Biemann Medal**

**Lingjun Li**  
University of Wisconsin-Madison

### THURSDAY, 4:45 - 5:30 PM

#### PLENARY LECTURE

Exhibit Hall AB, level 1



**How the Genome Folds**

**Erez Lieberman Aiden**  
Baylor College of Medicine and  
Rice University

#### DON'T MISS

##### • ASMS MEETING, WEDNESDAY, 4:45 - 5:30 PM

Ballroom I, level 4

Enjoy a beverage while you applaud awards, hear about new initiatives, and more!

##### • CLOSING EVENT, THURSDAY, 6:30 - 9:00 PM

National Aquarium

*Let's celebrate!* Enjoy all the aquarium has to offer including an Imax film and a dolphin event. Complete your tour with music provided by a talented group of your colleagues. Ticket is required, \$30.



**ORAL SESSIONS** are 8:30 - 10:30 am and 2:30 - 4:30 pm on Monday through Thursday.

Session A (MOA, TOA, WOA, ThOA) ..... Exhibit Hall AB, level 1  
 Session B (MOB, TOB, WOB, ThOB).... Room 307-308, level 3  
 Session C (MOC, TOC, WOC, ThOC)... Room 309-310, level 3  
 Session D (MOD, TOD, WOD, ThOD)... Room 314-317, level 3  
 Session E (MOE, TOE, WOE, ThOE)..... Ballroom I, level 4  
 Session F (MOF, TOF, WOF, ThOF)..... Ballroom II, level 4  
 Session G (MOG, TOG, WOG, ThOG)..... Ballroom III, level 4  
 Session H (MOH, TOH, WOH, ThOH)..... Ballroom IV, level 4

**ORAL PRESENTATIONS** are projected from ASMS computers running Microsoft Office 2010. Speakers are required to use the ASMS computers for their presentations.

**SPEAKERS** must load presentations at least one day prior to their talks. The speaker room is 330 (behind conference registration area) and is open with a technician according to this schedule:

**Sunday:** 10:00 am - 8:00 pm  
**Monday through Wednesday:** 7:30 am - 5:00 pm

**POSTERS AND EXHIBIT BOOTHS** are in Exhibit Hall C-G. The Hall is open:

Sunday Reception ..... 7:45 pm - 9:00 pm  
 Monday - Wednesday ..... 7:30 am - 8:00 pm  
 Thursday ..... 7:30 am - 3:00 pm

**POSTER SET-UP** is 7:30 am on the day scheduled and removal is 7:30 - 8:00 pm on the same day. Posters should not be removed early. Thursday posters must be removed by 3:30 pm.

**Refer to the poster numbers in this final program for board assignments.** Presenters should supply pushpins or Velcro to mount their posters.

**POSTER SESSIONS** are 10:30 am - 2:30 pm, Monday through Thursday. Special "themed refreshments" will be offered 1:30 - 2:30 pm daily.

**POSTER AUTHORS** must be present at posters on scheduled days at these times.

10:30 am - 1:00 pm ..... Odd-numbered posters  
 12:00 - 2:30 pm ..... Even-numbered posters

Presenters who must leave a poster unattended should post a return time. Presenters should wear "Poster Presenter" badges which are available at the poster supply counter.

Posters should not be removed before 7:30 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed at 2:30 pm.

**LUNCH CONCESSIONS** in the Poster/Exhibit Hall offer a variety of options to dine and network while taking a break from posters. Concessions are open 11:00 am - 2:00 pm, Monday through Thursday.

**EXHIBITORS** must staff exhibit booths as follows:

Sunday Reception ..... 7:45 pm - 9:00 pm  
 Monday - Thursday ..... 10:30 am - 2:30 pm

**WORKSHOPS** are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided in the pre-function area on level 3.

**DINNER BREAK, 7:00 - 8:00 PM** is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

### **SPECIAL PROGRAM FOR UNDERGRADUATE STUDENTS**

- **Poster competition**, 7:45 - 9:00 pm, Poster/Exhibit Hall
- **Breakfast Tutorial** "Make the Most of ASMS: What to See, Hear and Do!" 7:00 - 8:15 am, Monday, Room 319 (beverages and pastries provided)
- **Meet the Experts** at lunch tables reserved for undergraduate students, 12:00 - 1:00 pm, Monday, Poster/Exhibit Hall

**FREE WiFi Access** is provided in the Poster/Exhibit Hall. Computers are provided at stations throughout the convention center.

**CONFERENCE PROCEEDINGS** will be published online. Visit [www.asms.org](http://www.asms.org) after July 21 to view or download the Proceedings. Submission to the Proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker web casting slides will be printed to PDF and used for speakers who fail to submit.**

**WEB CASTING** includes tutorial lectures, plenary lectures, and oral sessions. Web casting will be available to conference attendees for three months after the conference. ASMS does not retain rights to material included in web castings. To access the presentations, go to [www.asms.org](http://www.asms.org), select "web casting" on the annual conference page, and enter your last name and the User ID printed on your conference name badge.

**CORPORATE HOSPITALITY SUITES** may be open 8:00 - 11 pm, Monday through Wednesday. Suites are located in the **Hilton Hotel**.

**CAREER CENTER** is located in the Poster/Exhibit Hall. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview booths must be reserved one day in advance.

Sunday ..... 7:45 - 9:00 pm  
 Monday - Wednesday ..... 7:30 am - 5:00 pm  
 Thursday ..... 7:30 am - 2:30 pm

**GUEST REGISTRATION** (\$10) includes designated name badge and entrance to the Sunday evening reception. The badge does not gain entrance to oral sessions or the Poster/Exhibit Hall.

**CONCIERGE DESK** in the conference registration area offers information on transportation, attractions and restaurants.

## GENERAL INFORMATION

**CORPORATE BREAKFAST SEMINARS** are hosted by some Corporate Members. Breakfast seminars are located in the convention center and start at 6:45 am on scheduled day. **Please reserve a seat at company exhibit booths.**

<b>MONDAY</b>	
<b>Company</b>	<b>Convention Center Location</b>
AB SCIEX	Room 343-344
AB SCIEX	Room 345-346
AB SCIEX	Room 347-348
Advanced Chemistry Development (ACD)	Room 328
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
EMD Millipore	Room 336
LECO	Room 327
Shimadzu	Room 337
<b>TUESDAY</b>	
<b>Company</b>	<b>Convention Center Location</b>
AB SCIEX	Room 343-344
AB SCIEX	Room 345-346
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
LECO	Room 327
New Objective	Room 328
Phenomenex	Room 329
Prosolia	Room 336
Shimadzu	Room 337
<b>WEDNESDAY</b>	
<b>Company</b>	<b>Convention Center Location</b>
AB SCIEX	Room 343-344
Agilent Technologies	Room 339-340
Bruker Daltonics	Room 338
LECO	Room 327
Phenomenex	Room 329
Protea Biosciences	Room 328
Shimadzu	Room 337
Tecan	Room 336
<b>THURSDAY</b>	
<b>Company</b>	<b>Convention Center Location</b>
Shimadzu	Room 337
Thermo Scientific	Room 339-340

### **MEDIA EVENTS**

Corporate media sessions are scheduled on Monday and Tuesday for members of the press and financial institutions.

<b>Company</b>	<b>Monday</b>	<b>Hilton Hotel Location</b>
Bruker Daltonics	8:00-9:00 am	Key Ballroom 6
Shimadzu	9:30-10:30 am	Holiday Ballroom 6
AB SCIEX	11:00 -12:00 pm	Key Ballroom 7
Agilent Technologies	1:30-2:30 pm	Key Ballroom 5
Thermo Scientific	3:00-4:00 pm	Holiday Ballroom 1-3
Waters Corporation	4:30-5:30 pm	Key Ballroom 8
<b>Company</b>	<b>Tuesday</b>	<b>Location</b>
PerkinElmer	9:30-10:30 am	Holiday Ballroom 4-5

### **CONFERENCE REGULATIONS**

- Name badge is required for all conference sessions, including the Poster/Exhibit Hall and the employment center.
- No smoking is permitted in the convention center.
- Cell phones must be turned off in oral sessions.
- No photography or recording is allowed in oral sessions or in the Poster/Exhibit Hall.
- Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without the express written authority of the author of the material presented. Such materials that are published in print or online must contain appropriate credits for all quotations and photographs.
- The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements. No signs on easels are permitted.
- Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.
- No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).
- Corporate or institutional logos on slides or posters may appear only one time in the presentation.

# HOTELS AND TRANSPORTATION



## CONFERENCE HOTELS

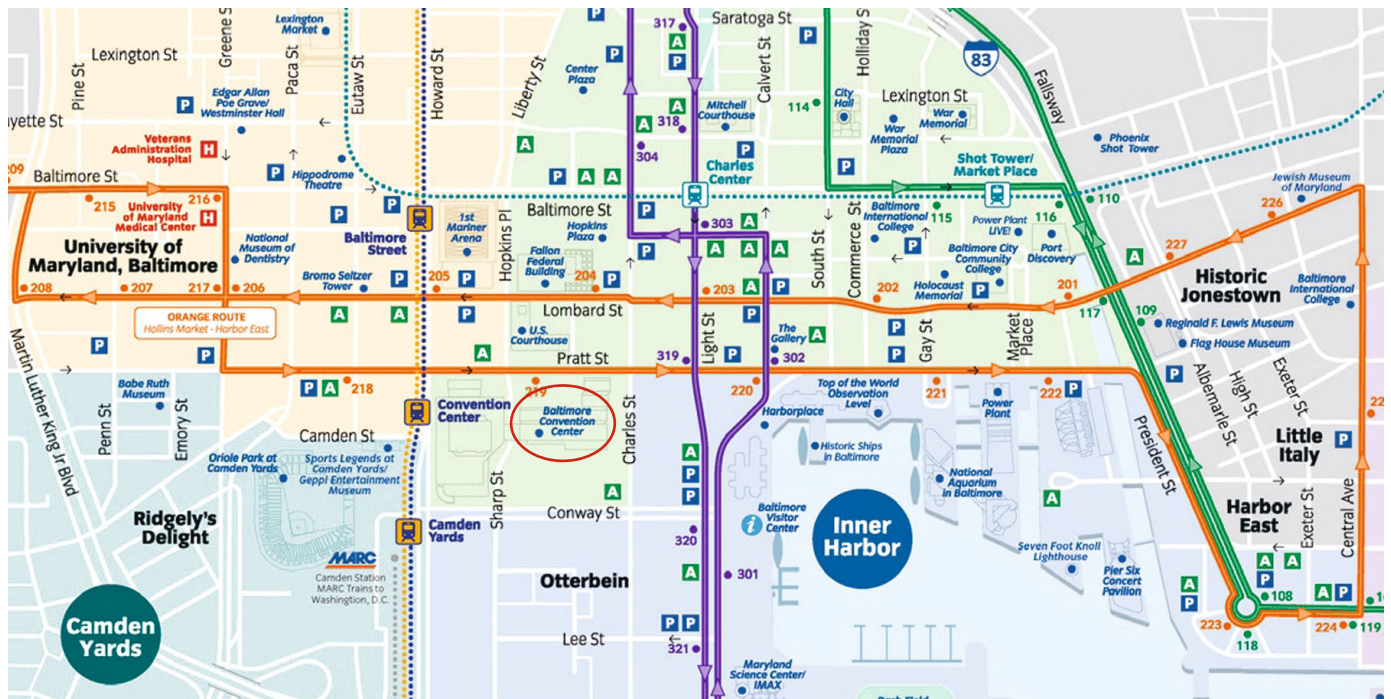
Hotel	Map No.	Telephone
Days Inn Inner Harbor	1	410-576-1000
Hampton Inn	2	410-685-5000
Hilton Baltimore	3	443-573-8700
Holiday Inn Inner Harbor	4	410 685-3500
Hyatt Regency	5	410 528 1234
Lord Baltimore	6	443 977-4092
Marriott Inner Harbor	7	410-962-0202
Monaco Baltimore	8	443-692-6170
Renaissance	9	410-547-1200
Sheraton City Center	10	410-752-1100
Sheraton Inner Harbor	11	410-962-8300

## HOTEL MAP



## TRANSPORTATION

Travel free throughout the heart of downtown Baltimore on the Charm City Circulator. The orange line connects many attractions and hotels to the Baltimore Convention Center. Image below shows bus stops.





*President*  
**Susan T. Weintraub**  
 University of Texas Health Science Center  
 San Antonio, TX



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 Purdue University  
 West Lafayette, IN



*Vice President for Programs*  
**Jenny Brodbelt**  
 University of Texas  
 Austin, TX



*Vice President for Arrangements*  
**Gary Valaskovic**  
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**Neil L. Kelleher**  
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**Rebecca A. Jockusch**  
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 East Lansing, MI



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 North Carolina State University  
 Raleigh, NC



*Member at Large for Digital Communications*  
**Michael J. MacCoss**  
 University of Washington  
 Seattle, WA

**Congratulations**

to these members who were elected to the ASMS Board

*Vice President for Programs*



**Vicki H. Wysocki**  
 Ohio State University  
 Columbus, OH

*Treasurer*



**Patrick R. Griffin**  
 The Scripps Research Institute  
 Jupiter, FL

*Member at Large for Education*



**Igor A. Kaltashov**  
 University of Massachusetts  
 Amherst, MA

*Member at Large for Digital Communications*



**Brian Searle**  
 Proteome Software, Inc.  
 Portland, OR

**Staff**

Judith A. Sjoberg, *Executive Director*  
 Jennifer Watson  
 Cindi Lilly, Miquela Sena  
 Marin Walker, Brent Watson

## ASMS INTEREST GROUPS AND COMMITTEES

### INTEREST GROUP COORDINATORS

<i>Analytical Laboratory Managers</i>	Brett Phinney
<i>Bioinformatics for MS</i>	Lucas Kall David Tabb
<i>Biotherapeutics</i>	Li Tao Arindam Roy
<i>Clinical Chemistry</i>	Cory Bystrom Brett Holmquist
<i>Data Independent Acquisition</i>	Yishai Levin
<i>DNA/RNA</i>	Norman Chiu Michael McGinley
<i>Drug Metabolism &amp; Pharmacokinetics</i>	Don McKenzie Mustafa Varoglu
<i>Energy, Petroleum &amp; Biofuels</i>	Patrick Hatcher Lateefah Stanford
<i>Environmental Applications</i>	Kerry Peru Chris Gill
<i>Flavor, Fragrance and Foodstuff</i>	Marc Engel Timothy Croley
<i>Forensics &amp; Homeland Security</i>	Glen Jackson Guido Verbeck
<i>FTMS</i>	Nathan Kaiser Franklin Leach
<i>Fundamentals</i>	George Khairallah Jos Oomens
<i>H/D Exchange, Covalent Labeling &amp; Cross Linking</i>	David Schriemer Joshua Sharp
<i>Imaging MS</i>	Liam McDonnell Zoltan Takats
<i>Ion Mobility MS</i>	Matthew Bush Erin Baker
<i>Ion Trap MS</i>	Daniel E. Austin Yu Xia
<i>Lipids &amp; Lipodomics</i>	Stephen Blanksby
<i>LC/MS Related Topics</i>	Amanda Berg Helene Cardasis
<i>Metabolomics</i>	Gary Patti Sunia Trauger
<i>Metal Ion Coordination Chemistry</i>	Benjamin Bythell Mike Van Stipdonk
<i>Peptide Fragmentation</i>	Sharon Pitteri
<i>Pharmaceuticals</i>	Brian Furmanski Shawna Hengel
<i>Photoionization MS</i>	Jack Syage Ralf Zimmerman
<i>Polymeric Materials</i>	William Erb Gyorgy Vas
<i>Quantitative Intact Proteomics</i>	Edward Dratz

<i>Regulated Bioanalysis</i>	Fabio Garofolo
<i>Undergraduate Research in MS</i>	J.C. Poutsma Elaine Marzluff
<i>Young Mass Spectrometrists</i>	Olga Friese Dian Su

### COMMITTEES

<i>Asilomar Conference (ACMS)</i>	Ryan Julian, Chair Glen Jackson Sharon Pitteri Scott McLuckey
<i>Corporate Liaison</i>	Gary Valaskovic, Chair Scott McLuckey Karen Anspach, Phenomenex Carla Marshall-Waggett, New Objective Bez Moghadam, Thermo Scientific Lance Nicolaysen, Waters Qihui Ni, EMD Millipore Johnny Cardenas, AB SCIEX
<i>Digital Communications</i>	Michael MacCoss, Chair Bin Ma Nathan Yates
<i>Education</i>	Gavin Reid, Chair Erin Carlson Michael Fitzgerald Elaine Marzluff Darrin Smith
<i>Nominating</i>	Barbara Larsen, Chair Hilkka Kenttamaa Joseph Loo Christine Miller Nathan Yates
<i>Publications</i>	David Muddiman, Chair Michelle Cilia Jessica Prenni Brandon Ruotolo Yu Xia Michael Gross ( <i>ex officio</i> )
<i>Sanibel Conference</i>	Jon Williams, Chair Neil Kelleher Erin Baker J.C. Poutsma

### ARCHIVIST

Michael Grayson

**AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY****2014 RECIPIENT: RICHARD M. CAPRIOLI****Award Lecture: 4:45 pm, Monday, Exhibit Hall AB, level 1**

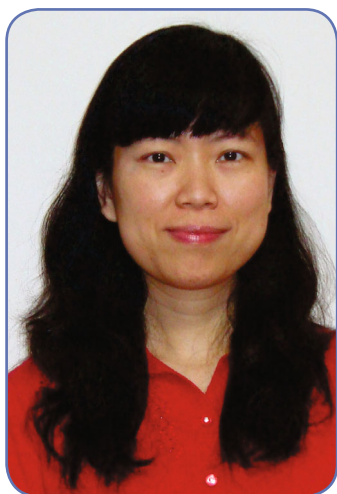
**Dr. Richard M. Caprioli** is awarded the 2014 ASMS Award for a Distinguished Contribution in Mass Spectrometry for the development of MALDI Imaging Mass Spectrometry and its application to molecular mapping of tissues in biology and medicine.

Professor Caprioli's work led to a new paradigm for molecular imaging of tissues, founded on the development of matrix assisted laser desorption ionization (MALDI) imaging mass spectrometry. This is now a burgeoning application of mass spectrometry whereby molecular measurements can be made directly from tissues, adding significantly to the information that can be obtained from these specimens.

This work has made significant contributions to the study of proteins, lipids, metabolites, and pharmaceutical compounds. Since publication of Professor Caprioli's seminal 1997 paper (Anal. Chem. 69(23), 4751-4760) showing the power of MALDI imaging mass spectrometry for tissue analysis, he has pioneered advancements in sample preparation, instrumentation, and informatics approaches that have considerably advanced the technology and made it accessible to hundreds of laboratories worldwide.

The impact of his work is evident in the numerous commercial platforms that employ this technology. Approximately 2,500 papers have been published to date on the subject of MALDI imaging mass spectrometry.

Dr. Caprioli is the Stanford Moore Chair in Biochemistry and Director of the Mass Spectrometry Research Center at Vanderbilt University. Scientist in the Biological Sciences Division and Director of Proteomics Research at Pacific Northwest National Laboratory (PNNL).

**BIEMANN MEDAL****2014 RECIPIENT: LINGJUN LI****Award Lecture: 4:45 pm, Tuesday, Exhibit Hall AB, level 1**

**Dr. Lingjun Li** is awarded the 2014 Biemann Medal for the number and depth of her contributions in the field of mass spectrometric study of neuropeptides and functional peptidomics.

Professor Lingjun Li's research program is focused on the development of novel and improved mass spectrometry (MS)-based tools in conjunction with microseparation techniques to study challenging neuroscience problems including functional discovery of neuropeptides and biomarker discovery in neurodegenerative diseases.

Dr. Li and her team have created several multi-faceted and integrated MS-based platforms that include high resolution *in-situ* peptide mapping, tissue imaging, *in vivo* microdialysis, high sensitivity micro-separation techniques coupled with tandem MS *de novo* sequencing, and new isotopic and isobaric labeling strategies, and improved bioinformatics tools to allow large-scale discovery and functional analysis of novel neuropeptides. More recently, the Li group also employed novel use of ion mobility MS to address several remaining technical challenges associated with peptidomic research. They developed a novel site-specific strategy to rapidly and precisely localize peptide epimers and new strategies to probe peptide sequence scrambling and peptide misidentification, and to improve isobaric tandem mass tag quantitation in QTOF based instrumentation.

Using these integrated platforms and multifaceted approaches, Professor Li and her group discovered more than 300 novel neuropeptides in crustacean model organisms whose genomic sequences are currently unavailable. These findings significantly expanded our knowledge about neuropeptides in these important model organisms and transformed current understanding of neuropeptide family organization and functional consequences of neuropeptide multiplicity.

Dr. Li is Professor of Pharmaceutical Sciences and Chemistry at the University of Wisconsin-Madison.





The Research Awards are fully funded by Thermo Scientific and Waters Corporation in the amount of \$35,000 each. Awards will be presented at the Biemann Medal Award Lecture, 4:45 pm, Tuesday, Exhibit Hall AB, level 1

Sponsored by  
THERMO SCIENTIFIC



**Kerry Pratt**  
University of Michigan

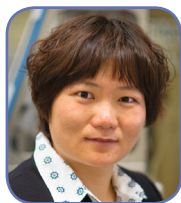
Sponsored by  
WATERS CORPORATION



**Zhibo Yang**  
University of Oklahoma

2014 POST-DOCTORAL AWARDS

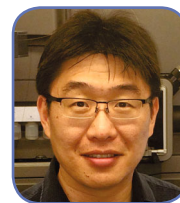
ASMS inaugurates the Post-Doctoral Awards in 2014. Three awards in the amount of \$10,000 each will be awarded annually. The purpose of the award is to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities envisioned for this award include, but are not limited to, conference and workshop attendance, travel to other mass spectrometry laboratories, purchase of books and/or software. The awards are open to ASMS members who are postdoctoral fellows within three years of completing a Ph.D. or equivalent degree. Applicants must be currently appointed as a postdoctoral fellow in North America (e.g., in academia, industry, a government or national laboratory or at a research institute). Details and an application are posted to [asms.org](http://asms.org).



**Huilin Li**  
University of California, Los Angeles



**Boone Prentice**  
Vanderbilt University



**Hao Zhang**  
Washington University at St Louis

RON A. HITES AWARD FOR OUTSTANDING RESEARCH PUBLICATION IN JASMS



The Ron Hites Award recognizes an outstanding presentation of original research. Selection is based on a paper's innovative aspects, technical quality, likely stimulation of future research, likely impact on future applications, and quality of presentation. The award is named in honor of Professor Ron Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS. The corresponding author receives a cash award of \$2,000 and all authors are acknowledged with certificates of commendation.

The 2014 award recognizes **Evan Williams** and co-authors Harry J. Sterling; Alexander F. Kintzer; Geoffrey K. Feld; Catherine A. Cassou; Bryan A. Krantz; for their paper **Supercharging Protein Complexes from Aqueous Solution Disrupts their Native Conformations**; *JASMS* 2012, vol. 23, pages 191 – 200.

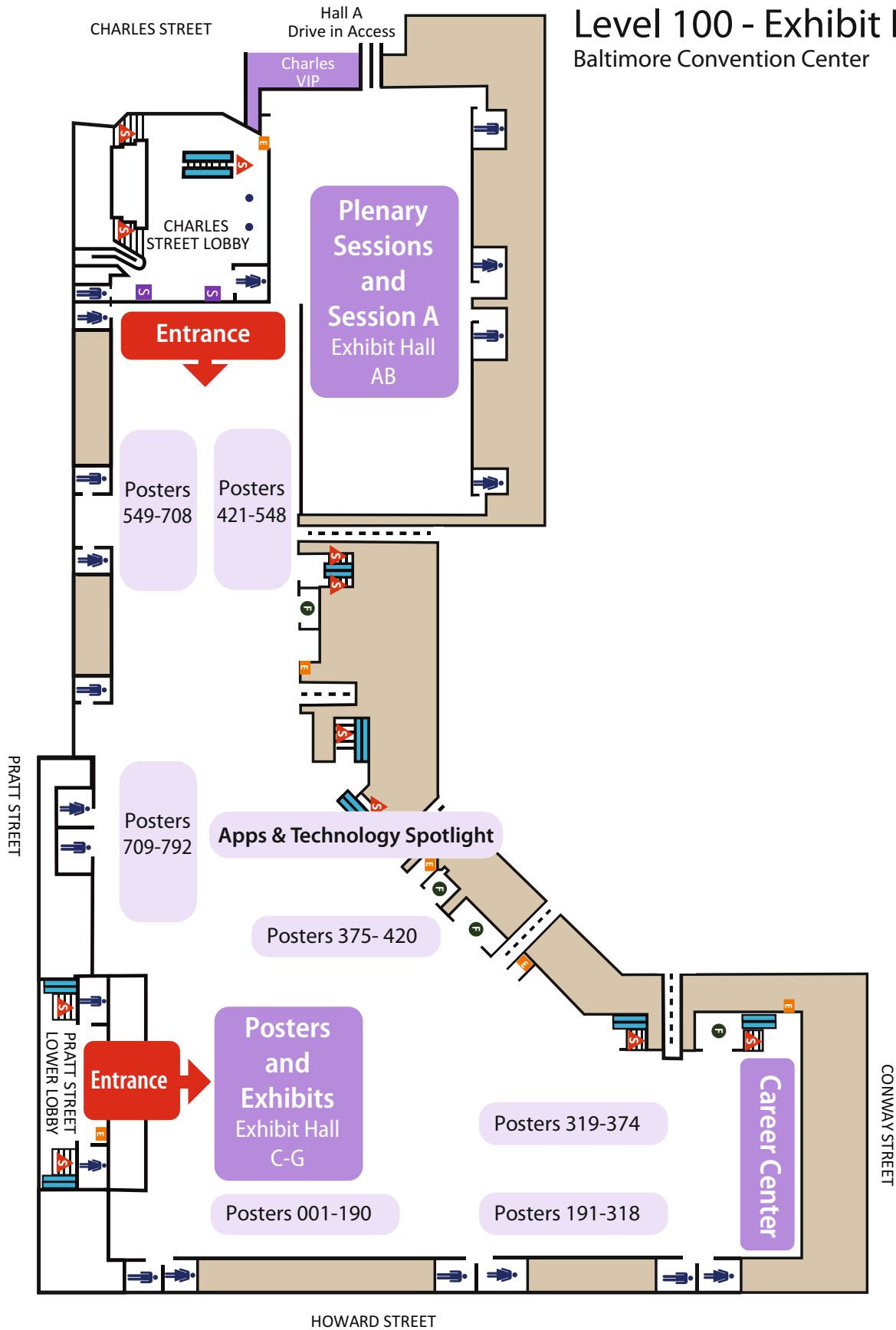


Left to right: Alexander F. Kintzer, Geoffrey K. Feld, Brian A. Krantz, Evan R. Williams, Catherine A. Cassou, and Harry J. Sterling



# Level 100 - Exhibit Halls

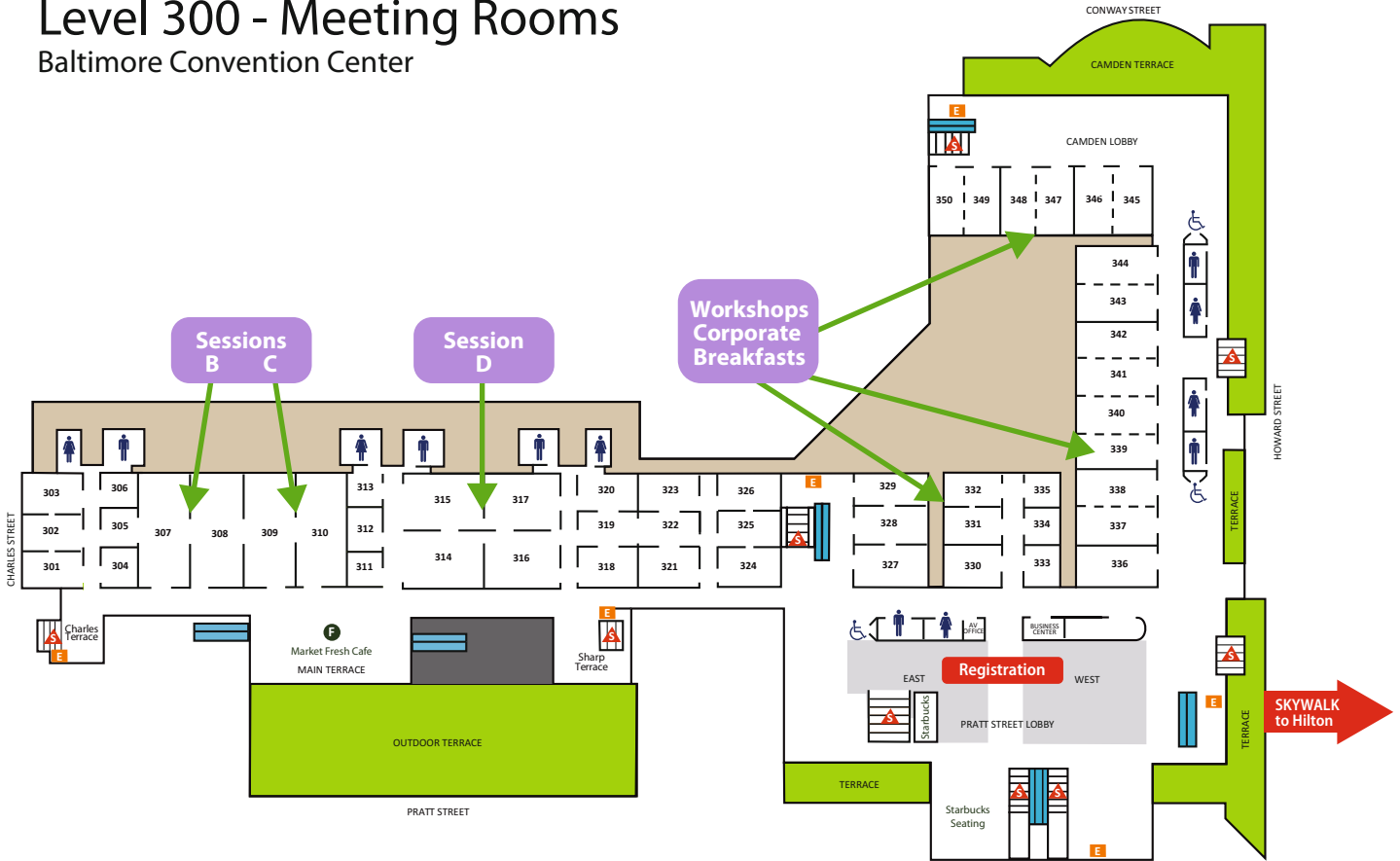
Baltimore Convention Center





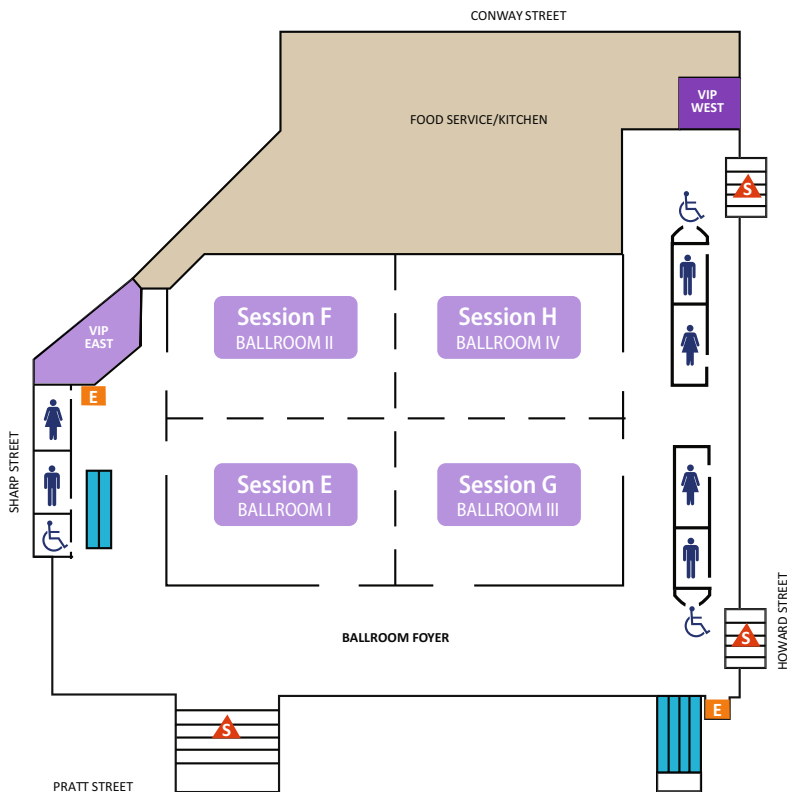
# Level 300 - Meeting Rooms

Baltimore Convention Center



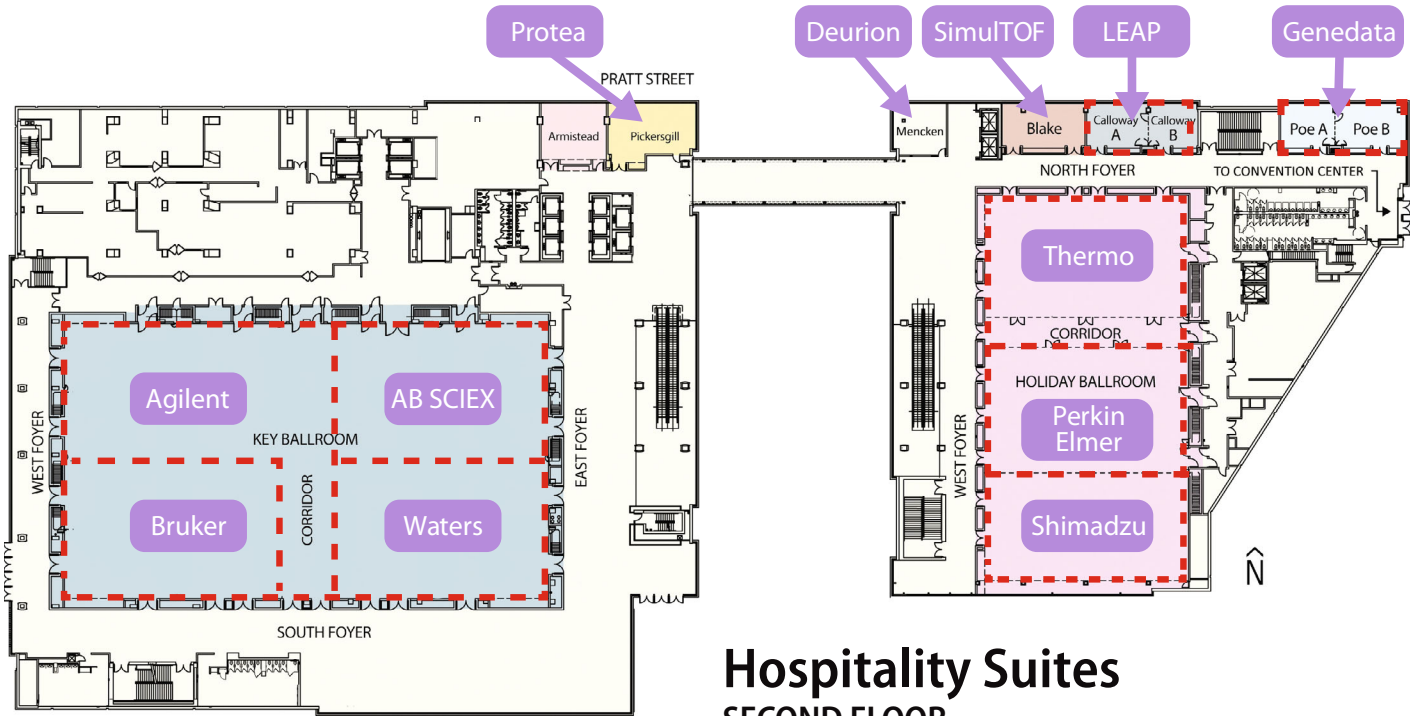
# Level 400 - Ballroom

Baltimore Convention Center





# HOSPITALITY SUITES IN HILTON HOTEL



## Hospitality Suites SECOND FLOOR Hilton Hotel



## ASMS CORPORATE MEMBERS



Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
AB SCIEX .....	160 .....		Key 7 .....	Rm 343/344, Mon-Wed; Rm 345/346 Mon-Tues; Rm 347/348 Mon
Advanced Chemistry Development (ACD/Labs) .....	36 .....	Poster .....		Room 328, Mon
Advion .....	176 .....			
Agilent Technologies .....	84 .....	Poster .....	Key 5 .....	Room 339/340, Mon-Wed
AIM Research Company .....	2 .....			
Alliance Pharma, Inc. ....	171 .....			
Analytical Chemistry .....		Library		
Analytical Sales & Services .....	87 .....	Poster		
Anasys Instruments .....	12 .....			
Antec .....	180 .....	Poster		
Apricot Designs, Inc. ....	76 .....			
Avanti Polar Lipids, Inc. ....	174 .....			
Bertin Technologies .....	17 .....			
BIOCRATES Life Sciences .....	143 .....			
Bioinformatics Solutions Inc. ....	42 .....	Poster		
Bioreclamation/VT .....	77 .....			
Biotage .....	33 .....			
Biotech Support Group .....	58 .....			
Bonna-Agela Technologies Ltd. ....	149 .....			
Bruker Daltonics .....	49 .....		Key 6 .....	Room 338, Mon-Wed
C&EN .....	155 .....			
CAMAG Scientific, Inc. ....	109 .....			
Cambridge Isotope Labs .....	62 .....			
Canadian Life Science .....	141 .....	Poster		
Cell Signaling Technology .....	15 .....			
Cerilliant .....		Poster		
Cerno Bioscience .....	63 .....			
Chemyx, Inc. ....	137 .....			
CovalX .....	28 .....			
CSS Analytical Co., Inc. ....	34 .....			
CTC Analytics .....	93 .....			
Denator AB .....	20 .....			
Detector Technology, Inc. ....	72 .....			
Deurion .....		Poster .....	Mencken	
Digital Proteomics .....		Poster		
Drummond Scientific .....	179 .....			
Edwards .....	164 .....			
EMCO High Voltage Corporation .....	133 .....			
EMD Millipore .....	40 .....	Poster .....		Room 336, Mon
ES Industries .....	75 .....	Poster		
ESI Source Solutions .....		Poster		
ETP Electron Multipliers .....	124 .....			
Exelis .....	55 .....	Poster		



## ASMS CORPORATE MEMBERS

Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
Extrel CMS .....	99 .....	Poster		
F.DGSI .....	102			
FLIR Systems, Inc. ....	73 .....	Poster		
Fluid Management Systems .....	165 .....	Poster		
Frontage Laboratories, Inc. ....	26			
Genedata .....	57 .....		Poe	
Genetic Engineering & Biotechnology News .....		Library		
Genovis .....	126 .....	Poster		
GenTech Scientific Inc. ....	48 .....			
GERSTEL, Inc. ....	71 .....	Poster		
GL Sciences .....	111 .....			
Glygen Corp. ....	106 .....	Poster		
Golden West Biologicals .....	154 .....			
Hamamatsu Corporation .....	39 .....	Poster		
Hamilton Robotics .....	7			
Harvard Apparatus .....	122			
HiTek Power .....	50			
Horizon Technology, Inc. ....	123			
HTX Technologies, LLC .....	136 .....	Poster		
Hudson Surface Technology .....	53 .....	Poster		
iChrom Solutions .....	103			
IDEX Health & Science .....	56 .....	Poster		
Imtakt USA .....	150			
Institute for Systems Biology .....	5			
INTAVIS, Inc. ....	91			
Integrated Analysis, Inc. ....	30 .....	Poster		
Integrated Proteomics Applications .....	25			
International Equipment Trading Ltd .....	115			
International Labmate .....		Library		
ionBench .....	140			
IONICS Mass Spectrometry .....	151			
IonSense, Inc. ....	120 .....	Poster		
IROA Technologies .....		Poster		
IsoSciences, LLC .....	145			
JEOL USA, Inc. ....	107			
JPT Peptide Technologies .....	97			
LEAP Technologies .....	14 .....	Poster	Calloway	
LECO Corporation .....	92 .....	Poster		Room 327, Mon-Wed
LNI Schmidlin .....	105			
M&M Mass Spec Consulting .....	128			
Mac-Mod Analytical .....	96			
MassTech, Inc. ....	29			
Matrix Science .....	22			
McKinley Scientific .....	89			
MestreLab Research .....	132			

## ASMS CORPORATE MEMBERS



Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
Metabolon, Inc.	156	Poster		
Microliter Analytical Supplies	16			
Microsaic Systems PLC	74	Poster		
Moeller Medical GmbH	59			
Molecular & Cellular Proteomics		Library		
Morpho Detection Inc.	44	Poster		
MS Bioworks	79			
MS Noise	35			
MS Vision	138			
MSParts Inc.	90			
mSPEC Group	95			
nanoLiter, LLC	135	Poster		
Nest Group, The		Poster		
New England Peptide	82			
New Objective, Inc.	88	Poster		Room 328, Tues
NIST	125			
Norgren, Inc.	130	Poster		
Oerlikon Leybold Vacuum	104			
OI Analytical	166			
Omni Enclosures	38			
Omni International	8	Poster		
Optimize Technologies	54	Poster		
Owlstone, Inc.	117			
Parker Hannifin	70	Poster		
PEAK Scientific	119	Poster		
Perfinity Biosciences, Inc.	159	Poster		
PerkinElmer, Inc.	112	Poster	Holiday 4 & 5	
Pfeiffer Vacuum	43	Poster		
Phenomenex, Inc.	116			Room 329, Tues-Wed
Phoenix S & T, Inc.	51			
PHOTONIS USA	170	Poster		
Physical Electronics				
Physikron		Poster		
Phytronix Technologies, Inc.	161			
PREMIER Biosoft	45			
Pressure BioSciences	66	Poster		
Promega Corp.	80			
Prosolia, Inc.	139	Poster		Room 336, Tues
Protea Biosciences, Inc.	46		Pickersgill	Room 328, Wed
Protein Metrics Inc.	100			
Proteome Software	78			
Proton Onsite	175			
Prozyme, Inc.	27			
PTM Biolabs, Inc.	69			
Qatar Foundation	3			



## ASMS CORPORATE MEMBERS

Company	Booth	Poster or Tabletop	Hilton Hotel Hospitality Suite	Breakfast Seminar
Research Scientific Services .....	52			
Restek Corporation.....	98			
RMI Laboratories LLC .....	41			
SAES Getters SpA.....	68			
Sage Science .....	67			
Sage-N Research, Inc. ....	83			
Samin Science Co., Ltd.....	61			
Science/AAAS .....		Library		
Scientific Instrument Services .....	1	Poster		
Scientific Systems, Inc.....	60			
Shimadzu.....	85	Poster	Holiday 6 .....	Room 337, Mon-Thur
Shrader Software Solutions.....	144			
Sierra Analytics.....	131			
Sigma-Aldrich .....	134	Poster		
Silantes GmbH .....	23			
Silicon Kinetics .....	142			
Spark Holland .....	114	Poster		
SpectralWorks Ltd. ....	31	Poster		
Spectroscopy Magazine .....	110			
Spellman High Voltage .....	47			
Springer Science + Business Media.....	4			
SunChrom GmbH.....	64			
Tandem Labs .....	129			
Tecan .....	118	Poster		Room 336, Wed
the Analytical Scientist.....		Library		
Thermo Scientific.....	127		Holiday 1-3 .....	Room 339/340, Thurs
Tofwerk / Mabritec .....	177			
Tomtec.....	24			
Tosoh Bioscience.....	21			
Trajan Scientific and Medical.....	121	Poster		
Trianja Technologies.....	19			
TSI Inc. ....	94			
United Sciences Corp.....	101			
Vaccubrand.....	9			
Veritomyx.....	32	Poster		
VICI Valco Instruments .....	108			
Virgin Instruments Corp / SimulTOF Systems.....	6		Blake	
Virscidian, Inc. ....	81	Poster		
Voltage Multipliers Inc.....	146			
VRS .....	86			
Vulcan Analytical .....	65			
Waters Corporation .....	113	Poster	Key 8	
Zef Scientific.....	37			
Zhejiang Haochuang Biotech .....	18			



## PROGRAM ACKNOWLEDGEMENTS



**Jenny Brodbelt**  
University of Texas, Austin  
*Vice President for Programs*

### STUDENT ASSISTANTS

Graduate students assist with many aspects of the conference, including registration, oral and poster sessions, and the Career Center. The students each receive a stipend to help with their conference travel expenses.

### PROGRAM COMMITTEE

---

Julia Aponte	Chris Crittenden	Carol Nilsson
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Michael Cammarata	Dustin Klein	Scott Robotham
Joe Cannon	Carolyn Mazzitelli	Michelle Robinson
Victoria Cotham		Junmei Zhang

### SESSION CHAIRS

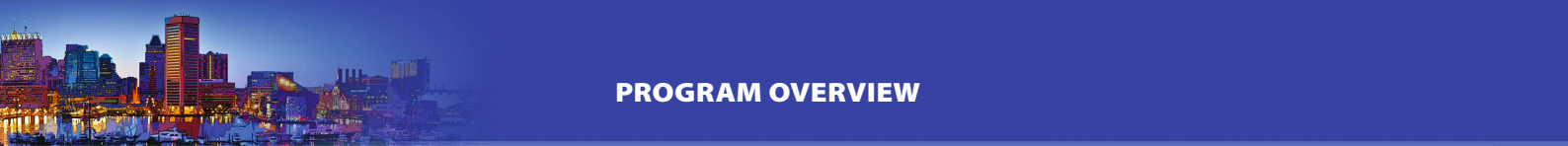
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Steve Blanksby	Maria Lorna A. De Leoz	Amanda Hummon	Kasper Rand
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Graham Cooks	Ying Ge	Jos Oomens	Nathan Yates
Matt Crowe	Chris Gill	Richard Perry	Renato Zenobi

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William Erb	Elaine Marzluff	Joshua Sharp	Nathan Yates
Olga Friese	Liam McDonnell	Don Smith	Ralf Zimmerman






# PROGRAM OVERVIEW

## SATURDAY

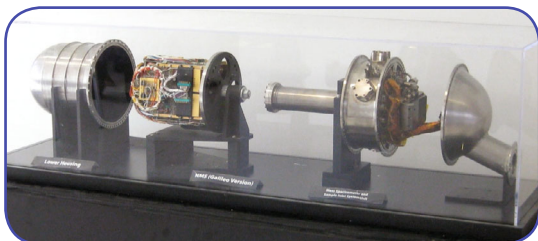
9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
2:00 - 5:00 PM	<b>REGISTRATION</b>

## SUNDAY

9:00 AM - 4:30 PM	<b>SHORT COURSES</b>
10:00 AM - 8:00 PM	<b>REGISTRATION</b>
5:00 - 6:30 PM	<p><b>TUTORIAL LECTURES</b>, Exhibit Hall AB, level 1</p> <div style="display: flex; align-items: flex-start;"> <div style="flex: 1;">  </div> <div style="flex: 2;"> <p><b>5:00 - 5:45 pm</b>  <b>Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know But Were Afraid to Ask</b></p> <p><b>Lucinda Cohen</b>  Merck Research Laboratories</p> </div> </div> <div style="display: flex; align-items: flex-start; margin-top: 10px;"> <div style="flex: 1;">  </div> <div style="flex: 2;"> <p><b>5:45 - 6:30 pm</b>  <b>Imaging Mass Spectrometry</b></p> <p><b>Ron M.A. Heeren</b>  FOM-AMOLF</p> </div> </div>
6:45 - 7:45 PM	<p><b>CONFERENCE OPENING</b>, Exhibit Hall AB, level 1  <b>Jenny Brodbelt</b>, <i>ASMS Vice President for Programs</i></p> <div style="display: flex; align-items: flex-start;"> <div style="flex: 1;">  </div> <div style="flex: 2;"> <p><b>7:00 - 7:45 pm</b></p> <p><b>The James Webb Space Telescope: From First Light to the Search for Earth 2.0</b></p> <p><b>Jason Kalirai</b>  Telescope Science Institute</p> </div> </div>
7:45 - 9:00 PM	<b>RECEPTION IN THE POSTER-EXHIBIT HALL</b>

### SPACEFLIGHT MASS SPECTROMETRY 1963 – 2018

A small exhibit featuring models of spaceflight mass spectrometers employed in the exploration of the Solar System over the past several decades is displayed in the Pratt Lobby. Mass spectrometers have contributed substantially to our understanding of planetary science and astrobiology, and their continued use has a bright future with new technologies under development. Displayed models



include engineering units, flight spares, and demonstration reproductions from robotic planetary missions to Venus, Jupiter, Saturn, Titan, and Mars. Experts will be on hand to answer questions about instrument design, mission science achievements, and future direction associated with these one-of-a-kind instruments.

The display has been coordinated by William B. Brinckerhoff, NASA GSFC, Greenbelt MD.



# PROGRAM OVERVIEW



## MONDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• MOA am: Emerging Environmental Contaminants, Exhibit Hall AB, level 1</li> <li>• MOB am: Instrumentation: New Developments in High Resolution and Mass Accuracy to Celebrate Alan Marshall's 70th Birthday, Room 307-308, level 3</li> <li>• MOC am: Nucleic Acids, Room 309-310, level 3</li> <li>• MOD am: Fundamentals: Reactions, Dynamics and Theory of Gas Phase Ions, Room 314-317, level 3</li> <li>• MOE am: Antibodies and Antibody-Drug Conjugates, Ballroom I, level 4</li> <li>• MOF am: H/D Exchange: New Developments in Technology, Ballroom II, level 4</li> <li>• MOG am: Informatics: Protein Identification, Ballroom III, level 4</li> <li>• MOH am: PTMs: Advances in Isolation, Enrichment, Derivatization and Separation, Ballroom IV, level 4</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<p><b>POSTER SESSION AND EXHIBITS</b>, Poster/Exhibit Hall, level 1</p> <p>Monday posters</p> <p>12:00 – 1:00 pm: <b>Undergraduate students</b> – look for reserved tables to <i>Meet the Experts</i></p>
<b>2:30 - 4:30 PM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• MOA pm: Polymer- and Packaging-Related Contaminants and Degradants in Consumer Products, Exhibit Hall AB, level 1</li> <li>• MOB pm: Instrumentation: Mini/Portable/Fieldable Mass Spectrometry, Room 307-308, level 3</li> <li>• MOC pm: Ion Mobility: Structures to Celebrate Mike Bowers' 75th Birthday, Room 309-310, level 3</li> <li>• MOD pm: Photoionization, Room 314-317, level 3</li> <li>• MOE pm: Characterization of Biologics and Biosimilars, Ballroom I, level 4</li> <li>• MOF pm: Quantitative Analysis in Drug Discovery and Development, Ballroom II, level 4</li> <li>• MOG pm: Informatics: Protein Quantification, Ballroom III, level 4</li> <li>• MOH pm: Imaging: Biomedical Applications, Ballroom IV, level 4</li> </ul>
<b>4:45 - 5:30 PM</b>	<p><b>AWARD LECTURE</b>, Exhibit Hall AB, level 1</p> <div style="display: flex; align-items: center;">  <div> <p><b>Award for a Distinguished Contribution in Mass Spectrometry</b></p> <p><b>Richard M. Caprioli</b> Vanderbilt University</p> </div> </div>
<b>5:45 - 7:00 PM</b>	<p><b>WORKSHOPS</b> All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> <li>1. Real World Applications of Photoionization; Room 307-308</li> <li>2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group); Room 309-310</li> <li>3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Room 314-317</li> <li>4. How to Succeed in Pharma without Really Trying; Room 327</li> <li>5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group); Room 336</li> <li>6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum &amp; Biofuels Interest Group); Room 337</li> <li>7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); Room 338</li> <li>8. ProteomicsDB; Room 339-340</li> <li>9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Room 341-342</li> <li>10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry (organized by Lipids and Lipidomics Interest Group); Room 343-344</li> <li>11. A State of the Union for Biomarker Translation (organized by Clinical Chemistry Interest Group); Room 345-346</li> <li>12. Antibody Drug Conjugates as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Room 347-348</li> <li>13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security (organized by Forensics and Homeland Security Interest Group); Room 349-350</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel

# PROGRAM OVERVIEW

## TUESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• TOA am: Integrated Qualitative and Quantitative LC-MS for Small Molecule Analysis, Exhibit Hall AB, level 1</li> <li>• TOB am: Instrumentation and Methods: FT, Ion Traps and Hybrid Instruments, Room 307-308, level 3</li> <li>• TOC am: Ion Mobility: Separations, Room 309-310, level 3</li> <li>• TOD am: Macromolecular Complexes: Activation and Dissociation, Room 314-317, level 3</li> <li>• TOE am: PK/PD Analysis of Biologics, Ballroom I, level 4</li> <li>• TOF am: H/D Exchange: Biological Applications, Ballroom II, level 4</li> <li>• TOG am: Phosphoproteomics in Disease, Ballroom III, level 4</li> <li>• TOH am: Imaging: Pharmaceuticals and Metabolomics, Ballroom IV, level 4</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<p><b>POSTER SESSION AND EXHIBITS</b>, Poster/Exhibit Hall</p> <p>Tuesday posters</p>
<b>2:30 - 4:30 PM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• TOA pm: Space Science, Astrobiology, and Atmospheric Chemistry, Exhibit Hall AB, level 1</li> <li>• TOB pm: Nano-Scale and Microfluidic Separations and Mass Spectrometry, Room 307-308, level 3</li> <li>• TOC pm: Protein-Protein and Protein-Ligand Interactions, Room 309-310, level 3</li> <li>• TOD pm: Fundamentals of Peptide Fragmentation, Room 314-317, level 3</li> <li>• TOE pm: Top-Down Protein Analysis, Ballroom I, level 4</li> <li>• TOF pm: Drug Target Discovery and Validation, Ballroom II, level 4</li> <li>• TOG pm: Clinical Diagnostics, Ballroom III, level 4</li> <li>• TOH pm: Imaging: Fundamentals, Instrumentation, and Method Development, Ballroom IV, level 4</li> </ul>
<b>4:45 - 5:30 PM</b>	<p><b>AWARD LECTURE</b>, Exhibit Hall A/B (lower level)</p> <div style="display: flex; align-items: center;">  <div> <p><b>Biemann Medal</b></p> <p><b>Lingjun Li</b> University of Wisconsin-Madison</p> </div> </div>
<b>5:45 - 7:00 PM</b>	<p><b>WORKSHOPS</b> All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> <li>1. H/D Exchange, Covalent Labeling and Crosslinking (organized by H/D Exchange, Covalent Labeling &amp; Cross Linking Interest Group); Room 307-308</li> <li>2. LC-MS System Performance Tracking in LC-MS Tracking in LC-MS (organized by LC/MS &amp; Related Topics Interest Group); Room 309-310</li> <li>3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis (organized by Regulated Bioanalysis Interest Group); Room 314-317</li> <li>4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment (organized by Analytical Lab Managers Interest Group); Room 336</li> <li>5. FTMS: ICR and Orbitrap (organized by FTMS Interest Group); Room 337</li> <li>6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry (organized by Environmental Applications Interest Group); Room 338</li> <li>7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess (organized by Fundamentals Interest Group); Room 339-340</li> <li>8. The NIH Review Process and Mock NIH Study Section; Room 341-342</li> <li>9. Imaging Mass Spectrometry vs. Histology (organized by Imaging MS Interest Group); Room 343-344</li> <li>10. Metabolomics: Emerging Technologies for Continued Innovation (organized by Metabolomics Interest Group); Room 345-346</li> <li>11. 50 Years of the British Mass Spectrometry Society: Past, Present &amp; Future; Room 347-348</li> <li>12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud; Room 349-350</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel

# PROGRAM OVERVIEW



## WEDNESDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• WOA am: Energy, Petroleum, and Biofuels: Advances in Sample Preparation and MS Interface Design, Exhibit Hall AB, level 1</li> <li>• WOB am: Ambient and Atmospheric Pressure Ionization: Fundamentals, Room 307-308, level 3</li> <li>• WOC am: The Triple Quadrupole: 35 Years of Evolution and Application to Celebrate Chris Enke's 80th Birthday, Room 309-310, level 3</li> <li>• WOD am: Quantitative Proteomics in Systems Biology/Cellular Pathway Analysis, Room 314-317, level 3</li> <li>• WOE am: Peptidomics, Ballroom I, level 4</li> <li>• WOF am: Pharmacoproteomics and Toxicoproteomics for Drug Development, Ballroom II, level 4</li> <li>• WOG am: PTMs: Comprehensive Analysis, Ballroom III, level 4</li> <li>• WOH am: Lipids and Profiling, Ballroom IV, level 4</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<p><b>POSTER SESSION AND EXHIBITS</b>, Poster/Exhibit Hall</p> <p>Wednesday posters</p>
<b>2:30 - 4:30 PM</b>	<p><b>ORAL SESSIONS</b></p> <ul style="list-style-type: none"> <li>• WOA pm: Energy, Petroleum, and Biofuels: Advances in MS Design and Informatics, Exhibit Hall AB, level 1</li> <li>• WOB pm: Ambient Ionization: Instrumentation and Applications, Room 307-308, level 3</li> <li>• WOC pm: Ecological and Human Health Environmental Chemistry and Toxicology, Room 309-310, level 3</li> <li>• WOD pm: Fundamentals: New Ion Activation Methods, Room 314-317, level 3</li> <li>• WOE pm: Plant "omics", Ballroom I, level 4</li> <li>• WOF pm: Proteomics: Infectious Diseases, Ballroom II, level 4</li> <li>• WOG pm: Targeted Quantification of Proteins and Post-translational Modifications, Ballroom III, level 4</li> <li>• WOH pm: Membrane Proteins, Ballroom IV, level 4</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>ASMS MEETING</b> , Ballroom I, level 4 Awards, board reports, wine, beer, soft drinks - and more!
<b>5:45 - 7:00 PM</b>	<p><b>WORKSHOPS</b> All workshops are located on level 3. There are light refreshments on level 3.</p> <ol style="list-style-type: none"> <li>1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Room 307-308</li> <li>2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Room 309-310</li> <li>3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Room 314-317</li> <li>4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Room 336</li> <li>5. Have Quadrupole Ion Traps Passed their Prime Time? (organized by Ion Trap Interest Group); Room 337</li> <li>6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Room 338</li> <li>7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Room 339-340</li> <li>8. Using Mass Spectrometry to Characterize the Exposome and Its Impact on Human Health; Room 341-342</li> <li>9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message; Room 343-344</li> <li>10. Quantitative Glycomics; Room 345-346</li> <li>11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS; Nalini Sadagopan, Room 347-348</li> <li>12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS (organized by Flavor Fragrance and Foodstuff Interest Group); Room 349-350</li> <li>13. Mass Spectrometry Applications in Art, Cultural Heritage, and Natural History, Room 327</li> </ol>
<b>7:00 - 8:00 PM</b>	<b>DINNER BREAK</b>
<b>AFTER 8:00 PM</b>	<b>CORPORATE HOSPITALITY SUITES</b> , Hilton Hotel

## PROGRAM OVERVIEW

### THURSDAY

<b>7:30 AM - 5:00 PM</b>	<b>REGISTRATION</b>
<b>8:30 - 10:30 AM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA am: Forensic Applications, Exhibit Hall AB, level 1</li> <li>• ThOB am: Instrumentation: New Developments in Ionization and Sampling, Room 307-308, level 3</li> <li>• ThOC am: FAIMS and DMS: New Developments and Applications, Room 309-310, level 3</li> <li>• ThOD am: Radical Ion Chemistry, Room 314-317, level 3</li> <li>• ThOE am: Biomarkers in Drug Discovery, Development and Diagnosis, Ballroom I, level 4</li> <li>• ThOF am: Covalent Labeling, Chemical Probes, and Crosslinking for Biomolecule Structural Characterization, Ballroom II, level 4</li> <li>• ThOG am: Informatics: Metabolomics, Ballroom III, level 4</li> <li>• ThOH am: Glycoproteins and Glycans: New MS Approaches, Ballroom IV, level 4</li> </ul>
<b>10:30 AM - 2:30 PM</b>	<b>POSTER SESSION AND EXHIBITS</b> , Poster/Exhibit Hall Thursday posters
<b>2:30 - 4:30 PM</b>	<b>ORAL SESSIONS</b> <ul style="list-style-type: none"> <li>• ThOA pm: Food Chemistry and Safety, Exhibit Hall AB, level 1</li> <li>• ThOB pm: Instrumentation: Time-of-Flight Mass Spectrometry, Room 307-308, level 3</li> <li>• ThOC pm: Mass Spectrometry in Structural Biology, Room 309-310, level 3</li> <li>• ThOD pm: Fundamentals: Ion Spectroscopy, Room 314-317, level 3</li> <li>• ThOE pm: Data Independent Acquisition, Ballroom I, level 4</li> <li>• ThOF pm: Epigenetic Modifications and Mechanisms, Ballroom II, level 4</li> <li>• ThOG pm: Metabolomics/Lipidomics: New MS Technologies and Applications, Ballroom III, level 4</li> <li>• ThOH pm: Carbohydrates: New MS Approaches, Ballroom IV, level 4</li> </ul>
<b>4:45 - 5:30 PM</b>	<b>PLENARY LECTURE</b> , Exhibit Hall AB, level 1  <div style="display: flex; align-items: center;">  <div> <p><b>How the Genome Folds</b></p> <p><b>Erez Lieberman Aiden</b>                          Baylor College of Medicine and Rice University</p> </div> </div>
<b>6:30 - 9:00 PM</b>	<b>CLOSING EVENT, National Aquarium.</b> Ticket required

All workshops are located on level 3. There are light refreshments on level 3.

### MONDAY WORKSHOPS, 5:45 - 7:00 PM

#### 1. Real World Applications of Photoionization;

Ralf Zimmerman and Jack Syage presiding  
Room 307-308

The workshop on Photoionization last year was a success with a standing room only crowd to the end. That workshop brought the mechanism of atmospheric pressure photoionization and vacuum photoionization up to date and stimulated significant discussion. This year we would like to focus more on applications as PI is expanding in its uses ranging from APPI in LC/MS in petroleums, food safety, and environmental monitoring to ambient analysis (DAPPI, DART/APPI, etc.) to its now becoming the preferred ionization source for explosives detection airport security detection systems (MS and IMS) potentially expanding the user base by yet another few thousand. This would be a great opportunity to get discussion and feedback on these new developments from the MS community and perhaps set the stage for a PI oral session in 2015 as these new developments mature.

#### 2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group);

Karl Clauser, Karl Mechtler, Lukas Käll, David Tabb presiding  
Room 309-310

The use of database search engines for identification of posttranslational modifications (PTMs) is common practice in most proteomics labs, but these identifications have been plagued by errors from two key sources. Karl Clauser will highlight the elevation of false discovery rates that results from allowing more degrees of freedom in identification, such as allowing for "blind PTM" searches or permitting too many modifiable sites in some peptides. Karl Mechtler will emphasize localization, the challenge of associating PTMs with the appropriate residue when multiple modifiable sites may be found in a peptide. Which PTM challenge merits more attention from the bioinformatics research community?

#### 3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Matthew Bush and Erin Baker presiding

Room 314-317

Results from ion mobility mass spectrometry studies are increasingly used to answer questions in biology, including applications to metabolomics, proteomics, targeted interactions, and large molecules. This is in part attributed to the increasing performance and selection of commercial ion mobility mass spectrometry instrumentation, which has made it easier to integrate ion mobility technologies into mass spectrometry workflows. In this workshop, we will showcase research that demonstrates the advantages of ion mobility for biological applications. There will also be opportunities to discuss the challenges that arise in different types of ion mobility studies, what is possible today, and opportunities for the future.

#### 4. How to Succeed in Pharma without Really Trying;

Lucinda Cohen presiding  
Room 327

This workshop will focus on advice to young scientists considering career choices after graduation. An expert panel consisting of current and former pharmaceutical scientists will engage in dialogue with the audience around their experiences job-hunting, changing positions, networking inside and outside the company, and thriving in today's ever-changing environment. Audience participation will be an essential driver for the workshop, with shared participant experiences being welcome. This workshop will continue the theme of the Sunday Tutorial Lecture by Lucinda Cohen, "Everything You Ever Wanted to Know about Mass Spectrometry in the Pharmaceutical Industry but Were Afraid to Ask." However, the focus will be pragmatic and offer insider perspectives on life in an industrial laboratory environment. Ultimately the intent is to help young mass spectrometrists connect with pharmaceutical industry veterans.

#### 5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group);

Norman Chiu and Michael McGinley presiding  
Room 336

The workshop will cover recent advances in MS characterization of oligonucleotides with an emphasis on recent development in sample preparation as well as MS data processing. While MS instrument development will likely be covered in other sessions, there have been several developments both in sample preparation of oligonucleotides as well as data analysis of collected data. The proposed workshop will have 4 short topic "primers" from thought leaders starting discussions; two about sample processing leading to oligonucleotide analysis using MS/MS as well as two discussing data interpretation of MS/MS data for oligonucleotides. Discussion should lead to some view of the current trends in analysis of oligonucleotides by MS.

#### 6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum & Biofuels Interest Group); Patrick Hatcher and Lateefah Stanford presiding

Room 337

The molecular complexity of biofuels and petroleum has offered an analytical challenge for those interested in assessing their composition. Advances in 2 dimensional GC x GC-MS, Fourier transform MS and Ion mobility MS are allowing for an exhaustive molecular characterization of these materials, to the point that a comprehensive molecular-level characterization of these mixtures is within reach. New developments in MS instrumentation and approaches are paving the way for advanced characterization of complex mixtures like petroleum and biofuels. The workshop will invite discussion leaders at the forefront of applications of these advanced MS approaches in the energy field to enlighten interested groups to venture into the arena.

#### 7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); JC Poutsma and Elaine Marzluff presiding

Room 338

Panel discussion with current undergrads, recent graduates, and faculty members at PUI institutions. This workshop is designed for undergraduates who are attending the ASMS meeting and will focus on how best to leverage their undergraduate research into success in graduate school and industry.

#### 8. ProteomicsDB; Bernhard Kuster and Mathias Wilhelm presiding

Room 339-340

There is a growing landscape of various databases and repositories for MS and proteomics. In this workshop, we would like to present ProteomicsDB, a free, professionally developed solution to store and analyze mass spectrometry-based proteomics data. ProteomicsDB has a strong focus on functionality and secondary use of proteomics and mass spectrometry data. We would like to discuss our motivations for initiating this effort, demonstrate typical use-cases for web interface and API, describe our short and long-term plans and generally encourage the involvement from the ASMS community.

#### 9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Douglas Sheeley, Charles Edmonds,

and Salvatore Sechi presiding  
Room 341-342

A major source of financial support for US research is the federal government. Unfortunately, researchers are sometimes not aware of the resources available to them. This two session workshop, to be held on consecutive evenings at the ASMS conference, will discuss the identification of appropriate agencies and programs, writing an effective application, responding to the criticisms of reviewers, and taking full

MONDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

advantage of guidance from program administrators. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on the new investigator. References to additional resources will be provided. A "mock" NIH study section presentation will provide additional insight into the review process at that agency, and an opportunity for discussion with NIH staff. Each session will allow substantial time for questions and staff will be available for one-on-one conversations afterward on both evenings.

**10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry** (organized by Lipids and Lipidomics Interest Group); Stephen Blanksby and Christer Ejsing presiding  
Room 343-344

The 61st ASMS conference in Minneapolis played host to the first workshop on "Lipid Mass Spectrometry and Lipidomics". This workshop was attended by ~190 participants and resulted in vibrant discussion. A recurring theme was the importance of developing guidelines for the uniform reporting of mass spectrometry-based lipid and lipidome data, particularly in terms of an abbreviation code that encapsulates the exact level to which lipids can be structurally defined and/or quantified when using a particular MS or MS/MS approach. This workshop will invite opinion on systems of annotation and reporting requirements from leaders in the field that will then be opened for discussion and input from all workshop participants. An expected outcome of this workshop will be the formation of a working group to collate and consider the ideas presented and to refine this into a series of recommendations for lipid mass spectrometrists.

**11. A State of the Union for Biomarker Translation** (organized by Clinical Chemistry Interest Group); Brian Rappold and Cory Bystrom presiding  
Room 345-346

With recent announcements from CPTAC and commercial companies that are offering novel diagnostics derived from proteomics research this presents an opportunity to review the problems that have been solved and the challenges that lie ahead. In this workshop, we will invite several guest speakers to give a brief assessment of the landscape from discovery to clinical utilization/commercialization which

will be followed by a moderated discussion. The co-chairs will also be soliciting ideas for future workshop topics so bring your ideas.

**12. Antibody Drug Conjugates as Pharmaceutical Agents** (organized by Pharmaceuticals Interest Group); Brian Furmanski and Shawna Hengel presiding  
Room 347-348

Due to the success of the 2013 pharmaceutical interest group workshop we will continue with a similar format being; the overview of the topic of antibody drug conjugates as pharmaceutical agents with a short informal presentation (10 min) by an academic/industrial leader. Following the presentation the panelists will be introduced along with three key questions to start of the discussion with the general audience. The short presentation is meant to capture the field in its current state, in addition give specific examples of challenging issues in the industry for the discovery and development of antibody drug conjugates. Potential areas of discussion may include characteristics of antibodies, drug antibody ratio (DAR) in vivo/ex vivo, strategies for sample prep/isolation, choice of mass analyzers and a comparison of complimentary tools to mass spectrometry including: ELISA, Luminex, page electrophoresis, Edman sequencing and surface plasmon resonance. To identify panelists, gauge the level of interest of the ASMS community and to tailor the discussion we will send out a survey of open ended questions in April.

**13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security** (organized by Forensics and Homeland Security Interest Group); Guido Verbeck and Glen Jackson presiding  
Room 349-350

Forensic-related applications of mass spectrometry has some unique challenges for researchers wishing to pursue a career in this field. We plan to stimulate an informative discussion between roundtable participants and audience members around the following topics: Funding; publishing; collaborating; job hunting; academic challenges. Roundtable participants will include knowledgeable and experienced members of the forensic and homeland security community, including representatives of funding agencies, crime labs, academia and publishers.

## TUESDAY WORKSHOPS, 5:45 - 7:00 PM

All workshops are located on level 3. There are light refreshments on level 3.

**1. H/D Exchange, Covalent Labeling and Crosslinking** (organized by H/D Exchange, Covalent Labeling & Cross Linking Interest Group); Joshua Sharp and David Schriemer presiding  
Room 307-308

The workshop will provide a forum for discussing the latest HDX, covalent labeling and crosslinking methods for protein analysis. Presentations will provide an opportunity to discuss MS-based methods, data analysis routines and applications with the attendees. The goal of these presentations will be to stimulate discussion and convey useful experimental detail you can take back to your lab.

**2. LC-MS System Performance Tracking in LC-MS** (organized by LC/MS & Related Topics Interest Group); Helene Cardasis presiding  
Room 309-310

While this group has previously hosted an annual workshop on LC-MS troubleshooting, this year we will take a more preventative approach. The workshop this year will focus on important aspects of whole-platform performance tracking with respect to defining data quality, understanding performance drift, and facilitating/ expediting troubleshooting when issues do arise. Discussion will touch on choice of QC sample, instrument method, frequency of measurement, key metrics and their interpretation, and QC data processing. We will also review and demo some of the freeware available for this purpose. As always, audience participation in the form of both questions and heated debate are encouraged!

**3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis** (organized by Regulated Bioanalysis Interest Group); Fabio Garofolo and Keyang Xu presiding  
Room 314-317

The purpose of this workshop is to provide an informal venue for the discussion of ADCs from a Regulated Bioanalytical point of view based on recent industry consensus. Dr. Keyang Xu (Genentech) will lead the discussion together with a recognized panel of bioanalytical experts in the field. As per the ASMS workshop format there will not be formal presentations but the participants will introduce the discussion topics for maximum of 10 minutes to engage the audience and encourage all to participate in a dynamic and productive discussion.

ADCs are generally complex heterogeneous mixtures of multiple species, these novel therapeutic products present unique challenges in Regulated Bioanalysis: Heterogeneity of the reference material (e.g.: lysine side chain-based conjugation; hydrazine-based); Heterogeneity impact on assay accuracy; In-vivo dynamicity and deconjugation (mixture of DAR); LC-MS high sensitivity for unconjugated drug detection. Multiple validated methods are need for well characterizing ADCs quantitation: Total antibody; Conjugated antibody; Antibody-conjugated drug; unconjugated/deconjugated drug. Interpretation of the bioanalytical data from these multiple assays can be complex. Discussion will also focus on regulatory expectations surrounding comparability studies for ADC.



TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

**4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment** (organized by Analytical Lab Managers Interest Group); Brett S. Phinney and Chris Colangelo presiding  
Room 336

Along with a panel of invited laboratory managers, we propose to discuss several topics related to controlling and measuring variation in sample preparation and Data analysis. These topics may include

- 1) How do you control variation in sample preparation
- 2) How do you measure variation in sample preparation
- 3) How to choose an appropriate QC standard, where to buy it or make it if necessary.
- 4) How to determine the appropriate number of replicates you need?
- 5) How to determine what amount of variation is due to sample preparation or biology
- 6) How do you control for variation in data analysis.
- 7) How to document variation and present it to core clientele

The session will discuss practical real world examples and implementations to measure and control for variation in core facilities. Audience members are encouraged to share their struggles and approaches for used in their own laboratories.

**5. FTMS: ICR and Orbitrap** (organized by FTMS Interest Group); Nathan Kaiser and Don Smith presiding  
Room 337

Recent advances in high resolution FTMS have focused on electric field control (e.g. high field Orbitrap and compensated/harmonized ICR cells) and new implementations of advanced data processing (e.g. absorption mode and eFT). These, as well as other new developments in FTMS instrumentation and fundamentals will be discussed. Fundamental and practical topics, as well as current instrument limitations will be open for interactive discussion.

**6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry** (organized by Environmental Applications Interest Group); Kerry Peru and Chris Gill presiding  
Room 338

Rapid expansion of hydrocarbon extraction, production and processing from nonconventional sources such as shale gas and oil sands has led to the need of determining the industry's impact on the environment by characterizing and monitoring associated contaminants. This year's Workshop is a continuation of last year's topic which drew considerable interest. Updates on analytical methodologies used for monitoring, identification and characterization of contaminants will be discussed along with an update of the state of the industry from an environmental perspective.

**7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess** (organized by Fundamentals Interest Group); George Khairallah and Jos Oomens presiding  
Room 339-340

This year marks a milestone for several researchers in the fundamentals field including Professor John Bartmess. We plan to honor this special occasion by providing a series of invited short presentations and discussions mainly in the research areas in which John was very active. In the yearly tradition of the fundamentals group, senior graduate students and postdoctoral scholars in research groups will give the presentations.

**8. The NIH Review Process and Mock NIH Study Section;** Douglas Sheeley, Charles Edmonds, and Salvatore Sechi presiding  
Room 341-342

A major source of financial support for US research is the federal government. Unfortunately, researchers are sometimes not aware of the resources available to them. This two session workshop, to be held on consecutive evenings at the ASMS conference, will discuss the

identification of appropriate agencies and programs, writing an effective application, responding to the criticisms of reviewers, and taking full advantage of guidance from program administrators. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on the new investigator. References to additional resources will be provided. A "mock" NIH study section presentation will provide additional insight into the review process at that agency, and an opportunity for discussion with NIH staff. Each session will allow substantial time for questions and staff will be available for one-on-one conversations afterward on both evenings.

**9. Imaging Mass Spectrometry vs. Histology** (organized by Imaging MS Interest Group); Liam McDonnell and Zoltan Takats presiding  
Room 343-344

The topic for discussion will concern the question of where imaging MS can have an impact in diagnostic and prognostic pathology, and what must be done for it to become a recognized clinical method. In order to encourage open discussion we will include a series of deliberately provocative 5-minute presentations.

- i) Imaging MS can replace histology.
- ii) Histology & diagnostics – mass spectrometrists underestimate its importance.
- iii) What is the added benefit of imaging MS in diagnostics?
- iv) In-surgery, *in-situ* analysis
- v) Open discussion – where can imaging MS make a difference?
- vi) What needs to be done for imaging MS to become a recognize clinical tool?

**10. Metabolomics: Emerging Technologies for Continued Innovation** (organized by Metabolomics Interest Group); Sunia Trauger and Gary Patti, presiding  
Room 345-346

This workshop will begin with a brief discussion of the most exciting technological advances in the field of metabolomics over the past year. The moderators will highlight 2-3 noteworthy metabolomic publications that they feel are particularly impressive achievements and survey the audience for their opinions. Three-four invited scientists with expertise in the technologies highlighted will serve as panelists and answer questions posed by the moderators and attendees. The workshop will close with a discussion among the panelists on their perspectives of emerging trends and the role that these technologies are playing in future development. Advances intended to be highlighted are: (i) software for post-processing of untargeted metabolomic data, (ii) innovative experimental designs using stable isotopes, (iii) shotgun approaches with ion mobility, and (iv) metabolite identification by in silico fragmentation.

**11. 50 Years of the British Mass Spectrometry Society: Past, Present & Future;** Helen Cooper, Sarah Hart, and Jackie Moseley presiding  
Room 347-348

- Presentation by BMSS President Professor John Monaghan on the history of BMSS.
- Three short talks on breaking developments in MS research from the UK
- BMSS travel grants for members to attend ASMS and plan was to select these talks from the recipients of that funding once allocated.
- Panel Q&A session to discuss future direction of BMSS

**12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud;** Andrey Bondarenko, Michael MacCoss, Christine Wu, and Nathan Yates presiding  
Room 349-350

The sharing, public dissemination, and analysis of mass spectrometry data has become a major challenge. We would like to present a community effort to provide a free, professionally developed solution

## TUESDAY WORKSHOPS, 5:45 - 7:00 PM *continued*

to the mass spectrometry field's needs. The application provides a "Google Docs" type interface optimized for mass spectrometry data. Data can be uploaded and kept private, shared with a group of collaborators, or made entirely public. Over the last year CHORUS has gained almost 400 users and these users have placed >9,000 mass spectrometry data files into the service. We have learned a lot

from user feedback. We would like to discuss improvements made to CHORUS over the last year and what new analysis capabilities have and are being added. We want to discuss our goals and get feedback from the community on our current and long-term priorities.

## WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM

**All workshops are located on level 3. There are light refreshments on level 3.**

### 1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Yishai Levin and Will Thompson presiding Room 307

The heated debate over data-dependent (DDA) versus data-independent (DIA) acquisition strategies shows no signs of abating. This workshop will focus on defining the experimental characteristics, specifically related to data acquisition, which would make up the "perfect" strategy for 'omic analyses. Facilitators will prime the discussion with some simple use-cases for 'omics analysis, then experts and novices alike will gather to share views on the most important attributes of data acquisition in this space. The goal of the discussion will then be a critical evaluation of current approaches against that "perfect" strategy, with an eye towards features that should exist in the next generation of tools.

### 2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Don McKenzie and Mustafa Varoglu presiding Room 309-310

One of the challenges faced by mass spectrometrists is the ability to efficiently gather and process data across multiple software platforms. Many scientists consider the advantages of having multiple types of mass spectrometers to leverage the benefits that each platform provides in data collection. Considerations like ion source diversity, trap vs. ToF vs. triple technology, degree and specificity of product ion formation etc. play into the strategy of building a high quality laboratory. With this in mind, it is common to equip laboratories with instrumentation from various vendors. However, many times a preferred procedure for data collection and/or processing can be limited or unavailable depending upon which vendor based set of hardware is employed. Reasons for this disparity can range from differences in vendor specific software capabilities to data collection and/or processing limitations incurred via patent restrictions. Further, having to train staff in the utilization of the various platforms can be time consuming and tie up limited resources. This workshop will focus on the various mechanisms used across labs to overcome software limitations as well as explore the idea of open source coding for DMPK mass spectrometry data analysis.

### 3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Li Tao and Arindam Roy presiding Room 314-317

This would be a forum to discuss current technical challenges and solutions for the characterization of protein therapeutics by mass spectrometry. Development of new methodologies to improve efficiency and robustness of mass spectrometric analysis will be discussed in this forum. Background information on several topics will be provided to initiate the discussion. Example of some topics for discussion would be

- (1) Molecular variants analysis
- (2) Degradation pathway identification
- (3) Quantitative analysis of glycosylation
- (4) Improving the speed of LC/MS analysis

### 4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Olga Friese and Dian Su presiding Room 336

The workshop features a panel discussion on professional development. Topics will be focused on career planning and management, fundamental training, industrial internship, job search tools and interview strategies. The panel, consisting of representatives from government, industrial and academic organizations, will share their knowledge and practices on career prospects.

### 5. Have Quadrupole Ion Traps Passed their Prime Time? (organized by Ion Trap Interest Group); Yu Xia presiding Room 337

In this workshop we will discuss the current status and possible future advancement of quadrupole ion traps, with relevance to the development of various types of mass analyzers. The following questions will be asked: 1. As a mass analyzer, how will ion traps compete with others and what are the critical technical advancements? 2. Structural confirmation by MS/MS vs. high resolution MS, any chance at all? 3. Ion trap as a reaction/storage vessel – what new capabilities are coming out of in research and what should be transferred to commercial instrument?

### 6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Gyorgy Vas and William Erb presiding Room 338

This workshop will focus on updating the group on recent work and challenges faced in the various fields such as academic, government, and industry. The focus of this group is polymer and material analysis utilizing various mass spectrometric techniques. This workshop will explore the various ways that polymers and materials are not only analyzed themselves but also how they interact with other materials such as patients, products, etc.

### 7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Tim Griffin presiding Room 339-340

The open source Galaxy software framework is gaining momentum as a tool to solve biological MS informatics problems. It offers unique features such as flexibility to integrate disparate software programs into effective workflows, and the ability to share complete workflows with other researchers. In this workshop, expert developers and users of Galaxy for biological MS data analysis will present practical tutorials. Presentations will be aimed at informing both software developers and biologists/analytical chemists on how they can make effective use of the Galaxy framework in their research.

## WEDNESDAY WORKSHOPS, 5:45 - 7:00 PM continued

**8. Using Mass Spectrometry to Characterize the Exposome and Its Impact on Human Health;** Michael J. Van Stipdonk and H. M. Skip Kingston, Anthony Macherone presiding  
Room 341-342

Two-thirds of global mortality is due to chronic disease with cardiovascular disease and cancers as the major causes. Investigations into the underlying factors for disease through genome-wide association studies and data mining have determined that the genetic heritability for these deaths is about 10%. This suggests that majority of causative factors for chronic human disease is not genetic but rather exposure to external and internal chemical entities and of these; only about 50% have been identified. The human exposome represents the totality of these exposures over individuals' lifetime and is a quantity of critical importance needed to understand their impact on disease. This workshop will define and encourage discussions on the human exposome and strategies for its measurement using multi-omics tools within the exposomics paradigm, with an emphasis on use of the exposomic information in guiding research to identify and validate new biomarkers of exposure and disease.

**9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message;** Ikumi Kayama, MA Medical & Scientific Illustrator presiding  
Room 343-344

Clarity in visual communication is as important to scientific meetings as clarity in writing is to journal articles. Most professors and researchers use PowerPoint to create presentations, but very few have taken a course in presentation design or layout. This workshop will offer PowerPoint design tips and tricks to make your presentation better-looking, easier to understand, and more memorable.

One of the most common misuses of PowerPoint slides are as a reading card or a vehicle for information overload. Some presenters make it more difficult to share their work because of hard-to-read slides/graphs and poor visuals. A professional illustrator and scientific communication specialist will teach simple yet effective ways to improve PowerPoint presentations to help professors, researchers, and students present their work more efficiently with better results.

**10. Quantitative Glycomics;** Yehia Mechref presiding  
Room 345-346

Glycosylation of proteins and lipids is one of the most prevalent posttranslational modification with various biological attributes. The functions of many proteins are modulated by glycosylation while anomalous glycosylation has been associated with various mammalian diseases and biological processes. Therefore, the demands to understand the roles of glycans and to monitor the development and progression of diseases have necessitated the development of reliable quantitative glycomics and glycoproteomics methods. A critical discussion of the state-of-the-art glycomics and glycoproteomics methods will be presented at this workshop. Application of these methods to understanding diseases and biological processes will be also presented and discussed. Reliable quantitative glycomics and glycoproteomics is facilitated by bioinformatics tools, an overview of which will be presented.



**11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS;** Nalini Sadagopan, Susan Abbatiello, Dawn Dufield presiding  
Room 347-348

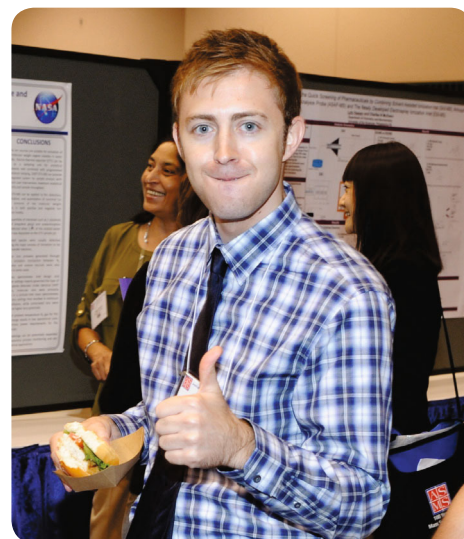
With increase in focus on biologic/biotherapeutic drugs by the pharmaceutical industry and also an increase in need for biomarkers (efficacy and safety) the deployment of LC-MS based techniques is on the rise primarily due to the speed in method development, and specificity of the technique. Scientists are finding new ways of doing sample prep to increase sensitivity/specificity, address reproducibility issues associated with enzymatic digestion and mass spectrometric methods to address specificity. The forum will provide a platform to share common themes, issues on these fronts and perhaps to surface newer needs in software, mass spec design, and automation.

**12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS** (organized by Flavor Fragrance and Foodstuff Interest Group);  
Marc Engel and Timothy Croley presiding  
Room 349-350

In the past 10 years there have been many developments in the instrumentation for the analysis of small molecules. With the evolution of GC QQQ and GC HRMS instrumentation, the confidence of quantification and identification of both constituents and contaminants found in flavors and fragrance agents and foodstuffs has increased significantly. After a few brief presentations we will discuss how we can use this instrumentation to improve our analyses.

**13. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History;** Mehdi Moini, presiding  
Room 327

The purpose of this workshop is to discuss the application of mass spectrometry (MS) to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to the application of MS to art and natural history specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of proteinaceous and organic specimens such as silk and wool textiles, leather and animal guts objects, bone and tissues, ink, paper, paint, coatings, binders, and wood. 2) Analysis of the fundamental factors that cause degradation and aging of natural history and art objects; identification of their deterioration markers, using degradation markers as clocks for dating objects, and studying environmental factors that affect deterioration. 3) Application of MS to paleo-organic matter such as fossilomics, amino acid racemization, and ancient DNA. 4) Forensic archeology. 5) Determination of the authenticity of art objects. 6) To be determined.



5:00 - 6:30 PM, SUNDAY  
TUTORIAL SESSION  
Jenny Brodbelt (University of Texas), presiding  
Exhibit Hall AB



5:00 - 5:45 pm  
**Mass Spectrometry in the Pharmaceutical Industry: Everything You Ever Wanted to Know But Were Afraid to Ask**

**Lucinda Cohen**  
Merck Research Laboratories



5:45 - 6:30 pm  
**Imaging Mass Spectrometry**

**Ron M.A. Heeren**  
FOM-AMOLF

6:45 - 7:45 PM, SUNDAY  
CONFERENCE OPENING  
Jenny Brodbelt (University of Texas), presiding  
Exhibit Hall AB

**Welcome, Jenny Brodbelt**  
ASMS Vice President for Programs



**The James Webb Space Telescope: From First Light to the Search for Earth 2.0**

**Jason Kalirai**  
Telescope Science Institute

7:45 - 9:00 PM, SUNDAY  
WELCOME RECEPTION  
Poster/Exhibit Hall  
Conference name badge is required.

8:30 - 10:30 AM, MONDAY MORNING  
EMERGING ENVIRONMENTAL CONTAMINANTS  
Matthew Crowe (Dow Chemical), presiding  
Exhibit Hall AB

MOA am 08:30 **Environmental Petroleomics: Characterization of 10<sup>5</sup> Biotic and Abiotic Petroleum Transformation Products 4-Years after the Deepwater Horizon Disaster**; Ryan P. Rodgers<sup>1,4</sup>; Brian M. Ruddy<sup>3</sup>; Vladislav V. Lobodin<sup>2,4</sup>; Amy M. McKenna<sup>4</sup>; Huan Chen<sup>4</sup>; David C. Podgorski<sup>2,4</sup>; Steven M. Rowland<sup>1</sup>; Jie Lu<sup>2,4</sup>; Yuri E. Corilo<sup>2,4</sup>; Alan G. Marshall<sup>1,4</sup>; <sup>1</sup>*FSU Department of Chemistry and Biochemistry, Tallahassee, FL*; <sup>2</sup>*Future Fuels Institute, Tallahassee, FL*; <sup>3</sup>*Taxon Biosciences Inc., Tiburon, CA*; <sup>4</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*

MOA am 08:50 **Subtractive Proteomics Reveals Novel Enzymes Induced in Rare Caffeine-Degrading Microorganisms**; Chi Li Yu<sup>1</sup>; Ryan Summers<sup>2</sup>; Yalan Li<sup>1</sup>; Sujit Mohanty<sup>2</sup>; Mani Subramanian<sup>3</sup>; Marshall Pope<sup>1</sup>; <sup>1</sup>*Proteomics Facility, Univ. of Iowa, Iowa City, IA*; <sup>2</sup>*Dept. of Chemical and Biochemical Engineering, Iowa City, IA*; <sup>3</sup>*CTR Biocatalysis & Bioprocessing, Univ. of Iowa, Iowa City, IA*

MOA am 09:10 **Silicon is a Nearly Ubiquitous Component of Ambient Nanoparticles**; Bryan Bzdek; Ross Pennington; Andrew Horan; Christopher Zordan; Murray Johnston; *University of Delaware, Newark, DE*

MOA am 09:30 **Identification of Environmental Metabolites using Combined High Resolution UPLC- QqTOF and Ultra High Resolution NanoLC-QqITOT Based Approaches**; Jeffrey Gilbert; Jesse Balcer; Yelena Adelfinskaya; Suresh Annangudi; David McCaskill; Pete Johnson; Gerrit Deboer; Mike Hastings; *Dow AgroSciences, Indianapolis, IN*

MOA am 09:50 **Terminal and Internal Alkyne Functionalities in Asphaltenes**; James Riedeman<sup>1</sup>; Xingyu Shen<sup>1</sup>; Huaming Sheng<sup>1</sup>; David Borton<sup>2</sup>; Matthew Hur<sup>3</sup>; Hilikka Kenttämaa<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*LECO, St Joseph, MI*; <sup>3</sup>*Chevron, Richmond, CA*

MOA am 10:10 **Detection of Water-Borne 4-Methylcyclohexanemethanol (MCHM) via Purge & Trap and Transportable, On-Site GC/MS**; Phil Tackett; Cynthia Liu; Mitch Wells; Dennis Barket; *FLIR Systems, Inc., West Lafayette, IN*

**INSTRUMENTATION: NEW DEVELOPMENTS IN HIGH RESOLUTION AND MASS ACCURACY IN HONOR OF ALAN MARSHALL'S 70th BIRTHDAY**

Patrick Limbach (University of Cincinnati), presiding  
Room 307-308

MOB am 08:30 **Precision Mass Spectrometry on Short-lived Nuclides: New Methods and Results**; Lutz Schweikhard<sup>1</sup>; for the SHIPTRAP collaboration<sup>2</sup>; and the ISOLTRAP collaboration<sup>3</sup>; <sup>1</sup>*University of Greifswald, Greifswald, Germany*; <sup>2</sup>*GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany*; <sup>3</sup>*ISOLDE/CERN, Geneva, Switzerland*



MOB am 08:50 **Further Characterization and Applications of Dynamically Harmonized FT ICR Cell;** Eugene Nikolaev<sup>1,2</sup>; Gleb Vladimirov<sup>1</sup>; Oleg Kharybin<sup>3</sup>; Matthias Witt<sup>4</sup>; Jochen Friedrich<sup>4</sup>; Roland Jertz<sup>4</sup>; Goekhan Baykut<sup>4</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, RAS, Moscow, Russia; <sup>3</sup>Orekhovich Institute of Biomedical Chemistry, RAMS, Moscow, Russia; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany

MOB am 09:10 **Pushing the Limits: Using Isotopic Fine Structure Mass Spectrometry to Assist the Understanding of <sup>17</sup>O labelled Peptides in NMR;** Juan Wei<sup>1</sup>; Oleg Antzutkin<sup>1,2</sup>; Mark Barrow<sup>1</sup>; Ray Dupree<sup>1</sup>; Steven Brown<sup>1</sup>; Peter B. O'connor<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>Luleå University of Technology, Luleå, Sweden

MOB am 09:30 **Unexplored Reserves of Resolution in Fourier Transform Mass Spectrometry;** Anton N. Kozhinov; Konstantin O. Nagornov; Daniel Ayoub; Yury O. Tsybin; *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

MOB am 09:50 **High-Field FTICR MS for Imaging Applications: Combining Ultra-High Resolving Power and Mass Accuracy with High Spatial Resolution and Throughput;** Jeffrey Spraggins; Raf Van De Plas; Junhai Yang; Richard Caprioli; *Vanderbilt University, Nashville, TN*

MOB am 10:10 **Development of an FT-ICR Mass Spectrometer in Preparation for 21 Telsa;** Nathan Kaiser<sup>1</sup>; Chad Weisbrod<sup>1</sup>; John Quinn<sup>1</sup>; Greg T. Blakney<sup>1</sup>; Steve Beu<sup>2</sup>; Tong Chen<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>S C Beu Consulting, Austin, TX; <sup>3</sup>Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL

**8:30 – 10:30 AM, MONDAY MORNING  
NUCLEIC ACIDS**

**Kathrin Breuker (University of Innsbruck), presiding  
Room 309-310**

MOC am 08:30 **Single-Molecule Force Spectroscopy and MS Studies of the Determinants of Duplex Stability;** Papa Nii Asare Okai; William Stephenson; Alan Chen; Pan Li; Daniele Fabris; *The RNA Institute, University at Albany, Albany, NY*

MOC am 08:50 **The Effects of Modifications on Glycosidic Bond Stability of Protonated and Sodium Cationized Nucleosides;** Mary T. Rodgers; Yanlong Zhu; *Wayne State University, Detroit, MI*

MOC am 09:10 **LC-MS/MS for the Sensitive Detection of  $\beta$ -Glucosyl-hydroxymethyluracil (Base J) in Genomic DNA of *Trypanosoma brucei*;** Shuo Liu<sup>1</sup>; Robert Sabatini<sup>2</sup>; Yinsheng Wang<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA; <sup>2</sup>University of Georgia, Athens, Georgia

MOC am 09:30 **Electrospray Mass Spectrometry of Telomeric DNA G-quadruplexes in Potassium;** Adrien Marchand<sup>1,2</sup>; Valérie Gabelica<sup>1,2</sup>; <sup>1</sup>Inserm, U869 ARNA, Bordeaux, France; <sup>2</sup>Université de Bordeaux, IECB, Pessac, France

MOC am 09:50 **Fluorescence Measurements of DNA-dye Complexes in the Gas Phase;** Stephen Sciuto<sup>1</sup>; Rebecca A. Jockusch<sup>2</sup>; <sup>1</sup>The University of Toronto, Toronto, Canada; <sup>2</sup>University of Toronto, Toronto, ON

MOC am 10:10 **Conformational Dynamics of DNA G-Quadruplex in Solution Studied by Kinetic Capillary Electrophoresis Coupled On-line with Mass Spectrometry;** Gleb Mironov; Victor Okhonin; Nasrin Khan; Maxim Berezovski; *University of Ottawa, Ottawa, Canada*

**8:30 – 10:30 AM, MONDAY MORNING  
FUNDAMENTALS: REACTIONS, DYNAMICS AND THEORY OF  
GAS PHASE IONS**

**John Poutsma (College of William and Mary), presiding  
Room 314-317**

MOD am 08:30 **Is It a Barrier or Endothermic? The Interesting Cases of Sm<sup>+</sup> Oxidation by O<sub>2</sub>, CO<sub>2</sub>, NO, and CO;** Richard Cox<sup>1</sup>; Shaun Ard<sup>2</sup>; Joshua Melko<sup>2</sup>; Nicholas Shuman<sup>2</sup>; Al Viggiano<sup>2</sup>; Ryan Johnson<sup>3</sup>; Hua Guo<sup>3</sup>; Peter Armentrout<sup>1</sup>; <sup>1</sup>University of Utah, Salt Lake City, UT; <sup>2</sup>Air Force Research Laboratory, Mesa, AZ; <sup>3</sup>University of New Mexico, Albuquerque, NM

MOD am 08:50 **Heterometallic Coinage Metal Clusters – Synthesis and Gas-Phase Reactivity;** George N. Khairallah<sup>1</sup>; Richard A. J. O'Hair<sup>2</sup>; <sup>1</sup>Bio21 Inst, Uni of Melbourne, Melbourne, Australia; <sup>2</sup>University of Melbourne, Victoria, Australia

MOD am 09:10 **Exploring Electron and Proton Transfer Timescales in the Gas Phase with Multiscale Pump-Probe Action Spectroscopy Experiments;** Luke MacAleese<sup>1</sup>; Sylvain Hermelin<sup>2</sup>; Luigi Bonacina<sup>2</sup>; Rodolphe Antoine<sup>1</sup>; Jean-Pierre Wolf<sup>2</sup>; Philippe Dugourd<sup>1</sup>; <sup>1</sup>ILM-UMR5306 Université Lyon 1 - CNRS, Villeurbanne, France; <sup>2</sup>GAP-Biophotonics, Université de Genève, Genève, Switzerland

MOD am 09:30 **Determining Masses, Separating Mixtures, and Probing Structures of Native-Like Ions using Selected Cation to Anion Proton Transfer (SCAPT) Reactions;** Kenneth J. Laszlo; Matthew F. Bush; *University of Washington, Seattle, WA*

MOD am 09:50 **Charges in Protein Electrospray Ionization: Like or Opposite?;** Rachel R. Ogorzalek Loo; Joseph A. Loo; *UCLA, Los Angeles, CA*

MOD am 10:10 **Structures and Energetics of Alkali Metal-Bound Clusters of 9-Ethylguanine;** Mohammad Azargun; Travis Fridgen; *Memorial University of NL, St. John's, Canada*

**8:30 – 10:30 AM, MONDAY MORNING  
ANTIBODIES AND ANTIBODY-DRUG CONJUGATES**  
**Beatrix Ueberheide (New York University), presiding  
Ballroom I, level 4**

MOE am 08:30 **Middle-down Primary Structure Assessment and PTM-profiling of Monoclonal Antibody by "Size-controlled" Proteolysis and Online Tandem Mass Spectrometry;** Weihan Wang<sup>1</sup>; Lichao Zhang<sup>1</sup>; Michelle English<sup>1</sup>; Dina Bai<sup>1</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald F. Hunt<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, University of Virginia, Charlottesville, VA; <sup>2</sup>Department of Pathology, University of Virginia, Charlottesville, VA

## MONDAY MORNING ORAL SESSIONS

MOE am 08:50 **Middle-Down and Extended Bottom-Up Mass Spectrometry for In-Depth and Rapid Characterization of Immunoglobulins and Their Mixtures**; [Daniel Ayoub](#)<sup>1</sup>; Luca Fornelli<sup>1</sup>; Kristina Srzentic<sup>1</sup>; Unige Laskay<sup>1</sup>; Alain Beck<sup>2</sup>; Yury O. Tsybin<sup>1</sup>; <sup>1</sup>*Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*; <sup>2</sup>*Centre d'Immunologie Pierre Fabre, Saint Julien-en-Genevois, France*

MOE am 09:10 **Informatics for mAb Analysis from Top to Bottom**; [Chris Becker](#)<sup>1</sup>; Wilfred Tang<sup>1</sup>; Yong Kil<sup>1</sup>; Marshall Bern<sup>1</sup>; John Schiel<sup>2</sup>; Lisa Kilpatrick<sup>2</sup>; Trina Formolo<sup>2</sup>; <sup>1</sup>*Protein Metrics Inc., San Carlos, CA*; <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*

MOE am 09:30 **An Optimized MS-based Pipeline for Producing Repertoires of Recombinant High Affinity Nanobodies**; [Yinyin Li](#)<sup>1</sup>; Peter Fridy<sup>1</sup>; Sarah Keegan<sup>2</sup>; Mary Thompson<sup>1</sup>; Ilona Nudelman<sup>1</sup>; David Fenyó<sup>2</sup>; Michael Rout<sup>1</sup>; Brian Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*New York University, New York, NY*

MOE am 09:50 **Native MS and IM-MS for Antibody Drug Conjugate Characterization**; François Debaene<sup>1</sup>; Amandine Boeuf<sup>2</sup>; Elsa Wagner-Rousset<sup>2</sup>; Nathalie Corvaia<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Alain BECK<sup>2</sup>; [Sarah Cianferani](#)<sup>1</sup>; <sup>1</sup>*LSMBO - IPHC, Strasbourg, France*; <sup>2</sup>*CIPF, Saint Julien en Genevois, France*

MOE am 10:10 **Mass Spectrometry-Based Proteomics in the Development of Antibody Drug Conjugates for Cancer Treatment**; [Jeremy Myers](#); Bingwen Lu; Kim Arndt; *Oncology Research, Pfizer WRD, Pearl River, New York*

**8:30 – 10:30 AM, MONDAY MORNING  
H/D EXCHANGE: NEW DEVELOPMENTS IN TECHNOLOGY  
Kasper Rand (University of Copenhagen), presiding  
Ballroom II, level 4**

MOF am 08:30 **HDsite: Hydrogen/deuterium Exchange by MS at Amino Acid Resolution**; [Zhong-yuan Kan](#); Wenbing Hu; Benjamin Walters; Leland Mayne; Walter Englander; *University of Pennsylvania, Philadelphia, PA*

MOF am 08:50 **Model-Free Analysis of Millisecond H/D Exchange Reveals Residual Helicity in ACTR, an Intrinsically Disordered Protein**; Theodore Keppel<sup>1,2</sup>; [David Weis](#)<sup>1</sup>; <sup>1</sup>*University of Kansas, Lawrence, KS*; <sup>2</sup>*Washington University School of Medicine, St. Louis, MO*

MOF am 09:10 **Targeted and Data-Independent Acquisition of Hydrogen/Deuterium Exchange using ETD**; [Vladimir Sarpe](#); David Schriemer; *University of Calgary, Calgary, Canada*

MOF am 09:30 **Conformational Changes in Peripheral Membrane Proteins using Langmuir Monolayers and Hydrogen-Deuterium Exchange Mass Spectrometry**; [Gregory F. Pirrone](#)<sup>1</sup>; Michael S. Kent<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Sandia National Laboratories, Albuquerque, NM*

MOF am 09:50 **Characterizing Protein Oligomer Structure and Dissociation Kinetics by Hydrogen/Deuterium Exchange Mass Spectrometry**; [Zhe Zhang](#); Richard Vachet; *University of Massachusetts, Amherst, MA*

MOF am 10:10 **Strategies for Minimizing Spurious In-Source CID for Peptides during ESI-MS**; [Siavash Vahidi](#); Lars Konermann; *Univ. of Western Ontario, London, ON*

**8:30 – 10:30 AM, MONDAY MORNING  
INFORMATICS: PROTEIN IDENTIFICATION  
David Tabb (Vanderbilt University), presiding  
Ballroom III, level 4**

MOG am 08:30 **Use of Personalized Sequence Databases for Peptide MS/MS Spectrum Matching in the Proteogenomic Analysis of 105 TCGA Breast Tumors**; [Karl R. Clauser](#)<sup>1</sup>; David Fenyó<sup>2</sup>; Kelly V. Ruggles<sup>2</sup>; Philipp Mertins<sup>1</sup>; Jana W. Qiao<sup>1</sup>; D. R. Mani<sup>1</sup>; Michael A. Gillette<sup>1</sup>; Sherri R. Davies<sup>3</sup>; Christopher Maher<sup>3</sup>; Li Ding<sup>3</sup>; Matthew J. Ellis<sup>3</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*NYU Langone Medical Center, New York, NY*; <sup>3</sup>*Washington University, St. Louis, MO*

MOG am 08:50 **Approaching the "Perfect" Database: Single-Molecule, Full-Length Transcript Sequencing to Create Sample-Specific, Full-Length Protein Databases**; [Gloria M. Sheynkman](#); Mark Scalf; Michael R. Shortreed; Brian L. Frey; Anthony J. Cesnik; Lloyd M. Smith; *University of Wisconsin, Madison, WI*

MOG am 09:10 **Novel Galaxy Workflows Combining RNA-seq and Proteomic MS/MS Reveal New Insights into Non-Model Organisms**; Jun Fan<sup>1</sup>; Vanessa Evans<sup>2</sup>; Gary Barker<sup>2</sup>; Kate Heesom<sup>2</sup>; Shyamasee Saha<sup>1</sup>; David Matthews<sup>2</sup>; [Conrad Bessant](#)<sup>1</sup>; <sup>1</sup>*Queen Mary University of London, London, UK*; <sup>2</sup>*University of Bristol, Bristol, UK*

MOG am 09:30 **Blind Spectral Alignment with Adaptive Penalties**; [Laurence E. Bernstein](#); Nuno Bandeira; *Univeristy of California, San Diego, La Jolla, CA*

MOG am 09:50 **Pecan: Peptide Identification Directly from Data-Independent Acquisition (DIA) MS/MS Data**; [Ying Sonia Ting](#)<sup>1</sup>; Jarrett Egerton<sup>1</sup>; Brendan Maclean<sup>1</sup>; Sangtae Kim<sup>2</sup>; Samuel H Payne<sup>2</sup>; William Stafford Noble<sup>1</sup>; Michael J. Maccoss<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*

MOG am 10:10 **Doubling Peptide Identification Efficiency in Complex Shotgun Proteomics by Deconvolution and Identification of Multiple Precursors in MS/MS**; [Bo Zhang](#); Mohammad Pirmoradian; Alexey Chernobrovkin; Roman Zubarev; *Karolinska Institutet, Stockholm, Sweden*

**8:30 – 10:30 AM, MONDAY MORNING  
PTMS: ADVANCES IN ISOLATION, ENRICHMENT,  
DERIVATIZATION AND SEPARATION  
Jen Grant (University of Wisconsin-Stout), presiding  
Ballroom IV, level 4**

MOH am 08:30 **A Multi-Functionalized Chemical Reagent Capable of Both Gel-Based Detection of Phosphoproteins and Enrichment of Phosphopeptides for Mass Spectrometric Analysis**; [Linna Wang](#); Li Pan; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*

MOH am 08:50 **Characterization of Lipid Modifications on Regulator of G Protein Signaling 4 (RGS4) from Sf9 Cells by Mass Spectrometry**; [Yuhuan Ji](#); Minjing Liu; Markus M. Bachschmid; Catherine E.

## MONDAY MORNING AND AFTERNOON ORAL SESSIONS

- Costello; Cheng Lin; *Boston University School of Medicine, Boston, MA*
- MOH am 09:10 **A Site-Specific Strategy for Localization of D-Amino Acids in Bioactive Peptides;** Chenxi Jia; Qing Yu; Christopher Lietz; Lingjun Li; *University of Wisconsin-Madison, Madison, Wisconsin*
- MOH am 09:30 **Simultaneous Quantitation of S-nitrosylation and Sulfenation Changes in Escherichia coli under Mild Oxidative Stress;** Katarzyna Wojdyła; James Williamson; Peter Roepstorff; Adelina Rogowska-Wrzęsinska; *University of Southern Denmark, Odense, Denmark*
- MOH am 09:50 **Protein S-Nitrosylation: Novel Detection, Redox Regulation and Stoichiometry;** Jaimoen Majumdar; Brent Martin; *University of Michigan, Ann Arbor, Michigan*
- MOH am 10:10 **New Methodology for the Enrichment and Characterization of O-GlcNAcylated Peptides;** Stacy Malaker<sup>1</sup>; Sarah Penny<sup>2</sup>; Dina Bai<sup>1</sup>; Weihang Wang<sup>1</sup>; Mark Cobbold<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald Hunt<sup>1</sup>; <sup>1</sup>*University of Virginia, Charlottesville, Virginia*; <sup>2</sup>*University of Birmingham, Birmingham, UK*

**10:30 AM – 2:30 PM, MONDAY  
MONDAY POSTER SESSION**  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm  
**12:00 – 1:00 pm**  
Undergraduate Students  
Meet the Experts at tables reserved for you.

## MONDAY AFTERNOON ORAL SESSIONS

- 2:30 – 4:30 PM, MONDAY AFTERNOON  
ANALYSIS OF POLYMER- AND PACKAGING-RELATED  
CONTAMINANTS AND DEGRADANTS IN  
CONSUMER PRODUCTS**  
Avinash Dalmia (PerkinElmer), presiding  
Exhibit Hall AB
- MOA pm 2:30 **Top-Down Mass Spectrometry of Hybrid Materials with Hydrophobic Peptide and Hydrophilic Polymer Blocks;** Chrys Wesdemiotis<sup>1</sup>; Ahlam Alalwiat<sup>1</sup>; Sarah E. Grieshaber<sup>2</sup>; Bradford A. Paik<sup>2</sup>; Xinqiao Jia<sup>2</sup>; <sup>1</sup>*The University of Akron, Akron, OH*; <sup>2</sup>*University of Delaware, Newark, DE*
- MOA pm 2:50 **An Application of Mass Spectrometry for the Detection of Chemical Markers for Product Traceability;** Evan Parker; Carlito Lebrilla; *UC Davis, Davis, CA*
- MOA pm 3:10 **Innovative Approaches for Complex Polymer Analysis with the Combination of DART-MS, Thermal Control and a Search Algorithm for Chaotic Spectra;** Kazumasa Kinoshita<sup>2</sup>; Yuki Kudou<sup>1</sup>; Kazuyuki Takama<sup>1</sup>; Haruo Shimada<sup>3</sup>; Yuka Noritake<sup>3</sup>; Yasuo Shida<sup>1</sup>; <sup>1</sup>*Bio Chromato, Inc, Fujisawa, Japan*; <sup>2</sup>*DirectAnalysis, Inc, Fujisawa, Japan*; <sup>3</sup>*Shiseido Research Center, Yokohama, Japan*
- MOA pm 3:30 **MALDI-TOF/TOF CID Study of Polycarbodiimide Branching Reactions;** Anthony P. Gies; William Heath; *Dow Chemical Company, Freeport, TX*
- MOA pm 3:50 **Matrix Segregation as a Major Cause for Sample Inhomogeneity using the Dried Droplet Sample Preparation Method for MALDI-MSI;** Steffen M. Weidner<sup>1</sup>; Stefan Johannes Gabriel<sup>1</sup>; Clemens Schwarzingger<sup>2</sup>; Ulrich Panne<sup>1</sup>; <sup>1</sup>*Fed. Inst. f. Mat. Research, Berlin, Germany*; <sup>2</sup>*Johannes Kepler University, Linz, At*
- MOA pm 4:10 **Utilization of GC-TOFMS and GC-High Resolution-TOFMS for Characterization of Contaminants and Degradation Products in Consumer Product Packaging Materials;** Ray Marsili<sup>1</sup>; Joe Binkley<sup>2</sup>; <sup>1</sup>*Marsili Consulting Group, Rockford, IL*; <sup>2</sup>*LECO Corporation, St. Joseph, MI*
- 2:30 – 4:30 PM, MONDAY AFTERNOON  
INSTRUMENTATION: MINI/PORTABLE/FIELDABLE  
MASS SPECTROMETRY**  
Christopher Gill (Vancouver Island University), presiding  
Room 307-308
- MOB pm 2:30 **Systematic Testing and Optimization of Subsystems for Development of a Handheld MS;** Mitch Wells; Brent Rardin; Kevin Rosenbaum; Leonard Rorrer; Adam Keil; Dennis Barket; Gary Gentry; *FLIR Systems, West Lafayette, IN*
- MOB pm 2:50 **Development of a Synchronized Discharge Ionization Probe for Direct Analysis of Non-volatile Chemicals on Surfaces Using Handheld Mass Spectrometers;** Xiao Wang; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- MOB pm 3:10 **Handheld Mass Spectrometry Enabled by Ultrahigh Pressure Operation using Air Buffer Gas;** Kevin Schultze; Kenion Blakeman; J. Michael Ramsey; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MOB pm 3:30 **A Loeb-Eiber Mass Filter for Miniature Mass Spectrometry Applications;** William D. Hoffmann; Feng Jin; Glen P. Jackson; *West Virginia University, Morgantown, WV*
- MOB pm 3:50 **Mobile Autonomous Underwater Mass Spec and Sampler System – Opening up the Entire Underwater Chemical Space;** David Fries<sup>1</sup>; Geran Barton<sup>1</sup>; David Millie<sup>2</sup>; Robert Ulrich<sup>3</sup>; John Paul<sup>3</sup>; <sup>1</sup>*USF, Tampa, Florida*; <sup>2</sup>*Michigan Technological University, Ann Harbor, MI*; <sup>3</sup>*USF, St. Petersburg, FL*
- MOB pm 4:10 **Utilizing a Novel Compact Mass Spectrometer (CMS) for the Detection and Quantification of Chemical Compounds Related to Cannabis;** Daniel Eikel<sup>1</sup>; Simon J. Prosser<sup>2</sup>; <sup>1</sup>*Advion Inc., Ithaca, NY*; <sup>2</sup>*Advion, Inc., Ithaca, NY*

## MONDAY AFTERNOON ORAL SESSIONS

### 2:30 – 4:30 PM, MONDAY AFTERNOON ION MOBILITY STRUCTURES IN HONOR OF MIKE BOWERS' 75TH BIRTHDAY Gert Von Helden (Fritz-Haber University), presiding Room 309-310

- MOC pm 2:30 **Are Disulfide Bridges Opened by ETD ?**; Emeline Hanozin; Denis Morsa; Philippe Massonnet; Loic Quinton; [Edwin De Pauw](#); *Mass spectrometry Laboratory, University of Liege, Liege, Belgium*
- MOC pm 2:50 **Substance P from Solution to the Gas Phase: Factors that Stabilize Kinetically Trapped Conformations**; [Kyle L. Fort](#)<sup>1</sup>; Joshua A. Silveira<sup>1</sup>; Kelly A. Servage<sup>1</sup>; Nicholas A. Pierson<sup>2</sup>; David E. Clemmer<sup>2</sup>; David H. Russell<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Indiana University Bloomington, Bloomington, IN
- MOC pm 3:10 **Utilizing High Throughput IMS-MS Measurements to Analyze Small Molecules and Their Noncovalent Interactions with Macromolecular Complexes**; [Erin Baker](#)<sup>1</sup>; Ryan Kelly<sup>1</sup>; Alex Apffel<sup>2</sup>; Kristin Burnum-Johnson<sup>1</sup>; Young-Mo Kim<sup>1</sup>; Yehia Ibrahim<sup>1</sup>; Daniel Orton<sup>1</sup>; Kevin Crowell<sup>1</sup>; Matthew Monroe<sup>1</sup>; Thomas Metz<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Alex Mordehai<sup>2</sup>; Ed Darland<sup>2</sup>; George Stafford<sup>2</sup>; Gordon Anderson<sup>1</sup>; Richard Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- MOC pm 3:30 **Supercharging of Native Protein Complexes: Effects of Polarity and Evidence for Multiple Mechanisms**; [Samuel J. Allen](#); Christiane N. Stachl; Matthew F. Bush; *University of Washington, Seattle, WA*
- MOC pm 3:50 **Ion Mobility and Solution Studies Show Specific Competitive Binding of Homo- and Heteromultimer Receptor:Protein:Carbohydrate Binding**; [Julie A. Leary](#); Youjin Seo; *UC Davis, Davis, CA*
- MOC pm 4:10 **Projected Superposition Approximation: A Novel Parameter Set for Prediction of Cross Sections in Nitrogen as a Drift Gas**; [Christian Bleiholder](#)<sup>1</sup>; Thomas Wyttenbach<sup>2</sup>; Michael T. Bowers<sup>2</sup>; <sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>University of California, Santa Barbara, CA

### 2:30 – 4:30 PM, MONDAY AFTERNOON PHOTOIONIZATION Helene Cardasis (Thermo Scientific), presiding Room 314-317

- MOD pm 2:30 **Evaluation of the Optimization Space for Atmospheric Pressure Photoionization (APPI)**; [Andreas Fredenhagen](#); Jürgen Kühnöl; *Novartis, Basel, Switzerland*
- MOD pm 2:50 **Highly Time-Resolved Mapping of Combustion Product-Concentrations in Dynamic Solid-Fuel Combustion Processes by Photoionisation Mass Spectrometry: Looking into a Burning Cigarette**; [Ralf Zimmermann](#)<sup>1</sup>; Romy Hertz-Schuenemann<sup>1</sup>; Sven Ehler<sup>1</sup>; Kevin McAdam<sup>2</sup>; Steven Coburn<sup>2</sup>; Chuan Liu<sup>2</sup>; Thorsten Streibel<sup>1</sup>; <sup>1</sup>University of Rostock, Rostock, Germany; <sup>2</sup>GR&D, BAT Ltd., Southampton, UK
- MOD pm 3:10 **Investigating the Ionization of Sulfur-Containing Compounds within Petroleum using Atmospheric Pressure Photoionization Fourier Transform Ion**

**Cyclotron Resonance Mass Spectrometry**; Holly Chan; [Mark Barrow](#); *University of Warwick, Coventry, UK*

- MOD pm 3:30 **Fluorophore-Assisted Laser Desorption/Ionization Mass Spectrometry (FALDI-MS) of biomolecules**; [Dragan Isailovic](#); Raymond West; Eric Finsden; *The University of Toledo, Toledo, OH*
- MOD pm 3:50 **Laser Desorption VUV Lamp Ionization for Quadrupole Ion Trap Mass Spectrometry**; [Qinghao Wu](#); Richard Zare; *Stanford University, Stanford, CA*
- MOD pm 4:10 **Analytical Performance of a Novel, Dopant-Free GC-APPI Source with Femtogram-Level Sensitivity for Quadrupole-Orbitrap GC/MS**; [Amelia C. Peterson](#)<sup>1</sup>; Hendrik Kersten<sup>2</sup>; Dirk Krumwiede<sup>1</sup>; Scott Quarmby<sup>3</sup>; Kyle D'Silva<sup>1</sup>; Kai Kroll<sup>2</sup>; Kirsten Haberer<sup>2</sup>; Maciej Bromirski<sup>1</sup>; Alexander Makarov<sup>1</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany; <sup>2</sup>University of Wuppertal, Wuppertal, Germany; <sup>3</sup>Thermo Fisher Scientific, Austin, TX

### 2:30 – 4:30 PM, MONDAY AFTERNOON CHARACTERIZATION OF BIOLOGICALS AND BIOSIMILARS James Madsen (Momena Pharmaceuticals), presiding Ballroom I, level 4

- MOE pm 2:30 **Sequence Variant Analysis with Increased Specificity and Meaningful Confidences**; [Sean L. Seymour](#); Ignat V. Shilov; Joe Durant; Bret Pehrson; Eric Johansen; *AB SCIEX, Redwood City, CA*
- MOE pm 2:50 **Size-Based Enrichment and 1D Proteomics of Low ppm Levels of Host Cell Proteins in High-Concentration Therapeutic Antibodies**; Gang Xiao; Da Ren; [Pavel Bondarenko](#); *Amgen, Inc., Thousand Oaks, CA*
- MOE pm 3:10 **Interleukin-23 Binding to Adnectin: An Approach to Correlating Molecular Structure with Hydrogen/Deuterium Exchange Mass Spectrometry**; [Roxana E. Iacob](#)<sup>1</sup>; Guodong Chen<sup>2</sup>; Stanley R. Krystek<sup>2</sup>; Hui Wei<sup>2</sup>; Richard Huang<sup>2</sup>; Li Tao<sup>2</sup>; Zheng Lin<sup>2</sup>; Paul E. Morin<sup>2</sup>; Michael L. Doyle<sup>2</sup>; Adrienne A. Tymiak<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Bristol-Myers Squibb, Princeton, NJ
- MOE pm 3:30 **New Workflows for Identification and Profiling of Disulfide Bonds in Biopharmaceuticals**; Jan Wiesner; Antje Kozicki; Anja Resemann; Rainer Paape; Lars Vorwerg; Kristina Marx; Andrea Kiehne; Ralf Hartmer; Carsten Baessmann; Detlev Suckau; [Wolfgang Jabs](#); *Bruker Daltonik GmbH, Bremen, Germany*
- MOE pm 3:50 **System Suitability Metrics for Analysis of Protein Therapeutics by LC-MS**; [Mowei Zhou](#); Ashley Gucinski; Michael Boyne; *U.S. FDA, Division of Pharmaceutical Analysis, St Louis, MO*
- MOE pm 4:10 **Biopharmaceutical Characterization: Evaluation of the NIST Monoclonal Antibody Reference Material.**; [John Schiel](#)<sup>1</sup>; Meiyao Wang<sup>1</sup>; Trina Formolo<sup>1</sup>; Lisa Kilpatrick<sup>1</sup>; Mark Lowenthal<sup>1</sup>; Henning Stockmann<sup>2</sup>; Karen Phinney<sup>1</sup>; Justin Prien<sup>6</sup>; Darryl Davis<sup>4</sup>; Oleg Borisov<sup>3</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>NIBRT, Dublin, Ireland; <sup>3</sup>Novavax, Gaithersburg, MD; <sup>4</sup>Janssen, Malvern, PA; <sup>5</sup>Amgen, West Greenwich, RI



2:30 – 4:30 PM, MONDAY AFTERNOON  
**QUANTITATIVE ANALYSIS IN  
 DRUG DISCOVERY AND DEVELOPMENT**  
**Brian Furmanski (GlaxoSmithKline), presiding**  
**Ballroom II, level 4**

MOF pm 2:30 **Digestion of Some Model Proteins for Therapeutic Proteins in Blood Plasma with Thermolysin and Quantification of the Peptides by LC/LC-MS/MS**; Aljona Saleh; *Stockholm university, Analytical Chemistry, Stockholm, Sweden*

MOF pm 2:50 **High-Throughput, Dual-Stream UHPLC/MS/MS Bioanalysis and Data-Deconvolution for Rapid Drug Discovery Applications**; Brendon Kapinos<sup>1</sup>; John Janiszewski<sup>1</sup>; Mary Piotrowski<sup>1</sup>; Wayne Lootsma<sup>2</sup>; Steve Ainley<sup>2</sup>; Nick Levitt<sup>3</sup>; <sup>1</sup>*Pfizer Inc., Groton, CT*; <sup>2</sup>*Sound Analytics, Niantic, CT*; <sup>3</sup>*Two Center Technologies, Cambridge, MA*

MOF pm 3:10 **Single Cell Drug Discovery**; Sachiko Date<sup>1</sup>; Hajime Mizuno<sup>1</sup>; Tsuyoshi Esaki<sup>1</sup>; Ai Fujita<sup>1</sup>; Tsutomu Masujima<sup>1</sup>; Haruo Iwabuchi<sup>2</sup>; Makoto Takei<sup>2</sup>; Hideo Takakusa<sup>2</sup>; Takashi Izumi<sup>2</sup>; Setsuko Fujita<sup>3</sup>; Shuichi Matsuda<sup>3</sup>; Motohiko Morihara<sup>3</sup>; Kiyoko Bando<sup>4</sup>; Jiro Deguchi<sup>4</sup>; Yasunori Fukuda<sup>5</sup>; Naoki Tarui<sup>5</sup>; <sup>1</sup>*Quantitative Biology Center (QBiC), RIKEN, Suita, Osaka, Japan*; <sup>2</sup>*Daiichi Sankyo Co. Ltd., Shinagawa, Tokyo, JP*; <sup>3</sup>*Ono Pharmaceutical Co., Ltd., Shimamoto, Osaka, JP*; <sup>4</sup>*Dainippon Sumitomo Pharma Co. Ltd., Osaka, JP*; <sup>5</sup>*Takeda Pharmaceutical Co., Ltd, Fujisawa, Kanagawa, JP*

MOF pm 3:30 **A Novel Selective Peptide Derivatization Strategy for Sensitivity Enhancement for the LC-MS/MS Bioanalysis of Protein Therapeutics in Serum**; Long Yuan<sup>1</sup>; Anna Mai<sup>2</sup>; Anne-Françoise Aubry<sup>1</sup>; Mark Arnold<sup>1</sup>; Qin Ji<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*Columbia University, New York, NY*

MOF pm 3:50 **Label-Free Quantification of GeLC-MALDI Data with a Novel Software Reveals Pancreatic Ductal Adenocarcinoma Subtype-Specific Protein Signatures**; Wiebke Nadler<sup>1,3</sup>; Alexander Kerner<sup>1,3</sup>; Sabrina Hanke<sup>1,3</sup>; Christoph Roesli<sup>1,2</sup>; <sup>1</sup>*Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany*; <sup>2</sup>*Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany*; <sup>3</sup>*Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany*

MOF pm 4:10 **Total Plasma 3-chloro-tyrosine and Methionine Sulfoxide are Biomarkers of Oxidative Stress Events in Humans**; Matthew Blatnik<sup>1</sup>; Rick Steenwyk<sup>1</sup>; Paul Huang<sup>2</sup>; Buckbinder Leonard<sup>3</sup>; <sup>1</sup>*Pfizer Inc., Groton, CT*; <sup>2</sup>*Massachusetts General Hospital and Harvard Medical, Boston, MA*; <sup>3</sup>*Pfizer Inc., Cambridge, MA*

2:30 – 4:30 PM, MONDAY AFTERNOON  
**INFORMATICS: PROTEIN QUANTIFICATION**  
**Nathan Yates (University of Pittsburgh), presiding**  
**Ballroom III, level 4**

MOG pm 2:30 **Proteome-Wide Analysis of Diversity Outbred Mouse Liver Protein Expression in Relation to Genetic and Environmental Variability**; Joel M. Chick<sup>1</sup>; Steven Ciciotte<sup>2</sup>; Steven C. Munger<sup>2</sup>; Daniel M. Gatti<sup>2</sup>; Karen L. Svenson<sup>2</sup>; Gary A. Churchill<sup>2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>*Harvard medical school, Boston, MA*; <sup>2</sup>*The Jackson Laboratory, Bar Harbor, MA*

MOG pm 2:50 **Streamlining Sequence Variant and Modification Analysis of Therapeutic Proteins**; Yong Kil<sup>1</sup>; Chris Becker<sup>1</sup>; Oleg Borisov<sup>2</sup>; Boyan Zhang<sup>3</sup>; Michael Kim<sup>4</sup>; Richard Seipert<sup>4</sup>; <sup>1</sup>*Protein Metrics Inc., San Carlos, CA*; <sup>2</sup>*Novavax, Inc., Gaithersburg, MD*; <sup>3</sup>*Beijing Mabworks Biotech Co., Ltd., Beijing, China*; <sup>4</sup>*Genentech, South San Francisco, CA*

MOG pm 3:10 **CONSTAND : A Normalization Method for Isobaric Labeled Spectra by Constrained Programming**; Evelyne Maes<sup>1,2</sup>; Wahyu Hadiwikarta<sup>1,2</sup>; Inge Mertens<sup>1</sup>; Geert Baggerman<sup>1,3</sup>; Jef Hooyberghs<sup>1,4</sup>; Dirk Valkenburg<sup>1,4</sup>; <sup>1</sup>*VITO, Mol, Belgium*; <sup>2</sup>*KULeuven, Leuven, Belgium*; <sup>3</sup>*Antwerpen, Antwerpen, Belgium*; <sup>4</sup>*UHasselt, Hasselt, Belgium*

MOG pm 3:30 **Proteform Quantitation through the IQ Framework**; Grant Fujimoto; Sangtae Kim; Kevin Crowell; Nikola Tolic; Charles Ansong; Si Wu; Ljiljana Pasa-Tolic; Richard D. Smith; Joshua Adkins; Sam Payne; *Pacific Northwest National Laboratory, Richland, WA*

MOG pm 3:50 **Statistical Elimination of Spectral Features with Large Between-Run Variation Enhances Quantitative Protein-Level Conclusions in Experiments with Data-Independent Spectral Acquisition**; Lin-Yang Cheng<sup>1</sup>; Yansheng Liu<sup>2</sup>; Ching-Yun Chang<sup>1</sup>; Hannes Roest<sup>2</sup>; Ruedi Aebersold<sup>2,3</sup>; Olga Vitek<sup>1,4</sup>; <sup>1</sup>*Department of Statistics, Purdue University, West Lafayette, IN*; <sup>2</sup>*Department of Biology, ETH, Zurich, Switzerland*; <sup>3</sup>*Faculty of Science, University of Zurich, Zurich, Switzerland*; <sup>4</sup>*Department of Computer Science, Purdue University, West Lafayette, IN*

MOG pm 4:10 **Public Sharing of Complex MS-based Qualitative and Quantitative Proteomic Data Analysis Workflows: Adding Value to big Data Repositories**; Tim Griffin<sup>1</sup>; Pratik Jagtap<sup>1</sup>; James Johnson<sup>2</sup>; Trevor Wennblom<sup>2</sup>; Bart Gottschalk<sup>2</sup>; Yue Chen<sup>1</sup>; <sup>1</sup>*University of Minnesota, Minneapolis, MN*; <sup>2</sup>*Minnesota Supercomputing Institute, Minneapolis, MN*

2:30 – 4:30 PM, MONDAY AFTERNOON  
**IMAGING: BIOLOGICAL APPLICATIONS**  
**Richard Perry (University of Illinois), presiding**  
**Ballroom IV, level 4**

MOH pm 2:30 **Advanced MALDI Imaging Techniques for the Study of Renal Disease**; Megan M. Gessel<sup>1</sup>; Jeffrey Spraggins<sup>1</sup>; Raf Van De Plas<sup>1</sup>; Dale Abrahamson<sup>2</sup>; Billy Hudson<sup>1</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University School of Medicine, Nashville, TN*; <sup>2</sup>*University of Kansas Medical Center, Kansas City, KS*

MOH pm 2:50 **Chronic Ethanol Consumption Profoundly Disrupts Regional Brain Ceramide-Sphingomyelin Content in a Mouse Model**; Amina S. Woods<sup>1</sup>; Aurelie Roux<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Ludovic Muller<sup>1</sup>; J. Albert Schultz<sup>2</sup>; Joseph R. O'Rourke<sup>3</sup>; Panayotis K. Thanos<sup>3</sup>; Nora D Volkow<sup>1</sup>; <sup>1</sup>*NIDA-IRP, NIH, Baltimore, MD*; <sup>2</sup>*Ionwerks, Inc., Houston, TX*; <sup>3</sup>*Stony Brook University, Stony Brook, NY*

MOH pm 3:10 **Spatially Resolved Rapid Evaporative Ionization Mass Spectrometry (REIMS) for Database Population and In-Theatre Classification of Excised Tissues**; Emrys A Jones; Ottmar Gof; Nicole Strittmatter; Abigail Speller; Zoltan Takats; *Imperial College London, London, UK*

## MONDAY AFTERNOON AND TUESDAY MORNING ORAL SESSIONS

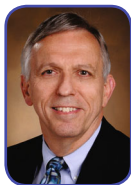
MOH pm 3:30 **Molecular Signatures and Implications of Focal Cerebral Ischemia Revealed using Nanospray Desorption Electrospray Ionization Mass Spectrometry Imaging;** [Ingela Lanekoff](#)<sup>1,3</sup>; Susan Stevens<sup>2</sup>; Mary Stenzel-Poore<sup>2</sup>; Julia Laskin<sup>1,3</sup>; <sup>1</sup>PNNL, Richland, WA; <sup>2</sup>Oregon Health & Science University, Portland, OR; <sup>3</sup>Pacific NW National Laboratory, Richland, WA

MOH pm 3:50 **Combining Magnetic Resonance Spectroscopic Imaging and Mass Spectrometric Imaging Reveals Protein Biomarkers of Aggressive Breast Cancer;** [Lu Jiang](#)<sup>1</sup>; Kamila Chughtai<sup>2</sup>; Tiffany Greenwood<sup>1</sup>; Zaver Bhujwala<sup>1</sup>; Venu Raman<sup>1</sup>; Gert Eijkel<sup>2</sup>; Ron Heeren<sup>2</sup>; Kristine Glunde<sup>1</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>FOM-Institute AMOLF, Amsterdam, The Netherlands

MOH pm 4:10 **3D Molecular Cartography of Humans;** [Amina Bouslimani](#)<sup>1</sup>; Carla Porto Da Silva<sup>1</sup>; Christopher M Rath<sup>1</sup>; Mingxun Wang<sup>1</sup>; Guo Yurong<sup>1</sup>; Antonio Gonzalez<sup>2</sup>; Donna Berg-Lyon<sup>2</sup>; Gail Ackermann<sup>2</sup>; Gitte Julie Moeller Christensen<sup>3</sup>; Nakatsuji Teruaki<sup>1</sup>; Lingjuan Zhang<sup>1</sup>; Andrew Borkowski<sup>1</sup>; Michael Meehan<sup>1</sup>; Kathleen Dorrestein<sup>1</sup>; Richard Gallo<sup>1</sup>; Nuno Bandeira<sup>1</sup>; Rob Knight<sup>2</sup>; Theodore Alexandrov<sup>4</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>Univ. of California at San Diego, La Jolla, CA; <sup>2</sup>University of Colorado at Boulder, Boulder, CO; <sup>3</sup>Aarhus University, Aarhus, Denmark; <sup>4</sup>University of Bremen, Bremen, Germany

### 4:45 – 5:30 PM, MONDAY AFTERNOON AWARD LECTURE

**Susan T. Weintraub (Univ. of Texas HSC, San Antonio), presiding  
Exhibit Hall AB**



**Award for a Distinguished Contribution in Mass Spectrometry**

**Richard M. Caprioli**  
Vanderbilt University

### 5:45 – 7:00 PM, MONDAY AFTERNOON WORKSHOPS Level 3

#### Light refreshments, level 3

1. Real World Applications of Photoionization; Room 307-308
2. Taming Errors for Peptides with Post-Translational Modifications (organized by Bioinformatics for MS Interest Group); Room 309-310
3. Applying Ion Mobility to Biological Problems (organized by Ion Mobility MS Interest Group); Room 314-317
4. How to Succeed in Pharma without Really Trying; Room 327
5. Discussion on MS Analysis of Oligonucleotides: Methodology and Informatics (organized by DNA/RNA Interest Group); Room 336
6. Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum (organized by Energy, Petroleum & Biofuels Interest Group); Room 337
7. Getting the Most out of Undergraduate Mass Spectrometry Research (organized by Undergraduate Research in MS Interest Group); Room 338
8. ProteomicsDB; Room 339-340
9. Working with Federal Agencies to Obtain Research Support. Session I: Counsel and Resources for Interactions with Federal Funding Agencies; Room 341-342
10. Systems of Annotation and Reporting Requirements for Lipid Mass Spectrometry (organized by Lipids and Lipidomics Interest Group); Room 343-344
11. A State of the Union for Biomarker Translation (organized by Clinical Chemistry Interest Group); Room 345-346
12. Antibody Drug Conjugates as Pharmaceutical Agents (organized by Pharmaceuticals Interest Group); Room 347-348
13. Roundtable Discussion on Research Challenges in Forensics and Homeland Security (organized by Forensics and Homeland Security Interest Group); Room 349-350

**AFTER 8:00 PM, MONDAY EVENING  
CORPORATE HOSPITALITY SUITES  
Hilton Hotel**

## TUESDAY MORNING ORAL SESSIONS

### 8:30 – 10:30 AM, TUESDAY MORNING INTEGRATED QUALITATIVE AND QUANTITATIVE LC-MS FOR SMALL MOLECULE ANALYSIS

**Alison Danell (East Carolina University), presiding  
Exhibit Hall AB**

TOA am 08:30 **Probing Dynamics of Plant Specialized Metabolism through Stable Isotopic Labeling and Nonselective Collision-Induced Dissociation;** [Zhenzhen Wang](#); A. Daniel Jones; Michigan State University, East Lansing, MI

TOA am 08:50 **Characterizing Chemical Composition of SOM using Graduated Extractions, Deep Fractionation and LCMS to Detect/Quantify a Broad Range of Compounds;** [Kristyn Roscioli](#)<sup>1</sup>; Yufeng Shen<sup>2</sup>; Thomas Fillmore<sup>1</sup>; Rui Zhao<sup>1</sup>; Nikola Tolic<sup>1</sup>; Brian Anderson<sup>2</sup>; Nancy J Hess<sup>1</sup>; Ljiljana Paša-Tolić<sup>1</sup>; Errol W Robinson<sup>1</sup>; <sup>1</sup>Environmental Molecular Sciences Laboratory, PNNL, Richland, WA; <sup>2</sup>Biological Sciences Division, PNNL, Richland, Washington

TOA am 09:10 **Analysis of Enantiomeric Amino Acids in Biological Samples via Capillary Electrophoresis Coupled with Mass Spectrometry;** [Takayuki Kawai](#); Stanislav Rubakhin; Jonathan Sweedler; University of Illinois at Urbana-Champaign, Urbana-Champaign, IL

TOA am 09:30 **Characterization of Alkylpolyglucoside Surfactants with Liquid Chromatography/Mass Spectrometry and Evaporative Light Scattering Detection: Total Characterization without a Reference Standard;** [Matthew Crowe](#); Katherine Davis; Janet Windisch; Dow Chemical Company, Collegeville, PA

TOA am 09:50 **Application of Qualitative and Quantitative Analysis of HRMS to Fast Identification of Major Drug Metabolic Pathways and Drug-Metabolizing Enzymes;** [Qian Ruan](#); Li Ma; Mingshe Zhu; Dept. of Biotransformation, Bristol-Myers Squibb, Princeton, NJ

TOA am 10:10 **Combining Derivatization and SWATH for the Integrated Quantification and Identification of Aldehydes and Ketones in Biological Samples;** David Siegel<sup>1</sup>; Anne Meinema<sup>1</sup>; Hjalmar Permentier<sup>1</sup>; Gerard Hopfgartner<sup>2</sup>; Rainer Bischoff<sup>1</sup>; <sup>1</sup>University of Groningen, Groningen, Netherlands; <sup>2</sup>University of Geneva, Geneva, Switzerland

**8:30 – 10:30 AM, TUESDAY MORNING  
INSTRUMENTATION AND METHODS: FT, ION TRAPS AND  
HYBRID INSTRUMENTS**

**Ryan Danell (Danell Consulting), presiding  
Room 307-308**

TOB am 08:30 **Hybrid Electron Transfer/Ultraviolet Photodissociation for Characterization of Intact Proteins;** Joe Cannon; Dustin Holden; Jennifer Brodbelt; University of Texas, Austin, TX

TOB am 08:50 **Absolute Pressure in FTICR/MS Using “CRAFTI” Technique For Measuring Collision Cross Sections;** Chad Jones; David V. Dearden; Brigham Young University, Provo, UT

TOB am 09:10 **A New Method for Isolating Ions in Quadrupole Ion Traps Using an Excitation Waveform Generated by Frequency Modulation and Upconversion;** Ryan T. Hilger; Robert E. Santini; Boone M. Prentice; Scott A. McLuckey; Purdue University, West Lafayette, IN

TOB am 09:30 **Dual-Trap Configuration for High Efficiency Tandem Mass Spectrometry Analysis;** Linfan Li; Xiaoyu Zhou; Zheng Ouyang; Purdue University, West Lafayette, IN

TOB am 09:50 **Lossless Ion Trapping in Structures for Lossless Ion Manipulation (SLIM);** Xinyu Zhang; Sandilya V.B. Garimella; Spencer A. Prost; Ian K. Webb; Randolph V. Norheim; Brian L. LaMarch; Tsung-Chi Chen; Aleksey V. Tolmachev; Gordon A. Anderson; Yehia M. Ibrahim; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA

TOB am 10:10 **Setting New Speed Records for Orbitrap Mass Spectrometry;** Alexander Makarov; Jan-Peter Hauschild; Eduard Denisov; Amelia Peterson; Oliver Lange; Eugen Damoc; Mathias Mueller; Konstantin Ayzikov; Andreas Wieghaus; Markus Kellmann; Thermo Fisher Scientific, Bremen, Germany

**8:30 – 10:30 AM, TUESDAY MORNING  
ION MOBILITY: SEPARATIONS**

**Stephen Valentine (West Virginia University), presiding  
Room 309-310**

TOC am 08:30 **Progress in the Development of Structures for Extended and Lossless Ion Separations and Manipulations;** Richard D. Smith; Xinyu Zhang; Ian Webb; Tsung-Chi Chen; Sandilya Garimella; Aleksey Tolmachev; Yehia Ibrahim; Gordon Anderson; Erin Baker; PNNL, Richland, WA

TOC am 08:50 **Ion Mobility Spectrometry of Foldamers;** Frédéric Rosu<sup>1</sup>; Christian Klein<sup>2</sup>; Xuesong Li<sup>3,4</sup>; Victor Maurizot<sup>3,4</sup>; Ivan Huc<sup>3,4</sup>; Valérie Gabelica<sup>4,5</sup>; <sup>1</sup>CNRS UMS 3033, Inserm U001, IECB, Pessac, France; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>CNRS, UMR 5284, CBMN, Pessac, France; <sup>4</sup>Université de Bordeaux, IECB, Pessac, France; <sup>5</sup>Inserm, U869 ARNA, Bordeaux, France

TOC am 09:10 **Accuracy in Ion Mobility Spectrometry: Requirements and Results;** Brian Hauck<sup>1</sup>; Bill Siems<sup>1</sup>; Charles Harden<sup>2</sup>; Vincent McHugh<sup>3</sup>; Herbert Hill, Jr.<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>LEIDOS - US Army ECBC Operations, Gunpowder, MD; <sup>3</sup>U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD

TOC am 09:30 **Ion Mobility Mass Spectrometry Differentiates Multiprotein Complex Structures formed in Solution and in Electrospray Droplets;** Linjie Han; Brandon Ruotolo; University of Michigan, Ann Arbor, MI

TOC am 09:50 **Structural Characterization of Methylenedianiline Regioisomers by Ion Mobility-Mass Spectrometry, Tandem Mass Spectrometry, and Computational Strategies;** Sarah M. Stow<sup>1</sup>; Jay G. Forsythe<sup>1</sup>; Tiffany M. Onifer<sup>1</sup>; Hartmut Nefzger<sup>2</sup>; Nicholas W. Kwiecien<sup>3</sup>; Jody C. May<sup>1</sup>; David M. Hercules<sup>1</sup>; John A. McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Bayer MaterialScience AG, Leverkusen B108, Germany; <sup>3</sup>University of Wisconsin, Madison, WI

TOC am 10:10 **IR Spectroscopy of IMS-MS Selected Protein Ions;** Stephan Warnke; Kevin Pagel; Gert von Helden; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

**8:30 – 10:30 AM, TUESDAY MORNING  
MACROMOLECULAR COMPLEXES: ACTIVATION AND  
DISSOCIATION**

**Brian Bothner (Montana State University), presiding  
Room 314-317**

TOD am 08:30 **Multi-Step Sequencing and Confident Identification of Native Protein Complexes with an Orbitrap Mass Spectrometer;** Mikhail Belov<sup>1,3</sup>; Eugen Damoc<sup>3</sup>; Eduard Denisov<sup>3</sup>; Philip Compton<sup>2</sup>; Neil L. Kelleher<sup>2</sup>; Alexander Makarov<sup>3</sup>; <sup>1</sup>Spectrograph LLC, Kennewick, WA; <sup>2</sup>Northwestern University, Evanston, IL; <sup>3</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany

TOD am 08:50 **Protein Complexes: Breaking Up is Hard to Do (Unless You Have an FTMS);** Huilin Li; Jiang Zhang; Piriya Wongkongkathap; Rachel R. Ogorzalek Loo; Joseph A. Loo; UCLA, Los Angeles, CA

TOD am 09:10 **Surface Induced Dissociation (SID) and Collision Induced Dissociation (CID) Characterization of Human Nucleosomes;** Yun Zhang; Xin Ma; Morgan Bernier; Cecil Howard; Michael Poirier; Jennifer Ottesen; Vicki Wysocki; The Ohio state university, Columbus, OH

TOD am 09:30 **Probing Protein Stability, Unfolding and Dissociation with Variable Temperature Mass Spectrometry and Variable Temperature Ion Mobility Mass Spectrometry;** Kamila Pacholarz<sup>1</sup>; Perdita Barran<sup>2</sup>; <sup>1</sup>University of Edinburgh, Edinburgh, UK; <sup>2</sup>University of Manchester, Manchester, UK

TOD am 09:50 **Top-Down Characterization of Non-Covalent Protein Complexes via Ultraviolet Photodissociation Mass Spectrometry;** John O'Brien; Jennifer Brodbelt; University of Texas, Austin, TX

- TOD am 10:10 **Association of the Dual Specificity Phosphatase DUSP12 with Various Messenger Ribonucleoprotein Particles Revealed by Interactome Analysis**; Panayiotis Vacratsis; *University of Windsor, Windsor, Canada*
- 8:30 – 10:30 AM, TUESDAY MORNING  
PK/PD ANALYSIS OF BIOLOGICS  
John Schiel (NIST), presiding  
Ballroom I, level 4**
- TOE am 08:30 **Transitioning to High-Resolution MS for Bioanalytical Study Support: Comparison of High Resolution MS Technologies**; John Kellie; Jonathan Kehler; Matthew Szapacs; *GSK, King Of Prussia, PA*
- TOE am 08:50 **In vivo Quantitation of Endosome-Disruptive Peptides using High-Resolution Mass Spectrometry to Support Pharmacokinetic Studies**; Bao-Jen Shyong; Rob Burke; Rubina Parmar; Elizabeth Mahan; Suzie Yeh; Rena Zhang; Mark Cancilla; *Merck & Co. Inc., West Point Plant, PA*
- TOE am 09:10 **Expanding the Possibilities of LC-MS/MS for the Quantification of (Therapeutic) Proteins in Complex Biological Matrices**; Kees Bronsema<sup>1,2</sup>; Rainer Bischoff<sup>1</sup>; Nico van de Merbel<sup>1,2</sup>; <sup>1</sup>*University of Groningen, Groningen, The Netherlands*; <sup>2</sup>*PRA, Assen, The Netherlands*
- TOE am 09:30 **Applying Acid Dissociation in LC-MS/MS Analysis of A PEGylated Anti-CD28 Domain Antibody in Human Serum**; Chao Gong; Jianing Zeng; Billy Akinsanya; Hao Jiang; Johanna Mora; Shannon Chilewski; Janice Gambardella; Alban Allentoff; Carol Gleason; Anne-Francoise Aubry; Binodh DeSilva; Mark Arnold; *Bristol-Myers Squibb, Princeton, NJ*
- TOE am 09:50 **LC-MS/MS Approaches to Support Clinical Studies of an Extended Half-Life Bioactive Peptide Fused to an Albumin-Binding Domain Antibody**; Chester L Bowen; Jonathan Kehler; Thomas Mencken; Bonnie Orr; Matthew Szapacs; *GlaxoSmithKline, King Of Prussia, PA*
- TOE am 10:10 **Biodistribution Studies of Transferrin-Based Drug in Animal Models by Inductively Coupled Plasma Mass Spectrometry (ICP-MS)**; Son N. Nguyen; Hanwei Zhao; Shunhai Wang; Cedric Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- 8:30 – 10:30 AM, TUESDAY MORNING  
H/D EXCHANGE: BIOLOGICAL APPLICATIONS  
Derek Wilson (York University), presiding  
Ballroom II, level 4**
- TOF am 08:30 **Setting the Stage: Recent Developments in HDX/MS for Exploring Protein Folding, Structure, Dynamics, and Interactions**; Lars Konermann; *Univ. of Western Ontario, London, Canada*
- TOF am 08:50 **Elucidating the Mechanisms of Antibody Neutralization of HIV Env by H/D Exchange**; Miklos Guttmann<sup>1</sup>; Jean-Philippe Julien<sup>2</sup>; Al Cupo<sup>3</sup>; Rogier Sanders<sup>3</sup>; Ian Wilson<sup>2</sup>; John Moore<sup>3</sup>; Kelly Lee<sup>1</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*Scripps Research Institute, La Jolla, CA*; <sup>3</sup>*Weill Medical College of Cornell University, New York, NY*
- TOF am 09:10 **Deubiquitinase-Induced Stabilization of Proteasomal Subunit Rpn1 Revealed by Hydrogen Exchange Mass Spectrometry**; Bradley Stocks<sup>1</sup>; Geng Tian<sup>2</sup>; Suzanne Elsasser<sup>2</sup>; Daniel Finley<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- TOF am 09:30 **Investigating the Interaction of an IgG<sub>1</sub> Antibody with the Neonatal Fc Receptor by HDX-MS and ETD**; Pernille Foged Jensen<sup>1</sup>; Vincent Larraillet<sup>2</sup>; Maximiliane Hilger<sup>2</sup>; Kasper D. Rand<sup>1</sup>; <sup>1</sup>*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Pharma Research, Roche Diagnostics GmbH, Penzberg, Germany*
- TOF am 09:50 **HDX Analysis of RGS-Gα and Multimeric Protein Complexes; Use of Isotopic Labeling**; Devrishi Goswami<sup>1</sup>; Nicole Brown<sup>2</sup>; Bruce Pascal<sup>1</sup>; Steve Tusky<sup>3</sup>; Eddy Arnold<sup>3</sup>; John Hepler<sup>2</sup>; Patrick Griffin<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, Scripps Florida, Jupiter, FL*; <sup>2</sup>*Emory University, Atlanta, Georgia*; <sup>3</sup>*Rutgers University, Piscataway, New Jersey*
- TOF am 10:10 **Implementing H/DX-MS in Therapeutic Protein Formulation Development**; Jun Zhang; Douglas Banks; Michael Treuheit; Gerald Becker; *Amgen, Inc, Seattle, WA*
- 8:30 – 10:30 AM, TUESDAY MORNING  
PHOSPHOPROTEOMICS IN DISEASE  
Ying Ge (University of Wisconsin), presiding  
Ballroom III, level 4**
- TOG am 08:30 **Proteogenomic Analysis of Human Breast Cancer Connects Genetic Alterations to Phosphorylation Networks**; Philipp Mertins<sup>1</sup>; Jana Qiao<sup>1</sup>; Karl R. Clauser<sup>1</sup>; D. R. Mani<sup>1</sup>; Michael Gillette<sup>1</sup>; Kelly Ruggles<sup>2</sup>; David Fenyó<sup>3</sup>; Sherri Davies<sup>4</sup>; Pei Wang<sup>5</sup>; Ping Yan<sup>6</sup>; Chenwei Lin<sup>6</sup>; Sean Wang<sup>6</sup>; Yuzheng Zhang<sup>6</sup>; Michael McLellan<sup>4</sup>; Henry Rodriguez<sup>7</sup>; Reid Townsend<sup>4</sup>; Li Ding<sup>4</sup>; Amanda Paulovich<sup>6</sup>; Matthew Ellis<sup>4</sup>; Steven A. Carr<sup>1</sup>; *Clinical Proteomic Tumor Analysis Consortium (CPTAC)*<sup>7</sup>; <sup>1</sup>*The Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*NYU Langone Medical Center, New York, NY*; <sup>3</sup>*New York University, New York, NY*; <sup>4</sup>*Washington University, St. Louis, MO*; <sup>5</sup>*Icahn School of Medicine at Mount Sinai, New York, NY*; <sup>6</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>7</sup>*National Cancer Institute, Bethesda, MD*
- TOG am 08:50 **Identification of Post-translational Modifications of Human Desmoplakins in Regulating Interactions with Intermediate Filaments**; Lichao Zhang<sup>1</sup>; Lauren Albrecht<sup>2</sup>; Kathleen Green<sup>2,3</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald Hunt<sup>1,4</sup>; <sup>1</sup>*Department of Chemistry, University of Virginia, Charlottesville, VA*; <sup>2</sup>*Department of Pathology, Northwestern University, Chicago, IL*; <sup>3</sup>*Department of Dermatology, Northwestern University, Chicago, IL*; <sup>4</sup>*Department of Pathology, University of Virginia, Charlottesville, VA*
- TOG am 09:10 **Quantitative Phosphoproteomic Analysis of the PTEN Signaling Pathway**; Saddiq Zahari; Jacqueline Douglass; Min Sik Kim; Patrick Shaw; Derese Getnet; Ben Park; Xinyan Wu; Akhilesh Pandey; *Johns Hopkins School of Medicine, Baltimore, MD*
- TOG am 09:30 **Phosphoproteome Profiling of Toll-Like Receptor Response to Different Ligand Stimulation in Macrophages; Role of MARCKS Ser163 Phosphorylation**; Virginie Sjoelund; Margery Smelkinson; Iain Fraser; Aleksandra Nita-Lazar; *NIH, Bethesda, MD*

## TUESDAY MORNING AND AFTERNOON ORAL SESSIONS

- TOG am 09:50 **Multi-Notch MS3-Based 10-Plex TMT Quantification of Human Colorectal Cancer Cells Reveals Distinct Temporal Phosphoproteomic Profiles in Wnt Signaling;** Mark P. Jedrychowski; Ryan Kunz; Robert A. Everley; David P. Nusinow; Leonid Peshkin; Marc W. Kirschner; Steven P. Gygi; *Harvard Medical School, Boston, MA*
- TOG am 10:10 **Drug-based Phosphoproteomic Study of Human Insulin Receptor Phosphorylation with Nano-flow UPLC-MS and UPLC-MS/MS;** Jason X. Tang; Zhongping Liao; John Beals; *Eli Lilly & Company, Indianapolis, IN*
- 8:30 – 10:30 AM, TUESDAY MORNING IMAGING: PHARMACEUTICALS AND METABOLOMICS**  
**Lingjun Li (University of Wisconsin-Madison), presiding**  
**Ballroom IV, level 4**
- TOH am 08:30 **Pharmaceutical Mass Spectrometry Imaging: A Cross Platform Approach for Both Targeted and Untargeted Molecular Histology;** Richard Goodwin<sup>1</sup>; John Swales<sup>1</sup>; Anna Nilsson<sup>2</sup>; C. Logan Mackay<sup>3</sup>; Per Andren<sup>2</sup>; Jennifer Sasaki<sup>4</sup>; Peter Webbom<sup>1</sup>; Anshul Gupta<sup>4</sup>; <sup>1</sup>*AstraZeneca, Macclesfield, UK*; <sup>2</sup>*Uppsala University, Uppsala, Sweden*; <sup>3</sup>*University of Edinburgh, Edinburgh, UK*; <sup>4</sup>*AstraZeneca, Waltham, MA*
- TOH am 08:50 **Mapping HIV Drugs in Tissue using IR-MALDESI MSI Coupled to the Q Exactive with Several Acquisition Modes;** David C. Muddiman<sup>1</sup>; Jeremy Barry<sup>1</sup>; Guillaume Robichaud<sup>1</sup>; Mark Bokhart<sup>1</sup>; Corbin Thompson<sup>2</sup>; Craig Sykes<sup>2</sup>; Angela Kashuba<sup>2</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*UNC Chapel Hill, Chapel Hill, NC*
- TOH am 09:10 **Multimodal Biomarkers Discovery in Kidney Disease using High Spatial and Spectral Resolution Mass Spectrometry Imaging;** Satoshi Miyamoto<sup>2,3</sup>; Gregory Hamm<sup>1</sup>; David Bonnell<sup>1</sup>; Kumar Sharma<sup>2,3</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>*ImaBiotech, MS Imaging Dept., LOOS, France*; <sup>2</sup>*Institute of Metabolomic Medicine, San Diego, CA*; <sup>3</sup>*Center for Renal Translational Medicine, Division, San Diego, CA*
- TOH am 09:30 **Tracking Metabolomic Dynamics during Corn Seed Germination using MALDI Mass Spectrometry Imaging;** Adam Feenstra<sup>1,2</sup>; Korte<sup>1,2</sup>; Young-Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames Laboratory, Ames, IA*
- TOH am 09:50 **Spatial Metabolomics of Alzheimer's Disease Brains using LAESI-MS;** Greg Kilby<sup>2</sup>; Callee Walsh<sup>2</sup>; Pamela Cantrell<sup>2</sup>; Greg Boyce<sup>2</sup>; James Langridge<sup>1</sup>; Giuseppe Astarita<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Protea Biosciences, Morgantown, WV*
- TOH am 10:10 **Imaging Mass Spectrometry of 3D Cell Cultures: Novel Approach to Evaluate the Penetration of New Therapeutics and Apoptotic Imaging Probes;** Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*

**10:30 AM – 2:30 PM, TUESDAY**  
**TUESDAY POSTER SESSION**  
**Poster/Exhibit Hall**  
Lunch concessions are open 11:00 am – 2:00 pm

## TUESDAY AFTERNOON ORAL SESSIONS

- 2:30 – 4:30 PM, TUESDAY AFTERNOON SPACE SCIENCE, ASTROBIOLOGY, AND ATMOSPHERIC CHEMISTRY**  
**Jos Oomens (Radboud University), presiding**  
**Exhibit Hall AB**
- TOA pm 2:30 **Detection of Organics in Geological Samples Containing Perchlorate with the MOMA Linear Ion Trap Mass Spectrometer;** Ricardo Arevalo Jr.<sup>1</sup>; Xiang Li<sup>2</sup>; Veronica Pinnick<sup>2</sup>; Friso H.W. Van Amerom<sup>3</sup>; Ryan M. Danell<sup>4</sup>; Stephanie Getty<sup>1</sup>; Lars Hovmand<sup>5</sup>; Paul Mahaffy<sup>1</sup>; William Brinckerhoff<sup>1</sup>; Fred Goesmann<sup>6</sup>; Harald Steingger<sup>6</sup>; <sup>1</sup>*NASA GSFC, Greenbelt, MD*; <sup>2</sup>*University of Maryland, Baltimore County, Greenbelt, MD*; <sup>3</sup>*SRI International, Hyattsville, MD*; <sup>4</sup>*Danell Consulting, Inc., Winterville, NC*; <sup>5</sup>*Linear Labs LLC, Washington, DC*; <sup>6</sup>*MPS, Lindau, Germany*
- TOA pm 2:50 **Label-Free Quantitation and Dynamic SILAC to Investigate the Effects of Microgravity on Primary Cardiac Cells;** J. Will Thompson<sup>1</sup>; Bryan J. Feger<sup>1</sup>; Laura G. Dubois<sup>1</sup>; Matthew W. Foster<sup>1</sup>; Lisa Scott Carnell<sup>2</sup>; Dawn E. Bowles<sup>1</sup>; M. Arthur Moseley<sup>1</sup>; <sup>1</sup>*Duke University School of Medicine, Durham, NC*; <sup>2</sup>*NASA Langley Research Center, Hampton, VA*
- TOA pm 3:10 **Identification and Separation of Oxidized Organic Aerosol Precursors using a Novel Field-Deployable High Resolution Ion Mobility Time-of-Flight Mass Spectrometer (IMS-TOF);** Jordan Krechmer<sup>1</sup>; Manjula Canagaratna<sup>2</sup>; Joel Kimmel<sup>2,3</sup>; Heikki Junninen<sup>4</sup>; Richard Knochenmuss<sup>3</sup>; Mike Cubison<sup>3</sup>; Paola Massoli<sup>2</sup>; Harald Stark<sup>1,2</sup>; John T. Jayne<sup>2</sup>; Jason Surratt<sup>5</sup>; Jose L. Jimenez<sup>1</sup>; Douglas Worsnop<sup>2,4</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*; <sup>2</sup>*Aerodyne Research Inc., Billerica, MA*; <sup>3</sup>*Tofwerk, AG, Thun, Switzerland*; <sup>4</sup>*University of Helsinki, Helsinki, Finland*; <sup>5</sup>*University of North Carolina, Chapel Hill, NC*
- TOA pm 3:30 **Proteome Expression Profiling of Hypergravity Exposure in *Drosophila*: Preparing for a NASA Space Mission;** Ravikumar Hosamani<sup>2</sup>; Chris Adams<sup>1</sup>; Shilpa R. Bhardwaj<sup>2</sup>; Anna Okumu<sup>1</sup>; Allis S. Chien<sup>1</sup>; Sharmila Bhattacharya<sup>2</sup>; <sup>1</sup>*Stanford University Mass Spectrometry, Stanford, CA*; <sup>2</sup>*NASA Ames, Sunnyvale, CA*
- TOA pm 3:50 **Reactions of N-containing PAH Anions with N and O atom: A DFT Study of Processes of Interstellar Interest;** Zhechen Wang<sup>1,2</sup>; Veronica M. Bierbaum<sup>1,2</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*; <sup>2</sup>*University of Colorado, Boulder, CO*

## TUESDAY AFTERNOON ORAL SESSIONS

- TOA pm 4:10 **Prebiological Evolution of Macromolecules. Investigation of the Abiogenic Peptide Formation at the Different Conditions by High Resolution Mass Spectrometry;** Alexey Kononikhin<sup>1,2</sup>; Olga Demina<sup>1</sup>; Igor Popov<sup>1,2</sup>; Natalia Starodubtseva<sup>1,2</sup>; Alexey Boldyrev<sup>2</sup>; Andrey Khodonov<sup>1</sup>; Sergey Varfolomeev<sup>1</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>*Emanuel Institute of Biochemical Physics, Moscow, Russia*; <sup>2</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russia*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
NANO-SCALE AND MICROFLUIDIC SEPARATIONS AND MASS SPECTROMETRY**  
Bryan Fonslow (Scripps Research Institute), presiding  
Room 307-308
- TOB pm 2:30 **Next Generation Blood Sampling For Mass Spectral Analysis Of Proteins and Metabolites;** Fred Regnier<sup>1</sup>; Tim Woenker<sup>2</sup>; JinHee Kim<sup>2</sup>; Jiri Adamec<sup>3</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Novilytic Laboratories, West Lafayette, Indiana*; <sup>3</sup>*University of Nebraska, Lincoln, NE*
- TOB pm 2:50 **Peering into Biology from the Outside: Exometabolic Microfluidics-Based Platforms Integrated with Structural Mass Spectrometry for Systems, Synthetic, and Chemical Biology;** John A. Mclean; Stacy D. Sherrod; Cody R. Goodwin; Virginia Pensabene; John P. Wiksw; *Vanderbilt University, Nashville, TN*
- TOB pm 3:10 **High Peak Capacity Ultranarrow PLOT LC Columns Coupled to Mass Spectrometry for Proteomic Analysis of Vanishingly Small Samples;** Barry L. Karger<sup>1</sup>; Siyang Li<sup>1</sup>; Xianzhe Wang<sup>1</sup>; Shashi K. Murthy<sup>1</sup>; David Fenyo<sup>2</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>*Barnett Institute, Northeastern University, Boston, MA*; <sup>2</sup>*New York University, New York, NY*
- TOB pm 3:30 **High Resolution HILIC for Proteomic LC-MS;** Kanta Horie<sup>1,2</sup>; Takeo Kamakura<sup>1</sup>; Suguru Ichihara<sup>1</sup>; Masaki Wakabayashi<sup>1</sup>; Nobuo Tanaka<sup>3</sup>; Yasushi Ishihama<sup>1</sup>; <sup>1</sup>*Kyoto University, Kyoto, Japan*; <sup>2</sup>*Eisai Co., Kawashima, Japan*; <sup>3</sup>*GL Sciences, Iruma, Japan*
- TOB pm 3:50 **Capillary Zone Electrophoresis-Electrospray Ionization-Tandem Mass Spectrometry for Highly Sensitive Shotgun Proteomics;** Liangliang Sun; Guijie Zhu; Xiaojing Yan; Si Mou; Norman J. Dovichi; *University of Notre Dame, South Bend, IN*
- TOB pm 4:10 **A Hybrid Microchip/Capillary Electrophoresis Mass Spectrometry Platform for Rapid and Ultrasensitive Bioanalysis;** Ryan T. Kelly<sup>1</sup>; Chengcheng Wang<sup>2</sup>; Cheng S. Lee<sup>2</sup>; Richard D. Smith<sup>1</sup>; Keqi Tang<sup>1</sup>; <sup>1</sup>*Pacific NW National Laboratory, Richland, WA*; <sup>2</sup>*University of Maryland, College Park, MD*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
PROTEIN-PROTEIN AND PROTEIN-LIGAND INTERACTIONS**  
Renato Zenobi, (ETH Zurich), presiding  
Room 309-310
- TOC pm 2:30 **Sheathless Capillary Electrophoresis Coupled with Mass Spectrometry in Analysis of Native Proteins and Protein Complexes;** Alexander R. Ivanov<sup>1</sup>; Rosa Viner<sup>3</sup>; Marcia R. Santos<sup>2</sup>; David Horn M. <sup>3</sup>; David R. Bush<sup>1</sup>; Arseniy M. Belov<sup>1</sup>; Barry L. Karger<sup>1</sup>; <sup>1</sup>*Barnett Institute, Northeastern University, Boston, MA*; <sup>2</sup>*Sciex Separations, Brea, CA*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- TOC pm 2:50 **Nanodiscs and CaR-ESI-MS: A Novel Method for the Discovery of Protein-Glycosphingolipid Interactions;** Aneika Leney; Xuxin Fan; Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- TOC pm 3:10 **Using Ion Mobility-Mass Spectrometry to Study the Interactions between Human Histone Deacetylase 8 and Poly-r(C)-binding Protein 1;** Shuai Niu; Byung Chul Kim; Carol Fierke; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- TOC pm 3:30 **The Attainment of Low-Charge State HK97 Bacteriophage Capsid at 13 MTh using STJ Cryodetection MALDI Time-of-Flight Mass Spectrometry;** Jonathan Feldman<sup>1</sup>; Robert Duda<sup>2</sup>; Roger Hendrix<sup>2</sup>; Mark E. Bier<sup>1</sup>; <sup>1</sup>*Carnegie Mellon University, Pittsburgh, PA*; <sup>2</sup>*University of Pittsburgh, Pittsburgh, Pennsylvania*
- TOC pm 3:50 **Electron Transfer Dissociation of Native Protein Complexes on a Quadrupole/Ion Mobility/TOF Instrument;** Frederik Lermlyte<sup>1,2</sup>; Albert Konijnenberg<sup>1</sup>; Jonathan P. Williams<sup>3</sup>; Jeff Brown<sup>3</sup>; Dirk Valkenborg<sup>2,4</sup>; Frank Sobott<sup>1,2</sup>; <sup>1</sup>*University of Antwerp, Antwerpen, Belgium*; <sup>2</sup>*CFP-CeProMa, University of Antwerp, Antwerp, Belgium*; <sup>3</sup>*Waters Corporation, Manchester, UK*; <sup>4</sup>*VITO, Mol, Belgium*
- TOC pm 4:10 **Towards a Molecular “Microscope”: MS-Based Identification of Endogenous Protein-Protein Interactions and Proximities using Global Chemical Stabilization in the Cellular Milieu;** Roman Subbotin; Brian Chait; *The Rockefeller University, New York, NY*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
FUNDAMENTALS OF PEPTIDE FRAGMENTATION**  
Yu Xia (Purdue University), presiding  
Room 314-317
- TOD pm 2:30 **IRMPD Spectroscopy of Ammonia Complexes of Peptide Fragments;** Oscar Hernandez<sup>2</sup>; Philippe Maitre<sup>2</sup>; Bela Paizs<sup>1</sup>; <sup>1</sup>*Bangor University, Bangor, UK*; <sup>2</sup>*Université Paris Sud, Paris, France*
- TOD pm 2:50 **ETD Performance Comparison among Benzyl/ Methyl/ n-Butylguanidine-Tagged Peptides;** Chang Xue; Jan Urban; František Tureček; *University of Washington, Department of Chemistry, Seattle, WA*
- TOD pm 3:10 **Radical Additions to Aromatic Residues in Peptides Facilitate Unexpected Side Chain and Backbone Losses;** Xing Zhang; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- TOD pm 3:30 **Understanding the Electron Capture Dissociation of Phosphopeptides by Use of Ion Mobility Mass Spectrometry and Molecular Dynamics Simulations;** Helen J. Cooper<sup>1</sup>; Andrew W. Jones<sup>1</sup>; Andrew J. Creese<sup>1</sup>; Doyong Kim<sup>2</sup>; David H. Russell<sup>2</sup>; <sup>1</sup>*University of Birmingham, Birmingham, UK*; <sup>2</sup>*Texas A&M University, College Station, Texas*
- TOD pm 3:50 **Enhanced Loss of Phosphate from Isobarically Tagged Phosphotyrosine Peptides: Impact on Site Localization Assignment, Immonium Ion Formation and MS/MS Interpretation;** Robert A. Everley<sup>1</sup>; Edward L. Huttlin<sup>1</sup>; Sean A. Beausoleil<sup>2</sup>; Steven P. Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Cell Signaling Technology, Danvers, MA*

- TOD pm 4:10 **Applying Arginylation for Proteomics;** H. Alexander Ehardt; Ruedi Aebersold; *ETH Zurich, Zurich, CH*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
TOP-DOWN PROTEIN ANALYSIS**  
**Jeff Agar (Northeastern University), presiding  
Ballroom I, level 4**
- TOE pm 2:30 **Top Down Ultraviolet Photodissociation For Confirmation of Linkage Specificity of Polyubiquitin Chains;** Joe R. Cannon; Kirby Martinez-Fonts; Andreas Matouschek; Jennifer S. Brodbelt; *Univ. of Texas at Austin, Austin, TX*
- TOE pm 2:50 **Intact Protein Characterization using Ultraviolet Photodissociation in a FT-ICR Mass Spectrometer;** Jared B. Shaw; Franklin E. Leach III; Tzu-Yung Lin; Si Wu; Errol W. Robinson; David W. Koppelaar; Ljiljana Paša-Tolić; *Pacific Northwest National Laboratory, Richland, WA*
- TOE pm 3:10 **Probing the Structures of Protein Complexes up to 800 kDa by Native Top-Down Tandem Mass Spectrometry with FT-ICR;** Huilin Li<sup>1</sup>; Jeremy Wolff<sup>2</sup>; Steve L. Van Orden<sup>2</sup>; Iain D G Campuzano<sup>3</sup>; Piriya Wongkongkathep<sup>1</sup>; Rachel R. Ogorzalek Loo<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>*UCLA, Los Angeles, CA*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*; <sup>3</sup>*Amgen Inc., Thousand Oaks, CA*
- TOE pm 3:30 **Quantitation of Proteoform-Level Responses in Oncogene-Induced Senescence using Label-free Top Down Proteomics and Advanced Data Acquisition;** Kenneth Durbin; Ryan Fellers; Paul Thomas; Philip Compton; Neil L. Kelleher; *Northwestern University, Evanston, IL*
- TOE pm 3:50 **Investigating Redox Regulation in the Apoptotic Pathway using High Resolution Mass Spectrometry;** Sophie Thurlow; David Clarke; Pat Langridge-Smith; C. Logan Mackay; Colin Campbell; *Edinburgh University, Edinburgh, UK*
- TOE pm 4:10 **Quantitation of Histones H2A/H2B and Their Changes during Biological Events by Top-Down FT-ICR MS/MS Analysis;** Xibei Dang<sup>1</sup>; Brian D. Spetman<sup>1</sup>; Krystal D. Nolan<sup>2</sup>; Jennifer S. Isaacs<sup>2</sup>; Jonathan H. Dennis<sup>1</sup>; Alan G. Marshall<sup>3</sup>; Nicolas L. Young<sup>3</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL*; <sup>2</sup>*Medical University of South Carolina, Charleston, SC*; <sup>3</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
DRUG TARGET DISCOVERY AND VALIDATION**  
**Jim Glick (Novartis BioMedical Research Institute), presiding  
Ballroom II, level 4**
- TOF pm 2:30 **Dissecting the Binding Mode of Low Affinity Phage Display Ligands by Hydrogen/Deuterium Exchange Mass Spectrometry;** Ulrike Leurs<sup>1</sup>; Rasmus Clausen<sup>1</sup>; Brian Lohse<sup>1</sup>; Jesper Kristensen<sup>1</sup>; Kasper D. Rand<sup>2</sup>; <sup>1</sup>*University of Copenhagen, Copenhagen, Denmark*; <sup>2</sup>*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*
- TOF pm 2:50 **Impacting Translation of Biotherapeutics with Immunoaffinity LC-MS/MS Quantification of Protein Targets;** Joe Palandra; Hendrik Neubert; *Pfizer, Andover, MA*
- TOF pm 3:10 **Central Dogma of Proteomics Provides Identification of Protein Targets, Action Mechanisms and Cellular Death Pathways of Small Molecule Anticancer Drugs;** Consuelo Marin Vicente<sup>1,2</sup>; Mohammad Pirmoradian<sup>1</sup>; Bo Zhang<sup>1</sup>; Alexey Chernobrovkin<sup>1</sup>; Neus Visa<sup>2</sup>; Roman Zubarev<sup>1</sup>; <sup>1</sup>*Karolinska Institute, Stockholm, Sweden*; <sup>2</sup>*Stockholm University, Stockholm, Sweden*
- TOF pm 3:30 **Affinity Selection - High Resolution Mass Spectrometry Screening to Rapidly Assess Druggability in the NF-kappaB Pathway;** Christine L. Andrews; Victoria Kutilek; Matthew Richards; Elliott Nickbarg; Michael Ziebell; Ryan Boinay; Chad Chamberlin; Patrick Curran; Peter Saradjian; Berengere Sauvagnat; Xianshu Yang; Nadya Smotrov; Zangwei Xu; Peter Dandliker; Ilona Kariv; Bruce Beutel; *Merck, Boston, MA*
- TOF pm 3:50 **Ion Mobility-Mass Spectrometry for Screening Amyloid Formation Inhibitors within Rationally-Designed Bifunctional Small Molecule Libraries;** Richard Kerr<sup>1</sup>; Jeffrey S. Derrick<sup>1</sup>; Michael W. Beck<sup>1</sup>; Younwoo Nam<sup>2</sup>; Mi Hee Lim<sup>2</sup>; Brandon Ruotolo<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Ulsan National Institute of Science and Technology, Ulsan, South Korea*
- TOF pm 4:10 **Successful High-Throughput Affinity-Selection Mass Spectrometry Assays of Mixtures of 200 Compounds by Time-of-Flight LCMS;** Mark Bean; Christopher Kwiatkowski; Sunny Hung; Stacy O'Neil Slawacki; Matt Kowalski; Geoffrey Quinke; Larry Szewczuk; Matt Zajac; *GlaxoSmithKline, Collegetown, PA*
- 2:30 – 4:30 PM, TUESDAY AFTERNOON  
CLINICAL DIAGNOSTICS**  
**Tim Garrett (University of Florida), presiding  
Ballroom III, level 4**
- TOG pm 2:30 **Development of on-Cartridge Enzyme Activity Assay for Cholinesterase in Human Whole Blood using Paper Spray Mass Spectrometry;** Yue Ren; Morgan McLuckey; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- TOG pm 2:50 **Targeted Metabolomics in Clinical Research Labs using LC-HRMS: Longitudinal Metabotype Determination for Individualized Biology in Healthy Volunteers;** Amélie Favre<sup>1</sup>; Ronan Euzen<sup>1</sup>; Marko Krstic<sup>1</sup>; Olaf Scheibner<sup>2</sup>; Maciej Bromirski<sup>2</sup>; Pierre-Edouard Sottas<sup>3</sup>; Frédéric Schütz<sup>4</sup>; Bertrand Rochat<sup>1</sup>; <sup>1</sup>*CHUV University Hospital, Lausanne, Switzerland*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>3</sup>*BioKaizen, Monthey, Switzerland*; <sup>4</sup>*Swiss Institute of Bioinformatics, Lausanne, Switzerland*
- TOG pm 3:10 **Validation of an Automated Immuno-MALDI Assay for the Clinical Measurement of Plasma Renin Activity;** Robert Popp<sup>1</sup>; David Malmstrom<sup>1</sup>; Alex Camenzind<sup>1</sup>; Andrew Chambers<sup>1</sup>; J Grace van der Gugten<sup>2</sup>; Daniel Holmes<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*St. Paul's Hospital, UBC, Vancouver, Canada*; <sup>3</sup>*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*

TOG pm 3:30 **Translational Bionformatics Platform for Next Generation Histology by Imaging Mass Spectrometry;** Kirill Veselkov<sup>1</sup>; Reza Mirnezami<sup>1</sup>; Nicole Strittmatter<sup>1</sup>; James Kinross<sup>1</sup>; Abigail Speller<sup>1</sup>; Tigran Abramov<sup>2</sup>; James McKenzie<sup>1</sup>; Emrys Jones<sup>1</sup>; Ara Darzi<sup>1</sup>; Robert Goldin<sup>1</sup>; Elaine Holmes<sup>1</sup>; Jeremy Nicholson<sup>1</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College, London, London; <sup>2</sup>Sevastopol National Technical University, Sevastopol, Ukraine

TOG pm 3:50 **An Empirically Driven Approach for the Identification of Optimal Peptides for Tandem Mass Spectrometry Experiments on Dried Blood Spots;** James G. Bollinger; Clark M. Henderson; Andrew N. Hoofnagle; Michael J. MacCoss; University of Washington, Seattle, WA

TOG pm 4:10 **Universal Calibration: Populations Don't Lie, People Do;** Matthew Crawford<sup>1</sup>; Christopher Shuford<sup>1</sup>; Stacy Dee<sup>1</sup>; Yvonne Wright<sup>1</sup>; Martin Green<sup>1</sup>; Patricia Holland<sup>1</sup>; Mary Morr<sup>1</sup>; Brian Rappold<sup>2</sup>; Russell Grant<sup>1</sup>; <sup>1</sup>LabCorp, Burlington, NC; <sup>2</sup>Essential Testing, LLC, St. Louis, MO

**2:30 – 4:30 PM, TUESDAY AFTERNOON  
IMAGING: FUNDAMENTALS, INSTRUMENTATION, AND  
METHOD DEVELOPMENT**

**Francisco Fernandez Lima (Florida International Univ.), presiding  
Ballroom IV, level 4**

TOH pm 2:30 **High-Resolution Tandem Mass Spectrometry Imaging;** Bernhard Spengler; Dhaka Ram Bhandari; Andreas Römpf; Analytical Chemistry, Giessen, Germany

TOH pm 2:50 **New Developments in Nanospray Desorption Electrospray Ionization Mass Spectrometry: Compensation for Matrix Effects and Shotgun-like Quantification;** Julia Laskin<sup>1,2</sup>; Ingela Lanekoff<sup>1,2</sup>; <sup>1</sup>Pacific NW National Laboratory, Richland, WA; <sup>2</sup>Pacific NW National Laboratory, Richland, WA

TOH pm 3:10 **Multimodal Imaging for Biological Applications: X-ray microCT and Mass Spectrometry Imaging;** Anne Bruinen<sup>1</sup>; Shane Ellis<sup>1</sup>; Enrico Schioppa<sup>2</sup>; Josef Uher<sup>3</sup>; Ron M.A. Heeren<sup>1</sup>; Jan Visser<sup>2</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, Netherlands; <sup>2</sup>FOM institute Nikhef, Amsterdam, the Netherlands; <sup>3</sup>Amsterdam Scientific Instruments, Amsterdam, the Netherlands

TOH pm 3:30 **Coupling Atomic Force Microscopy with Biological Mass Spectrometry for High Spatial Resolution Imaging;** Suman Ghorai; Chinthaka A. Seneviratne; Kermit K. Murray; Louisiana State University, Baton Rouge, LA

TOH pm 3:50 **Multi-modality 3-D Imaging of a Human Carotid Atherosclerotic Plaque: Correlating in vivo Ultrasound and Imaging Mass Spectrometry;** Heath Patterson<sup>1</sup>; Martin Dufresne<sup>1</sup>; Aurelien Thomas<sup>2</sup>; Robert James Doonan<sup>3</sup>; Stella Daskalopoulou<sup>3</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>University of Montreal, Montreal, Canada; <sup>2</sup>University of Lausanne, Lausanne, Switzerland; <sup>3</sup>McGill University Health Centre, Montreal, Canada

TOH pm 4:10 **Soft-landing Ion Mobility Metal Deposition for MALDI-MS Imaging of Forensic and Biological Samples;** Barbara Walton; Drew Sturtevant; Kent Chapman; Guido Verbeck; University of North Texas, Denton, TX

**4:45 – 5:30 PM, TUESDAY AFTERNOON  
AWARD LECTURE**

**Susan T. Weintraub (Univ. of Texas HSC, San Antonio), presiding  
Exhibit Hall AB**



**Biemann Medal**

**Lingjun Li**  
University of Wisconsin-Madison

**5:45 – 7:00 PM, TUESDAY AFTERNOON  
WORKSHOPS**

**Level 3**

**Light refreshments, level 3**

1. H/D Exchange, Covalent Labeling and Crosslinking (organized by H/D Exchange, Covalent Labeling & Cross Linking Interest Group); Room 307-308
2. LC-MS System Performance Tracking in LC-MS Tracking in LC-MS (organized by LC/MS & Related Topics Interest Group); Room 309-310
3. Antibody-Drug Conjugates (ADC) - A Complex Problem in Regulated Bioanalysis (organized by Regulated Bioanalysis Interest Group); Room 314-317
4. Controlling and Measuring Variation in Sample Preparation and Data Analysis in a Core Facility Environment (organized by Analytical Lab Managers Interest Group); Room 336
5. FTMS: ICR and Orbitrap (organized by FTMS Interest Group); Room 337
6. Environmental Impacts and Implications of Hydrocarbon Extraction and Processing – The Role of Mass Spectrometry (organized by Environmental Applications Interest Group); Room 338
7. Gas Phase Ion Chemistry – Thermochemistry, Kinetics and Structures. In Honor of John Bartmess (organized by Fundamentals Interest Group); Room 339-340
8. The NIH Review Process and Mock NIH Study Section; Room 341-342
9. Imaging Mass Spectrometry vs. Histology (organized by Imaging MS Interest Group); Room 343-344
10. Metabolomics: Emerging Technologies for Continued Innovation (organized by Metabolomics Interest Group); Room 345-346
11. 50 Years of the British Mass Spectrometry Society: Past, Present & Future; Room 347-348
12. CHORUS – A Community Solution for the Storage, Visualization, Sharing, and Analysis of Mass Spectrometry Data on the Cloud; Room 349-350

**AFTER 8:00 PM, TUESDAY EVENING  
CORPORATE HOSPITALITY SUITES  
Hilton Hotel**



8:30 – 10:30 AM, WEDNESDAY MORNING  
ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN SAMPLE  
PREPARATION AND MS INTERFACE DESIGN

Mark Lowenthal (NIST), presiding  
Exhibit Hall AB

- WOA am 08:30 **Combining Metal Ion Complexation and Ultrahigh Resolution Mass Spectrometry for the Selective Analysis of Nitrogen Compounds in Asphaltenes;** Wolfgang Schrader; Sami Lababidi; *Max-Planck Inst für Kohlenforschung, Mülheim / Ruhr, Germany*
- WOA am 08:50 **A Combined Experimental and Computational Study on the Reaction Pathways of Fast Pyrolysis of Cellobiose;** Mckay Easton; John Degenstein; Priya Murria; John J. Nash; Hilka I. Kenttamaa; *Purdue University, West Lafayette, IN*
- WOA am 09:10 **Detailed Characterization of Crude Oil and Its Fractions, Is Mass Spectrometry Sufficient?;** Michael T. Cheng; Matthew Hurt; *Chevron Research, Richmond, CA*
- WOA am 09:30 **Separation-Enhanced Characterization of Oxygenated Petroleum Compounds by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS);** Steven M. Rowland<sup>1</sup>; Winston K. Robbins<sup>2</sup>; Yuri E. Corilo<sup>3,4</sup>; Alan G. Marshall<sup>1,4</sup>; Ryan P. Rodgers<sup>3,4</sup>; <sup>1</sup>*FSU Department of Chemistry and Biochemistry, Tallahassee, FL*; <sup>2</sup>*Consultant, Future Fuels Institute, FSU, Tallahassee, FL*; <sup>3</sup>*Future Fuels Institute, Florida State University, Tallahassee, FL*; <sup>4</sup>*Ion Cyclotron Resonance Program, NHMFL, FSU, Tallahassee, FL*
- WOA am 09:50 **Characterization and Quantification of Fermentation Inhibitors in Biomass Hydrolysates for Biofuel Production;** Arne Ulbrich; Alan J. Higbee; Samantha Austin; Daniel R. Noguera; John Ralph; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- WOA am 10:10 **Isomer Distribution Analysis for Improved Hydrocarbon Mixtures Characterization;** Aviv Amirav<sup>1,2</sup>; Tal Alon<sup>1,2</sup>; Alexander Fialkov<sup>1</sup>; <sup>1</sup>*Tel-Aviv University, Tel-Aviv, Israel*; <sup>2</sup>*Aviv Analytical Ltd, Tel Aviv, Israel*

8:30 – 10:30 AM, WEDNESDAY MORNING  
AMBIENT AND ATMOSPHERIC PRESSURE  
IONIZATION: FUNDAMENTALS

Brian Clowers (Washington State University), presiding  
Room 307-308

- WOB am 08:30 **Evaluation of Nanopipette Emitters with Orifice Diameters Less Than 100 Nanometers for Use in Electrospray Ionization Mass Spectrometry;** Steven Ray<sup>1</sup>; Elizabeth Yuill<sup>1</sup>; Alicia Friedman<sup>1</sup>; Anumita Saha<sup>1</sup>; Chris Enke<sup>2</sup>; Gary Hieftje<sup>1</sup>; Lane Baker<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*University of New Mexico, Albuquerque, NM*
- WOB am 08:50 **Fundamental Spray Characteristics and Complex Formation using SAWN and Other Spray Techniques;** Bob Hommersom<sup>1</sup>; Shane R. Ellis<sup>1</sup>; Tiffany Porta<sup>1</sup>; Marc C. Duursma<sup>1</sup>; Yue Huang<sup>2</sup>; Scott R. Heron<sup>2</sup>; David R. Goodlett<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>*FOM Institute AMOLF, Amsterdam, Nederland*; <sup>2</sup>*University of Maryland, Baltimore, MD*

WOB am 09:10 **Supercharging Techniques for Protein Desalting and Structural Characterization from Native Aqueous Solutions;** Catherine A. Cassou; Evan R. Williams; *University of California, Berkeley, Berkeley, CA*

WOB am 09:30 **Evolution of Ions from Charged Droplets Studied by Pulsed Nanospray Coupled to Ion Mobility-Mass Spectrometry;** Carina Minardi; Kaveh Jorabchi; *Georgetown Univ., Washington, DC*

WOB am 09:50 **Surprising New Ionization Methods for Mass Spectrometry, Mechanistic Insights and Potential Practical Utility;** Sarah Trimpin; Corinne Lutomski; Tarick El-Baba; Beixi Wang; Lorelie Imperial; Daniel Woodall; Ruby Kumar; Bryan Harless; Casey Foley; Chih-Wei Liu; Ellen Inutan; *Wayne State University, Detroit, MI*

WOB am 10:10 **Optical Spectroscopic Comparisons of Helium Plasma Ambient Desorption/Ionization Sources for Mass Spectrometry;** Paul Farnsworth<sup>1</sup>; Wade Ellis<sup>1</sup>; Charlotte Reininger<sup>1</sup>; Joel Keelor<sup>2</sup>; Adam Kaylor<sup>2</sup>; <sup>1</sup>*Brigham Young University, Provo, UT*; <sup>2</sup>*Georgia Institute of Technology, Atlanta, GA*

8:30 – 10:30 AM, WEDNESDAY MORNING  
THE TRIPLE QUADRUPOLE 35 YEARS ON EVOLUTION AND  
APPLICATIONS TO CELEBRATE CHRIS ENKE'S 80TH BIRTHDAY  
R. Graham Cooks (Purdue University), presiding  
Room 309-310

- WOC am 08:30 **The Triple Quadrupole: An Historical Perspective;** Richard A. Yost; *University of Florida, Gainesville, FL*
- WOC am 08:50 **The Secret Identity of Phase-Space 'Ellipses' – Are They Misnamed?;** David P.A. Kilgour<sup>1</sup>; David R. Goodlett<sup>1</sup>; John F.J. Todd<sup>2</sup>; <sup>1</sup>*School of Pharmacy, University of Maryland, Baltimore, MD*; <sup>2</sup>*School of Physical Sciences, University of Kent, Canterbury, UK*
- WOC am 09:10 **Mass Selective Axial Ejection in a Low Pressure Linear Ion Trap in the presence of Nonlinear RF Fields;** Mircea Guna; *AB Sciex, Concord, Canada*
- WOC am 09:30 **Moore's Law and the Consequence of Technological Change;** Alan Schoen; *Thermo Fisher Scientific, San Jose, CA*

WOC am 09:50 **Performance Investigation and Mass Resolution Enhancement of an Electrospray Ionization Quadrupole Mass Spectrometer with a Position Sensitive Detector;** Sarfaraz Syed; Gert Eijkel; Shane Ellis; Donald Smith; Ron Heeren; *FOM Institute AMOLF, Amsterdam, The Netherlands*

WOC am 10:10 **Room for Improvement;** Christie G. Enke; *University of New Mexico, Placitas, NM*

8:30 – 10:30 AM, WEDNESDAY MORNING  
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY/CELLULAR  
PATHWAY ANALYSIS  
Michael Fitzgerald (Duke University), presiding  
Room 314-317

WOD am 08:30 **Metastatic Potential of Osteosarcoma Cells Mapped through Kinase Networks;** Ievgen Motorykin; Milan Milovancev; Shay Bracha; Marcus Weinman; Claudia Maier; *Oregon State University, Corvallis, OR*

WOD am 08:50 **Measuring Reduced-Representation Phosphorylation Profiles with a High-Throughput MS Assay Produces a “Connectivity Map” of Signaling Responses to Drug Perturbations;** Jennifer G. Abelin; Jinal Patel; Lola Fagbami; Xiaodong Lu; Steven A. Carr; Jacob D. Jaffe; *Broad Institute of MIT and Harvard, Cambridge, MA*

WOD am 09:10 **Integration of Ribosome Profiling with Label-Free Quantitative Proteomics;** Andy Kong; Chih-Chiang Tsou; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*

WOD am 09:30 **Transformation of Mouse Embryonic Stem Cells to extra-Embryonic Endoderm (XEN) cells: A Proteomic Investigation of Early Cell Fate Decision Making;** Claire Mulvey<sup>1,2</sup>; Christian Schröter<sup>2</sup>; Laurent Gatto<sup>1</sup>; Mike Deery<sup>1</sup>; Kathy Niakan<sup>3</sup>; Alfonso Martinez-Arias<sup>2</sup>; Kathryn S. Lilley<sup>1</sup>; <sup>1</sup>*Dept. of Biochemistry, University of Cambridge, Cambridge, U.K.*; <sup>2</sup>*Dept. of Genetics, University of Cambridge, Cambridge, U.K.*; <sup>3</sup>*MRC NIMR, Mill Hill, London, U.K.*

WOD am 09:50 **Cross-Omics: Global Phosphoproteomics and Metabolomics Reveals a Connection between Kinase Inhibition and RNA Processing in BCR-ABL H929 Myeloma Cells;** Susanne Breikopf<sup>1,2</sup>; Min Yuan<sup>1</sup>; Katja Helenius<sup>1,2</sup>; Costas Lyssiotis<sup>3</sup>; John M Asara<sup>1</sup>; <sup>1</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*; <sup>3</sup>*Weill Cornell Medical College, New York, NY*

WOD am 10:10 **NeuCode Mouse: Multiplexed Proteomic Analysis Reveals Tissue Specific Effects of Deubiquitinase Deletion;** Christopher M. Rose<sup>1</sup>; Joshua M. Baughman<sup>2</sup>; Timothy W. Rhoads<sup>1</sup>; Clay E. Williams<sup>1</sup>; Anna E. Merrill<sup>1</sup>; Donald S. Stapleton<sup>1</sup>; Mark P. Keller<sup>1</sup>; Alexander S. Hebert<sup>1</sup>; Michael W. Westphall<sup>1</sup>; Alan D. Attie<sup>1</sup>; Donald S. Kirkpatrick<sup>2</sup>; Anwasha Dey<sup>2</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Genentech, South San Francisco, CA*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
PEPTIDOMICS**

**Amanda Hummon (University of Notre Dame), presiding  
Ballroom I, level 4**

WOE am 08:30 **Distinct Peptidome Signatures of Triple Negative Breast Cancer Revealed by Large-Scale Comparative Peptidomic Analysis;** Chaochao Wu; Zhe Xu; Fang Xie; Athena Schepmoes; Thomas Fillmore; Rosalie Chu; Gordon Slys; Matthew Monroe; Ronald Moore; Yufeng Shen; Nikola Tolic; Samuel Payne; David Camp; Tao Liu; Richard Smith; *Pacific Northwest National Laboratory, Richland, WA*

WOE am 08:50 **Peptidomics of Human Milk during Lactation and Mastitis;** Stephanie Contreras; Andres Guerrero; Dave Dallas; Lauren Wu; Jennifer Smilowitz; Daniela Barile; Bruce German; Carlito Lebrilla; *University of California, Davis, Davis, CA*

WOE am 09:10 **Mass Spectral Investigation of Circadian Rhythm-Related Neuropeptide Secretion in Crustacean via *in vivo* Microdialysis;** Zhidan Liang<sup>1</sup>; Claire Schmerberg<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>*UW-Madison, Madison, Wisconsin*; <sup>2</sup>*Duke University, Durham, NC*

WOE am 09:30 **Investigating Mechanism of Preeclampsia by Probing Low Molecular Weight (LMW) Placental Proteome using Capillary Liquid Chromatography-Time-Of-Flight Mass Spectrometer (cLC/Q-ToF);** Komal Kedia; Steven Graves; Craig Thulin; Bruce Jackson; *BYU, Provo, Utah*

WOE am 09:50 **Analytical Strategy for the High-Throughput Sequencing of Venom Peptides (1-10kDa) Combining Cutting-Edge Technologies of Proteomics, Transcriptomics and Bioinformatics;** Loic Quinton<sup>1</sup>; Michel Degueudre<sup>1</sup>; Julien Echterbille<sup>1</sup>; Marion Verdenaud<sup>2</sup>; Madeleine Boulanger<sup>1</sup>; Charlotte Gouin<sup>3</sup>; Jordi Durban<sup>4</sup>; Raquel Rodriguez<sup>4</sup>; Rebeca Minambres<sup>4</sup>; Frederic Ducancel<sup>2</sup>; Nicolas Gilles<sup>3</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>*Laboratory of mass spectrometry, ULg, Liège, Belgique*; <sup>2</sup>*iBiTEc S/SPI Antibody Eng. for Health, Gif-sur-Yvette, France*; <sup>3</sup>*iBiTEcS, SIMOPRO, Gif-sur-Yvette, France*; <sup>4</sup>*Sistemas Genomicos Ltd, Valencia, Spain*

WOE am 10:10 **Expanding the Detectable HLA Peptide Repertoire using Electron-Transfer / Higher-Energy Collision Dissociation (ETHcD);** Geert P.M. Mommen<sup>1</sup>; Christian K. Frese<sup>2</sup>; Hugo D. Meiring<sup>1</sup>; Jacqueline van Gaans-van den Brink<sup>3</sup>; Ad P.J.M. de Jong<sup>1</sup>; Cecile A.C.M. van Els<sup>3</sup>; Albert J.R. Heck<sup>2</sup>; <sup>1</sup>*Intravacc, Bilthoven, Netherlands*; <sup>2</sup>*Utrecht University, Utrecht, Netherlands*; <sup>3</sup>*RIVM, Bilthoven, Netherlands*

**8:30 – 10:30 AM, WEDNESDAY MORNING  
PHARMACOPROTEOMICS AND TOXICOPROTEOMICS FOR  
DRUG DEVELOPMENT**

**Alexander Ivanov (Northeastern University), presiding  
Ballroom II, level 4**

WOF am 08:30 **High Resolution LC/MS-based Background Subtraction for Toxicoproteomic Profiling: Application to Differentiate Microsomal Protein Bindings of Acetaminophen versus Those of 3-hydroxyacetanilide;** Haiying Zhang; Jinping Gan; Yue-Zhong Shu; W. Griffith Humphreys; *Bristol-Myers Squibb R&D, Princeton, NJ*

WOF am 08:50 **Absolute Quantitation of NAPQI-modified Serum Albumin from Rat Plasma Samples by LC-MS/MS: Monitoring Acetaminophen Toxicity;** André Leblanc; Tze Chieh Shiao; René Roy; Lekha Sleno; *UQAM, Montreal, Canada*

WOF am 09:10 **Direct Monitoring of Protein-Protein Inhibition Using Nano Electrospray Ionization Mass Spectrometry;** Dragana Cubrilovic<sup>1</sup>; Konstantin Barylyuk<sup>1</sup>; Daniela Hofmann<sup>1</sup>; Martin Gräber<sup>2</sup>; Thorsten Berg<sup>2</sup>; Gerhard Wider<sup>1</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*Universität Leipzig, Leipzig, Germany*

WOF am 09:30 **Tandem Mass-Spectrometry on Native Non-Reduced and Reduced Antibody-Drugs Conjugates using an Orbitrap Mass Spectrometer Equipped with a High-Mass Quadrupole;** Andrey Dyachenko<sup>1,2</sup>; Sara Rosati<sup>1,2</sup>; Mike Belov<sup>3</sup>; Eugen Damoc<sup>3</sup>; Eduard Denisov<sup>3</sup>; Alexander Makarov<sup>1,3</sup>; Albert Heck<sup>1,2</sup>; <sup>1</sup>*University of Utrecht, Utrecht, Netherlands*; <sup>2</sup>*Netherlands Proteomics Center, Utrecht, Netherlands*; <sup>3</sup>*ThermoFisher Scientific, Bremen, Germany*

WOF am 09:50 **More from Less: Straightforward Turn-Key Workflow Enables Combined Pharmacokinetic and Integrated “Omic” Studies from Limited Tissue;** Jon Reed<sup>1,2</sup>; Gogce Crynen<sup>1,2</sup>; Laila Abdullah<sup>1,2</sup>; Ariel Hart<sup>1</sup>; Prashanthi Vallabhaneni<sup>1</sup>; Rosa Joy<sup>1</sup>; Daniel Paris<sup>1,2</sup>; Fiona Crawford<sup>1,2</sup>; <sup>1</sup>Roskamp Institute, Sarasota, Florida; <sup>2</sup>SRQ Bio, Sarasota, Florida

WOF am 10:10 **Full Structure Elucidation of Elapid Snake Venom Proteins Targeting the Acetylcholine Receptor using the latest Quadrupole-Orbitrap Mass Spectrometer;** Martijn Pinkse<sup>1</sup>; Jeroen Kool<sup>2</sup>; Laurens van Herpen<sup>1</sup>; Tabiwang Arrey<sup>3</sup>; Markus Kellmann<sup>3</sup>; Peter D. Verhaert<sup>1</sup>; <sup>1</sup>Delft University of Technology, Delft, Netherlands; <sup>2</sup>VU University Amsterdam, Amsterdam, Netherlands; <sup>3</sup>Thermo Fisher Scientific, Bremen, Germany

**8:30 – 10:30 AM, WEDNESDAY MORNING  
PTMS: COMPREHENSIVE ANALYSIS**

**Saiful Chowdhury (University of Texas, Arlington), presiding  
Ballroom III, level 4**

WOG am 08:30 **Middle-Down Proteomics Reveals Interdependency of Histone Marks and Assists Their Functional Characterization;** Simone Sidoli<sup>1</sup>; Veit Schwämmle<sup>1</sup>; Xudong Wu<sup>2</sup>; Chung-Fan Lee<sup>2</sup>; Kristian Helin<sup>2</sup>; Ole Nørregaard Jensen<sup>1</sup>; <sup>1</sup>University of Southern Denmark, Odense, Denmark; <sup>2</sup>Centre for Epigenetics, BRIC, Copenhagen, Denmark

WOG am 08:50 **Global Ubiquitylome Profiling for the Identification of Oncogenic Effector Substrates and Drug Targets in Cancer;** Namrata Udeshi<sup>1</sup>; Jean-Philippe Theurillat<sup>1,2</sup>; Jan Krönke<sup>3</sup>; Tanya Svinkina<sup>1</sup>; Monica Schenone<sup>1</sup>; Benjamin Ebert<sup>1,3</sup>; Levi Garraway<sup>1,2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>The Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA; <sup>3</sup>Brigham and Woman's Hospital, Boston, MA

WOG am 09:10 **An Ultra-tolerant Database Search Identifies Hundreds of Thousands of Modified Peptides;** Joel Chick; David Nusinow; Bo Zhai; Steven P. Gygi; Harvard medical school, Boston, MA

WOG am 09:30 **Comprehensive Monitoring of Dynamic Phosphorylation on Intact Proteins by Native MS on an Extended Mass Range Orbitrap;** Michiel Van De Waterbeemd<sup>1</sup>; Philip Lössl<sup>1</sup>; Violette Gautier<sup>1</sup>; Masami Yamashita<sup>2</sup>; Elena Conti<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Max Planck Institute of Biochemistry, Martinsried, Germany

WOG am 09:50 **Lysine 2-Hydroxyisobutyrylation is a New and Widely Distributed Histone Modification with Important Biological Functions;** Lunzhi Dai<sup>1</sup>; Chao Peng<sup>1</sup>; Emilie Montellier<sup>2</sup>; Zhike Lu<sup>1</sup>; Yue Chen<sup>1</sup>; Haruhiko Ishii<sup>4</sup>; Alexandra Debernardi<sup>2</sup>; Thierry Buchou<sup>2</sup>; Sophie Rousseaux<sup>2</sup>; Fulai Jin<sup>4</sup>; Benjamin R. Sabari<sup>3</sup>; Zhiyou Deng<sup>1</sup>; He Huang<sup>1</sup>; C. David Allis<sup>3</sup>; Bing Ren<sup>4</sup>; Saadi Khochbin<sup>2</sup>; Yingming Zhao<sup>1</sup>; <sup>1</sup>University of Chicago, Chicago, Illinois; <sup>2</sup>Université Joseph Fourier, La Tronche Cedex, France; <sup>3</sup>The Rockefeller University, New York, NY; <sup>4</sup>University of California, San Diego, La Jolla, CA

WOG am 10:10 **Novel Acyl-Lysine Modifications in a Bacterial Proteome Elucidate Substrate Metabolism;** Hong Hanh Nguyen<sup>1</sup>; Yanan Yang<sup>1</sup>; Robert Gunsalus<sup>1</sup>; Michael McInerney<sup>2</sup>; Joseph Loo<sup>1</sup>; Rachel Ogorzalek Loo<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>The University of Oklahoma, Norman, OK

**8:30 – 10:30 AM, WEDNESDAY MORNING  
LIPIDS AND PROFILING**

**Kim Ekroos (Zora Biosciences), presiding  
Ballroom IV, level 4**

WOH am 08:30 **Functional Lipidomics - From Structural Characterization to Regulation of Lipid Metabolic Networks;** Christer Ejsing; *Department Of Biochemistry And Molecular Biology, Odense, Denmark*

WOH am 08:50 **Stable Isotope Labeling in Cell Culture of Short-, Medium- and Long-Chain acyl-Coenzyme A Thioesters for SID-LC-MS/MS Analysis;** Nathaniel W. Snyder; Sankha S. Basu; Zinan Zhou; Andrew J. Worth; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*

WOH am 09:10 **Biosynthetic Pathway of 12-hydroxyheptadecatrienoic Acid Revealed by LC-MS/MS System;** Toshiaki Okuno<sup>1</sup>; Takehiko Matsunobu<sup>2</sup>; Takehiko Yokomizo<sup>1</sup>; <sup>1</sup>Department of Biochemistry, Juntendo University, Tokyo, Japan; <sup>2</sup>Medical Biochemistry, Kyushu University, Fukuoka, Japan

WOH am 09:30 **Method Development for Comprehensive Analysis of Lysophospholipid Molecular Species by Shotgun Lipidomics;** Chunyan Wang; Miao Wang; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*

WOH am 09:50 **Single-Cell Nanomanipulation to Identify Lipid Heterogeneity in Mammalian Cells at the Cancer Forefront;** Jason Hamilton; Mandy Phelps; Guido Verbeck; *University of North Texas, Denton, TX*

WOH am 10:10 **Glucosylceramide and Glucosylsphingosine Quantitation by Liquid Chromatography-Tandem Mass Spectrometry to Enable Studies of Neuronopathic Gaucher Disease;** Rick Hamler; Nastry Brignol; Sean Morrison; Hui Chang; Leo Dungan; Robert Boyd; Sean Clark; Richie Khanna; John Flanagan; Kenneth Valenzano; Elfrida Benjamin; *Amicus Therapeutics, Cranbury, New Jersey*

**10:30 AM – 2:30 PM, WEDNESDAY  
WEDNESDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm**

2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
ENERGY, PETROLEUM, AND BIOFUELS: ADVANCES IN  
MS DESIGN AND INFORMATICS

Michael Freitas (Ohio State University), presiding  
Exhibit Hall AB

WOA pm 2:30 **Elucidating Structures of Compounds in Complex Mixture by a Combination of Ion Mobility and Ultrahigh-Resolution MS and Collisional Cross-Section Calculation;** [Sunghwan Kim](#)<sup>1</sup>; Ahmed Arif<sup>1</sup>; Eleanor Riches<sup>2</sup>; Kevin Giles<sup>2</sup>; Yunju Cho<sup>1</sup>; Hugh I Kim<sup>3</sup>; Jong Wha Lee<sup>3</sup>; Cheol Ho Choi<sup>1</sup>; <sup>1</sup>Chemistry Department, Kyungpook National University, Daegu, South Korea; <sup>2</sup>Waters Corporation, Manchester, N/A; <sup>3</sup>Pohang University of Science and Technology, Pohang, Republic of Korea

WOA pm 2:50 **Ion Mobility Petroleomics: Towards Isomeric Compositional Space Elucidation via New Software and Methods;** [Eleanor Riches](#)<sup>1</sup>; Priscilla Lalli<sup>2</sup>; Ryan P. Rodgers<sup>2,3</sup>; Yuri Corilo<sup>2,3</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Future Fuels Institute, Tallahassee, FL

WOA pm 3:10 **Analysis of Crude Oil Samples on the Multi Reflecting High Resolution TOF at resolution over 160,000;** [George Tikhonov](#)<sup>1</sup>; Viatcheslav Artaev<sup>1</sup>; Boris Kozlov<sup>2</sup>; Kevin Siek<sup>1</sup>; Anatoly Verenchikov<sup>2</sup>; <sup>1</sup>LECO Corporation, Saint Joseph, MI; <sup>2</sup>MS Consulting, Bar, Montenegro

WOA pm 3:30 **Direct Analysis of Crude Oil using Orbitrap Mass Spectrometry with Resolving Powers above 1,000,000;** Eduardo M. Schmidt<sup>1</sup>; Marcos A. Pudenzi<sup>1</sup>; Jandyson M. Santos<sup>1</sup>; Eugen Damoc<sup>2</sup>; Eduard Denisov<sup>2</sup>; Alexander Makarov<sup>2</sup>; [Marcos N. Eberlin](#)<sup>1</sup>; <sup>1</sup>ThermoFisher Mass Spectrometry Laboratory, Campinas, Brazil; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany

WOA pm 3:50 **Spectroscopic and FT-ICR Mass Spectral Analysis of Asphaltene Subfractionation by N-Methyl-2-pyrrolidone;** [Mmili M. Mapolelo](#)<sup>1</sup>; Simon I. Andersen<sup>1</sup>; Amy M. McKenna<sup>2</sup>; Jacqueline M. Jarvis<sup>2</sup>; Ryan P. Rodgers<sup>2</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>Schlumberger, Edmonton, Canada; <sup>2</sup>Natl High Magnetic Field Laboratory, Tallahassee, FL

WOA pm 4:10 **Use of 2D GC-MS and ESI-FTICR-MS to Characterize Quality Crude Oil Produced from Aliphatic Coal via Hydrous Pyrolysis;** [Blaine Hartman](#); Patrick Hatcher; Old Dominion University, Norfolk, VA

Maréchal<sup>2</sup>; Denis Falconet<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>George Washington University, Washington, District Of Columbia; <sup>2</sup>CEA-CNRS-INRA-Univ. Grenoble Alpes, Grenoble, France

WOB pm 3:10 **Single-probe Sampling and Ionization Technique for Single Cell Mass Spectrometry Analysis: Development and Applications;** [Ning Pan](#); Anthony Burgett; Naga Rama Kothapalli; Zhibo Yang; University of Oklahoma, Norman, OK

WOB pm 3:30 **High Repetition-Rate, Fiber-Based Laser Vaporization, Electrospray Ionization Mass Spectrometry (Fiber-LEMS);** Paul Flanagan<sup>1</sup>; Fengjian Shi<sup>1</sup>; Jieutonne Archer<sup>1</sup>; Andrew Mills<sup>2</sup>; Martin Fermann<sup>2</sup>; [Robert Lewis](#)<sup>1</sup>; <sup>1</sup>Temple University, Philadelphia, PA; <sup>2</sup>IMRA America, Inc., Ann Arbor, MI

WOB pm 3:50 **Direct Quantification of Chemical Warfare Agent Related Compounds using Active Capillary Inlet and SESI Mass Spectrometry;** [Jan-Christoph Wolf](#)<sup>1</sup>; Pablo Martinez-Lozano Sinues<sup>1</sup>; Martin Schaefer<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, CH; <sup>2</sup>SPIEZ Laboratory, Spiez, CH

WOB pm 4:10 **jigSAWN: A Self-optimizing SAWN Control Interface;** [Erik Nilsson](#)<sup>2</sup>; Michael Wilson<sup>1</sup>; Yue Huang<sup>1</sup>; Scott Heron<sup>1</sup>; David Kilgour<sup>1</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, Baltimore, MD; <sup>2</sup>Deurion LLC, Seattle, WA

2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
ECOLOGICAL AND HUMAN HEALTH ENVIRONMENTAL  
CHEMISTRY AND TOXICOLOGY

J. Will Thompson (Duke University), presiding  
Room 309-310

WOC pm 2:30 **Comprehensive Characterization of Mixed-Halogen Dioxins and Furans Generated in Fire Debris Using GCxGC-TOFMS and APGC-TQS;** [Kari Organtini](#)<sup>1</sup>; Anne Myers<sup>2</sup>; Karl Jobst<sup>3</sup>; Eric Reiner<sup>3</sup>; Jack Cochran<sup>4</sup>; Adam Ladak<sup>5</sup>; Douglas Stevens<sup>5</sup>; Frank Dorman<sup>1</sup>; <sup>1</sup>Penn State University, University Park, PA; <sup>2</sup>University of Toronto, Toronto, Canada; <sup>3</sup>Ontario Ministry of the Environment, Toronto, ON; <sup>4</sup>Restek Corporation, Bellefonte, PA; <sup>5</sup>Waters Corporation, Beverly, MA

WOC pm 2:50 **Characterization of Paralytic Shellfish Poisons by HILIC-IM-MS coupling;** [Salomé Poyer](#)<sup>1</sup>; Corinne Loutelier-Bourhis<sup>1</sup>; Florence Mondegue<sup>2</sup>; Julien Enche<sup>3</sup>; Gael Coadou<sup>1</sup>; Anne Bossée<sup>3</sup>; Philipp Hess<sup>2</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>University of Rouen, Mont Saint Aignan, France; <sup>2</sup>IFREMER, Nantes, France; <sup>3</sup>DGA Maitrise NRBC, Vert Le Petit, France

WOC pm 3:10 **Fast Identification and Quantification of Major Protein Carbonyls α-amino adipic and γ-glutamic semialdehydes---A New Pronase Hydrolysis Methodology;** [Lin Huang](#)<sup>1</sup>; Jacob Raber<sup>2</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, OR; <sup>2</sup>Oregon Health & Science University, Portland, OR

WOC pm 3:30 **Supercritical Fluid Chromatography Coupled to Orbitrap Mass Spectrometry for Analysis of Oil Sands Process-Affected Water;** [Alberto Pereira](#); Jonathan Martin; University of Alberta, Edmonton, Canada

2:30 – 4:30 PM, WEDNESDAY AFTERNOON

AMBIENT IONIZATION: INSTRUMENTATION AND APPLICATIONS

Demian Ifa (York University), presiding  
Room 307-308

WOB pm 2:30 **Data-Independent Ion Correlations by Dynamic Sample Introduction Ambient MS;** Ezequiel M. Morzan<sup>1</sup>; Rachel V. Bennett<sup>2</sup>; [Facundo M. Fernandez](#)<sup>2</sup>; <sup>1</sup>Universidad de Buenos Aires, Buenos Aires, Argentina; <sup>2</sup>Georgia Institute of Technology, Atlanta, GA

WOB pm 2:50 **Metabolic Response to Altered Light Conditions in Genetically Modified Chlamydomonas by LAESI Mass Spectrometry with Ion Mobility Separation;** [Sylvia Stopka](#)<sup>1</sup>; Bindesh Shrestha<sup>1</sup>; Éric



WOC pm 3:50 **A Highly Sensitive, Fully Automated, High Throughput Method to Analyze Nicotine Metabolites in Human Serum using HPLC-APCI-Tandem Mass Spectrometry**; [Kristin Dortch](#); Kevin Caron; Hunter Ronald; Luo Zuzheng; Alexander Ricky; Akins Ricky; McGahee Ernest; Connie Sosnoff; Lanqing Wang; *Centers for Disease Control and Prevention, Atlanta, GA*

WOC pm 4:10 **Identification and Quantification of Fourteen N-Nitrosamines in Canadian Drinking Water Systems using SPE-HPLC-MS/MS Methods**; [Yichao Qian](#); Minghuo Wu; Jessica Boyd; Steve Hrudehy; Xing-Fang Li; *University of Alberta, Edmonton, Canada*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
FUNDAMENTALS: NEW ION ACTIVATION METHODS  
Hao Chen (Ohio University), presiding  
Room 314-317**

WOD pm 2:30 **Improvement of the Low Mass Cutoff Effect using Digital Ion Trap Technology**; Fuxing Xu; [Chuanfan Ding](#); *Fudan University, Shanghai, China*

WOD pm 2:50 **“Flow-Through” Electron Capture Dissociation in a Novel Branched Radio-Frequency Ion Trap for High Throughput Mass Spectrometry**; [Takashi Baba](#); J. Larry Campbell; Yves Le Blanc; Jim. W. Hager; Bruce A. Thomson; *AB Sciex, Concord, Canada*

WOD pm 3:10 **Effects of Sodium Cationization on Electron Detachment Dissociation Fragments of Heparin Oligosaccharides**; [Isaac Agyekum](#)<sup>2</sup>; Muchena J. Kailemia<sup>2</sup>; Lingyun Li<sup>3</sup>; Robert J. Linhardt<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*University of Georgia, Chemistry Department, Athens, GA*; <sup>3</sup>*Rensselaer Polytechnic University, Troy, NY*

WOD pm 3:30 **UV Photogeneration of Peptidic Carbenes and UV Photodissociation of ETD Fragmentation Products**; [Christopher Shaffer](#); Ales Marek; Robert Pepin; Frantisek Turecek; *University of Washington, Seattle, Washington*

WOD pm 3:50 **Effect of Conformational Flexibility on Gas-Phase Unfolding of Noncovalent Protein Homodimers Probed by CID and SID**; [Yang Song](#); Yun Zhang; Royston Quintyn; Mowei Zhou; Vicki Wysocki; *The Ohio State University, Columbus, OH*

WOD pm 4:10 **Gas-Phase Structural Effects in Negative Ion Electron Capture Dissociation (niECD)**; [Ning Wang](#); Kristina Hakansson; *University of Michigan, Ann Arbor, MI*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
PLANT“OMICS”  
Ron Cerny (University of Nebraska), presiding  
Ballroom I, level 4**

WOE pm 2:30 **Living Without Our Daily Bread – Towards Solutions for Sufferers of Gluten Intolerance**; [Michelle Colgrave](#)<sup>1,2</sup>; Keren Byrne<sup>1,2</sup>; Hareshwar Goswami<sup>1,2</sup>; Greg Tanner<sup>2,3</sup>; Crispin Howitt<sup>2,3</sup>; <sup>1</sup>*CSIRO Animal, Food & Health Science, St Lucia, Australia*; <sup>2</sup>*CSIRO Food Futures Flagship, Canberra, Australia*; <sup>3</sup>*CSIRO Plant Industry, Black Mountain, Australia*

WOE pm 2:50 **Targeted and Nontargeted Apple Metabolomics using 96-blade LC-MS**; [Sanja Risticvic](#); Fatemeh Mousavi; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*

WOE pm 3:10 **Structural Identification of N-glycoproteins and Stress Signaling in Arabidopsis Thaliana**; Jun Ma; Qianqian Li; Guochen Qin; [Yi-Min She](#); *Shanghai Center for Plant Stress Biology, Shanghai, P. R. China*

WOE pm 3:30 **Nuclear Proteins Controlling Soybean Rust Resistance**; Bret Cooper; *USDA-ARS, Beltsville, MD*

WOE pm 3:50 **A Quantitative Systems Approach to Understand Differences in Geminivirus-induced Senescence in Arabidopsis thaliana**; [Laura Edwards](#); Inna Kulikova; Sophia Yang; Mariana Franco-Ruiz; Caroline Bryan; Elise Braswell; Lisa Rightmyer; Kevin Blackburn; Michael B. Goshe; Jose Trinidad Ascencio-Ibanez; *North Carolina State University, Raleigh, NC*

WOE pm 4:10 **Alteration of the Root Microbiome using Plant Mutants Affecting Root Carbon Allocation**; [Ljiljana Pasa-Tolic](#)<sup>1</sup>; Charles Ansong<sup>1</sup>; Joshua Aldrich<sup>1</sup>; Heather Brewer<sup>1</sup>; Alice Dohnalkova<sup>1</sup>; Richard Ferrieri<sup>2</sup>; Susannah Green Tringe<sup>3</sup>; Michael Sadowsky<sup>4</sup>; Chanlan Chun<sup>4</sup>; Lihui Song<sup>5</sup>; Yaya Cui<sup>6</sup>; Vania Pankiewicz<sup>5,6</sup>; Fernanda do Amaral<sup>5,7</sup>; Karina Freire d’Eça Nogueira Santos<sup>5,6</sup>; Emanuel de Souza<sup>5</sup>; Fabio Pedrosa<sup>5</sup>; Gary Stacey<sup>5</sup>; <sup>1</sup>*Pacific NW Nat’l Lab, Richland, WA*; <sup>2</sup>*Brookhaven National Laboratory, Upton, NY*; <sup>3</sup>*DOE Joint Genome Institute, Walnut Creek, CA*; <sup>4</sup>*BioTechnology Institute, University of Minnesota, St. Paul, MN*; <sup>5</sup>*University of Missouri, Columbia, MO*; <sup>6</sup>*Federal University of Parana, Curitiba, Brazil*; <sup>7</sup>*Federal University of Santa Catarina, Florianopolis, Brazil*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
PROTEOMICS: INFECTIOUS DISEASES  
Rena Robinson (University of Pittsburgh), presiding  
Ballroom II, level 4**

WOF pm 2:30 **Identification of HLA-DR-Presented Peptides in Synovial Tissue and Fluid, and PBMCs from Patients with Rheumatoid Arthritis or Antibiotic-Refractory Lyme Arthritis**; [Qi Wang](#)<sup>1</sup>; Elise E. Drouin<sup>2</sup>; Chunxiang Yao<sup>1</sup>; Jiyang Zhang<sup>1,3</sup>; Yu Huang<sup>1</sup>; Allen C. Steere<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Massachusetts General Hospital, Boston, MA*; <sup>3</sup>*National University of Defense Technology, Changsha, Hunan Province, China*

WOF pm 2:50 **Viral-induced Changes in the Liver Proteome**; Dijana Vitko; Anannya Bhattacharya; Katrin Hoermann; Katja Parapatics; André C. Mueller; Jacques Colinge; Andreas Bergthaler; [Keiryn L. Bennett](#); *CeMM Research Center for Molecular Medicine, Vienna, Austria*

WOF pm 3:10 **Revealing Essential Metabolic Enzymes for Mycobacterium Tuberculosis Survival using a Targeted Quantitation Strategy on a Q Exactive Mass Spectrometer**; [John D. Leszyk](#); Subhalaxmi Nambi; Scott A. Shaffer; Christopher Sasseti; *University of Massachusetts Medical School, Worcester, MA*

WOF pm 3:30 **Proteomic Identification of Interspecies Host-Pathogen Interactions by Protein Crosslinking: *Acinetobacter baumannii* Infection of Human Lung Epithelia;** Devin Schweppe; Juan Chavez; James Bruce; *University of Washington, Seattle, WA*

WOF pm 3:50 **Human Immune Defense versus Viral Immune Evasion: Emerging Roles for Phosphorylation and Acetylation in Virus-Host Dynamics;** Tuo Li; Benjamin Diner; Jin Chen; Ileana M. Cristea; *Princeton University, Princeton, NJ*

WOF pm 4:10 **Glycoproteomic Analysis of Plasmas from HIV Infected Individuals of Post-Seroconversion, with Developed AIDS, HAART and Elite Suppression;** Weiming Yang<sup>1</sup>; Oliver Laeyendecker<sup>1,3</sup>; Sarah Wendel<sup>3</sup>; Shisheng Sun<sup>1</sup>; Jian-Ying Zhou<sup>1</sup>; Minghui Ao<sup>1</sup>; Joel Blankson<sup>2</sup>; Richard Moore<sup>2</sup>; George Seage III<sup>4</sup>; Connie Celum<sup>5</sup>; Deborah Donnell<sup>7</sup>; Susan Buchbinder<sup>6</sup>; Matthew Cousins<sup>1</sup>; Hui Zhang<sup>1</sup>; Jay Brooks Jackson<sup>1</sup>; <sup>1</sup>*Department of Pathology, Johns Hopkins University, Baltimore, MD;* <sup>2</sup>*Department of Medicine, Johns Hopkins University, Baltimore, MD;* <sup>3</sup>*NIAID, National Institutes of Health, Bethesda;* <sup>4</sup>*Department of Epidemiology, Harvard SPH, Boston, MA;* <sup>5</sup>*Department of Medicine, University of Washington, Seattle, WA;* <sup>6</sup>*Statistical Center for HIV/AIDS Research and Pre, Seattle, WA;* <sup>7</sup>*San Francisco Department of Public Health, San Francisco, CA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
TARGETED QUANTIFICATION OF PROTEINS AND POST-TRANSLATIONAL MODIFICATIONS**

**Yishai Levin (Weizmann Institute of Science), presiding  
Ballroom III, level 4**

WOG pm 2:30 **Going Wide with Targeted Quantification of PTMs: Proteomic Connectivity Maps of Drugs, Disease, Genomics, and Beyond;** Jacob D. Jaffe; Jennifer Abelin; Jinal Patel; Jordan Taylor; Lola Fagbami; Amanda Creech; Caitlin Feeney; Xiaodong Lu; Roger Hu; Aravind Subramanian; Steven A. Carr; *The Broad Institute, Cambridge, MA*

WOG pm 2:50 **High Sensitivity Targeted Quantification of ERK Phosphorylation Dynamics and Stoichiometry without Affinity Enrichment;** Tujin Shi; Tao Liu; Matthew Gaffrey; Yuqian Gao; William Chrisler; Thomas Fillmore; Carrie Nicora; Marina Gritsenko; Chaochao Wu; Jintang He; Jia Guo; Rui Zhao; Ronald Moore; Richard Smith; David Camp, II; Karin Rodland; Steven Wiley; Wei-Jun Qian; *Pacific Northwest National Laboratory, Richland, WA*

WOG pm 3:10 **Development of a Novel 2D LC/MRM-MS Approach for Deeper and Broader Quantitation of Putative Protein Biomarkers in Human Plasma;** Romain Simon<sup>1</sup>; Andrew Percy<sup>1</sup>; Andrew Chambers<sup>1</sup>; <sup>1</sup>*Christoph Borchers*<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada;* <sup>2</sup>*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*

WOG pm 3:30 **Targeted Quantitation of Post-Translational Modifications and Protein-Protein Interactions of Human Nitric Oxide Synthase 2 in Airway Epithelial Cells;** Erik J Soderblom; J. Will Thompson; Kurren Mehta; Loretta G. Que; Harvey E. Marshall; M. Arthur Moseley; Matthew W. Foster; *Duke University Medical Center, Durham, NC*

WOG pm 3:50 **A Multiplex PRM Assay for Assessing Regulatory Mechanisms of Cell Death in Breast Cancer Xenografts;** Matthew R. Meyer<sup>1</sup>; John A. Wrobel<sup>3</sup>; Kelly V. Ruggles<sup>2</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Robert Kitchens<sup>1</sup>; Jacqueline Snider<sup>1</sup>; Jeremy Hoog<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>1</sup>; David Fenyo<sup>2</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO;* <sup>2</sup>*New York University, New York, NY;* <sup>3</sup>*University of North Carolina, Chapel Hill, NC*

WOG pm 4:10 **Rapid Processing of Large Scale Quantitative Proteomics Projects: Integration of Skyline with the CHORUS Cloud;** Brendan MacLean<sup>1</sup>; Andrey Bondarenko<sup>2</sup>; Nick Shulman<sup>1</sup>; Oleksii Tymchenko<sup>3</sup>; Christine Wu<sup>2</sup>; Nathan Yates<sup>4</sup>; Michael J. Maccoss<sup>1</sup>; <sup>1</sup>*Univ of Washington, Seattle, WA;* <sup>2</sup>*Stratus Biosciences, Seattle, WA;* <sup>3</sup>*TeamDev, Kharkov, Ukraine;* <sup>4</sup>*University of Pittsburgh, Pittsburgh, PA*

**2:30 – 4:30 PM, WEDNESDAY AFTERNOON  
MEMBRANE PROTEINS**

**Stephen Eyles (University of Massachusetts-Amherst), presiding  
Ballroom IV, level 4**

WOH pm 2:30 **Applications of Mass Spectrometry-based Strategies for Structural Studies of 7-Transmembrane Receptors and other Membrane Proteins;** Graham M West; Bruce Pascal; Michael Chalmers; Pat Griffin; *The Scripps Research Institute, Scripps Florida, Jupiter, FL*

WOH pm 2:50 **Probing the Membrane Protein Interaction Network of *Pseudomonas aeruginosa* Cells by Chemical Cross-Linking Mass Spectrometry;** Arti Navare; Richard Siehnel; Kirsten Beck; Alejandro Wolf-Yadlin; Pradeep Singh; James E. Bruce; *University of Washington, Seattle, WA*

WOH pm 3:10 **Amphipols Outperform Detergents in the Stabilization of Membrane Protein Structure in the Gas Phase;** Antonio N. Calabrese; Tom G. Watkinson; Peter J. F. Henderson; Sheena E. Radford; Alison E. Ashcroft; *University of Leeds, Leeds, UK*

WOH pm 3:30 **The Fragmentation of Gaseous Integral Membrane Proteins;** Owen Skinner; Adam Catherman; Bryan Early; Paul Thomas; Philip Compton; Neil L. Kelleher; *Northwestern University, Evanston, IL*

WOH pm 3:50 **The Release of Membrane Protein from Detergent Micelles in the Gas Phase – Mechanistic Insights and New Detergents;** Idlir Liko; Eamonn Reading; Timothy Allison; Arthur Laganowsky; Carol V. Robinson; *University of Oxford, Oxford, Oxfordshire*

WOH pm 4:10 **Exosome Surface Proteins: Enrichment and Identification by Mass Spectrometry;** Rebecca Rose<sup>1</sup>; Nathan Edwards<sup>3</sup>; Suzanne Ostrand-Rosenberg<sup>2</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>*University of Maryland, College Park, MD;* <sup>2</sup>*University of Maryland, Baltimore County, MD;* <sup>3</sup>*Georgetown University, Georgetown, Washington, D.C.*

4:45 – 5:30 PM, WEDNESDAY AFTERNOON  
ASMS MEETING

Susan T. Weintraub, ASMS President, presiding  
Enjoy a beverage and hear the latest ASMS news.  
Ballroom I, level 4

5:45 – 7:00 PM, WEDNESDAY AFTERNOON  
WORKSHOPS

Level 3

Light refreshments, level 3

1. The DIA Primer (organized by Data Independent Acquisition Interest Group); Room 307-308
2. Mechanisms to Process Data Given Software Restrictions Across Vendors (organized by DMPK Interest Group); Room 309-310
3. Characterization of Biologics by Mass Spectrometry (organized by Biotherapeutics Interest Group); Room 314-317
4. Get Ready to Become a MS Rising Star (organized by Young Mass Spectrometrists Interest Group); Room 336
5. Have Quadrupole Ion Traps Passed their Prime Time (organized by Ion Trap Interest Group); Room 337
6. Advancements and Discussion of Mass Spectrometry Technology and Challenges within the Polymer and Material Fields (organized by Polymeric Materials Interest Group); Room 338
7. The Galaxy Framework for Biological MS Informatics: Practical Tips for Software Developers and Users; Room 339-340
8. Using Mass Spectrometry to Characterize the Exosome and Its Impact on Human Health; Room 341-342
9. PowerPoint Design Tips and Tricks: How Your Slides Could be Hurting Your Talk and Your Message; Room 343-344
10. Quantitative Glycomics; Room 345-346
11. Current Trends, Gaps, and Needs in Workflows for Absolute Protein Quantitation by LC-MS; Nalini Sadagopan, Room 347-348
12. Modern GCMS for Flavor, Fragrance and Foodstuffs Analysis: GC QQQ and GC HRMS (organized by Flavor Fragrance and Foodstuff Interest Group); Room 349-350
13. Mass Spectrometry Applications in Art, cultural Heritage, and Natural History; Room 327

AFTER 8:00 PM, WEDNESDAY EVENING  
CORPORATE HOSPITALITY SUITES  
Hilton Hotel

THURSDAY MORNING ORAL SESSIONS

8:30 – 10:30 AM, THURSDAY MORNING  
FORENSIC APPLICATIONS

Lisa Jones (Indiana Univ.-Purdue Univ. Indianapolis), presiding  
Exhibit Hall AB

- ThOA am 08:30 **Qualitative Analysis of Commercially Available Household and Agrochemicals using Miniature Mass Spectrometry Coupled with Ambient Ionization**; Christopher Pulliam; Ryan Bain; Graham Cooks; *Purdue University, West Lafayette, IN*
- ThOA am 08:50 **Simultaneous Measurement of Creatinine and 11-nor-9-Carboxy-THC in Urine by Paper Spray-Mass Spectrometry for Illicit Drug Screening**; Nicholas Manicke; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- ThOA am 09:10 **Development of Hand Portable GC/MS for Onsite Arson Investigation and Screening for Toxic Chemicals on Firefighter PPE Gear**; Andrew Byrnes<sup>1</sup>; John DeHaan<sup>2</sup>; David Matthew<sup>3</sup>; Nickesha Chung<sup>4</sup>; Ed Kissel<sup>4</sup>; Andy Saksa<sup>4</sup>; Eric Diken<sup>4</sup>; Gareth Dobson<sup>4</sup>; <sup>1</sup>Utah Valley University Emergency Services, Orem, UT; <sup>2</sup>Fire-Ex Forensics, Vallejo, CA; <sup>3</sup>Fire Service Consulting, Napa, CA; <sup>4</sup>Smiths Detection, Danbury, CT
- ThOA am 09:30 **Direct Identification of ANFO Explosive on Real Crime Scene Samples: Banknotes and ATM Explosion Residues**; Vinicius Veri<sup>1</sup>; Jandyson Machado<sup>1</sup>; Jose Perez<sup>1</sup>; Marcos Franco<sup>1</sup>; Rodrigo Borges<sup>2</sup>; Wanderley Souza<sup>2</sup>; Jorge Zacca<sup>3</sup>; Deleon Correa<sup>4</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>University of Campinas - Unicamp, Campinas, Brazil; <sup>2</sup>Inmetro, Rio de Janeiro, Brazil; <sup>3</sup>Brazilian Federal Police, Brasília, Brazil; <sup>4</sup>Technical-Scientific Police Superintendency, São Paulo, Brazil
- ThOA am 09:50 **A Novel Forensic Approach towards Determining Time of Death Utilizing Saliva Glycosylation**; Bum Jin Kim<sup>1</sup>; Chanyoung Han<sup>1</sup>; Jong-Soon Choi<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>GRASST, Chungnam National University, Daejeon, Korea; <sup>2</sup>Korea Basic Science Institute, Daejeon, Korea
- ThOA am 10:10 **Analysis of Phenethylamine Street Drugs for Psychoactive Compounds and Impurities**; Maura McGonigal<sup>1</sup>; Noelle Elliott<sup>2</sup>; Philip Smith<sup>1</sup>; Frank Dorman<sup>1</sup>; <sup>1</sup>Penn State, University Park, PA; <sup>2</sup>Perkin Elmer, Shelton, CT
- 8:30 – 10:30 AM, THURSDAY MORNING  
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING  
Michael Bereman (North Carolina State University), presiding  
Room 307-308
- ThOB am 08:30 **Controlled-Resonant Surface Tapping-Mode Scanning Probe Electro spray Ionization Mass Spectrometry Imaging**; Matthias Lorenz; Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThOB am 08:50 **Gas Chromatography Plasma-Assisted Reaction Chemical Ionization Mass Spectrometry for Quantification of Organobromines**; Ninghang Lin<sup>1</sup>; Haopeng Wang<sup>1</sup>; Kaveh Kahen<sup>2</sup>; Hamid Badiei<sup>2</sup>; Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>Georgetown Univ., Washington, DC; <sup>2</sup>PerkinElmer Inc., Woodbridge, Canada
- ThOB am 09:10 **Metabolic Profiling of Single Arabidopsis Cells by Capillary Microsampling and ESI Mass Spectrometry with Ion Mobility Separation**; Linwen Zhang<sup>1</sup>; Daniel P. Foreman<sup>1</sup>; Paaqua A. Grant<sup>1</sup>; Bindesh Shrestha<sup>1</sup>; Sally A. Moody<sup>1</sup>; Florent Villiers<sup>2</sup>; June M. Kwak<sup>2,3</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>The George Washington University, Washington, DC; <sup>2</sup>Maryland University, College Park, MD; <sup>3</sup>Institute for Basic Science, Daegu, Republic of Korea
- ThOB am 09:30 **DMSO Enhances Electro spray Response and Boosts Sensitivity of Proteomic Experiments – Lessons Learnt from a Variety of Mass Spectrometers**; Hannes Hahne; Fiona Pacht; Benjamin Ruprecht; Susan Klaeger; Dominic Helm; Heiner Koch; Bernhard Kuster; *Technische Universität München, Freising, Germany*

ThOB am 09:50 **Development of Rapid Bedside Diagnosis Tool by Coupling of Bio-Compatible Solid Phase Microextraction (SPME) Devices to Mass Spectrometry**; German Augusto Gómez-Ríos; Barbara Bojko; Fatemeh Mirnaghi; [Janusz Pawliszyn](#); *University of Waterloo, Waterloo, Canada*

ThOB am 10:10 **Rectangular Ion Funnel (RIF): Conceptualization and Analytical Performance of a New ESI-MS Interface for Structures for Lossless Ion Manipulations (SLIM)**; [Tsunq-Chi Chen](#); Ian Webb; Marques Harrer; Spencer Prost; Sandilya Garimella; Xinyu Zhang; Jonathan Cox; Randy Norheim; Brian Lamarche; Erin Baker; Aleksey Tolmachev; Gordon Anderson; Keqi Tang; Yehia Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*

**8:30 – 10:30 AM, THURSDAY MORNING  
FAIMS AND DMS: NEW DEVELOPMENTS AND APPLICATIONS  
Randy Purves (University of Saskatchewan), presiding  
Room 309-310**

ThOC am 08:30 **Improved Detection of SUMOylated Peptides in Large Scale Proteomic Analyses using High Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS)**; [Eric Bonnell](#); Frederic Lamoliatte; Pierre Thibault; *Université de Montréal, Montréal, QC*

ThOC am 08:50 **Differential Mobility Spectrometry of Derivatized Steroid Hormones: Examining the Relationships between Structures and Solvation**; [Chang Liu](#)<sup>1</sup>; J. Larry Campbell<sup>1</sup>; J.C. Yves Leblanc<sup>1</sup>; Subhakar N. Dey<sup>2</sup>; Subhasish Purkayastha<sup>2</sup>; Tim L. Hoffman<sup>1</sup>; <sup>1</sup>AB SCIEX, Concord, ON, Canada; <sup>2</sup>AB SCIEX, Framingham, MA

ThOC am 09:10 **Fast Separation of Hydroxytestosterone Isomers using Chip-Based FAIMS Combined with Mass Spectrometry for High-Throughput Drug Assays**; [Robert Smith](#)<sup>1</sup>; Dora Santos<sup>2</sup>; Yongmin Li<sup>2</sup>; Weichao Chen<sup>2</sup>; Kari Schlicht<sup>3</sup>; Danielle Toutoungi<sup>1</sup>; Colin Creaser<sup>4</sup>; Sam Sperry<sup>5</sup>; <sup>1</sup>Owlstone Ltd, Cambridge, UK; <sup>2</sup>Vertex Pharmaceuticals Incorporated, San Diego, CA; <sup>3</sup>Agilent Technologies Inc, Wakefield, MA; <sup>4</sup>Loughborough University, Loughborough, UK; <sup>5</sup>Effector Therapeutics, San Diego, CA

ThOC am 09:30 **Improvement in the Detection of Leukemia Antigens with Differential Ion Mobility Spectrometry Coupled to Tandem Mass Spectrometry**; [Samantha Isenberg](#); Udara Dharmasiri; Paul Armistead; Gary Glish; *University of North Carolina, Chapel Hill, NC*

ThOC am 09:50 **High Throughput Analysis using Guard-Column UHPLC-DMS-MS/MS to screen Veterinary Drug Residues in Animal Tissues**; [Steven Lehotay](#)<sup>1</sup>; Alan Lightfield<sup>1</sup>; Marilyn Schneider<sup>1</sup>; Paul C. Winkler<sup>2</sup>; <sup>1</sup>USDA ARS, Wyndmoor, PA; <sup>2</sup>AB Sciex, Golden, CO

ThOC am 10:10 **Evaluation of Two FAIMS Configurations for Improved Speed, Selectivity, and Sensitivity in Targeted Peptide Quantitation**; [Susan E. Abbatiello](#); Lindsay Pino; Steven A. Carr; *The Broad Institute of MIT and Harvard, Cambridge, MA*

**8:30 – 10:30 AM, THURSDAY MORNING  
RADICAL ION CHEMISTRY**

**Benjamin Bythell (University of Missouri-St. Louis), presiding  
Room 314-317**

ThOD am 08:30 **Kinetic Ion Thermometers (KIT) for the Determination of Internal Energy in Transient Peptide Cation-Radicals Formed by Electron Transfer**; [Frantisek Turecek](#); Robert Pepin; *University of Washington, Seattle, WA*

ThOD am 08:50 **Formation and Reaction of Methoxy Radical with Disulfide Linked Peptides in a NanoESI Plume: Chemistry and Utility**; [Kirt L. Durand](#); Craig Stinson; Xiaoxiao Ma; Chasity Love; Yu Xia; *Purdue University, West Lafayette, IN*

ThOD am 09:10 **“How Sweet It Is”: Development of a New Method for Generating Sugar Radical Cations via Non-Covalent Complexes**; [Sandra Osburn](#); Spencer J. Williams; Richard A.J. O’Hair; *University of Melbourne, Parkville, Australia*

ThOD am 09:30 **Radical Delivery and Radical Fragmentation with Crown Ether Attachment for Structural Analysis of Biomolecules**; [Huong T \(Nicole\) Pham](#); Ryan R. Julian; *University of California, Riverside, CA*

ThOD am 09:50 **Identification of the Presence of Isomeric Reactant Ions Based on their Ion-Molecule Reaction Kinetics**; [Ashley Wittrig](#); Hilkka Kenttamaa; *Purdue University, West Lafayette, IN*

ThOD am 10:10 **Tuning Radical Reactivity by Polarity Switching in Gas Phase Distonic Ions**; David Marshall<sup>2</sup>; Lifu Ma<sup>2</sup>; Benjamin Kirk<sup>3</sup>; Adam Trevitt<sup>2</sup>; [Stephen J Blanksby](#)<sup>1</sup>; <sup>1</sup>Queensland University of Technology, Brisbane, Australia; <sup>2</sup>University of Wollongong, Wollongong, Australia; <sup>3</sup>Lawrence Berkeley National Laboratory, Berkeley, CA

**8:30 – 10:30 AM, THURSDAY MORNING  
BIOMARKERS IN DRUG DISCOVERY,  
DEVELOPMENT AND DIAGNOSIS  
Nathalie Agar (Harvard Medical Center), presiding  
Ballroom I, level 4**

ThOE am 08:30 **Identification of Translational Biomarkers in Drug Discovery: Animal Model Optimization and Experimental Design**; [Petia Shipkova](#); Joelle Onorato; Dong Cheng; Anthony Azzara; Don Robertson; *Bristol Myers Squibb, Princeton, NJ*

ThOE am 08:50 **Rapid Assessment of Apoptotic Signaling to Study Synergy of Cancer Chemotherapeutics**; [Robert Sprung](#)<sup>1</sup>; Mark Meads<sup>1</sup>; Luis Saavedra-Roman<sup>2</sup>; Elizabeth Wood<sup>1</sup>; Wei Guan<sup>1</sup>; David Britton<sup>3</sup>; Ian Pike<sup>3</sup>; Kenneth Shain<sup>1</sup>; John Koomen<sup>1</sup>; <sup>1</sup>H. Lee Moffitt Cancer Center, Tampa, FL; <sup>2</sup>University of South Florida, Tampa, FL; <sup>3</sup>Proteome Sciences, London, UK

ThOE am 09:10 **Tracer Methodologies for Measuring Triglyceride Metabolism in Pharmaceutical Research & Development: How to Get the Skinny on Fat**; [David McLaren](#); Steven Stout; Dan Xie; Ying Chen; Seongah Han; Jinqi Liu; Sheng-Ping Wang; Raymond Rosa; Vivienne Mendoza; Olga Berejnaia; Gowri Bhat; Paul Miller; Pan Yi; Kithsiri Herath; Ablatt Mahsut; Vinit Shah; Dunlu Chen; Beth Ann Murphy; Karen Akinsanya; Hayes Danksy; Jose Castro-Perez; Shirley Pinto; Douglas Johns; Stephen Previs; Thomas Roddy; *Merck & Co., Inc., Kenilworth, NJ*



ThOE am 09:30 **Understanding Uptake and Trafficking Pathways Taken by Liver-Targeted siRNAs by Looking for Metabolite Breadcrumbs using High Resolution Mass Spectrometry**; Christopher Kochansky; Kristen Kwasnjuk; Michael Lyman; BaoJen Shyong; Kristin Geddes; Heather Trexler; Charles Thompson; Mark Cancilla; *Merck Research Labs, West Point, PA*

ThOE am 09:50 **Serum Protein Biomarkers to Monitor Duchenne Muscular Dystrophy Disease Progression and Response to Therapy**; Ramya L Marathi<sup>1</sup>; Sree Rayavarapu<sup>1</sup>; Aiping Zhang<sup>1</sup>; Haeri Seol<sup>1</sup>; Kristy J Brown<sup>1</sup>; Heather Gordish-Dressman<sup>1</sup>; Kanneboyina Nagaraju<sup>1</sup>; Eric P Hoffman<sup>1</sup>; Erik Henricson<sup>2</sup>; Craig McDonald<sup>2</sup>; Yetrib Hathout<sup>1</sup>; <sup>1</sup>*Children's National Medical Center, Washington D.C., DC*; <sup>2</sup>*University of California, Davis School of Medicine, Davis, CA*

ThOE am 10:10 **Integrated Analysis of Proteomic and Genomic Data from Breast Cancer Tumor Profiles**; D. R. Mani<sup>1</sup>; Philipp Mertins<sup>1</sup>; Pei Wang<sup>2,3</sup>; Karl R. Clauser<sup>1</sup>; Michael A. Gillette<sup>1</sup>; Jana W. Qiao<sup>1</sup>; Xianglong Wang<sup>2</sup>; Yuzheng Zhang<sup>2</sup>; Ping Yan<sup>2</sup>; Chenwei Lin<sup>2</sup>; Amanda Paulovich<sup>2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*Fred Hutchinson Cancer Research Center, Seattle, WA*; <sup>3</sup>*Mount Sinai School of Medicine, New York, NY*

**8:30 – 10:30 AM, THURSDAY MORNING  
COVALENT LABELING, CHEMICAL PROBES, AND  
CROSSLINKING FOR BIOMOLECULE  
STRUCTURAL CHARACTERIZATION**

**Simin Maleknia (University of New South Wales), presiding  
Ballroom II, level 4**

ThOF am 08:30 **Extending the Cross-Linking/MS Strategy: Monitoring Protein Conformations by Incorporation of Unnatural Amino Acids, Photo-Cross-Linking, and MS**; Rico Schwarz; Knut Koelbel; Philip Loessl; Christian Ihling; Andrea Sinz; *Martin Luther University Halle, Halle, Germany*

ThOF am 08:50 **Structural Characterization using Chemical Cross-linking and Hydrogen/Deuterium Exchange: Resource for Novel Model of Human Haptoglobin**; Zdenek Kukacka<sup>1,2</sup>; Petr Man<sup>1,2</sup>; Petr Novak<sup>1,2</sup>; Petr Pompach<sup>1,2</sup>; <sup>1</sup>*Institute of Microbiology ASCR, Prague, Czech Republic*; <sup>2</sup>*Faculty of Science, Charles University, Prague, Czech Republic*

ThOF am 09:10 **A Novel Bioorthogonal and Clickable Cross-Linker for improved Protein/Protein Interaction Analysis**; Catherine Nury<sup>1,2</sup>; Virginie Redeker<sup>3</sup>; Sébastien Dautry<sup>4</sup>; Anthony Romieu<sup>4</sup>; Guillaume Van der Rest<sup>5</sup>; Pierre-Yves Renard<sup>4</sup>; Ronald Melki<sup>3</sup>; Julia Chamot-Rooke<sup>1,2</sup>; <sup>1</sup>*CNRS UMR 3528, Institut Pasteur, Paris, France, Paris, France*; <sup>2</sup>*Institut Pasteur, Structural MS & Proteomics Unit, Paris, France*; <sup>3</sup>*Laboratoire Enzymologie et Biochimie Structurales, Gif sur Yvette, France*; <sup>4</sup>*Université de Rouen - UMR 6014 CNRS, Mont Saint Aignan, France*; <sup>5</sup>*Université Paris Sud, Lab. Chimie Physique, Orsay, France*

ThOF am 09:30 **Mass-Spectrometry-Based Footprinting to Map the Precursor tRNA Binding Sites in a Protein-Only RNase P Variant**; Tien-Hao Chen; Akiko Tanimoto; Xin Ma; Wei Zhou; Jikang Wu; Venkat Gopalan; Vicki Wysocki; *The Ohio State University, Columbus, OH*

ThOF am 09:50 **High Resolution Measurement of Protein Topography by Covalent Carbene Labeling Induced by Single-Shot Laser Irradiation**; Joshua Buse<sup>1</sup>; Ryan Bomgarden<sup>2</sup>; John Rogers<sup>2</sup>; Chris Etienne<sup>2</sup>; David C. Schriemer<sup>1</sup>; <sup>1</sup>*University of Calgary, Calgary, Alberta*; <sup>2</sup>*Thermo Fisher Scientific, Rockford, Illinois*

ThOF am 10:10 **Probing the Conformational Change of Orange Carotenoid Protein during Photo-Activation in Cyanobacteria**; Hao Zhang; Haijun Liu; Jeremy King; Mindy Prado; Michael L. Gross; Robert E. Blankenship; *Washington University, St Louis, MO*

**8:30 – 10:30 AM, THURSDAY MORNING  
INFORMATICS: METABOLOMICS**

**Pieter Dorrestein (University of California, San Diego), presiding  
Ballroom III, level 4**

ThOG am 08:30 **Searching PubChem with Tandem Mass Spectrometry Data: Teaming Molecular Fingerprint Prediction and Fragmentation Trees**; Sebastian Böcker<sup>1</sup>; Huibin Shen<sup>2</sup>; Kai Dührkop<sup>1</sup>; Juho Rousu<sup>2</sup>; <sup>1</sup>*Friedrich-Schiller-University Jena, Jena, Germany*; <sup>2</sup>*Aalto University, Helsinki, Finland*

ThOG am 08:50 **ramclustR: post-XCMS Feature Clustering for Data Reduction and Spectral Matching-Based Annotation**; Corey Broeckling<sup>1</sup>; Fayyaz-ul-Amir Afsar Minhas<sup>1</sup>; Asa Ben-Hur<sup>1</sup>; Jessica Prenni<sup>1</sup>; Steffen Neumann<sup>2</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*Leibniz Institute of Plant Biochemistry, Halle, Germany*

ThOG am 09:10 **Multivariate Analysis, Visualization and Network Tools for Biological Interpretation of Metabolomic Data**; Dmitry Grapov<sup>1,2</sup>; Oliver Fiehn<sup>1,2</sup>; <sup>1</sup>*NIH West Coast Metabolomics Center, Davis, CA*; <sup>2</sup>*University of California, Davis, Davis, CA*

ThOG am 09:30 **Database Driven Molecular Annotation of Imaging Mass Spectrometry**; Andrew D. Palmer<sup>1</sup>; Michael Becker<sup>2</sup>; Janina Oetjen<sup>3</sup>; Ilya Chernyavsky<sup>1</sup>; Dmitry N. Kozlov<sup>1</sup>; Theodore Alexandrov<sup>1,4</sup>; <sup>1</sup>*University of Bremen, Bremen, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>3</sup>*MALDI Imaging Lab, University of Bremen, Bremen, Germany*; <sup>4</sup>*SCiLS GmbH, Bremen, Germany*

ThOG am 09:50 **Mass Spectrometry Based Metabolomics Work Area and Data Management Software "From Sample to Metabolic Pathways"**; Bernd Haas; Martin Buratti; Nicole Huber; Hannes Pedevilla; Therese Koal; *Biocrates Life Sciences AG, Innsbruck, Österreich*

ThOG am 10:10 **Lifeline-S.O.S: "Crowd Curation" of Unidentified GC-(EI)MS spectra through Social Online Spectrometry**; Manor Askenazi<sup>1</sup>; Yuri Mirokhin<sup>2</sup>; Stephen Stein<sup>2</sup>; <sup>1</sup>*Biomedical Hosting LLC, Arlington, MA*; <sup>2</sup>*NIST, Gaithersburg, MD*

**8:30 – 10:30 AM, THURSDAY MORNING  
GLYCOPROTEINS AND GLYCANS: NEW MS APPROACHES**  
**Ronghu Wu (Georgia Tech), presiding  
Ballroom IV, level 4**

ThOH am 08:30 **Determination of the False Discovery Rate in Glycopeptide Identifications using GlycoPep Evaluator**; Zhikai Zhu; Xiaomeng Su; Eden Go; Heather Desaire; *University of Kansas, Lawrence, KS*

## THURSDAY MORNING AND THURSDAY AFTERNOON ORAL SESSIONS

ThOH am 08:50 **Method for Analysis of Glycan Degradation Products in the Feces of Breast-Fed Newborns;** Jasmine C. C. Davis; Sarah M. Totten; Carlito B. Lebrilla; *UC Davis, Davis, CA*

ThOH am 09:10 **Relative Quantification of Glycans using Multiplexed Carbonyl-Reactive Tandem Mass Tags and CE-ESI-MS;** Xuefei Zhong<sup>1</sup>; Yan Liu<sup>2</sup>; Sergei Snovida<sup>3</sup>; John Rogers<sup>3</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>*University of Wisconsin Madison, Madison, WI*; <sup>2</sup>*Xiamen University, Xiamen, P.R.China*; <sup>3</sup>*Thermo Fisher Scientific, Rockford, IL*

ThOH am 09:30 **Stable Isotope Labeling Strategies for Quantitative UPLC-MS Based Glycomics;** Silvia Millan Martin<sup>1</sup>; Simone Albrecht<sup>1</sup>; Margaret Doherty<sup>1</sup>; Cedric Delporte<sup>1</sup>; Niaobh McLoughlin<sup>1</sup>; Natalia Navas<sup>2</sup>; Jonathan Bones<sup>1</sup>; <sup>1</sup>*NIBRT, Dublin, Ireland*; <sup>2</sup>*University of Granada, Granada, Spain*

ThOH am 09:50 **Quantitative LC-MS/MS Glycomic Analysis using Tandem Mass Tag (TMT);** Shiyue Zhou<sup>1</sup>; Yunli Hu<sup>1</sup>; Sergei Snovida<sup>2</sup>; John C. Rogers<sup>2</sup>; Julian Saba<sup>3</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>*Texas Tech University, Lubbock, TX*; <sup>2</sup>*Thermo Fisher Scientific, Rockford, IL*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*

ThOH am 10:10 **A Novel Method for Quantitative Analysis of Sialylated Glycopeptides;** Punit Shah; Shadi Toghi Eshghi; Weiming Yang; Jing Chen; Lijun Chen; Hui Zhang; *Johns Hopkins University School of Medicine, Baltimore, MD*

10:30 AM – 2:30 PM, THURSDAY  
THURSDAY POSTER SESSION  
Poster/Exhibit Hall  
Lunch concessions are open 11:00 am – 2:00 pm

## THURSDAY AFTERNOON ORAL SESSIONS

### 2:30 – 4:30 PM, THURSDAY AFTERNOON FOOD CHEMISTRY AND SAFETY Clifton K. Fagerquist (USDA), presiding Exhibit Hall AB

ThOA pm 2:30 **Integrated Targeted and Untargeted Analysis of Ergot Alkaloids in Cereals using UHPLC – TripleTOF MS;** José Diana Di Mavungu; Sarah De Saeger; *Ghent University, Ghent, Belgium*

ThOA pm 2:50 **The Molecular Architecture of an Edible Biofilm;** Laura Sanchez<sup>1</sup>; Julie Button<sup>2</sup>; Theodore Alexandrov<sup>3</sup>; Benjamin Wolfe<sup>2</sup>; Rachel Dutton<sup>2</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>*University of California, San Diego, Skaggs school, La Jolla, CA*; <sup>2</sup>*Harvard FAS Center for Systems Biology, Cambridge, MA*; <sup>3</sup>*University of Bremen, Bremen, Germany*

ThOA pm 3:10 **Ion Mobility Studies of Isomeric Species Lycopene,  $\beta$ -carotene, and  $\alpha$ -carotene and the Retention of Trans and Cis Conformation;** Matthew Bernier; Rachel Kopec; Steven Schwartz; Vicki Wysocki; *The Ohio State University, Columbus, OH*

ThOA pm 3:30 **Simultaneous Quantitative Determination of Melamine, Ammeline, Ammelide, Cyanuric acid and Dicyandiamide in Infant Formula and Other Foods by UHPLC-MS/MS with Fast Polarity Switching;** Hui Zhao; Katerina Mastovska; James Stark; Brent Rozema; John Austad; *Covance, Madison, WI*

ThOA pm 3:50 **Evaluating terroir - Revealing the Chemical Basis of Organoleptic Properties of Cabernet Sauvignon Wine with Untargeted LC and GC/QTOF Workflows;** Stephan Baumann<sup>1</sup>; Susan Ebeler<sup>2</sup>; Frank David<sup>3</sup>; Mark Sartain<sup>1</sup>; Sofia Aronova<sup>1</sup>; Kawaljit Tandon<sup>4</sup>; <sup>1</sup>*Agilent Technologies, Inc., Santa Clara, CA*; <sup>2</sup>*UC Davis Department of Viticulture and Enology, Davis, CA*; <sup>3</sup>*Research Institute for Chromatography, Kortrijk, Belgium*; <sup>4</sup>*Constellation Brands, Inc., Madera, CA*

ThOA pm 4:10 **Application of Wheat-Specific Peptide Markers for the Detection of Gluten in an incurred Cornbread Model using Mass Spectrometry;** Katherine L. Fiedler<sup>1</sup>; Sara C. McGrath<sup>1</sup>; Lauren S. Jackson<sup>2</sup>; Mark M. Ross<sup>1</sup>; <sup>1</sup>*U.S. FDA, CSFAN, College Park, MD*; <sup>2</sup>*U.S. FDA, CFSAN, Bedford Park, IL*

### 2:30 – 4:30 PM, THURSDAY AFTERNOON INSTRUMENTATION: TIME-OF-FLIGHT MASS SPECTROMETRY William Brinckerhoff (NASA), presiding Room 307-308

ThOB pm 2:30 **Space- and Time-Resolved Detection of Ions and Neutrals in MALDI-TOF-MS Using an Active Pixel Detector;** Shane R. Ellis; Ron M.A. Heeren; *FOM Institute AMOLF, Amsterdam, Netherlands*

ThOB pm 2:50 **MALDI-TOF-MS-Analysis of Intact High Mass Proteins by Phonon-Assisted Field Emission in Silicon Nanomembranes;** Diana Hildebrand<sup>1</sup>; Hyun-Cheol Shin Shin<sup>1,2</sup>; Hyunseok Kim Kim<sup>2</sup>; Jonghoo Park<sup>3</sup>; Zlatan Aksamija Aksamija<sup>4</sup>; Robert Blick<sup>1,2</sup>; <sup>1</sup>*University of Hamburg, Hamburg, Germany*; <sup>2</sup>*University of Wisconsin-Madison, Madison, WI*; <sup>3</sup>*Kyungpook National University, Daegu, Korea*; <sup>4</sup>*University of Massachusetts-Amherst, Amherst, MA*

ThOB pm 3:10 **High Resolution Multi-Reflecting TOFMS with Ion Trap Converter;** Viatcheslav Artaev<sup>1</sup>; Sergey Kirillov<sup>2</sup>; Boris Kozlov<sup>2</sup>; Mikhail Yavor<sup>2</sup>; Anatoly Verenchikov<sup>2</sup>; <sup>1</sup>*LECO Corporation, St Joseph, MI*; <sup>2</sup>*Mass Spectrometry Consulting, Bar, Montenegro*

ThOB pm 3:30 **Instrumentation, Statistics and Inference in TOFMS;** Andreas Ipsen; *Swansea University, Swansea, UK*

ThOB pm 3:50 **Perfect Timing: Fragment Ion Mobility Based Performance Increase on a qTOF Instrument;** Dominic Helm<sup>1</sup>; Christopher J Hughes<sup>2</sup>; Johannes PC Vissers<sup>2</sup>; Benjamin Ruprecht<sup>1</sup>; Hannes Hahne<sup>1</sup>; Isabelle Becher<sup>3</sup>; Markus Bantscheff<sup>3</sup>; James I Langridge<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>*Technische*

Universität München, Freising, Germany; <sup>2</sup>Waters Corporation, Manchester, UK; <sup>3</sup>Cellzome, Heidelberg, Germany

- ThOB pm 4:10 **Transient Sample Introduction with Laser Ablation Coupled to an Inductively Coupled Plasma Distance-of-Flight Mass Spectrometer (ICP-DOFMS);** Elise A. Dennis<sup>1</sup>; Alexander W. Gundlach-Graham<sup>1</sup>; Christie G. Enke<sup>2</sup>; Steven J. Ray<sup>1</sup>; Charles J. Barinaga<sup>3</sup>; David W. Koppenaal<sup>3</sup>; Gary M. Hieftje<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>University of New Mexico, Placitas, NM; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
MASS SPECTROMETRY IN STRUCTURAL BIOLOGY**  
**Christian Bleiholder (Florida State University), presiding**  
**Room 309-310**

- ThOC pm 2:30 **Integrating Native Mass Spectrometry with (Quantitative) Proteomics and Comparative Chemical Cross-linking – Insights into the Assembly of Key Protein Complexes;** Carla Schmidt; Yuliya Gordiyenko; Nina Morgner; Min Zhou; Carol Robinson; *University of Oxford, Oxford, UK*
- ThOC pm 2:50 **Using Surface Induced Dissociation-Ion Mobility (SID-IM) to Distinguish the Different Interfaces that Exist in Tetrameric Protein Complexes;** Royston Quintyn; Jing Yan; Vicki Wysocki; *The Ohio State University, Columbus, Ohio*
- ThOC pm 3:10 **Metabolic Pulse Chase Labeling of Rodents Shows that the Protein Cores of Some Intracellular Protein Machines Last a Lifetime;** Jeffrey Savas<sup>1</sup>; Brandon Toyama<sup>2</sup>; Varda Levram-Ellisman<sup>3</sup>; Roger Tsien<sup>3</sup>; Martin Hetzer<sup>2</sup>; John Yates<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Salk Institute for Biological Studies, La Jolla, CA; <sup>3</sup>University of California at San Diego, La Jolla, CA
- ThOC pm 3:30 **Charge Detection Mass Spectrometry Measures Mass Distribution of Virus Capsids above 20 MDa and Resolves Intermediates in Virus Assembly;** David Keifer; *Indiana University, Bloomington, IN*
- ThOC pm 3:50 **Large Scale Protein-Protein Complex Structure Prediction with *in vivo* Cross-Linking Data;** Chunxiang Zheng; Juan Chavez; Arti Navare; Xia Wu; James Bruce; *University of Washington, Seattle, WA*
- ThOC pm 4:10 **Droplet Sizes, Electrospray Currents, and Nonspecific Aggregation in Electrokinetically Controlled Native Nanoelectrospray Ionization;** Kimberly Davidson<sup>1</sup>; Derek Oberreit<sup>2</sup>; Christopher Hogan<sup>2</sup>; Matthew Bush<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>University of Minnesota, Minneapolis, MN

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
FUNDAMENTALS: ION SPECTROSCOPY**  
**Elaine Marzluff (Grinnell College), presiding**  
**Room 314-317**

- ThOD pm 2:30 **Fluorescence Resonance Energy Transfer Measurements for the Structural Characterization of Gaseous Proteins Generated by Electrospray Ionization;** Martin F. Czar<sup>1</sup>; Arash Zarrine-Afsar<sup>2</sup>; Franziska Zosel<sup>2</sup>; Iwo König<sup>2</sup>; Benjamin Schuler<sup>2</sup>; Rebecca A. Jockusch<sup>1</sup>; <sup>1</sup>University of Toronto, Toronto, Canada; <sup>2</sup>Universität Zürich, Zürich, Switzerland

- ThOD pm 2:50 **Action-EET Based Dissociation of Disulfide Bonds with Tryptophan as a Donor in the Gas Phase;** Nathan Hendricks<sup>1</sup>; Nichole M. Lareau<sup>2</sup>; John A. Mclean<sup>2</sup>; Ryan R. Julian<sup>1</sup>; <sup>1</sup>University of California, Riverside, Riverside, CA; <sup>2</sup>Vanderbilt University, Nashville, TN

- ThOD pm 3:10 **Conformer-Specific Infrared Spectroscopy of Cyclic  $b_6$  and  $b_8$  Fragments Produced by Collision-Induced Dissociation of Peptides;** Oleg Aseev; Marta Perez; Ursula Röthlisberger; Thomas Rizzo; *École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

- ThOD pm 3:30 **Gas-phase Conformation of Polyproline Peptides and the  $b_2$  Fragment by IRMPD Spectroscopy;** Jonathan Martens<sup>1</sup>; Josipa Grzetic<sup>1</sup>; Giel Berden<sup>1</sup>; Jos Oomens<sup>1,2</sup>; <sup>1</sup>Radboud University Nijmegen, Nijmegen, Netherlands; <sup>2</sup>University of Amsterdam, Amsterdam, Netherlands

- ThOD pm 3:50 **Infrared Multiple Photon Dissociation Spectroscopy of a Gas-Phase Oxo-Molybdenum Complex with 1,2-dithiolene Ligands;** Michael J. Van Stipdonk<sup>1</sup>; John K. Gibson<sup>2</sup>; Giel Berden<sup>3</sup>; Jos Oomens<sup>3,4</sup>; <sup>1</sup>Duquesne University, Pittsburgh, PA; <sup>2</sup>Lawrence Berkeley Laboratory, Berkeley, CA; <sup>3</sup>Radboud University Nijmegen, Nijmegen, The Netherlands; <sup>4</sup>University of Amsterdam, Amsterdam, The Netherlands

- ThOD pm 4:10 **Soft Landing of Mass-Selected Polyoxometalate Anions onto Self-Assembled Monolayers;** Don Gunaratne; Grant Johnson; Amity Andersen; Dan Du; Weiyang Zhang; Yuehe Lin; Julia Laskin; *Pacific Northwest National Laboratory, Richland, WA*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
DATA INDEPENDENT ACQUISITION**  
**Paul West (Biomarker Discovery), presiding**  
**Ballroom I, level 4**

- ThOE pm 2:30 **Comparison of Shotgun Proteomics with Data Independent Acquisition in Terms of Number of Identified Peptides;** Roland M. Bruderer; Oliver M. Bernhardt; Saša M. Miladinović; Tejas Gandhi; Oliver Rinner; Lukas Reiter; *BiognoSYS AG, Zurich, Switzerland*

- ThOE pm 2:50 **Multiphase-cHiPLC Coupled SWATH Profiling of Metastatic Melanoma Cells Reveals MAPK Pathway Mutation Specific Protein Expression;** Christoph Krisp<sup>1</sup>; Robert Parker<sup>1</sup>; Matthew McKay<sup>1</sup>; Dana Pascovici<sup>1</sup>; Hao Yang<sup>2</sup>; Remco van Soest<sup>2</sup>; Tina Settineri<sup>2</sup>; Mark P. Molloy<sup>1</sup>; <sup>1</sup>Australian Proteome Analysis Facility, Sydney, Australia; <sup>2</sup>Eksigent, part of AB SCIEX, Redwood City, CA

- ThOE pm 3:10 **Systematic Investigation on Suitability of LC-QqTOF with SWATH Acquisition for Routine Forensic Screenings-Comparison with IDA and Targeted MRM Approaches;** Andreas T. Roemmelt; Andrea E. Steuer; Michael Poetzsch; Thomas Kraemer; *Zurich Institute of Forensic Medicine, UZH, Zurich, Switzerland*

ThOE pm 3:30 **Harnessing the Power of SWATH-MS for Unbiased Identification of O-GlcNacylated Proteins;** Christine Jelinek; Genaro Ramirez-Correa; Guanghui Han; David Colquhoun; Alexey Lyashkov; Gerald Hart; David Graham; Jennifer Van Eyk; Anne Murphy; *Johns Hopkins School of Medicine, Baltimore, MD*

ThOE pm 3:50 **Increasing Depth of Coverage in Data Independent Acquisition with Acquisition Improvements and Higher Sample Loads;** Christie L. Hunter<sup>1</sup>; Ben Collins<sup>2</sup>; Ludovic Gillet<sup>2</sup>; Ruedi Aebersold<sup>2</sup>; <sup>1</sup>AB SCIEX, Redwood City, CA; <sup>2</sup>ETH Zurich, Zurich, Switzerland

ThOE pm 4:10 **Establishment of DIA-based Methods in Urine Biomarker Discovery - A Comparative Study to Discover an Early Stage Chronic Pancreatitis Biomarker;** Jan Muntel<sup>1</sup>; Saima Ahmed<sup>1</sup>; Melena Bellin<sup>2</sup>; Vivek Kadiyala<sup>3</sup>; Shadeah L. Suleiman<sup>3</sup>; Linda S. Lee<sup>3</sup>; Peter A. Banks<sup>3</sup>; Darwin L. Conwell<sup>4</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>Boston Children's Hospital, Boston, MA; <sup>2</sup>University of Minnesota, Minneapolis, MN; <sup>3</sup>Brigham and Women's Hospital, Boston, MA; <sup>4</sup>Ohio State University Wexner Medical Center, Columbus, OH

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
EPIGENETIC MODIFICATIONS AND MECHANISMS**  
**Maria Person (University of Texas, Austin), presiding**  
**Ballroom II, level 4**

ThOF pm 2:30 **Stable Isotope labeled Histone Peptide Library for Histone Post-Translational Modification and Variant Quantification by Mass Spectrometry;** Shu Lin<sup>1</sup>; Samuel Wein<sup>1</sup>; Michelle Gonzales-Cope<sup>1,2</sup>; Gabriel L. Otte<sup>1</sup>; Leila Afjehi-Sadat<sup>1</sup>; Tobias Maile<sup>3</sup>; Shelley L. Berger<sup>1</sup>; John Rush<sup>4</sup>; Jennie Lill<sup>3</sup>; David Amott<sup>3</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Princeton University, Princeton, NJ; <sup>3</sup>Genentech Inc., South San Francisco, CA; <sup>4</sup>Cell Signaling Technology Inc., Danvers, MA

ThOF pm 2:50 **Differential Analysis of histone Post Translational Modifications in MEL Cells using WCX-HILIC Coupled to Middle-Down ECD Mass Spectrometry;** Annie Moradian<sup>1</sup>; Michael Sweredoski<sup>1</sup>; Anastasia Kalli<sup>2</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>California Institute of Technology, Pasadena, CA; <sup>2</sup>Children's Hospital Los Angeles, Los Angeles, CA

ThOF pm 3:10 **Top Down MS/MS Analysis of Dynamic Changes in Histone Sequence Variants and Post-Translational Modifications during HIV Activation;** Yu Chen<sup>1</sup>; Xibei Dang<sup>1</sup>; Brian D. Spetman<sup>2</sup>; Jonathan H. Dennis<sup>2</sup>; Alan G. Marshall<sup>1,2</sup>; Nicolas L. Young<sup>1</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University, Tallahassee, FL

ThOF pm 3:30 **Dynamic and Combinatorial Landscape of Histone Modifications through Plasmodium falciparum Life Cycle;** Anita Saraf<sup>1</sup>; Serena Cervantes<sup>2</sup>; Evelien Bunnik<sup>2</sup>; Nadia Ponts<sup>2</sup>; Mihaela Sardi<sup>1</sup>; Duk-Won Chung<sup>2</sup>; Jacques Prudhomme<sup>2</sup>; Zhihui Wen<sup>1</sup>; Joseph Varberg<sup>1</sup>; Michael Washburn<sup>1</sup>; Karine Le Roch<sup>2</sup>; Laurence Florens<sup>1</sup>; <sup>1</sup>Stowers Institute for Medical Research, Kansas City, MO; <sup>2</sup>University of California Riverside, Riverside, CA

ThOF pm 3:50 **Quantitative Profiling of Chromatome Dynamics Reveals the Regulatory Switches of Epigenome in Hypoxia-Induced Oncogenesis;** Bamaprasad Dutta; Siu Kwan Sze; *Nanyang Technological University, Singapore, Singapore*

ThOF pm 4:10 **Protein Profiling Reveals Dynamic H1 Expression and Identifies H3 K9me/S10p/K14ac tri-modification Forms in Monocyte Differentiation;** Hui Tang; Kangling Zhang; *University of Texas Medical Branch at Galveston, Galveston, TX*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
METABOLOMICS/LIPIDOMICS:  
NEW MS TECHNOLOGIES AND APPLICATIONS**  
**Stephen Blanksby (Queensland University), presiding**  
**Ballroom III, level 4**

ThOG pm 2:30 **Comprehensive Lipidome Profiling Enables Functional Studies to Determine the Role of Aberrant Lipid Metabolism in Metastatic Colorectal Cancer Cells;** Cassie Phaner; Gavin E. Reid; *Michigan State University, East Lansing, MI*

ThOG pm 2:50 **Integration of Supercritical Fluid Chromatography with Ion Mobility-Mass Spectrometry (SFC-IM-MS) for Metabolomics and Lipidomics;** Rafael Montenegro Burke<sup>1</sup>; Cody Goodwin<sup>1</sup>; Libin Xu<sup>1</sup>; Zeljka Korade<sup>2</sup>; Brian Bachmann<sup>1</sup>; Ned Porter<sup>1</sup>; John A. Mclean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt Kennedy Center, Nashville, Tennessee

ThOG pm 3:10 **Applications and Performance of the GC/ quadrupole-Orbitrap MS in Discovery Metabolomics;** Allison Balloun<sup>1</sup>; Jason Cole<sup>3</sup>; Taylor Wahlig<sup>1</sup>; Amelia Petersen<sup>2</sup>; Jens Griep-Raming<sup>2</sup>; Michael Westphal<sup>1</sup>; Jean-Michel Ane<sup>1</sup>; Michael Sussman<sup>1</sup>; Joshua Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Fisher Scientific, Austin, TX

ThOG pm 3:30 **Accurate Quantification of Polyunsaturated Glycerophospholipids by Shotgun Lipidomics;** Kai Schuhmann; Andrej Shevchenko; *MPI-CBG, Dresden, Germany*

ThOG pm 3:50 **Facile Determination of C=C Bonds within Lipids by On-Line Paternò-Büchi Reaction and Tandem Mass Spectrometry;** Xiaoxiao Ma; Yuan Su; Zheng Ouyang; Yu Xia; *Purdue University, West Lafayette, IN*

ThOG pm 4:10 **A Sensitive Mass Spectrometry Platform Providing Ozone Induced Dissociation for High Throughput Lipid Structure Characterization;** Qibin Zhang; Yehia Ibrahim; Karl Weitz; Ronald Moore; Richard D. Smith; Keqi Tang; *Pacific Northwest National Laboratory, Richland, WA*

**2:30 – 4:30 PM, THURSDAY AFTERNOON  
CARBOHYDRATES: NEW MS APPROACHES**  
**Maria Lorna De Leoz (NIST), presiding**  
**Ballroom IV, level 4**

ThOH pm 2:30 **Application of Selected Accumulation Ion Mobility Spectrometry-Electron Activated Dissociation Tandem Mass Spectrometry in Structural Analysis of Isomeric Glycans;** Yi Pu<sup>1</sup>; Rebecca S. Glaskin<sup>2</sup>; Cheng Lin<sup>2</sup>; Catherine E. Costello<sup>1,2</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Boston University School of Medicine, Boston, MA



ThOH pm 2:50 **Comparing the LC-MS of Permethylated and Native Glycans on Reversed-Phase and Porous Graphitic Carbon Columns;** Yunli Hu; Shiyue Zhou; James Blackmer; Yehia Mechref; *Texas Tech University, Lubbock, TX*

ThOH pm 3:10 **Exploring the Brain Glycome using Tissue Cell Membrane Capture and Nanoflow Liquid Chromatography/Mass Spectrometry;** Injung Ji<sup>1</sup>; Serenus Hua<sup>1</sup>; Jong-Soon Choi<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*AGRS, Chungnam National University, Daejeon, Korea;* <sup>2</sup>*Division of Life Science, KBSI, Daejeon, Korea*

ThOH pm 3:30 **Oligosaccharide MSn and Spectral Library Matching: Instrumental and Collision Energy Comparisons;** Andrew Hanneman<sup>1</sup>; David Ashline<sup>1,2</sup>; Hailong Zhang<sup>2</sup>; Vernon Reinhold<sup>2</sup>; <sup>1</sup>*Glycan Connections, Lee, NH;* <sup>2</sup>*University of New Hampshire, Durham, NH*

ThOH pm 3:50 **Fully Automated Annotation and Identification of Glycosaminoglycan MS/MS Spectra;** Jiana Duan; Jon Amster; *University of Georgia, Athens, GA*

ThOH pm 4:10 **Discovery of a Novel Peeling Reaction that Contributes to the Underestimation of 3-O-sulfation in Heparan Sulfate;** Yu Huang<sup>1</sup>; Yang Mao<sup>1</sup>; Chengli Zhong<sup>2</sup>; Geert-Jan Boons<sup>2</sup>; Cheng Lin<sup>1</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA;* <sup>2</sup>*University of Georgia, Athens, GA*

4:45 – 5:30 PM, THURSDAY AFTERNOON  
PLENARY LECTURE

Jenny Brodbelt (University of Texas, Austin), presiding  
Exhibit Hall AB



How The Genome Folds

Erez Lieberman Aiden  
Baylor College of Medicine and Rice University

6:30 – 9:00 PM, THURSDAY  
CLOSING EVENT  
National Aquarium  
Ticket is required.



7:30 – 8:00 am..... Set up all Monday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 7:30 – 8:00 pm..... Remove all Monday posters

Imaging MS: Method Development .....	001-018
Imaging MS: Software .....	019-030
Informatics: Workflow and Data Management.....	031-049
Informatics: Small Molecule Identification & Characterization..	050-062
Proteins: General.....	063-087
Proteins: PTMs.....	088-122
Proteins: Membranes .....	123-138
Intact Proteins: Sequence Analysis .....	139-149
Proteins: Complexes .....	150-165
Proteins: Covalent Labeling.....	166-179
Intact Proteins: Non-Covalent Interactions.....	180-185
Peptides: General.....	186-199
Peptides: Sequence Analysis .....	200-207
Proteomics: New Approaches .....	208-224
Epigenetic Modifications / Histones.....	225-237
Lipids: General .....	238-253
Systems Biology: General .....	254-279
Toxicology: Therapeutic Drug Monitoring/Drugs of Abuse.....	280-294
Ionization Mechanisms.....	295-316
Ion Structure/Energetics.....	319-329
Geochemistry .....	330-333
Isotope Ratio MS.....	334-335
Food Safety.....	336-359

Component Source Determination for Drugs, Pharmaceuticals, and Homeland Security Applications ...	360-365
Accelerator Mass Spectrometry .....	366
Biomimetic / Catalytic Systems .....	367
History of Mass Spectrometry .....	368
Ambient Ionization: Instrumentation .....	375-404
Plant"omics".....	405-419
Biomarkers: Discovery.....	421-445
Disease Biomarkers .....	446-467
Small Molecule: Qualitative Analysis.....	468-484
Small Molecule Quantitation.....	485-519
Homeland Security .....	520-531
High Throughput Analytics / Robotics.....	532-540
Environmental Analysis: Hydrocarbon and DOM .....	549-557
Energy: Biofuels and Algae .....	558-577
Metabolomics: Untargeted Metabolite Profiling.....	578-605
Metabolomics: Identification of Unknown Metabolites.....	606-630
Metabolomics: Sample Preparation.....	631-638
Drug Metabolism: Qualitative Analysis .....	639-647
High Accuracy / High Performance MS: Instrumentation .....	648-660
Instrumentation: New Concepts .....	661-676
LCMS: Software .....	677-683
Photoionization: Instrumentation and Applications.....	684-686
Instrumentation: New Developments in Mass Analyzers.....	687-707
LCMS: Instrumentation.....	709-726
LCMS: Chromatography.....	727-752
LCMS: Sample Preparation (Drugs and Metabolites) .....	753-786

These special posters will be displayed all week.

Special **The Analytical Triple-Quadrupole Mass Spectrometer and Low-Energy CID: Beginnings, Offshoots, and Current Applications;** [Michael A. Grayson](#)<sup>1</sup>; [Christie G. Enke](#)<sup>2</sup>; [Richard A. Yost](#)<sup>3</sup>; <sup>1</sup>*Retired, St Charles, MO*; <sup>2</sup>*University of New Mexico, Placitas, NM*; <sup>3</sup>*University of Florida, Gainesville, FL*

Special **The British Mass Spectrometry Society: The first 50 years;** [Alison E. Ashcroft](#)<sup>1</sup>; [Susan Crosland](#)<sup>2</sup>; [Keith R Jennings](#)<sup>3</sup>; <sup>1</sup>*University of Leeds, Leeds, United Kingdom*; <sup>2</sup>*Syngenta, Jealott's Hill, Bracknell, UK*; <sup>3</sup>*2 Meadow Croft Drive, Bishop Monkton, UK*

Special **Call for Participants for the iPRG 2015 Study: Label-Free Quantitative Proteomics Data Analysis**

**Imaging MS: Method Development, 001 - 018**

MP 001 **Systematic Study of Stage Raster Speed, Laser Repetition Rate and Pulse Energy in MALDI MSI;** [Rory T. Steven](#); [Ian S. Gilmore](#); [Josephine Bunch](#); *National Physical Laboratory, London, UK*

MP 002 **High Throughput Spatially Resolved Peptide Identification using Hydrogel Digestion and Electro-Elution;** [Erin H. Seeley](#); [Gregory Boyce](#); [Linda Prengaman](#); [Greg W. Kilby](#); *Protea Biosciences, Inc., Morgantown, WV*

MP 003 **Quality Measures of MALDI MS imaging;** [Oskar Karlsson](#); [Malin Andersson](#); *Uppsala University, Uppsala, Sweden*

MP 004 **Multicenter MALDI Mass Spectrometry Imaging Identifies Proteomic Markers of Stromal Activation in Breast Cancer;** [Tim Dekker](#)<sup>1</sup>; [Benjamin Balluff](#)<sup>1</sup>; [Emrys Jones](#)<sup>1</sup>; [Cedrik Schoene](#)<sup>2</sup>; [Michaela Aubele](#)<sup>2</sup>; [Manfred Schmitt](#)<sup>3</sup>; [Judith Kroep](#)<sup>1</sup>; [Vincent Smit](#)<sup>1</sup>; [Rob Tollenaar](#)<sup>1</sup>; [André Deelder](#)<sup>1</sup>; [Wilma Mesker](#)<sup>1</sup>; [Axel Walch](#)<sup>2</sup>; [Liam McDonnell](#)<sup>1</sup>; <sup>1</sup>*Leiden University Medical Center, Leiden, Netherlands*; <sup>2</sup>*Helmholtz Zentrum Muenchen, Munich, Germany*; <sup>3</sup>*Klinikum rechts der Isar, Munich, Germany*

MP 005 **Imaging Mass Spectrometry and Depth Profiling for the Organic Thin Film using Laser Desorption Ionization;** [Takaya Satoh](#)<sup>1</sup>; [Masahide Shima](#)<sup>1</sup>; [Hironobu Niimi](#)<sup>1</sup>; [Yoji Nakajima](#)<sup>2</sup>; [Makiko Fujii](#)<sup>3</sup>; [Toshio Seki](#)<sup>3</sup>; [Jiro Matsuo](#)<sup>3</sup>; [Robert DiPasquale](#)<sup>4</sup>; <sup>1</sup>*JEOL Ltd., Akishima, Japan*; <sup>2</sup>*Asahi Glass Co., Ltd., Yokohama, Japan*; <sup>3</sup>*Kyoto Univ., Kyoto, Japan*; <sup>4</sup>*JEOL USA Inc., Peabody, MA*

MP 006 **Using MALDI-IMS and Membrane Microarrays for Tissue Classification;** [Roberto Fernández](#)<sup>1</sup>; [Tarson Tolentino-Cortez](#)<sup>2</sup>; [Sergio Lage](#)<sup>3</sup>; [Jone Garate](#)<sup>1</sup>; [Izaskun Erguido](#)<sup>1</sup>; [Rafael Rodríguez-Puertas](#)<sup>1</sup>; [Egoitz Astigarraga](#)<sup>2</sup>; [Gabriel Barreda-Gómez](#)<sup>2</sup>; [José A. Fernández](#)<sup>1</sup>; <sup>1</sup>*University of Basque Country, Leioa, Spain*; <sup>2</sup>*IMG Pharma Biotech, Leioa, Spain*; <sup>3</sup>*Cruces University Hospital, Barakaldo, Spain*

MP 007 **Sensitive Imaging of Essential Elements in a Rat Cerebellum using an Optimized LA/ICP-MS Setup Including a Collision Reaction Interface;** [Rebecca Niehaus](#); [Christoph Alexander Wehe](#); [Michael Sperling](#); [Uwe Karst](#); *Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

MP 008 **In-depth Identification of Protein Images by Combining High Mass Resolution MALDI FTICR Imaging and High Performance qTOF nLC-MS/MS;** [Shannon Cornett](#); [Sergei Dikler](#); [Matt Willetts](#); *Bruker Daltonics Inc., Billerica, MA*

MP 009 **Integration and Application of Separation Strategies to Multiplex Imaging Mass Spectrometry for Complex Neuropeptide Analysis;** [Shan Jiang](#); [Zichuan Zhang](#); [Lingjun Li](#); *UW-Madison, Madison, WI*

MP 010 **High Resolution and High Mass Accuracy Multiply Charged MALDI Technique for in situ Protein Characterization – Sequencing, Identification and Visualization;** [Bingming Chen](#)<sup>1</sup>; [Christopher Lietz](#)<sup>2</sup>; [Anh Van](#)<sup>1</sup>; [Lingjun Li](#)<sup>1,2</sup>; <sup>1</sup>*School of Pharmacy, UW-Madison, Madison, WI*; <sup>2</sup>*Department of Chemistry, UW-Madison, Madison, WI*

MP 011 **Optimization of the Analysis of Proteins Found in Paint Cross-sections from Works of Art by MALDI MSI;** [Emily O'Neill](#)<sup>1</sup>; [Marcel Powers](#)<sup>2</sup>; [Julie Arslanoglu](#)<sup>3</sup>; [John Allison](#)<sup>2</sup>;

- Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>The College of New Jersey, Ewing, NJ; <sup>3</sup>The Metropolitan Museum of Art, New York, NY
- MP 012 **Development of Imaging MS Methods to Monitor the Molecular Composition of Latent Fingermarks;** Nidia Lauzon<sup>1</sup>; Matthew Howland<sup>2</sup>; Martin Dufresne<sup>1</sup>; Vinita Chauhan<sup>2</sup>; Pierre Chaurand<sup>1</sup>; <sup>1</sup>Université de Montréal, Montreal, Canada; <sup>2</sup>Health Canada, Ottawa, Canada
- MP 013 **Increasing the Specificity and Sensitivity in Imaging Mass Spectrometry: Regiospecific Transfer of Proteins from Tissue Sections to Functionalized Surfaces;** Erik Fournaise; Pierre Chaurand; Department of Chemistry, Université de Montréal, Montreal, QC, Canada
- MP 014 **Multiplexed Molecular Imaging Mass Spectrometry: Analysis of Different Molecular Types on a Single Tissue Section;** Domenico Taverna<sup>1,2</sup>; Erin H Seeley<sup>2,3</sup>; Jeremy L Norris<sup>2</sup>; Raf Van de Plas<sup>2</sup>; Giovanni Sindona<sup>1</sup>; Richard M Caprioli<sup>2</sup>; <sup>1</sup>University of Calabria, Arcavacata Di Rende, Italy; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Protea Bioscience, Inc., Morgantown, WV
- MP 015 **Top-Down and Bottom-Up Analyses of Proteins on the Same Tissue Section using High Mass Resolution Imaging Mass Spectrometry;** David G. Rizzo; Jeffrey M. Spraggins; Kristie L. Rose; Richard M. Caprioli; Vanderbilt University MSRC, Nashville, TN
- MP 016 **Low Molecular Weight Proteins Revealed by Virtual 2D Gels;** Karen Lohnes; Robert Gunsalus; Joseph A. Loo; Rachel O. Loo; UCLA, Los Angeles, CA
- MP 017 **Single-step Process for Coupling *in situ* Protease Digestion with MALDI IMS: Pre-coated Trypsin Targets for High-throughput Analysis of FFPE Tissues;** Faizan Zubair; Junhai Yang; Richard Caprioli; Paul Laibinis; Vanderbilt University, Nashville, TN
- MP 018 **Tuning the Selectivity of MALDI Imaging Mass Spectrometry through Control of the Sample Preparation Parameters of Alternative Matrix Deposition Techniques;** Brian Malys; Kevin Owens; Elsa Gorre; Drexel University, Philadelphia, PA
- Imaging MS: Software, 019 - 030**
- MP 019 **CARDINAL: Open-source R Package for Statistical Analysis of 2D and 3D Mass Spectrometry Imaging Experiments;** Kyle Bemis<sup>1</sup>; Livia Eberlin<sup>1</sup>; Christina Ferreira<sup>1</sup>; Stephanie van de Ven<sup>2</sup>; Parag Mallick<sup>2</sup>; Mark Stollowitz<sup>2</sup>; Olga Vitek<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Stanford School of Medicine, Palo Alto, CA
- MP 020 **Topographical Surface Imaging Mass Spectrometry;** Theodore Alexandrov<sup>1,2</sup>; Christopher M Rath<sup>3</sup>; Amina Bouslimani<sup>1</sup>; Carla Porto Da Silva<sup>1</sup>; Yi Zeng<sup>1</sup>; Neha Garg<sup>1</sup>; Cliff Kapon<sup>1</sup>; Tal Luzzatto Knaan<sup>1</sup>; Katherine Duncan<sup>4</sup>; Laura Sanchez<sup>1</sup>; Alexey Melnik<sup>1</sup>; Kathleen Dorrestein<sup>1</sup>; Pieter Dorrestein<sup>1</sup>; <sup>1</sup>Skaggs School of Pharmacy, UCSD, La Jolla, CA; <sup>2</sup>University of Bremen, Bremen, Germany; <sup>3</sup>Novartis Institute for Biomedical Research, Emeryville, CA; <sup>4</sup>Scripps Institution of Oceanography, UCSD, La Jolla, CA
- MP 021 **3D MALDI Imaging of Mouse Heart after Myocardial Infarction;** Michael Becker<sup>1</sup>; Lena Hauberg-Lotte<sup>2</sup>; Judith Berger<sup>3</sup>; Janina Oetjen<sup>2</sup>; Dennis Trede<sup>9</sup>; Michaela Aichler<sup>6</sup>; Wolfgang Dreher<sup>7</sup>; Moritz Wildgruber<sup>8</sup>; Klaus Steinhörst<sup>5</sup>; Jan Hendrik Kobarg<sup>5</sup>; Stefan Schiffer<sup>9</sup>; Stefan Heldmann<sup>3</sup>; Herbert Thiele<sup>3</sup>; Peter Maass<sup>4</sup>; Axel Walch<sup>6</sup>; Theodore Alexandrov<sup>4</sup>; <sup>1</sup>Brüker Daltonik GmbH, Bremen, Germany; <sup>2</sup>MALDI Imaging Lab, University of Bremen, Bremen, Germany; <sup>3</sup>Fraunhofer MEVIS Project Group Image Registration, Lübeck, Germany; <sup>4</sup>Center for Industrial Mathematics, Bremen, Germany; <sup>5</sup>Steinbeis Innovation Center SCiLS Research, Bremen, Germany; <sup>6</sup>Research Unit Analytical Pathology, HMGU München, Oberschleissheim, Germany; <sup>7</sup>University of Bremen, Bremen, Germany; <sup>8</sup>Klinikum Rechts der Isar, TU München, München, Germany; <sup>9</sup>SCiLS GmbH, Bremen, Germany
- MP 022 **Automated Differential Analysis Between Tissue Samples Measured by Imaging Mass Spectrometry;** Nico Verbeeck<sup>1,2</sup>; Yousef El Aalamat<sup>1,2</sup>; David M. Anderson<sup>3</sup>; Zsolt Ablonczy<sup>4</sup>; Yiannis Koutalos<sup>4</sup>; Rosalie Crouch<sup>4</sup>; Kevin L. Schey<sup>3</sup>; Richard M. Caprioli<sup>3</sup>; Bart De Moor<sup>1,2</sup>; Etienne Waelkens<sup>5</sup>; Raf Van de Plas<sup>3</sup>; <sup>1</sup>KU Leuven, ESAT - STADIUS, Leuven, Belgium; <sup>2</sup>KU Leuven, iMinds Department Medical IT, Leuven, Belgium; <sup>3</sup>Vanderbilt University, MSRC, Nashville, TN; <sup>4</sup>Medical University of South Carolina, Charleston, SC; <sup>5</sup>KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium
- MP 023 **Capitalizing on Multi-Modal Imaging: Deeper Insights Through Fusion of Mass Spectrometry and Other Imaging Technologies;** Raf Van de Plas; Junhai Yang; Jeffrey Spraggins; Richard M. Caprioli; Vanderbilt University, Nashville, TN
- MP 024 **OpenMSI: A Web-Based Portal for Rapid Processing of Size-Independent, Next-Generation Mass Spectrometry Imaging Experiments;** Ben Bowen; Annette Greiner; Shreyas Cholia; Katherine Louie; Wes Bethel; Trent Northen; Oliver Ruebel; Lawrence Berkeley National Lab, Berkeley, CA
- MP 025 **Large MSI Datasets Analysis and Normalization using a "BigData" Platform: Proof-of- Concept in Hunting Biomarkers of Pulmonary Arterial Hypertension;** Sébastien J. Dumas; Raphael Legouffe<sup>2</sup>; Fabien Pamelard<sup>2</sup>; David Bonnel<sup>2</sup>; Youssef Oulamine<sup>2</sup>; Gaël Picard De Muller<sup>2</sup>; Gregory Hamm<sup>2</sup>; Elie Fadel<sup>1,3</sup>; Marc Humbert<sup>1,4</sup>; Sylvia Cohen-kaminsky<sup>1</sup>; Jonathan Stauber<sup>2</sup>; <sup>1</sup>INSERM UMR-S 999, Univ Paris-Sud, LabEx LERMIT, Le Plessis Robinson, France; <sup>2</sup>ImaBiotech, MS Imaging Dept., LOOS, France; <sup>3</sup>Hôpital Marie Lannelongue, Département de chirurgie, Le Plessis Robinson, France; <sup>4</sup>Service de Pneumologie, Centre National de Referen, Le Kremlin Bicêtre, France
- MP 026 **Data Management for Handling Large Data Sets in msiQuant Software for Mass Spectrometry Imaging;** Patrik Kallback; Mohammadreza Shariatgorji; Anna Nilsson; Per E. Andren; Uppsala University, Uppsala, Sweden
- MP 027 **Registration of Mass Spectrometry Imaging datasets to the Allen Brain Atlas;** Ricardo J. Carreira<sup>1</sup>; Walid M. Abdelmoula<sup>2</sup>; Reinald Shyti<sup>3</sup>; Benjamin Balluff<sup>1</sup>; René J. M. van Zeijl<sup>1</sup>; Else Tolner<sup>3,4</sup>; Arn M.J.M. van den Maagdenberg<sup>3,4</sup>; Boudewijn F.P. Lelieveldt<sup>2,5</sup>; Jouke Dijkstra<sup>2</sup>; Liam McDonnell<sup>1</sup>; <sup>1</sup>Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands; <sup>2</sup>Department of Radiology, LUMC, Leiden, Netherlands; <sup>3</sup>Department of Human Genetics, LUMC, Leiden, Netherlands; <sup>4</sup>Department of Neurology, LUMC, Leiden, Netherlands; <sup>5</sup>Faculty of EEMCS, Delft University of Technology, Delft, Netherlands
- MP 028 **Compositional Hierarchies for Spectral Segmentation of Mass Spectrometry Imaging Data Sets for Redundancy Reduction and Improved Interpretation;** Alan M. Race<sup>1</sup>; Josephine Bunch<sup>2</sup>; Aleš Leonardiš<sup>1</sup>; Iain B. Styles<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>National Physical Laboratory, London, UK
- MP 029 **Efficient Noise Reduction in Imaging Mass Spectrometry Data using Robust PCA;** Yousef El Aalamat<sup>1,2</sup>; Nico Verbeeck<sup>1,2</sup>; Junhai Yang<sup>3</sup>; Bart De Moor<sup>1,2</sup>; Richard M. Caprioli<sup>3</sup>; Etienne Waelkens<sup>4</sup>; Raf Van de Plas<sup>3</sup>; <sup>1</sup>KU Leuven, ESAT-STADIUS, Leuven, Belgium; <sup>2</sup>KU Leuven, iMinds Department Medical IT, Leuven, Belgium; <sup>3</sup>Vanderbilt University, MSRC, Nashville, TN; <sup>4</sup>KU Leuven, Dept. Cellular and Molecular Medicine, Leuven, Belgium

MP 030 **Correcting Mass Shifts: Lock Mass-Free Recalibration Procedure for Mass Spectrometry Imaging;** [Purva Kulkarni](#)<sup>1,2</sup>; [Philipp Kynast](#)<sup>1,2</sup>; [Filip Kaftan](#)<sup>2,3</sup>; [Vladimír Vrkoslav](#)<sup>4</sup>; [Josef Cvačka](#)<sup>3,4</sup>; [Markus Knaden](#)<sup>2</sup>; [Aleš Svatoš](#)<sup>2,3</sup>; [Sebastian Böcker](#)<sup>1</sup>; <sup>1</sup>*Lehrstuhl für Bioinformatik, FSU, Jena, Germany*; <sup>2</sup>*Max Planck Institute for Chemical Ecology, Jena, Germany*; <sup>3</sup>*Inst. of Organic Chemistry & Biochemistry, AS CR, Prague, Czech Republic*; <sup>4</sup>*Dept. of Analytical Chemistry, Charles University, Prague, Czech Republic*

**Informatics: Workflow & Data Management, 031 - 049**

MP 031 **PROCESS – PROteomics Data Collection, Software and Standards to Support Open Access and Long Term Management of Data;** [Simon Perkins](#)<sup>1</sup>; [Henning Hermjakob](#)<sup>2</sup>; [Andrew Jones](#)<sup>1</sup>; <sup>1</sup>*University of Liverpool, Liverpool, UK*; <sup>2</sup>*European Bioinformatics Institute, Cambridge, UK*

MP 032 **Collecting and mining Mass Spectrometry Quality Control Data for Proteomics;** [Wout Bittremieux](#)<sup>1</sup>; [Pieter Kelchtermans](#)<sup>2</sup>; [Dirk Valkenburg](#)<sup>3</sup>; [Lennart Martens](#)<sup>2</sup>; [Bart Goethals](#)<sup>1</sup>; [Kris Laukens](#)<sup>1</sup>; <sup>1</sup>*University of Antwerp, Antwerp, Belgium*; <sup>2</sup>*Ghent University, Ghent, Belgium*; <sup>3</sup>*VITO, Mol, Belgium*

MP 033 **Community-based Development and Evaluation of Biological Mass Spectrometry Software via the Galaxy Tool Shed;** [Bart Gottschalk](#)<sup>2</sup>; [Pratik Jagtap](#)<sup>1</sup>; [Harald Barsnes](#)<sup>3</sup>; [Marc Vaudel](#)<sup>3</sup>; [Ira Cooke](#)<sup>4</sup>; [James Johnson](#)<sup>2</sup>; [John Chilton](#)<sup>5</sup>; [Leeann Higgins](#)<sup>1</sup>; [Todd Markowski](#)<sup>1</sup>; [Trevor Wennblom](#)<sup>2</sup>; [Anne-Francoise Lamblin](#)<sup>2</sup>; [Yue Chen](#)<sup>6</sup>; [Sangtae Kim](#)<sup>7</sup>; [Lennart Martens](#)<sup>9</sup>; [Tim Griffin](#)<sup>6</sup>; <sup>1</sup>*Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN*; <sup>2</sup>*Minnesota Supercomputing Institute, UMN, Minneapolis, MN*; <sup>3</sup>*University of Bergen, Bergen, Norway*; <sup>4</sup>*La Trobe University, Melbourne, Australia*; <sup>5</sup>*PennState University, University Park, PA*; <sup>6</sup>*University of Minnesota, Minneapolis, MN*; <sup>7</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>8</sup>*Ghent University, Ghent, Belgium*

MP 034 **KYSS: Mass Spectrometry Data Quality Assessment for Protein Analysis and Large-Scale Proteomics;** [Gerard Such-Sanmartin](#); [Simone Sidoli](#); [Estela Ventura-Espejo](#); [Ole Jensen](#); *University of Southern Denmark, Odense, DK*

MP 035 **Modular Software for Visualization, Analysis and Interpretation of Mass-Spectrometry Data;** [Dmitry Avtonomov](#); [Chih-Chiang Tsou](#); [Alexander Raskind](#); [Alexey Nesvizhskii](#); *University of Michigan, Ann Arbor, MI*

MP 036 **Using Maxquant on Amazon Cloud EC2: Pros and Cons;** [John Philip](#); [Ronald Hendrickson](#); *Memorial Sloan-Kettering Can, New York, NY*

MP 037 **Scientific Workflows for Automated, Documented and Reproducible Data Analysis in Bottom-up and Targeted Proteomics;** [Yassene Mohammed](#)<sup>1,2</sup>; [Suzanne van der Plas-Duivesteyn](#)<sup>1</sup>; [Dominik Domanski](#)<sup>3</sup>; [Christoph Borchers](#)<sup>2,4</sup>; [Magnus Palmblad](#)<sup>1</sup>; <sup>1</sup>*Center for Proteomics and Metabolomics, Leiden Univ, Leiden, The Netherlands*; <sup>2</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>3</sup>*Instit. of Biochem & Biophys, Polish Acad of Sci, Warsaw, Poland*; <sup>4</sup>*UVic Dept of Biochemistry and Biophysics, Victoria, Canada*

MP 038 **Bioanalytical Laboratory Data Flow Strategy for Electronic Notebook and Laboratory Information Data Systems;** [Michael J. Hayes](#); [Jennifer Davis](#); [Timothy Bedman](#); [Jimmy Flarakos](#); *Novartis Institutes for Biomedical Research, East Hanover, NJ*

MP 039 **Instrument Management and Tracking System Developed for The University of Maryland Baltimore Mass Spectrometry Center;** [Michael C. Wilson](#); [Young Ah Goo](#); [Maureen A. Kane](#); [Jace W. Jones](#); [Bao Q. Tran](#);

[Scott Heron](#); [David R. Goodlett](#); *University of Maryland, Baltimore, Baltimore, MD*

MP 040 **Computational Infrastructure for Mining “Big” Proteomic Data;** [Himanshu Grover](#); [David Fenyo](#); *New York University, New York, NY*

MP 041 **ProteomicsDB: Show Cases for Rapid Meta-Analysis of Thousands of Mass Spectrometry Data Sets;** [Mathias Wilhelm](#)<sup>1</sup>; [Judith Schlegl](#)<sup>2</sup>; [Hannes Hahne](#)<sup>1</sup>; [Amin Moghaddas Gholami](#)<sup>1</sup>; [Marcus Lieberenz](#)<sup>2</sup>; [Emanuel Ziegler](#)<sup>2</sup>; [Lars Butzmann](#)<sup>2</sup>; [Siegfried Gessulat](#)<sup>2</sup>; [Harald Marx](#)<sup>1</sup>; [Mikhail Savitski](#)<sup>3</sup>; [Karsten Schnatbaum](#)<sup>4</sup>; [Ulf Reimer](#)<sup>4</sup>; [Holger Wenschuh](#)<sup>4</sup>; [Marcus Bantscheff](#)<sup>3</sup>; [Anja Gerstmair](#)<sup>2</sup>; [Franz Faerber](#)<sup>2</sup>; [Bernhard Kuster](#)<sup>1</sup>; <sup>1</sup>*Technische Universität München, Freising, DE*; <sup>2</sup>*SAP AG Germany, Walldorf, DE*; <sup>3</sup>*Cellzome, Heidelberg, DE*; <sup>4</sup>*JPT Peptide Technologies, Berlin, DE*

MP 042 **RAId’s Knowledge Integrated Databases;** [Gelio Alves](#); [Aleksy Ogurtsov](#); [Yi-Kuo Yu](#); *National Center for Biotechnology Information, NLM, Bethesda, MD*

MP 043 **Enabling Reusable Crowdsourced Annotation of All Mass Spectrometry Data;** [Jeremy Carver](#)<sup>1</sup>; [Mingxun Wang](#)<sup>1,2</sup>; [June Snedecor](#)<sup>1,2</sup>; [Seungjin Na](#)<sup>1,2</sup>; [Adrian Guthals](#)<sup>1,2</sup>; [Nuno Bandeira](#)<sup>1,2</sup>; <sup>1</sup>*Center for Computational Mass Spectrometry, La Jolla, CA*; <sup>2</sup>*University of California, San Diego, La Jolla, CA*

MP 044 **Improving Dynamic Offline Lockmass to Tolerate High Mass Shift;** [Ying Zhang](#); [Zhihui Wen](#); [Michael Washburn](#); [Laurence Florens](#); *Stowers Institute for Medical Research, Kansas City, MO*

MP 045 **Quality By Design Method Development with Mass Detection;** [Sean Mccarthy](#); [Margaret Maziarz](#); *Waters, Milford, MA*

MP 046 **Tracking Chromatographic Peaks with Mass Detection during Method Development;** [Margaret Maziarz](#); [Sean Mccarthy](#); *Waters, Milford, MA*

MP 047 **Automated Collision Cross Section Calculation for Traveling Wave Ion Mobility Spectrometry Instruments;** [Brett Harper](#)<sup>1</sup>; [Matthew Brantley](#)<sup>2</sup>; [Michael Pettit](#)<sup>1</sup>; [Touradj Solouki](#)<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*; <sup>2</sup>*University of Texas at Tyler, Tyler, TX*

MP 048 **A Method for Creating Libraries of Recurring Unidentified Mass Spectra from Large Metabolic Data Sets;** [Wm. Gary Mallard](#)<sup>1</sup>; [N. Rabe Andriamaharavo](#)<sup>1</sup>; [Yuri Mirokhin](#)<sup>1</sup>; [John M. Halket](#)<sup>2</sup>; [Stephen Stein](#)<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*; <sup>2</sup>*Mass Spectrometry Facility, King’s College, London, UK*

MP 049 **Characterizing Molecular Mechanisms of Mammalian Hibernation via Non-Model Organism Quantitative Proteogenomics;** [Katie Vermillion](#)<sup>1</sup>; [Pratik Jagtap](#)<sup>2</sup>; [Todd Markowski](#)<sup>2</sup>; [LeeAnn Higgins](#)<sup>2</sup>; [James Johnson](#)<sup>2</sup>; [Matthew Andrews](#)<sup>1</sup>; [Timothy Griffin](#)<sup>2</sup>; <sup>1</sup>*University of Minnesota, Duluth, MN*; <sup>2</sup>*University of Minnesota, Minneapolis, MN*

**Informatics: Small Molecule Identification and Characterization, 050 - 062**

MP 050 **Isomer-Specific Fragmentation Pathways of Gaseous Anions Derived from Isomeric Hydroxybenzyl Alcohols (HBAs);** [Hanxue Xia](#); [Upul Nishshanka](#); [Carl Weisbecker](#); [Athula B. Attygalle](#); *Stevens Institute of Technology, Hoboken, NJ*

MP 051 **Improved and Extended Tandem Mass Spectral Library with Multiple Precursor Types for More Robust and Flexible Metabolite Identification;** [Xiaoyu Yang](#); [Pedatsur Neta](#); [Yuxue Liang](#); [Stephen Stein](#); *National Institute of Standards and Technology, Gaithersburg, MD*



- MP 052 **Large-Scale Analysis of Non-Targeted LC-MS Metabolomics Data with OpenMS in the Compound Discoverer Platform;** Fabian Aichele<sup>1</sup>; Timo Sachsenberg<sup>1</sup>; Erhan Kenar<sup>1</sup>; Sebastian Kusch<sup>2</sup>; Hans Grensemann<sup>2</sup>; Oliver Kohlbacher<sup>1</sup>; <sup>1</sup>Center for Bioinformatics, Tübingen, Germany; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, Germany
- MP 053 **Application of Fragmentation Analysis in Annotation of Ions in Creation of LC/MS Libraries from Accurate Mass Spectrometry in Global Metabolomics;** Hongping Dai; Corey DeHaven; Anne Evans; *Metabolon, Inc., Durham, NC*
- MP 054 **Combined Isotopic Enrichment, High-Resolution MS, and Advanced Software Tools to Aid in the Identification of Trace-Level Environmental Metabolites by LC/MS;** Jesse L. Balcer<sup>1</sup>; Jeffrey R. Gilbert<sup>1</sup>; Yelena A. Adelfinskaya<sup>1</sup>; Leah Luna<sup>2</sup>; Jeffrie Godbey<sup>1</sup>; Pete L. Johnson<sup>1</sup>; Gerrit J. DeBoer<sup>1</sup>; Ayanna U. Jackson<sup>1</sup>; Amber R. Mahan<sup>1</sup>; <sup>1</sup>Dow AgroSciences, Indianapolis, IN; <sup>2</sup>The Dow Chemical Company, Midland, MI
- MP 055 **Web-Based Toolkit for Interpretation of High Accuracy Mass-Spectrometry Data;** Alexander Raskind; *University of Michigan, Ann Arbor, MI*
- MP 056 **Enabling High Throughput Compound Discovery via Global Natural Products Social Molecular Networking;** Mingxun Wang<sup>1</sup>; Yao Peng<sup>1</sup>; Jeremy Carver<sup>1</sup>; Vanessa Phelan<sup>1</sup>; Laura Sanchez<sup>1</sup>; Jeramie Watrous<sup>1</sup>; Clifford Capono<sup>1</sup>; Don Nguyen<sup>1</sup>; Tal Knaan<sup>1</sup>; Neha Garg<sup>1</sup>; Carla Porto Da Silva<sup>1</sup>; Amina Bouslimani<sup>1</sup>; Alexey Melnik<sup>1</sup>; Michael Meehan<sup>1</sup>; Wei-ting Liu<sup>2</sup>; Anne Lamsa<sup>1</sup>; Paul Boudreau<sup>1</sup>; Evgenia Glukhov<sup>1</sup>; Eduardo Esquenazi<sup>4</sup>; Hailey Houson<sup>4</sup>; Venkat Macherla<sup>4</sup>; Mario Sandoval-Calderon<sup>5</sup>; Pep Charusanti<sup>1</sup>; Brendan Duggan<sup>1</sup>; Marcelino Gutierrez<sup>6</sup>; Xueting Liu<sup>3</sup>; Lixin Zhang<sup>3</sup>; Bradley Moore<sup>1</sup>; William Gerwick<sup>1</sup>; Pieter Dorrestein<sup>1</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>University of California, San Diego, La Jolla, CA; <sup>2</sup>Stanford University, Stanford, CA; <sup>3</sup>IMCAS, Beijing, PRC; <sup>4</sup>Sirenas Marine Discovery, San Diego, CA; <sup>5</sup>National Autonomous University of Mexico, Mexico City, Mexico; <sup>6</sup>INDICASAT, Clayton, City of Knowledge, Panama
- MP 057 **Towards Comprehensive, Reliable and Accurate Mass Spectral Data Repositories;** Eva Duchoslav<sup>1</sup>; Lyle Burton<sup>1</sup>; Emmanuel Varesio<sup>2</sup>; Ron Bonner<sup>1</sup>; Gérard Hopfgartner<sup>2</sup>; <sup>1</sup>AB Sciex, Concord, Canada; <sup>2</sup>University of Geneva, Geneva, Switzerland
- MP 058 **Spectral Deconvolution of Multiplex Fragmentation Data without the use of a non-Fragmentation Scan;** Thomas McClure; David Wright; Michael Athanas; *Thermo Fisher Scientific, San Jose, CA*
- MP 059 **Machine Classification Consistent with LipidMaps Ontology: Bringing Classifications to the Unknowns;** Ryan Taylor; Ryan Miller; John Prince; *Brigham Young University, Provo, UT*
- MP 060 **Msplinter: A Molecular Model of Lipid Fragmentation;** Ryan Taylor; Ryan Miller; John Prince; *Brigham Young University, Provo, UT*
- MP 061 **XPeak: Quantitation and Characterization of the Metabolic Profile of Colorectal Cancer Relapse;** Jordan Kruger; Amrita Cheema; Subha Madhavan; Nathan Edwards; *Georgetown University Medical Center, Washington, District of Columbia*
- MP 062 **Power of Isotopic Fine Structure for Unambiguous Determination of Metabolite Elemental Compositions: in silico Evaluation and Metabolomic Application;** Daisuke Miura<sup>1</sup>; Tatsuhiko Nagao<sup>1</sup>; Daichi Yukihira<sup>1</sup>; Yoshinori Fujimura<sup>2</sup>; Kazunori Saito<sup>3</sup>; Katsutoshi Takahashi<sup>4</sup>; <sup>1</sup>Kyushu University, Fukuoka, Japan; <sup>2</sup>ICMRN, Kyushu University, Fukuoka, Japan; <sup>3</sup>Bruker Daltonics K.K., Kanagawa, Japan; <sup>4</sup>National Institute of Advanced Industrial Science, Tsukuba, Japan
- Proteins: General, 063 - 087**
- MP 063 **Development of an Asp-N Peptide Mapping Method for a Therapeutic Growth Factor;** Hung-Yu Lin; Kenneth Moore; Jenny Heidbrink Thompson; WenJun (David) Mo; *MedImmune, Inc., Gaithersburg, MD*
- MP 064 **Global Effects of Protease Inhibitors on Protein Identification and Quantification;** John Mangrum; Adam Hawkrige; *Virginia Commonwealth University, Richmond, VA*
- MP 065 **Simple Protein Fractionation Enhances Peptide-based Protein Quantitation in Experiments using Metabolic Labeling;** James Moresco<sup>1</sup>; Antonio Pinto<sup>2</sup>; Jolene Diedrich<sup>1</sup>; Patricia Tu<sup>1</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>CAPES Foundation, Brasilia, Brazil
- MP 066 **Effects of Aptamer End Groups on Linkage to Support Material for Specific Enrichment of Proteins;** Funda Yıldırım<sup>1</sup>; Ülkü Güler<sup>1</sup>; Burak Tavşanlı<sup>2</sup>; Ömür Çelikbıçak<sup>1</sup>; Bekir Salih<sup>1</sup>; <sup>1</sup>Hacettepe University, Department of Chemistry, Ankara, Turkey; <sup>2</sup>Istanbul Tech. University, Department of Chemistry, Istanbul, Turkey
- MP 067 **Characterization by nano-LC/ESI-MS/MS of Highly Degraded Collagen Detected in 4,400-year-old Egyptian Wall Paintings of the Idout Tomb;** Shunsuke Fukakusa<sup>1</sup>; Kazuki Kawahara<sup>2</sup>; Ahmed Sayed Shoeib<sup>3</sup>; Abel Akarish<sup>4</sup>; Hideya Kawasaki<sup>5</sup>; Hiroshi Suita<sup>5</sup>; Ryuichi Arakawa<sup>5</sup>; Takashi Nakazawa<sup>1</sup>; <sup>1</sup>Nara Women's University, Nara, Japan; <sup>2</sup>Osaka University, Osaka, Japan; <sup>3</sup>Cairo University, Cairo, Egypt; <sup>4</sup>National Research Center, Cairo, Egypt; <sup>5</sup>Kansai University, Osaka, Japan
- MP 068 **The Study of Protein/Pigment Interactions in Art Materials from Replica Paints with an Integrated ELISA and Proteomics Approach;** Natalya Atlasevich<sup>1</sup>; Caroline Tokarski<sup>3</sup>; Brian Baade<sup>2, 5</sup>; John Loike<sup>4</sup>; Julie Arslanoglu<sup>1</sup>; <sup>1</sup>Metropolitan Museum of Art, New York, NY; <sup>2</sup>University of Delaware, Newark, DE; <sup>3</sup>USR CNRS 3290 MSAP, Villeneuve D'ascq, France; <sup>4</sup>Columbia University, New York, NY; <sup>5</sup>University of Delaware, Newark, DE
- MP 069 **Analysis of Centipede, Spider, and Snake Venoms by Electrospray and MALDI Mass Spectrometry;** Chip Cochran; Allen Cooper; Eric Gren; Wayne Kelln; David Nelsen; Ben Gardner; William Hayes; Gerard Fox; *Loma Linda University, Loma Linda, CA*
- MP 070 **High-throughput Scheduled MRM for Multiplexed Analysis of Activity-based Probe Labeled Enzymes in Human Cells;** Song Li; Yu Shi; Christian Malapit; Amy Howell; Xudong Yao; *University of Connecticut, Storrs, CT*
- MP 071 **A Comparative Study of Human Whey Colostral Protein Levels from Women With and Without Gestational Diabetes Mellitus (GDM);** Darren Weber<sup>1</sup>; Jennifer T. Smilowitz<sup>2, 3</sup>; Dmitry Grapov<sup>4</sup>; Brett S. Phinney<sup>1</sup>; <sup>1</sup>Proteomics Core Facility, UC Davis, Davis, CA; <sup>2</sup>Foods for Health Institute, UC Davis, Davis, CA; <sup>3</sup>Department of Food Science and Technology, UC Davis, Davis, CA; <sup>4</sup>West Coast Metabolomics Center, UC Davis, Davis, CA
- MP 072 **MS Analyses of Proteins Associated with Autoimmune Diseases;** Leesa Deterding; Jeffrey F. Kuhn; Katina Johnson; Rachelle Bienstock; Jinglan Wang; Erin Hopper; Shyamal Peddada; Frederick Miller; Kenneth B. Tomer; *NIEHS, Research Triangle Park, NC*
- MP 073 **Identification of ERK2 Substrates using Label-Free Approach;** Farzin Gharahdaghi; *Astrazeneca, Waltham, MA*

- MP 074 **Evaluation of a Universal LC-MS/MS Assay for Bioanalysis of Human IgG4 Subclass Monoclonal Antibody Protein Drugs;** Craig Titsch; Hao Jiang; Weifeng Xu; Jianing Zeng; Michael Furlong; Mark Arnold; Anne-Francoise Aubry; *Bristol-Myers Squibb, Lawrenceville, NJ*
- MP 075 **Simultaneously Probing Lipoprotein and Lipid Kinetics in Humans using a Practical Oral Tracer Procedure;** Haihong Zhou<sup>1</sup>; Gissette Reyes-Soffer<sup>2</sup>; Tiffany Thomas<sup>2</sup>; Kithsiri Heratch<sup>1</sup>; Ablatt Mahsut<sup>1</sup>; Yi Pan<sup>1</sup>; Gowri Bhat<sup>1</sup>; Kristian Jensen<sup>1</sup>; David Kelley<sup>1</sup>; Henry Ginsberg<sup>2</sup>; Stephen Previs<sup>1</sup>; Thomas Roddy<sup>1</sup>; <sup>1</sup>*Merck & Co., Inc., Rahway, NJ*; <sup>2</sup>*Columbia University, New York, NY*
- MP 076 **Protective Effects of Flavonoids on Cytochrome c Oxidation in Continuous Stirred Tank Reactor Coupled with Electrospray Ionization Mass Spectrometry;** Hui Fan; Veronica Waybright; Jeremy Barnes; Kevin Schug; *The University of Texas at Arlington, Arlington, TX*
- MP 077 **Differential Analysis by SIEVE for sequence Variant Analysis (SVA) of High-Cell-Age Material;** Georg Drabner; Verena Niggeloh; *Roche Diagnostics GmbH, Penzberg, Germany*
- MP 078 **Capillary Electrophoresis Separation and Fractionation Combined with MALDI-MS for Analysis of Reproduction Proteins from Pieridae Butterflies;** Måns Ekelöf; Maria Khihon Rokhas; Johan Jacksén; Åsa Emmer; *Royal Institute of Technology, Stockholm, Sweden*
- MP 079 **Automatic Capillary Isoelectric Focusing – Electrospray Ionization – Mass Spectrometry for Protein Separation and Characterization;** Shuai Sherry Zhao; *University of British Columbia, Vancouver, Canada*
- MP 080 **Capillary Zone Electrophoresis–Electrospray Ionization-Tandem Mass Spectrometry for Top-Down Characterization of the *Mycobacterium marinum* Secretome;** Yimeng Zhao<sup>1</sup>; Liangliang Sun<sup>1</sup>; Matthew Champion<sup>1</sup>; Michael Knierman<sup>2</sup>; Norman Dovichi<sup>1</sup>; <sup>1</sup>*University of Notre Dame, South Bend, IN*; <sup>2</sup>*Eli Lilly and Company, Indianapolis, IN*
- MP 081 **On the Stabilization of Noncovalent Protein Complexes via Vapor Treatment of Electrospray Droplets;** J. Corinne DeMuth; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- MP 082 **Determination of Novel Copper Binding Sites in MEK1 by Metal-Catalyzed Oxidation Based Mass Spectrometry Analysis;** Xiaoji Yao; Donita Brady; Christopher Counter; Kunhong Xiao; *Duke University Medical Center, Durham, NC*
- MP 083 **Top Down Protein Analysis Applied to Ancient Photographs;** Austin Nevin<sup>2</sup>; Fabrice Bray<sup>1</sup>; Christian Rolando<sup>1</sup>; Caroline Tokarski<sup>1</sup>; <sup>1</sup>*Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France*; <sup>2</sup>*Politecnico di Milano, Milano, Italy*
- MP 084 **Front-End Electron Transfer Dissociation Coupled to 14.5 T FT-ICR MS for Top-Down Protein MS/MS Analysis;** Chad R. Weisbrod<sup>1</sup>; A. Michelle English<sup>2</sup>; Nathan K. Kaiser<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Greg T. Blakney<sup>1</sup>; Xiaoyan Guan<sup>1</sup>; John E. P. Syka<sup>3</sup>; Lee Earley<sup>3</sup>; Christopher Mullen<sup>3</sup>; Donald F. Hunt<sup>2</sup>; Alan G. Marshall<sup>1,4</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*University of Virginia, Charlottesville, VA*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>4</sup>*Florida State University, Tallahassee, FL*
- MP 085 **Semi-preparative Purification and Characterization of Lysozyme Modified with Poly Ethylene Glycol (PEG);** M Sundaram Palaniswamy<sup>1</sup>; N.S Lakshmi<sup>1</sup>; Ravindra Gudihai<sup>1</sup>; Ning Tang<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Bangalore, India*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- MP 086 **Effect of Centrifugation on Tryptic Digestion;** Jihyeon Lee; Taehee Kim; Jeongkwon Kim; *Chungnam National University, Daejeon, South Korea*
- MP 087 **Systematic and Quantitative Comparison of Digest Efficiency and Specificity Reveals the Impact Of Trypsin Quality on MS-based Proteomics;** Julia Maria Burkhart; Albert Sickmann; *Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
- Proteins: PTMs, 088 - 122**
- MP 088 **Complete Trimethylation of Proteins and its Application to the Quantification of Lysine Methylation at Specific Residues using Mass Spectrometry;** Steven Toth; *Toledo, OH*
- MP 089 **Measuring Protein-Bound Glutathione (PSSG) : Critical Correction for Cytosolic Glutathione Species;** Michael Bukowski; Matthew Picklo; *USDA-ARS Human Nutrition Research Center, Grand Forks, ND*
- MP 090 **Improved Detection of Acidic Post-translational Modifications Utilizing Negative Ion Mode with Alkaline Liquid Chromatography/Fourier Transform-Ion Cyclotron Resonance Mass Spectrometry;** Phillip McCloskey; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- MP 091 **Quantitative Study of Protein Carbonylation in Human Blood Samples;** Chelsea Coffey; Suresh Narayanasamy; David Simpson; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- MP 092 **Methylation Artefacts Introduced during Standard Proteomics Sample Preparation Workflows and Its Impact on Histone PTM Analysis;** Florian Richter<sup>1,2</sup>; Aneliya Yoveva<sup>1</sup>; Gerhard Mittler<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Immunobiology & Epigenetics, Freiburg, Germany*; <sup>2</sup>*Functional Proteomics SFB 815 Goethe-University, Frankfurt am Main, Germany*
- MP 093 **Controlled Reduction of Disulfide Bonds in Biopharmaceuticals using an Electrochemical Reactor Cell Online with LC/MS;** Jean-Pierre Chervet; Agnieszka Kraj; Hendrik-Jan Brouwer; Nico Reinhoud; *Antec, Zoeterwoude, Netherlands*
- MP 094 **Characterization of the Degradation Products of a Color-Changed Monoclonal Antibody: Tryptophan-Derived Chromophores;** Yiming Li<sup>1</sup>; Alla Polozova<sup>2</sup>; Flaviu Gruia<sup>1</sup>; Jinhua Feng<sup>1</sup>; <sup>1</sup>*MedImmune, Gaithersburg, MD*; <sup>2</sup>*Amgen, West Greenwich, RI*
- MP 095 **Linking Epidermal Growth Factor Signaling to Dynamic Chromatin Modifications;** Rosalynn Molden<sup>1</sup>; Daniel Thomas<sup>3</sup>; Susan Janicki<sup>2</sup>; Benjamin A. Garcia<sup>3</sup>; <sup>1</sup>*Princeton University, Princeton, NJ*; <sup>2</sup>*The Wistar Institute, Philadelphia, PA*; <sup>3</sup>*University of Pennsylvania, Philadelphia, PA*
- MP 096 **Mass Spectrometric Characterization of Aldehyde-Mediated N-terminal Epimerization in Protein;** Tomoyuki Oe; Ryo Kajita; Seon Hwa Lee; Takaaki Goto; *Tohoku University, Sendai, Japan*
- MP 097 **Analysis of Monoclonal Antibody Oxidation using Capillary Electrophoresis coupled to Quadrupole Time-of-Flight Mass Spectrometry;** Suresh Babu CV; Ravindra Gudihai; *Agilent Technologies, Bangalore, India*
- MP 098 **Modifications of Albumin Isolated from Patients with Multi-Morbid Disease;** Melissa Grant; Iain Chapple; Parth Narendran; Paul Cockwell; Andrew Creese; *University of Birmingham, Birmingham, UK*
- MP 099 **High Resolution is Not a Strict Requirement for Characterization and Quantification of Histone PTMs;** Kelly R. Karch; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*

- MP 100 **Proteome-wide Light/Dark Modulation of Protein Thiol Oxidation in Cyanobacteria Revealed by Quantitative Site-Specific Redox Proteomics**; Jia Guo<sup>1</sup>; Amelia Y. Nguyen<sup>3</sup>; Dian Su<sup>1,4</sup>; Matthew J. Gaffrey<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Jon M. Jacobs<sup>1</sup>; Richard D. Smith<sup>1,2</sup>; David W. Koppenaal<sup>2</sup>; Himadri B. Pakrasi<sup>3</sup>; Wei-Jun Qian<sup>1</sup>; <sup>1</sup>*Biological Sciences Division, PNNL, Richland, WA*; <sup>2</sup>*Environmental Molecular Sciences Laboratory, PNNL, Richland, WA*; <sup>3</sup>*Department of Biology, Washington University, St. Louis, MO*; <sup>4</sup>*Genentech Inc, South San Francisco, CA*
- MP 101 **Global Analysis of Absolute and Relative Quantification of SUMOylated Proteins in *Saccharomyces cerevisiae* by Data-Independent Acquisition using LC/MS<sup>e</sup>**; Armann Andaya; Nikhil Bhagwat; Youjin Seo; Neil Hunter; Julie A. Leary; *UC Davis, Davis, CA*
- MP 102 **Quantitative Redox Proteomics using Cysteine Specific Isobaric Tags**; Kumaran Sivagnanam; Leslie M. Hicks; *University of North Carolina, Chapel Hill, NC*
- MP 103 **Analysis of TOR's Role in Lipid Droplet Accumulation in *Chlamydomonas reinhardtii***; Emily Werth<sup>1</sup>; Silas P. Rodrigues<sup>1,2</sup>; Leslie M. Hicks<sup>1</sup>; <sup>1</sup>*University of North Carolina at Chapel Hill, Chapel Hill, NC*; <sup>2</sup>*Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*
- MP 104 **Rapid Profiling of Proteomes and Sub-Proteomes on the Orbitrap Tribrid Mass Spectrometer**; Steven Danielson<sup>1</sup>; Todd Markowski<sup>2</sup>; LeeAnn Higgins<sup>2</sup>; Pratik Jagtap<sup>2</sup>; Tim Griffin<sup>2,3</sup>; Yue Chen<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Center for Mass Spectrometry and Proteomics, UMN, St. Paul, MN*; <sup>3</sup>*Dept. of Biochemistry, University of Minnesota, Minneapolis, MN*
- MP 105 **Comprehensive Screening of lipid Peroxidation-Derived Modifications to Protein using Isotope Data Dependent Scan**; Ryo Takahashi; Seon Hwa Lee; Takaaki Goto; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 106 **Analysis of Glycosylation Sites within the Polypeptide Encoded by Exon 7 of Mouse ZP3 protein (ZP3E7)**; Armand Ngounou; Izabela Sokolowska; Urmi Roy; Alisa Woods; Costel Darie; *Clarkson University, Potsdam, NY*
- MP 107 **Oxidative Stress-Derived Formation and Transamination of N-terminal Alpha-Ketoamide Peptides/Proteins**; Seon Hwa Lee; Hyunsook Kyung; Ryo Yokota; Takaaki Goto; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 108 **Simultaneous Mass Spectrometric Analysis of Various Chemical Modifications on Human Serum Albumin: Strategies for Clean-Up, Sequence Coverage, and Identification**; Takaaki Goto; Yuta Kudo; Kazuyuki Murata; Seon Hwa Lee; Tomoyuki Oe; *Tohoku University, Sendai, Japan*
- MP 109 **Unravelling the Drugable ALK Signaling Pathway in Neuroblastoma by Quantitative Proteomics**; Dorte B. Bekker-Jensen; Kristina B. Emdal; Chiara Francavilla; Jesper V. Olsen; *NNF Center for Protein Research, Copenhagen, Denmark*
- MP 110 **Top-down Mass Spectrometry Reveals Molecular Heterogeneity in the Swine Heart**; Zachery Gregorich<sup>1</sup>; Wei Guo<sup>2</sup>; Timothy Hacker<sup>1</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>*UW Madison, Madison, WI*; <sup>2</sup>*University of Wyoming, Laramie, WY*
- MP 111 **Characterization of Cyanobacterial Photosystem II Proteins from Wild-Type and Mutant Cells by Top-Down Mass Spectrometry**; Daniel A. Weisz; Haijun Liu; Weidong Cui; Hao Zhang; Michael L. Gross; Himadri B. Pakrasi; *Washington University in St. Louis, St. Louis, MO*
- MP 112 **Stability of Nitration and Oxidation in Hemoglobin Extracted from Dried Blood Spot by Nanoflow Liquid Chromatography Tandem Mass Spectrometry**; Chih-Huang Fan; Hauh-Jyun Candy Chen; *National Chung Cheng Univ., Ming-Hsiung, Chia-Yi, Taiwan*
- MP 113 **Identification and Functional Characterization of a Novel Phosphorylation Site in DDB2**; Qian Cai; Yinsheng Wang; *University of California at Riverside, Riverside, CA*
- MP 114 **Determining the Redox Proteome of Photosynthetic Organisms**; William Slade; Leslie Hicks; *University of North Carolina, Chapel Hill, NC*
- MP 115 **Use of Proteomics Techniques in the Study in Animal Model Proteins Expression upon Exposure to 2, 3 Butanedione**; Leticia Dias Lima Jedlicka<sup>1</sup>; Sheila Guterres<sup>1</sup>; Richard G. Landgraf<sup>1</sup>; Bernadete de Faria<sup>1</sup>; Etelvino J. H. Bechara<sup>1,2</sup>; Assuncao Nilson A. <sup>1</sup>; <sup>1</sup>*UNIFESP, São Paulo, Brasil*; <sup>2</sup>*USP, Sao Paulo, SP Brazil*
- MP 116 **Analysis by Mass Spectrometry of the Phospho-State of Tau using a Novel Microtubule Affinity Column**; Robert Pelot<sup>1</sup>; Jon Reed<sup>1,3</sup>; Gogce Crynen<sup>1</sup>; Corbin Bachmeier<sup>2</sup>; Laila Abdullah<sup>1</sup>; James Evans<sup>1</sup>; Mike Mullan<sup>1</sup>; Fiona Crawford<sup>1,3</sup>; <sup>1</sup>*Roskamp Institute, Sarasota, FL*; <sup>2</sup>*The Open University, Milton Keynes, UK*; <sup>3</sup>*The Veterans Administration, Tampa, FL*
- MP 117 **Proteomic Profile of Lipid Peroxidation in Human Cardiomyopathy**; Mark Jeong; Wes Blakeslee; Don Backos; Timothy McKinsey; Kristofer Fritz; *University of Colorado Anschutz Medical Campus, Aurora, CO*
- MP 118 **Identification of a Novel Post-Translational Modification, Methylated Diphthine, in Diphthamide Biosynthetic Pathway**; Wei Chen; Zhewang Lin; Xiaoyang Su; Bo Ci; Sheng Zhang; Hening Lin; *Cornell University, Ithaca, NY*
- MP 119 **Characterizing Phosphorylation and Ubiquitination Cross-talk in *Magnaporthe oryzae***; Jennifer L. Parker; Yeonyee Oh; David C. Muddiman; Ralph A. Dean; *North Carolina State University, Raleigh, NC*
- MP 120 **Western Diet Causes Metabolic Disorder in Mouse Heart**; Stephen A. Whelan; Jean L. Spencer; Chunxiang Yao; Jessica B. Behring; Christian Heckendorf; Deborah A. Siwick; Wilson S. Colucci; Richard A. Cohen; Markus M. Bachschmid; Catherine E. Costello; Mark E. Mccomb; *Boston University School of Medicine, Boston, Ma*
- MP 121 **Stoichiometric Determination of Global Protein Acetylation by Stable Isotope Labeling and Mass Spectrometry**; Josue Baeza<sup>1</sup>; James Dowell<sup>1</sup>; Michael Smallegan<sup>1</sup>; Zia Khan<sup>2</sup>; John Denu<sup>1</sup>; <sup>1</sup>*University of Wisconsin Madison, Madison, WI*; <sup>2</sup>*University of Maryland College Park, College Park, MD*
- MP 122 **An Improved Immunoaffinity Reagent for Quantitative Profiling of Lysine Acetylation**; Jeffrey C. Silva; Ailan Guo; Anthony Couvillon; Rami Najjar; Daniel Mulhern; Kimberly A. Lee; Jian-Min Ren; Jia Xiaoying; Hongbo Gu; *Cell Signaling Technology, Danvers, MA*
- Proteins: Membranes, 123 - 138**
- MP 123 **Analysis of *Helicobacter pylori* cell surface proteins**; Bradley J. Voss; W. Hayes Mcdonald; Timothy L. Cover; *Vanderbilt University, Nashville, TN*
- MP 124 **Profiling of Cell Surface Proteome and Secreted Metabolome from an *in-vitro* Model System, using LC-MS technologies**; Ravi K. Krovvidi<sup>1</sup>; Leo Bonilla<sup>2</sup>; Syed Salman Lateef<sup>1</sup>; Arunkumar Padmanaban<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Bangalore, India*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- MP 125 **Exploring the Surface Proteins of Myeloid Derived Suppressor Cells**; Sitara Chauhan<sup>1</sup>; Steve Danielson<sup>2</sup>; Rebecca Rose<sup>1</sup>; Susan Ostrand-Rosenberg<sup>3</sup>; Nathan Edwards<sup>4</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>*University of Maryland, College Park, MD*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*University of Maryland, Baltimore County, MD*; <sup>4</sup>*Georgetown University Medical Center, Washington D.C., DC*

- MP 126 **Quantification of Membrane Bound Drug Transporter Proteins at the Blood-Brain Barrier;** Thomas Lau<sup>1,2</sup>; Jean-Pierre Eliane<sup>3</sup>; Lauren Gauthier<sup>2</sup>; Bo Feng<sup>3</sup>; Patrick Trapa<sup>4</sup>; Jennifer Liras<sup>4</sup>; Hendrik Neubert<sup>2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>Broad Institute, Cambridge, MA; <sup>2</sup>Pfizer Inc, Andover, MA; <sup>3</sup>Pfizer Inc, Groton, CT; <sup>4</sup>Pfizer Inc, Cambridge, MA
- MP 127 **Proteomic Analysis of the Membrane Proteins in Human Placenta;** Jong-Sun Lim<sup>1</sup>; Hyoung-Joo Lee<sup>1</sup>; Keun Na<sup>1</sup>; Min Jung Lee<sup>1</sup>; Han-Ho Lee<sup>1</sup>; Ja-Young Kwon<sup>2</sup>; Young-Ki Paik<sup>1</sup>; <sup>1</sup>YPRC, Seoul, South Korea; <sup>2</sup>Collage of Medicine, Yonsei University, Seoul, South Korea
- MP 128 **Characterization of the Membrane Proteome and N-glycoproteome in BV-2 Mouse Microglia by Liquid Chromatography-Tandem Mass Spectrometry;** Dohyun Han<sup>1,3</sup>; Sungyoon Moon<sup>1,2</sup>; Jongmin Woo<sup>1,4</sup>; Youngsoo Kim<sup>2,3</sup>; <sup>1</sup>Seoul National University College of medicine, Seoul, South Korea; <sup>2</sup>Departments of Biomedical Engineering, SNU, Seoul, South Korea; <sup>3</sup>Institute of Medical & Biological Engineering, SNU, Seoul, South Korea; <sup>4</sup>Department of Biomedical Science, Seoul, South Korea
- MP 129 **Life on the Edge: Exploring the Superficial Interface between *Ignicoccus hospitalis* and *Nanoarchaeum equitans* using 2D LC-MS/MS-based Proteomics;** Richard J. Giannone; Louie L. Wurch; Zamin Yang; Mircea Podar; Robert Hettich; Oak Ridge National Laboratory, Oak Ridge, TN
- MP 130 **Enhanced MALDI-MS using Alkylated Trihydroxyacetophenone as a Matrix for Hydrophobic Peptides in Membrane Protein Analysis;** Yuko Fukuyama<sup>1</sup>; Chihiro Nakajima<sup>1</sup>; Shunsuke Izumi<sup>2</sup>; Koichi Tanaka<sup>1</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Hiroshima University, Higashi-Hiroshima, Japan
- MP 131 **Affinity Screening of Purified GPCRs on the Automated Ligand Identification System (ALIS): Protein Expression, Characterization, and Screening Results for CXCR4;** Charles E. Whitehurst<sup>1</sup>; Zhiping Yao<sup>3</sup>; Denise Murphy<sup>4</sup>; Mingzuan Zhang<sup>5</sup>; Shane Taremi<sup>2</sup>; Lisa Wojcik<sup>6</sup>; Julie M. Strizki<sup>8</sup>; Jack D. Bracken<sup>7</sup>; Cliff C. Cheng<sup>8</sup>; Xianshu Yang<sup>2</sup>; Gerald W. Shipp, Jr.<sup>9</sup>; Michael Ziebell<sup>2</sup>; Elliott Nickbar<sup>2</sup>; <sup>1</sup>Boehringer Ingelheim, Ridgefield, CT; <sup>2</sup>Merck Pharmaceuticals Inc., Boston, MA; <sup>3</sup>Novartis Institute for Biomedical Research, Cambridge, MA; <sup>4</sup>Pfizer Global Biotherapeutics, Cambridge, MA; <sup>5</sup>Biogen Idec Hemophilia Therapeutic, Inc., Waltham, MA; <sup>6</sup>Merck Research Laboratory, West Point, PA; <sup>7</sup>University of California, Los Angeles, CA; <sup>8</sup>Central Research Institute, Shanghai, China; <sup>9</sup>The New Venture Fund, Washington, DC
- MP 132 **In-depth Mapping of the Cell Surface Proteome of Cancer Cells Expressing Specific Alleles of KRas;** Xiaoying Ye; DaRue A. Prieto; Gordon Whiteley; Josip Blonder; Fredrick National Laboratory for Cancer Research, Frederick, MD
- MP 133 **A Comparison of Plasma Membrane and Whole Proteome Profiling Across 10 Cell Lines on an Orbitrap Fusion;** David Nusinow; Michael Weekes; Mark Jedrychowski; Robert Everley; Steven Gygi; Harvard Medical School, Boston, MA
- MP 134 **Examining Ligand Induced Conformational Changes in the Human Erythrocyte Glucose Transporter, GLUT1, through Chemical Crosslinking and Mass Spectrometry;** Kenneth Lloyd; John Leszyk; Scott A. Shaffer; Anthony Carruthers; UMASS Medical School, Worcester, MA
- MP 135 **A proteomic Approach for Monitoring the Dynamic Response of the Female Oviductal Epithelium Surface to Male Gametes;** Konstantin Artemenko<sup>1</sup>; Jana Horáková<sup>1,4</sup>; Birgit Steinberger<sup>2,3</sup>; Urban Besenfelder<sup>3</sup>; Gottfried Brem<sup>2</sup>; Jonas Bergquist<sup>1</sup>; Corina Mayrhofer<sup>2,3</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>University of Veterinary Medicine, Vienna, Austria; <sup>3</sup>University of Nat.Resources &Applied Life Sciences, Tulln, Austria; <sup>4</sup>Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
- MP 136 **Interrogation of the Ubiquitinated Proteome of Exosomes Shed by Myeloid-derived Suppressor Cells;** Meghan Burke<sup>1</sup>; Maria Oei<sup>1</sup>; Suzanne Ostrand-Rosenberg<sup>2</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>University of Maryland College Park, College Park, MD; <sup>2</sup>University of Maryland Baltimore County, Baltimore, MD
- MP 137 **Identification and Post-Translational Modifications of Intact Proteins in Exosomes Shed by Murine Myeloid-Derived Suppressor Cells;** Lucia Geis-Asteggiane<sup>1</sup>; Avantika Dhabaria<sup>1</sup>; Nathan J. Edwards<sup>2</sup>; Suzanne Ostrand-Rosenberg<sup>3</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD - Maryland; <sup>2</sup>Georgetown University Medical Center, Washington, DC; <sup>3</sup>University of Maryland Baltimore County, Baltimore, MD
- MP 138 **Multiple Dissociation Pathways of Ganglioside-Toxin Complexes Revealed by Collision Induced Dissociation and Surface Induced Dissociation in the Gas Phase;** Yue Ju; Yun Zhang; Vicki Wysocki; The Ohio State University, Columbus, OHIO
- Intact Proteins: Sequence Analysis, 139 - 149**
- MP 139 **Sequence Variant Analysis of Therapeutic Proteins using LC/MS/MS;** Ning Tang; Agilent Technologies, Santa Clara, CA
- MP 140 **Probing Disulfide Bonds with Top-Down Mass Spectrometry;** Jeremy J. Wolff; Christopher J. Thompson; J. Paul Speir; Bruker Daltonics, Billerica, MA
- MP 141 **Fourier Transform Ion Cyclotron Resonance Top-Down Mass Spectrometry of Intact and Reduced Antibodies;** Jeremy J. Wolff; Christopher J. Thompson; Bruker Daltonics, Billerica, MA
- MP 142 **Extracting Complementary Protein Sequence Information using Sequential Ion Mobility Resolved Electron Transfer Dissociation and Collision Induced Dissociation;** Deepali Rathore; Forouzan Aboufazel; Eric D. Dodds; University of Nebraska, Lincoln, NE
- MP 143 **Determination of the Number of Methionine Residues in Proteins via Gas-Phase Ion/Ion Reactions for Improved Sequence Analysis;** Alice Pilo; Yang Gao; Scott McLuckey; Purdue University, West Lafayette, IN
- MP 144 **Strategies for Mass Spectrometry-Based de novo Sequencing of a Critical Monoclonal Antibody Reagent;** Lawrence Dick; Van Hoang; Merck & Company, West Point, PA
- MP 145 **Combining UV Laser Irradiation and IR Activated-Ion Electron Capture Dissociation to Enhance Disulfide Bond Cleavage for Protein Top-Down MS;** Piriya Wongkongkathep<sup>1</sup>; Huilin Li<sup>1</sup>; Xing Zhang<sup>2</sup>; Ryan R. Julian<sup>2</sup>; Rachel O. Loo<sup>1</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>University of California, Riverside, Riverside, CA
- MP 146 **Extending Top-Down Intact Protein Sequence Coverage using ETD, Ion-Ion Proton Transfer (IIPT) Reactions and Parallel Ion Parking;** A. Michelle English<sup>1</sup>; John E. P. Syka<sup>2</sup>; Christopher Mullen<sup>2</sup>; Lee Earley<sup>2</sup>; Jeffrey Shabanowitz<sup>1</sup>; Donald F. Hunt<sup>1</sup>; <sup>1</sup>University of Virginia, Charlottesville, VA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 147 **Inclusion of Internal Fragment Ions in Spectral Analysis to Increase Sequence Coverage in Top-Down Mass Spectrometry;** David R. Bush; Jared R. Auclair; Alexander R. Ivanov; Jeffrey N. Agar; Barry L. Karger; Barnett Institute, Northeastern University, Boston, MA

- MP 148 **Characterization of Rare Hemoglobin Mutants with Top-Down High Resolution Mass Spectrometry and Semi-Automated Data Analysis;** Didia Coelho Graça<sup>1</sup>; Ralf Hartmer<sup>2</sup>; Photis Beris<sup>3</sup>; Kaveh Samii<sup>4</sup>; Lorella Clerici<sup>5</sup>; Wolfgang Jabs<sup>2</sup>; Carsten Stoermer<sup>2</sup>; Denis Hochstrasser<sup>1,5</sup>; Pierre Lescuyer<sup>1,5</sup>; Alexander Scherl<sup>1,5</sup>; <sup>1</sup>DHPS, Faculty of medicine, University of Geneva, Geneva, Switzerland; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Laboratoire Unilabs Coppet, Geneva, Switzerland; <sup>4</sup>Division of Hematology, Geneva University Hospital, Geneva, Switzerland; <sup>5</sup>DGLM, Geneva University Hospitals, Geneva, Switzerland
- MP 149 **Top Down Analysis of Protein Classes with Incomplete Genomes;** David Morgenstern<sup>1</sup>; Marshall W. Bern<sup>2</sup>; Chris Becker<sup>2</sup>; David Fenyó<sup>1</sup>; Baldomera Olivera<sup>3,4</sup>; Julita Imperial<sup>3</sup>; Beatrix Ueberheide<sup>1</sup>; <sup>1</sup>NYU, New York City, NY; <sup>2</sup>Protein Metrics Inc., San Carlos, CA; <sup>3</sup>University of Utah, Salt Lake City, UT; <sup>4</sup>The Howard Hughes Medical Institute, Chevy Chase, MD
- Proteins: Complexes, 150 - 165**
- MP 150 **Characterization of the TAP Tag Affinity-Purified Mouse RNA Exosome Complex with Data-Independent MS<sup>E</sup> with Ion Mobility;** Veronika Grinstein<sup>2</sup>; Lewis M. Brown<sup>1</sup>; David Chen<sup>1</sup>; Uttiya Basu<sup>2</sup>; <sup>1</sup>Columbia University, New York, NY; <sup>2</sup>Columbia University Medical Center, New York, NY
- MP 151 **System Wide Characterisation of *Trypanosoma brucei* Cytoplasmic Protein Complexes Utilising Chromatography and Proteomics;** Thomas Crozier; Mark Larence; Lucia Guther; Michael Ferguson; Angus Lamond; University of Dundee, Dundee, UK
- MP 152 **Turnover and Complex Assembly of the Yeast Oligosaccharyl transferase by dynamic SILAC and Targeted Mass Spectrometry;** Susanne Mueller<sup>1</sup>; Asa Wahlander<sup>2</sup>; Nathalie Selevsek<sup>2</sup>; Robert Gauss<sup>1</sup>; Markus Aebi<sup>1</sup>; <sup>1</sup>Institute of Microbiology, ETH Zurich, Zurich, Switzerland; <sup>2</sup>Functional Genomics Center Zurich, Zurich, Switzerland
- MP 153 **Investigation of *P. aeruginosa* Lipopolysaccharide Transporter Subunit LptA Oligomerization by Chemical Crosslinking and LC-tandem Mass Spectrometry;** Rong Fang Gu; Adam Shapiro; Stephania Livchak; AstraZeneca, Waltham, MA
- MP 154 **Exploring the Experimental Controls Used for Identifying Transcription Factor Associated Proteins by Mass Spectrometry;** Charles Banks; Zachary Lee; Gina Boanca; Michael Washburn; Stowers Institute, Kansas City, MO
- MP 155 **Intact Mass Analysis of PEGylated Therapeutic Proteins using TripleTOF® System;** Faraz Rashid<sup>1</sup>; Annu Uppal<sup>1</sup>; Dipankar Malakar<sup>1</sup>; Anita Krishnan<sup>2</sup>; <sup>1</sup>ABSCIEX, Gurgaon, India; <sup>2</sup>LUPIN Limited Biotech Division, G O Square Mall, Pune, Maharashtra, IN
- MP 156 **A Mass Spectrometry Based Proteomics Approach to Analyze the Modularity of the Chromatin Remodeling Swr1 Complex;** Mahadevan Lakshminarasimhan<sup>1</sup>; Gaye Hattem<sup>1</sup>; Mihaela Sardu<sup>1</sup>; Sreenivasa Ramisetty<sup>2</sup>; Michael Washburn<sup>1</sup>; <sup>1</sup>Stowers Institute for Medical Research, Kansas City, MO; <sup>2</sup>Indexx Laboratories, Westbrook, ME
- MP 157 **Increasing Transfer Efficiency in Native Mass Spectrometry of Supermolecular Protein Complexes with a Modified Dual-Funnel QTOF ;** Ralf Hartmer<sup>1</sup>; Peter Brechlin<sup>1</sup>; Werner Imhoff<sup>1</sup>; Anja Wiechmann<sup>1</sup>; Wolfgang Jabs<sup>1</sup>; Pierre-Olivier Schmitt<sup>2</sup>; Françoise Debaene<sup>3</sup>; Alain Van Dorselaer<sup>3</sup>; Sarah Cianferani<sup>3</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Bruker Daltonique, Wissembourg, France; <sup>3</sup>LSMBO Université de Strasbourg, Strasbourg, France
- MP 158 **A Proteomic Profile of Deleted in Breast Cancer 1 (DBC1) and its Role in Transcriptional Regulation;** Preeti Joshi; Amanda Guise; Olivia Quach; Sophie Giguere; Jeffrey Kong; Ileana M. Cristea; Princeton University, Princeton, NJ
- MP 159 **Interactome of *Bacillus subtilis* Cell Division Machinery;** Livia Goto Silva<sup>1</sup>; Jimmy Rodriguez Murillo<sup>1</sup>; Micaella P. da Fonseca<sup>2</sup>; Agnelo Rodrigues de Souza<sup>2</sup>; Gilberto Barbosa Domont<sup>1</sup>; Federico Gueiros-Filho<sup>3</sup>; Magno Junqueira<sup>1</sup>; <sup>1</sup>Federal University of Rio de Janeiro, Rio De Janeiro, Brazil; <sup>2</sup>University of Brasilia, Brasilia, DF-Brazil; <sup>3</sup>University of Sao Paulo-USP, Sao Paulo, Sao Paulo-Brazil
- MP 160 **A Robust Platform for Routine Analysis of Endogenous Protein Complexes with Ion Exchange Chromatography Coupled to Native Electrospray Mass Spectrometry;** Paul Dominic B. Olinares; Zachary T. Quinkert; Julio C. Padovan; Brian T. Chait; The Rockefeller University, New York, NY
- MP 161 **Characterization of Bound HSV-2 Peptides in a Heat Shock Protein Based Vaccine;** Joseph Connolly; Zhenyu Li; Jesse Martin; Shiwen Lin; Stephen Monks; Agenus, Inc., Lexington, MA
- MP 162 **Comparative proteomic Analysis Reveals Novel Components at the Plasma Membrane of Differentiated HepaRG Cells;** Catalina Petreanu<sup>2</sup>; Izabela Sokolowska<sup>1</sup>; Alina Macovei<sup>2</sup>; Alisa G. Woods<sup>1</sup>; Lucian G Radu<sup>2</sup>; Costel Darie<sup>1</sup>; Norica Brinza-Nichita<sup>2</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>Institute of Biochemistry, Bucharest, Romania
- MP 163 **Defining Interacting Proteins of the Retinoic Acid Receptor Responder Protein-1 using TAP-TAG Affinity and SILAC Titration Strategy;** Haeri Seol; Kristy J Brown; Yetrib Hathout; Children's National Medical Center, Washington, DC
- MP 164 **Strategies for Identifying Specific Constituents of Protein Complexes and Benefits of Combining Bead Matrices for Immunoaffinity & Mass Spectrometric Applications;** Aman Tyagi<sup>1</sup>; Ken Oh<sup>1</sup>; Ebbing deJong<sup>2</sup>; Sricharan Bandhakavi<sup>1</sup>; Michael Early<sup>1</sup>; <sup>1</sup>Bio-Rad Laboratories, Hercules, CA; <sup>2</sup>University of Minnesota, Minneapolis, MN
- MP 165 **Accurate Stoichiometry Determination of a Very Large Molecular Machine: The 50 MDa Yeast Nuclear Pore Complex;** Wenzhu Zhang; Javier Fernandez-Martinez; Michael P. Rout; Brian T. Chait; The Rockefeller University, New York, NY
- Proteins: Covalent Labeling, 166 - 179**
- MP 166 **Elucidating the Interaction of Resveratrol with Amyloid-β (1-40) using Labeling Electrospray Deposition and Mass Spectrometry;** Jeddiah Griffin; Paul Martino; Carson-Newman University, Jefferson City, TN
- MP 167 **Rapid Gas-Phase Carbene Labeling and Top-Down Mass Spectrometry Provides Topographical Structural Information;** Daniel Therrien<sup>2</sup>; Douglas Steiner<sup>2</sup>; Elizabeth Campbell<sup>1</sup>; Mark Carver<sup>1</sup>; Emily Hammer<sup>1</sup>; Margaret Cothorn<sup>1</sup>; Paul Martino<sup>1</sup>; <sup>1</sup>Carson-Newman University, Jefferson City, TN; <sup>2</sup>Martino Labs, Inc., Kalispell, MT
- MP 168 **Chemo-Enzymatic Derivatization and Enrichment of Protein Post-Translational Modifications: Methylation and Isoaspartic Acid;** Zhaohui Zhou; Northeastern University, Boston, MA
- MP 169 **Structural Analysis of Fibrillar and Prefibrillar Oligomeric Forms of Amyloid Abeta at the Level of Single Residue by Covalent Labeling;** Janna Kiselar<sup>1</sup>; Alexandra Klinger<sup>2</sup>; Sergei Ilchenko<sup>1</sup>; Mark R Chance<sup>1</sup>; Paul Axelsen<sup>2</sup>; <sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>University of Pennsylvania, Pennsylvania, PA

- MP 170 **Identification of Phosphorylation of Tyrosines on Tubulin Following Exposure to Organophosphorus Pesticides using LC-MS/MS;** Michael G. Bartlett<sup>1</sup>; Pei Li<sup>1</sup>; Alvin Terry<sup>2</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Georgia Regents University, Augusta, GA
- MP 171 **Standardization of Hydroxyl Radical Protein Footprinting Data - High Resolution Footprint of Galectin-1;** Boer Xie; *Complex Carbohydrate Research Center, The University of Georgia, Athens, GA*
- MP 172 **Epitope Mapping of EGFR Binding to an Adnectin by Fast Photochemical Oxidation of Proteins (FPOP);** Yuetian Yan<sup>1</sup>; Guodong Chen<sup>2</sup>; Hui Wei<sup>2</sup>; Richard Huang<sup>2</sup>; Jingjie Mo<sup>2</sup>; Don Rempel<sup>1</sup>; Adrienne Tymiak<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>Washington University, Saint Louis, MO; <sup>2</sup>Bristol-Myers Squibb, Princeton, NJ
- MP 173 **FPOP Dosimetry Experiment in Building a More Quantitative FPOP Platform;** Ben Niu; Hao Zhang; Daryl Giblin; Don Rempel; Michael Gross; *Washington University, Saint Louis, MO*
- MP 174 **Development of an *in vivo* Protein Footprinting Method for the Structural Analysis of Proteins;** Lisa M. Jones; *Indiana University-Purdue University Indianapolis, Indianapolis, IN*
- MP 175 **Efficient Quantitation of Hydroxyl Radical-Mediated Protein Footprinting using Proteome Discoverer;** Aimee Rinas<sup>1</sup>; Lisa Jones<sup>2</sup>; <sup>1</sup>Indiana University Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Indiana University-Purdue University Indianapolis, Indianapolis, IN
- MP 176 **Characterization of Robo1 IG 1-2 Protein and Robo1-Heparin Complex by High Structural Resolution Hydroxyl Radical Protein Footprinting;** Zixuan Li; Heather Moniz; Annapoorani Ramiah; Kelley Moremen; Joshua Sharp; *Complex Carbohydrate Research Center UGA, Athens, GA*
- MP 177 **Structural Analysis of HIV-1 gp120 and its Complex with Neutralizing Immunoglobulin G1 b12 using Hydroxyl Radical Protein Footprinting;** Xiaoyan Li; Joshua S. Sharp; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- MP 178 **Method for the Specific Quantification of Oxidative Stress Based on Metal Tags in Proteins;** Ahmed H. El-Khatib; Diego Esteban-Fernández; Michael Linscheid; *Humboldt-Universität zu Berlin, Berlin, Germany*
- MP 179 **Methods for Determining Site-Specificity of Reversible Thiol Modifications in Ras GTPases;** G. Aaron Hobbs; Harsha P. Gunawardena; Minh V. Huynh; Xian Chen; Sharon L. Campbell; *Biochemistry & Biophysics, UNC-Chapel Hill, NC*
- Intact Proteins: Covalent Interactions, 180 - 185**
- MP 180 **Use of Nano-electrospray Ionization/Mass Spectrometry for the Studies of Non-covalent Interactions Between Indoleamine 2, 3-dioxygenase and Small Molecule Inhibitors;** Hui Wei; John Newitt; Aaron Balog; Adrienne Tymiak; Guodong Chen; *Bristol-Myers Squibb, Princeton, NJ*
- MP 181 **Advances in Native Mass Spectrometry-based Methods for the Analysis of Non-Covalent Protein Complexes;** Jonathan P. Williams; Malcolm Anderson; Lidia Jackson; Kevin Giles; Jeff Brown; *Waters Corporation, Manchester, UK*
- MP 182 **Investigating the Catalytic Mechanism of Serine Palmitoyltransferase using Native Mass Spectrometry and Top-Down Fragmentation;** David J. Clarke; John Wadsworth; C. Logan Mackay; Dominic Campopiano; *University of Edinburgh, Edinburgh, UK*
- MP 183 **Molecular Self-Assembly of Bacterial Stress-Response Protein WrbA Studied by Mass Spectrometry;** Alan Kadek<sup>1,2</sup>; Zdenek Kukacka<sup>1,2</sup>; Julien Marcoux<sup>3</sup>; Ondrej Vanek<sup>2</sup>; Olga Ettrichova<sup>4,5</sup>; Rudiger Ettrich<sup>4,5</sup>; Carol Robinson<sup>3</sup>; Petr Man<sup>1,2</sup>; Petr Novak<sup>1,2</sup>; <sup>1</sup>Institute of Microbiology ASCR, Prague, Czech Republic; <sup>2</sup>Faculty of Science, Charles University in Prague, Prague, Czech Republic; <sup>3</sup>Department of Chemistry, University of Oxford, Oxford, UK; <sup>4</sup>Global Change Research Centre ASCR, Nove Hradky, Czech Republic; <sup>5</sup>Faculty of Science, University of South Bohemia, Ceske Budejovice, Czech Republic
- MP 184 **Nanodisc Characterization by Tandem Mass Spectrometry, Ion Mobility and Atomic Force Microscopy;** Iain D.G. Campuzano<sup>1</sup>; Huilin Li<sup>2</sup>; Joseph A. Loo<sup>2</sup>; George Svitel<sup>1</sup>; Paul D. Schnier<sup>1</sup>; <sup>1</sup>Amgen Inc., Thousand Oaks, CA; <sup>2</sup>UCLA, Los Angeles, CA
- MP 185 **Monitoring the Proteolytic Degradation of  $\beta$ 2-Microglobulin Oligomers and Amyloid Fibrils using Mass Spectrometry;** William Warren<sup>1,2</sup>; Jill Graham<sup>1,2</sup>; Peter Chien<sup>1,2</sup>; Richard Vachet<sup>1,2</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>University of Massachusetts, Amherst, MA
- Peptides: General, 186 - 199**
- MP 186 **Improvements in Shotgun Proteomics using a Benchtop Quadrupole High Field Orbitrap;** Tabiwang N. Arrey<sup>1</sup>; Eugen Damoc<sup>1</sup>; Kai Scheffler<sup>2</sup>; Yue Xuan<sup>1</sup>; Maciej Bromirski<sup>1</sup>; Markus Kellmann<sup>1</sup>; Thomas Moehring<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Dreieich, Germany
- MP 187 **Identification and Quantification of a Hydrophobic C-terminal Amidated Peptide in Ocular Fluid Extracts;** Tatiana N. Boronina<sup>1</sup>; Niranjan Pandey<sup>2</sup>; Aleksander S. Popel<sup>2</sup>; Robert O'meally<sup>1</sup>; Robert N. Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>BME, Johns Hopkins School of Medicine, Baltimore, MD
- MP 188 **A Novel 6x5 Peptide Mixture for Instrument Performance Monitoring;** Michael Rosenblatt; Ethan Strauss; Marjeta Urh; *Promega Corporation, Madison, WI*
- MP 189 **MS<sup>n</sup> Characterization of Phosphothreonine Peptide Isomers;** Christopher C. Lai; Wen-Jian Qian; Terrence R. Burke, Jr; James A. Kelley; *NCI/NIH, Frederick, MD*
- MP 190 **Detection of Metal Binding Sites in Peptides and Proteins using Ultrahigh Performance Liquid Chromatography High Resolution Mass Spectrometry (UHPLC-HRMS);** Rutika Patel; Fred Asante; Dil Ramanathan; *Kean University, Union, NJ*
- MP 191 **Comparison of C18 Reversed-Phase Column Material for Shotgun Proteomics;** Fiona Pachtl<sup>1</sup>; Hannes Hahne<sup>1</sup>; Bernhard Kuster<sup>2</sup>; <sup>1</sup>Technische Universität München, Freising, Germany; <sup>2</sup>Technical University Munich, Freising, Germany
- MP 192 **Enhancing MS Identification of Tryptic Peptides with Heavy Mass Tagging on Solid Phase;** Ioannis Pikalov; Chang Xue; Frantisek Turecek; *University of Washington, Seattle, WA*
- MP 193 **SpikeMix™ Peptides – A Novel Approach for Synthetic Preparation of Low Cost & Small Scale Peptide Pools for Large Scale Proteomics;** Karsten Schnatbaum<sup>1</sup>; Johannes Zerweck<sup>1</sup>; Maren Eckey<sup>1</sup>; Larry Eckler<sup>1</sup>; Holger Wenschuh<sup>1</sup>; Hannes Hahne<sup>2</sup>; Bernhard Kuster<sup>2</sup>; Ulf Reimer<sup>1</sup>; <sup>1</sup>JPT Peptide Technologies GmbH, Berlin, Germany; <sup>2</sup>Technische Universität München, Freising, Germany
- MP 194 **Development of a High Resolution Data Independent Acquisition Method for Detecting Organophosphorus Nerve Agents as Butyrylcholinesterase Inhibitors;** Caroline Watson<sup>1</sup>; Melissa Carter<sup>2</sup>; Brian Crow<sup>2</sup>; Brooke



- Pantazides<sup>2</sup>; Jonas Perez<sup>3</sup>; Darryl Johnson<sup>1</sup>; Thomas Blake<sup>2</sup>; Rudolph Johnson<sup>2</sup>; <sup>1</sup>ORISE Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>CDC, Atlanta, GA; <sup>3</sup>Battelle, Atlanta, GA
- MP 195 **Investigating the Use of Alternative Solvent Systems for Maximizing Sensitivity for Bottom-Up Proteomics on a Q Exactive Plus;** Mark Szewc<sup>1</sup>; Joshua Nicklay<sup>1</sup>; Tara Schroeder<sup>1</sup>; Scott Peterman<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific BRIMS, Cambridge, MA
- MP 196 **Targetted Analysis of Peptides in Live Single-Cell Mass Spectrometry;** Ai Fujita<sup>1</sup>; Hajime Mizuno<sup>1</sup>; Iwao Sakane<sup>2</sup>; Tsutomu Masujima<sup>1</sup>; <sup>1</sup>Quantitative Biology Center (QBiC), RIKEN, Suita, Japan; <sup>2</sup>ITO-EN Ltd, Makinohara, Japan
- MP 197 **A New Strategy for Sensitive and Selective Quantitation of Membrane Proteins using Differential Mobility Spectrometry and MRM Cubed Technology;** Li Ma<sup>1</sup>; Yaofeng Cheng<sup>1</sup>; Yuan-qing Xia<sup>2</sup>; Jeff Miller<sup>2</sup>; Elliot Jones, Jr<sup>2</sup>; Mingshe Zhu<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>AB Sciex, Framingham, MA
- MP 198 **Implementation of Hybrid QqToF Data in MaxQuant Software for the Processing of SILAC Experiments;** Christof Lenz<sup>1,2</sup>; Jasmin Corso<sup>1</sup>; Juergen Cox<sup>3</sup>; Joerg Dojahn<sup>4</sup>; Thomas Oellerich<sup>5</sup>; Henning Urlaub<sup>1,2</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>University Medical Center, Goettingen, Germany; <sup>3</sup>Max Planck Institute of Biochemistry, Martinsried, Germany; <sup>4</sup>AB SCIEX, Darmstadt, Germany; <sup>5</sup>Goethe University, Frankfurt am Main, Germany
- MP 199 **Single Bead Peptide Microarrays Characterized by Laser Ablation Electrospray Ionization Mass Spectrometry Imaging (LAESI-MSI);** Holly Henderson<sup>1</sup>; Vladislav Bergo<sup>2</sup>; Benjamin Mildenberg<sup>2</sup>; Greg Kilby<sup>1</sup>; Matthew Powell<sup>1</sup>; <sup>1</sup>Protea Biosciences Group, Inc., Morgantown, WV; <sup>2</sup>Adeptix, Boston, MA
- Peptides: Sequence Analysis, 200 - 207**
- MP 200 **Rapid Disulfide Bond Recognition in Proteins through HIFU Generated Proteolytic Peptides Exhibiting Giant Triplet Signal Signatures;** Serge Chesnov; Rene Brunisholz; <sup>1</sup>Functional Genomics Center Zurich, Zurich, Switzerland
- MP 201 **De novo Sequencing of Peptides in Free Radial Initiated Peptide Sequencing (FRIPS) Mass Spectrometry;** Han Bin Oh; <sup>1</sup>Sogang Univ. Dept. of Chemistry, Seoul, South Korea
- MP 202 **Characterization of Photo-switchable bZIP Domains: Sequencing of Internally Cross-linked Peptides via Collision-induced Dissociation Tandem Mass Spectrometry;** Ahmed M. Ali; Matthew W. Forbes; G. Andrew Woolley; <sup>1</sup>Department of Chemistry, University of Toronto, Toronto, Canada
- MP 203 **Identification of Selenocysteine Sites in Selenoproteins using HPLC and Low Energy CID;** Stephen Chan; Fei Li; <sup>1</sup>University of Delaware, Newark, DE
- MP 204 **Protease-Containing Membranes for Antibody Digestion Prior to Middle-Down Sequencing;** Yongle Pang<sup>1</sup>; Gavin Reid<sup>1,2</sup>; Merlin Bruening<sup>1</sup>; <sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Department of Biochemistry & Molecular Biology, East Lansing, MI
- MP 205 **Peptide Sequencing using Q-TOF and MALDI TOF/TOF Mass Spectrometry in Combination with Different Software Tools;** Lena von Sydow; Anja Ekdahl; Gustaf Hedlund; Pernilla Korsgren; <sup>1</sup>AstraZeneca R&D, Mölndal, Sweden
- MP 206 **Combining NeuCode with LysC and LysN Digestion for de novo Sequencing Applications;** Robert Cunningham<sup>1</sup>; Ryan Bomgarden<sup>1</sup>; Christine Johnson<sup>2</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>Northwestern University, Evanston, IL
- MP 207 **Application of Multiple Protease Digestion with SPS de novo Approach to the Characterization of Hemoglobin Variants;** Jane Yang<sup>1</sup>; Adrian Guthals<sup>1</sup>; Jesse Meyer<sup>1</sup>; Majid Ghassemian<sup>1</sup>; Elizabeth Komives<sup>1</sup>; Nuno Bandeira<sup>1</sup>; David Herold<sup>2</sup>; <sup>1</sup>UCSD, San Diego, CA; <sup>2</sup>VAMC/ UCSD, San Diego, CA
- Proteomics: New Approaches, 208 - 224**
- MP 208 **Cysteine-selective Combined Precursor Isotopic Labeling and Isobaric Tagging (cPILOT);** Liqing Gu; Adam Evans; Renā Robinson; <sup>1</sup>Department of Chemistry, University of Pittsburgh, Pittsburgh, PA
- MP 209 **Absolute Signal Intensity as a Metric for Surrogate Peptides Selection and Ion Ratio Thresholds for Absolute Quantification Mass Spectrometry;** Phillip Loziuk; Wei Li; Jack Wang; Quanzi Li; Ronald Sederoff; Vincent Chiang; Dave Muddiman; <sup>1</sup>North Carolina State University, Raleigh, NC
- MP 210 **Protein Turnover Rate in Gastrointestinal Tract;** Liisa Arike<sup>1</sup>; Sjoerd van der Post<sup>1</sup>; Andrus Seiman<sup>2</sup>; Gunnar C. Hansson<sup>1</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Competence Center of Food and Fermentation Technol, Tallinn, Estonia
- MP 211 **Protein Turnover and Quantification Determination in Mice using a Combination of Both Metabolic and Chemical Labeling;** Liisa Arike; Gunnar C Hansson; Sjoerd Van Der Post; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden
- MP 212 **Application of Quantitative Proteomics and RNA-Seq to Study the Evolution of Primate Transcript and Protein Expression Levels;** Zia Khan<sup>1</sup>; Michael Ford<sup>2</sup>; Darren Cusanovich<sup>3</sup>; Amy Mitranos<sup>3</sup>; Jonathan Pritchard<sup>3</sup>; Yoav Gilad<sup>3</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>MS Bioworks LLC, Ann Arbor, MI; <sup>3</sup>University of Chicago, Chicago, IL; <sup>4</sup>Stanford University, Stanford, CA
- MP 213 **Nano Flow UPLC-MS Analyses of Insulin Receptor Site-Specific Phosphorylation Induced by Insulin and Insulin Mimetic Peptide;** Zhongping Liao; Jason X. Tang; John Beals; <sup>1</sup>Eli Lilly & Company, Indianapolis, IN
- MP 214 **A Targeted in vivo SILAC Approach for Quantification of Drug Metabolism Enzymes;** Kenneth MacLeod; Tuo Zang; Zoe Riches; Colin Henderson; Roland Wolf; Jeffrey Huang; <sup>1</sup>Medical Research Institute, University of Dundee, Dundee, UK
- MP 215 **Cell-selective Labeling using Amino Acid Precursors for Proteomic Studies of Multicellular Environments and Biomarker Discovery;** Nicholas Gauthier<sup>1</sup>; Boumediene Soufi<sup>2</sup>; Boris Macek<sup>3</sup>; Chris Sander<sup>1</sup>; Martin Miller<sup>1</sup>; <sup>1</sup>Memorial Sloan-Kettering Cancer Center, New York, NY; <sup>2</sup>Proteome Center Tuebingen, Tuebingen, Germany; <sup>3</sup>University of Tuebingen, Tubingen, Germany
- MP 216 **Sensitivity Increased MultiPLEX (SIMPLEX) SILAC for Quantitative Proteomics;** Duc Duong<sup>1</sup>; Eric Dammer<sup>1</sup>; Ron Trolard<sup>2</sup>; Nicholas Seyfried<sup>1</sup>; <sup>1</sup>Emory University, Atlanta, GA; <sup>2</sup>Cambridge Isotope Laboratories, Cambridge, MA
- MP 217 **Development of a 20-plex Method for Profiling Total Proteome and Proteome turnover in Yeast;** Yanling Yang; Haiyan Tan; Zhiping Wu; Hong Wang; Junmin Peng; <sup>1</sup>St. Jude Children's Research Hospital, Memphis, TN
- MP 218 **SILAC Labeling of Mitophagy-Inhibited C. elegans;** Michelle Henderson<sup>1</sup>; Hope Henderson<sup>2</sup>; Suzanne Wolff<sup>2</sup>; Andrew Dillin<sup>2</sup>; Edgar Arriaga<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of California, Berkeley, Berkeley, CA

- MP 219 **Development and Characterization of a Proteomics Normalization Standard Consisting of 1,000 Stable Isotope Labeled Peptides**; Christopher M. Colangelo<sup>1</sup>; Lisa M. Chung<sup>1</sup>; Craig Dufresne<sup>2</sup>; David Hawke<sup>3</sup>; Alexander R. Ivanov<sup>4</sup>; Antonius Koller<sup>5</sup>; Brendan Maclean<sup>6</sup>; Brett Phinney<sup>7</sup>; Kristie Rose<sup>8</sup>; Paul Rudnick<sup>9</sup>; Brian C. Searle<sup>10</sup>; Vagisha Sharma<sup>6</sup>; Scott A. Shaffer<sup>11</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Thermo Fisher Scientific, West Palm Beach, FL; <sup>3</sup>UT- M.D. Anderson Cancer Center, Houston, TX; <sup>4</sup>Barnett Institute, Northeastern University, Boston, MA; <sup>5</sup>Stony Brook University, Stony Brook, NY; <sup>6</sup>University of Washington, Seattle, WA; <sup>7</sup>University of California, Davis, CA; <sup>8</sup>Vanderbilt University, Nashville, TN; <sup>9</sup>Spectragen Informatics, Rockville, MD; <sup>10</sup>Proteome Software Inc., Portland, OR; <sup>11</sup>University of Massachusetts Medical School, Worcester, MA
- MP 220 **Global Equalization of Peptide Abundance through Limited Digestion and Depletion Improves Quantitation Sensitivity and Accuracy of Whole Proteomes**; Bryan Fonslow; Jeffrey Savas; Navin Rauniyar; John R. Yates III; The Scripps Research Institute, La Jolla, CA
- MP 221 **Multiphase Trap Chips for Improved Protein Identification and Quantitation in Discovery and Targeted Proteomics**; Christoph Krisp<sup>1</sup>; Hao Yang<sup>2</sup>; Remco van Soest<sup>2</sup>; Mark P. Molloy<sup>1</sup>; <sup>1</sup>Macquarie University, Sydney, Australia; <sup>2</sup>Eksigent, part of AB SCIEX, Redwood City, CA
- MP 222 **Comparative Proteomics-Based in Silico Analyzes Further our Understanding of Mouse Spermatogenesis and Fertility**; Tanxi Cai; Yongqiang Wang; Jiejian Luo; Taijiao Jiang; Fuquan Yang; *Institute of Biophysics, CAS, Beijing, China*
- MP 223 **Selective Isolation of Genome-Associated Proteins Reveals Dynamics of Chromatin Composition in Stem Cells**; Mahmoud-Reza Rafiee; Jeroen Krijgsveld; *EMBL Heidelberg, Heidelberg, Germany*
- MP 224 **An Ion-Current-Based, Proteomic Investigation of Schwann Cells Radial Sorting Revealed New Insights into Directional Cell Migration and Neural Developments**; Jun Li; Shichen Shen; Xiaomeng Shen; Jun Qu; *University at Buffalo SUNY, Buffalo, NY*
- Epigenetic Modifications/Histones, 225 - 237**
- MP 225 **A Tool for Quantifying and Visualizing High-Resolution MS/MS and MS Spectra from Data-Independent Acquisition Experiments**; Michael J Sweredoski; Jenny Broeker; Annie Moradian; Sonja Hess; *Caltech, Pasadena, CA*
- MP 226 **Data-Independent ETD Mass Spectrometry for Middle-Down Histone Post-Translational Modifications Analysis**; Michael J Sweredoski<sup>1</sup>; Tonya Pekar-Second<sup>2</sup>; Annie Moradian<sup>1</sup>; Sonja Hess<sup>1</sup>; <sup>1</sup>Caltech, Pasadena, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 227 **Utilizing Targeted Proteomics to Determine the Factors that Influence the Specificity of Rtt109 Histone Acetylation**; Yin-Ming Kuo; Ryan Henry; Andrew Andrews; *Fox Chase Cancer Center, Philadelphia, PA*
- MP 228 **Harnessing Proteomics to Study the Role of Histone Deacetylases in T-Cell Receptor Signalling and T-Cell Proliferation**; Dijana Vitko<sup>1</sup>; Lisa Göschl<sup>2</sup>; Florian Breitwieser<sup>1</sup>; Roland Tschisnarov<sup>2</sup>; Nicole Boucheron<sup>2</sup>; Christian Seiser<sup>3</sup>; Jacques Colinge<sup>1</sup>; Wilfried Ellmeier<sup>2</sup>; Keiryn L. Bennett<sup>1</sup>; <sup>1</sup>CeMM Research Center for Molecular Medicine, Vienna, Austria; <sup>2</sup>Institute of Immunology, Vienna, Austria; <sup>3</sup>Max F. Perutz Laboratories, Vienna, Austria
- MP 229 **Histone H1 Phosphorylation in Human Breast Cancer**; Michael E. Hoover<sup>1,6</sup>; Sean W. Harshman<sup>1,6</sup>; Chengsi Huang<sup>2</sup>; Owen E. Branson<sup>2</sup>; Sarah B. Chaney<sup>3</sup>; Carolyn M. Cheney<sup>4,6</sup>; Thomas J. Rosol<sup>3</sup>; Charles L. Shapiro<sup>5,6</sup>; Vicki H. Wysocki<sup>2</sup>; Kay Huebner<sup>5,6</sup>; Michael A. Freitas<sup>5,6</sup>; <sup>1</sup>Biomedical Sciences Graduate Program, Columbus, OH; <sup>2</sup>OSU Department of Chemistry & Biochemistry, Columbus, OH; <sup>3</sup>OSU College of Veterinary Medicine, Columbus, OH; <sup>4</sup>Department of Internal Medicine, Columbus, OH; <sup>5</sup>Comprehensive Cancer Center, Columbus, OH; <sup>6</sup>The Ohio State University Wexner Medical Center, Columbus, OH
- MP 230 **Confidence Metrics for Identification of Proteins, Post-translational Modifications (PTMs) and Proteoforms**; Naomi Brownstein<sup>1</sup>; Nicolas L. Young<sup>2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>NHMFL / FSU, Tallahassee, FL
- MP 231 **Multiplexed Parallel Reaction Monitoring-Targeting Histone Modifications on the Q-Exactive Mass Spectrometer**; Hui Tang; Kangling Zhang; *University of Texas Medical Branch at Galveston, Galveston, TX*
- MP 232 **Infection of Borna Disease Virus Impacts Proteome and Histone Lysine Acetylation in Human Oligodendroglia Cells**; Xia Liu<sup>1,2</sup>; Xiaojun Peng<sup>3</sup>; Zhongyi Cheng<sup>3</sup>; Peng Xie<sup>1,2</sup>; <sup>1</sup>Institute of Neuroscience, Chongqing Medical Univ, Chongqing, CN; <sup>2</sup>The First Affiliated Hospital, Chongqing Medical U, Chongqing, CN; <sup>3</sup>PTM Biolabs, Inc, Hangzhou, China
- MP 233 **Characterization of Global Patterns of 5-Methylcytosine and 5-Hydroxymethylcytosine in the Vascular Endothelium using LC-MS/MS**; Apurva Shirodkar<sup>1,2</sup>; Michelle E. Young<sup>1</sup>; Jacquie Lu<sup>2</sup>; Philip Marsden<sup>1,2</sup>; <sup>1</sup>University of Toronto, Toronto, Canada; <sup>2</sup>St. Michael's Hospital, Toronto, Canada
- MP 234 **Identification of Histone Post-translational Modifications in Alzheimer's Disease Brain**; Kyle Anderson<sup>1,2</sup>; Ilarion Turko<sup>1,2</sup>; <sup>1</sup>IBBR, Rockville, MD; <sup>2</sup>NIST, Gaithersburg, MD
- MP 235 **Dynamic Changes in Histone Post-Translational Modifications: A New Global MS-based Profiling Approach**; Raphaël Bilgraer<sup>1</sup>; Sylvie Gillet<sup>1</sup>; Sophie Gil<sup>2</sup>; Danièle Evain-Brion<sup>2</sup>; Olivier Laprèvote<sup>1,3</sup>; <sup>1</sup>CNRS UMR 8638, Université Paris Descartes, Paris, France; <sup>2</sup>INSERM U1139, Université Paris Descartes, Paris, France; <sup>3</sup>Toxicologie Biologique, Hôpital Lariboisière, APHP, Paris, France
- MP 236 **Investigating the Specificity of Histone Acetyltransferase Activity for Producing Rare Modifications on Histones using Mass Spectrometry**; Amanda Hu<sup>1</sup>; Laura-Mae Britton<sup>2</sup>; Benjamin A. Garcia<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Princeton University, Princeton, NJ
- MP 237 **Identification of Serine and Threonine O-Acetyltransferases**; Laura-Mae Britton<sup>1</sup>; Benjamin Garcia<sup>2</sup>; <sup>1</sup>Princeton University, Princeton, NJ; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- Lipids: General, 238 - 253**
- MP 238 **Automatic Characterization of Lipids using Charge Remote Fragmentation Ions and Peaks Characteristic of Fatty Acid Fragmentation From MALDI MS/MS Data**; Ningombam Sanjib Meitei<sup>1</sup>; Arun Apte<sup>2</sup>; Dietmar Waidelich<sup>3</sup>; Fadi Abdi<sup>4</sup>; Matthias Glueckmann<sup>3</sup>; <sup>1</sup>PREMIER Biosoft, Indore, India; <sup>2</sup>PREMIER Biosoft, Palo Alto, U.S.A.; <sup>3</sup>AB SCIEX, Darmstadt, Germany; <sup>4</sup>AB SCIEX, Framingham, U.S.A.
- MP 239 **Identification of Novel Serum Lipid Biomarkers Predicting Preeclampsia using a Shotgun Lipidomics Approach**; Swati Anand<sup>1</sup>; Sydney Young<sup>1</sup>; sean esplin<sup>2</sup>; Craig Thulin<sup>3</sup>; Bruce Jackson<sup>1</sup>; Steven Graves<sup>1</sup>; <sup>1</sup>BYU, Provo, UT; <sup>2</sup>University of Utah, Salt lake city, UT; <sup>3</sup>Utah valley university, orem, UT



- MP 240 **Lipidomic Analysis and Comparison of Young and Old Rat Skeletal Muscles using UHPLC-HRMS**; Yu-Hsuan Tsai<sup>1,2</sup>; Timothy Garrett<sup>1,3</sup>; Christy Carter<sup>1,4</sup>; Richard A. Yost<sup>1,2</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Dept. of Chemistry, Gainesville, Florida; <sup>3</sup>Dept. of Pathology, Gainesville, Florida; <sup>4</sup>Dept. Aging & Geriatric Research, Gainesville, Florida
- MP 241 **Phospholipidomics of Yeast Lipidome and Marine Lecithin by Single Run LC/MS/MS**; Corinne Bure; Maud Cansell; Alexandre Pinsolle; Sophie Aycirieux; Jean-Marie Schmitter; University of Bordeaux, Bordeaux, France
- MP 242 **Comprehensive Investigation of Reversed-phase LC Methodology for Global Lipidomics Analyses using High-Resolution Accurate Mass LC-MS/MS**; Kevin J. McHale<sup>1</sup>; Josef Ruzicka<sup>1</sup>; David A. Peake<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific, Carmel, IN
- MP 243 **Data Acquisition Parameters Optimization of Quadrupole Orbitrap for Global Lipidomics on LC-MS/MS time frame**; Josef Ruzicka<sup>1</sup>; Kevin J. Mchale<sup>1</sup>; David A. Peake<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- MP 244 **Tandem Mass Tag hydrazide - A New Derivative for Oxosteroid Analysis**; Katarina Rigdova<sup>2</sup>; Yuqin Wang<sup>2</sup>; Malcolm Ward<sup>1</sup>; William James Griffiths<sup>2</sup>; Ian Pike<sup>1</sup>; <sup>1</sup>Proteome Sciences plc, London, UK; <sup>2</sup>Swansea University, Swansea, UK
- MP 245 **Comparison of Experimental MALDI Mass Spectrometric and Computer Modeling Investigation of Protonated and Cationized Phosphatidylcholines**; Vitaliy Chagovets; Michal Holcapek; Miroslav Lisa; University of Pardubice, Pardubice, Czech Republik
- MP 246 **Comprehensive LC/sCID-MS and GC/MS Lipidomic Platform for In-Depth Characterization of Diverse Lipids: Application in Biological Target Identification for Drug Discovery**; Laila Abdullah<sup>1</sup>; James Evans<sup>1</sup>; Jon Reed<sup>1,2</sup>; Gogce Crynen<sup>1,2</sup>; Corbin Bachmeier<sup>1</sup>; Hannah Montague<sup>1</sup>; Ariel Gonzalez<sup>1</sup>; Madison Crocker<sup>1</sup>; Tanja Emmerich<sup>1</sup>; Robert Pelot<sup>2</sup>; Michael Mullan<sup>1</sup>; Fiona Crawford<sup>1,2</sup>; <sup>1</sup>Roskamp Institute, Sarasota, FL; <sup>2</sup>SRQ Bio, Sarasota, FL
- MP 247 **Live Single-cell Mass Spectrometry for Direct Lipid Analysis of a Stimulated Allergy Cell**; Hajime Mizuno; Yosuke Kawai; Tsutomu Masujima; Quantitative Biology Center (QBiC), RIKEN, Suita, Japan
- MP 248 **Gas Phase Discrimination of Phosphatidylcholines and Phosphatidylethanolamines using Charge-Inversion Ion/Ion Reactions**; Stella Rojas-Betancourt<sup>1</sup>; John Stutzman<sup>1</sup>; Stephen J Blanksby<sup>2</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Queensland University of Technology, Brisbane, Australia
- MP 249 **Molecular Differentiation of *Escherichia coli* Strains as a Function of Antibiotic Stress**; Alyssa Garabedian<sup>1</sup>; Emily Schenk<sup>1</sup>; Diana Hernandez<sup>1</sup>; Christopher Thompson<sup>2</sup>; Yuk-Ching Tse-Dinh<sup>1</sup>; Francisco Fernandez-Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA
- MP 250 **Global Lipid Profiling of Mucosa from Patients with Chronic Sinusitis and Otitis Media and Controls**; Farbod Fazlollahi<sup>1</sup>; Kessiri Kongmanas<sup>2</sup>; Nongnuij Tanphaichitr<sup>2</sup>; Kym Faull<sup>1</sup>; Jeffrey Suh<sup>1</sup>; Quinton Gopen<sup>1</sup>; <sup>1</sup>UCLA, Los Angeles, CA; <sup>2</sup>University of Ottawa, Ottawa, Canada
- MP 251 **Mass Spectrometry Study of Non-Glycerol Lipids Hydrolysis by Phospholipase A2**; Reza Nemati<sup>1</sup>; Emily Anstadt<sup>2</sup>; Vahid Farrokhi<sup>1</sup>; Robert Clark<sup>2</sup>; Xu Wang<sup>3</sup>; Xudong Yao<sup>1</sup>; Frank Nichols<sup>4</sup>; <sup>1</sup>Department of Chemistry, University of Connecticut, Storrs, CT; <sup>2</sup>Department of Medicine, University of Connecticut, Farmington, CT; <sup>3</sup>AB SCIEX, Framingham, MA; <sup>4</sup>University of Connecticut School Dental Medicine, Farmington, CT
- MP 252 **Phospholipid Oxidation Products as Biomarkers for Oxidative Stress in Inflammatory Liver Disease**; Beate Fuchs; Jürgen Schiller; University of Leipzig, Leipzig, Germany
- MP 253 **The Use of Glycerol for Enhanced Lipid Signal in Liquid Extraction Surface Analysis Mass Spectrometry of Thin Tissue Sections**; Alexander Dexter<sup>1</sup>; Josephine Bunch<sup>2</sup>; Iain B. Styles<sup>1</sup>; Helen J. Cooper<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>National Physical Laboratory, London, UK
- Systems Biology: General, 254 - 279**
- MP 254 **Confetti: A Multi-protease Map of the HeLa Proteome for Comprehensive Proteomics**; Hamid Mirzaei<sup>1</sup>; David Trudgian<sup>1</sup>; Xiaofeng Guo<sup>2</sup>; Andrew Lemoff<sup>1</sup>; Sivaramakrishna Yadavalli<sup>1</sup>; <sup>1</sup>UT Southwestern, Dallas, TX; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- MP 255 **A Draft Map of the Human Proteome**; Min-Sik Kim<sup>1</sup>; Sneha M. Pinto<sup>1,2</sup>; Derese Getnet<sup>1</sup>; Raja Sekhar Nirujogi<sup>1,2</sup>; Srikanth S. Manda<sup>1,2</sup>; Raghothama Chaerkady<sup>1</sup>; Anil Madugundu<sup>2</sup>; Dhanashree S. Kelkar<sup>2</sup>; Ruth Isserlin<sup>3</sup>; Shobhit Jain<sup>3</sup>; Joji K. Thomas<sup>2</sup>; Babylakshmi Muthusamy<sup>2</sup>; Nandini A. Sahasrabudhe<sup>2</sup>; Praveen Kumar<sup>2</sup>; Pamela Leal Rojas<sup>1</sup>; Lavanya Balakrishnan<sup>2</sup>; Jayshree Advani<sup>2</sup>; Bijesh George<sup>2</sup>; Santosh Renuse<sup>2</sup>; Lakshmi Dhevi N. Selvan<sup>2</sup>; Arun H. Patil<sup>2</sup>; Vishalakshi Nanjappa<sup>2</sup>; Aneesha Radhakrishnan<sup>2</sup>; Tejaswini Subbannayya<sup>2</sup>; Rajesh Raju<sup>2</sup>; Manish Kumar<sup>2</sup>; Sreelakshmi Sreenivasamurthy<sup>2</sup>; Arivusudar Marimuthu<sup>2</sup>; Gajanan J. Sathe<sup>2</sup>; Sandip Chavan<sup>2</sup>; Keshava K. Datta<sup>2</sup>; Yashwanth Subbannayya<sup>2</sup>; Apeksha Sahu<sup>2</sup>; Soujanya D. Yelamanchi<sup>2</sup>; Savita Jayaram<sup>2</sup>; Pavithra Rajagopalan<sup>2</sup>; Jyoti Sharma<sup>2</sup>; Krishna R. Murthy<sup>2</sup>; Aafaque A. Khan<sup>2</sup>; Sartaj Ahmed<sup>2</sup>; Nazia Syed<sup>2</sup>; Gourav Dey<sup>2</sup>; Aditi Chatterjee<sup>2</sup>; Tai-Chung Huang<sup>1</sup>; Jun Zhong<sup>4</sup>; Xinyan Wu<sup>1</sup>; Patrick G. Shaw<sup>4</sup>; Muhammad S. Zahari<sup>1</sup>; Henry Lam<sup>5</sup>; Christopher J. Mitchell<sup>1</sup>; John T. Schroeder<sup>1</sup>; Ravi Sirdeshmukh<sup>2</sup>; Anirban Maitra<sup>1</sup>; Steven D. Leach<sup>1</sup>; Charles G. Drake<sup>1</sup>; Marc K. Halushka<sup>1</sup>; T. S. Keshava Prasad<sup>2</sup>; Ralph H. Hruban<sup>1</sup>; Candace L. Kerr<sup>6</sup>; Gary D. Bader<sup>3</sup>; Christine A. Iacobuzio-Donahue<sup>1</sup>; Harsha Gowda<sup>2</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Johns Hopkins University SOM, Baltimore, MD; <sup>2</sup>Institute of Bioinformatics, Bangalore, India; <sup>3</sup>The Donnelly Centre, University of Toronto, Toronto, Canada; <sup>4</sup>Johns Hopkins University, Baltimore, MD; <sup>5</sup>The Hong Kong University of Science and Technology, Clear Water Bay, Hongkong; <sup>6</sup>University of Maryland, Baltimore, Maryland
- MP 256 **Integrative Omics Analysis Reveals Distinct Gene and Protein Expression Signatures across Multiple Tissues in an Individual**; Srikanth S. Manda<sup>1,3</sup>; Min-Sik Kim<sup>2</sup>; Raja Sekhar Nirujogi<sup>1,3</sup>; Premendu P. Mathur<sup>3</sup>; Harsha Gowda<sup>1</sup>; Akhilesh Pandey<sup>1,2</sup>; <sup>1</sup>Institute of Bioinformatics, Bangalore, India; <sup>2</sup>Johns Hopkins University SOM, Baltimore, MD; <sup>3</sup>Center for Bioinformatics, Pondicherry University, Puducherry, India
- MP 257 **High-Coverage High-Throughput Characterization of Breast Cancer Cell Lines through the Use of Synchronous Precursor Selection MS3-based 10-plexed Quantitative Proteomics**; John Lapek<sup>1</sup>; Jessica Biosvert<sup>1</sup>; Cyril Benes<sup>1,2</sup>; Wilhelm Haas<sup>1,2</sup>; <sup>1</sup>MGH Cancer Center, Charlestown, MA; <sup>2</sup>Harvard Medical School, Charlestown, MA
- MP 258 **Construction of a Physical Map of a Human Cell**; Anne-Claude Gingras<sup>1</sup>; Christopher Go<sup>1</sup>; Wade H Dunham<sup>1</sup>; James DR Knight<sup>1</sup>; Étienne Coyaud<sup>2</sup>; Geoffrey Hesketh<sup>1</sup>; Jean-Philippe Lambert<sup>1</sup>; Payman Samavarchi-Tehrani<sup>1</sup>; Amber L. Couzens<sup>1</sup>; Andy Kong<sup>3</sup>; Laurence Pelletier<sup>1</sup>; Hyungwon Choi<sup>4</sup>; Alexey Nesvizhskii<sup>3</sup>; Brian Raught<sup>2</sup>;

- <sup>1</sup>Lunenfeld-Tanenbaum Research Institute, Toronto, Canada; <sup>2</sup>Ontario Cancer Institute, Toronto, Canada; <sup>3</sup>University of Michigan, Ann Arbor, MI; <sup>4</sup>National University of Singapore, Singapore
- MP 259 **The Nuclear Proteome of a Vertebrate; Martin Wuehr**; Thomas Guettler; Leonid Peshkin; Graeme C. McAlister; Aaron C. Groen; Timothy J. Mitchison; Marc W. Kirschner; Steven P. Gygi; *Harvard Medical School, Boston, MA*
- MP 260 **Protein Quantitative Trait Locus (pQTL) Analysis in a Mouse Genetic Reference Population using Targeted Mass Spectrometry Methods; Yibo Wu**<sup>1</sup>; Evan Williams<sup>2</sup>; Sander Houten<sup>3</sup>; Carmen Argmann<sup>3</sup>; Witold Wolski<sup>1</sup>; Johan Auwerx<sup>2</sup>; Ruedi Aebersold<sup>1, 4</sup>; <sup>1</sup>IMSB, Zurich, Switzerland; <sup>2</sup>EPFL, Lausanne, Switzerland; <sup>3</sup>University of Amsterdam, Amsterdam, Netherland; <sup>4</sup>University of Zurich, Zurich, Switzerland
- MP 261 **A Systems Approach to the Characterization of Toll-Like Receptor Response to Different Ligand Stimulation in Macrophages; Virginie Sjoelund**; Arthur Nuccio; Zachary Benet; Jessica Mann; Marijke Koppenol-Raab; Alisa Bochnowski; Nathan Manes; Bhaskar Dutta; Iain Fraser; Aleksandra Nita-Lazar; *NIH/NIAID/LSB, Bethesda, MD*
- MP 262 **Dynamic Analysis of Pure HIV-1 Infected and Bystander Monocyte Derived Macrophages (MDMs); Isabel Martinez Ferrando**<sup>1</sup>; Alexandre Deshiere<sup>2</sup>; Alexey Lyashkov<sup>1</sup>; Ceereena Mohien<sup>1</sup>; David Colquhoun<sup>1</sup>; Michel Ouellet<sup>2</sup>; Michel Tremblay<sup>2</sup>; David R. Graham<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>Laval University, Quebec city, Quebec
- MP 263 **Advanced Ti4+-IMAC (Phospho)proteomics to Identify Novel Melanoma Companion Drug Targets and Uncover Phosphorylation Dynamics and Pathway Dependence in Senescence Signaling; Erik L. de Graaf**<sup>1</sup>; Gianluca Maddalo<sup>1</sup>; Joanna Kaplon<sup>2</sup>; Marjon A. Smit<sup>2</sup>; Daniel S. Peeper<sup>2</sup>; Albert J.R. Heck<sup>1</sup>; A.F. Maarten Altelaar<sup>1</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>The Netherlands Cancer Institute, Amsterdam, The Netherlands
- MP 264 **Enhanced Informatics Methods for Enriching Protein Identifications in the Metaproteome Characterization of the Human Gut Microbiome; Robert Hettich**<sup>1</sup>; Alison Erickson<sup>1</sup>; J Chai<sup>1</sup>; Chongle Pan<sup>2</sup>; Rachel Adams<sup>1</sup>; Brandi Cantarel<sup>3</sup>; Claire Fraser-Liggett<sup>3</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>3</sup>University of Maryland, Baltimore, MD
- MP 265 **A Data Independent Strategy for a Multi-omic Approach to Investigate Obesity Treatment within a Mouse Model; Gertjan Kramer**<sup>1</sup>; Nicholas Dekker<sup>1</sup>; Lee A Gethings<sup>2</sup>; Victoria Lee<sup>3</sup>; Robert J Beynon<sup>3</sup>; James I Langridge<sup>2</sup>; Johannes P.C. Vissers<sup>2</sup>; Johannes M.F.G. Aerts<sup>1</sup>; <sup>1</sup>Academic Medical Centre, University of Amsterdam, Amsterdam, Netherlands; <sup>2</sup>Waters, Manchester, UK; <sup>3</sup>University of Liverpool, Liverpool, UK
- MP 266 **Hypothesis Driven Approach to Integrated Lipidomic and Proteomic Data Analysis; Gogce Crynen**<sup>1,2</sup>; Laila Abdullah<sup>1,2</sup>; Jon Reed<sup>1,2</sup>; James Evans<sup>1</sup>; Hannah Montague<sup>1</sup>; Ariel Hart<sup>1</sup>; Ariel Gonzalez<sup>1</sup>; Madison Crocker<sup>1</sup>; Tanja Emmerich<sup>1</sup>; Robert Pelot<sup>1</sup>; Michael Mullan<sup>1</sup>; Fiona Crawford<sup>1,2</sup>; <sup>1</sup>Roskamp Institute, Sarasota, Florida; <sup>2</sup>SRQ Bio, Sarasota, Florida
- MP 267 **Comprehensive Analysis of Alterations in Lipid and Bile Acid Metabolism by Carbon Tetrachloride using Integrated Transcriptomics and Metabolomics; Jinchun Sun**<sup>1</sup>; Thomas Schmitt<sup>1</sup>; Laura Schnackenberg<sup>1</sup>; Lisa Pence<sup>1</sup>; Yosuke Ando<sup>1,2</sup>; James Greenhaw<sup>1</sup>; Xi Yang<sup>1</sup>; Svetoslav Slavov<sup>1</sup>; William Salminen<sup>1,3</sup>; Donna Mendrick<sup>1</sup>; Richard Beger<sup>1</sup>; <sup>1</sup>NCTR / USFDA, Jefferson, AR; <sup>2</sup>Daiichi Sankyo Co., Ltd, Tokyo, Japan; <sup>3</sup>PAREXEL International, Boston, MA
- MP 268 **LC-MS Chemoplexing for the Direct Measurement of Apparent Catalytic Efficiency of Enzyme Systems; Richard King**<sup>1</sup>; Bonnie Baker<sup>1</sup>; Victoria King<sup>2</sup>; Carmen Fernandez-Metzler<sup>1</sup>; <sup>1</sup>PharmaCadence Analytical Services, LLC, Hatfield, PA; <sup>2</sup>Northeastern University, Boston, MA
- MP 269 **Chemokine and Sphingosine-1-Phosphate Signaling in RAW 264.7 Cells Quantitated using Targeted Proteomics and Simulated using Simmune; Nathan Manes**<sup>1</sup>; Marijke Koppenol-Raab<sup>1</sup>; Eunkyung An<sup>1</sup>; Virginie Sjoelund<sup>1</sup>; Jing Sun<sup>1</sup>; Bastian Angermann<sup>1</sup>; Masaru Ishii<sup>2</sup>; Martin Meier-Schellersheim<sup>1</sup>; Ronald Germain<sup>1</sup>; Aleksandra Nita-Lazar<sup>1</sup>; <sup>1</sup>National Institutes of Health, Bethesda, MD; <sup>2</sup>Osaka University, Osaka, Japan
- MP 270 **Integrated Transcriptomic and Proteomic Analysis of an Indian Malaria Vector –Anopheles stephensi; Sreelakshmi Sreenivasamurthy**<sup>1,2</sup>; Ajeet Kumar Mohanty<sup>3</sup>; Manish Kumar<sup>1,2</sup>; Gourav Dey<sup>1,2</sup>; Sneha Pinto<sup>1,4</sup>; Raja Sekhar Nirujogi<sup>1,4</sup>; Anil Madugundu<sup>1</sup>; Arun Patil<sup>1</sup>; Jayshree Advani<sup>1</sup>; Sutopa Dwivedi<sup>1</sup>; Manoj Kumar Gupta<sup>1,2</sup>; Dhanashree Kelkar<sup>1</sup>; Chris Mitchell<sup>4</sup>; Charles Wang<sup>5</sup>; Harsha Gowda<sup>1</sup>; T. S. Keshava Prasad<sup>1</sup>; Zhijian Tu<sup>6</sup>; Ashwani Kumar<sup>3</sup>; Akhilesh Pandey<sup>4</sup>; <sup>1</sup>Institute of Bioinformatics, Bangalore, India; <sup>2</sup>Manipal University, Manipal, India; <sup>3</sup>National Institute of Malaria Research, Goa, India; <sup>4</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>5</sup>School of Medicine, Loma Linda University, Loma Linda, CA; <sup>6</sup>Department of Biochemistry, Virginia Tech, Blacksburg, VA
- MP 271 **Dysregulation of Nitric Oxide Metabolism in Host Erythrocytes Following Plasmodium falciparum Infection; Simon A. Cobbold**<sup>1</sup>; David H. Perlman<sup>2</sup>; Manuel Llinás<sup>3</sup>; Kiaran Kirk<sup>4</sup>; <sup>1</sup>Bio21 Institute, University of Melbourne, Melbourne, Australia; <sup>2</sup>Princeton University, Princeton, NJ; <sup>3</sup>The Pennsylvania State University, University Park, PA; <sup>4</sup>The Australian National University, Acton, Australia
- MP 272 **Absolute Quantification of Over 1000 Yeast Proteins Provides Insights into Translational Control; Stephen W. Holman**<sup>1</sup>; Craig Lawless<sup>2</sup>; Philip Brownridge<sup>1</sup>; Karin Lanthaler<sup>2</sup>; Victoria M. Harman<sup>1</sup>; Dean E. Hammond<sup>1</sup>; Rebecca L. Miller<sup>1</sup>; Rachel H. Watkins<sup>2</sup>; Paul F. G. Sims<sup>2</sup>; Christopher M. Grant<sup>2</sup>; Claire E. Evers<sup>1</sup>; Robert J. Beynon<sup>1</sup>; Simon J. Hubbard<sup>2</sup>; <sup>1</sup>The University of Liverpool, Liverpool, UK; <sup>2</sup>The University of Manchester, Manchester, UK
- MP 273 **Proteomic Analysis of Environmental Stress in Oysters; Paul Haynes**<sup>1</sup>; Emma Thompson<sup>2</sup>; Sridevi Muralidharan<sup>1</sup>; Wayne O'Connor<sup>3</sup>; David Raftos<sup>2</sup>; <sup>1</sup>Department of Chemistry and Biomolecular Sciences, Macquarie University, Sydney, NSW Australia; <sup>2</sup>Department of Biological Sciences, Macquarie University, NSW Australia; <sup>3</sup>NSW Department of Primary Industries, Taylors Beach, NSW Australia
- MP 274 **An Integrated Metabolomics and Proteomics Approach to Understand Chemically Mediated Diatom Competition; Christina M. Jones**<sup>1</sup>; Kelsey L. Poulson-Ellestad<sup>1</sup>; Brook L. Nunn<sup>2</sup>; Jessie Roy<sup>1</sup>; Facundo M. Fernández<sup>1</sup>; Julia Kubanek<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>University of Washington, Seattle, WA
- MP 275 **Multiple Nutrient Stresses at Intersecting Pacific Ocean Biomes Detected by Protein Biomarkers; Mak Saito**<sup>1</sup>; Matthew McIlvin<sup>1</sup>; Dawn Moran<sup>1</sup>; Tyler Goepfert<sup>1</sup>; Giacomo DiTillio<sup>2</sup>; Carl Lamborg<sup>1</sup>; <sup>1</sup>Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; <sup>2</sup>College of Charleston, Charleston, SC
- MP 276 **Integrated Omics Analysis of the Interaction Between Ignicoccus hospitalis and Nanoarchaeum equitans; Timothy Hamerly**<sup>1</sup>; Brian P. Tripet<sup>1</sup>; Richard Giannone<sup>2</sup>; Robert Hettich<sup>2</sup>; Mircea Podar<sup>2</sup>; Valerie Copie<sup>1</sup>; Brian

- Bothner<sup>1</sup>; <sup>1</sup>Montana State University, Bozeman, MT; <sup>2</sup>Oak Ridge National Laboratory, Oak Ridge, TN
- MP 277 **Characterization of the Core and Unique Proteome of *Anaeromyxobacter dehalogenans* 2CP-C Grown With Various Electron Acceptors;** Xiaoxin Liu<sup>1,2</sup>; Silke Nissen<sup>1,2</sup>; Karuna Chourey<sup>1</sup>; Frank Löffler<sup>1,2</sup>; Robert Hettich<sup>1,2</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>The University of Tennessee, Knoxville, TN
- MP 278 **Targeted Proteogenomic Characterization of the *Shewanella oneidensis* MR-1 Extracellular Proteome;** William Judson Hervey IV<sup>1</sup>; Erinn C. Howard<sup>2</sup>; Emily R. Peterson<sup>3</sup>; Dagmar Hajkova Leary<sup>1</sup>; Anthony P. Malanoski<sup>1</sup>; Jinny L. Liu<sup>1</sup>; Justin C. Biffinger<sup>1</sup>; Sarah M. Glaven<sup>1</sup>; Baochuan Lin<sup>1</sup>; Lisa A. Fitzgerald<sup>1</sup>; Gary J. Vora<sup>1</sup>; Bradley R. Ringeisen<sup>1</sup>; <sup>1</sup>Naval Research Laboratory, Washington, DC; <sup>2</sup>West Virginia Wesleyan College, Buckhannon, WV; <sup>3</sup>Nova Research, Inc., Alexandria, VA
- MP 279 **Metaproteomic Analysis of an Electricity Consuming Biocathode Biofilm;** Dagmar Hajkova Leary<sup>1</sup>; Anthony Malanoski<sup>1</sup>; William Judson Hervey, IV.<sup>1</sup>; Zheng Wang<sup>1</sup>; Brian Eddie<sup>2</sup>; Gary Vora<sup>1</sup>; Leonard Tender<sup>1</sup>; Baochuan Lin<sup>1</sup>; Sarah Glaven<sup>1</sup>; <sup>1</sup>Naval Research Laboratory, Washington, DC; <sup>2</sup>National Research Council, Washington, DC
- Toxicology: Therapeutic Drug Monitoring / Drugs of Abuse, 280 - 294**
- MP 280 **Verification of an LC-MS/MS Method for 19 Opioids, Opiates, and Their Metabolites in Human Urine without Hydrolysis;** Sarah Fair-Wandland; Kerry Hassell; Joseph L. Herman; ThermoFisher Scientific, Franklin, MA
- MP 281 **Analysis of Pain Panel Medications in Urine on Raptor™ Biphenyl by LC-MS/MS;** Sharon Lupo; Frances Carroll; Paul Connolly; Ty Kahler; Restek, Bellefonte, PA
- MP 282 **Comparison of LDTD with Traditional LCMS for Quantitative Screening of Urine Drugs of Abuse using Benchtop Quadrupole Orbitrap Mass Spectrometer;** Kristine Van Natta; Marta Kozak; Thermo Fisher Scientific, San Jose, CA
- MP 283 **Evaluation of Sample Preparation Methods for Semi-Quantitative Ultra-High Throughput Urine Screening using LDTD HR/AM MS technique;** Marta Kozak; Kristine Van Natta; Thermo Fisher Scientific, San Jose, CA
- MP 284 **Ultra Fast Analysis of 13 Benzodiazepines by LDTD-MS/MS Cross Validated with LC-MS/MS for 200 Real Urine Samples;** Alex Birsan; Serge Auger; Annick Dion; Pierre Picard; Jean Lacoursiere; Phytronix Technologies Inc., Quebec, QC
- MP 285 **Evaluation of a Novel High-Throughput Screening Method for Drugs of Abuse in Urine with Paper-Spray Triple Quadrupole Mass Spectrometry;** Bradley Hart<sup>1</sup>; Maria C. Prieto Conaway<sup>1</sup>; Kristine van Natta<sup>1</sup>; Nicholas E. Manicke<sup>2</sup>; Marta Kozak<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Dept of Chemistry, Indiana Univ-Purdue Univ, Indianapolis, IN
- MP 286 **Rapid LC-MS/MS Analysis of Opiates and Benzodiazepines in Urine using a Partially Porous C-18 Stationary Phase;** J. Fred Banks; Ammon Analytical Laboratory, Linden, NJ
- MP 287 **Challenges and Solutions for High Throughput TFC-LC-MS/MS in Clinical Toxicology;** Yvonne Wright; Christopher Shuford; Matthew Crawford; Patricia Holland; Stacy Dee; Martin Green; Russell Grant; LabCorp, Burlington, NC
- MP 288 **Development of a New Toxicological Drug Screening Method for More than 800 Compounds in Biological Matrices using a UPLC-QToF MS;** Gilles Provencher; Nicolas Caron; Michel Lefebvre; Normand Fleury; INSPQ, Quebec, Canada
- MP 289 **Applying Enhanced Confirmation Criteria for Reducing False Positive Rates (FPR) in Toxicology Screening using High Resolution, LC-QToF, Accurate Mass Analysis;** Petra Decker<sup>1</sup>; Karin Wendt<sup>1</sup>; Carsten Baessmann<sup>1</sup>; Christian Albers<sup>1</sup>; Tony Drury<sup>2</sup>; Laura Huppertz<sup>3</sup>; Juergen Kempf<sup>3</sup>; Volker Auwaerter<sup>3</sup>; Anna Pelander<sup>4</sup>; Mira Sundström<sup>4</sup>; Ilkka Ojanperä<sup>4</sup>; Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker UK Ltd., Coventry, UK; <sup>3</sup>University Medical Center, Forensic Toxicology, Freiburg, Germany; <sup>4</sup>Hjelt-Institute, University of Helsinki, Helsinki, Finland
- MP 290 **Quantitation of Pain Management Drugs using Ultra-Fast Liquid Chromatography/Mass Spectrometry in Human Plasma Utilizing Positive/Negative Polarity Switching;** Steven R. McGown<sup>1</sup>; Robert D. English<sup>1</sup>; Chris Denicola<sup>2</sup>; Nataliya Bulayeva<sup>3</sup>; Rob Freeman<sup>2</sup>; Kevin Rosenblatt<sup>3</sup>; Ben Figard<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Houston, TX; <sup>2</sup>Restek Corporation, Bellefonte, PA; <sup>3</sup>UT-Health Science Center, Houston, TX
- MP 291 **Increased Throughput for the Analysis of delta-9-THC in Oral Fluids using Triple Quadrupole Mass Spectrometry coupled to Automated Dual-Channel HPLC;** Kevin McCann; Andre Szczesniewski; Agilent Technologies, Santa Clara, CA
- MP 292 **Comprehensive Screening for Drugs of Abuse in Urine by LC-MSn Combined with MS Spectral Library Matching;** Zoltan Czentnar<sup>2</sup>; Andrea Kiehne<sup>2</sup>; Markus Meyer<sup>2</sup>; Michael D. Timmons<sup>1</sup>; <sup>1</sup>Bruker Daltonics Inc., Billerica, MA; <sup>2</sup>Bruker Daltonik GmbH, Bremen, DE
- MP 293 **A Workflow-driven High-throughput Screening Method for Synthetic Cannabinoids and Metabolites in Urine with Q-TOF Mass Spectrometer and Multiplexed LCs;** Xiang He; Zhaoxiang (Sean) Wu; Jenny Moshin; Alexandre Wang; AB SCIEX, Redwood City, CA
- MP 294 **Quantification of Illicit Drugs in Urine for Confirmatory Analysis in Routine Laboratories using Ion Trap LC-MS<sup>n</sup>;** Julian Philips; Markus Peer; Birgit Schneider; Bruker Daltonik, Bremen, Germany
- Ionization Mechanisms, 295 - 316**
- MP 295 **Nitrilium Cations in the Spectra of N-Methyl-N-Perfluoroacyl- Amino Acids and Their Alkyl Esters;** Nino G. Todua; Kirill V. Tretyakov; Anzor I. Mikaia; National Institute of Standards and Technology, Gaithersburg, MD
- MP 296 **Ionization Mechanism in Radio-Frequency Ionization (RFI);** Abayomi D. Olaitan; Behrooz Zekavat; Touradj Solouki; Baylor University, Waco, TX
- MP 297 **Detection of Light vs. Heavy Atoms with a Laser Induced Plasma Ionization Source for Single Particle Analysis;** Andrew Horan; Murray Johnston; University of Delaware, Newark, DE
- MP 298 **Ion Chemistry in the APPI Source Studied by Ion-Molecule Reactions in Q2 of a Triple Quadrupole Mass Spectrometer;** Annie van Dam; Andries P. Bruins; University of Groningen, Groningen, Netherlands
- MP 299 **Ionization of Gaseous Compounds in Direct and Dopant-Assisted Atmospheric Pressure Photoionization;** Tiina J Kauppila<sup>1</sup>; Hendrik Kersten<sup>2</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>University of Helsinki, Helsinki, N/A; <sup>2</sup>University of Wuppertal, Wuppertal, Germany
- MP 300 **Mechanistic Understanding on Why a Number of Compounds with High Gas Phase Basicity Produce Mostly Molecular Ions by (+) APPI-MS;** Arif Ahmed<sup>1</sup>; Cheol Ho Choi<sup>1,2</sup>; Younghwan Kim<sup>3</sup>; Sunghwan Kim<sup>1,2</sup>; <sup>1</sup>Kyungpook National University, Daegu, South Korea; <sup>2</sup>Green-Nano Materials Research Center, Daegu, South Korea; <sup>3</sup>Korea Basic Science Institute, Daejeon, South Korea

- MP 301 **Ionization from Freezing Water: Why it Should be Expected;** Charles N. McEwen<sup>2</sup>; Beixi Wang<sup>1</sup>; Vincent Pagnotti<sup>2</sup>; Shubhashis Chakrabarty<sup>2</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>University of the Sciences, Philadelphia, PA
- MP 302 **Experimental and Theoretical Investigations of Positron Ionization Mass Spectrometry with Biological Molecules;** Panagiotis Papoulias<sup>1</sup>; Indika Wanniarachchi<sup>1</sup>; Caroline Morgan<sup>1</sup>; Alan Sebastian<sup>1</sup>; Larry Burggraf<sup>2</sup>; Rod Greaves<sup>3</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>Air Force Institute of Technology, Dayton, OH; <sup>3</sup>First Point Scientific, Inc., Agoura Hills, CA
- MP 303 **Ion-Velocity Distribution of MALDI Ions Measured in an Internal Source Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry;** Vladimir Frankevich<sup>1</sup>; Vitaliy Chagovets<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich, Zurich, Switzerland; <sup>2</sup>University of Pardubice, Pardubice, Czech Republic
- MP 304 **Large Biomolecule Clusters Detection using MALDI Ion Trap Mass Spectrometer with Charge Detector;** Yung-Kun Chuang; Szu-Hsueh Lai; Jung-Lee Lin; Chung-Hsuan Chen; Academia Sinica, Taipei, Taiwan
- MP 305 **Ion-to-Neutral Ratios and Thermal Proton Transfer Reactions in Matrix-Assisted Laser Desorption/Ionization;** I-Chung Lu<sup>1</sup>; Kuan Yu Chu<sup>1,2</sup>; Chih-Yuan Lin<sup>1</sup>; Yuri A. Dyakov<sup>1</sup>; Hsu Chen Hsu<sup>1</sup>; Yuan-Tseh Lee<sup>1,2</sup>; Chi-Kung Ni<sup>1,3</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan; <sup>2</sup>National Taiwan University, Taipei, Taiwan; <sup>3</sup>National Tsinghua University, Hsinchu, Taiwan
- MP 306 **Ion Intensity and Thermal Proton Transfer Reactions in Matrix-Assisted Laser Desorption/Ionization;** Chuping Lee<sup>1,3</sup>; I-Chung Lu<sup>1</sup>; Hui-Yuan Chen<sup>1</sup>; Hou-Yu Lin<sup>1,3</sup>; Sheng-Wei Hung<sup>1</sup>; Yuri Dyakov<sup>1</sup>; Kuo-Tung Hsu<sup>2</sup>; Chih-Yu Liao<sup>2</sup>; Yin-Yu Lee<sup>2</sup>; Cheng-Ming Tseng<sup>5</sup>; Yuan Tseh Lee<sup>1,3</sup>; Chi-Kung Ni<sup>1,4</sup>; <sup>1</sup>Academia Sinica, Taipei, Taiwan; <sup>2</sup>National Synchrotron Radiation Research Center, Hsinchu, Taiwan; <sup>3</sup>National Taiwan University, Taipei, Taiwan; <sup>4</sup>National Tsing Hua University, Hsinchu, Taiwan; <sup>5</sup>National Chiao Tung University, Hsinchu, Taiwan
- MP 307 **Excited State Lifetime and Fluorescence Properties of UV-MALDI Matrices;** Hou-Yu Lin<sup>1</sup>; Botao Song<sup>1</sup>; I-Chung Lu<sup>1</sup>; Kuo-Tung Hsu<sup>2</sup>; Chih-Yu Liao<sup>2</sup>; Yin-Yu Lee<sup>2</sup>; Cheng-Ming Tseng<sup>3</sup>; Yuan-Tseh Lee<sup>1,4</sup>; Chi-Kung Ni<sup>1,5</sup>; <sup>1</sup>Institute of Atomic and Molecular Sciences, Academ, Taipei, Taiwan; <sup>2</sup>National Synchrotron Radiation Research Center, Hsinchu, Taiwan; <sup>3</sup>National Chiao Tung University, Hsinchu, Taiwan; <sup>4</sup>National Taiwan University, Taipei, Taiwan; <sup>5</sup>National Tsing Hua University, Hsinchu, Taiwan
- MP 308 **Relation of Excited State Lifetimes and Ion Yields for Common MALDI Matrices;** Kristopher Kirmess; Gary R. Kinsel; Southern Illinois University at Carbondale, Carbondale, Illinois
- MP 309 **Variation of Alkali Metal Ion Distribution with MALDI Sample Composition Investigated with Dual-Polarity Time-of-Flight Imaging Mass Spectrometer;** Yin-Hung Lai; Hsun Lee; Yi-Sheng Wang; Genomics Research Center, Academia Sinica, Taipei, Taiwan
- MP 310 **One Method Might Not be Enough – Investigating Ionization of Peptides and Their Modifications;** Wiebke Nadler<sup>1,3</sup>; Dietmar Waidelich<sup>4</sup>; Alexander Kerner<sup>1,3</sup>; Christoph Roesli<sup>1,2</sup>; <sup>1</sup>Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany; <sup>2</sup>Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany; <sup>3</sup>Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany; <sup>4</sup>AB SCIEX, Darmstadt, Germany
- MP 311 **In-Source Reactions of Catechol During Oxidative Positive Ion Electrospray Mass Spectrometric Analysis;** Luis Sojo; Xenon Pharmaceutical, Burnaby, Canada
- MP 312 **Protonation and Desolvation as Limiting Factors in the Linear Dynamic Range of Electrospray Ionization Mass Spectrometry;** Clint M. Alfaro; Agbo-Oma Uwakweh; Daniel A. Todd; Brandie M. Ehrmann; Nadja B. Cech; University of North Carolina at Greensboro, Greensboro, NC
- MP 313 **Predicting Concentrations of Small Molecules without Standard Substances in LC/API/MS via Ionization Efficiency Scales;** Anneli Kruve; Jaanus Liigand; Piia Burk; Karl Kaupmees; Riin Rebane; Ivo Leito; Koit Herodes; Merit Oss; University of Tartu, Tartu, Estonia
- MP 314 **Supercharging Reagents as Mobile Phase Additives in the LC-MS Analysis of Intact Proteins;** Michael Nshanian<sup>1</sup>; Rachel R. Ogorzalek Loo<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>UCLA, Department of Chemistry and Biochemistry, Los Angeles, CA; <sup>2</sup>UCLA, Department of Biological Chemistry, Los Angeles, CA
- MP 315 **Atmospheric Pressure Laser Ionization with a Novel Highly Sensitive Atmospheric Pressure Ionization Interface for Gas Chromatography-Mass Spectrometry;** Thorsten Benter<sup>1</sup>; Tiina J Kauppila<sup>2</sup>; Hendrik Kersten<sup>1</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany; <sup>2</sup>University of Helsinki, Helsinki, N/A
- MP 316 **A Model for the Supercharging of Proteins in the Positive and Negative Ion Modes Based on Gas-Phase Basicities;** Kevin Douglass; Andre Venter; Western Michigan University, Kalamazoo, MI

Ion Structure / Energetics, 319 - 329

- MP 319 **Gas-Phase Acidities of Amino Acid Amides;** Chelsea E. Plummer; Michele L. Stover; David A. Dixon; Carolyn J. Cassidy; The University of Alabama, Tuscaloosa, AL
- MP 320 **Understanding Conformational Effects on Proton Affinity of Peptides Containing Lysine and Its Unnatural Homologs;** Patrickhenry Batoon; Jianhua Ren; University of the Pacific, Stockton, CA
- MP 321 **Gas-phase Acidities of Nitrated Azole Species from the Extended Kinetic Method;** Charles Nichols<sup>1,2</sup>; W. Carl Lineberger<sup>1,2</sup>; Veronica M. Bierbaum<sup>1,2</sup>; <sup>1</sup>University of Colorado, Boulder, CO; <sup>2</sup>JILA, Boulder, CO
- MP 322 **Metal Ion/Peptide Binding at Nitrogen Sites: The Histidine Rule;** Robert C. Dunbar<sup>1</sup>; Giel Berden<sup>2</sup>; Jos Oomens<sup>2</sup>; <sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>Radboud University Nijmegen, Nijmegen, Netherlands
- MP 323 **Unimolecular Dissociation of Penicillamine Sulfinyl Radical Ions;** Chasity B. Love; Joseph S. Francisco; Yu Xia; Purdue University, Lafayette, IN
- MP 324 **Fragmentation Studies of Tetracene-dienophile Adducts by Different Ionization Methods and Time-of-Flight Mass Spectrometry;** Daryl Giblin<sup>2</sup>; Brittni A. Qualizza<sup>1</sup>; Jacob W. Ciszek<sup>1</sup>; M. Paul Chiarelli<sup>1</sup>; Michael L. Gross<sup>2</sup>; <sup>1</sup>Loyola University, Chicago, IL; <sup>2</sup>Washington University, St Louis, MO
- MP 325 **Investigation of an Unusual Rearrangement of Certain Protonated Anilide Analogs with Collision Induced Dissociation Mass Spectrometry;** Chengli Zu; Shijing Xia; Patrick Hanley; Bruce Bell; Dow Chemical Company, Midland, MI
- MP 326 **Investigation of the Fragmentation Processes of Amines by VisPD Experiments in an FT-ICR MS;** Claus Gernert; Sarah Seulen; Jurgen Grotemeyer; Christian-Albrechts-Univ, Kiel, Germany
- MP 327 **Influence of Heating Rate and Pyrolysis Temperature on the Internal Energy and Composition of Organic Aerosols;** Sandra Spencer; Gary L. Glish; University of North Carolina, Chapel Hill, NC

- MP 328 **Base-Pairing Energies of Proton-Bound Dimers of Cytosine and Methylated Cytosines: Implications for the Stability of DNA *i*-Motif Conformations;** Bo Yang<sup>1</sup>; Aaron Moehlig<sup>2</sup>; Thomas Morton<sup>2</sup>; M.T. Rodgers<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>University of California, Riverside, CA
- MP 329 **Probing Gold-Catalyzed Alkyne Hydration Reaction by Mass Spectrometry: Evidence for Dinuclear Gold Intermediates and Dual Activation of Substrates;** Mei Lu<sup>1</sup>; Yijin Su<sup>2</sup>; Xiaodong Shi<sup>2</sup>; Eric Masson<sup>1</sup>; Fengyao Li<sup>1</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Ohio University, Athens, OH; <sup>2</sup>West Virginia University, Morgantown, WV
- Geochemistry, 330 - 333**
- MP 330 **Thermal Ionization Time-of-Flight Mass Spectrometry as a Tool for Uranium Exploration;** Dongfa Guo<sup>1</sup>; Shengkai Xie<sup>1</sup>; Jinying Li<sup>2</sup>; Jing Tan<sup>1</sup>; Zengwei Fan<sup>1</sup>; Guifang Liu<sup>1</sup>; Chen Dong<sup>1</sup>; Jianyong Cui<sup>1</sup>; <sup>1</sup>Beijing Research Institute of Uranium Geology, Beijing, China; <sup>2</sup>China Institute of Atomic Energy, Beijing, China
- MP 331 **Gas-Phase Fragmentation of Metal Adducts of Alkali-Metal Carbonate Salts;** Robert Hale; Athula B. Attygalle; Carl Weisbecker; *Stevens Institute of Technology, Hoboken, NJ*
- MP 332 **LC-MS/MS for Quantitative Analysis of Geochemically Important Sterols in Sediments from Antarctica and Brazil;** Giovana Bataglion<sup>1</sup>; Eduardo Meurer<sup>1</sup>; Ana Cecília Rizatti<sup>2</sup>; Márcia Bicego<sup>2</sup>; Rolf Weber<sup>2</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>University of Campinas (Unicamp), Campinas, Brazil; <sup>2</sup>University of São Paulo (USP), São Paulo, Brazil
- MP 333 **Improved Resolution and Precision for High Quality Elemental Imaging of tissue Samples using Laser Ablation - ICP-MS;** René Chemnitzer<sup>1</sup>; Andrew Toms<sup>2</sup>; Meike Hamester<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Milton, Canada
- Isotope Ratio MS, 334 - 335**
- MP 334 **Ultratrace Determination of <sup>137</sup>Cs and <sup>137</sup>Cs/<sup>133</sup>Cs Isotope Ratios Measurements in Environmental Soil Samples byCRC-ICP-MS/MS;** Saeed H. Al-Meer; Mohamed A. Amr; Muneera T. Al-Qahtani; *Qatar University, Doha, QATAR*
- MP 335 **GC-Pyrolysis-GC Coupled to Combustion Isotope Ratio Mass Spectrometry for Position Specific Isotope Analysis;** Herbert Tobias; Joseph Ruesch; Tom Brenna; *Cornell University, Ithaca, NY*
- Food Safety, 336 - 359**
- MP 336 **The Analysis of Food and Calcium Supplements for Lead by ICP MS;** Marc E. Engel; *FDACS, Tallahassee, FL*
- MP 337 **Analysis of Addictive Alkaloids from Opium Poppy in Hot Pot by UHPLC Tandem Triple Quadrupole Mass Spectrometry;** Peibin Hu<sup>1</sup>; Chang Jiang<sup>1</sup>; Tao Bo<sup>2</sup>; <sup>1</sup>Agilent Technologies, Chengdu, China; <sup>2</sup>Agilent technologies, Beijing, China
- MP 338 **Advances in Screening Capability for the Detection of Residues and Contaminants in Complex Samples using Accessible Mass Detection;** Sara Stead<sup>2</sup>; Howard Read<sup>2</sup>; Kevin Cook<sup>1</sup>; Eimear McCall<sup>2</sup>; Veronica Lattanzio<sup>3</sup>; Dominic Roberts<sup>2</sup>; Jennifer Burgess<sup>1</sup>; Ramesh Rao<sup>2</sup>; Mark Benvenuti<sup>2</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>Waters corp, Manchester, UK; <sup>3</sup>Institute of Sciences of Food Production (ISPA), Bari, Italy
- MP 339 **Sensitive Quantification of Multi-Mycotoxin by LC-MS/MS;** Sha Joshua Ye; Changtong Hao; Hui Qiao; Lisa Cousins; *IONICS Mass Spectrometry Gro, Bolton, Canada*
- MP 340 **Analysis of Macrolides in Food by UPLC-MS/MS;** Pavel Metalnikov; Renat Selimov; Ilya Batov; Alexandre Komarov; Alexandre Panin; *VGNKI, Moscow, Russian Federation*
- MP 341 **Extraction of Acrylamide from Coffee and Potato Chips (Crisps) using Supported Liquid Extraction (SLE+) Prior to LC-MS/MS Analysis;** Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Geoff Davies<sup>1</sup>; Adam Senior<sup>1</sup>; Rhys Jones<sup>1</sup>; Helen Lodder<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, N/A; <sup>2</sup>Biotage LLC, Charlotte, NC
- MP 342 **High Sensitivity Analysis of Acrylamide in Potato Chips by LC/MS/MS with Modified QuEChERS Sample Pre-treatment Procedure;** Zhi Wei Ting<sup>1</sup>; Yin Ling Chew<sup>2</sup>; Jing Cheng Ng<sup>2</sup>; Jie Xing<sup>1</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; <sup>2</sup>Department of Chemistry, National University of Singapore, Singapore
- MP 343 **Detection of di-(2-ethylhexyl)phthalate (DEHP) Metabolites in Human Hair by Automated Online Solid Phase Exaction Coupled with LC-MS/MS;** Yan Zin Chang; *Taichung, Taiwan*
- MP 344 **Rapid and Simultaneously Screening and Quantitation of Mycotoxins in Different Matrix using High Resolution MSMS Instrument;** Michael Sulyok<sup>2</sup>; Detlev Schleuder<sup>1</sup>; Stephen Lock<sup>3</sup>; Jianru Stahl-Zeng<sup>1</sup>; <sup>1</sup>AB SCIEX, Darmstadt, Germany; <sup>2</sup>IFA Tulln, Department of Agrobiotechnology, Tulln, Austria; <sup>3</sup>AB SCIEX, Warrington, UK
- MP 345 **Highly Sensitive and Rapid Simultaneous Method for 32 Mycotoxins in Baby Food Samples by UHPLC-MS/MS using Fast Polarity Switching;** Stephane Moreau<sup>1</sup>; Mikael Levi<sup>2</sup>; <sup>1</sup>SHIMADZU Europe, Albert-Hahn Strasse 6-10, Duisburg, Germany; <sup>2</sup>SHIMADZU France, Bd Salvador Allende, Marne La Vallée, France
- MP 346 **Determination of N-nitrosamines in Elastomeric Feeding Bottle Teats using Liquid Chromatography-Atmospheric Pressure Chemical Ionization Tandem Mass Spectrometry with Dynamic MRM;** Shao-Zhen Wang<sup>1</sup>; Dai-Yong Huang<sup>2</sup>; Shan-An Chan<sup>3</sup>; <sup>1</sup>Agilent, Shanghai, China; <sup>2</sup>Agilent, Hong-Kong, China; <sup>3</sup>Agilent, Taipei, Taiwan
- MP 347 **GC-MS/MS Analysis of 2-Acetyl-1-pyrroline (2AP) in Rice Kernels;** Helene Hopfer<sup>1</sup>; Farman Jodari<sup>3</sup>; Philip Wylie<sup>2</sup>; Florence Zakharov<sup>1</sup>; Susan Ebeler<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Agilent Technologies, Little Falls, Delaware; <sup>3</sup>California Rice Research Foundation, Biggs, CA
- MP 348 **Simultaneous Detection of 21 Multi-Family Plant Growth Regulators in Fruits by High Performance Liquid Chromatography Coupled with Tandem Mass Spectrometry;** Dunming Xu<sup>1</sup>; Hehe Huang<sup>1</sup>; Yu Zhou<sup>1</sup>; Meiling Lu<sup>2</sup>; Shan Zhou<sup>2</sup>; <sup>1</sup>Xiamen Entry-Exit Bureau of Inspect. & Quarantine, Xiamen, China; <sup>2</sup>Agilent Technologies, Beijing, China
- MP 349 **Simultaneous Determination of 2- and 4-methylimidazoles in Beverages using a Fast Filter and Shoot Method;** Xiaoqian Wang; Greg France; Michael Telepchak; *UCT, Bristol, PA*
- MP 350 **Rapid Analysis of Sudan and Other Prohibited Dyes in Chilli Powder using Ultra Performance Liquid Chromatography and Tandem Mass Spectrometry;** Dimple Shah; Evelyn Goh; Thomas C. Beaty; *Waters Corporation, Milford, MA*
- MP 351 **Highly Sensitive and Robust LC/MS/MS Method for Quantitative Analysis of Six Artificial Sweeteners in Beverages and Foods;** Jie Xing<sup>1</sup>; Zhi Wei Ting<sup>1</sup>; Yin Ling Chew<sup>2</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; <sup>2</sup>Department of Chemistry, Faculty of Science, National University of Singapore, Singapore

- MP 352 **Detection and Quantification of  $\beta$ -N-methylamino-L-alanine in Food Mussels using Dansyl Chloride Chemical Derivatization and Tandem Mass Spectrometry;** [Matilda Lampinen Salomonsson](#)<sup>1</sup>; Elisabeth Fredriksson<sup>1</sup>; Annelie Hansson<sup>2</sup>; Ulf Bondesson<sup>1</sup>; <sup>1</sup>The National Veterinary Institute (SVA), Uppsala, Sweden; <sup>2</sup>Uppsala University, Uppsala, Sweden
- MP 353 **Quantitative Analysis of Algal Toxins in Shellfish and Algae by Isotope Dilution LC-MS/MS using Differential Isotope Labeling Derivatization;** [Daniel Beach](#); Michael Quilliam; National Research Council Canada, Halifax, Canada
- MP 354 **Development of a Quantitative LC-MS/MS Method for Regulating Diarrhetic Shellfish Toxins in the United States;** [Whitney L. Stutts](#); Sara C. McGrath; Stephen M. Conrad; Jonathan R. Deeds; FDA/CFR, College Park, MD
- MP 355 **Rapid Direct Detection of the Major Fish Allergen by Selected MS/MS Ion Monitoring Mass Spectrometry;** [Monica Carrera](#)<sup>1</sup>; Benito Cañas<sup>2</sup>; Lorena Barros<sup>1</sup>; Jose Manuel Gallardo<sup>1</sup>; <sup>1</sup>Spanish National Research Council (CSIC), Vigo, Spain; <sup>2</sup>Complutense University, Madrid, Spain
- MP 356 **Chemometric Identification of Non-Altered Protein Sequences in Processed Food and Their Application for Relative Quantitation using Triple Quadrupole LC/MS;** Martin Roeder<sup>2</sup>; Nick Gundermann<sup>2</sup>; Wolfgang Weber<sup>2</sup>; Joachim Thiemann<sup>1</sup>; [Thomas Glauner](#)<sup>1</sup>; <sup>1</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>2</sup>IFP Institut fuer Produktqualitaet, Berlin, Germany
- MP 357 **Identification of Diethyl Phthalate in Waste Cooking Oil on a Portable Rectilinear Ion Trap Mass Spectrometer;** [Eric Handberg](#)<sup>1</sup>; Jie Jiang<sup>2</sup>; Jing Gao<sup>2</sup>; Guo Xiaotun<sup>1</sup>; Wenge Qu<sup>2</sup>; Dongdong Zhang<sup>2</sup>; Shunsheng Zhang<sup>1</sup>; Tao Chen<sup>1</sup>; Yongqi Sang<sup>1</sup>; Xiaofeng Dong<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>East China Institute of Technology, Nanchang, China; <sup>2</sup>Harbin Institute of Technology at Weihai, Weihai, China; <sup>3</sup>Wego, Weihai, China
- MP 358 **A Sensitive and Accurate LC/MS/MS Approach for Detection of Porcine Biomarkers in Halal Food Commodities;** [Wan Noor Faradalila Wan Jamaluddin](#)<sup>1</sup>; Venkatesha Gaddemane<sup>2</sup>; Fanny Widjaja<sup>2</sup>; Chee Sian Gan<sup>2</sup>; Dzulkifly Mat Hashim<sup>1</sup>; <sup>1</sup>Universiti Putra Malaysia, Serdang, Malaysia; <sup>2</sup>Agilent Technologies, Singapore, Singapore
- MP 359 **LC-DMS-MS/MS Detection of MCPD Esters in Edible Oils;** [Shaun Macmahon](#); Timothy Begley; FDA Center for Food Safety, College Park, MD
- Component Source Determination for Drugs Pharmaceutical, and Homeland Security Applications, 360 - 365**
- MP 360 **Determination of Fentanyl in Human Plasma by LC-MS/MS and Pharmacokinetic Study in Healthy Korean Male Volunteers;** [Young-Rim Jung](#)<sup>1</sup>; Ji-Young Lee<sup>2</sup>; Mi-Young Kim<sup>2</sup>; Hye-Seoung Shin<sup>2</sup>; <sup>1</sup>Gyeonggi Science High School for the Gifted, Suwon, South Korea; <sup>2</sup>Seoul Pharma Laboratories, CrystalGenomics Inc., Seoul, South Korea
- MP 361 **Screening of Adulterated Heparin by Simplified Peroxide Digestion and RPIP-LC-MS;** [Hongli Li](#)<sup>1</sup>; Peter Nemes<sup>1,2</sup>; <sup>1</sup>US Food and Drug Administration, Silver Spring, Maryland; <sup>2</sup>George Washington University, Washington, DC
- MP 362 **Evaluation of Allergenic Preservatives in Cosmetics using Mass Spectrometry;** [Soraya El Khatib](#); Rosana M. Alberici; Renan S. Galaverna; Marcos N. Eberlin; *Unicamp, Campinas, Brasil*
- MP 363 **Analysis of Potential Genotoxic Impurities in the Drug Development Process using GC-MS/MS;** Christine (Chunang) Gu<sup>1</sup>; [Helen \(Qingyu\) Sun](#)<sup>2</sup>; Kefei Wang<sup>2</sup>; <sup>1</sup>Genentech, South San Francisco, CA; <sup>2</sup>Bruker Daltonics, Fremont, CA
- MP 364 **High-Throughput Sample Preparation and Liquid Chromatography/Tandem Mass Spectrometry Method for Quantitation of Sulfur Mustard (HD) Metabolites in Human Urine;** [KesavaReddy Muntha](#)<sup>1</sup>; Christopher Nixon<sup>1</sup>; Shane Wyatt<sup>1</sup>; Timothy Croley<sup>2</sup>; <sup>1</sup>DCLS, Commonwealth of Virginia, Richmond, US; <sup>2</sup>Food and Drug Administration Center, College Park, MD, US
- MP 365 **Enabling Direct Sample Analysis of Sorbent-based Microextraction fibers with DART-MS for Rapid Generation of Unique Chemical Attribute Signature Results;** [Brian D. Musselman](#); Joseph Lapointe; Robert Goguen; *IonSense, Inc., Saugus, MA*
- Accelerator Mass Spectrometry, 366**
- MP 366 **Use of Accelerated Mass Spectrometry (AMS) to Characterize Placental Transfer of Therapeutic Proteins;** [Jian Wang](#)<sup>1</sup>; Lifei Wang<sup>1</sup>; Eliza Fung<sup>1</sup>; Jiachang Gong<sup>1</sup>; Brad Maxwell<sup>1</sup>; Mark Arnold<sup>1</sup>; MaryEllen Mc Nerney<sup>2</sup>; Anne Aubry<sup>1</sup>; Lakshmi Sivaraman<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Bristol-Myers Squibb, New Brunswick, NJ
- Biomimetic / Catalytic Systems, 367**
- MP 367 **ESI-MS Investigation of Reaction Intermediates and Catalytic Cycle of a Ligand-Free Heck-Matsuda Arylation Reaction;** [Alexandre F. Gomes](#); Francisco de Azambuja; Carlos R. D. Correia; Fabio C. Gozzo; *Institute of Chemistry - University of Campinas, Campinas, SP, Brazil*
- History of Mass Spectrometry, 368**
- MP 368 **History of Mass Spectrometry Mapped by Bibliometric Methods;** [Cathelijn Waaijer](#)<sup>1</sup>; Magnus Palmblad<sup>2</sup>; <sup>1</sup>Centre for Science and Technology Studies, Leiden, Netherlands; <sup>2</sup>Leiden University Medical Center, Leiden, Netherlands
- Ambient Ionization: Instrumentation, 375 - 404**
- MP 375 **Evaluation of Fieldable Gas Sources for DART Mass Spectrometry;** [William A. Harris](#); Yvette R. Hudson; Johnny K. Ho; Douglas B. Henderson; Danielle N. Dickinson; *Northrop Grumman, Linthicum Heights, MD*
- MP 376 **Targeted Analysis of Single Micro-Droplets using Extractive Electrospray Ionization with Tandem Mass Spectrometry;** [Christopher D. Chouinard](#)<sup>1</sup>; Dieter M. Drexler<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Bristol-Myers Squibb Company, Wallingford, CT
- MP 377 **Estimation of the Formation Rates of Polyatomic Species of Metals in Plutonium Analyses using Multicollector ICP-MS with a Desolvating Nebulizer;** [Alexandre Mitroshkov](#); Khris Olsen; May-Lin Thomas; *PNNL, Battelle, Richland, WA*
- MP 378 **Rapid Analysis of Pentose and Hexose using Direct Analysis in Real Time Mass Spectrometry;** [He Cui](#)<sup>1</sup>; Jiamin Ma<sup>1,2</sup>; Wenhao Zhang<sup>2</sup>; Zong Yang<sup>3</sup>; Echo W. Jia<sup>3</sup>; Xiaokun Duan<sup>3</sup>; Charles C. Liu<sup>3</sup>; <sup>1</sup>Shandong Extry-Exit Inspection & Quarantine Bureau, Qingdao, China; <sup>2</sup>Qingdao University, Qingdao, China; <sup>3</sup>ASPEC Technologies Limited, Beijing, China
- MP 379 **Optical and Mass Spectrometric Characterization of AC/DC Plasma Discharges for Laser Ablation Mass Spectrometry;** [Joel Keelor](#)<sup>1</sup>; Adam Kaylor<sup>1</sup>; Charlotte Reininger<sup>2</sup>; Paul Farnsworth<sup>2</sup>; Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>Brigham Young University, Provo, UT

- MP 380 **Increased Sensitivity in LAESI-MS Analyses using a Heated Extension Tube for the Analysis of Plant and Animal Tissues;** Brent Reschke; Holly Henderson; Trust Razunguzwa; Scott Mathess; Callee Walsh; Pamela Williams; Matthew Powell; *Protea Biosciences Group, Inc., Morgantown, WV*
- MP 381 **The Importance of Tool Choice for Numerical Analysis of Ion Transport in Mass Spectrometers Spanning Multiple Gas Dynamic Regimes;** Sergey Gimelshein<sup>1</sup>; Natalia Gimelshein<sup>2</sup>; Taylor Lilly<sup>3</sup>; Rebecca Webb<sup>3</sup>; Eugene Moskovets<sup>4</sup>; <sup>1</sup>University of Southern California, Los Angeles, CA; <sup>2</sup>Gimel Inc, Montrose, CA; <sup>3</sup>University of Colorado at Colorado Springs, Colorado Springs, CO; <sup>4</sup>MassTech Inc, Columbia, MD
- MP 382 **Multiple Solid Phase Microextraction (m-SPME) Coupled with Ambient Mass Spectrometry (AMS) for Rapidly Quantifying Trace Emerging Pollutants in ppt Level;** Jo-Han Chou; Min Zong Huang; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 383 **Continuum/Kinetic Approach for Ion Transport Modeling in Atmospheric and Intermediate Pressure Interfaces of the ESI/MS Systems;** Natalia Gimelshein<sup>1</sup>; Sergey Gimelshein<sup>2</sup>; Taylor Lilly<sup>3</sup>; Eugene Moskovets<sup>4</sup>; Berk Oktem<sup>4</sup>; <sup>1</sup>Gimel Inc., Montrose, CA; <sup>2</sup>University of Southern California, Los Angeles, CA; <sup>3</sup>University of Colorado at Colorado Springs, Colorado Springs, CO; <sup>4</sup>MassTech Inc, Columbia, MD
- MP 384 **Introducing Internal Calibrants for High Performance Liquid Chromatography/Fourier Transform-Ion Cyclotron Resonance (HPLC/FT-ICR) by Ambient Laser Desorption;** Yu-Min Huang; Chu-Nian Cheng; Hung Su; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- MP 385 **Filling the Ambient Ionization Toolbox: Complementary Ion Sources on the Same Platform;** Robert B. Cody<sup>1</sup>; John Dane<sup>1</sup>; Jason Shepard<sup>2</sup>; Mehmet Yigit<sup>2</sup>; <sup>1</sup>JEOL USA, Inc., Peabody, MA; <sup>2</sup>University at Albany, Albany, NY
- MP 386 **DART - High Performance Ion Mobility Spectrometry (HPIMS) for Rapid Chemical Identification;** Ching Wu<sup>1</sup>; Anthony Midey<sup>1</sup>; Robert Jackson<sup>1</sup>; Joe Tice<sup>2</sup>; Paul Danis<sup>2</sup>; Brian Musselman<sup>2</sup>; <sup>1</sup>Excellims Corporation, Acton, MA; <sup>2</sup>IonSense Inc., Saugus, MA
- MP 387 **Pulsed Desorption Electrospray Ionization Mass Spectrometry Imaging;** Troy J. Comi; Richard H. Perry; *University of Illinois, Urbana-Champaign, IL*
- MP 388 **Pulsed Optically Induced Chemical Gas Phase Ionization at Low Pressure using an UV-LED;** Jens Langejuergen; Christian-Robert Raddatz; Stefan Zimmermann; *Leibniz University Hannover, Hannover, Germany*
- MP 389 **Simultaneous Detection of Polar and Nonpolar Compounds by Pyrolysis/Electrospray+Atmospheric Pressure Chemical Ionization/Mass Spectrometry (Py/ESI+APCI/MS);** Sy-Chyi Cheng; Siou-Sian Jhang; Ruei-Hung Hung; Jentaie Shiea; *National Sun Yat-Sen Univ., Kaohsiung, TAIWAN*
- MP 390 **Pesticides Screening in Bee using Venturi-Assisted Laser Desorption (VALDI) for Ambient Ionization Mass Spectrometry;** Andrea Machado<sup>1</sup>; Marcos Franco<sup>2</sup>; Nicolas Schwab<sup>2</sup>; Marcos Eberlin<sup>2</sup>; <sup>1</sup>NSF Bioensaios, Viamão, Brazil; <sup>2</sup>Institute of Chemistry, University of Campinas, Campinas, Brazil
- MP 391 **An Effective Ambient Desorption/Ionization Source using Hydrogen-Doped Argon as the Support Gas;** Wade C Ellis; Anna P Openshaw; Paul B Farnsworth; *Brigham Young University, Provo, UT*
- MP 392 **Droplets + Electric Fields -> Intense ESI and MALDI Mass Spectra;** Drew Sauter<sup>1</sup>; Andrew D Sauter III<sup>1</sup>; Gary Groenewold<sup>2</sup>; Roy Helmy<sup>3</sup>; Robert Ross<sup>4</sup>; Patrick Limbach<sup>4</sup>; <sup>1</sup>Nanoliter, LLC, Henderson, NV; <sup>2</sup>Idaho National Lab, Idaho City, ID; <sup>3</sup>Merck Research Lab, Rahway, NJ; <sup>4</sup>University of Cincinnati, Cincinnati, OH
- MP 393 **A Closer Look to Sonic Spray Ionization;** Abdil Ozdemir<sup>2</sup>; Jung-Lee Lin<sup>1</sup>; Yi Sheng Wang<sup>1</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>Academia Sinica Genomic Research Center, Taipei, Taiwan; <sup>2</sup>Sakarya University Chemistry Department, Sakarya, TURKEY
- MP 394 **Ion Manipulation in Air: Separations, Reactions, and Product Collection;** Pu Wei; Zane Baird; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- MP 395 **Ion Dynamics of an Atmospheric Pressure Inlet for a Compact Mass Spectrometer;** Chaminda M. Gamage; Jamey Jones; Jack Henion; Simon J. Prosser; *Advion, Inc., Ithaca, NY*
- MP 396 **Coupling of Ultrafast LC Separation with Mass Spectrometry by DESI;** Yi Cai; *Ohio University, Athens, OH*
- MP 397 **Active Pixel Detector: A New Detection System for the Characterization of Native-Like Protein and DNA Complexes by Electrospray Ionization;** Tiffany Pona; Shane R. Ellis; Bob Hommersom; Ron M.A. Heeren; *FOM Institute AMOLF, Amsterdam, The Netherlands*
- MP 398 **Improved Molecular Coverage in Negative Ion Mode and Reactive Laser Ablation Electrospray Ionization Mass Spectrometry;** Hang Li; Akos Vertes; *George Washington University, Washington, DC*
- MP 399 **Paper Assisted Ultrasonic Spray Ionization for Direct Screening of Complicated Matrixes with Mass Spectrometry;** Guangming Huang; Hongying Zhu; Gongyu Li; *University of Science and Technology of China, Hefei, China*
- MP 400 **Plasma-based Ambient Sampling/Ionization/Transmission Integrated Source for Mass Spectrometry;** Yueming Zhou<sup>1,2</sup>; Yiming Zhang<sup>3</sup>; Ning Zhang<sup>1</sup>; Yafeng Li<sup>1</sup>; Caiqiao Xiong<sup>1</sup>; Suming Chen<sup>1</sup>; Xiang Pan<sup>3</sup>; Li Zhou<sup>3</sup>; Zhaogui Liu<sup>3</sup>; Zongxiu Nie<sup>1,4</sup>; <sup>1</sup>Institute of Chemistry Chinese Academy of Sciences, Beijing, China; <sup>2</sup>East China Institute of Technology, Nanchang, Jiangxi, China; <sup>3</sup>Jiangsu Skyray Instrument Inc., Kunshan, Jiangsu, China; <sup>4</sup>Beijing Center for Mass Spectrometry, Beijing, China
- MP 402 **Thermal Desorption/Electrospray and Plasma Ionization/Mass Spectrometry for Simultaneously Detecting Polar and Nonpolar Compounds in Complex Mixtures;** Min Zong Huang; Siou-Sian Jhang; Jentaie Shiea; *Dep. of Chemistry National Sun Yat-Sen University, Kaohsiung, Taiwan*
- MP 403 **A Modified Direct Sample Analysis (DSA) Ionization Source for the Direct Analysis of Thin-Layer Chromatography (TLC) Plates;** Greg Winter; Joshua Wilhide; William R. LaCourse; *UMBC, Baltimore, MD*
- MP 404 **A Novel Atmospheric Interface for the Analysis of Tissue using Rapid Evaporative Ionization Mass Spectrometry (REIMS);** Cristina Guallar-Hoyas<sup>1</sup>; Ottmar Golf<sup>1</sup>; Lajos Gödörházy<sup>2</sup>; Dániel Szalay<sup>2</sup>; Tamás Karancsi<sup>2</sup>; Steven Pringle<sup>3</sup>; Mike Morris<sup>3</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Medimass, Budapest, Hungary; <sup>3</sup>Waters Corporation, Manchester, UK

## Plant"omics" 405 - 419

- MP 405 **Multifaceted Investigation of Metabolites During Nitrogen Fixation in the Medicago truncatula-Sinorhizobium meliloti Symbiosis via High Resolution MALDI-MS Imaging and ESI-MS;** Erin Gemperline<sup>1</sup>; Junko

- Maeda<sup>2</sup>; Muthusubramanian Venkateshwaran<sup>3</sup>; Jean-Michel Ané<sup>2</sup>; Lingjun Li<sup>1,4</sup>; <sup>1</sup>Department of Chemistry, UW-Madison, Madison, WI; <sup>2</sup>Department of Agronomy, UW-Madison, Madison, WI; <sup>3</sup>School of Agriculture, UW-Platteville, Platteville, WI; <sup>4</sup>School of Pharmacy, UW-Madison, Madison, WI
- MP 406 **An Untargeted and Targeted Analysis of Early ABA-Induced Phosphoproteomic Changes in Wildtype and Quadruple ABA Receptor Mutant *A. thaliana* Strains;** Benjamin Minkoff; Kelly Stecker; Michael Sussman; University of Wisconsin, Madison, WI
- MP 407 **Role of the RCAR3 gene in ABA-induced Signaling in *Arabidopsis thaliana*;** Chhaya Patole; Jim Dunwell; Rainer Cramer; University of Reading, Reading, UK
- MP 408 **Analysis of Resin Acids in Seedlings and Resin-Soaked Loblolly Pine using MALDI-MS/MS and LC-MS/MS;** Michelle Reid<sup>1</sup>; Rainey Patterson<sup>1</sup>; Gary F. Peter<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>Chemistry Department, University of Florida, Gainesville, FL; <sup>2</sup>Genetics Institute, University of Florida, Gainesville, FL
- MP 409 **In vitro Validation of Barley Endoprotease B2 Specificity by the Degradation of Multiple Endogenous Substrates and Label Free Differential LC-MS;** Joanne B. Connolly<sup>1</sup>; Hanne Damgaard Poulsen<sup>2</sup>; Jesper Christiansen<sup>3</sup>; Henrik Brinch-Pedersen<sup>3</sup>; Giuseppe Dionisio<sup>2</sup>; <sup>1</sup>Waters, Manchester, UK; <sup>2</sup>Aarhus University, Slagelse, Denmark; <sup>3</sup>Aarhus University, Tjele, Denmark
- MP 410 **Proteomic Analysis of Brassinolide Treated *Arabidopsis* Seedlings under Salt Stress by LC/MS/MS;** Isha Sharma<sup>1</sup>; Kevin Blackburn<sup>1</sup>; Tara E. Nash<sup>1</sup>; Pratap Pati<sup>2</sup>; Michael B. Goshe<sup>1</sup>; Steven D. Clouse<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>Guru Nanak Dev University, Punjab, India
- MP 411 **Determining the Phosphorylation Motif(s) of GRIK-activated SnRK1 using LC/MS/MS;** Laura Greeley; Linda Hanley-Bowdoin; Michael Goshe; NCSU, Raleigh, NC
- MP 412 **<sup>13</sup>CO<sub>2</sub> Growth Chamber Enabling High Enrichment in vivo Labeling over Complete Plant Life Cycle for Metabolic Flux Analysis;** Calvin Peters; Jerry Cohen; Adrian D. Hegeman; University of Minnesota, Saint Paul, MN
- MP 413 **Identification of Potential Chemical Giraffe-Feeding Deterrents in *Acacia Robusta* using Untargeted Metabolomics with LC-ESI-HRMS;** Stephen A. Brockman; Megan Strauss; Dana M. Freund; Jerry D. Cohen; Adrian D. Hegeman; University of Minnesota, Saint Paul, MN
- MP 414 **A Novel Platform for the Identification of Plant Bioactive Peptides;** Brian Kelly<sup>1</sup>; Christine Kirkpatrick<sup>1</sup>; Awais Altaf<sup>2</sup>; Sumaira Kousar<sup>2</sup>; Amer Jamil<sup>2</sup>; Leslie Hicks<sup>1</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>University of Agriculture, Faisalabad, Pakistan
- MP 415 **Targeted Metabolomics Approach to Unravel the Production of Hydroxy Fatty Acids in *Physaria fendleri*, a Promising Industrial Crop;** Jean-Christophe Cocuron; Brooke Anderson; Alison Boyd; Ana Paula Alonso; The Ohio State University, Columbus, OH
- MP 416 **Nutrient Deficiency Responses of Potato (*Solanum tuberosum* L.) Revealed by Combined Proteomics and Metabolomics Approaches;** Anna Maria Jozefowicz<sup>1</sup>; Nadja Arens<sup>1</sup>; Andrea Matros<sup>1</sup>; Manuela Peukert<sup>1</sup>; Stefanie Döll<sup>1</sup>; Stephanie Kaspar<sup>2</sup>; Hans-Peter Mock<sup>1</sup>; <sup>1</sup>Institute of Plant Genetics & Crop Plant Research, Gatersleben, Germany; <sup>2</sup>Brüker Daltonik GmbH, Bremen, Germany
- MP 417 **Spatial Analysis of Phototropic Metabolites in a Plant Cell by Live Single-cell Mass Spectrometry;** Takashi Fujii; Tsuyoshi Esaki; Sachiko Date; Hajime Mizuno; Tsutomu Masujima; Quantitative Biology Center (QBiC), RIKEN, Suita, Osaka, Japan
- MP 418 **A Novel Microflow UPLC-MS/MS Multiplexed Assay for the Absolute Quantitation of 13 Phytohormones in Plants;** Jay Kirkwood; Lisa Wolfe; Hend Ibrahim; Cory Broeckling; Jessica Prenni; CSU Proteomics and Metabolomics Facility, Fort Collins, CO
- MP 419 **Phytohormone Profiling: Obtaining Highest Sensitivity and Throughput;** Catherine Rawlinson<sup>2</sup>; Lars Kamphuis<sup>5</sup>; Kar-Chun Tan<sup>6</sup>; Riki Kitano<sup>7</sup>; Bruce Fraser<sup>3</sup>; John Hewetson<sup>4</sup>; Karam Singh<sup>5</sup>; Robert Trengove<sup>2</sup>; Paul Wynne<sup>1</sup>; <sup>1</sup>Shimadzu, Park Orchards, Australia; <sup>2</sup>Murdoch University, Perth, Australia; <sup>3</sup>Shimadzu Scientific Instruments, Palmerston North, New Zealand; <sup>4</sup>Shimadzu Australasia, Sydney, Australia; <sup>5</sup>CSIRO Plant Industry, Perth, Australia; <sup>6</sup>Curtin University, Perth, Australia; <sup>7</sup>Shimadzu Corporation, Kyoto, Japan
- Biomarkers: Discovery, 421 - 445**
- MP 421 **Potential Prognostic Indicators of Oral Squamous Cell Carcinoma Associated with Patient Outcomes - Using Systems Biology Approach;** Thomas Harris<sup>1</sup>; Nicole Kawachi<sup>1</sup>; Peicheng Du<sup>2</sup>; Thomas Belbin<sup>1</sup>; Edward Nieves<sup>1</sup>; Richard Smith<sup>1</sup>; Ruth Angeletti<sup>1</sup>; Michael Prystowsky<sup>1</sup>; Jihyeon Lim<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY; <sup>2</sup>Dept. Information Systems and Technology, UMDNJ, Newark, NJ
- MP 422 **Using Breast Milk to Assess Breast Cancer Risk: The Role of Mass Spectrometry-Based Proteomics;** Roshanak Aslebagh<sup>1</sup>; Armand G. Ngounou Wetie<sup>1</sup>; Sallie S. Schneider<sup>2</sup>; Susan R. Sturgeon<sup>3</sup>; Kathleen F. Arcaro<sup>3</sup>; Costel C. Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>Pioneer Valley Life Sciences Institute, Springfield, MA; <sup>3</sup>University of Massachusetts, Amherst, MA
- MP 424 **Development of Urinary and Kidney Biomarkers to Monitor Oligomer Treatment in Duchenne Muscular Dystrophy;** Aiping Zhang; Kitipong Jaesoontachoon; Conner Shaughnessy; Sree Rayavarapu; Kristy J Brown; Patricio Ray; Kanneboyina Nagaraju; John N. van den Anker; Eric P Hoffman; Yetrib Hathout; Children's National Medical Center, Washington, DC
- MP 425 **Change in IgGs Fc N-linked Glycosylation in Human Disease;** Hsi-Chang Shih<sup>1,3</sup>; Yu-Ting Chang<sup>2</sup>; Ming-Chu Chang<sup>2</sup>; Chein-Hung Chen<sup>3</sup>; Ya-Po Kuo<sup>3</sup>; Chung-Hsuan Chen<sup>1,3</sup>; <sup>1</sup>Dept. of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Dept. of Internal Medicine, NTU Hospital, Taipei, Taiwan; <sup>3</sup>The Genomics Research Center, Academia Sinica, Taipei, Taiwan
- MP 426 **Stop Enzymatic Activity and Preserve the Molecular Integrity of Tissue Samples by Heat Stabilization;** Ulla Sollenberg; Marcus Söderquist; Mats Borén; Karl Skold; Denator AB, Uppsala, Sweden
- MP 427 **In-depth Analysis of Glioma Stem Cells through an Integrative Genomics-Proteomics Approach;** Huiling Liu<sup>1</sup>; Dong Wang<sup>2</sup>; Qianghu Wang<sup>2</sup>; Alexander S. Shavkunov, <sup>1</sup>; Erik Philip Sulman<sup>2</sup>; Charles A Conrad<sup>2</sup>; Frederick F Lang Jr<sup>2</sup>; Carol L. Nilsson<sup>1</sup>; <sup>1</sup>University of Texas Medical Branch, Galveston, TX; <sup>2</sup>The University of Texas M.D. Anderson Cancer Cent, Houston, Texas
- MP 428 **Identification of Glioblastoma A Priori Bevacizumab Response Biomarkers by Mass Spectrometry-Based Label-Free Quantitative Proteomics;** Maxime Heroux<sup>1</sup>; Marla Chesnik<sup>1</sup>; Brian Halligan<sup>1</sup>; Mona Al-Gizawiy<sup>1</sup>; Jennifer Connelly<sup>1</sup>; Wade Mueller<sup>1</sup>; Scott Rand<sup>1</sup>; Elizabeth Cochran<sup>1</sup>; Peter LaViolette<sup>1</sup>; Mark Malkin<sup>2</sup>; Kathleen Schmainda<sup>1</sup>; Shama Mirza<sup>1</sup>; <sup>1</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>2</sup>Virginia Commonwealth University, Richmond, VA



- MP 429 **Large-Scale Quantitative Proteomic/Metaproteomic Platform Discovers Target Pathways and Promising Biomarkers of COPD-associated Lung Cancer**; Brian Sandri<sup>1</sup>; Andy Limper<sup>2</sup>; Pratik Jagtap<sup>4</sup>; Ping Yang<sup>2</sup>; Ola Larsson<sup>3</sup>; Peter Bitterman<sup>1</sup>; Tim Griffin<sup>4</sup>; Leeann Higgins<sup>4</sup>; Todd Markowski<sup>4</sup>; Chris Wendt<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Mayo Clinic, Rochester, MN; <sup>3</sup>Karolinska Institutet, Solna, Sweden; <sup>4</sup>Mass Spectrometry and Proteomics, UMN, Minneapolis, MN
- MP 430 **Multi-Platform Analysis of Metabolic Perturbations in Diabetic NOD Mice: Evaluation of the Metabolome, Lipidome and Signaling Mediators**; Johannes Fahrman<sup>1</sup>; Dmitry Grapov<sup>1</sup>; Jun Yang<sup>1</sup>; Bruce Hammock<sup>1</sup>; Oliver Fiehn<sup>1</sup>; Manami Hara<sup>2</sup>; <sup>1</sup>University of California, Davis, Davis, CA; <sup>2</sup>Department of Medicine, The University of Chicago, Chicago, IL
- MP 431 **Label-free Quantitative Proteomics Analysis of Hepatocellular Carcinoma with Different Grading Reveals Potential Prognostic Marker**; Wael Naboulsi<sup>1</sup>; Dominik Megger<sup>1</sup>; Thilo Bracht<sup>1</sup>; Kristin Rosowski<sup>1</sup>; Birgit Korte<sup>1</sup>; Stephanie Tautges<sup>1</sup>; Marvin Voss<sup>1</sup>; Michael Kohl<sup>1</sup>; Maike Ahrens<sup>1</sup>; Martin Eisenacher<sup>1</sup>; Katja Kuhlmann<sup>1</sup>; Helmut Meyer<sup>1</sup>; Andreas Hoffmann<sup>4</sup>; Frank Weber<sup>4</sup>; Joerg Schlaak<sup>3</sup>; Hideo Baba<sup>2</sup>; Barbara Sitek<sup>1</sup>; <sup>1</sup>Medizinisches Proteom-Center, Bochum, Germany; <sup>2</sup>Pathologie, Universitätsklinikum Essen, Essen, Germany; <sup>3</sup>Hepatologie, Universitätsklinikum Essen, Essen, Germany; <sup>4</sup>Medicine, Universitätsklinikum Essen, Essen, Germany
- MP 432 **Discovery of Glycoprotein Signatures for Aggressive Prostate Cancer via SWATH Mass Spectrometry**; Yansheng Liu<sup>1</sup>; Chen Jing<sup>2</sup>; Atul Sethi<sup>1</sup>; Qing K Li<sup>2</sup>; Geroge Steven Bova<sup>3</sup>; Lijun Chen<sup>2</sup>; Ben Collins<sup>1</sup>; Ludovic CJ Gillet<sup>1</sup>; Bernd Wollscheid<sup>1</sup>; Hui Zhang<sup>2</sup>; Ruedi Aebersold<sup>1,4</sup>; <sup>1</sup>Institute of Molecular Systems Biology ETH, Zurich, Switzerland; <sup>2</sup>Johns Hopkins University, Baltimore, DE; <sup>3</sup>University of Tampere, Tampere, Finland; <sup>4</sup>Faculty of Science University of Zurich, Zurich, Switzerland
- MP 433 **A Novel Platform for Plasma Biomarker Discovery with super-SILAC Quantification of Microparticle Proteomes**; Michal Harel<sup>1</sup>; Yuval Shaked<sup>2</sup>; Tamar Geiger<sup>1</sup>; <sup>1</sup>Tel Aviv University, Tel Aviv, Israel; <sup>2</sup>Technion, Haifa, Israel
- MP 434 **Novel Orbitrap-Based Two-Dimensional LC-MS/MS Workflows to Qualitatively and Quantitatively Analyze Native Human Peptides in Complex Secretome Samples**; Baozhen Shan<sup>2</sup>; Martijn Pinkse<sup>1</sup>; Bharath Kumar Raghuraman<sup>1</sup>; Cassandra Wigmore<sup>2</sup>; Peter D. Verhaert<sup>1</sup>; <sup>1</sup>Delft University of Technology, Delft, Netherlands; <sup>2</sup>BSI, Waterloo, Ontario, Canada
- MP 435 **Biomarker Discovery of CD14, a Soluble Endotoxin Receptor for Diagnosis of Stable Coronary Artery Disease**; Thomas S.-H. Chiou<sup>1</sup>; Min-Yi Lee<sup>1</sup>; Chao-Jen Kuo<sup>1</sup>; Wen-Jen Chen<sup>1</sup>; Chun-Hao Huang<sup>1</sup>; Chen-Lung Steve Lin<sup>1</sup>; Wen-Ter Lai<sup>2</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>Kaohsiung Medical University Hospital, Kaohsiung, Taiwan
- MP 436 **Environmental Exposure to Xenobiotic Agents in Breast Cancer**; Maria Hassis<sup>1</sup>; George Lemieux<sup>2</sup>; Namrata Prasad<sup>1</sup>; Susan Fisher<sup>1</sup>; Zena Werb<sup>2</sup>; Katherine Williams<sup>1</sup>; <sup>1</sup>Department of Ob/Gyn & Reproductive Sciences, UCSF, San Francisco, CA; <sup>2</sup>Department of Anatomy, UCSF, San Francisco, CA
- MP 437 **A Comparative Proteomics Study of Cerebrospinal Fluid from Smith-Lemli-Opitz Syndrome Patients**; Stephanie M. Cologna; Christopher A. Wassif; Sandra K. Conley; Peter S. Backlund; Alfred L. Yergey; Forbes D. Porter; *National Institutes of Health, Bethesda, MD*
- MP 438 **Biomarkers of Dietary Intake to Gauge Health and the Onset of Disease**; Simin D. Maleknia; Russell Bonduriansky; *University of New South Wales, Sydney, Australia*
- MP 439 **Metabolic Profiling of Autistic Brain Tissue Analysis by Laser Ablation Electrospray Ionization**; Rachelle Jacobson; Jessica Stolee; Valerie Hu; Akos Vertes; *George Washington University, Washington, District of Columbia*
- MP 440 **Phosphoproteomics Reveals Activation of FAK Kinase Signaling Pathway in Tamoxifen-Resistant Breast Cancer**; Xinyan Wu<sup>1</sup>; Muhammad Zahari<sup>1</sup>; Santosh Renuse<sup>2</sup>; Nandini Sahasrabudde<sup>2</sup>; Min-Sik Kim<sup>1</sup>; Raghothama Chaerkady<sup>1</sup>; Saraswati Sukumar<sup>1</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Institute of Bioinformatics, Bangalore, India
- MP 441 **Down-scaling Tissues Proteomics, toward Precious FFPE Tissue Sample Preparation**; Rémi Longuespée<sup>1</sup>; Gabriel Mazzucchelli<sup>1</sup>; Nicolas Smargiasso<sup>1</sup>; Dominique Baiwir<sup>2</sup>; Florence Quesada Calvo<sup>3</sup>; Marie Alice Meuwis<sup>3</sup>; Philippe Delvenne<sup>4</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>Mass Spectrometry Laboratory, University of Liège, Belgium; <sup>2</sup>GIGA Proteomic Facilities, University of Liège, Liège, Belgium; <sup>3</sup>Hepato-Gastroenterology and Digestive Oncology, Liège, Belgium; <sup>4</sup>Laboratory of Experimental Pathology, Liège, Belgium
- MP 442 **Development of a Diagnostic Proteomic Profiling Platform for Differentiating Thoracic Tumors**; Linan Wang<sup>1,2</sup>; Konstantin Shilo<sup>1,3</sup>; Charles Hitchcock<sup>1,3</sup>; Michael A. Freitas<sup>1,2</sup>; <sup>1</sup>Ohio State University, Columbus, OH; <sup>2</sup>Molecular Virology, Immunology & Medical Genetics, Columbus, OH; <sup>3</sup>College of Medicine Pathology, Columbus, OH
- MP 443 **Colorectal Cancer Screening using Targeted LC-MS/MS-Based Metabolic Profiling of Human Serum**; Danijel Djukovic<sup>1</sup>; Jiangjiang Zhu<sup>1</sup>; Lingli Deng<sup>1</sup>; Haiwei Gu<sup>1</sup>; Farhan Himmati<sup>1</sup>; Gabriela Chiorean<sup>1,3</sup>; Daniel Raftery<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>3</sup>Indiana University Melvin and Bren Simon Cancer Ce, Indianapolis, IN
- MP 444 **Discovery of Lipid Biomarkers of Stroke and Cerebral Injury**; Anthony Iavarone<sup>1</sup>; Sunil Sheth<sup>2</sup>; Raymond Swanson<sup>3,4</sup>; <sup>1</sup>UC Berkeley, Berkeley, CA; <sup>2</sup>UCLA, Los Angeles, CA; <sup>3</sup>UCSF, San Francisco, CA; <sup>4</sup>San Francisco Veterans Affairs Medical Center, San Francisco, CA
- MP 445 **Hitting the Target: Novel Reagents for the Chemical-Proteomics Based Identification of Vascular Accessible Biomarkers**; Sabrina Hanke<sup>1,3</sup>; Alexander Kerner<sup>1,3</sup>; Yixin Zhang<sup>4</sup>; Christoph Roesli<sup>1,2</sup>; <sup>1</sup>Junior Research Group Biomarker Discovery, DKFZ, Heidelberg, Germany; <sup>2</sup>Biomarker Discovery, HI-STEM gGmbH, Heidelberg, Germany; <sup>3</sup>Helmholtz Int. Grad. School for Cancer Research, Heidelberg, Germany; <sup>4</sup>B CUBE Center for Molecular Bioengineering, Dresden, Germany
- Disease Biomarkers, 446 - 467**
- MP 446 **A Glycoprotein Biomarker Panel for Pancreatic Cancer Discovered by Quantitative Mass Spectrometry**; Song Nie<sup>1</sup>; Andy Lo<sup>1</sup>; Jing Wu<sup>1</sup>; Jianhui Zhu<sup>1</sup>; Zhijing Tan<sup>1</sup>; Diane M. Simeone<sup>1</sup>; Michelle A. Anderson<sup>2</sup>; Kerby A. Shedden<sup>3</sup>; Mack T. Ruffin<sup>4</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>Surgery department, Ann Arbor, MI; <sup>2</sup>Department of Internal, Ann Arbor, Michigan; <sup>3</sup>Department of Statistics, University of Michigan, Ann Arbor, Michigan; <sup>4</sup>Department of Family Medicine, University of Michigan, Ann Arbor, Michigan
- MP 447 **Quantitative Targeted Proteomics-Based Personalized Molecular Target Chemotherapy for Recurrent Brain Tumor**; Sumio Ohtsuki<sup>1</sup>; Wataru Obuchi<sup>2</sup>; Mitsutoshi Nakata<sup>3</sup>; Jun-ichiro Hamada<sup>2</sup>; Tetsuya Terasaki<sup>2</sup>; <sup>1</sup>Kumamoto University, Kumamoto, Japan; <sup>2</sup>Tohoku University, Sendai, Japan; <sup>3</sup>Kanazawa University, Kanazawa, Japan

- MP 448 **Identification and Comparison of Protein Candidate Biomarkers from Lower Urinary Tract Symptoms (LUTS) in Mouse Models and Human Patients;** Tyler Greer<sup>1</sup>; Anatoliy Nechyporenko<sup>2</sup>; Ling Hao<sup>2</sup>; Chad Vezina<sup>3</sup>; Will Ricke<sup>4</sup>; Paul Marker<sup>2</sup>; Dale Bjorling<sup>3</sup>; Wade Bushman<sup>4</sup>; Lingjun Li<sup>2</sup>; <sup>1</sup>Department of Chemistry UW-Madison, Madison, WI; <sup>2</sup>School of Pharmacy UW-Madison, Madison, WI; <sup>3</sup>School of Veterinary Medicine UW-Madison, Madison, WI; <sup>4</sup>Department of Urology UW-Madison, Madison, WI
- MP 449 **Targeted and Discovery Proteomic Comparisons of Thyroid Neoplasms Reveals Differential Protein Expression;** Juan Martinez-Aguilar<sup>1</sup>; Roderick Clifton-Bligh<sup>2</sup>; Mark Molloy<sup>1,3</sup>; <sup>1</sup>Macquarie University, Sydney, Australia; <sup>2</sup>Kolling Institute of Medical Research, Sydney, Australia; <sup>3</sup>Australian Proteome Analysis Facility, Sydney, Australia
- MP 450 **SRM as a New Efficient Detection Tool for the Early Diagnosis of the Lyme Disease;** Gilles Schnell<sup>1</sup>; Amandine Boeuf<sup>1</sup>; Benoît Westermann<sup>1</sup>; Benoît Jaulhac<sup>2</sup>; Nathalie Boulanger<sup>2</sup>; Laurence Ehret-Sabatier<sup>1</sup>; <sup>1</sup>LSMBO, Strasbourg, France; <sup>2</sup>EA7290, Groupe Borréliose de Lyme, Strasbourg, France
- MP 451 **Detection of Amyloid  $\beta$ -peptides in Cerebrospinal Fluid and Blood Plasma with Immunoprecipitation-MALDI-TOF-MS, using Micropillar Targets on a Silicon Chip;** Johan Jacksén<sup>1</sup>; Patrik EK<sup>1</sup>; Patrick Öeckl<sup>3</sup>; Bernd Baumann<sup>3</sup>; Jens Wiltfang<sup>2</sup>; Markus Otto<sup>3</sup>; Johan Roeraade<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology, Stockholm, Sweden; <sup>2</sup>Georg-August-Universität Göttingen, Göttingen, Germany; <sup>3</sup>University of Ulm, Ulm, Germany
- MP 452 **Evaluation of Drug Induced Toxicity on Cultured Primary Hepatocytes using MS-based Quantitative Proteomics;** Laxmikanth Kollipara<sup>1</sup>; Lisa Dietz<sup>1</sup>; Patricio Godoy<sup>2</sup>; Jan Hengstler<sup>2</sup>; Albert Sickmann<sup>1</sup>; <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften –, Dortmund, Germany; <sup>2</sup>Leibniz-Institut für Arbeitsforschung (IfADo), Dortmund, Germany
- MP 453 **Quantitative Profiling of N-linked Glycoproteins from Normal Breast Epithelia and Breast Cancer Cells;** Ten-Yang Yen; Roger Yen; Moe Thein; Yejin Yoo; Alejandro Corona; Judi Wong; Leslie Timpe; Bruce Macher; *San Francisco State University, San Francisco, CA*
- MP 454 **Elevated Peptides in Lung Lavage Fluid Associated with Bronchiolitis Obliterans Syndrome;** Stephen B. Harvey; *University of Minnesota, Minneapolis, MN*
- MP 455 **Analysis of Bone Marrow Derived Multipotent Stromal Cell Secretome** Miljan Kuljanin, David Hess, Gilles A. Lajoie; Miljan Kuljanin; *Western University, London, Canada*
- MP 456 **Systematic Analysis of Tissue Glycoprotein Expression for the Early Detection of Pancreatic Cancer;** Hua Xiao<sup>2</sup>; Evelyn Kim<sup>1</sup>; David Misek<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Shanghai Jiao Tong University, Shanghai, China
- MP 457 **A Combined FASP and TMT Approach (iFASP) for the Identification of CSF Biomarker Candidates for Alzheimer's Disease;** Omar Barnaby<sup>1,2</sup>; Adam Boxer<sup>3</sup>; Hanno Steen<sup>1,2</sup>; Judith Steen<sup>1,2</sup>; <sup>1</sup>Boston Children's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>University of California, San Francisco, CA
- MP 458 **Characterizing the Nodal-regulated Breast Cancer Secretome and Its Role in Human Bone Marrow Mesenchymal Stem Cell Mediated Tumorigenesis;** Dylan Dieters-Castator<sup>1</sup>; Gilles Lajoie<sup>1</sup>; Lynne-Marie Postovit<sup>2</sup>; <sup>1</sup>University of Western Ontario, London, Canada; <sup>2</sup>University of Alberta, Edmonton, Canada
- MP 459 **Evaluation of a Protein Marker for Amyotrophic Lateral Sclerosis;** Melinda Beccari<sup>1</sup>; Miguel Mitne-Neto<sup>2</sup>; Valdemir Melechco Carvalho<sup>2</sup>; Gabriela Venturini<sup>3</sup>; Mayana Zatz<sup>1</sup>; <sup>1</sup>Human Genome and Stem Cell Research Center, São Paulo, Brazil; <sup>2</sup>Fleury Group, São Paulo, Brazil; <sup>3</sup>Instituto do Coração, São Paulo, Brazil
- MP 460 **High Performance Mass Spectrometry Revealing Phosphorylation-Dependent Regulation of GATA-2 Function;** Chenxi Yang; Koichi Katsumura; Emery Bresnick; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*
- MP 461 **Effect of Fluoride in Insulin Resistance of Gastrocnemium Muscle in Diabetic Rats: A Proteomic Analysis;** Aline Lima Leite<sup>1,2</sup>; Tatiana Martini<sup>1</sup>; Fernanda Zucki<sup>1</sup>; Heloísa Aparecida Barbosa da Silva Pereira<sup>2</sup>; Marília Afonso Rabelo Buzalaf<sup>1</sup>; <sup>1</sup>Bauru dental School, Bauru, SP; <sup>2</sup>Federal University of São Carlos, São Carlos, SP
- MP 462 **A Sensitive LC/MS/MS Method for the Quantification of Free T3/T4 in Serum, using a Simple Ultrafiltration Sample Preparation Procedure;** Evelyn McClure; *AB SCIEX, Concord, Canada*
- MP 463 **The Role of Proteomics in Deciphering the Intracellular Mechanism of Diuresis by the Insect Vector of Chagas' Disease *Rhodnius prolixus*;** Noman Hassan; Rachit Batta; Paula Gioino; Juan Ianowski; George Katselis; *College of Medicine, University of Saskatchewan, Saskatoon, Saskatchewan, Canada*
- MP 464 **Penile Squamous Cell Carcinoma: Searching for Protein Profiles by Imaging Mass Spectrometry;** Elisângela Silva<sup>1</sup>; Adriana Bulgarelli<sup>1</sup>; Bernadete Faria<sup>2</sup>; Isabela Cunha<sup>1</sup>; Rafael Rocha<sup>1</sup>; Stenio Zequi<sup>1</sup>; Gustavo Guimarães<sup>1</sup>; Fernando Soares<sup>1</sup>; Nilson Assunção<sup>2</sup>; Jose Vassallo<sup>3</sup>; <sup>1</sup>AC Camargo Cancer Center, São Paulo, SP-Brazil; <sup>2</sup>Federal University of São Paulo, São Paulo, SP-Brazil; <sup>3</sup>State University of Campinas Medical School, Campinas, SP-Brazil
- MP 465 **Catalase Corrected Metabolic Syndrome Induced Protein/PTM Changes in a Mouse Model of CVD;** Mark E. Mccomb; Stephen A. Whelan; Chunxiang Yao; Jessica B. Behring; Jean L. Spencer; Christian Heckendorf; Deborah A. Siwik; Wilson S. Colucci; Richard A. Cohen; Markus M. Bachschmid; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- MP 466 **Metabolite Profiling of Foodborne Disease Significance – Case study *Escherichia coli* O157;** Ann Perera<sup>1</sup>; Indira Kudva<sup>2</sup>; Preeti Bais<sup>3</sup>; Manohar John<sup>4</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>USDA-ARS-NADC, Ames, IA; <sup>3</sup>The Jackson Laboratory, Farmington, CT; <sup>4</sup>Pathovacs Inc, Ames, IA
- MP 467 **Defining Post-Translational Proteolysis Important in Biology and Medicine through N-terminal Labeling;** Reid O'Brien Johnson; Sean Shen; Rachel Ogorzalek Loo; Joseph A. Loo; *University of California, Los Angeles, CA*
- Small Molecule: Qualitative Analysis, 468 - 484**
- MP 468 **Identification of Plasmodium Falciparum Thioredoxin Reductase (PfTrxR) Inhibitors from Malaria Box using LC-MS Functional Assay;** Angela Calderon<sup>1</sup>; Neil Tiwari<sup>1</sup>; Katja Becker<sup>2</sup>; <sup>1</sup>Auburn University, Auburn, AL; <sup>2</sup>Justus Liebig University, Giessen, Germany
- MP 469 **Application of a Molecular Feature Extraction Algorithm to Detect Co-Eluting Species in Degraded Pharmaceuticals;** Fatkhulla K. Tadjimukhamedov; Tsion Billig; Qun Xu; Robyn Powell; Jennifer L. Belsky; John T. Simpson; *United States Pharmacopeia, Rockville, MD*



- MP 470 **Identification of Cooling Agents in Aerosols of an E-Cigarette from Unit Mass Resolution Spectra Enhanced to High Mass Accuracy**; Serban Moldoveanu; Karen Kilby; *Winston-Salem, NC*
- MP 471 **Development of an Ultrafast Screen for Synthetic Cannabinoids using a RapidFire-MS/MS System**; Jennifer Cottine Hitchcock; Ayodele Morris; Gregory McIntire; *Ameritox, Ltd., Greensboro, NC*
- MP 472 **New Approach For Compound Identification using Fine Isotopic Pattern Search**; Caroline Ding<sup>1</sup>; Tim Stratton<sup>1</sup>; Hans Pfaff<sup>2</sup>; Hans Gensemann<sup>2</sup>; Christoph Henrich<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- MP 473 **Large-Scale Nanoparticle Screening for Nanoparticle Assisted Laser Desorption Ionization Mass Spectrometry of Plant Metabolites**; Gargey Yagnik<sup>1,2</sup>; Andrew Korte<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames lab US DOE, Ames, IA*
- MP 474 **My ZAB is Dying! Exact Mass Determinations of ESI Invisible Molecules on Qtofs with TAPCI, Toluene Atmospheric Pressure Chemical Ionization**; Todd Williams<sup>1</sup>; Larry Seib<sup>1</sup>; Robert Drake<sup>1</sup>; Jared Mays<sup>2</sup>; <sup>1</sup>*University of Kansas, Lawrence, KS*; <sup>2</sup>*Augustana College, Sioux Falls, SD*
- MP 475 **Small Molecule Analysis using Laser Desorption/Ionization-Mass Spectrometry on Maldi Matrix Incorporated Sol-Gel Film**; Ömür Celikbıçak; Bekir Salih; *Hacettepe University, Department of Chemistry, Ankara, Turkey*
- MP 476 **Surface Analysis of Permanent Wave Processing Hair using DART-MS**; Shoji Takigami<sup>1</sup>; Erika Ikeda<sup>1</sup>; Yuta Takagi<sup>1</sup>; Jun Watanabe<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; <sup>1</sup>*Gunma University, Kiryu, Japan*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>3</sup>*AMR, Inc., Tokyo, Japan*
- MP 477 **Mass Spectrometric Analysis of Oxidation Products generated in an Electrochemical Artificial Kidney**; Maria Viehoff<sup>1</sup>; Lars Büter<sup>1</sup>; Karin G. F. Gerritsen<sup>2</sup>; Frank Simonis<sup>3</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>*University of Muenster, Muenster, D*; <sup>2</sup>*University Medical Center Utrecht, Utrecht, The Netherlands*; <sup>3</sup>*Nanodialysis B.V., Oirschot, The Netherlands*
- MP 478 **Collision Induced Dissociation Mass Spectra of Protonated Alkyl Dihydrocinnamates**; Sihang Xu; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- MP 479 **Development of a Fast UPLC-MS/MS Screen for Common Drugs of Abuse**; Erin C. Strickland; Gregory McIntire, Ph.D; *Ameritox, Ltd., Greensboro, NC*
- MP 480 **Development of a Qualitative Screen for Select Non-Tricyclic Antidepressants by UPLC/TOF**; Jeremy P. Smith; Erin C. Strickland; Gregory McIntire, Ph.D; *Ameritox, Ltd, Greensboro, NC*
- MP 481 **Software Assisted Rapid Screening and Identification of Potential Genotoxic Degradation Products**; Siji Joseph; Syed Salman Lateed; Vinayak Azhakaprakalam; Sreelakshmy Menon; *Agilent technologies, Bangalore, India*
- MP 482 **Environmental Marker Profiling of Landfill Leachate in Carcass Disposal**; Ryu Ji-Jeong; Seo Jungju; Hwang Geum Sook; *Korea Basic Science Institute(KBSI), Seoul, Korea*
- MP 483 **Characterization of Metabolites of biib028, a Heat Shock Protein 90 Inhibitor, in Rats and Dogs, by High Resolution Mass Spectrometry**; Natalia Penner; Chandra Prakash; *Biogen Idec, Cambridge, MA*
- MP 484 **Identification of Persistent Pd-containing Impurities using LC-MS/MS and LC-ICP-MS**; Wendy Zhong; Qiang Tu; Ryan Cohen; Renee Dermenjian; *Merck, Rahway, New Jersey*
- MP 485 **Avoiding Potential Interferences by Choosing the Right LCMSMS Transition for Midazolam Analysis**; Eric Morin; Jason Bilodeau; Nathalie Pelletier; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 486 **Combined Method for the Analysis of Darunavir, Ritonavir and Lopinavir in Human EDTA Plasma by LCMSMS**; Pierre-Yves Caron; Sylvain Lachance; François Viel; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- MP 487 **A Novel WCX Micro SPE Plate and Its Application in the Sample Extraction for LC-MS/MS Quantitation Method Development**; Guotao Lu<sup>1</sup>; Manik Desai<sup>2</sup>; Dawei Zhou<sup>2</sup>; Wan Wang<sup>3</sup>; Jerry Wang<sup>1</sup>; <sup>1</sup>*Bonna-Agela Technologies, Inc., Wilmington, DE*; <sup>2</sup>*XenoBiotic Laboratories, Inc., Plainsboro, NJ*; <sup>3</sup>*Bonna-Agela Technologies, Ltd., Tianjin, China*
- MP 488 **Inhibition of Inter-Conversion between Pitavastatin and its Lactone Metabolite for Application in Clinical Studies using LCMSMS**; Guy Havard; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- MP 489 **Solving Linearity Issue at High Concentration for the Determination of Gemcitabine using LCMSMS**; François Viel; Guy Havard; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Quebec, Canada*
- MP 490 **Highly Selective and Sensitive Determination of Betamethasone-17,21-Dipropionate, Bethamethasone-17-Propionate and Betamethasone by LCMSMS**; Nadia Smith; Philippe Belanger; François Samson-Thibault; Marie-Josée Marcoux; Marie-Claude Theberge; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 491 **Unique Liquid Chromatography Separation of Calcifediol and its 3-epimer analog using Dimethylpentafluorophenyl Propyl Column on a LCMSMS**; Guy Havard; Nicolas Jean; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 492 **Investigation of the Impact of Light on the Determination of Lurasidone in Human Serum by LCMSMS**; Valérie Montminy; Nathalie Pelletier; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 493 **Improved Performance with Column Back-Flushing between Injections: Two Case Studies**; Jason Bilodeau; Nicolas Jean; Marie-Claude Theberge; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 494 **Evaluation of Matrix Effect when Matrix Factor is not Enough for LCMSMS Bioanalytical Method**; Jason Bilodeau; Nadine Lafontaine; Pierre-Yves Caron; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 495 **Resolution of Sildenafil-d8 Ionization Dependence on Sildenafil Concentrations**; Pierre-Yves Caron; Audrey Wilmott; Nancy Lampron; François Viel; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 496 **Lower Limit of Quantitation at Sub-endogenous Compound Level and the Challenge of Low Quality Control Samples Preparation**; Marie-Claude Theberge; Jason Bilodeau; Guy Havard; François Viel; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*

- MP 497 **Improvement of Sensitivity and Robustness of an LCMSMS Quantitation Method for Digoxin, Controlling the Reactivity of the Deuterated Internal Standard;** Luc Bouchard; Carine Levesque; Nathalie Pelletier; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 498 **Investigation of a Clinical Methodology for Sample Collection for the Determination of Inosine in Human Plasma by LC/MS/MS;** Luc Bouchard; Nathalie Pelletier; Sylvain Lachance; Nadine Boudreau; Ann Levesque; *inVentiv Health Clinical, Quebec, Canada*
- MP 499 **Quantative Analysis of Docetaxel in NCR Nude Mice Fat by LC-MS/MS;** Yung-Hsiang Chen; Jason Oeh; Bianca Liederer; Marcel Hop; Brian Dean; Xiao Ding; *Genentech Inc., South San Francisco, CA*
- MP 500 **Application of HILIC Mode to Improve LC/ESI/MS Sensitivity of Opiates and Metabolites;** Anne Mack; William Long; Xiaoli Wang; *Agilent Technologies, Wilmington, DE*
- MP 501 **Stability Investigation on Dimethyl Fumarate in Rat Blood by LC-MS/MS: Insight Into Pharmacokinetics and Metabolic Fate In Vivo;** Venkatraman Junnotula; Hermes Licea Perez; *GSK, King Of Prussia, PA*
- MP 502 **A Highly Selective, Fast and Robust LC/MS/MS Method for the Quantification of Poloxamer 188 in Rat Plasma;** Aihua Liu; Brandon Wilcock; Laixin Wang; Scott Reuschel; Min Meng; *Tandem Labs, Salt Lake City, UT*
- MP 503 **Improving Sensitivity and Throughput for the Quantification of Buprenorphine, Norbuprenorphine, and Naloxone in Human Plasma using LC/MS/MS Assay;** Sherry Liu; Chad Moore; Laixin Wang; Scott Reuschel; Min Meng; *Tandem Labs, Salt Lake City, UT*
- MP 504 **Method Development of a Simultaneous Fast Quantitation of Niacin, Nicotinamide and Nicotinic Acid using HPLC Tandem Mass Spectrometry;** Todd Lusk; *Quintiles Bioanalytical and ADME Labs, Ithaca, NY*
- MP 505 **Challenges on Method Development for the Quantitation of Beclomethasone Dipropionate and Beclomethasone-17-monopropionate in Human Plasma by UPLC®-MS/MS;** Nancy Zheng; Marking G Peay; Michael Waldron; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- MP 506 **Simultaneous Low Level Determination of Ascorbic and Dehydroascorbic Acids using Newly Developed HILIC Stationary Phases and Tandem Mass Spectrometry;** William E. Cotham<sup>1</sup>; Audrey M. Howard<sup>2</sup>; Michael D. Walla<sup>1</sup>; Norma Frizzell<sup>2</sup>; John W. Baynes<sup>2</sup>; Matthew Przybyciel<sup>3</sup>; <sup>1</sup>*University of South Carolina, Dept. of Chemistry, Columbia, SC*; <sup>2</sup>*University of South Carolina School of Medicine, Columbia, SC*; <sup>3</sup>*ES Industries, West Berlin, NJ*
- MP 507 **A General Approach to Eliminating Downfield Interference in Bioanalysis of Amines by SCX Chromatography - Application to Oxybutynin and NNAL;** A Dzerk; P Miller; D Grafelman; E Sarajlic; C Kafonek; *Celerion, Inc, Lincoln, NE*
- MP 508 **Development and Validation of a Rapid and Sensitive LC-MS/MS Method for Quantification of CSUOH0901, an Antitumor Agent;** Ramakrishna Reddy Voggu; Xiang Zhou; Bin Su; Baochuan Guo; *Cleveland State University, Cleveland, Ohio*
- MP 509 **A Novel Derivatization Strategy to Enhance Stability and Sensitivity of LC-MS Detection of Catechol Estrones Extracted from Human Serum;** Lisa Bottalico<sup>1,2</sup>; Clementina Mesaros<sup>1,2</sup>; Qingqing Wang<sup>1,2</sup>; Kannan Rangiah<sup>3</sup>; Ian A. Blair<sup>1,2</sup>; <sup>1</sup>*University of Pennsylvania School of Medicine, Philadelphia, PA*; <sup>2</sup>*Center for Cancer Pharmacology, Philadelphia, PA*; <sup>3</sup>*C-CAMP, Bangalore, INDIA*
- MP 510 **A Single Method for the Quantitation of Sirolimus (Rapamycin) in Whole Blood and Multiple Tissues;** Donald Gray; Tyler DeGraw; Rachel Sun; *BASi, West Lafayette, IN*
- MP 511 **Direct Analysis of Carbodiimides in Pharmaceutical Compounds by High Performance Liquid Chromatography Mass Spectrometry;** Timothy Nowak; Ryan Cohen; Lin Wang; Vincent Antonucci; *Merck, Rahway, NJ*
- MP 512 **Modeling of in vitro Activity with Rat Pharmacokinetics to Remove the Need for in vivo Screening of RIP2 Inhibitors;** Michael Reilly; David Lipshutz; Bart Votta; Helen Sun; Elizabeth Rivera; Mukesh Mahajan; Rakesh Nagilla; Barb Swift; Carol Capriotti; Scott Berger; Linda Casillas; Peter Gough; Robert Marquis; John Bertin; *GlaxoSmithKline, Collegeville, PA*
- MP 513 **A Novel Device for Plasma Micro-Sampling Technique Developed for Bioanalysis;** Ji Zhang; David Lok; Jesse Gray; Matt Jones; *Takeda Pharmaceutical International, Cambridge, MA*
- MP 514 **Method Development and Validation for the Quantitation of ManNAc in Human Plasma using HILIC LC-MS/MS;** Yifan Shi<sup>1</sup>; Meng Fang<sup>1</sup>; Michael Zhang<sup>1</sup>; Yinghe Li<sup>1</sup>; Amy Wang<sup>2</sup>; Ed Kerns<sup>2</sup>; Nuria Carrillo-Carrasco<sup>2</sup>; Xin Xu<sup>2</sup>; Selwyn Yorke<sup>3</sup>; Bradley Gillespie<sup>4</sup>; <sup>1</sup>*Alliance Pharma, Malvern, PA*; <sup>2</sup>*TRND, NCATS, NIH, Rockville, MD*; <sup>3</sup>*New Zealand Pharmaceuticals, Palmerston North, New Zealand*; <sup>4</sup>*Leidos Biomedical Research Inc., Frederick, MD*
- MP 515 **Quantitation and Comparison of A Durg by using Whole Blood Assay and Plasma Assay;** Megan Mimnaugh; John Yu; Jeffrey Duggan; Jennifer Bleecker; Heln Luo; *Boehringer Ingelheim Pharma, Inc., Ridgefield, CT*
- MP 516 **Quantification of Tryptophan and Its Major Kynurenine Metabolites in Human Plasma;** Farid Jahouh; Fang Qian; Rong Wang; *Icahn School of Medicine at Mount Sinai, New York, NY*
- MP 517 **Development of an Ultrasensitive Microflow LC/MS/MS Method for Vitamin D Metabolites Analysis using Amplifex Diene Derivatization Reagent;** Jenny Dai<sup>1</sup>; Subhakar Dey<sup>2</sup>; Eric Battaglioli<sup>3</sup>; Bruce Stanley<sup>1</sup>; Robin Wilson<sup>3</sup>; <sup>1</sup>*Section of Research Resources, Penn State Univ, Hershey, PA*; <sup>2</sup>*AB SCIEX, Chemistry and Consumables R&D, Framingham, MA*; <sup>3</sup>*Department of Public Health Sciences, Penn State, Hershey, PA*
- MP 518 **Quantitative Analysis of Microcystins using A Newly Developed Triple Quadrupole Instrument;** Yanan Yang<sup>1</sup>; Cindy Tsai<sup>2</sup>; Anabel Fandino<sup>1</sup>; Cameron George<sup>1</sup>; Cynthia Hahn<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc, Santa Clara, CA*; <sup>2</sup>*San Jose State University Research Foundation, Gold River, CA*
- MP 519 **Post-column Mobile Phase Adjustment: A Strategy to Eliminate the Contradiction between Liquid Chromatography and Mass Spectrometry in Determining Flavonoids;** Shirui Zheng; *Zhejiang University, Hangzhou, China*
- Homeland Security, 520 - 531**
- MP 520 **Adaptation of U.S. EPA Method 538 Conditions and QC Approach for EA2192 Analysis by Liquid Chromatography/Tandem Mass Spectrometry;** Terry O'Neill<sup>1</sup>; Sandip Chattopadhyay<sup>2</sup>; Stuart Willison<sup>3</sup>; Matthew Magnuson<sup>3</sup>; <sup>1</sup>*MRIGlobal, Kansas City, MO*; <sup>2</sup>*Tetra Tech, Inc., Cincinnati, OH*; <sup>3</sup>*U.S. Environmental Protection Agency, Cincinnati, OH*

- MP 521 **Portable Membrane Inlet Mass Spectrometer for Rapid Detection of Drugs, Explosives and Chemical Weapons;** Stamatiou Giannoukos; Boris Brkić; Stephen Taylor; *University of Liverpool, Liverpool, UK*
- MP 522 **Extractive Electrospray Mass Spectrometry of Triacetone Triperoxide Vapour in the Presence of Ionic Liquids;** Alex R. Hill; James C. Reynolds; Martin B. Smith; Paul F. Kelly; Colin S. Creaser; *Loughborough University, Loughborough, UK*
- MP 523 **Detection and Characterization of Chemical Attribution Signatures from Smokeless Powders by Direct Analysis in Real Time – Mass Spectrometry;** Frederick Li<sup>1</sup>; Andrew Horsley<sup>1</sup>; Joseph Tice<sup>2</sup>; Brian Musselman<sup>2</sup>; Adam Hall<sup>3</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*IonSense, Inc., Saugus, MA*; <sup>3</sup>*Northeastern University, Boston, MA*
- MP 524 **Application of Capillary Atmospheric Pressure Electron Capture Ionization (CAPECI) for the Ultra-Sensitive Detection of Explosives, Drugs and Environmental Toxins;** Valerie Dergmann; David Mueller; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 525 **On-site Identification of Volatile Chemical Warfare Agents by Portable Gas-Chromatography Mass Spectrometry Instrument;** Hisayuki Nagashima<sup>1</sup>; Tomohide Kondo<sup>1</sup>; Tomoki Nagoya<sup>1</sup>; Takeshi Ohmori<sup>1</sup>; Mieko Kanamori-Kataoka<sup>1</sup>; Kouichiro Tsuge<sup>1</sup>; Isaac Ohsawa<sup>1</sup>; Yasuo Seto<sup>1</sup>; Toru Ikeda<sup>2</sup>; Naoko Kurimata<sup>2</sup>; Shohei Unoke<sup>2</sup>; Manabu Sodeyama<sup>3</sup>; <sup>1</sup>*National Research Institute of Police Science, Kashiwa, Japan*; <sup>2</sup>*INFICON Co., Ltd., Yokohama, Japan*; <sup>3</sup>*Teikoku-Sen-i Co., Ltd., Tokyo, Japan*
- MP 526 **On-site Detection of Chemical Warfare Agents by Atmospheric Pressure Chemical Ionization Counterflow-Introduction Ion-Trap Mass Spectrometry with Swab Sampling Mode;** Yasuo Seto<sup>1</sup>; Hisayuki Nagashima<sup>1</sup>; Tomoki Nagoya<sup>1</sup>; Takeshi Ohmori<sup>1</sup>; Mieko Kanamori-Kataoka<sup>1</sup>; Koichiro Tsuge<sup>1</sup>; Isaac Ohsawa<sup>1</sup>; Susumu Watanabe<sup>2</sup>; Hiroaki Hashimoto<sup>2</sup>; Akihiko Okumura<sup>3</sup>; <sup>1</sup>*National Research Institute of Police Science, Kashiwa, Japan*; <sup>2</sup>*Hitachi High-Tech Solutions Co., Mito, Japan*; <sup>3</sup>*Hitachi Ltd., Kokubunji, Japan*
- MP 527 **Multiplex Quantification of Microbial and Plant Protein Toxins in Complex Matrices by Immuno-Extraction And High Resolution Targeted Mass Spectrometry;** Mathieu Dupre<sup>1</sup>; Francois FENAILLE<sup>1</sup>; Cécile Feraudet-Tarisse<sup>1</sup>; Patricia Lamourette<sup>1</sup>; Hervé Volland<sup>1</sup>; Stéphanie Simon<sup>1</sup>; Christophe Junot<sup>1</sup>; Virginie Brun<sup>2</sup>; Francois Becher<sup>1</sup>; <sup>1</sup>*CEA, iBiTec-S, SPI, Gif Sur Yvette, France*; <sup>2</sup>*CEA, DSV, iRTSV, U1038 INSERM, EDyP, 38054 Grenoble, France*
- MP 528 **Exploration of a Top-Down Absolute Quantification Approach of Staphylococcal enterotoxins by High Resolution Targeted Mass Spectrometry on the Q-Exactive Instrument;** Mathieu Dupre<sup>1</sup>; Alexandre Seyer<sup>1</sup>; Francois Fenaille<sup>1</sup>; Patricia Lamourette<sup>1</sup>; Hervé Boutal<sup>1</sup>; Hervé Volland<sup>1</sup>; Christophe Junot<sup>1</sup>; Virginie Brun<sup>2</sup>; Francois Becher<sup>1</sup>; <sup>1</sup>*CEA, iBiTec-S, SPI, 91191 Gif-sur-Yvette, France*; <sup>2</sup>*CEA, DSV, iRTSV, U1038 INSERM, EDyP, 38054 Grenoble, France*
- MP 529 **Mass Spectrometric Forensic Analysis of Botulinum Neurotoxin Type A Isolated from Infant Formula and Patient Stool;** Suzanne R. Kalb; Jakub Baudys; John R. Barr; *CDC, Atlanta, GA*
- MP 530 **Optimization of a Mass Spectrometer for Detection of Trace and Bulk Explosives and Narcotics;** Ross Harper; Rakesh Patel; Adam Keil; Mitch Wells; Dennis Barket; *FLIR Systems, West Lafayette, IN*
- MP 531 **Characterization of Analytical Markers in Seized Opium Samples using an Enhanced Ion Mobility Spectrometry-Mass Spectrometry Method;** Peter Liuni<sup>1</sup>; Vladimir Romanov<sup>2</sup>; Marie-Josée Binette<sup>3</sup>; Hafid Zaknoun<sup>3</sup>; Maggie Tam<sup>3</sup>; Pierre Pilon<sup>3</sup>; Jan Hendrikse<sup>2</sup>; Derek Wilson<sup>1</sup>; <sup>1</sup>*York University, Toronto, ON*; <sup>2</sup>*Smiths Detection, Mississauga, ON*; <sup>3</sup>*Canada Border Services Agency, Ottawa, ON*
- High Throughput Analysis / Robotics, 532 - 540**
- MP 532 **Evaluation of the SPEware Cerex ALD-III 192 for Use in Automating SPE and SLE Methods in Validated LC-MS/MS Assays;** Patricia L Holland; Christopher M Shuford; Martin K Green; Stacy Dee; Matthew Crawford; Russell P Grant; *LabCorp, Burlington, NC*
- MP 533 **On-line Automated Protein Precipitation Preparation Followed by LC-MS/MS Analysis and LTD-MS/MS Cross Validation;** Pascal Belisle; Sylvain Letarte; Serge Auger; Pierre Picard; *Phytrox Technologies, Quebec, Canada*
- MP 534 **Automated SAIL on an Orbitrap Exactive;** Andrew Harron<sup>1</sup>; Khoa Hoang<sup>1</sup>; Milan Pophristic<sup>1</sup>; Charles N. Mcewen<sup>2</sup>; <sup>1</sup>*University of Sciences, Philadelphia, PA*; <sup>2</sup>*Univ. of the Sciences, Philadelphia, PA*
- MP 535 **Development and Validation of Direct Analysis Method for Screening and Quantitation of Amphetamines in Urine by LC/MS/MS;** Zhaoyi Zhan<sup>1</sup>; Zhe Sun<sup>1</sup>; Jie Xing<sup>1</sup>; Helmy Rabaha<sup>2</sup>; Swee Chin Lim<sup>2</sup>; <sup>1</sup>*Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, Singapore*; <sup>2</sup>*Department of Scientific Services, Ministry of Health, Brunei Darussalam*
- MP 536 **Mass Spectrometry Based Hit Triage: A Case Study on a Protease using RapidFire Mass Spectrometry;** Juncai Meng<sup>1</sup>; Gregory Adam<sup>1</sup>; Keith Rickert<sup>1</sup>; Edward Hudak<sup>1</sup>; Ming-Tain Lai<sup>2</sup>; Jay Grobler<sup>2</sup>; Paul Zuck<sup>1</sup>; Eric Johnson<sup>1</sup>; Jeffrey Hermes<sup>1</sup>; <sup>1</sup>*Screening and Protein Sciences, Merck Research Lab, North Wales, PA*; <sup>2</sup>*Infectious Disease, Merck Research Labs, West Point, PA*
- MP 537 **Investigation of Semi-Automated Serum Processing for High-Throughput N-Glycan Profiling by MALDI-TOF MS;** Yongha In<sup>1</sup>; Seounghee Song<sup>1</sup>; Jeesu Kim<sup>1</sup>; Kyu Hwan Park<sup>1</sup>; Yangsun Kim<sup>2</sup>; <sup>1</sup>*Applied Surface Technology, Suwon, Korea*; <sup>2</sup>*Hudson Surface Technology, Old Tappan, NJ*
- MP 538 **High-Throughput Analysis and Characterization of Small and Large Molecules by Matrix Assisted Ionization Vacuum Ion Mobility Spectrometry Mass Spectrometry;** Daniel Woodall; Beixi Wang; Tarick El-Baba; Ellen Inutan; Sarah Trimpin; *Wayne State University, Detroit, MI*
- MP 540 **Utilizing RapidFire Technology Coupled with MS/MS for Label-Free Biochemical Mechanistic Evaluation of Multiple Epigenetic and Metabolism Targets and Inhibitors;** Patrick Bingham; Karen Maegley; Cody Krivacic; *Pfizer, San Diego, CA*
- Environmental Analysis: Hydrocarbon and DOM, 549 - 557**
- MP 549 **Extraction and Molecular Characterization of Water-Soluble Organic Matter in Marine Sediments;** Frauke Schmidt<sup>2</sup>; Matthias Witt<sup>1</sup>; Jens Fuchser<sup>1</sup>; Boris P. Koch<sup>3</sup>; Kai-Uwe Hinrichs<sup>2</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, Germany*; <sup>2</sup>*MARUM, Bremen, Germany*; <sup>3</sup>*AWI, Bremerhaven, Germany*
- MP 550 **Temporal Characterization of Petroleum Residue in Louisiana Salt Marsh Sediments after the Deepwater Horizon Oil Spill by FT-ICR Mass Spectrometry;** Huan Chen<sup>1</sup>; Aixin Hou<sup>2</sup>; Nabanita Bhattacharyya<sup>2</sup>; Rui Zhang<sup>2</sup>; Rebecca L. Beasley<sup>1</sup>; Ryan P. Rodgers<sup>1,3</sup>; Alan G. Marshall<sup>1,3</sup>; Amy Mckenna<sup>1</sup>; <sup>1</sup>*Nat'l High Magnetic Field Lab, Tallahassee, FL*; <sup>2</sup>*Louisiana State University, Baton Rouge, LA*; <sup>3</sup>*Florida State University, Tallahassee, FL*

- MP 551 **Rapid Screening and Confirmation Analysis of Polycyclic Aromatic Hydrocarbons (PAHs) with DART Mass Spectrometry;** Yu Takabayashi<sup>1</sup>; Jun Watanabe<sup>2</sup>; Motoshi Sakakura<sup>3</sup>; Teruhisa Shiota<sup>3</sup>; <sup>1</sup>SHIMADZU TECHNO-Research, INC., Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>AMR, Inc., Tokyo, Japan
- MP 552 **Fast and Automated EPH Fractionation and Clean Up;** Kambiz Sadeghi; Rudolf Addink; *Fluid Management Systems, Watertown, MA*
- MP 553 **Integration of an *in situ* Mass Spectrometer with an Autonomous Underwater Vehicle for Characterization of Dissolved Hydrocarbon Distributions;** Tim Short; Strawn Toler; John Kloske; Steve Untiedt; Mark Ryder; Andres Cardenas-Valencia; Charles Cullins; *SRI International, St Petersburg, FL*
- MP 554 **Molecular Analysis of Aircraft-collected Atmospheric Particles and Cloud Water by nano-DESI and ESI High Resolution Mass Spectrometry;** Eric Boone<sup>1</sup>; Alexander Laskin<sup>2</sup>; Julia Laskin<sup>2</sup>; Christopher Wirth<sup>3</sup>; Paul B. Shepson<sup>3</sup>; Brian Stirm<sup>3</sup>; Kerri Pratt<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Pacific NW National Laboratory, Richland, WA; <sup>3</sup>Purdue University, West Lafayette, IN
- MP 555 **Photochemically-Induced Leaching of Water-Soluble Organics from Macondo Crude Oil into the Environment;** David C. Podgorski<sup>1,2</sup>; Phoebe Z. Ray<sup>3</sup>; Huan Chen<sup>1</sup>; Amy M. McKenna<sup>1</sup>; Ryan P. Rodgers<sup>1,4</sup>; Alan G. Marshall<sup>1,4</sup>; Matthew A. Tarr<sup>3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Tallahassee, FL; <sup>3</sup>UNO Department of Chemistry, New Orleans, LA; <sup>4</sup>FSU Department of Chemistry and Biochemistry, Tallahassee, FL
- MP 556 **Condensed Phase Membrane Introduction Mass Spectrometry (CP-MIMS) for the Real Time, Trace Level Measurement of Naphthenic Acids;** Kyle D. Duncan<sup>1,3</sup>; Gregory W. Vandergriff<sup>1</sup>; Dane R. Letourneau<sup>1,3</sup>; Dietrich A. Volmer<sup>1,2</sup>; Erik T. Krogh<sup>1,3</sup>; Christopher G. Gill<sup>1,3</sup>; <sup>1</sup>Applied Environmental Research Laboratories (AERL), VIU, Nanaimo, BC, Canada; <sup>2</sup>Saarland University, Saarbrücken, Germany; <sup>3</sup>Chemistry Department, University of Victoria, Victoria, BC, Canada
- MP 557 **Direct Quantification by Isotope Dilution-Mass Spectrometry of Hydrophobic Analytes Extracted from Wastewater by Stir Bar Sorptive Extraction;** Andrew Boggess; H.M. Skip Kingston; *Duquesne University, Pittsburgh, PA*
- Energy: Biofuels and Algae, 558 - 577**
- MP 558 **Systems-Wide Investigation of Photosynthetic Algae during a Shift from Excess- to Limiting- Light Conditions using Multi-Platform Metabolomics and Proteomics;** Nathan Sindt; Graham Peers; Jessica Prenni; *Colorado State University, Ft. Collins, CO*
- MP 559 **A Potential Alternate Synthetic Route to Lignin Thioacidolysis Standards and Their Characterization by GC-MS;** Dawn Kato; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- MP 560 **Elucidation of Synthetic Lignin Oligomers by Tandem Mass Spectrometry;** Fan Huang; Bert C. Lynn; *University of Kentucky, Lexington, KY*
- MP 561 **A GC/MS Procedure for the Rapid Characterization of Algal Liquefaction Products and Process Optimization;** Anna Caldwell<sup>1</sup>; Christian Richard<sup>2</sup>; Bhavish Patel<sup>2</sup>; John M. Halket<sup>1,3</sup>; <sup>1</sup>King's College London, London, UK; <sup>2</sup>Imperial College London, London, UK; <sup>3</sup>Specialist Bioanalytical Services Limited, Egham, UK
- MP 562 **Metaproteomic Approaches for Target Discovery of Glycoside Hydrolases and Auxiliary Activities in the Digestome of Lower Termite *Coptotermes gestroi*;** Fabio Squina<sup>1</sup>; Macelo Falsarella Carazzolle<sup>2</sup>; Ana Maria Costa-Leonardo<sup>4</sup>; Ramon Oliveira Vidal<sup>2</sup>; Gonçalo Guimarães Pereira<sup>2</sup>; Adriana Franco Paes Leme<sup>3</sup>; João Paulo Franco Cairo<sup>1</sup>; <sup>1</sup>CTBE - CNPEM, Campinas, Brazil; <sup>2</sup>UNICAMP, Campinas, Brazil; <sup>3</sup>LNBio - CNPEM, Campinas, Brazil; <sup>4</sup>UNESP, Rio Claro, Brazil
- MP 563 **Effects of Inhibitory Compounds of Lignocellulosic Hydrolysates in Cultivation of Lipid-Producing Bacteria;** Yohannes H. Rezenom; Baixin Wang; Kun-Ching Cho; Janessa L. Tran; Jason Gill; Ryland Young; David H. Russell; Kung-Hui Chu; *Texas A&M University, College Station, TX*
- MP 564 **Profiling of Novel Saponins in Switchgrass using Ultrahigh Performance Liquid Chromatography and Tandem Mass Spectrometry;** Afrand Kamali Sarvestani<sup>1,4</sup>; Aaron Joseph Garoutte<sup>2,4</sup>; Leonardo Dacostasousa<sup>3,4</sup>; Venkatesh Balan<sup>3,4</sup>; Bruce E Dale<sup>3,4</sup>; James Tiedje<sup>2,4</sup>; A. Daniel Jones<sup>1,4</sup>; <sup>1</sup>Michigan State University Department of Chemistry, East Lansing, MI; <sup>2</sup>MSU Department of Microbiology and Molecular Genet, East Lansing, MI; <sup>3</sup>MSU Department of Chemical Engineering, East Lansing, MI; <sup>4</sup>Great Lakes Bioenergy Research Center, East Lansing, MI
- MP 565 **Temporal Resolution and Product Distribution From Glucose to Cellulose using Thin-film Pyrolysis High Resolution Mass Spectrometry;** Daniel Cole; Carolyn Hutchinson; Young Jin Lee; *Iowa State Univ Chemistry Dept, Ames, IA*
- MP 566 **Exploring Molecular Structures using In-source CID on  $\mu$ Py-GC-APCI-TOF Mass Spectrometry;** Nathan Bond<sup>1</sup>; Daniel Cole<sup>2</sup>; Allison Kvam<sup>1</sup>; Carolyn Hutchinson<sup>2</sup>; Young Jin Lee<sup>2</sup>; *1*Iowa State University, Ames, IA; *2*Iowa State Univ Chemistry Dept, Ames, IA
- MP 567 **Negative APPI Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Analysis of Fast Pyrolysis Bio-Oils;** Carolyn Hutchinson; Kaitlin Heinen; Young Jin Lee; *Iowa State University, Ames, IA*
- MP 568 **An LC/MS/MS Investigation Of Chemical Reactions Causing Instability in Wood-Derived Pyrolysis Bio-Oils;** Matthew Rasmussen<sup>1</sup>; Jincy Joseph<sup>2</sup>; Brian Frederick<sup>2</sup>; Elizabeth A. Stemmler<sup>1</sup>; <sup>1</sup>Bowdoin College, Brunswick, ME; <sup>2</sup>University of Maine, Orono, ME
- MP 569 **Structure and Function of Microbial Communities: Integrating 'Meta-omics' Data Sets;** Eric Huang<sup>1</sup>; Frank Aylward<sup>2</sup>; Paul Piehowski<sup>1</sup>; Young-Mo Kim<sup>1</sup>; Thomas Metz<sup>1</sup>; Cameron Currie<sup>2</sup>; Stephen Lindemann<sup>1</sup>; Margaret Romine<sup>1</sup>; William Nelson<sup>1</sup>; Jim Fredrickson<sup>1</sup>; Richard D. Smith<sup>1</sup>; Kristin Kristin Burnum-Johnson<sup>1</sup>; Mary Lipton<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>UW-Madison, Madison, WI
- MP 570 **Oxidation of Biodiesel under Electrospray Ionization Process;** Maira Fasciotti<sup>1</sup>; Viviane Fernandes da Silva<sup>1</sup>; Samantha Ribeiro Campos da Silva<sup>1</sup>; Thays Vieira da Costa Monteiro<sup>1</sup>; Paulo Roque Martins Silva<sup>1</sup>; Werickson Fortunato de Carvalho Rocha<sup>1</sup>; Valnei Smarcaro Cunha<sup>1</sup>; Romeu José Daroda<sup>1</sup>; Marcos Nogueira Eberlin<sup>2</sup>; <sup>1</sup>INMETRO, Duque De Caxias, Brazil; <sup>2</sup>University Of Campinas, Campinas, SP, Brazil
- MP 571 **Metaproteomics and the Ecology of Algal Blooms;** Jags Pandhal; *Sheffield, UK*
- MP 572 **Proteomic and Transcriptomic Analysis of a Solvent Producing Bacterium *Clostridium acetobutylicum* ATCC 824;** Lie Min<sup>1,2</sup>; Keerthi Venkataramanan<sup>1,2</sup>; Shuyu Hou<sup>1,2</sup>; E. Terry Papoutsakis<sup>1,2</sup>; Kelvin H. Lee<sup>1,2</sup>; <sup>1</sup>University of Delaware, Newark, DE; <sup>2</sup>Delaware Biotechnology Institute, Newark, DE

- MP 573 **Advanced MS Analysis of a Novel Biodiesel Production Method**; Derek Waggoner; Patrick Hatcher; *Old Dominion University, Norfolk, VA*
- MP 574 **Small Anhydrooligosaccharides Represent Key Intermediates in Cellulose Fast Pyrolysis**; John Degenstein<sup>1</sup>; Priya Murria<sup>1</sup>; Matthew Hurt<sup>2</sup>; James Riedeman<sup>1</sup>; McKay Easton<sup>1</sup>; Linan Yang<sup>1</sup>; John Nash<sup>1</sup>; Rakesh Agrawal<sup>1</sup>; W. Nicholas Delgass<sup>1</sup>; Fabio Ribeiro<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*Chevron, Richmond, CA*
- MP 575 **Liquid Chromatography/Tandem Mass Spectrometric Method for Quantitative Characterization of Bio-oil from Fast Pyrolysis of Biomass**; Alex Dow; Vinod Kumar Venkatakrishnan; John Degenstein; James Riedeman; Tiffany Jarrell; Christopher Marcum; Ximeng You; Hilikka Kenttamaa; *Purdue University, West Lafayette, IN*
- MP 576 **Characterization of Biomass and Biochar by LDI-FTICRMS**; Thierry Ghislain<sup>1,2</sup>; Vincent Carré<sup>3</sup>; Yann Le Brech<sup>2</sup>; Guillaïn Mauviel<sup>2</sup>; Anthony Dufour<sup>1,2</sup>; Frédéric Aubriet<sup>3</sup>; <sup>1</sup>*CNRS, Nancy, France*; <sup>2</sup>*Université de Lorraine, Nancy, France*; <sup>3</sup>*Université de Lorraine, Metz, France*
- MP 577 **On-Line Mass Spectrometric Analysis of the Primary Fast Pyrolysis Products of Synthetic Lignin Oligomers with  $\beta$ -O-4 and 5-5 Linkages**; Priya Murria<sup>1</sup>; Huaming Sheng<sup>1</sup>; John Degenstein<sup>1</sup>; Weijuan Tang<sup>1</sup>; Matthew Hurt<sup>2</sup>; Ian Klein<sup>1</sup>; Hilikka Kenttämää<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, U.S.*; <sup>2</sup>*Chevron, Richmond, CA*
- Metabolomics: Untargeted Metabolite Profiling, 578 - 605**
- MP 578 **Sensitivity Increases in Microflow Chromatography for Untargeted Metabolomics in Biomedicine**; Sigurður V. Smáráson<sup>1</sup>; Jason Causon<sup>2</sup>; Baldur Bragi Sigurðsson<sup>1</sup>; Baljit Ubhi<sup>3</sup>; <sup>1</sup>*Center for Biomedicine, European Academy Bozen/Bol, Bolzano, Italy*; <sup>2</sup>*AB SCIEX, Warrington, UK*; <sup>3</sup>*AB SCIEX, Redwood City, CA*
- MP 579 **Development of a Redoxome Platform to Quantify COPD Patient Plasmas for Relative Severity of Oxidative Stress**; Qiuying Chen; Jane Penrose; Ruba Deeb; Crystal Ronald; Steven Gross; *Weill Cornell Medical College, New York, NY*
- MP 580 **Analysis of Metabolites in Human Plasma using GC-TOF MS**; Cristina Di Poto; Yue Luo; Mohammad R Nezami Ranjbar; Rency Varghese; Chi Zhang; Mahlet Tadesse; Habtom Ressom; *Georgetown University, Washington, DC*
- MP 581 **LC-HRMS and Data Mining Tools for the Combined Metabolomic and Lipidomic Serum Profiling of Human Cohorts**; Samia Boudah<sup>1,2</sup>; Etienne Thévenot<sup>3</sup>; Alexandre Seyer<sup>4</sup>; Simon Broudin<sup>4</sup>; Lydie Oliveira<sup>1</sup>; Florence Castelli<sup>1</sup>; Jean-Claude Tabet<sup>5</sup>; Benoit Colsch<sup>1</sup>; Christophe Junot<sup>1</sup>; <sup>1</sup>*LEMM-CEA-Saclay, Gif-Sur-Yvette, France*; <sup>2</sup>*GlaxoSmithKline - Centre de recherche F.Hyafil, Villebon-sur-Yvette, France*; <sup>3</sup>*DRT/LIST/DM2I/LADIS-CEA-Saclay, Gif-sur-Yvette, France*; <sup>4</sup>*Profilomic SA, Boulogne-Billancourt, France*; <sup>5</sup>*LCSOB-UPMC, Paris, France*
- MP 582 **Discriminant Biomarkers of ARDS Associated to H1N1 Influenza Identified by Metabolomics HPLC-QTOF-MS/MS platform**; Alessia Ferrarini<sup>1</sup>; Laura Righetti<sup>1,2</sup>; Francisco J. Rupérez<sup>1</sup>; MPaz Martínez<sup>1</sup>; Federica Pellati<sup>2</sup>; José A. Lorente<sup>3</sup>; Nicolás Nin<sup>3,4</sup>; Coral Barbas<sup>1</sup>; <sup>1</sup>*CEMBIO, San Pablo CEU University, Madrid, Spain*; <sup>2</sup>*Università degli Studi di Modena e Reggio Emilia, Modena, Italy*; <sup>3</sup>*Hospital Universitario de Getafe, CIBERES, Getafe, Madrid, Spain*; <sup>4</sup>*Hospital Universitario de Torrejón, Torrejón, Madrid, Spain*
- MP 583 **UPLC-MS Placental Profiling to Investigate Diseases of Pregnancy**; Elizabeth J Want<sup>1</sup>; Leanne Nye<sup>1</sup>; Julia Langer<sup>1</sup>; Catherine Williamson<sup>2</sup>; Peter Dixon<sup>2</sup>; <sup>1</sup>*Imperial College, London, UK*; <sup>2</sup>*Kings College, London, UK*
- MP 584 **Effect of Ventilation in an Animal Model of Sepsis through a Multiplatform Lung Fingerprinting Approach: From Method Development to Application**; Shama Naz<sup>1</sup>; Yeny Rojas<sup>2</sup>; Leticia Martínez-Caro<sup>3</sup>; Nicolas Nin<sup>4</sup>; Miguel A. de La Cal<sup>2</sup>; Antonia García<sup>1</sup>; José A. Lorente<sup>3</sup>; Coral Barbas<sup>1</sup>; <sup>1</sup>*CEMBIO, Universidad CEU San Pablo, Boadilla, Madrid, Spain*; <sup>2</sup>*Hospital Universitario de Getafe-CIBERES, Madrid, Spain*; <sup>3</sup>*H.U. Getafe-CIBERES, Universida Europea, Madrid, Spain*; <sup>4</sup>*H.U. Getafe-CIBERES, H.U. de Torrejón, Madrid, Spain*
- MP 585 **Strategies for the Interrogation of Dynamic Exometabolomic Profiles from Mock-Organ Bioreactors**; Cody Goodwin<sup>1</sup>; Katrin Zeilinger<sup>4</sup>; Marc Luebberstedt<sup>4</sup>; Ed Darland<sup>6</sup>; Emma Rennie<sup>5</sup>; Rashi Iyer<sup>3</sup>; Srinivas Iyer<sup>3</sup>; John Wikswow<sup>2</sup>; John A. Mclean<sup>2</sup>; <sup>1</sup>*Vanderbilt Univ Dept of Chem, Nashville, TN*; <sup>2</sup>*Vanderbilt University, Nashville, TN*; <sup>3</sup>*Los Alamos National Lab, Los Alamos, NM*; <sup>4</sup>*Charite University, Berlin, Germany*; <sup>5</sup>*Agilent Technologies, Santa Clara, CA*
- MP 586 **Urinary Metabolomics Analysis Reveals the Impact of the Experimental, Surgical Menopause in Rats**; John Cutts; Stephen Barnes; Landon Wilson; Helen Kim; *University of Alabama at Birmingham, Birmingham, AL*
- MP 587 **Development of a Standard Protocol for High-Throughput Metabolome Profiling of Urine using FIA- and nano-ESI Coupled with FT/ICR-MS**; Baivi Xue<sup>1</sup>; Sandra Alves<sup>2</sup>; Francois Fenaille<sup>3</sup>; Benoit Colsch<sup>2</sup>; Jean-Claude Tabet<sup>2</sup>; Richard B. Cole<sup>2</sup>; Alain Paris<sup>4</sup>; Christophe Junot<sup>3</sup>; Estelle Rathahao-Paris<sup>1</sup>; <sup>1</sup>*INRA, AgroParisTech, Equipe IAQA, UMR 1145 Ingéni, Paris, France*; <sup>2</sup>*Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*; <sup>3</sup>*CEA, iBiTec-S, SPI, Gif Sur Yvette, France*; <sup>4</sup>*INRA, AgroParisTech, Mét@ risk, Paris, France*
- MP 588 **Metabolomics and Lipidomics Analysis of Murine Plasma and Aortic Tissue in Low Carbohydrate High Protein Diet in Apolipoprotein E-knockout Mice**; Dajana Vuckovic; Mathilde Triguineaux; Olivia Koury; Andreas Bergdahl; *Concordia University, Montreal, Canada*
- MP 589 **A Data-Independent MS/MS Approach to Metabolomics Profiling**; Anne E. Blackwell<sup>1</sup>; Mark J. Sartain<sup>2</sup>; Daniel Cuthbertson<sup>3</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*; <sup>3</sup>*Agilent Technologies, Denver, CO*
- MP 590 **Comparative Metabolomics Analyses with IMS-MS Techniques to Determine Molecular Changes in Plasma Upon Exposing Rats to TiO<sub>2</sub> Nanoparticles**; Hossein Maleki; Gregory Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- MP 591 **Comparison of LC/MS Data Processing Methods For Lipidomic Data using MZmine 2.10 and Agilent Profinder**; Stephanie Samra; Brian DeFelice; Ingrid Gennity; Oliver Fiehn; *UC Davis, Davis, CA*
- MP 592 **Metabolomic Studies Reveal that Huntingtin Protein is Essential for Mitochondrial Metabolism, Bioenergetics and Structure in Murine Embryonic Stem Cells**; Steven Gross<sup>1</sup>; Qiuying Chen<sup>1</sup>; Ismail Ismailoglu<sup>1</sup>; Lili Yang<sup>1</sup>; Melissa Popowski<sup>2</sup>; Ali Brivanlou<sup>2</sup>; <sup>1</sup>*Weill Cornell Medical College, New York, NY*; <sup>2</sup>*The Rockefeller University, New York, NY*
- MP 593 **Metabolic Signature of Autism Spectrum Disorders Revealed by High Performance Isotope Labeling LC-MS**; Yiman Wu<sup>1</sup>; Chiao-Li Tseng<sup>1</sup>; Sidney Tam<sup>2</sup>; Kelvin SY Leung<sup>3</sup>; Liang Li<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*; <sup>2</sup>*Dept. of Clinical Biochemistry, Queen Mary Hospital, Hong Kong, PR China*; <sup>3</sup>*Hong Kong Baptist University, Hong Kong, PR China*

- MP 594 **Metabolomic Analysis of Human Serum using Isotopic Labeling and High-resolution LC-MS for Parkinson's Disease Biomarker Discovery;** Wei Han; Shraddha Sapkota; Richard Camicioli; Roger Dixon; Liang Li; *University of Alberta, Edmonton, Canada*
- MP 595 **Ion Mobility-MS-Based Metabolic Profiling to Distinguish Cancerous and Non-cancerous Breast Tissue Diseases;** Kelly Hines<sup>1</sup>; Billy Ballard<sup>2</sup>; Dana Marshall<sup>2</sup>; Emma Rennie<sup>3</sup>; John McLean<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Meharry Medical College, Nashville, TN*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- MP 596 **Metabolomic Profiling of Anionic Metabolites in Oral Cancer Cells by Capillary Ion Chromatography HR/AM Mass Spectrometry;** Junhua Wang<sup>1</sup>; Terri Christison<sup>2</sup>; Kaori Misuno<sup>3</sup>; Shen Hu<sup>3</sup>; Ralf Tautenhahn<sup>1</sup>; Linda Lopez<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Sunnyvale, CA*; <sup>3</sup>*School of Dentistry and Jonsson Compre. Cancer Ctr, Los Angeles, CA*
- MP 597 **Creation of Reproducible UHPLC-MS/MS Methodology and Compound Libraries for Clinical Metabolomic Applications;** Li Zhang<sup>1</sup>; Anna Mathew<sup>2</sup>; Jaeman Byun<sup>1</sup>; Kari Bonds<sup>1</sup>; Heidi Baum<sup>1</sup>; Sasha Raskind<sup>1</sup>; Stephen Brown<sup>1</sup>; Charles Burant<sup>1</sup>; Subramaniam Pennathur<sup>2</sup>; <sup>1</sup>*University of Michigan, MRC2, Ann Arbor, MI*; <sup>2</sup>*University of Michigan, Department of Internal Med, Ann Arbor, MI*
- MP 598 **Untargeted Metabolomics Reveals that Ascorbic Acid Attenuates Glycerol Trinitrate-Mediated Activation of the (hypo)Xanthine/Xanthine Oxidase System;** Jaewoo Choi<sup>1</sup>; Eunice Lee<sup>2</sup>; Cristobal L. Miranda<sup>1</sup>; Jan F. Stevens<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*University of Notre Dame, Notre Dame, IN*
- MP 599 **A Serum Metabolomic *in vitro* Diagnostic Multivariate Index Assay for Prostate Cancer Detection;** Xiaoling Zang<sup>1</sup>; Christina Jones<sup>1</sup>; Tran Long<sup>1</sup>; María Eugenia Monge<sup>1,2</sup>; Manshui Zhou<sup>1</sup>; L. DeEtte Walker<sup>1</sup>; Roman Mezencev<sup>1</sup>; Alexander Gray<sup>1</sup>; John McDonald<sup>1</sup>; Facundo Fernández<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*CIBION-CONICET, Ciudad de Buenos Aires, Argentina*
- MP 600 **Metabolomic Study of the Rice Blast Fungus *Magnaporthe oryzae* by GC x GC x QTOFMS;** William Ledford<sup>1</sup>; Margarita Marroquin-Guzman<sup>1</sup>; Richard Wilson<sup>1</sup>; Qingping Tao<sup>2</sup>; Stephen Reichenbach<sup>2</sup>; Zhanpin Wu<sup>3</sup>; Edward Ledford<sup>3</sup>; Sofia Aronova<sup>4</sup>; Jennifer Gushue<sup>4</sup>; Harry Prest<sup>4</sup>; <sup>1</sup>*University of Nebraska at Lincoln, Lincoln, NE*; <sup>2</sup>*GC Image LLC, Lincoln, NE*; <sup>3</sup>*Zoex Corporation, Houston, TX*; <sup>4</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- MP 601 **Examination of Human Serum Samples from Subjects with and without a Chronic Neurodegenerative Disorder;** Jason Winnike<sup>1</sup>; Simon Gregory<sup>1,2</sup>; Xiang Zhang<sup>3</sup>; <sup>1</sup>*David H. Murdock Research Institute, Kannapolis, NC*; <sup>2</sup>*Duke Molecular Physiology Institute, Durham, NC*; <sup>3</sup>*University of Louisville, Louisville, KY*
- MP 602 **Optimizing and Benchmarking Untargeted Metabolomics - Quantitative Evaluation of Instrumentation and Methodology to Allow Cross-Lab Comparisons;** Nathaniel G. Mahieu; Amanda Chen; Kevin Cho; Gary J. Patti; *Washington University, St. Louis, MO*
- MP 603 **Effect of Cinnamaldehyde as an Antibacterial Agent on *E. coli* Growth using 96-blade SPME;** Fatemeh Mousavi; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- MP 604 **Global Profiling of *E. coli* Metabolites using Liquid Chromatography- and Gas Chromatography-Mass Spectrometry;** Kelly H. Telu; Nirina R. Andriamaharavo; Ramesh Marupaka; Xinjian Yan; Yamil Simón-Manso; Stephen E. Stein; *NIST, Gaithersburg, MD*
- MP 605 **Untargeted Metabolomics of *Neurospora crassa* Wild Type and the Os-2 Mutant under Heat Shock Stress and 2-deoxyglucose Treatment;** Yuan Xu; Dana M. Freund; Nora Plesofsky; Robert Brambl; Stephen Brockman; Adrian D. Hegeman; Jerry D. Cohen; *University of Minnesota, St. Paul, MN*
- Metabolomics: Identification of Unknown Metabolites, 606 - 630**
- MP 606 **Identification of Unknown Metabolites in *Chlamydomonas reinhardtii* with Accurate Mass GC-QTOF Mass Spectrometry;** John Meissen<sup>1</sup>; Kohei Takeuchi<sup>2</sup>; Zipora Tietel<sup>1</sup>; Mine Palazoglu<sup>1</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>*UC Davis, Davis, CA*; <sup>2</sup>*Kao Corporation, Tokyo, Japan*
- MP 607 **Characterization of Metabolites from *Medicago truncatula* using Gas Chromatography High Resolution Time-of-Flight Spectrometry – Knowns and Unknowns;** Jeffrey Patrick<sup>1</sup>; Joe Binkley<sup>1</sup>; David Alonso<sup>1</sup>; David Huhman<sup>2</sup>; Feng Qiu<sup>2</sup>; Dennis Fine<sup>2</sup>; Lloyd W. Sumner<sup>2</sup>; <sup>1</sup>*LECO Corporation, St. Joseph, MI*; <sup>2</sup>*Samuel Roberts Noble Foundation, Ardmore, OK*
- MP 608 **Electron and Chemical Ionization on a Novel GC High Resolution Mass Spectrometer – Tools for the Identification of Unknown Metabolites;** Lorne Fell<sup>1</sup>; Jeffrey Patrick<sup>1</sup>; Oliver Fiehn<sup>2</sup>; John Meissen<sup>2</sup>; <sup>1</sup>*LECO Corporation, St. Joseph, MI*; <sup>2</sup>*UC Davis, Davis, CA*
- MP 609 **Targeting and Identifying Trace Metal Metabolites;** Rene Boiteau<sup>1,2</sup>; Daniel Repeta<sup>2</sup>; <sup>1</sup>*Massachusetts Institute of Technology, Cambridge, Massachusetts*; <sup>2</sup>*Woods Hole Oceanographic Institution, Woods Hole, MA*
- MP 610 **Analysis of Flavonoids from Lotus Leaves by Combining Macroporous Resin Chromatography and LC-MS/MS;** Mingzhi Zhu<sup>1</sup>; Lili Jiao<sup>2</sup>; Wei Wu<sup>2</sup>; Mingquan Guo<sup>1,3</sup>; <sup>1</sup>*Wuhan Botanical Garden, Chinese Academy of Science, Wuhan, China*; <sup>2</sup>*Changchun University of Chinese Medicine, Changchun, China*; <sup>3</sup>*University of Southern California, Alhambra, CA*
- MP 611 **Indole Metabolomics: A Facile Means for the Identification of Indolic Compounds from Plant Tissues;** Peng Yu<sup>1</sup>; Janet P. Slovin<sup>2</sup>; Adrian D. Hegeman<sup>1</sup>; Jerry D. Cohen<sup>1</sup>; <sup>1</sup>*University of Minnesota, Saint Paul, MN*; <sup>2</sup>*USDA/ARS, Beltsville, MD*
- MP 612 **Tracking the Cryptic Biochemistry of Specialized Metabolites in the Medicinal Plant *Camptotheca acuminata* using <sup>13</sup>C Isotopic Labeling;** Sujana Pradhan; *Michigan State University, East Lansing, US*
- MP 613 **Development of Compound Identification Technique for Conjugated Unknown Compounds using Ion Trap Time-of-Flight Mass Spectrometry;** Tairo Ogura<sup>1,2</sup>; Akihiro Tai<sup>3</sup>; Takeshi Bamba<sup>2</sup>; Eiichiro Fukusaki<sup>2</sup>; <sup>1</sup>*Shimadzu corporation, Kyoto, Japan*; <sup>2</sup>*Osaka University, Osaka, Japan*; <sup>3</sup>*Prefectural University of Hiroshima, Hiroshima, Japan*
- MP 614 **Development of Tandem Mass Spectral Libraries for Plant Metabolomics and Metabolite Identifications;** Dennis D. Fine<sup>1</sup>; Feng Qiu<sup>1</sup>; Sandy Yates<sup>2</sup>; Romano Hebel<sup>3</sup>; Aiko Barsch<sup>3</sup>; Lloyd W. Sumner<sup>1</sup>; <sup>1</sup>*Plant Biology Division, The Noble Foundation, Ardmore, OK*; <sup>2</sup>*Bruker Daltonics, Fremont, CA*; <sup>3</sup>*Bruker Daltonics, Bremen, Germany*
- MP 615 **Mass Spectral Based Strategies for Rapid Identification of Novel Metabolites Unraveling Evolutionary Patterns of HGL-DTG Biosynthesis in the genus *Nicotiana*;** Sven Heiling<sup>1</sup>; Emmanuel Gaquerel<sup>2</sup>; Aiko Barsch<sup>3</sup>; Arnd Ingendoh<sup>3</sup>; Ian T. Baldwin<sup>1</sup>; <sup>1</sup>*Max Planck Institute for Chemical Ecology, Jena, Germany*; <sup>2</sup>*Centre for Organismal Studies Heidelberg, Heidelberg, Germany*; <sup>3</sup>*Bruker Daltonics, Bremen, Germany*





- MP 616 **Structural Characterization and Fragmentation Rule Generation of Flavonoids using Fragmentation Trees;** Arpana Vaniya; Yan Ma; Tobias Kind; Oliver Fiehn; *UC Davis, Davis, CA*
- MP 617 **De novo Metabolite Identification in the Soil Bacterium *Acinetobacter baylyi* ADP1 using H/D Exchange, ESI/HRMS and MS<sup>n</sup>;** Lucille Stuani<sup>1</sup>; Christophe Lechaplais<sup>1</sup>; Ekaterina Darii<sup>1</sup>; Marcel Salanoubat<sup>1</sup>; Alain Perret<sup>1</sup>; Jean-Claude Tabet<sup>2</sup>; <sup>1</sup>CEA-Genoscope/UMR8030, Evry, France; <sup>2</sup>UPMC-IPCM/CSOB/UMR7201, Paris, France
- MP 618 **Structure Elucidation of Novel Natural Products of Streptomycetes by Molecular Networking and Ion-Mobility Spectrometry;** Andrew R. Johnson<sup>1</sup>; Chan Gao<sup>2</sup>; Marie Elliott<sup>2</sup>; Erin E. Carlson<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>McMaster University, Hamilton, ON, Canada
- MP 619 **LC-TOF MS Profiling of Glutathione Conjugates of Endogenous Oxylipins in *Arabidopsis* leaves;** Jiangyin Bao; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- MP 620 **The Electrochemical Simulation of Selegiline Metabolism Leads to Generation of Amphetamines;** Przemyslaw Mielczarek<sup>1</sup>; Marek Smoluch<sup>1</sup>; Krzysztof Labuz<sup>2</sup>; Piotr Suder<sup>1</sup>; Jerzy Silberring<sup>1,3</sup>; <sup>1</sup>AGH University of Science and Technology, Krakow, Poland; <sup>2</sup>The Rydygier Hospital, Addiction Outpatient Clinic, Krakow, Poland; <sup>3</sup>Centre of Polymer and Carbon Materials, PAN, Gliwice, Poland
- MP 621 **Mapping Distribution of Sulfur-containing Metabolites in Health-promoting Crops by S-omics using Ultrahigh Performance Mass Spectrometry;** Ryo Nakabayashi<sup>1</sup>; Kazuki Saito<sup>1,2</sup>; <sup>1</sup>RIKEN Center for Sustainable Resource Science, Yokohama, Japan; <sup>2</sup>Chiba University, Chiba, Japan
- MP 622 **Cyclic Peptide Substructures Automatically Assigned using Exact Mass ESI/MSMS Data and the MASSPEC Algorithm;** Marshall M. Siegel<sup>1</sup>; Gary Walker<sup>1</sup>; Eugene Ciccimaro<sup>2</sup>; Serhiy Hnatyshyn<sup>2</sup>; <sup>1</sup>MS Mass Spec Consultants, Fair Lawn, NJ; <sup>2</sup>Bristol-Myers Squibb, Lawrenceville, NJ
- MP 623 **Addressing Identification Ambiguity in Untargeted Metabolomics by Processing Raw Spectra into a High Quality Reference Data;** Juraj Lutisan<sup>1</sup>; Yingying Huang<sup>2</sup>; Mark Sanders<sup>2</sup>; Eric Genin<sup>3</sup>; Robert Mistrík<sup>1</sup>; <sup>1</sup>HighChem, Bratislava, Slovakia; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Thermo Fisher Scientific, Villebon sur Yvette, France
- MP 624 **iElement: New UHRMS Signal Handling Approach for More Accurate Elemental Composition Determination;** Wei-Hung Chang<sup>1</sup>; Yu-Chen Huang<sup>1</sup>; Han-Jia Lin<sup>2</sup>; Yet-Ran Chen<sup>1</sup>; <sup>1</sup>Academia Sinica, Taipei, TAIWAN; <sup>2</sup>National Taiwan Ocean University, Keelung, Taiwan
- MP 625 **A New HPLC Retention Database of Metabolites that is Accurate Regardless of the Method or Instrument Used;** Josh Hewitt; Daniel Abate; Baijie Peng; Paul Boswell; *University of Minnesota, St. Paul, MN*
- MP 626 **Template-Based Aligner: A Toolbox for GC-MS Data Analysis;** Yi Yi; Farbod Fazlollahi; Jeffrey Gornbein; Kym Faull; Yingnian Wu; *University of California, Los Angeles, Los Angeles, CA*
- MP 627 **MIDAS: A Database-Searching Algorithm for Metabolite Identification in Metabolomics;** Yingfeng Wang<sup>1</sup>; Ben Bowen<sup>2</sup>; Chongle Pan<sup>1</sup>; <sup>1</sup>Oak Ridge National Lab, Oak Ridge, TN; <sup>2</sup>Lawrence Berkeley National Lab, Berkeley, CA
- MP 628 **Rapid Characterization of Xenometabolome by Direct Introduction Fourier Transform Mass Spectrometry (FTMS) Combined with Post-Acquisition Data Filtering;** Estelle Rathahao-Paris<sup>1</sup>; Sandra Alves<sup>2</sup>; Alain Paris<sup>3</sup>; <sup>1</sup>INRA, UMR 1145 GENIAL, Paris, France; <sup>2</sup>UPMC-IPCM-UMR8232, Paris, France; <sup>3</sup>Muséum National d'Histoire Naturelle, UMR7245, Paris, France
- MP 629 **SWATH Libraries and Common Fragment Libraries for Metabolites Identification in Urine;** Gerard Hopfgartner<sup>1</sup>; Emmanuel Varesio<sup>1</sup>; Lyle Burton<sup>2</sup>; Eva Duchoslav<sup>2</sup>; Ron Bonner<sup>2</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>AB SCIEX, Concord, ON
- MP 630 **Electron Ionization Accurate Mass GC-MS Fragmentation Rules;** Zijuan Lai; Oliver Fiehn; *UC Davis, Davis, CA*
- Metabolomics: Sample Preparation, 631 - 638**
- MP 631 **Comparison of Extraction Methods for Untargeted Lipid Analysis by Liquid Chromatography - Mass Spectrometry (LC-MS);** Rainey Patterson<sup>1</sup>; Richard A. Yost<sup>1</sup>; Timothy Garrett<sup>2</sup>; <sup>1</sup>Chemistry Department, University of Florida, Gainesville, FL; <sup>2</sup>Department of Pathology, University of Florida, Gainesville, FL
- MP 632 **Integrated Metabolic Platform Including Automated Bligh and Dyer Extraction and Dual-Columns UHPLC-MS/MS Separations for the Analyses of Tissues and Cells;** Emmanuel Varesio<sup>1</sup>; Guenter Boehm<sup>2</sup>; Sandra Jahn<sup>1</sup>; Sandrine Cudre Correia De Almeida<sup>1</sup>; Renzo Piconi<sup>2</sup>; Gerard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>CTC Analytics AG, Zwingen, Switzerland
- MP 633 **Assessment of Relative Efficiency and Selectivity of Extraction Methods for Global Metabolomics by LC-MS;** Dmitri Sitnikov; Dajana Vuckovic; *Concordia University, Montreal, CA*
- MP 634 **Pathway Targeted Metabolomics Analysis in Oral Cancer Cells using Capillary Ion Chromatography Coupling to a New HR/AM Mass Spectrometer;** Junhua Wang<sup>1</sup>; Terri Christison<sup>2</sup>; Kaori Misuno<sup>3</sup>; Shen Hu<sup>3</sup>; Linda Lopez<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Sunnyvale, CA; <sup>3</sup>School of Dentistry and Jonsson Comprehensive Canc, Los Angeles, CA
- MP 635 **Solid Liquid Extraction-Determination of levonorgestrel in Plasma by Liquid Chromatography-tandem Mass Spectrometry Method;** Ting Guan<sup>1</sup>; Guotao Lu<sup>2</sup>; <sup>1</sup>Bonna Agela Technologies. Ltd, Tianjin, China; <sup>2</sup>Bonna Agela Technologies. Inc, Wilmington, DE
- MP 636 **Metabolomics of Mammalian Tissues: Optimizing Mode of Anesthesia, Tissue Collection and Extraction Strategies;** Charles Evans; Katherine Overmyer; Nathan Qi; Charles Burant; *University of Michigan, Dept. of Internal Medicine, Ann Arbor, MI*
- MP 637 **Improved Methodology for Quantitative SRM Based LC-MS/MS for the Analysis of AcylCoAs for Rational Design of Synthetic Biology Processes;** Alex Apffel<sup>1</sup>; Laurakay Bruhn<sup>1</sup>; Jeff Hanson<sup>2</sup>; Michelle Chang<sup>2</sup>; <sup>1</sup>Agilent Laboratories, Santa Clara, CA; <sup>2</sup>Dept. of Chemistry, UC Berkeley, Berkeley, CA
- MP 638 **A Novel Sampling Method to Perform Metabolomics Studies Based on Mass Spectrometry Detection for Bio-Processing Applications;** Elie Flux; Jonny Nachtigall; Michael Herold; Ralf Looser; *metanomics GmbH, Berlin, Germany*
- Drug Metabolism: Qualitative Analysis, 639 - 647**
- MP 639 **Cross Platform Comparison of Data Acquisition and Processing using MassMetaSite for Metabolic Soft Spot Identification;** Ismael Zamora<sup>1</sup>; Gisela Backfish<sup>2</sup>; Natasha Penner<sup>3</sup>; Wilson Shou<sup>4</sup>; Anthony Paiva<sup>4</sup>; Don Richards<sup>5</sup>; Matt Willets<sup>5</sup>; Andreas Brink<sup>6</sup>; Thomas Ramp<sup>6</sup>; John Janiszewski<sup>7</sup>; Veronica Zelesky<sup>7</sup>; Carrie Funk<sup>7</sup>; Esra Nurten Cece<sup>8</sup>; Laura Goracci<sup>9</sup>; Diane E. Grotz<sup>10</sup>; Kerry Fillgrove<sup>11</sup>;

- Somang Kim<sup>11</sup>; Kevin Bateman<sup>11</sup>; <sup>1</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; <sup>2</sup>AbbVie, Ludwigshafen, Germany; <sup>3</sup>Biogen Idec, Cambridge, MA; <sup>4</sup>Bristol-Myers Squibb Company, Wallingford, CT; <sup>5</sup>Bruker, Billerica, MA; <sup>6</sup>F. Hoffmann-La Roche Ltd, Basel, Switzerland; <sup>7</sup>Pfizer Inc., Groton, CT; <sup>8</sup>Pompeu Fabra University, Barcelona, Spain; <sup>9</sup>University of Perugia, Perugia, Italy; <sup>10</sup>Merck Research Labs, Kenilworth, NJ; <sup>11</sup>Merck & Co., West Point, PA
- MP 640 **Characterization of Major Metabolites of Victrelis (SCH 503034) in Bile Samples by Extensive Tandem MS Analysis;** Li-Kang Zhang; Merck Research Laboratories, Kenilworth, NJ
- MP 641 **Rapid and Confident Metabolite Profiling and Identification using Bench-Top Orbitrap Q Exactive and New Software;** Kate Comstock<sup>1</sup>; Caroline Ding<sup>1</sup>; Tim Stratton<sup>1</sup>; Kelly Wang<sup>2</sup>; Gene Eiserberg<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Gilead Sciences, Foster City, CA
- MP 642 **Swath MSMS: Smart Data Acquisition Workflows for Metabolite Identification;** Natalia Penner<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Chandra Prakash<sup>1</sup>; <sup>1</sup>Biogen Idec, Cambridge, MA; <sup>2</sup>AB SCIEX, Concord, ON
- MP 643 **Identification of NADPH-Independent GSH Conjugates of Acetylene-Containing Positive Allosteric Modulators of Metabotropic Glutamate Receptor Subtype 5;** Xiaoliang Zhuo; Xiaohua Huang; Andrew Degnan; Lawrence Snyder; Fukang Yang; Huang Hong; Yue-Zhong Shu; Benjamin Johnson; Bristol-Myers Squibb, Wallingford, CT
- MP 644 **Fast Detection of Reactive Metabolites Trapped as GSH Conjugates using Polarity Switching and UHPLC on a Triple Quadrupole Mass Spectrometer;** Lingyi Huang; Ke Huang; Richard B van Breemen; University of Illinois College of Pharmacy, Chicago, IL
- MP 645 **Utilization of AMS and HRMS for Metabolite Profiling and Identification of [<sup>14</sup>C]SSP-002358 in a Human Microtracer Phase 1 study;** Sudheer Bobba<sup>1</sup>; Jie Ding<sup>1</sup>; Goutam Chowdhury<sup>1</sup>; Kristen Cardinal<sup>1</sup>; Randall Press<sup>1</sup>; Claudine Oelke<sup>2</sup>; Todd Pankratz<sup>3</sup>; Marie Croft<sup>3</sup>; Graeme Scarfe<sup>4</sup>; <sup>1</sup>Covance Laboratories Inc., Madison, WI; <sup>2</sup>Covance Clinical Development Services, Madison, WI; <sup>3</sup>Xceleron Inc, Germantown, MD; <sup>4</sup>Shire, Basingstoke, UK
- MP 647 **In Source Fragments? Real Metabolites?;** Min Lin; Jill Pirhalla; Gordon Dear; GlaxoSmithKline, King Of Prussia, PA
- High Accuracy / High Performance MS: Instrumentation, 648 - 660**
- MP 648 **Effect of Extraction Electric Field on Radial Ion Confinement in a Linear Quadrupole Ion Trap Equipped with Angled-Wire Extraction Electrodes;** Steve C. Beu<sup>1</sup>; Yu Chen<sup>2</sup>; Christopher L. Hendrickson<sup>2</sup>; Nathan K. Kaiser<sup>2</sup>; Alan G. Marshall<sup>2,3</sup>; <sup>1</sup>S C Beu Consulting, Austin, TX; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL
- MP 649 **Continuous Atmospheric Pressure Interface Miniature Mass Spectrometer;** Yanbing Zhai<sup>1</sup>; Cunjuan Bian<sup>1</sup>; Yuzhuo Wang<sup>1</sup>; Xiaohua Zhang<sup>2</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology, Beijing, China; <sup>2</sup>Purkinje General, Beijing, China
- MP 650 **Mass-Selective Ion Transmission and Accumulation within an Ion Trap Array;** Yuzhuo Wang<sup>1</sup>; Xiaohua Zhang<sup>2</sup>; You Jiang<sup>3</sup>; Xiang Fang<sup>3</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology, Beijing, China; <sup>2</sup>Beijing Purkinje General Instrument Co.,Ltd, Beijing, China; <sup>3</sup>National Institute of Metrology, Beijing, China
- MP 651 **Fast Ion Mobility Spectrometry and High Resolution TOF MS;** Boris Kozlov<sup>1</sup>; Vasily Makarov<sup>1</sup>; Igor Kurmin<sup>2</sup>; Anatoly Verenchikov<sup>1</sup>; <sup>1</sup>MS Consulting, Bar, Montenegro; <sup>2</sup>Institute for Analytical Instrumentation, RAS, St. Petersburg, Russia
- MP 652 **Achieving the Highest Performance for Protein Identification and SILAC Relative Quantitation on a Benchtop Quadrupole High Field Orbitrap Mass Spectrometer;** Xiaoyue Jiang<sup>1</sup>; Ryan Bomgarden<sup>2</sup>; Daniel Lopez Ferrer<sup>1</sup>; Andreas Huhmer<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Thermo Fisher Scientific, Rockford, IL
- MP 653 **New Developments on a Benchtop Quadrupole-Orbitrap Mass Spectrometer;** Jan-Peter Hauschild; Eduard Denisov; Amelia Peterson; Oliver Lange; Alexander Makarov; Eugen Damoc; Mathias Mueller; Andreas Wieghaus; Markus Kellmann; Thermo Fisher Scientific, Bremen, Germany
- MP 654 **Comprehensive Evaluation of Pre-amplifier Configurations and Performance Parameters for Fourier Transform Ion Cyclotron Resonance Mass Spectrometry at 21 Tesla;** Tzu-Yung Lin<sup>1</sup>; Gordon A. Anderson<sup>1</sup>; Randolph V. Norheim<sup>1</sup>; Franklin E. Leach III<sup>1</sup>; Jared B. Shaw<sup>1</sup>; Aleksey V. Tolmachev<sup>1</sup>; Kristyn M. Roscioli<sup>1</sup>; Peter B. O'Connor<sup>2</sup>; David W. Koppenaal<sup>1</sup>; Errol W. Robinson<sup>1</sup>; Ljiljana Paša-Tolić<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Warwick, Coventry, U.K.
- MP 655 **Utilizing Hydrogen Carrier Gas for High Throughput Gas Chromatography - High Resolution Time of Flight Mass Spectrometry (GC-HRT): Application Compendium;** Joe Binkley; David Alonso; LECO Corporation, St. Joseph, MI
- MP 656 **Towards Routine Anion Isobar Separation for Accelerator Mass Spectrometry;** Jean-François Alary<sup>1</sup>; Reza Javahery<sup>2</sup>; William E. Kieser<sup>3</sup>; Lisa M. Cousins<sup>2</sup>; <sup>1</sup>Isobarex Corp., Bolton ON, CA; <sup>2</sup>IONICS Mass Spectrometry, Bolton ON, CA; <sup>3</sup>University of Ottawa, Ottawa ON, CA
- MP 657 **Design and Evaluation of Two Channel Off-axis Ion Funnel Trap (TCOAIFT) in FTICR Mass Spectrometer;** T-W. Dominic Chan; Liulin Deng; The Chinese University of Hong Kong, Hong Kong, China
- MP 658 **Comparison of V-shape Ion Funnel (V-IF) and Two Channel Off-axis Ion Funnel (TCOAIF) in FTICR Mass Spectrometer;** Liulin Deng; T-W. Dominic Chan; The Chinese University of Hong Kong, Hong Kong, China
- MP 659 **Flying Droplets, Streams using Inductive Electric Fields. How To Do It. Why You Want To;** Drew Sauter; Andrew Sauter III; Nanoliter, LLC, Henderson, NV
- MP 660 **Lipid Profile Coverage Achieved by LC-TOFMS and Direct TOFMS Analysis at 50k, 100k, and 200k Resolution;** Kevin Siek; Viatcheslav Artaev; George Tikhonov; Roza Wojcik; LECO Corporation, Saint Joseph, MI
- Instrumentation: New Concepts, 661 - 676**
- MP 661 **Simultaneous FAIMS Detection without Scanning Compensation Voltage;** Yuichiro Hashimoto; Hideki Hasegawa; Hiroyuki Satake; Masao Suga; Hitachi, Ltd, Central Research Lab, Kokubunji, Tokyo, Japan
- MP 662 **Simulation Study for A Periodic Field Multi-stage Differential Mobility Analyzer (DMA) for Enhanced Resolution;** Jiagi Shen<sup>1</sup>; Kent Gillig<sup>2</sup>; Chung-Hsuan Chen<sup>2</sup>; Wenjian Sun<sup>1</sup>; <sup>1</sup>Shimadzu Research Laboratory of Shanghai, Shanghai, China; <sup>2</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan

- MP 663 **Development and Applications of a Combined FastGC Proton-Transfer-Reaction Mass Spectrometry Instrument;** Lukas Fischer<sup>1</sup>; Alfons Jordan<sup>1</sup>; Andrea Romano<sup>2</sup>; [Christian Lindinger](#)<sup>1</sup>; Jens Herbig<sup>1</sup>; Lukas Märk<sup>1</sup>; Eugen Hartungen<sup>1</sup>; Gernot Hanel<sup>1</sup>; Philipp Sulzer<sup>1</sup>; Franco Biasioli<sup>2</sup>; Tilmann D. Märk<sup>1,3</sup>; <sup>1</sup>*IONICON Analytik GmbH., Innsbruck, AUSTRIA*; <sup>2</sup>*Research and Innovation Centre, FEM, San Michele, Italy*; <sup>3</sup>*University of Innsbruck, Innsbruck, Austria*
- MP 664 **A Real Dual-Source System for Triple Quadrupole Mass Spectrometer;** [Gang Li](#); Gangqiang Li; Hang Zhou, China
- MP 665 **Enhanced Detection Capabilities in Speciation Analysis using HPLC-ICP-MS;** [Peio Riss](#)<sup>1</sup>; Rene Chemnitzer<sup>2</sup>; Meike Hamester<sup>2</sup>; Andrew Toms<sup>3</sup>; <sup>1</sup>*Bruker France, Paris, France*; <sup>2</sup>*Bruker Germany, Bremen, Germany*; <sup>3</sup>*Bruker Canada, Milton, Ontario*
- MP 666 **Improved Performance of Elemental Composition Determination through True Internal Calibration on a Compact MS System;** [Simon J. Prosser](#)<sup>1</sup>; Nigel Sousou<sup>1</sup>; Ming Gu<sup>2</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>*Advion, Inc., Ithaca, NY*; <sup>2</sup>*Cerno Bioscience, Norwalk, CT*
- MP 667 **Laser Ablation APCI-MS for Direct Molecular Analysis of Thin-Layer Chromatography Separations;** [Tim Elseberg](#); Christina Herdering; Michael Sperling; Uwe Karst; *University of Münster, Münster, Germany*
- MP 668 **The Aerolens: An Evaluation Study Based on Computational Methods and Mass Spectrometric Tests;** [Dimitris Papanastasiou](#)<sup>1</sup>; Diamantis Kounadis<sup>1</sup>; Alexander Lekkas<sup>1</sup>; Athanasios Zacharos<sup>2</sup>; Ioannis Nikolos<sup>2</sup>; Ioannis Orfanopoulos<sup>1</sup>; Emmanuel Raptakis<sup>1</sup>; <sup>1</sup>*Fasmatech, Athens, Greece*; <sup>2</sup>*Technical University of Crete, Chania, Greece*
- MP 669 **Tandem Mass Spectrometry using Linear Ion Guides and Digital Waveform Manipulation;** [Peter Ta Reilly](#); Liang Wang; Nathan Hoffman; Gregory Brabeck; *Washington State University, Pullman, WA*
- MP 670 **Duty Cycle Based Ion Isolation and Preconcentration in a Digitally Driven Linear Ion Trap;** [Gregory Brabeck](#); Nathan Hoffman; Liang Wang; Peter Ta Reilly; *Washington State University, Pullman, WA*
- MP 671 **Versatile Solutions to Current Demands for Automated Sample Cleanup, High Throughput, and High Resolution Chromatography on a Single LC-MS Platform;** Catherine Lafontaine<sup>1</sup>; Keeley Murphy<sup>2</sup>; [Joseph DiBussolo](#)<sup>1</sup>; Francois Espourteille<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Franklin, MA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- MP 672 **A Dual Split Gate for Improved Ion Injection;** [Michael W. Senko](#); Philip M Remes; Rexford T. Heller; *Thermo Fisher Scientific, San Jose, CA*
- MP 673 **The After-Life for Radially Ejected Ions in the Linear Ion Trap;** Viatcheslav V. Kovtoun; *Thermo Fisher Scientific, San Jose, CA*
- MP 674 **Tandem Mass Spectrometry using the Atmospheric Pressure-Electron Capture Dissociation (AP-ECD) Ion Source;** [Damon Robb](#)<sup>1</sup>; Jeff Brown<sup>2</sup>; Mike Morris<sup>2</sup>; Michael Blades<sup>1</sup>; <sup>1</sup>*University of British Columbia, Vancouver, Canada*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- MP 675 **Atmospheric Pressure Charge Stripping (AP-CS) for the ESI-MS Analysis of Polymeric Compounds;** Damon Robb<sup>1</sup>; [Jeff Brown](#)<sup>2</sup>; Mike Morris<sup>2</sup>; Michael W. Blades<sup>1</sup>; <sup>1</sup>*University of British Columbia, Vancouver, Canada*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- MP 676 **Development of an SDS and Matrix Removal Platform for On-Line GELFrEE Fractionation and Analysis of Histones with top-Down Mass Spectrometry;** [Ki Hun Kim](#); Philip Compton; Yupeng Zheng; John Tran; Neil L. Kelleher; *Northwestern University, Evanston, IL*
- LCMS Software, 677 - 683
- MP 677 **Dynamic Control of Structures for Lossless Ion Manipulation;** [Brian L. Lamarche](#); Spencer A. Probst; Kevin L. Crowell; Yehia M. Ibrahim; Erin S. Baker; Ian K. Webb; Xinyu Zhang; Tsung-Chi Chen; Sandilya Garimella; Aleksey V. Tolmachev; Keqi Tang; Jonathan T. Cox; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- MP 678 **A Novel Enterprise Quantitative Software Offering for LCMS Bioanalysis;** [Nicholas Duczak, Jr.](#); Ryo Komatsuzaki; Keeley Murphy; David M Brant; *Thermo Fisher Scientific, San Jose, CA*
- MP 679 **A Bayesian Fitness Measure To Score the Results From a Charge State Deconvolution;** Paul Gazis; *Thermo Fisher Scientific, San Jose, CA*
- MP 680 **To See or Not to See – How PPI Predicts the Detectability of Potentially Modified Peptides by Mass Spectrometry;** Jan Muntel<sup>1</sup>; Sarah W. Boswell<sup>2</sup>; [Shaojun Tang](#)<sup>1</sup>; Saima Ahmed<sup>1</sup>; Michael Springer<sup>2</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>*Boston Children's Hospital, Boston, MA*; <sup>2</sup>*Harvard Medical School, Boston, MA*
- MP 681 **MSALAD: A Computational Platform Combining LC, MS and Lectin Data from Glycan Arrays;** [Lisa Parsons](#); Ewa Jankowska; John Cipollo; *FDA, Bethesda, Md*
- MP 682 **A Snippet Wiki, Online Code Playground, and Tool Generator for Spectral Data Algorithms;** [Pieter Kelchtermans](#)<sup>1,2</sup>; Laurent Gatto<sup>3</sup>; Kris Laukens<sup>4</sup>; Dirk Valkenburg<sup>2</sup>; Lennart Martens<sup>1,5</sup>; <sup>1</sup>*UGent, Gent, BE*; <sup>2</sup>*VITO, Mol, BE*; <sup>3</sup>*University of Cambridge, Cambridge, UK*; <sup>4</sup>*Biomina, UAntwerpen, Antwerpen, BE*; <sup>5</sup>*VIB, Gent, BE*
- MP 683 **An Automated Web-Based Interface for the Analysis of LC-MS/MS Proteomic Data using R Scripting and DanteR;** [Jana D. Rucker](#); Lewis K. Pannell; *U. of South Alabama Mitchell Cancer Institute, Mobile, Alabama*
- Photoionization: Instrumentation and Applications, 684 - 686
- MP 684 **Progress in the Development of a GC-APPI Source with Femto Gram Sensitivity;** [Hendrik Kersten](#); Kirsten Haberer; Kai Kroll; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- MP 685 **Trace Analysis of Potential Genotoxic Impurities by Liquid Chromatography with Atmospheric Pressure Photoionization Mass Spectrometry (APPI-LC/MS);** Ryan Cohen; *Merck, Rahway, NJ*
- MP 686 **Evaluation of Atmospheric Pressure Photo Ionization (APPI) for the Measurement of Drugs of Abuse in Urine;** Robert D. Voyksner<sup>1</sup>; [Jack Syage](#)<sup>2</sup>; <sup>1</sup>*LCMS Limited, Durham, NC*; <sup>2</sup>*Morpho Deception Inc, Santa Anna, CA*
- Instrumentation: New Developments in Mass Analyzers, 687 - 707
- MP 687 **Simulations of Ion Motion in Toroidal Ion Traps;** [Jessica M. Higgs](#); Daniel E. Austin; *Brigham Young University, Provo, UT*
- MP 688 **A Mass Analyser Utilising a Toroidal DC Electrostatic Field: A Theoretical Approach;** Will Johnson; *Swansea University, Swansea, UK*
- MP 689 **Large and Small, See Them All. A Study of Dynamic, Signal Dependent Optimization of Detector Gain in Triple Quad MS;** [Felician Muntean](#); Barry Nesmith; Zicheng Yang; Ed George; Desmond Kaplan; *Bruker Daltonics, Fremont, CA*
- MP 690 **Using a Fourier-Transform Quadrupole Ion Trap Operating with Advanced Ion Excitation Methods for High Performance Mass Analysis of Organic Hydrocarbons;** [Michael Schmidt](#)<sup>1</sup>; Albrecht Brockhaus<sup>1</sup>;

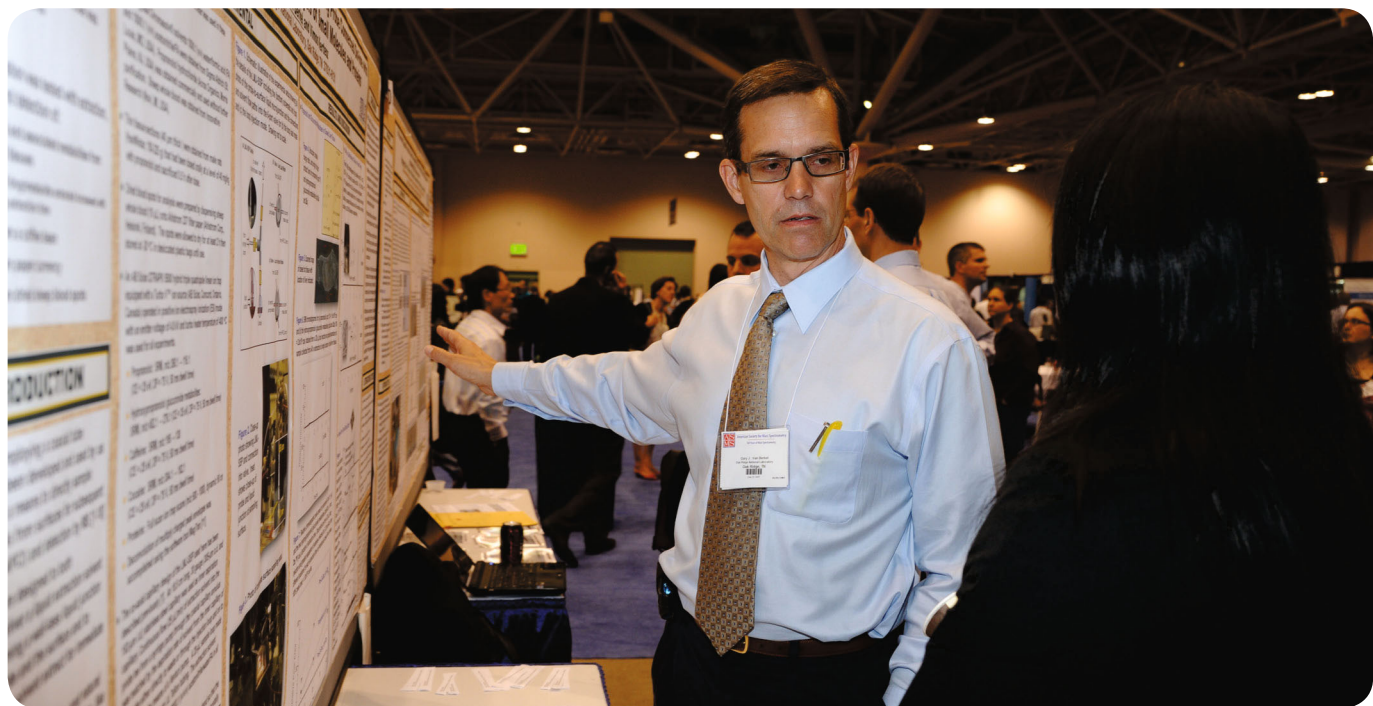
- Klaus Brockmann<sup>1</sup>; Thorsten Benter<sup>1</sup>; Alexander Laue<sup>2</sup>; Michel Aliman<sup>2</sup>; <sup>1</sup>University of Wuppertal, Wuppertal, Germany; <sup>2</sup>Carl Zeiss AG, Oberkochen, Germany
- MP 691 **Microfabricated Silicon Ion Traps for Portable, High Pressure Mass Spectrometry;** Kenion Blakeman; Tina Stacy; Craig Cavanaugh; J. Michael Ramsey; *University of North Carolina, Chapel Hill, NC*
- MP 692 **Tandem Mass Spectrometry using Miniature Cylindrical Ion Traps Operated at Ultra High Pressures;** Andrew Hampton; J. Michael Ramsey; *UNC - Chapel Hill, Chapel Hill, NC*
- MP 693 **Study of the Impact of Gas Flow in a Microscale Ion Trap Operated at High Pressure;** Bruno Coupier; Dmitriy Chernookiy; Sorin Mitran; J. Michael Ramsey; *UNC Chapel Hill, Chapel Hill, NC*
- MP 694 **Optimization of the Cylindrical Ion Trap Geometry USING Mesh Endcaps;** Dmitriy Chernookiy; Bruno Coupier; J. Michael Ramsey; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- MP 695 **An Investigation of the Space of Trajectories in a Novel oa-TOF Geometry;** Keith Richardson; John B Hoyes; *Waters Corporation, Manchester, UK*
- MP 696 **Toroidal Multipole Expansion for the Design of Circular Ion Traps;** Steve Lammert<sup>1</sup>; Ed Lee<sup>1</sup>; Joe Oliphant<sup>1</sup>; Randy Waite<sup>1</sup>; Daniel Austin<sup>2</sup>; Dennis Tolley<sup>2</sup>; Karl Warnick<sup>2</sup>; <sup>1</sup>Torion Technologies, Inc, American Fork, UT; <sup>2</sup>Brigham Young University, Provo, UT
- MP 697 **Development of a Miniature Laser Desorption TOF-MS for Field Portable, High Confidence Detection of Low- and Non-volatile Samples;** Timothy Cornish<sup>1</sup>; Scott Ecelberger<sup>1</sup>; William Brinckerhoff<sup>2</sup>; Stephanie Getty<sup>2</sup>; <sup>1</sup>C&E Research, Inc., Columbia, MD; <sup>2</sup>NASA GSFC, Greenbelt, MD
- MP 698 **Improved Electrostatic Ion Trap for Charge Detection Mass Spectrometry;** Deven Shinholt; Martin Jarrold; *IU Chemistry Dept., Bloomington, IN*
- MP 699 **Simulation, Construction and Experimental Characterization of A Modified Dynamically Harmonized FT-ICR Cell;** Tong Chen<sup>1</sup>; Nathan K. Kaiser<sup>1</sup>; Chad R. Weisbrod<sup>1</sup>; Steven C. Beu<sup>2</sup>; Gregory T. Blakney<sup>1</sup>; John P. Quinn<sup>1</sup>; Daniel G. McIntosh<sup>1</sup>; Vaughan Williams<sup>1</sup>; Christopher L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>S C Beu Consulting, Austin, TX; <sup>3</sup>Dept. of Chem. and Biochem., Florida State Univ., Tallahassee, FL
- MP 700 **Theory and Application of Instantaneous Frequency in FTMS;** Oleg Yu. Tsybin<sup>1</sup>; Anton N. Kozhinov<sup>2</sup>; Konstantin O. Nagornov<sup>2</sup>; Yury O. Tsybin<sup>2</sup>; <sup>1</sup>Saint-Petersburg State Polytechnical University, Saint-Petersburg, Russia; <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- MP 701 **Mapping Ion Cloud Dynamics Reveals Optimal Operation Regimes in FT-ICR MS;** Konstantin O. Nagornov; Anton N. Kozhinov; Yury O. Tsybin; *Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
- MP 702 **Bringing Triple Quadrupole Detection Limits to a New Standard – in Theory and in Practice;** Michael Ugarov<sup>1</sup>; Anabel Fandino<sup>1</sup>; Michael Flanagan<sup>1</sup>; Thomas Glauner<sup>2</sup>; László Toelgyesi<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Agilent Technologies, Waldbronn, Germany
- MP 703 **Accurate Simulation of Image Charge Effects in Cylindrical and Harmonized FT-ICR Cells via Particle-in-Cell Method;** Joshua Driver<sup>2</sup>; Jon Amster<sup>1</sup>; Andriy Kharchenko<sup>1</sup>; Ron M.A. Heeren<sup>3</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Univ of Georgia, Athens, GA; <sup>3</sup>FOM Institute AMOLF, Amsterdam, Netherlands
- MP 704 **Investigation of Image Charge Effects in Electrostatic FT Mass-Analyzers by Computer Simulations;** Gleb Vladimirov<sup>1,2</sup>; Andriy Kharchenko<sup>4,5</sup>; Ron M.A. Heeren<sup>4</sup>; Eugene Nikolaev<sup>1,3</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, RAS, Moscow, Russia; <sup>3</sup>Orekhovich Institute of Biomedical Chemistry, RAMS, Moscow, Russia; <sup>4</sup>FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands; <sup>5</sup>Glushkov Institute of Cybernetics of NAS, Kyiv, Ukraine
- MP 706 **Miniaturized Planar Electrode Linear Ion Trap (LIT) Mass Analyzer;** Ailin Li; Brett J. Hansen; Andrew T. Powell; Yuan Tian; Aaron R. Hawkins; Daniel E. Austin; *Brigham Young University, Provo, UT*
- MP 707 **How Far Can Ion Trap Miniaturization Go? Space-Charge Limits and Scaling Parameters for Very Small Cylindrical Ion Traps (CITs);** Yuan Tian; Daniel Austin; *Brigham Young University, Provo, UT*
- LCMS: Instrumentation, 709 - 726**
- MP 709 **Identification and Quantification of Electrochemically Generated Metabolites of Thyroxine (T4) by Means of LC-ESI-MS and LC-ICP-MS with Counter Gradient Elution;** Chun Kong Mak<sup>1,2</sup>; Christoph A. Wehe<sup>1</sup>; Michael Sperling<sup>1,3</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Muenster, Muenster, Germany; <sup>2</sup>NRW Graduate School of Chemistry, Muenster, Germany; <sup>3</sup>EVISA, Muenster, Germany
- MP 710 **Maximizing Nanoflow Spray Stability and Sensitivity using Automated Emitter Rinsing;** Amanda Berg; Helena Svobodova; Gary A. Valaskovic; *New Objective, Inc., Woburn, MA*
- MP 711 **Validation of an In-Source Micro Flow LC-MS/MS Method for Bioanalysis;** Casey Johnson; Chad Christianson; Shane Needham; Sharon DeChenne; *Alturas Analytics, Moscow, ID*
- MP 712 **Continuous Sampling System for Liquid Chromatography-Mass Spectrometry-Based Detection of Intact Proteins and Small Molecules;** Kendra R. Evans; Braydon L. Dymm; Dominick J. Alton; *University of Detroit Mercy, Detroit, U.S.*
- MP 713 **Preparative Two Dimensional LC-SFC/MS Techniques for the Purification of Organic Compounds from the Complex Mixtures;** Zahid Ali; Mary Ababat; Lu Zeng; *Takeda California, San Diego, CA*
- MP 714 **Applications of Supercritical Fluid Chromatography for Chiral Metabolite Separations in a DMPK Bioanalytical Laboratory;** Hermes Licea Perez<sup>1</sup>; Dana Knecht<sup>1</sup>; Christopher Evans<sup>1</sup>; Mark Wrona<sup>2</sup>; Paul Rainville<sup>2</sup>; <sup>1</sup>Bioanalysis / GSK, King Of Prussia.; <sup>2</sup>Waters, Milford, MA
- MP 715 **A Novel Hybrid SFC/UHPLC/MS System Optimized for Low Peak Dispersion;** Patric Hoerth<sup>1</sup>; Rick Wikfors<sup>2</sup>; Tom A. van de Goor<sup>1</sup>; <sup>1</sup>Agilent Technologies R&D, Waldbronn, Germany; <sup>2</sup>Agilent Technologies, Toughkenamon, PA
- MP 716 **Intelligent Algorithm for Multidimensional Optimization of Time of Flight Instrumentation;** Javier Satulovsky; Huy Bui; Brian Smart; William Frazer; Maithilee Samant; George Stafford; Gregor Overney; *Agilent Technologies, Santa Clara, CA*
- MP 717 **Exploring the Uncharted Depths of the Complex Human Proteome using the Orbitrap Fusion Mass Spectrometer;** Graeme Mcalister; Jesse D. Canterbury; Philip M Remes; Shannon Eliuk; Vlad Zabrouskov; Michael W. Senko; *Thermo Fisher Scientific, San Jose, CA*
- MP 718 **Q-Exactive Plus and Orbitrap Fusion: Determination of Optimal Settings for Peptide and Phosphopeptide Identification;** Thiago Verano-Braga; James Williamson; Alistair Edwards; Ole Nørregaard Jensen; Frank Kjeldsen;

- Martin Røssel Larsen; *University of Southern Denmark, Odense, Denmark*
- MP 719 **Qualitative and Quantitative Comparison of Q Exactive Plus and Orbitrap Fusion for Label Free and Isobaric Tag Based Quantification;** James Williamson; Thiago Verano-Braga; Alistair Edwards; Ole Nørregaard Jensen; Frank Kjeldsen; Martin Røssel Larsen; *University of Southern Denmark, Odense, Denmark*
- MP 720 **Robustness Study of Peptides in Plasma using Novel Technologies in an LC-MS Instrument;** Karen Salomon; Maurizio Splendore; Louis Maljers; Zicheng Yang; Steven Schachterle; *Bruker, Fremont, CA*
- MP 721 **Extending Inter Scan Linear Dynamic Range on a QqTOF platform;** Feng Zhong; Doug Simmons; J.C. Yves Leblanc; Nic Bloomfield; *AB SCIEX, Concord, On, Canada*
- MP 722 **Electron Ionization in LC-MS: Increasing Selectivity and Sensitivity;** Achille Cappiello<sup>1</sup>; Hanno Evard<sup>2</sup>; Giorgio Famiglioni<sup>1</sup>; Pierangela Palma<sup>1</sup>; Veronica Termopoli<sup>1</sup>; <sup>1</sup>*University of Urbino, Urbino, Italy*; <sup>2</sup>*University of Tartu, Tartu, Estonia*
- MP 723 **Improved Sensitivity for Shotgun Proteomics on an ES TOF Instrument through a Combination of Acetonitrile Dopant and Zero Dead-Volume CaptiveSpray;** Scarlet Beck<sup>1</sup>; Igor Paron<sup>1</sup>; Annette Michalski<sup>2</sup>; Stephanie Kaspar<sup>2</sup>; Markus Lubeck<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Juergen Cox<sup>1</sup>; Matthias Mann<sup>1</sup>; <sup>1</sup>*Max Planck Institute of Biochemistry, Martinsried, Germany*; <sup>2</sup>*Bruker Daltonik GmbH, Bremen, Germany*
- MP 724 **Coupling Laser Ablation Sample Transfer and LC-ESI-MS for tissue imaging;** Fabrizio Donnarumma; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- MP 725 **Capillary Exit Voltage-Induced vs. CID Fragmentation Behavior of Four Antiviral Drugs in an Agilent Ion Trap Mass Spectrometer;** Mohamed W Attwa; Nasser Salem; Ali S. Abdelhameed; A. F. M. Motiur Rahman; Adnan A. Kadi; *King Saud University, Riyadh, Saudi Arabia*
- MP 726 **A Comparative Study of Chalcones Fragmentation: Induced In-source Fragmentation in ESI-Triple Quadrupole with MS3 in ESI-Ion Trap;** Adnan A Kadi; Mohamed W. Attwa; A. F. M. Motiur Rahman; *King Saud University, Riyadh, Saudi Arabia*
- LCMS Chromatography, 727 - 752**
- MP 727 **Spectroscopic Investigation in Differentiating Random from Block Polyether Copolymers using Reversed-Phase LC Coupled with ELSD or MS;** Robielyn Ilagan; Shenmin Pan; Ernest Long; *MacDermid Electronics Solutions, Waterbury, CT*
- MP 728 **Combining Mass Spectra with UV Spectra for Orthogonal Chromatographic Detection and Peak Identification;** Thomas E. Wheat<sup>1</sup>; Aparna Chavali<sup>2</sup>; Sean McCarthy<sup>2</sup>; Paula Hong<sup>2</sup>; Patricia McConville<sup>2</sup>; <sup>1</sup>*Waters Corporation, Hopedale, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- MP 729 **Routine MS Detection Applied to USP Chromatographic Methods;** Thomas E. Wheat<sup>1</sup>; Daniel Root<sup>2</sup>; Aparna Chavali<sup>2</sup>; Patricia McConville<sup>2</sup>; <sup>1</sup>*Waters Corporation, Hopedale, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- MP 730 **Applicability of novel Supercritical Fluid Chromatography Tandem Quadrupole-Time of Flight Mass Spectrometry;** Jianzhong Li; Ying Meng; Tao Bo; Rong An; *Agilent Technologies(China), Beijing, China*
- MP 731 **Coupling of HPLC with ESI-MS for Studying the Aging of Ultrasmall Multimodal Nanoparticles;** Charles Truillet; François Lux; Olivier Tillement; Philippe Dugourd; Rodolphe Antoine; *Institut Lumière Matière, UMR5306 Université Lyon, Villeurbanne, France*
- MP 732 **Sensitivity of Detection of 12 Aminoglycoside Antibiotics by Positive ESI – Comparison between HILIC and Reverse Phase Methods;** Olga Shimelis; Emily Barrey; Dave Bell; Craig Aurand; *Sigma-Aldrich, Bellefonte, PA*
- MP 733 **Orthogonal Fast and Ultra-Fast Reverse Phase Chiral LC/MS Methods for the Analysis of Stereoisomeric Pharmaceutical Compounds;** Alfonso Espada; Cristina Anta; *Lilly S.A., Alcobendas, Spain*
- MP 734 **Improved LC-MS/MS Method for the Quantitation of the Plant Hormones Abscisic Acid and Indole-3-Acetic Acid;** Yongxin Nie<sup>1</sup>; Yinggao Liu<sup>1</sup>; Hongxia Jiang<sup>1</sup>; Ron Orlando<sup>2</sup>; <sup>1</sup>*ShanDong Agricultural University, Taian, SD*; <sup>2</sup>*University of Georgia, Athens, GA*
- MP 735 **Development of a Sensitive LC/MC/MS Assay for the Analysis of Total Testosterone and Steroids in Human Serum;** Liming Peng<sup>1</sup>; Cheni Krishnan<sup>2</sup>; Eric Davis<sup>2</sup>; Xiaohong Chen<sup>1</sup>; Bhasin Shalender<sup>1</sup>; <sup>1</sup>*Brigham and Women's Hospital, Boston, Massachusetts*; <sup>2</sup>*AB Sciex, Foster City, CA*
- MP 736 **The Application of Multiple LC/MS Methods to Help Determine the m/z of a Low Level Impurity in a Drug Product;** Wendy Hengwen Zhong; Michael Matchett; Randy Wilhelm; *Mallinckrodt, Saint Louis, MO*
- MP 737 **Selection of Negative Mode Standard in LC-MS under Neutral Condition for Assessing Solvent Quality;** Subhra Bhattacharya; Deva H. Puranam; Stephen C. Roemer; *Thermo Fisher Scientific, Fair Lawn, NJ*
- MP 738 **Improved Automated Reversed-Phase HPLC-MS Methods for Quantitative Amino Acid Analysis;** Keely Glass<sup>1</sup>; Jen Skerritt<sup>1</sup>; Carol Jiang<sup>1</sup>; Roman Lin<sup>1</sup>; George Dubai<sup>1</sup>; Amy Huang<sup>1</sup>; John Simon<sup>1,2</sup>; <sup>1</sup>*Duke University, Durham, NC*; <sup>2</sup>*Univeristy of Virginia, Charlottesville, VA*
- MP 739 **Analysis of D- and L-amino Acids using Automated Pre-Column Derivatization and Liquid Chromatography-Electrospray Ionization Mass Spectrometry;** Kenichiro Tanaka<sup>1</sup>; Hidetoshi Terada<sup>2</sup>; Yoshiko Hirao<sup>2</sup>; Kiyomi Arakawa<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>*Shimadzu Scientific Instruments, Inc., Columbia, MD*; <sup>2</sup>*Shimadzu Corporation, Kyoto, Japan*
- MP 740 **Development of a Novel Amino Acids Analysis Column for LC-MS without Derivatization;** Itaru Yazawa; Hiroshi Tachikawa; *Imtakt Corporation, Kyoto, Japan*
- MP 741 **LC-MS Analysis of "Dirty" Food and Pharma Samples with Monolithic Silica Columns;** Stephan Altmaier; Egidijus Machtejevas; Karin Cabrera; *Merck Millipore, Merck KGaA, Darmstadt, Germany*
- MP 742 **Full Optimization of LCMS Methods to Increase Robustness of Complicated Matrix Containing Samples using Active Flow Management Chromatography;** Eric Stover<sup>1</sup>; Mark Dreyer<sup>1</sup>; Mary Blackburn<sup>1</sup>; Luisa Pereira<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Runcorn, Cheshire, UK*
- MP 743 **Analyzing Highly Organic Samples, Polar Analytes, and Large Volume Injections using Microflow Chromatography Coupled with Mass Spectroscopy;** Subodh Nimkar<sup>1</sup>; Khaled Mriziq<sup>1</sup>; Leo Wang<sup>2</sup>; <sup>1</sup>*SCIEX Separations, Division of AB SCIEX, Redwood City, CA*; <sup>2</sup>*AB SCIEX, Redwood City, CA*
- MP 744 **Fabrication of Stage-Frit NanoLC column for Proteomic Analysis;** Ming-Yueh Hsieh; He-Hsuan Hsiao; *NCHU, Department of Chemistry, Taichung, Taiwan*
- MP 745 **Advancing Host Cell Protein Analyses through Improved Microscale Peptide Separations and 2D UHPLC Chromatography;** Matthew Lauber; Catalin Doneanu; Stephan Koza; Weibin Chen; Kenneth Fountain; *Waters Corporation, Milford, MA*

- MP 746 **Design and Evaluation of a Modified Salt Pulse Scheme for Increased Measurement Depth in a MudPIT Proteome Experiment;** Ramsunder Iyer<sup>1,2</sup>; Richard J. Giannone<sup>1</sup>; Robert Hettich<sup>1</sup>; <sup>1</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*; <sup>2</sup>*University of Tennessee, Knoxville, TN*
- MP 747 **Finding the Appropriate LC Setup for Proteomics Experiments Depending on the Sample Complexity using Chip-Based Columns;** Jan Muntel<sup>1</sup>; Helena Svobodova<sup>2</sup>; Gary A. Valaskovic<sup>2</sup>; Saima Ahmed<sup>1</sup>; Kevin Broadbelt<sup>1</sup>; Omar Barnaby<sup>1</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>*Boston Children's Hospital, Boston, MA*; <sup>2</sup>*New Objective, Woburn, MA*
- MP 748 **Improved Protein Identification by nanoLC/MS/MS using Chip Based Columns with Integrated Post-Column Addition of DMSO for Increased Sensitivity;** Remco van Soest<sup>1</sup>; Christie Hunter<sup>2</sup>; Hao Yang<sup>1</sup>; <sup>1</sup>*Sciex Separations, Redwood City, CA*; <sup>2</sup>*AB SCIEX, Redwood City, CA*
- MP 749 **Normal Phase LC/MS Post Additive Infusion for Vitamin D3 EP Method 01/2013:0072 With No LC Modifications;** Keith Rippel; *Pfizer Consumer Healthcare, Richmond, VA*
- MP 750 **Enhancing MS Sensitivity in Negative Electrospray Mode by Post-Column Addition of a Modifier;** Angela Doneanu<sup>1</sup>; James Murphy<sup>2</sup>; <sup>1</sup>*Waters, Milford, MA*; <sup>2</sup>*Waters Corporation, Milford, MA*
- MP 751 **Optimization of Intact Protein RP-LC-MS Analysis using a Characterized Standard Protein Mix;** Benjamin Cutak; Jim Blasberg; Gordon Nicol; Kevin Ray; *Sigma-Aldrich, Saint Louis, MO*
- MP 752 **Assessment of the Effects of Intact Protein Mass Measurements by On-Line Liquid Chromatography Coupled with Mass Spectrometry;** Jinghua Zhu; Qishan Lin; *State University of New York at Albany, Rensselaer, NY*
- LCMS Sample Preparation I (Drugs and Metabolites), 753 - 786**
- MP 753 **Automating On-Line Extraction, Derivatization and Cleanup with LC-MS to Measure Estrogens in Biological Fluids;** Jennifer Poshkus<sup>1</sup>; Heather Heilman<sup>1</sup>; Joseph Di Bussolo<sup>2</sup>; <sup>1</sup>*West Chester University of Pennsylvania, West Chester, PA*; <sup>2</sup>*Thermo Fisher Scientific, West Chester, PA*
- MP 754 **LC-MS/MS with Novel Online Cleanup Valving Solution for Quantitative Analysis of Testosterone in Serum;** Andre Szczesniowski; Sheher Bano Mohsin; *Agilent Technologies, Schaumburg, IL*
- MP 755 **Analysis of Vitamin D3 in Dietary Supplements by 2-dimensional LC System;** Taku Tsukamoto; Kazuhiro Sonomura; Keiko Yamabe; Kiyomi Arakawa; Yoshihiro Hayakawa; *Shimadzu Corporation, Kyoto, Japan*
- MP 756 **A Reduced Workflow Method for the Extraction of Vitamin B7 from Human Serum with No Drydown Prior to Mixed-Mode LC-MS/MS;** Frank Kero; Victor Vandell; Lee Williams; Geoff Davies; Adam Senior; Rhys Jones; Helen Lodder; Elena Gairloch; Claire Desbrow; Wendy Hartsock; *Biotage, Charlotte, NC*
- MP 757 **Comparison of SPE Approaches for the Extraction of Thyroid Hormones: T3, rT3 and T4 prior to LC-MS/MS Analysis;** Lee Williams<sup>1</sup>; Helen Lodder<sup>1</sup>; Adam Senior<sup>1</sup>; Rhys Jones<sup>1</sup>; Alan Edgington<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage LLC, Charlotte, NC*
- MP 758 **Supported Liquid Extraction of Vitamin D Metabolites: 25-hydroxy and 1 $\alpha$ ,25-dihydroxy Vitamin D<sub>2</sub>/D<sub>3</sub> using PTAD Derivatization Prior to LC-MS/MS Analysis;** Rhys Jones<sup>1</sup>; Alan Edgington<sup>1</sup>; Lee Williams<sup>1</sup>; Adam Senior<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>*Biotage GB Limited, Cardiff, UK*; <sup>2</sup>*Biotage LLC, Charlotte, NC*
- MP 759 **Vitamin D Metabolites in Serum: Extraction using Phospholipid Depletion Technology (PLD) Prior to UPLC-MS/MS Analysis;** Victor Vandell<sup>1</sup>; Lee Williams<sup>2</sup>; Alan Edgington<sup>2</sup>; Frank Kero<sup>1</sup>; Elena Gairloch<sup>1</sup>; Rhys Jones<sup>2</sup>; Adam Senior<sup>2</sup>; <sup>1</sup>*Biotage, Charlotte, NC*; <sup>2</sup>*Biotage GB Limited, Cardiff, N/A*
- MP 760 **Extraction of Antiepileptic Drugs from Biological Fluids using Supported Liquid Extraction (ISOLUTE® SLE+) in 96-Well Plate Prior to LC-MS-MS Analysis;** Victor Vandell<sup>1</sup>; Frank Kero<sup>1</sup>; Elena Gairloch<sup>1</sup>; Lee Williams<sup>2</sup>; Adam Senior<sup>2</sup>; Rhys Jones<sup>2</sup>; Geoff Davies<sup>2</sup>; Alan Edgington<sup>2</sup>; <sup>1</sup>*Biotage, Charlotte, NC*; <sup>2</sup>*Biotage GB Limited, Cardiff*
- MP 761 **Extraction of Mycophenolic Acid and Mycophenolic Acid Metabolite from Serum using Supported Liquid Extraction Prior to LC-MS-MS Analysis;** Victor Vandell<sup>1</sup>; Frank Kero<sup>1</sup>; Elena Gairloch<sup>1</sup>; Lee Williams<sup>2</sup>; Adam Senior<sup>2</sup>; Rhys Jones<sup>2</sup>; Geoff Davies<sup>2</sup>; Alan Edgington<sup>2</sup>; Martin Cherrier<sup>1</sup>; <sup>1</sup>*Biotage, Charlotte, NC*; <sup>2</sup>*Biotage GB Limited, Cardiff, N/A*
- MP 762 **Single Step Separation of Plasma from Whole Blood without the Need for Centrifugation Applied to the Quantitative Analysis of Warfarin;** Alan J Barnes<sup>1</sup>; Adam McMahon<sup>2</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*WMIC, University of Manchester, Manchester, UK*
- MP 763 **Fully Automated Analysis of Immunosuppressant Drugs with ZinMass-200 Clinical LC-MS/MS Analyzer;** Murat Celik; Huseyin Awni Cavdar; *ZIVAK Technologies, Istanbul, Turkey*
- MP 764 **Challenges and Strategies in Developing an Ultrafiltration/LC/MS/MS Assay for Quantitation of Unbound Paclitaxel in Human Plasma Following Abraxane Treatment;** Linge Li; Michael P. Waldron; Bruce Hidy; Rand Jenkins; *PPD, Richmond, VA*
- MP 765 **Troubleshooting of Low Recovery of LC-MS Method for 2-Hydroxypyridine-N-oxid (HOPO) in a Drug Candidate Substance during Technical Transfer;** Gang Tang; Qinggang Wang; Peter Tattersal; *Bristol-Myers Squibb, New Brunswick, NJ*
- MP 766 **Removal of Phospholipids using Phosphate-Selective Sorbent;** Chiaki Aoyama; Shigenori Ota; Yuko Yui; Kosuke Osaka; Masakazu Takahashi; Masayoshi Ohira; *GL Sciences Inc., Shinjuku-Ku, Japan*
- MP 767 **Extraction of Telmisartan from Human Plasma using an Improved Capacity Supported Liquid Extraction (SLE) 96-well Plate;** Matthew Cleeve; Tina Ovitt; *Kinesis, St Neots, UK*
- MP 768 **Extraction of Indomethacin and Ibuprofen from Small Volume Biological Fluid Samples using a New Versatile  $\mu$ Elution SPE 96-well Plate Format;** Matthew Cleeve; *Kinesis, St Neots, UK*
- MP 769 **Quantification of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL) in Urine using Solid-Phase Extraction and UPLC-ES/MS/MS;** Kellie Woodling<sup>1</sup>; Frank Kero<sup>2</sup>; Victor Vandell<sup>2</sup>; Goncalo Gamboa da Costa<sup>1</sup>; <sup>1</sup>*NCTR, Jefferson, AR*; <sup>2</sup>*Biotage, Charlotte, NC*
- MP 770 **High-Throughput SPME-UPLC-MS as a Convenient Method for the Simultaneous Determination of Various Prohibited Substances in Urine and Plasma;** Nathaly Reyes-Garcés; Ezel Boyaci; Krzysztof Gorynski; Ángel Rodríguez-Lafuente; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- MP 771 **A New Approach to Automated Method Development for LC-MS/MS Sample Preparation;** Guy Burssens<sup>1</sup>; Roland Geyer<sup>1</sup>; Jeffrey Enders<sup>2</sup>; <sup>1</sup>*Tecan, Männedorf, Switzerland*; <sup>2</sup>*Ameritox, Ltd., Greensboro, TN*



- MP 772 **Automated Hydrolysis, DPX Extraction and LC/MS/MS Analysis of Pain Management Drugs from Urine;** Fred Foster<sup>1</sup>; Oscar Cabrices<sup>1</sup>; John Stuff<sup>1</sup>; Edward Pfannkoch<sup>1</sup>; William Brewer<sup>2</sup>; <sup>1</sup>Gerstel, Inc., Linthicum, MD; <sup>2</sup>University of South Carolina, Columbia, SC
- MP 773 **Utilizing Beta Glucuronidase Enzymatic Digest for LC/MS Analysis for Glucuronide Metabolites;** Craig Aurand; Dave Bell; Emily Barrey; Olga Shimelis; *Sigma Aldrich, Bellefonte, PA*
- MP 774 **Aminoglycoside Analysis in Pork Muscle using Molecularly Imprinted Polymer Cleanup and LC-MS/MS Detection;** Emily Barrey; Olga Shimelis; Carmen Santasania; Xiaoning Lu; *Sigma-Aldrich, Bellefonte, PA*
- MP 775 **Identification and Quantification of Lignin Degradation Products in Highly Saline Mixtures by Two-Stage HPLC Coupled with ESI Tandem Mass Spectrometry;** Hanyu Zhu<sup>1</sup>; Christopher Marcum<sup>1</sup>; Christopher Gulvik<sup>2</sup>; Alison Buchan<sup>2</sup>; Hilikka Kenttämää<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>University of Tennessee, Knoxville, TN
- MP 776 **A New Fully Automated Online SPE/HPLC-MS/MS Method for the Determination of Phenoxycarboxylic Acids in Water;** Franziska Chmelka<sup>1</sup>; Oscar Cabrices<sup>2</sup>; Edward Pfannkoch<sup>2</sup>; <sup>1</sup>Labor Dr. Helle GmbH & Co.KG, Bremerhaven, Germany; <sup>2</sup>Gerstel Inc., Linthicum, MD
- MP 777 **Simplified Dioxin Sample Preparation using a Novel Carbon Adsorbent;** Dr. Conor Smith; *United Science Corp, Minneapolis, MN*
- MP 778 **Removing Phthalate Contamination from Organic Solvents using a Novel Carbon Sorbent;** Doug Fryer; *United Science Corp, Minneapolis, MN*
- MP 779 **New Solvent Grade Targeted for Trace Analysis by UHPLC-MS;** Subhra Bhattacharya; Deva H. Puranam; Stephen C. Roemer; *Thermo Fisher Scientific, Fair Lawn, NJ*
- MP 780 **Aminopyrene and Aminopyrene-based GUMBOS as Novel Matrices for MALDI-MS;** Hashim Alghafly; Kermit K. Murray; Isiah M. Warner; *Baton Rouge, LA*
- MP 781 **Bioanalytical Considerations for Utilizing a Capillary Micro-sampling Device for Plasma Collection and Isolation with LC-MS Detection;** Sharon Boram<sup>1</sup>; Chester L Bowen<sup>1</sup>; Jim Kenney<sup>2</sup>; Joseph Siple<sup>2</sup>; <sup>1</sup>GlaxoSmithKline, King Of Prussia, PA; <sup>2</sup>Drummond Scientific, Broomall, PA
- MP 782 **A Simplified Load-Wash-Elute Solid Phase Extraction Protocol for the Oasis® HLB µElution Plate;** Xin Zhang; Pamela Iraneta; Frank Marszalkowski; *Waters Corp, Milford, MA*
- MP 783 **Evaluation of a Novel 96-well Filter Plate for the Effective Removal of Serum Protein and Phospholipids prior to LC-MS/MS Analysis;** Lee Williams<sup>1</sup>; Helen Lodder<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Plant<sup>1</sup>; Adam Senior<sup>1</sup>; Alan Edgington<sup>1</sup>; Rhys Jones<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, UK; <sup>2</sup>Biotage, Charlotte, NC
- MP 784 **Assessing Efficiency of Matrix Cleanup using Concise LC-QQQ Methods of Lipid Detection;** Irina Dioumaeva<sup>1</sup>; Bruce Richter<sup>2</sup>; <sup>1</sup>Agilent Technologies, Inc., Lake Forest, CA; <sup>2</sup>Agilent technologies, Inc., Little Falls, DE
- MP 785 **Evaluation of Electrospray Ionization Effects on Jurkat-T Human Leukemia Cell Washing Buffers & Lipid Extraction Methods by LC-MS;** Candice Ulmer<sup>1</sup>; Jing Chen<sup>2</sup>; Timothy Garrett<sup>3</sup>; Clayton Matthews<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>Dept. of Chemistry, Univ of Florida, Gainesville, FL; <sup>2</sup>Immunology & Laboratory Science, Univ of Florida, Gainesville, FL; <sup>3</sup>CTSI, Dept. of Pathology, Univ of Florida, Gainesville, FL
- MP 786 **The Impact of Euthanasia Methods and Preanalytical Sample Handling in Lipid Analysis;** Fredrik Jernerén<sup>4</sup>; Jörg Hanrieder<sup>2</sup>; Marcus Söderquist<sup>3</sup>; Oskar Karlsson<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Chalmers Tech. University, Gothenburg, Sweden; <sup>3</sup>Denator, Uppsala, Sweden; <sup>4</sup>University of Oxford, Oxford, UK



7:30 – 8:00 am..... Set up all Tuesday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 7:30 – 8:00 pm..... Remove all Tuesday posters

Imaging MS: Method Development .....001-013  
 Imaging MS: Small Molecules and Drugs.....014-046  
 Imaging MS: Disease Markers .....047-073  
 Informatics: Peptide Identification and Characterization .....074-091  
 Informatics: Post-Translational Modifications .....092-100  
 Proteins: MTMS .....101-131  
 Proteins: Complexes .....132-147  
 Protein Therapeutics: Structural Characterization .....148-161  
 Phosphopeptides: Sequence Analysis .....162-164  
 Peptidomics .....165-172  
 Peptides: Quantitative Analysis (New Approaches to Data Acquisition and Analysis).....173-186  
 Proteomics: New Approaches .....187-208  
 Microorganisms: Identification and Characterization.....209-232  
 Antibodies and Antibody: Drug Conjugates .....233-252  
 Biosimilars .....253-266  
 Food Safety .....267-285  
 Lipids: Identification and Structural Analysis .....286-299  
 Toxicology .....300-312

Carbohydrates .....319-337  
 Ion/Molecule, Ion/Ion, Ion/Electron Interactions .....338-360  
 Ion Spectroscopy .....361-372  
 Ambient Ionization: Instrumentation .....373-379  
 Ambient Ionization: Applications .....380-409  
 MALDI Sample Preparation .....410-420  
 Biomarkers: Discovery .....421-442  
 Disease Biomarkers .....443-458  
 Biomarkers: Quantitative Analysis .....459-488  
 Small Molecule Quantitation .....489-523  
 Small Molecules Qualitative Analysis .....524-535  
 H/D Exchange: Hardware, Software, and Methodology .....536-547  
 Environmental Analysis: Pharmaceuticals and Pesticides .....549-583  
 Energy: Hydrocarbon and Petrochemical .....584-610  
 Drug Metabolism: Qualitative Analysis .....611-636  
 Metabolomics: Untargeted Metabolite Profiling .....637-666  
 Plant"omics" .....667-680  
 Approaches to Quantitation .....681-694  
 Instrumentation: New Concepts .....709-724  
 Instrumentation: New Developments in Ionization and Sampling .....725-745  
 GCMS: Instrumentation and Applications .....746-772  
 Polymers .....773-792

**Imaging MS: Method Development, 001 - 013**

- TP 001 **High-Throughput Single Cell Profiling via Optically-Guided MALDI-TOF MS;** Ta-Hsuan Ong; David Kissick; Stanislav Rubakhin; Jonathan Sweedler; *University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 002 **Imaging of Lipids in Kidney using Silver Nanoparticles;** Shelley N Jackson<sup>1</sup>; Ajay Kailas<sup>1</sup>; Ludovic Muller<sup>1</sup>; Aurelie Roux<sup>1</sup>; J Albert Schultz<sup>2</sup>; Amina S. Woods <sup>1</sup>; <sup>1</sup>*NIDA-IRP, NIH, Baltimore, MD*; <sup>2</sup>*Ionwerks Inc, Houston, TX*
- TP 003 **Imaging of N-linked Glycans from Formalin-fixed Paraffin-embedded Tissue Sections Using MALDI Mass Spectrometry;** Shadi Toghi Eshghi; Shuang Yang; Punit Shah; Jered Pasay; Xingde Li; Hui Zhang; *Johns Hopkins University, Baltimore, MD*
- TP 004 **Lipid Visualisation and Identification through collision Cross Section Aided Correlation of MALDI Imaging and MS/MS Fragmentation Data Sets;** Mark Towers; Emmanuelle Claude; Johannes Pc Vissers; *Waters Corporation, Manchester, UK*
- TP 005 **Comprehensive Characterization of the Mouse Brain Proteome Sampled in Mass Spectrometry Imaging studies;** Bram Heijis<sup>1</sup>; Ricardo J. Carreira<sup>1</sup>; Reinald Shyti<sup>2</sup>; Arn van den Maagdenberg<sup>2</sup>; Peter van Veelen<sup>3</sup>; Liam McDonnell<sup>1</sup>; <sup>1</sup>*Center for Proteomics and Metabolomics, LUMC, Leiden, The Netherlands*; <sup>2</sup>*Department of Human Genetics, LUMC, Leiden, The Netherlands*; <sup>3</sup>*Dept of Immunohematology & Blood Transfusion, LUMC, Leiden, The Netherlands*
- TP 006 **Correlated Imaging Mass Spectrometry and Raman Spectroscopy for Oncology and Drug Resistance;** Dorothy Ahlf<sup>1</sup>; Amanda B. Hummon<sup>2</sup>; Paul Bohn<sup>2</sup>; <sup>1</sup>*University of Notre Dame, South Bend, IN*; <sup>2</sup>*University of Notre Dame, Notre Dame, IN*
- TP 007 **On-Chip Characterization of Brain Tumor Heterogeneity and Single-Cell Drug Susceptibility Analysis by Mass Spectrometry Imaging;** David Calligaris<sup>1</sup>; Denis Loginov<sup>2</sup>; Revaz Machaidze<sup>1</sup>; Isaiah Norton<sup>1</sup>; Daniel R. Feldman<sup>3</sup>; John A. Alberta<sup>4</sup>; Charles D. Stiles<sup>4</sup>; Christopher J. Love<sup>2</sup>; Nathalie Y. R. Agar<sup>1</sup>; <sup>1</sup>*Department of Neurosurgery, BWH/HMS, Boston, MA*; <sup>2</sup>*Department of Chemical Engineering, MIT, Cambridge, MA*; <sup>3</sup>*Department of Pathology, BWH/HMS, Boston, MA*; <sup>4</sup>*Department of Cancer Biology, DFCI/HMS, Boston, MA*

- TP 008 **Improved Spatial Resolution in the Analysis of FFPE Tissue after Tryptic Digestion;** Janine Beckmann<sup>1</sup>; Nannan Tao<sup>2</sup>; Janina Oetjen<sup>3</sup>; Detlev Suckau<sup>1</sup>; Theodore Alexandrov<sup>4</sup>; Michael Becker<sup>1</sup>; <sup>1</sup>*Bruker Daltonik GmbH, Bremen, GERMANY*; <sup>2</sup>*Bruker Daltonics Inc., Fremont, CA*; <sup>3</sup>*MALDI Imaging Lab, University of Bremen, Bremen, Germany*; <sup>4</sup>*Center for Industrial Mathematics, Bremen, Germany*
- TP 009 **Assessment of Blood-Brain Barrier Crossing using MSI: New Predictive Tools for CNS Targeted Drug Efficacy Study;** Gregory Hamm; Fabien Pamelard; David Bonnel; Raphael Legouffe; Guillaume Hochart; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, FRANCE*
- TP 010 **3D Imaging of TiO<sub>2</sub> Nanoparticle Exposure Effects on Tetrahymena pyriformis;** Tina B. Angerer; John S. Fletcher; *University of Gothenburg, Gothenburg, Sweden*
- TP 011 **Toward Quantitative Infrared Matrix Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Mass Spectrometry Imaging of Biological Tissue;** Mark Bokhart<sup>1</sup>; Guillaume Robichaud<sup>1</sup>; Jeremy Barry<sup>1</sup>; Angela Kashuba<sup>2</sup>; Craig Sykes<sup>2</sup>; David Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*The University of North Carolina, Chapel Hill, NC*
- TP 012 **Quantitative Laser Desorption Ionization Mass Spectrometry Imaging of Elements Directly in Histological Tissue Sections;** Jinrui Gan; Mohammadreza Shariatgorji; Anna Nilsson; Patrik Kallback; Per E. Andren; *Uppsala University, Uppsala, Sweden*
- TP 013 **On tissue Chemical Derivatization of Primary Amines: Application to Quantitative MALDI-MS Imaging of Neuropeptides and Amino Acids;** Mohammadreza Shariatgorji<sup>1</sup>; Oskar Karlsson<sup>1</sup>; Anna Nilsson<sup>1</sup>; Henrik Lodén<sup>1</sup>; Xiaoqun Zhang<sup>2</sup>; Per Svenningsson<sup>2</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>*Uppsala University, Uppsala, Sweden*; <sup>2</sup>*Karolinska Institutet, Stockholm, Sweden*

**Imaging MS: Small Molecules and Drugs, 014 - 046**

- TP 014 **Quercetin as a Highly Efficient MALDI Matrix for Negative-Ion Tissue Imaging by FTICR-MS;** Xiaodong Wang<sup>1</sup>; Jun Han<sup>1</sup>; Juncong Yang<sup>1</sup>; Jingxi Pan<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*



- TP 015 **Mass Spectrometry Imaging Data Co-Registered with Allen Brain Atlas Reveals the Accumulation of fatty Acids in the Hindbrain of MFP-2 Deficient Mice;** Karolina Škrášková<sup>1,2</sup>; Gert Eijkel<sup>1</sup>; Myriam Baes<sup>3</sup>; Paul P. Van Veldhoven<sup>4</sup>; Stephanie de Munter<sup>3</sup>; Artem Khmelinski<sup>5,6</sup>; Walid M. Abdelmoula<sup>6</sup>; Jouke Dijkstra<sup>6</sup>; Ron M.A. Heeren<sup>1,2</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, The Netherlands; <sup>2</sup>TI-COAST, Amsterdam, The Netherlands; <sup>3</sup>Laboratory of Cellular Metabolism, KU Leuven, Leuven, Belgium; <sup>4</sup>LIPIT, KU Leuven, Leuven, Belgium; <sup>5</sup>Percuro B.V., Enschede, The Netherlands; <sup>6</sup>Department of Radiology, LUMC, Leiden, The Netherlands
- TP 016 **Quantitative Molecular Imaging of Neurotransmitters Measured Directly from Histological Tissue Sections in Experimental Models of Parkinson's Disease;** Mohammadreza Shariatgorji<sup>1</sup>; Anna Nilsson<sup>1</sup>; Nicoletta Schintu<sup>2</sup>; Richard J. A. Goodwin<sup>1</sup>; Xiaoqun Zhang<sup>2</sup>; Alan Crossman<sup>3</sup>; Erwan Bezdard<sup>4</sup>; Per Svenningsson<sup>2</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Karolinska Institutet, Stockholm, Sweden; <sup>3</sup>University of Manchester, Manchester, UK; <sup>4</sup>University of Bordeaux 2, Bordeaux, France
- TP 017 **Detection of Ammonia on Human Colon Cancer-Bearing Livers of Superimmunodeficient NOG Mice by MALDI MS Imaging;** Akiko Kubo<sup>1,2</sup>; Mitsuyo Ohmura<sup>1</sup>; Tsuyoshi Nakanishi<sup>3</sup>; Makoto Suematsu<sup>1,2</sup>; <sup>1</sup>Keio University, Tokyo, Japan; <sup>2</sup>ERATO Suematsu gas biology project, Tokyo, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan
- TP 018 **Food-induced Changes of Lipids and Vitamins in Rat Neuronal and Intestinal Tissue Visualized by Imaging ToF-SIMS;** Masoumeh Dowlatshahpour<sup>2</sup>; Eva Jennische<sup>3</sup>; Stefan Lange<sup>3</sup>; Per Malmberg<sup>1</sup>; Andrew Ewing<sup>1</sup>; <sup>1</sup>University of Gothenburg, Gothenburg, Sweden; <sup>2</sup>Chalmers University of Technology, Gothenburg, Sweden; <sup>3</sup>Institute of Biomedicine, Gothenburg, Sweden
- TP 019 **Characterizing the Chemotypic Landscape of Polymicrobial Biofilms;** Vanessa Phelan<sup>1</sup>; Julieta Aguilar<sup>1</sup>; Kit Pogliano<sup>1</sup>; Pieter Dorrestein<sup>2</sup>; <sup>1</sup>UC, San Diego, La Jolla, CA; <sup>2</sup>University of California, San Diego, Skaggs school, La Jolla, CA
- TP 020 **High Resolution Mass Spectrometry Imaging of Plant Tissues: Towards a Plant Metabolome Atlas;** Andreas Roempp<sup>1</sup>; Dhaka Bhandari<sup>1</sup>; Wolfgang Friedt<sup>2</sup>; Sven Gottwald<sup>2</sup>; Bernhard Spengler<sup>1</sup>; <sup>1</sup>Analytical Chemistry, Justus Liebig University, Giessen, Germany; <sup>2</sup>Plant Breeding, Justus Liebig University, Giessen, Germany
- TP 021 **MALDI/LDI-FTICR Mass Spectrometry Imaging for Plant Tissue Analysis to Distinguish Changes in Metabolite Distributions under Different Stimulus Environments;** Katsutoshi Takahashi; *Nat'l Institute Advan. Indus. Sci Tech, Tokyo, Japan*
- TP 022 **Chemical Interface of Plant-Pathogen Interactions Explored by MALDI MS Imaging;** Adam Klein<sup>1,2</sup>; Gargey Yagnik<sup>1,2</sup>; Rebecca Hansen<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames Laboratory-USDOE, Ames, IA
- TP 023 **Biopsy Analysis Using Flowprobe Mass Spectrometry;** Mariam S Elnaggar<sup>1</sup>; Brendan Prideaux<sup>2</sup>; Veronique Dartois<sup>2</sup>; Justin Wiseman<sup>1</sup>; <sup>1</sup>Prosolia, Inc., Indianapolis, IN; <sup>2</sup>PHRI, Newark, NJ
- TP 024 **Investigating Absolute Quantitation of Small Molecule Drugs Profiled in Tissue Sections using Liquid Extraction Surface Analysis (LESA)-MRM analysis;** Edward Takach; Tom Clinckemaillie; Thomas O'Shea; Hanlan Liu; *Sanofi, Waltham, MA*
- TP 025 **ESI-MS Fingerprinting and HPTLC/DESI-MS Imaging of the Crude Extract from the Peels of *Citrus aurantium* L. (*Rutaceae*);** Bianca Bagatela<sup>1,2</sup>; Andrey Lopes<sup>1,2</sup>; Elaine Cristina Cabral<sup>1</sup>; Fábio Perazzo<sup>2</sup>; Demian Iffa<sup>1</sup>; <sup>1</sup>York University, Toronto, ON, Canada; <sup>2</sup>UNIFESP, São Paulo, SP, Brazil
- TP 026 **Imaging and Spatial Profiling of Anti-Tuberculosis Drugs in Tissue using Liquid Microjunction Surface Extraction, MALDI-MS Imaging, and Micro-Dissection LC-MS/MS;** Brendan Prideaux<sup>1</sup>; Mariam S Elnaggar<sup>2</sup>; Jansy Sarathy<sup>1</sup>; Matthew Zimmerman<sup>1</sup>; Justin Wiseman<sup>2</sup>; Veronique Dartois<sup>1</sup>; <sup>1</sup>Public Health Research Institute, Rutgers, Newark, NJ; <sup>2</sup>Prosolia, Inc., Indianapolis, IN
- TP 027 **High Sensitive Quantitation of Raclopride in Rat Brain by Liquid Extraction Surfaced Analysis Mass Spectrometry;** Jun Tadano; Toichiro Yamada; Kenichi Watanabe; Tetsuya Nakagawa; Masashi Yabuki; *Dainippon Sumitomo Pharma Co., Ltd., Suita, Japan*
- TP 028 **Drug Distribution and Pharmacokinetics in an Orthotopic Brain Tumor Model by MS Imaging and LCMS;** Stacey R. Oppenheimer<sup>1</sup>; Matt Teague<sup>1</sup>; Justine Lam<sup>2</sup>; Jinwei Wang<sup>2</sup>; Konstantinos Tsaparikos<sup>2</sup>; Hui Wang<sup>2</sup>; Justin Stroh<sup>1</sup>; Emily Miller<sup>1</sup>; Wei Song<sup>1</sup>; Tod Smeal<sup>2</sup>; Ted W. Johnson<sup>2</sup>; <sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>Pfizer, La Jolla, CA
- TP 029 **A Nano-PALDI Approach for Absolute Quantitation of Anticancer Drugs in Tumor Tissues;** Enrico Davoli; Roberta Pastorelli; Massimo Zucchetti; Silvia Giordano; Lavinia Morosi; *IRCCS Istituto Mario Negri, Milano, Italy*
- TP 030 **Spatially Correlated Quantitative MALDI Analyses of Rifampicin in Liver;** Chad W. Chumbley<sup>1</sup>; Michelle L. Reyzer<sup>1</sup>; Gwendolyn A. Marriner<sup>2</sup>; Laura E. Via<sup>2</sup>; Clifton E. Barry, III<sup>2</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>NIAID, National Institutes of Health, Bethesda, MD
- TP 031 **Imaging LA-ICP-MS as a Powerful Tool for the Investigation of Toxic Mercury Species in *Drosophila melanogaster*;** Ann-Christin Niehoff<sup>1</sup>; Stefanie Fingerhut<sup>2</sup>; Sabrina Kröger<sup>2</sup>; Oliver Bolle Bauer<sup>2</sup>; Jacqueline Schulz<sup>4</sup>; Sören Meyer<sup>1</sup>; Michael Sperling<sup>2</sup>; Astrid Jeibmann<sup>4</sup>; Tanja Schwerdtle<sup>3</sup>; Uwe Karst<sup>2</sup>; <sup>1</sup>NRW Graduate School of Chemistry, Münster, Germany; <sup>2</sup>Westfälische Wilhelms-Universität Münster, Münster, Germany; <sup>3</sup>Universität Potsdam, Nuthetal, Germany; <sup>4</sup>University Hospital Münster, Münster, Germany
- TP 032 **Quantitative LA-ICP-MS Imaging of Silver in Different Target Organs of Rats after Intratracheal Instillation of Silver Nanoparticles;** Franziska Blaske; Olga Reifschneider; Mandy Grossgarten; Michael Sperling; Uwe Karst; *Westfälische Wilhelms-Universität Münster, Muenster, GERMANY*
- TP 033 **Effects of Oral Administration of Methylphenidate on *Drosophila* Brain Studied by Imaging Mass Spectrometry;** Nhu Phan<sup>1</sup>; Amir Mohammadi<sup>2</sup>; Masoumeh Pour<sup>2</sup>; Jörg Hanrieder<sup>2</sup>; John Fletcher<sup>1</sup>; Andrew Ewing<sup>1,2</sup>; <sup>1</sup>Gothenburg University, Gothenburg, Sweden; <sup>2</sup>Chalmers University of Technology, Gothenburg, Sweden
- TP 034 **PET Ligand distribution in rat brain by MALDI Imaging: Impact of the tissue preparation on Raclopride distribution;** Emeline Faloux; David Bonnel; Gregory Hamm; Jonathan Stauber; *ImaBiotech, MS Imaging Dept., Loos, France*
- TP 035 **Visualizing First Pass Hepatic Metabolism of Amodiaquine using MALDI Mass Spectrometry Imaging;** Stephanie Dale<sup>3</sup>; Beth DiTondo<sup>1</sup>; Kerstin Strupat<sup>2</sup>; Patrick Rudewicz<sup>3</sup>; <sup>1</sup>AB SCIEX, Framingham, MA; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Novartis, Emeryville, CA
- TP 036 **Identification of the Neuroanatomical Substrate Involved in ICVNPY Inhibitory Effects on Reinstatement of Cocaine-Induced Behavior in Rats by MALDI IMSite;** Leila Hosseinzadehshahri; *Student, Buffalo, NY*

- TP 037 **Visualization of Lipids and Small Metabolites in *Arabidopsis thaliana* Seed by MALDI-MS imaging;** María Dueñas<sup>1,2</sup>; Andrew Korte<sup>1,2</sup>; Kent Chapman<sup>3</sup>; Drew Sturtevant<sup>3</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames Laboratory US Dept. of Energy, Ames, IA; <sup>3</sup>University of North Texas, Denton, TX
- TP 038 **Mapping Regional Localization in Rat Brain of Reduced Lipoic Acid by Laser Ablation Electrospray Ionization Tandem Mass Spectrometry (LAESI-MS/MS);** Marina Galvez-Peralta<sup>1</sup>; Callee M. Walsh<sup>2</sup>; Aric F. Logsdon<sup>1</sup>; Jason D. Huber<sup>1</sup>; Paul R. Lockman<sup>1</sup>; Patrick S. Callery<sup>1</sup>; <sup>1</sup>West Virginia University, Morgantown, WV; <sup>2</sup>Protea Biosciences, Morgantown, WV
- TP 039 **Mapping Metabolite and Protein Changes in the Cataractous Lens using MALDI Imaging Mass Spectrometry;** Mitchell G. Nye-Wood<sup>1</sup>; Jeffrey Spraggins<sup>2</sup>; Richard M. Caprioli<sup>2</sup>; Kevin L. Schey<sup>2</sup>; Paul J. Donaldson<sup>1</sup>; Angus C. Grey<sup>1</sup>; <sup>1</sup>University of Auckland, Auckland, New Zealand; <sup>2</sup>Vanderbilt University, Nashville, TN
- TP 040 **High Spatial Resolution Laser Microdissection LC-MS/MS analysis of rat liver histology samples;** Paul Moench; Christopher DeBenedetto; James Glick; Robert Johnson; Jimmy Flarakos; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- TP 041 **A Multidimensional Approach for Identification of Isobaric Lipids Detected in Direct MS Analysis and Imaging of Human Liver;** Joscelyn Sarsby<sup>1</sup>; Alan Race<sup>1</sup>; Patricia F. Lalor<sup>1</sup>; Josephine Bunch<sup>2</sup>; Helen Cooper<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>National Physical Laboratory, London, UK
- TP 042 **Strategies for Optimizing Detection of Endogenous Metabolites Directly from Tissue via MALDI MS;** Michelle L. Reyzer; Jeffrey Spraggins; Richard M. Caprioli; *Vanderbilt University, Nashville, TN*
- TP 043 **Finding Biomarkers in *Arabidopsis* FERONIA Receptor Kinase using MALDI-MSI;** Rebecca Hansen<sup>1,2</sup>; Gargey Yagnik<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>Iowa State University, Ames, IA; <sup>2</sup>Ames Laboratory-USDOE, Ames, IA
- TP 044 **Phenotype Determination of *Caenorhabditis Elegans* with Matrix-Assisted Laser Desorption/Ionization Mass Spectrometric Imaging;** Robert Menger; Chaevien Clendinen; Louis Searcy; Richard A. Yost; Arthur S. Edison; *University of Florida, Gainesville, FL*
- TP 045 **Characterizing the Novel Synthetic Cannabinoid, RCS-4's Metabolism – Human Hepatocytes Applicability in Clinical and Forensic Drug Testing;** Adarsh Gandhi<sup>1</sup>; Mingshe Zhu<sup>2</sup>; Shaokun Pang<sup>3</sup>; Ariane Wohlfarth<sup>4</sup>; Karl Scheidweiler<sup>4</sup>; Marilyn Huestis<sup>4</sup>; <sup>1</sup>Lundbeck Research USA Inc., Paramus, NJ; <sup>2</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>3</sup>AB SCIEX, San Diego, CA; <sup>4</sup>NIDA, NIH, Baltimore, MD
- TP 046 **Classification of Drug Induced Toxicology in Tissue Samples using MALDI Mass Spectrometry Imaging;** Anna Nilsson<sup>1</sup>; Richard Goodwin<sup>2</sup>; Benita Forngren<sup>3</sup>; Suzanne Iverson<sup>4</sup>; Johan Lindberg<sup>5</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>AstraZeneca, Macclesfield, UK; <sup>3</sup>former AstraZeneca, Södertälje, Sweden; <sup>4</sup>AstraZeneca, Göteborg, Sweden; <sup>5</sup>Swedish Toxicology Sciences Research Center, Södertälje, Sweden
- Imaging MS: Disease Markers, 047 - 073**
- TP 047 **Quantitative 3D MALDI-MS Imaging of Neurotransmitters and Metabolites in Aging Models of the Mouse Brain;** Mohammadreza Shariatgorji<sup>1</sup>; Anna Nilsson<sup>1</sup>; Dennis Trede<sup>2,3</sup>; Theodore Alexandrov<sup>2,4</sup>; Nicoletta Schintu<sup>5</sup>; Per Svenningsson<sup>6</sup>; Per E. Andren<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>SciLS GmbH, Bremen, Germany; <sup>3</sup>Steinbeis Innovation Center SciLS Research, Bremen, Germany; <sup>4</sup>University of Bremen, Bremen, Germany; <sup>5</sup>Karolinska Institutet, Stockholm, Sweden
- TP 048 **Spatial Metabolites and Lipids Profiling in a Rat Model of Experimental Autoimmune Myocarditis by Matrix-assisted Laser Desorption/Ionization Imaging Mass Spectrometry;** Jin Woo Jung<sup>1</sup>; Kwan Soo Hong<sup>2</sup>; Geum-Sook Hwang<sup>1</sup>; Jungju Seo<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Seoul, South Korea; <sup>2</sup>Korea Basic Science Institute, Ochang, South Korea
- TP 049 **Classification of Soft Tissue Sarcomas using MALDI Imaging Mass Spectrometry;** Sha Lou; Benjamin Balluff; Marieke A. de Graaf; Judith V.M.G. Bovée; Liam A. McDonnell; *Leiden University Medical Center, Leiden, the Netherlands*
- TP 050 **Importance of Tissue Suppression Effect on Biomarkers by MSI—Application to Mouse Xenografts;** Guillaume Hochart<sup>1</sup>; Fred Fack<sup>2</sup>; David Bonnel<sup>1</sup>; Olivier Keunen<sup>2</sup>; Simone P. Niclou<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>Norlux Neuro-Oncology Laboratory, CRP-Santé, Luxembourg, Luxembourg
- TP 051 **Discrimination of Metastasis from Breast and Pancreatic Cancer by MALDI Imaging;** Rita Casadonte<sup>1</sup>; Mark Kriegsmann<sup>3</sup>; Katrin Friedrich<sup>4</sup>; Gustavo Baretton<sup>4</sup>; Mike Otto<sup>1,2</sup>; Soeren Deininger<sup>5</sup>; Detlev Suckau<sup>5</sup>; Martin Schuerenberg<sup>6</sup>; Jörg Kriegsmann<sup>1,2</sup>; <sup>1</sup>Proteopath, Trier, Germany; <sup>2</sup>Center for Histology, Cytology & Mol. Diagnostics, Trier, Germany; <sup>3</sup>University of Heidelberg, Department of Pathology, Heidelberg, Germany; <sup>4</sup>University of Dresden, Department of Pathology, Dresden, Germany; <sup>5</sup>Bruker Daltonik GmbH, Bremen, Germany
- TP 052 **De Novo Discovery of Tumor Clones Linked to Metastasis and Poor Prognosis Using MALDI Imaging Mass Spectrometry;** Benjamin Balluff<sup>1</sup>; Christian Frese<sup>4</sup>; Stefan Maier<sup>5</sup>; Cedrik Schoene<sup>2</sup>; Bernhard Kuster<sup>3</sup>; Manfred Schmitt<sup>6</sup>; Michaela Aubele<sup>2</sup>; Heinz Hoefler<sup>2</sup>; André Deelder<sup>1</sup>; Albert Heck<sup>4</sup>; Johannes Morreau<sup>1</sup>; A.F. Maarten Altelaa<sup>4</sup>; Axel Walch<sup>2</sup>; Liam McDonnell<sup>1</sup>; <sup>1</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>2</sup>Helmoltz Zentrum Muenchen, Munich, Germany; <sup>3</sup>Technical University Munich, Freising, Germany; <sup>4</sup>Utrecht University, Utrecht, N/A; <sup>5</sup>TU Muenchen, Freising, Germany; <sup>6</sup>Klinikum Rechts der Isar, Munich, Germany
- TP 053 **Histodiagnostic Differentiation of Primary Mamma Carcinoma Tumor and Metastasis by MALDI-TOF Imaging and Intact Cell Mass Spectrometry;** Sophie Froehlich<sup>1</sup>; Donscho Kerjaschki<sup>2</sup>; Guenter Allmaier<sup>1</sup>; Martina Marchetti-Deschmann<sup>1</sup>; <sup>1</sup>Vienna University of Technology, Vienna, Austria; <sup>2</sup>Medical University Vienna, Vienna, Austria
- TP 054 **Validation of Mass Spectrometry Imaging as a Tool for the Detection of Cancer Tissue in Tissue Sections;** Olga Kraus<sup>1</sup>; Pierre Abramowski<sup>2</sup>; Kristoffer Riecken<sup>2</sup>; Boris Fehse<sup>2</sup>; Sascha Rohn<sup>3</sup>; Hartmut Schlüter<sup>1</sup>; <sup>1</sup>Clinical Chemistry, University Hamburg Eppendorf, Hamburg, Deutschland; <sup>2</sup>Research Department Cell and Gene Therapy, Clinic, Hamburg, uswählen (nur für USA / Kan. / Aus.); <sup>3</sup>Institute of Food Chemistry, University Hamburg, Hamburg, uswählen (nur für USA / Kan. / Aus.)
- TP 055 **Identification and Spatial Localization of Proteins from Mouse Brain Tumor Using a Combination of MALDI Imaging and LC-MALDI;** Sergei Dikler<sup>1</sup>; Daniel R. Feldman<sup>2</sup>; Jennifer L. Ide<sup>2</sup>; Mark A. Marchionni<sup>3</sup>; Charles D. Stiles<sup>3</sup>; Nathalie Y.R. Agar<sup>2,3</sup>; <sup>1</sup>Bruker Daltonics, Billerica, MA; <sup>2</sup>Brigham and Women's Hospital, HMS, Boston, MA; <sup>3</sup>Dana-Farber Cancer Institute, HMS, Boston, MA
- TP 056 **Proteomic Analysis of Formalin-Fixed Paraffin-Embedded Renal Amyloidosis Tissues using MALDI Imaging Mass Spectrometry;** Rita Casadonte<sup>1</sup>; Mark

- Kriegsmann<sup>2</sup>; Mike Otto<sup>1,3</sup>; Rainer Paape<sup>4</sup>; Detlev Suckau<sup>4</sup>; Sören-Oliver Deininger<sup>4</sup>; Kerstin Amann<sup>5</sup>; Jörg Kriegsmann<sup>1,3</sup>; <sup>1</sup>Proteopath GbR, Trier, Germany; <sup>2</sup>University of Heidelberg, Department of Pathology, Heidelberg, Germany; <sup>3</sup>Center for Histology, Cytology and Molecular Diagn, Trier, Germany; <sup>4</sup>Brüker Daltonik GmbH, Bremen, Germany; <sup>5</sup>University of Erlangen-Nuremberg, Erlangen, Germany
- TP 057 **Differences in the Proteomic Pattern of Colon and Pancreatic Carcinoma using High-Throughput Imaging Mass Spectrometry (IMS);** Jörg Kriegsmann<sup>1,5</sup>; Mark Kriegsmann<sup>2</sup>; Vanessa Schommer<sup>1</sup>; Daniela Aust<sup>3</sup>; Gustavo Baretton<sup>3</sup>; Sören-Oliver Deininger<sup>4</sup>; Detlev Suckau<sup>4</sup>; Mike Otto<sup>1,5</sup>; Rita Casadonte<sup>5</sup>; <sup>1</sup>Center for Histology, Cytology and Molecular Diagn, Trier, Germany; <sup>2</sup>University of Heidelberg, Department of Pathology, Heidelberg, Germany; <sup>3</sup>University of Dresden, Department of Pathology, Dresden, Germany; <sup>4</sup>Brüker Daltonik GmbH, Bremen, Germany; <sup>5</sup>Proteopath GbR, Trier, Germany
- TP 058 **Imaging Mass Spectrometry to Uncover Proteomic Differences in Non-Hodgkin's Lymphomas;** Kristina Schwamborn<sup>1</sup>; Martina Rudelius<sup>2</sup>; Richard Caprioli<sup>3</sup>; <sup>1</sup>Technical University Munich, Munich, Germany; <sup>2</sup>University of Würzburg, Würzburg, Germany; <sup>3</sup>Vanderbilt University, Nashville, TN
- TP 059 **Multimodal Imaging Mass Spectrometry for Probing the Protein-Lipid Interplay Underlying Amyloid-Beta Plaque Formation in Experimental Alzheimers Disease;** Jörg Hanrieder<sup>1,2</sup>; Stina Syvänen<sup>3</sup>; Andrew G. Ewing<sup>1,2</sup>; <sup>1</sup>Chalmers Tech. University, Gothenburg, Sweden; <sup>2</sup>National Center for Imaging Mass Spectrometry, Gothenburg, Sweden; <sup>3</sup>Uppsala University, Uppsala, Sweden
- TP 060 **MALDI Imaging of Lipid and Protein Changes in the Human Alzheimer's Disease Hippocampus;** Angus C. Grey; Lakshini Mendis; Richard L.M. Faull; Maurice A. Curtis; *Auckland University, Auckland, New Zealand*
- TP 061 **Tracking Cholesterol Distribution following Plaque Formation in a Mouse Model of Atherosclerosis using Dietary d6-cholesterol and MALDI Imaging Mass Spectrometry;** Nathan Hatcher<sup>1</sup>; Jose Castro-Perez<sup>2</sup>; Vivienne Mendoza<sup>2</sup>; Nana Kofi Karikari<sup>1</sup>; Karen Gagen<sup>2</sup>; Henry Shion<sup>3</sup>; Alan Millar<sup>3</sup>; John Shockcor<sup>3</sup>; David McLaren<sup>2</sup>; Vinit Shah<sup>2</sup>; Stephen Previs<sup>2</sup>; Karen Akinsanya<sup>2</sup>; Michele Cleary<sup>1</sup>; Thomas P Roddy<sup>2</sup>; Douglas G Johns<sup>2</sup>; Sheng-Ping Wang<sup>2</sup>; <sup>1</sup>Merck Research Labs, West Point, PA; <sup>2</sup>Merck Research Labs, Kenilworth, NJ; <sup>3</sup>Waters Corporation, Milford, MA
- TP 062 **Mass Spectrometry Imaging of Breast Tumor Hypoxia Using 2-Nitroimidazoles as Chemical Markers;** Nadine E. Mascini<sup>1</sup>; Asif Rizwan<sup>2</sup>; Lu Jiang<sup>2</sup>; Menglin Cheng<sup>2</sup>; Kristine Glunde<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM Institute AMOLF, Amsterdam, Netherlands; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- TP 063 **Imaging MS Sheds Light on What's Happening in Traumatic Brain Injury;** Ludovic Muller<sup>1,2</sup>; Aurelie Roux<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Brian M Cox<sup>3</sup>; J Albert Schultz<sup>4</sup>; Amina S Woods<sup>1</sup>; <sup>1</sup>NIH/NIDA-IRP, Baltimore, MD; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Uniformed Services University, Bethesda, MD; <sup>4</sup>Ionwerks, Houston, TX
- TP 064 **Profiling and Imaging of Lipids in Demyelinated Rat Spinal Cord Using Mass Spectrometry;** Roberto Fernandez<sup>1</sup>; Pau Gonzalez<sup>2</sup>; Javier Díez-García<sup>3</sup>; Begoña Castro<sup>3</sup>; Francisco J. Rodríguez<sup>2</sup>; Jose A. Fernandez<sup>1</sup>; <sup>1</sup>Universidad del País Vasco, Leioa, Spain; <sup>2</sup>Hospital Nacional de Paraplégicos, Toledo, Spain; <sup>3</sup>Histocell S. L., Derio, Spain
- TP 065 **Defining the Tissue Distribution of Glycosphingolipid Species in Model Tissue Systems using High Resolution MALDI Imaging Mass Spectrometry;** Ellen Jones<sup>1</sup>; Shaalee Dworski<sup>2</sup>; Mustafa Kamani<sup>3</sup>; Jeffrey Medin<sup>2,3</sup>; Tamara Nowling<sup>4</sup>; James Norris<sup>1</sup>; Richard Drake<sup>1</sup>; <sup>1</sup>Department of Cell and Molecular Pharmacology, MUSC, Charleston, South Carolina; <sup>2</sup>Institute of Medical Science University of Toronto, Ontario, Canada; <sup>3</sup>University Health Network, University of Toronto, Ontario, Canada; <sup>4</sup>Division of Rheumatology & Immunology, MUSC, Charleston, SC
- TP 066 **MALDI-IMS of Brain Tissue from a Mouse Model of Timothy Syndrome;** William Friesen; Brian Schultz; Sarbajit Banerjee; Troy Wood; *SUNY at Buffalo, Buffalo, NY*
- TP 067 **MALDI-MSI Lipidomic Investigation into the Delayed Effect of Acute Radiation Exposure: The Lung Syndrome and Efficacy of a Medical Countermeasure;** Claire L. Carter; Jace W. Jones; Isabel Jackson; Zeljko Vujaskovic; Stephanie Tabisz; Allison Gibbs; Jamie Haper; Kory Barrow; Ann M. Farese; Thomas J. MacVittie; Maureen A. Kane; *University of Maryland, Baltimore, MD*
- TP 068 **MALDI-IMS Profiling of N-Linked Glycans in FFPE Tissue Blocks and On-tissue Characterization of Glycan Structures;** Richard R Drake<sup>1</sup>; Powers Thomas<sup>1</sup>; Yuan Shao<sup>1</sup>; Haab Brian<sup>2</sup>; Anand Mehta<sup>3</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Van Andel Research Institute, Grand Rapids, MI; <sup>3</sup>Drexel University, Doylestown, PA
- TP 069 **A MALDI-IMS Workflow for Assessment of Global Changes in N-linked Glycan Profiles in Tumor Tissue Microarrays;** Thomas Powers<sup>1</sup>; Benjamin Neely<sup>1</sup>; Yuan Shao<sup>1</sup>; Raymond Lance<sup>2</sup>; Dean Troyer<sup>2</sup>; Anand Mehta<sup>3</sup>; Brian Haab<sup>4</sup>; Richard R Drake<sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>3</sup>Drexel University, Doylestown, PA; <sup>4</sup>Van Andel Research Institute, Grand Rapids, MI
- TP 070 **High Spatial and Mass Resolution Imaging of Human Age Matched Healthy and Age Related Macular Degenerated Retinal Tissue;** David M. Anderson<sup>1</sup>; Zsolt Ablonczy<sup>2</sup>; Jeffrey Spraggins<sup>1</sup>; Yannis Koutalos<sup>2</sup>; Rosalie Crouch<sup>2</sup>; Anne Hanneken<sup>3</sup>; Richard Caprioli<sup>1</sup>; Kevin Schey<sup>1</sup>; <sup>1</sup>Vanderbilt University School of Medicine, Nashville, TN; <sup>2</sup>Medical University of South Carolina, Charleston, SC; <sup>3</sup>The Scripps Research Institute, La Jolla, CA
- TP 071 **Mass Spectrometric Imaging in Malaria Research;** Saleh Mahmud Khalil; Andreas Römpf; Jette Pretzel; Katja Becker; Bernhard Spengler; *Giessen, GERMANY*
- TP 072 **Lipidomic analysis of Nipah Virus Infection in a Mouse Model by MALDI-MS Imaging;** Alexander Shavkunov<sup>1</sup>; Bjorn Nilsson<sup>1</sup>; Tatyana Yun<sup>2</sup>; Terry Juelich<sup>2</sup>; Jennifer Smith<sup>2</sup>; Alexander Freiberg<sup>2</sup>; Carol Nilsson<sup>1</sup>; <sup>1</sup>Department of Pharmacology and Toxicology, UTMB, Galveston, TX; <sup>2</sup>Department of Pathology, UTMB, Galveston, TX
- TP 073 **Oxidative Damage During Staphylococcus aureus Infection Revealed by High Mass Resolution MALDI Protein Imaging;** Jessica L. Moore<sup>1</sup>; Jeffrey Spraggins<sup>2</sup>; Neal D. Hammer<sup>3</sup>; Kristie Lindsey Rose<sup>1</sup>; Eric P. Skaar<sup>3</sup>; Richard M. Caprioli<sup>1</sup>; <sup>1</sup>Vanderbilt University MSRC, Nashville, TN; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Vanderbilt University Medical Center, Nashville, TN
- Informatics: Peptide Identification and Characterization, 074 - 091**
- TP 074 **Automated Parameter Setting for Protein Database Searches;** Wilfred Tang; Yong Joo Kil; Chris Becker; Marshall W. Bern; *Protein Metrics Inc., San Carlos, CA*
- TP 075 **MS Amanda Stand-Alone for Integration into Proteomic Workflows;** Viktoria Dorfer<sup>1</sup>; Peter Pichler<sup>2</sup>; Thomas

- Stranzl<sup>2</sup>; Stephan Winkler<sup>1</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>University of Applied Sciences Upper Austria, Hagenberg, Austria; <sup>2</sup>IMP Vienna, Austria
- TP 076 **Mixture Peptide Identifications with Proteomic Software from Complex Mixtures in Isolation Events from Hybrid and Tribrid Mass Spectrometers;** Leeann Higgins<sup>1</sup>; Todd Markowski<sup>1</sup>; Pratik Jagtap<sup>1</sup>; Susan K. Van Riper<sup>2</sup>; <sup>1</sup>University of Minnesota, St. Paul, MN; <sup>2</sup>University of Minnesota, Minneapolis, MN
- TP 077 **Identifying Novel Peptide Sequence Variants from High Throughput RNA-Seq Data Via Flexible Proteomic Database Generation using the Galaxy Framework;** James Johnson<sup>1</sup>; Gloria Sheynkman<sup>2</sup>; Pratik Jagtap<sup>3</sup>; Michael Shortreed<sup>2</sup>; Getiria Onsongo<sup>1</sup>; Lloyd Smith<sup>2</sup>; Tim Griffin<sup>3</sup>; <sup>1</sup>Minnesota Supercomputing Institute, Minneapolis, MN; <sup>2</sup>University of Wisconsin, Madison, WI; <sup>3</sup>University of Minnesota, Minneapolis, MN
- TP 078 **Towards a Novel Unprecedentedly Comprehensive Protein Identification Strategy, Mass Spectrometry and Ribosome Profiling: The Perfect Match;** Jeroen Crappé<sup>1</sup>; Alexander Koch<sup>1</sup>; Elvis Ndah<sup>1,2</sup>; Sandra Steyaert<sup>1</sup>; Daria Gawron<sup>1,2</sup>; Ellen De Meester<sup>1</sup>; Sarah De Keulenaer<sup>1</sup>; Petra Van Damme<sup>1,2</sup>; Gerben Menschaert<sup>1</sup>; <sup>1</sup>Ghent University, Ghent, Belgium; <sup>2</sup>VIB, Ghent, Belgium
- TP 079 **A Mutated Peptide Database for the Analysis of Aberrant Protein Sequences in Cancer;** Xu Yang; Iuliana Lazar; Department of Biological Sciences, Virginia Tech, Blacksburg, VA
- TP 080 **Accurate FDR (False Discovery Rate) Estimation for Database Searching in Proteogenomics Studies;** Yoonsung Joh<sup>1</sup>; Hyunwoo Kim<sup>1</sup>; Kyubaek Hwang<sup>2</sup>; Heejin Park<sup>1</sup>; Eunok Paek<sup>1</sup>; <sup>1</sup>Hanyang University, Seoul, KOREA; <sup>2</sup>Soongsil University, Seoul, KOREA
- TP 081 **Proteogenomic Approach to Cancer Cell Line Differentiation using Exome-Derived Variant Peptides: NCI-60 Panel Case Study;** Maria A. Karpova<sup>1</sup>; Dmitry S. Karpov<sup>1</sup>; Mark V. Ivanov<sup>2</sup>; Alexey L. Chernobrovkin<sup>1,3</sup>; Mikhail A. Pyatnitskiy<sup>1</sup>; Andrey V. Lisitsa<sup>1</sup>; Alexander I. Archakov<sup>1</sup>; Mikhail V. Gorshkov<sup>2</sup>; Sergei A. Moshkovskii<sup>1</sup>; <sup>1</sup>Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Karolinska Institutet, Stockholm, Sweden
- TP 082 **Assessing Depth of Proteome Coverage Required for Novel Peptide Detection in Breast Cancer using Patient Derived Xenograft Models;** Kelly Ruggles<sup>1</sup>; Zuojiang Tang<sup>1</sup>; Zuya Wang<sup>1</sup>; Jennifer Teubl<sup>1</sup>; Manor Askenazi<sup>2</sup>; Christopher Maher<sup>3</sup>; Song Cao<sup>3</sup>; Li Ding<sup>3</sup>; Michael McLellan<sup>3</sup>; Karl Clauser<sup>4</sup>; Philipp Mertins<sup>4</sup>; Robert Kitchens<sup>3</sup>; Charles Perou<sup>5</sup>; Steven Carr<sup>4</sup>; R. Reid Townsend<sup>3</sup>; Sherri Davies<sup>3</sup>; Matthew Ellis<sup>3</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>NYU Langone Medical Center, New York, NY; <sup>2</sup>Biomedical Hosting LLC, Arlington, MA; <sup>3</sup>Washington University, St. Louis, MO; <sup>4</sup>Broad Institute of MIT and Harvard, Boston, MA; <sup>5</sup>University of North Carolina, Chapel Hill, NC
- TP 083 **IC: A New Peptide Identification Tool for Both Data-Dependent and Data-Independent Acquisition;** Sangtae Kim<sup>1</sup>; Ying Sonia Ting<sup>2</sup>; Alex Hu<sup>2</sup>; Richard D. Smith<sup>1</sup>; William Stafford Noble<sup>2</sup>; Michael J. Maccoss<sup>2</sup>; Samuel H. Payne<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>University of Washington, Seattle, WA
- TP 084 **Peptide-Centric Database Search Engines Applied to Data Independent Acquisition UDMS<sup>e</sup> Data;** Pedro Navarro; Jennifer Hahlbrock; Jörg Kuharev; Ute Distler; Stefan Tenzer; Institute for Immunology, Univ. Medical Center, Mainz, Germany
- TP 085 **Direct Non-Targeted Protein Identification from Data Independent Acquisition (DIA) Data Using Database Search;** Ignat Shilov<sup>1</sup>; Sean L. Seymour<sup>1</sup>; Christie Hunter<sup>1</sup>; Stephen A Tate<sup>2</sup>; Gordana Ivosev<sup>1</sup>; Ahmad Hosseingholizadeh<sup>2</sup>; <sup>1</sup>AB Sciex, Redwood City, CA; <sup>2</sup>AB SCIEX, Concord, ON
- TP 086 **Optimized Spectral Library Generation for HRM/SWATH Acquisition as Implemented in Spectronaut;** Tejas Gandhi; Roland M. Bruderer; Magdalena Bober; Vito Zanotelli; Oliver M. Bernhardt; Oliver Rinner; Lukas Reiter; BiognoSYS AG, Zurich, Switzerland
- TP 087 **MSPLIT-SWATH: a New Spectral Library Search Algorithm for Data Independent Acquisition of Complex Protein Mixtures;** Jian Wang<sup>1</sup>; Monika Tucholska<sup>2</sup>; Jean Philippe Lambert<sup>2</sup>; Brett Larsen<sup>2</sup>; Stephen A Tate<sup>3</sup>; Anne-Claude Gingras<sup>2</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>UCSD, La Jolla, CA; <sup>2</sup>Lunenfeld-Tanenbaum Research Institute, Toronto, ON; <sup>3</sup>AB SCIEX, Concord, ON
- TP 088 **The Generating Function Approach for Peptide Identification in Spectral Networks;** Adrian Guthals<sup>1</sup>; Christina Boucher<sup>2</sup>; Nuno Bandeira<sup>1,3</sup>; <sup>1</sup>Department of Computer Science, UCSD, La Jolla, CA; <sup>2</sup>Department of Computer Science, CSU, Fort Collins, CO; <sup>3</sup>Skaggs School of Pharmacy and Pharm. Sci., UCSD, La Jolla, CA
- TP 089 **Spectral Library Searching for Samples where the Amount of Sample is Severely Limited;** Himanshu Grover<sup>1</sup>; Sarah Keegan<sup>1</sup>; Siyang Li<sup>2</sup>; Xianzhe Wang<sup>2</sup>; Shashi Murthy<sup>2</sup>; Barry L. Karger<sup>2</sup>; Alexander R. Ivanov<sup>2</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>New York University, New York, NY; <sup>2</sup>Barnett Inst., Northeastern University, Boston, MA
- TP 090 **A Better Scoring Function for Top-Down Spectral Deconvolution;** Qiang Kou<sup>1</sup>; Xiaowen Liu<sup>1,2</sup>; <sup>1</sup>Indiana University-Purdue University Indianapolis, Indianapolis, IN; <sup>2</sup>Indiana University School of Medicine, Indianapolis, IN
- TP 091 **Top-down Proteomics with a Bottom-up Algorithm;** Marshall W. Bern<sup>1</sup>; Yong J. Kil<sup>1</sup>; Wilfred Tang<sup>1</sup>; Chris Becker<sup>1</sup>; Xuemei Han<sup>2</sup>; John R. Yates, III<sup>2</sup>; Kristie Rose<sup>3</sup>; Dhananjay Sakrikar<sup>3</sup>; Kevin L. Schey<sup>3</sup>; Richard Caprioli<sup>3</sup>; <sup>1</sup>Protein Metrics Inc., San Carlos, CA; <sup>2</sup>The Scripps Research Institute, La Jolla, CA; <sup>3</sup>Vanderbilt University, Nashville, TN
- Informatics: Post-Translational Modifications, 092 - 100**
- TP 092 **A New N-linked Glycopeptide Identification Tool, for Large-Scale Glycoproteomics Analysis by Spectral Library Searching;** Yingwei Hu; Pei-Jing Pai; Henry Lam; The Hong Kong University of Science and Technology, Hong Kong, CHINA
- TP 093 **Data-Independent Mass Spectrometry for the Analysis of Red Blood Cell Protein Degradation and Aging;** Huisong Pak<sup>1</sup>; Pierre Lescuyer<sup>3</sup>; Markus Muller<sup>2</sup>; Alexander Scherl<sup>1</sup>; <sup>1</sup>University of Geneva, Geneva, Switzerland; <sup>2</sup>SIB, Geneva, Switzerland; <sup>3</sup>Geneva University Hospital, Geneva, Switzerland
- TP 094 **A Computational Framework for Mining MS1 Data for Post Translational Modifications;** Bruce D. Pascal; Graham M. West; Yelenis Mari; Patrick R. Griffin; The Scripps Research Institute, Scripps Florida, Jupiter, FL
- TP 095 **Software for Differential Characterization of PTMs: Approaches in Data Acquisition and Processing;** Jean L. Spencer; Vivek N. Bhatia; Amanuel Kehasse; Stephen A. Whelan; Christian F. Heckendorf; Catherine E. Costello; Mark E. McComb; Boston University School of Medicine, Boston, MA
- TP 096 **Simultaneous Localization and Assignment of Different Post-Translational Modifications using ptmRS;** Etienne Beltzung<sup>1</sup>; Thomas Taus<sup>2</sup>; Gerhard Dürnberger<sup>2,3</sup>; Johannes Stadlmann<sup>2</sup>; Dea Slade<sup>1</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>MFPL, Vienna, AT; <sup>2</sup>IMP/IMBA, Vienna, AT; <sup>3</sup>GMI, Vienna, AT

- TP 097 **Correction of Errors in Tandem Mass Spectrum Extraction Enhances Phosphopeptide Identification;** Piliang Hao; Yan Ren; James Tam; Siu Kwan Sze; *Nanyang Technological University, Singapore, Singapore*
- TP 098 **Algorithm for Accurate Estimation of False Localization Rates in Phosphoproteomics;** Thomas Taus<sup>1</sup>; Thomas Köcher<sup>1</sup>; Etienne Beltzung<sup>2</sup>; Gerhard Dürmberger<sup>1,3</sup>; Karl Mechtler<sup>1</sup>; <sup>1</sup>IMP/IMBA, Vienna, Austria; <sup>2</sup>MFPL, Vienna, Austria; <sup>3</sup>GMI, Vienna, Austria
- TP 099 **Evaluation of Accessible Database Searching Engines for Accurate Identification of Histone Post-Translational Modifications;** Zuofei Yuan; Shu Lin; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- TP 100 **SAHA Treatment Reveals the Link between Histone Lysine Acetylation and Proteome in Non-small Cell Lung Cancer A549 Cells;** Quan Wu<sup>1</sup>; Lejie Cao<sup>1</sup>; Xiaojun Peng<sup>2</sup>; Tieming He<sup>2</sup>; Zhongyi Cheng<sup>2</sup>; <sup>1</sup>Central Laboratory, Affiliated Provincial Hospital, Hefei, CN; <sup>2</sup>PTM Biolabs, Inc, Hangzhou, China
- Proteins: PTMs, 101 - 131**
- TP 101 **Functional Control of AP2 Transcription Factors in Plasmodium Falciparum is Mediated via acetyl-CoA Metabolism and Extensive Lysine Acetylation;** Simon A. Cobbold<sup>1</sup>; Joana Santos<sup>2</sup>; David H. Perlman<sup>3</sup>; Manuel Llinás<sup>2</sup>; <sup>1</sup>Bio21 Institute, University of Melbourne, Melbourne, Australia; <sup>2</sup>The Pennsylvania State University, University Park, PA; <sup>3</sup>Princeton University, Princeton, NJ
- TP 102 **Discovery of a Methylglyoxal (MGO) Modification in a Recombinant Monoclonal Antibody;** Chris Chumsae; *AbbVie Bioresearch Center, Worcester, MA*
- TP 103 **Quantification of Aspirin's Pharmacodynamic Effect by Targeted Mass Spectrometry Analysis of Platelet Cyclooxygenase-1 Acetylation;** Xuanwen Li; Susanne Fries; Ruizhi Li; John A. Lawson; Scott L. Diamond; Ian A. Blair; Garret A. FitzGerald; Tilo Grosser; *University of Pennsylvania, Philadelphia, PA*
- TP 104 **Narrow IEF Windows and Superficially Porous Liquid Chromatography MS Allow for Efficient Characterization and Stoichiometric Quantitation of Heterogeneous Proteins;** John Corbett; Daniel Plymire; Junmei Zhang; Steven Patrie; *University of Texas Southwestern Medical Center, Dallas, Texas*
- TP 105 **Multiple PTMs Play a Role in the Regulation of Platelets in Health and Disease;** Florian Beck<sup>1</sup>; Fiorella Solari<sup>1</sup>; Stefan Lorocho<sup>1</sup>; Saskia Venne<sup>1</sup>; Marc Vaudel<sup>2</sup>; Lennart Martens<sup>3</sup>; Ulrich Walter<sup>4</sup>; Johan Heemskerk<sup>5</sup>; Albert Sickmann<sup>1</sup>; René Zahedi<sup>1</sup>; <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; <sup>2</sup>Department of Biomedicine, University of Bergen, Bergen, Norway; <sup>3</sup>VIB Ghent University, Ghent, Belgium; <sup>4</sup>Center for Thrombosis and Hemostasis CTH, Mainz, Germany; <sup>5</sup>Cardiovascular Research Institute CARIM, Maastricht, The Netherlands
- TP 106 **Comprehensive Profiling of Lysine Acetylation in Staphylococcus aureus;** Yi Zhang<sup>1</sup>; Zhixiang Wu<sup>1</sup>; Xuelian Wan<sup>1</sup>; Ping Liu<sup>1</sup>; Yingming Zhao<sup>2</sup>; Minjia Tan<sup>1</sup>; <sup>1</sup>Shanghai Institute of Materia Medica, Shanghai, CHINA; <sup>2</sup>the University of Chicago, Chicago, IL
- TP 107 **Variability in the Glycosylation Patterns of gp120 proteins from Different Human Immunodeficiency Virus Type 1 Isolates Expressed in Different Cells;** Ehwang Song<sup>1</sup>; Samantha Rice-Williams<sup>2</sup>; Fan Jiang<sup>2</sup>; Ghalib Alkhatib<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Southern Research Institute, Birmingham, AL
- TP 108 **Large-Scale Analysis of Lysine SUMOylation by SUMO Remnant Immunoaffinity Profiling;** Frederic Lamoliatte<sup>1</sup>; Danielle Caron<sup>1</sup>; Chantal Durette<sup>1</sup>; Louiza Mahrouche<sup>1</sup>; Mohamed Ali Maroui<sup>2</sup>; Olivier Caron-Lizotte<sup>1</sup>; Eric Bonnell<sup>1</sup>; Mounira Chelbi-alix<sup>2</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>Institute for Research in Immunology and Cancer, Montréal, QC, CANADA; <sup>2</sup>CNRS FRE3235, Université Paris Descartes, Paris, France
- TP 109 **Automated Immunoaffinity-Based Proteomic Methods for the Study of Post-Translational Modification;** Matthew P. Stokes<sup>1</sup>; Jeffrey C. Silva<sup>1</sup>; Steven Murphy<sup>2</sup>; Jason Russell<sup>2</sup>; Jian Min Ren<sup>1</sup>; Kimberly Lee<sup>1</sup>; <sup>1</sup>Cell Signaling Technology, Danvers, MA; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- TP 110 **Protein and Glycoprotein LC/MS Using HILIC;** Barry Boyes<sup>1,2</sup>; Ron Orlando<sup>2</sup>; Stephanie Schuster<sup>1</sup>; Joseph Destefano<sup>1</sup>; <sup>1</sup>Advanced Materials Technology Inc., Wilmington, DE; <sup>2</sup>University of Georgia, Athens, GA
- TP 111 **A Phosphoproteomic Approach to Enrich and Identify Mono- and poly(ADP-ribosylation) Sites in Whole Cell Lysate;** Casey M. Daniels<sup>1</sup>; Shao-En Ong<sup>2</sup>; Anthony K.L. Leung<sup>1</sup>; <sup>1</sup>Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; <sup>2</sup>University of Washington, Seattle, WA
- TP 112 **The Novel Lysine Glutarylation Pathway, Its Regulatory Enzyme SIRT5, Its Substrates and Regulatory Role in Metabolism;** Minjia Tan<sup>1</sup>; Chao Peng<sup>2</sup>; Kristin A. Anderson<sup>3</sup>; Peter Chhoy<sup>3</sup>; Zhongyu Xie<sup>2</sup>; Lunzhi Dai<sup>2</sup>; Yi Zhang<sup>1</sup>; Matthew D. Hirschey<sup>3</sup>; Yingming Zhao<sup>2</sup>; <sup>1</sup>Shanghai Institute of Materia Medica, Shanghai, CHINA; <sup>2</sup>the University of Chicago, Chicago, IL; <sup>3</sup>Duke University Medical Center, Durham, NC
- TP 113 **Site-Specific Quantitation of Lysine Acetylation in Isomeric Peptides of Histones H3 and H4;** Nebiyu Abshiru<sup>1,2</sup>; Olivier Caron-Lizotte<sup>1,2</sup>; Roshan Elizabeth<sup>1,2</sup>; Alain Verreault<sup>1,2</sup>; Pierre Thibault<sup>1,2</sup>; <sup>1</sup>University de Montreal, Montreal, Canada; <sup>2</sup>Institute for Research in Immunology and Cancer, Montreal, QC
- TP 114 **Affinity-based Quantitative Proteomics Reveals Non-histone Substrates of Methyltransferases G9a/GLP in Human Breast Adenocarcinoma Cell MDA-MB-231;** Xing-Jun Cao; Benjamin A. Garcia; *University of Pennsylvania, Philadelphia, PA*
- TP 115 **A Cell Line-Specific Atlas of Protein Asp- and Glu-ADP-Ribosylation;** Yajie Zhang; Jianqi Wang; Ming Ding; Yonghao Yu; *UT Southwestern Medical Center, Dallas, TX*
- TP 116 **Structural and Functional Analysis of the Role of Multisite Phosphorylation in Irreversible Fatty Acylation by Mass Spectrometry;** Hongying Zhong; *Central China Normal University, Wuhan, CHINA*
- TP 117 **Simultaneous Monitoring of Protein Methylation and Acetylation Expands the Post-Translational Modification Network in a Human Gastric Cancer Cell Line;** Hongbo Gu; Charles L. Farnsworth; Kimberly A. Lee; Jianmin Ren; Xiaoying Jia; Jeffrey C. Silva; *Cell Signaling Technology, Danvers, MA*
- TP 118 **PTM Directed Re-Wiring and Their Networks in Oncogene Mutant and Knock-Out Cancer Cells;** Jing Song; Benlian Wang; Zhenghe Wang; Mark R. Chance; *Case Western Reserve University, Cleveland, OH*
- TP 119 **Glycan Site Mapping of Glycoproteins in Serum;** Qiuting Hong; Evan Parker; Ting Song; Carlito Lebrilla; *Chemistry, UC, Davis, Davis, CA*
- TP 120 **Comprehensive Mapping of Ribosomal Protein Post-Translational Modifications by LC-MS/MS Analysis of Tryptic and Microwave-Assisted HCL Partial Hydrolysates;** Yuwei Chang; Rueyhung Weng; Chen-Chung Liao; Wailap Ng; *National Yang Ming University, Taipei, Taiwan*

- TP 121 **Identification and Quantification of Reversible Cysteine Modification Sites in GPx7-deficient Mice using Multiplexed iodoTMT tags for Irreversible Labeling and Enrichment;** Yi-Yun Chen<sup>1</sup>; Ping-Kun Hsieh<sup>2</sup>; Suh-Yuen Liang<sup>1</sup>; Wen-Hwa Lee<sup>2</sup>; Tzu-Ching Meng<sup>1</sup>; Kay-Hooi Khoo<sup>1</sup>; <sup>1</sup>*Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- TP 122 **Lysine Acetylome in *Streptomyces roseosporus* Reveals the Roles of Lysine Acetylation in Regulating Biosynthesis of Secondary Metabolites;** Guojian Liao<sup>1</sup>; Xiaojun Peng<sup>2</sup>; Zhongyi Cheng<sup>2</sup>; Jianping Xie<sup>1</sup>; <sup>1</sup>*College of Pharmaceutical Sciences, Southwest Univ, Chongqing, CN*; <sup>2</sup>*PTM Biolabs, Inc, Hangzhou, China*
- TP 123 **Quantification of Lysine Acetylation in Human Oligodendroglia Cells in Response to Borna Disease Virus Infection;** Xia Liu<sup>1,2</sup>; Xiaojun Peng<sup>3</sup>; Zhongyi Cheng<sup>3</sup>; Peng Xie<sup>1,2</sup>; <sup>1</sup>*Institute of Neuroscience, Chongqing Medical Univ, Chongqing, CN*; <sup>2</sup>*The First Affiliated Hospital, Chongqing Medical U, Chongqing, CN*; <sup>3</sup>*PTM Biolabs, Inc, Hangzhou, China*
- TP 124 **A Comprehensive Workflow for Simultaneous Assessment of Multiple PTMs;** Martin R. Larsen; Alistair V.G. Edwards; Giuseppe Palmisano; *Univ. Southern Denmark, Odense, Denmark*
- TP 125 **Elucidation of Diverse and Divergent Post-Translational Modification of Proteins in Closely Related Bacteria in a Natural Microbial Community without Enrichment;** Zhou Li<sup>1,2</sup>; Yingfeng Wang<sup>2</sup>; Qiuming Yao<sup>3</sup>; Nicholas Justice<sup>4</sup>; Tae-Hyuk Ahn<sup>2</sup>; Dong Xu<sup>3</sup>; Robert Hettich<sup>1,2</sup>; Jillian Banfield<sup>4</sup>; Chongle Pan<sup>1,2</sup>; <sup>1</sup>*University of Tennessee, Knoxville, TN*; <sup>2</sup>*Oak Ridge National Lab, Oak Ridge, TN*; <sup>3</sup>*University of Missouri, Columbia, MO*; <sup>4</sup>*University of California, Berkeley, CA*
- TP 126 **Functional Proteomics Defines the Molecular Mechanisms underlying Receptor Tyrosine Kinases (RTKs) signaling specificity;** Chiara Francavilla<sup>1</sup>; Kristoffer T.G. Rigbolt<sup>2</sup>; Kristina B. Emdal<sup>1</sup>; Moreno Papetti<sup>1</sup>; Jesper V. Olsen<sup>1</sup>; Blagoy Blagoev<sup>3</sup>; <sup>1</sup>*NNF CPR, Copenhagen, Denmark*; <sup>2</sup>*FRIAS, University of Freiburg, Freiburg, Germany*; <sup>3</sup>*University of Southern Denmark, Odense, Denmark*
- TP 127 **Uncovering Novel Redox Regulated Cysteines in the Mitochondrial Proteome Governed by Distinct Sites of Reactive Oxygen Species Production;** Casey Quinlan<sup>1</sup>; Bradford Gibson<sup>2</sup>; Martin Brand<sup>2</sup>; Jason Held<sup>3</sup>; <sup>1</sup>*Pfizer, La Jolla, CA*; <sup>2</sup>*Buck Institute for Research on Aging, Novato, CA*; <sup>3</sup>*Washington University Medical School, St. Louis, MO*
- TP 128 **Phosphorylation Dynamics of PTH Receptor Signaling in Osteoblasts;** Grace Williams; Jennifer Bethard; Mary Berkaw; Louis Luttrell; Lauren Ball; *Medical Univ of S Carolina, Charleston, SC*
- TP 129 **Isomer Proteomics: A Case Study of Epimerization and Isomerization in Crystallins;** Yuanqi Tao; Ryan R. Julian; *University of California, Riverside, Riverside, CA*
- TP 130 **Probing the Regulation of Ubc9 Activity using a Mass Spectrometry-Based *in vitro* SUMOylation Assay;** Francis McManus<sup>1</sup>; Danielle Caron<sup>2</sup>; Frederic Lamoliatte<sup>1</sup>; Pierre Thibault<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montréal, Canada*; <sup>2</sup>*Université Laval, Québec, Canada*
- TP 131 **Evaluating the Relationship between N-glycosylation and Protein Stability in the Enteric Pathogen *Campylobacter jejuni*;** Joel Cain<sup>1</sup>; Nichollas Scott<sup>2</sup>; Nestor Solis<sup>1</sup>; Melanie White<sup>1</sup>; Stuart Cordwell<sup>1</sup>; <sup>1</sup>*The University of Sydney, Sydney, Australia*; <sup>2</sup>*University of British Columbia, Vancouver, BC*
- TP 132 **Robust and Sensitive Methodologies of Chemical Crosslinking and Mass Spectrometry for Hybrid Structural Characterization of Endogenous Protein Complexes;** Yi Shi<sup>1</sup>; Javier Fernandez-Martinez<sup>1</sup>; Riccardo Pellarin<sup>2</sup>; Peter Fridy<sup>1</sup>; Elina Tjioe<sup>2</sup>; Seung Joong Kim<sup>2</sup>; Qingjun Wang<sup>3</sup>; Andrej Sali<sup>2</sup>; Michael P. Rout<sup>1</sup>; Brian T. Chait<sup>1</sup>; <sup>1</sup>*The Rockefeller University, New York, NY*; <sup>2</sup>*University of California, San Francisco, CA*; <sup>3</sup>*University of Kentucky, Lexington, KY*
- TP 133 **Analysis of Ferritin and Apoferritin by MALDI-TOF with STJ Cryodetection;** Logan Plath<sup>1</sup>; Alexander Aksenov<sup>2</sup>; Abdil Ozdemir<sup>3</sup>; David Sipe<sup>1</sup>; Mark E. Bier<sup>1</sup>; <sup>1</sup>*Carnegie Mellon University, Pittsburgh, PA*; <sup>2</sup>*University of California - Davis, Davis, CA*; <sup>3</sup>*Sakarya University, Adapazari, Turkey*
- TP 134 **Study of the Mitochondrial Importome in *Trypanosoma brucei* using SILAC, RNAi and high resolution MS;** Silke Oeljeklaus<sup>1</sup>; Christian Peikert<sup>1</sup>; Jan Mani<sup>2</sup>; André Schneider<sup>2</sup>; Bettina Warscheid<sup>1</sup>; <sup>1</sup>*Faculty of Biology, University of Freiburg, Freiburg, Germany*; <sup>2</sup>*University of Bern, Bern, Switzerland*
- TP 135 **Binding Properties of Copper(II)-Human Amylin Complexes Revealed by Laser Ablation Electrospray Ionization Mass Spectrometry;** Emmeline Ha; Hang Li; Robert P. Donaldson; Aleksander Jeremic; Akos Vertes; *The George Washington University, Washington, DC*
- TP 136 **Optimizing an Orbitrap Mass Spectrometer for the High Resolution Analysis of Intact Mega Dalton Virus Capsids;** Joost Snijder<sup>1</sup>; Michiel van den Waterbeemd<sup>1</sup>; Eugen Damoc<sup>2</sup>; Eduard Denisov<sup>2</sup>; Dmitry Grinfeld<sup>2</sup>; Alexander Makarov<sup>1,2</sup>; Albert J.R. Heck<sup>1</sup>; <sup>1</sup>*Utrecht University, Utrecht, The Netherlands*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- TP 137 **The Monitoring of the Protein Complex Landscape in Response on Apoptosis using PCP-SILAC;** Nicholas Scott; Anders Kristensen; Leonard Foster; *University of British Columbia, Vancouver, Canada*
- TP 138 **Scoring Protein Interactions Using the CRAPome: A Contaminant Repository for Affinity Purification Mass Spectrometry Data;** Dattatreya Mellacheruvu<sup>1</sup>; Zachary Wright<sup>1</sup>; Anne-Claude Gingras<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>*University of Michigan, Ann Arbor, MI*; <sup>2</sup>*Samuel Lunenfeld Research Institute, Mount Sinai H, Toronto, ON*
- TP 139 **Identification of Protein Interaction Partners of Protein Phosphatase 2A Catalytic Subunit Using Quantitative Mass Spectrometry;** Divyasri Damacharla<sup>1</sup>; Xiangmin Zhang<sup>1</sup>; Danjun Ma<sup>1</sup>; Monique Lewis<sup>1</sup>; Michael Caruso<sup>1</sup>; Wissam Anteer<sup>1</sup>; Yue Qi<sup>1</sup>; zhao yang<sup>1</sup>; Rodney Berry<sup>1</sup>; Abdullah Mallisho<sup>1</sup>; Zaher Msallaty<sup>1</sup>; Sorin Draghici<sup>1</sup>; Jeffrey Horowitz<sup>2</sup>; Berhane Seyoum<sup>1</sup>; Zhengping Yi<sup>1</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*University of Michigan, Ann Arbor, MI*
- TP 140 **Identification of BK Protein Partners in Mouse Cerebellum using Proteomic Mass Spectrometry;** Lancia Darville; Bernd Sokolowski; *University of South Florida, Tampa, FL*
- TP 141 **New Interactors of the Peroxisomal Receptor Export Complex Revealed by Affinity Purification and SILAC Mass Spectrometry;** Jason Tonillo<sup>1</sup>; Sascha Steltgens<sup>1</sup>; Claudia Lindemann<sup>1</sup>; Thilo Lerari<sup>1</sup>; Helmut E. Meyer<sup>1</sup>; Ralf Erdmann<sup>2</sup>; Katja Kuhlmann<sup>1</sup>; <sup>1</sup>*Medical Proteome Center, Ruhr-University, Bochum, Germany*; <sup>2</sup>*Institute of Physiol. Chemistry, Ruhr-University, Bochum, Germany*
- TP 142 **The Mx1 Homeoprotein Regulates Target Gene Expression during Development by Forming Protein Complexes;** Jiange Yang; Jingqiang Wang; *Fudan University, Shanghai, P. R. China*

- TP 143 **Protein Phosphatase 1 Catalytic Subunit Protein Interaction Partners in Human Skeletal Muscle Revealed by Targeted Proteomics**; [Zhao Yang](#); Michael Caruso; Danjun Ma; Abdullah Mallisho; Berhane Seyoum; Monique Lewis; Xiangmin Zhang; Wissam Al-Janabi; Yue Qi; Divyarsi Damacharla; Rodney Berry; Zaher Msallaty; Sorin Draghici; Assia Shisheva; Zhengping Yi; *Wayne State University, Detroit, MI*
- TP 144 **Structural Probing of Calmodulin Interaction Network by Protein Engineering, Chemical Cross-Linking and Mass Spectrometry**; [Katarzyna Kulej](#); Morten Rasmussen; Simone Sidoli; Martin R. Larsen; *University of Southern Denmark, Odense M, Denmark*
- TP 145 **High-Throughput Proteomic Mapping of Protein Interaction Networks: Toward a Global View of the Human Interactome**; [Edward L. Huttlin](#)<sup>1</sup>; Lily Ting<sup>1</sup>; Raphael Bruckner<sup>1</sup>; Joao Paulo<sup>1</sup>; Melanie Gygi<sup>1</sup>; Ramin Rad<sup>1</sup>; Deepak Kolippakkam<sup>1</sup>; John Szpyt<sup>1</sup>; Gabriela Zarraga<sup>1</sup>; Stanley Tam<sup>1</sup>; Fana Gebreab<sup>1</sup>; Greg Colby<sup>1</sup>; Robert Obar<sup>1</sup>; Virginia Guarani-Pereira<sup>1</sup>; Timothy Harris<sup>2</sup>; Spyros Artavanis-Tsakonas<sup>1,2</sup>; Mathew Sowa<sup>1</sup>; J. Wade Harper<sup>1</sup>; Steven Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Biogen Idec, Boston, MA*
- TP 146 **Molecular Composition of HIV-1 Virion-Associated Lipid Rafts: Insights into Pathogenesis**; [David R Graham](#)<sup>1</sup>; Veronica Aquino<sup>1</sup>; Brandon Bullock<sup>1</sup>; Brian Agnew<sup>2</sup>; Rhoel Dinglasan<sup>1</sup>; David Colquhoun<sup>3</sup>; Ravi Tharakan<sup>4</sup>; Hung Trinh<sup>5</sup>; Katherine Bruner<sup>1</sup>; Ceereena Ubaida Mohien<sup>1</sup>; <sup>1</sup>*Johns Hopkins University, Baltimore, MD*; <sup>2</sup>*LifeTech, Eugene, Or*; <sup>3</sup>*Shimadzu Scientific Instr, Columbia, MD*; <sup>4</sup>*JHU, Baltimore, MD*; <sup>5</sup>*Walter Reed Army Institute of Research, Silver Spring, MD*
- TP 147 **Characterization of Membrane Protein Complexes in Photoreceptor Outer Segments using Size Fractionation-Based Protein Correlation Profiling**; [Nikolai Skiba](#); Vadim Arshavsky; *Duke University, Durham, NC*
- Protein Therapeutics: Structural Characterization, 148 - 161**
- TP 148 **Understanding N-terminal Variation in Therapeutic Proteins by High Resolution Mass Spectrometry: from Top-down to Bottom-up**; [Guilong \(Charles\) Cheng](#); Adriana Kita; Gomathinayagam Ponniah; Hongcheng Liu; Bruce Andrien; *Alexion Pharmaceutical Inc., Cheshire, CT*
- TP 149 **Middle-down and Bottom-Up Characterization of a Monoclonal Antibody Trastuzumab with Sheathless CESI-MS Coupled to the Orbitraps Mass Spectrometers**; [Marcia Santos](#)<sup>1</sup>; David Bush<sup>5</sup>; Hans Dewald<sup>1</sup>; Rosa Viner<sup>2</sup>; Alain Beck<sup>3</sup>; Antonius Heemskerck<sup>4</sup>; Barry Karger<sup>5</sup>; Alexander Ivanov<sup>5</sup>; <sup>1</sup>*AB Sciex LLC, Brea, CA*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*Centre d'Immunologie Pierre Fabre (CIPF), Saint-Julien-en-Genevois, France*; <sup>4</sup>*Leiden University Medical Center, Leiden, The Netherlands*; <sup>5</sup>*Barnett Institute, Northeastern University, Boston, MA*
- TP 150 **Rapid Identification and Characterization of Biopharmaceuticals using Capillary Electrophoresis – Mass Spectrometry Coupled with Supercharging**; [Rajeswari Lakshmanan](#)<sup>1</sup>; Chitra K. Ratnayake<sup>1</sup>; Rachel O. Loo<sup>2</sup>; Joseph A. Loo<sup>2</sup>; <sup>1</sup>*AB Sciex, Brea, CA*; <sup>2</sup>*UCLA, Los Angeles, CA*
- TP 151 **Primary Structure Characterization of a Therapeutic Protein by nano-LC-MS/MS to Elucidate Proteolytic Instability**; [Xian Huang](#); Dan Rock; *Amgen, Inc., Seattle, WA*
- TP 152 **Characterization of Disulfide Variants and Free Sulfhydryls by Mass Spectrometry Using Non-reduced Multi-Attribute Method**; [Yuling Zhang](#); Robert Bailey; Nancy Nightlinger; Alison Gillespie; Alain Bolland; Richard Rogers; *Amgen, Seattle, WA*
- TP 153 **Monosaccharide Profiling by Intact Mass Analysis - Method Qualification of a New Approach for the Characterization of Highly Glycosylated Biopharmaceuticals**; [Benjamin Mueller](#); Stefanie Fitzek; Stefanie Janzen; Elke Schwitulla; Andreas Wattenberg; *Protagen Protein Services, Dortmund, Germany*
- TP 154 **Advanced LC-MS Based Characterization for Determination of Critical Quality Attributes in Therapeutic Proteins**; Chen Li<sup>1</sup>; Anna Zhang<sup>2</sup>; Serah Liu<sup>2</sup>; Peter Li<sup>1</sup>; Julian Saba<sup>3</sup>; Zhiqi Hao<sup>3</sup>; [Shiaw-Lin Wu](#)<sup>1,2</sup>; <sup>1</sup>*BioAnalytix Inc., Cambridge, MA*; <sup>2</sup>*Barnett Institute, Northeastern University, Boston, MA*; <sup>3</sup>*ThermoFisher Scientific, San Jose, CA*
- TP 155 **Size Exclusion Isotope Dilution Mass Spectrometry: An Alternative Method for Influenza Vaccine Potency Determination**; [Jonathan Bundy](#); Zsuzsanna Kuklenyik; Yulanda Williamson; Maria Solano; Tracie Williams; John R. Barr; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 156 **Quantitative Profiling Glycoforms of Therapeutic mAb using Orthogonal Techniques: Comparison of subunit 1/2Fc analysis with the released glycan assay**; [Henry Shion](#)<sup>1</sup>; Mark Hilliard<sup>2</sup>; Ying-Qing Yu<sup>1</sup>; Weibin Chen<sup>1</sup>; Niaobh McLoughlin<sup>2</sup>; Pauline Rudd<sup>2</sup>; <sup>1</sup>*Waters Corp., Milford, MA*; <sup>2</sup>*NIBRT, Dublin, Ireland*
- TP 157 **Increasing the Confidence of Sequence Variant Identification by the Development of Integrated Mass Spectrometric and Informatics Workflow**; Stephane Houel<sup>1</sup>; Scott Geromanos<sup>1</sup>; Andrew Tudor<sup>2</sup>; Barry Dyson<sup>2</sup>; Ying Qing Yu<sup>1</sup>; [Weibin Chen](#)<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters Corporation, Manchester, UK*
- TP 158 **Automating Characterization of mAb Charge Variants Isolated by Cation Exchange Chromatography using Integrated LCMS Peptide Mapping and Informatics Workflow**; [Vera Ivleva](#); Robert Birdsall; Ying Qing Yu; Weibin Chen; *Waters Corporation, Milford, MA*
- TP 159 **Development of Fast Photochemical Oxidation of Protein (FPOP) Platform for Protein Therapeutics: Validation and Application**; [Ying Zhang](#)<sup>1</sup>; Aaron Wecksler<sup>2</sup>; Patricia Molina<sup>2</sup>; Galahad Deperalta<sup>2</sup>; Victor Ling<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO*; <sup>2</sup>*Genentech Inc., South San Francisco, CA*
- TP 160 **A Mass Spectrometry Toolbox for the Characterization of Defined CRM<sub>197</sub> Glycoconjugate Vaccines Candidates**; [Uwe Möginger](#)<sup>1,2</sup>; Anja Resemann<sup>3</sup>; Christopher E. Martin<sup>1,2</sup>; Eike Wamhoff<sup>1,2</sup>; Detlef Suckau<sup>3</sup>; Subramanian Govindan<sup>1</sup>; Sharavathi Parameswarappa<sup>1</sup>; Claney Lebev Pereira<sup>1</sup>; Peter H. Seeberger<sup>1,2</sup>; Chakkumkal Anish<sup>1</sup>; Daniel Kolarich<sup>1</sup>; <sup>1</sup>*Max Planck Institute for Colloids and Interfaces, Potsdam, Germany*; <sup>2</sup>*Freie University, Berlin, Germany*; <sup>3</sup>*Bruker Daltonics, Bremen, Germany*
- TP 161 **Structural Analysis of an Intact Monoclonal Antibody using On-Line Electrochemical Reduction of Disulfide Bonds and Ultrahigh Resolution FTICR-MS**; [Simone Nicolardi](#); André M. Deelder; Magnus Palmblad; Yuri E.M. van der Burg; *Leiden University Medical Center, Leiden, Netherlands*
- Phosphopeptides: Sequence Analysis, 162 - 164**
- TP 162 **Enhanced Characterization of Multiply Phosphorylated Peptides using Hydroxyapatite Enrichment and Ultraviolet Photodissociation**; [Michelle Robinson](#); Jennifer Brodbelt; *University of Texas at Austin, Austin, TX*
- TP 163 **Tandem Mass Spectrometry Sequencing of Post-Translationally Modified Peptides using Matrix Assisted Ionization Vacuum on an ESI Source**; [Ruby Kumar](#); Chih-Wei Liu; Corinne Lutomski; Ellen Inutan; Sarah Trimpin; *Wayne State University, Detroit, MI*

- TP 164 **Unblocking the Sink: Improved CID-Based Analysis of Phosphorylated Peptides by Enzymatic Removal of the Basic C-Terminal Residue**; Francesco Lanucara; Dave Chi Hoo Lee; Claire E. Evers; *University of Liverpool, Liverpool, UK*
- Peptidomics, 165 - 172**
- TP 165 **Sample Complexity Reduction Assisted Neuropeptidomics of the Rat Habenula through Liquid Chromatography Mass Spectrometry**; Ning Yang; Stanislav Rubakhin; Cong Wu; Jonathan Sweedler; *University of Illinois at Urbana Champaign, Urbana, IL*
- TP 166 **Development of Sequence Tag Library Search System for Peptidomics**; Masaki Murase<sup>1</sup>; Jingwen Yao<sup>1</sup>; Kentaro Morimoto<sup>1</sup>; Yoshihiro Yamada<sup>1</sup>; Sadanori Sekiya<sup>1</sup>; Shigeki Kajihara<sup>1</sup>; Shinichi Iwamoto<sup>1</sup>; Koichi Tanaka<sup>1</sup>; Kenji Nakayama<sup>2</sup>; Yu Miyazaki<sup>2</sup>; Naoki Terada<sup>2</sup>; Takahiro Inoue<sup>2</sup>; Osamu Ogawa<sup>2</sup>; <sup>1</sup>*Koichi Tanaka Lab of Adv. Sci. and Tech., Shimadzu, Kyoto, JAPAN*; <sup>2</sup>*Dept. Urology, Grad. Sch. Med., Kyoto University, Kyoto, Japan*
- TP 167 **Profiling of Precursor Processing Events using Single Cell Analysis**; Susanne Neupert; Christian Derst; Reinhard Predel; *University of Cologne - Biocenter, Cologne, Germany*
- TP 168 **Mass Spectrometric Characterization of the Neuropeptidome in the Mouse Lung (*Mus musculus*)**; Qing Yu; Kelsey Branchfield; Christopher Lietz; Jingxin Wang; Xin Sun; Lingjun Li; *University of Wisconsin-Madison, Madison, Wisconsin*
- TP 169 **Comprehensive Quantitative Analysis of Ovarian and Breast Cancer Tumor Peptidomes**; Zhe Xu<sup>1</sup>; Chaochao Wu<sup>1</sup>; Fang Xie<sup>1</sup>; Gordon W. Slys<sup>2</sup>; Nikola Tolic<sup>2</sup>; Matthew E. Monroe<sup>1</sup>; Vladislav A. Petyuk<sup>1</sup>; Samuel H. Payne<sup>1</sup>; Grant M. Fujimoto<sup>1</sup>; Ronald J. Moore<sup>1</sup>; Thomas L. Fillmore<sup>2</sup>; Athena A. Schepmoes<sup>1</sup>; Douglas A. Levine<sup>3</sup>; Reid Townsend<sup>4</sup>; Sherri R. Davies<sup>4</sup>; Shunqiang Li<sup>4</sup>; Matthew Ellis<sup>4</sup>; Karin D. Rodland<sup>1</sup>; Tao Liu<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>*Biological Sciences Division, PNNL, Richland, WA*; <sup>2</sup>*Environmental Molecular Sciences Laboratory, PNNL, Richland, WA*; <sup>3</sup>*Memorial Sloan-Kettering Cancer Center, New York, NY*; <sup>4</sup>*Department of Medicine, Washington University, St. Louis, MO*
- TP 170 **Analysis of the Cysteine-Containing Proteome and Peptidome in CSF using TMT and iodoTMT**; Fiona E. McAllister; Shellie Hyde; Karen Parker; Joshua E. Elias; *Stanford School of Medicine, Stanford, CA*
- TP 171 **Recent Advances in Mhc-Associated Peptide Proteomics (MAPPs) Technology for a Risk Assessment of Immunogenicity of Biotherapeutics**; Tatiana Pimenova; Axel Ducret; Denise Sauter; Paul Cutler; Thomas Weiser; Thomas Singer; Anja Langenkamp; *F. Hoffmann-La Roche Ltd, Basel, Switzerland*
- TP 172 **Enrichment of Amino Terminal Peptides from Formalin-Fixed Paraffin-Embedded Tissues**; Zon Lai<sup>1</sup>; Juliane Weisser<sup>1</sup>; Peter Bronsert<sup>2</sup>; Oliver Schilling<sup>1</sup>; <sup>1</sup>*University of Freiburg, Freiburg, Germany*; <sup>2</sup>*University Medical Center Freiburg, Freiburg, Germany*
- Peptides: Quantitative Analysis (New Approaches to Data Acquisition and Analysis), 173 - 186**
- TP 173 **Quantitative Proteomics Analysis by Parallel Reaction Monitoring MS of Inhibitor Enriched Kinases from Patient-derived Breast Cancer Xenografts**; Matthew R. Meyer<sup>1</sup>; John A. Wrobel<sup>3</sup>; Kelly V. Ruggles<sup>2</sup>; Petra Erdmann-Gilmore<sup>1</sup>; Lee M. Graves<sup>3</sup>; Jian Jin<sup>3</sup>; Jeremy Hoog<sup>1</sup>; Shunqiang Li<sup>1</sup>; Jacqueline Snider<sup>1</sup>; Robert Kitchens<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Matthew J. Ellis<sup>1</sup>; David Fenyo<sup>2</sup>; Gary L. Johnson<sup>3</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>*Washington University in St. Louis, St. Louis, MO*; <sup>2</sup>*New York University, New York, NY*; <sup>3</sup>*University of North Carolina, Chapel Hill, NC*
- TP 174 **Can Multiple Reaction Monitoring Cubed Solve Interference issues for the analysis of Tachykinin Related Peptides by LC-MS<sup>n</sup>**; Floriane Pailleux; Francis Beaudry; *Université de Montréal, St-Hyacinthe, Canada*
- TP 175 **An SRM Toolkit for "Faster-Better-Cheaper" Absolute Quantification of *Escherichia coli* Pathway Proteins**; Pragya Singh<sup>1</sup>; Tanveer Batth<sup>1</sup>; Vikram Ramakrishnan<sup>1</sup>; Mirta M. L. Sousa<sup>2</sup>; Leanne Jade Chan<sup>1</sup>; Jay D. Keasling<sup>1</sup>; Paul D. Adams<sup>1</sup>; Chris Petzold<sup>1</sup>; <sup>1</sup>*Lawrence Berkeley National Lab, Emeryville, CA*; <sup>2</sup>*Norwegian University of Science and Technology, Trondheim, Norway*
- TP 176 **SRM Vs. HR-MS Quantitative Proteomics: Matrix Effect and LOQ in Serum**; Dominique Baiwir<sup>1</sup>; Nicolas Smargiasso<sup>2</sup>; Gabriel Mazzucchi<sup>2</sup>; Edwin De Pauw<sup>2</sup>; <sup>1</sup>*University of Liege, GIGA Proteomic Facility, Liege, Belgium*; <sup>2</sup>*Univeristy of Liege, MS Lab - GIGA, Liege, Belgium*
- TP 177 **Toward Highly Multiplexed Immuno-Multiple Reaction Monitoring Mass Spectrometry Assays**; Paul Ippoliti<sup>1</sup>; Eric Kuhn<sup>1</sup>; Lola Fagbami<sup>1</sup>; Steve Murphy<sup>2</sup>; Jacob D. Jaffe<sup>1</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*Broad Institute of MIT and Harvard, Cambridge, MA*; <sup>2</sup>*Agilent Technologies, Madison, WI*
- TP 178 **Targeted Proteomics with an Extended Dynamic Range (EDR) Triple Quadrupole Mass Spectrometer**; Robert Maxwell<sup>1</sup>; Maurizio Splendore<sup>1</sup>; Stephen Zanon<sup>1</sup>; Milady Ninonuevo<sup>1</sup>; Karen Salomon<sup>1</sup>; Pierre-Olivier Schmit<sup>2</sup>; Desmond Kaplan<sup>1</sup>; <sup>1</sup>*Bruker CAM, Fremont, CA*; <sup>2</sup>*Bruker Daltonique S.A, Wissembourg, France*
- TP 179 **Enhanced Performance and Robustness in Peptide Quantitation Using a Newly Developed Triple Quadrupole Instrument**; Yanan Yang; Alex Zhu; Christine Miller; Anabel Fandino; *Agilent Technologies, Santa Clara, CA*
- TP 180 **Deep Proteomics of the *Xenopus Laevis* Egg using an mRNA-derived Reference Database**; Martin Wühr<sup>1</sup>; Robert M Freeman Jr<sup>1</sup>; Marc Presler<sup>1</sup>; Matthew Sonnett<sup>1</sup>; Marko E Horb<sup>2</sup>; Leonid Peshkin<sup>1</sup>; Marc W Kirschner<sup>1</sup>; Steven Gygi<sup>1</sup>; <sup>1</sup>*Harvard Medical School, Boston, MA*; <sup>2</sup>*Marine Biological Laboratory, Woods Hole, MA*
- TP 181 **Framework for the Automated Selection of Transitions and Peptides for Quantification by SWATH<sup>TM</sup>**; Stephen Tate<sup>1</sup>; Gordana Ivosev<sup>1</sup>; Jean-Philippe Lambert<sup>2</sup>; George Rosenberger<sup>3</sup>; Samuel Bader<sup>4</sup>; Anne-Claude Gingras<sup>2</sup>; Robert Moritz<sup>4</sup>; Ruedi Aebersold<sup>3</sup>; <sup>1</sup>*AB SCIEX, Concord, Canada*; <sup>2</sup>*LTRI, Toronto, Canada*; <sup>3</sup>*ETH-IMSB, Zurich, Switzerland*; <sup>4</sup>*ISB, Seattle, WA*
- TP 182 **Improved DIA Approaches to Address Sample Complexity**; Brett Larsen<sup>1</sup>; Stephen A Tate<sup>2</sup>; Jian Wang<sup>3</sup>; Nuno Bandeira<sup>3</sup>; Anne-Claude Gingras<sup>1</sup>; <sup>1</sup>*Lunenfeld-Tanenbaum Research Institute, Toronto, CANADA*; <sup>2</sup>*AB SCIEX, Concord, ON*; <sup>3</sup>*University of California, San Diego, La Jolla, CA*
- TP 183 **Optimization of Ion Libraries for Label Free SWATH Quantitation with Experimental and Hypothetical Transitions**; Peter D. McQueen<sup>1,3</sup>; Vic Spicer<sup>1,2</sup>; Oleg Krokhin<sup>1,3</sup>; David Levin<sup>1,4</sup>; Richard Sparling<sup>1,5</sup>; John Wilkins<sup>1,3</sup>; <sup>1</sup>*University of Manitoba, Winnipeg, Canada*; <sup>2</sup>*Department of Physics, Winnipeg, Canada*; <sup>3</sup>*Manitoba Centre for Proteomics and Systems Biology, Winnipeg, Canada*; <sup>4</sup>*Biosystems Engineering, Winnipeg, Canada*; <sup>5</sup>*Department of Microbiology, Winnipeg, Canada*
- TP 184 **A Novel SWATH-MS Platform for Comprehensive Characterization of Epigenetic Histone Modifications**; Benjamin A. Garcia<sup>1</sup>; Eric Johansen<sup>2</sup>; Sean Seymour<sup>2</sup>; Zuo-Fei Yuan<sup>1</sup>; Kelly R. Karch<sup>1</sup>; Christie L. Hunter<sup>2</sup>; Sahana Mollah<sup>2</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*AB Sciex, Redwood City, CA*



- TP 185 **High Throughput Peptide Mapping Using High Resolution Direct Infusion Nano-electrospray**; Gerald W. Becker; Jonathon Woodard; Vladimir Razinkov; Zhang Jun; *Amgen, Seattle, WA*
- TP 186 **Data Independent Analysis with Data Dependent Isolation Widths**; Yang Kang; Adam Lau; Stephen Tate; *AB Sciex, Concord, Canada*
- Proteomics: New Approaches, 187 - 208**
- TP 187 **A Novel Membrane-Based High-Throughput Sample Preparation Method for Bottom-Up Proteomics**; Sebastian Berger; Saima Ahmed; Nerea Cuevas Polo; Jan Muntel; Hanno Steen; *Harvard Medical School/Children's Hospital Boston, Boston, MA*
- TP 188 **Discovery of Multiple Native Cationic Antimicrobial Peptides with Hydrogel Microparticles and ETD De Novo Sequencing by Orbitrap Mass Spectrometry**; Paul Russo; Melanie Juba<sup>1,1</sup>; Megan Devine<sup>1</sup>; Stephanie Barksdale<sup>1</sup>; Carlos Rodriguez<sup>1</sup>; Myung Chung<sup>1</sup>; Kent Vliet<sup>2</sup>; Irina Tchernyshyov<sup>3</sup>; Jennifer Van Eyk<sup>3</sup>; Lissa Anderson<sup>4</sup>; Dina Bai<sup>4</sup>; Jeffrey Shabanowitz<sup>4</sup>; Donald Hunt<sup>4</sup>; Joel Schnur<sup>1</sup>; Monique Van Hoek<sup>1</sup>; Barney Bishop<sup>1</sup>; <sup>1</sup>George Mason University, Manassas, VA; <sup>2</sup>University of Florida, Gainesville, FL; <sup>3</sup>Johns Hopkins University, Baltimore, MD; <sup>4</sup>University of Virginia, Charlottesville, VA
- TP 189 **Single-tube Sample Preparation Workflows using Paramagnetic Beads for Ultra-sensitive Proteomics**; Christopher Hughes; Jeroen Krijgsveld; *EMBL, Heidelberg, Germany*
- TP 190 **A Universal Solid-phase Sample-preparation for Proteomics and Glycomics**; Hui Zhou<sup>1,2</sup>; Stephen Kostel<sup>1</sup>; Vivek Joshi<sup>3</sup>; Dave Brewster<sup>3</sup>; Richard Lee<sup>1,2</sup>; <sup>1</sup>Boston Children's Hospital, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>EMD Millipore Corp., Danvers, MA
- TP 191 **A MS-based Novel Chemical Method for Comprehensive Analysis of Protein N-glycosylation**; Weixuan Chen; Johanna Smeeckens; Ronghu Wu; *Georgia Tech, Atlanta, GA*
- TP 192 **Rethinking the Proteomics Experiment for LC/MS - Scaling for optimal results**; Tom Van De Goor; Stephan Buckenmaier; Monika Dittmann; *Agilent Technologies, Waldbronn, Germany*
- TP 193 **Study of a Preparation Method for a Highly Reproducible Monolithic Silica Capillary Column for Shotgun Proteomics**; Hiroshi Kobayashi; Mayu Ishida; Hiroo Wada; *Shinwa Chemical Industries Ltd, Kyoto, Japan*
- TP 194 **Bottom-up Proteomics of E. coli using Dynamic pH Junction Preconcentration and CZE-ESI-MS/MS**; Guijie Zhu; Liangliang Sun; Xiaojing Yan; Norman Dovichi; *University of Notre Dame, Notre Dame, IN*
- TP 195 **Exploration of the Use of Capillary Electrophoresis as an Augmentation or Replacement for Liquid Chromatography in Proteomic Analyses**; Ruth Alvarez<sup>1</sup>; Neloni Wijeratne<sup>1</sup>; Ahyoung Joo<sup>1</sup>; Chitra Ratnayake<sup>2</sup>; Paymaneh Malihi<sup>1</sup>; Kian Kani<sup>1</sup>; Jonathan Katz<sup>1</sup>; <sup>1</sup>CAMM/USC, Los Angeles, ca; <sup>2</sup>AB Sciex, Brea, CA
- TP 196 **Optimizing Capillary Electrophoresis for Top-Down Proteomics of 30-80 kDa proteins**; Yihan Li<sup>1</sup>; Philip D. Compton<sup>1</sup>; John C. Tran<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Genentech Inc., South San Francisco, CA
- TP 197 **Shotgun Proteomics on Volume-limited Neuron Cultures by CE and LC MS**; Camille Lombard; Rosemary M. Onjiko; M. Chiara Manzini; Peter Nemes; *George Washington University, Washington, DC*
- TP 198 **Proteomics Applications Using Matrix Assisted Ionization Vacuum-Ion Mobility Spectrometry/Mass Spectrometry**; Chih-Wei Liu<sup>1</sup>; Beixi Wang<sup>1</sup>; Ruby Kumar<sup>1</sup>; James Wager-Miller<sup>2</sup>; Ken Mackie<sup>2</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>Wayne State University, Detroit, MI; <sup>2</sup>Indiana University, Bloomington, IN
- TP 199 **Versatile Bio-applications of Argon Cluster Primary Ion Beam Use in ToF-SIMS**; Tae Lee<sup>1</sup>; Jin Gyeong Son<sup>1,2</sup>; Hyun Kyong Shon<sup>1</sup>; Sohee Yoon<sup>1</sup>; Ji-Won Park<sup>1</sup>; Jeong Hee Moon<sup>3</sup>; Sang Woo Han<sup>2</sup>; <sup>1</sup>KRISS, Daejeon, South Korea; <sup>2</sup>KAIST, Daejeon, South Korea; <sup>3</sup>KRIBB, Daejeon, South Korea
- TP 200 **The Effect of Chitosan Nanoparticle to Hepatic Cells – Is Chitosan Nanoparticle an Enhancer of AKT1/mTOR Pathway?**; Ming-Hui Yang<sup>1</sup>; Han-Pin You<sup>2</sup>; Yu-Chang Tyan<sup>2</sup>; <sup>1</sup>National Applied Research Laboratories, Hsinchu, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan
- TP 201 **Utilizing the Chemical Probe UNC1215 to Better Understand the Role of L3MBTL3 via SILAC Chemical Proteomics and Ligand-Directed Chemical Labeling**; Craig Wagner<sup>1</sup>; Mary Moyer<sup>1</sup>; Jon Williams<sup>1</sup>; Carrow Wells<sup>1</sup>; Brandon Turunen<sup>1</sup>; Tim Willson<sup>1</sup>; Stephen Frye<sup>2</sup>; Lindsey James<sup>2</sup>; <sup>1</sup>GlaxoSmithKline, Research Triangle Park, NC; <sup>2</sup>UNC Eshelman School of Pharmacy, Chapel Hill, NC
- TP 202 **New in vivo RNA-Binding Architectures Discovered by RBDmap**; Christian K. Frese; Alfredo Castello; Bernd Fischer; Sophia Foehr; Anne-Marie Alleaume; Tomaz Curk; Jeroen Krijgsveld; Matthias W. Hentze; *EMBL Heidelberg, Heidelberg, Germany*
- TP 203 **A Function-Based Intact Protein Analysis Workflow for Discovery of Novel Microbial Metal and Uranium Reductases in a Gram Positive Bacterium**; Anne Otwell<sup>1</sup>; Robert Sherwood<sup>1</sup>; Zhi Li<sup>1</sup>; Ornella Nelson<sup>1</sup>; Hening Lin<sup>1</sup>; Stephen Callister<sup>2</sup>; Ruth Richardson<sup>1</sup>; Sheng Zhang<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 204 **Identifying Reactive Metabolite Protein Targets in Liver Microsomes using Click Chemistry and Affinity Purification**; André Leblanc; Tze Chieh Shiao; René Roy; Lekha Sleno; *UQAM, Montreal, Canada*
- TP 205 **Tackling "Beadomics." Affinity Pulldowns using Two Different Bead Types**; Peter Hains<sup>1</sup>; Fiona Deane<sup>2</sup>; Andrew Lin<sup>2</sup>; Adam McCluskey<sup>2</sup>; Philip Robinson<sup>1</sup>; <sup>1</sup>Children's Medical Research Institute, Westmead, Australia; <sup>2</sup>University of Newcastle, Newcastle, Australia
- TP 206 **Identification of Functional Antibody Targets by Affinity Pulldowns and High Resolution Mass Spectrometry**; Maria Christina Malinao; Liping Hu; Dau Satpayev; Kendall Morrison; Vladimir Kery; *Agensys, Inc., Santa Monica, CA*
- TP 207 **Site-Specific Glutamine Seronylation by Mass Spectrometry-based Analysis**; Chi-Chi Chou; Jason Ching-Yao Lin; Chun-Hung Lin; Kay-Hooi Khoo; *Institute of Biological Chemistry, Academia Sinica, Taipei, Taiwan*
- TP 208 **Profiling Chicken Kinases with a MS Compatible Probe**; Xuan (Jo-Ann) Ding; Mariola Edelmann; *Mississippi State University, Mississippi State, MS*
- Microorganisms: Identification and Characterization, 209 - 232**
- TP 209 **Starvation-induced Changes in Lipid and Other Biomolecule Compositions in Dictyostelium discoideum Cells**; Kendra Adams<sup>1</sup>; John DeBord<sup>1</sup>; Richard Gomer<sup>2</sup>; Christopher Thompson<sup>3</sup>; Francisco Fernandez Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, Florida; <sup>2</sup>Texas A&M University, College Station, TX; <sup>3</sup>Bruker Daltonics Inc., Billerica, MA

- TP 210 **Two Shiga toxin 2 Subtypes in a Single Shiga Toxin-Producing Escherichia Coli Analyzed by RT-qPCR, MALDI-TOF-MS and Top-Down Proteomic Analysis;** Clifton K. Fagerquist; William J. Zaragoza; *USDA/ARS, Albany, CA*
- TP 211 **Quantitative Proteomics in Giardia Duodenalis: Investigating Host Origin, Assemblage and Isolate Variation;** Samantha Emery<sup>1</sup>; Ernest Lacey<sup>2</sup>; Paul Haynes<sup>1</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*Microbial Screening Technologies, Sydney, Australia*
- TP 212 **Rapid Detection of Bacterial Resistance by MALDI-TOF MS in Combination with Stable Isotope Labeling;** Jette Jung<sup>3</sup>; Sören Schubert<sup>3</sup>; Gary Kruppa<sup>2</sup>; Katrin Sparbier<sup>1</sup>; Christoph Lange<sup>1</sup>; Markus Kostrzewa<sup>1</sup>; <sup>1</sup>*Bruker Daltonics GmbH, Bremen, Germany*; <sup>2</sup>*Bruker Daltonics Inc., Billerica, MA*; <sup>3</sup>*Max-von-Pettenkofer Institute, Munich, Germany*
- TP 213 **Sequence Level and Dual-phase Flagella Antigen Identification of Salmonella by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS);** Keding Cheng; Angela Sloan; Julie Meakin; Stuart McCorrister; Morganne Jerome; Garrett Westmacott; Mike Drebot; Celine Nadon; J. David Knox; Gehua Wang; *Public Health Agency of Canada, Winnipeg, Canada*
- TP 214 **Study of MALDI Sample Preparation for Bacterial Identification;** Eun-kyeong Choi<sup>1</sup>; Hanyoung Jung<sup>1</sup>; Kyu Hwan Park<sup>1</sup>; Yongsun Kim<sup>2</sup>; <sup>1</sup>*Applied Surface Technology Inc., Suwon, KOREA*; <sup>2</sup>*Hudson Surface Technology Inc., Old Tappan, NJ*
- TP 215 **Recycling Old Software – Microbe Identification Using REIMS and MicrobeLynx;** Nicole Strittmatter<sup>2</sup>; Steven Pringle<sup>1,2</sup>; Keith Richardson<sup>1</sup>; Julia Balog<sup>2,3</sup>; Laurence Firth<sup>1</sup>; Zoltan Takats<sup>2</sup>; Lidia Cammack<sup>2</sup>; Mike Morris<sup>1,2</sup>; <sup>1</sup>*Waters Corporation, Manchester, UK*; <sup>2</sup>*Imperial College London, London, UK*; <sup>3</sup>*Medimass Ltd, Budapest*
- TP 216 **MALDI-TOF MS Detection of Carbapenem Resistant Enterobacteriaceae and Pseudomonas aeruginosa;** Patrick Chong<sup>1</sup>; Stuart McCorrister<sup>1</sup>; Mark Unger<sup>2</sup>; David Boyd<sup>1</sup>; Michael Mulvey<sup>1</sup>; Garrett R Westmacott<sup>1</sup>; <sup>1</sup>*Public Health Agency of Canada, Winnipeg, Canada*; <sup>2</sup>*University of Manitoba, Winnipeg, Canada*
- TP 217 **Serovar and Strain Level Bacterial Differentiation Capabilities for 36 Closely Related Outbreak Strains by Intact Protein LCMS;** Melinda McFarland; Denis Andrzejewski; Peter Evans; John Callahan; *US Food & Drug Administration, College Park, MD*
- TP 218 **Fatty Acid and Lipid Profiling of Arbuscular Mycorrhizal Fungi with LAESI-MS;** Gregory Boyce<sup>1</sup>; Callee Walsh<sup>1</sup>; Erin H. Seeley<sup>1</sup>; Joseph Morton<sup>2</sup>; Greg W. Kilby<sup>1</sup>; <sup>1</sup>*Protea Biosciences, Morgantown, WV*; <sup>2</sup>*West Virginia University, Morgantown, WV*
- TP 219 **Rapid Screening of Vancomycin-resistant Enterococcus (VRE) using Mass Spectrometry;** Yannick Charriert<sup>1,2</sup>; Elodie Degout-Charmette<sup>1</sup>; Tiphaine Cecchini<sup>1,2</sup>; Gilles Zambardi<sup>3</sup>; Xavier Lacoux<sup>1</sup>; Christine Franceschi<sup>3</sup>; Dominique Dechaume<sup>3</sup>; Tanguy Fortin<sup>1</sup>; Alain Theretz<sup>1</sup>; Arnaud Salvador<sup>2</sup>; Gaspard Gervasi<sup>4</sup>; Jerome Lemoine<sup>2</sup>; Jean-Philippe Charrier<sup>1</sup>; <sup>1</sup>*BIOMERIEUX, Marcy L'etoile, FRANCE*; <sup>2</sup>*ANABIO, UMR 5180, CNRS / Université de Lyon, Lyon-, Villeurbanne, France*; <sup>3</sup>*bioMérieux, La Balme les Grottes, France*; <sup>4</sup>*BioMérieux, Marcy L'etoile, N/A*
- TP 220 **A Rapid Fungal De-Replication/Identification Method Based on Laser Ablation Electrospray Ionization (LAESI) Mass Spectrometry Technology and Principle Component Analysis (PCA);** Lin Du<sup>1</sup>; Haddon Goodman<sup>2</sup>; Robert Cichewicz<sup>1</sup>; <sup>1</sup>*University of Oklahoma, Norman, OK*; <sup>2</sup>*Protea Biosciences, Inc., Morgantown, WV*
- TP 221 **Rapid Assays of Bacteria Binding to Oligosaccharides;** Qian Wang<sup>1</sup>; Zachery Lewis<sup>2,3</sup>; Andres Guerrero<sup>1</sup>; David Mills<sup>2,3</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*Department of Chemistry, UC Davis, Davis, CA*; <sup>2</sup>*Department of Viticulture & Enology, UC Davis, Davis, CA*; <sup>3</sup>*Department of Food Science & Technology, UC Davis, Davis, CA*
- TP 222 **An LC-MALDI Method for the Discovery and Identification of Markers of Antibiotic Resistance in Enterobacteriaceae;** Philippa Hart<sup>1</sup>; Emmanuel Wey<sup>2</sup>; Timothy McHugh<sup>3</sup>; Indran Balakrishnan<sup>2</sup>; Omar Belgacem<sup>1</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*Royal Free Hospital NHS Foundation Trust, London, UK*; <sup>3</sup>*UCL Centre for Clinical Microbiology, London, UK*
- TP 223 **The Structural Analysis of Oocyst Walls of Cryptosporidium, Toxoplasma, and Eimeria with Mass Spectrometry and Microscopy;** Edwin M. Motari<sup>1</sup>; G. Guy Bushkin<sup>2</sup>; Jitender P. Dubey<sup>3</sup>; Catherine E. Costello<sup>4</sup>; Phillips W. Robbins<sup>1</sup>; John Samuelson<sup>1</sup>; <sup>1</sup>*Boston University School of Dental Medicine, Boston, MA*; <sup>2</sup>*Massachusetts Institute of Technology, Cambridge, MA*; <sup>3</sup>*Animal Parasitic Diseases Laboratory, United State, Beltsville, MD*; <sup>4</sup>*Boston University School of Medicine, Boston, MA*
- TP 224 **Development of an LC-HRMS-based Metabolomic Approach to Study Methicillin-Resistant Staphylococcus aureus;** Sandrine Aros-Calt<sup>1,2</sup>; Bruno Muller<sup>2</sup>; Céline Ducruix<sup>1,2</sup>; Samia Boudah<sup>1,3</sup>; Guillaume L'hostis<sup>2</sup>; Gaspard Gervasi<sup>2</sup>; Christophe Junot<sup>1</sup>; François Fenaille<sup>1</sup>; <sup>1</sup>*LEMM-CEA-Saclay, Gif sur Yvette, France*; <sup>2</sup>*bioMérieux, Marcy l'Etoile, France*; <sup>3</sup>*GlaxoSmithKline - Centre de recherche F.Hyafil, Villebon-sur-Yvette, France*
- TP 225 **Identification and Characterization of Francisella Strains by MALDI-TOF Detection for Biodefense Purposes;** Emie Durighello<sup>1</sup>; Alain Lorphelin<sup>1</sup>; Marie-Anne Roncato<sup>2</sup>; Eric Ezan<sup>3</sup>; Laurent Bellanger<sup>2</sup>; Jean Armengaud<sup>1</sup>; <sup>1</sup>*CEA, DSV/IBEB/SBTN/LBSP, Bagnols Sur Cèze, France*; <sup>2</sup>*CEA, DSV/IBEB/SBTN/LICB, Bagnols sur Cèze, France*; <sup>3</sup>*CEA, DSV/IBEB/SBTN, Bagnols sur Cèze, France*
- TP 226 **A Shotgun Proteomics-based Method to Differentiate E. coli Strains for Microbial Source Tracking;** Wenguang Shao; Min Zhang; Stanley Lau; Henry Lam; *the Hong Kong University of Science and Technology, Hong Kong, China*
- TP 227 **Discovery and Validation of Invasive Aspergillois Protein Biomarkers in Human Bronchoalveolar Lavage Fluid;** Chengsi Huang<sup>1</sup>; Jason W. McCarthy<sup>2</sup>; Karen Wood<sup>1</sup>; Luke Herren<sup>1</sup>; Marta Feldmesser<sup>2</sup>; Vicki H. Wysocki<sup>1</sup>; <sup>1</sup>*The Ohio State University, Columbus, OH*; <sup>2</sup>*Albert Einstein College of Medicine, Bronx, NY*
- TP 228 **A Multi-Instrumental Targeted Proteomics Approach is Sufficient and Necessary for Comprehensive Analysis of Mycobacterial Protein Secretion;** Matthew M Champion; Emily Williams; George Kennedy; Patricia Digioseppe-Champion; *University of Notre Dame, Notre Dame, IN*
- TP 229 **AlignGF - Assessing the Statistical Significance of Pairwise Spectral Alignments in Spectral Networks;** Seungjin Na<sup>1</sup>; Stephen Callister<sup>2</sup>; Samuel Payne<sup>2</sup>; Nuno Bandeira<sup>1</sup>; <sup>1</sup>*University of California, San Diego, La Jolla, CA*; <sup>2</sup>*Pacific Northwest National Laboratory, Richland, WA*
- TP 230 **Escherichia Coli Outer Membrane Protein A (OMP-A) sequence differentiation by MALDI-TOF-TOF analyses of cyanogen bromide digestion products;** Leslie Harden; Michael Cooley; *USDA/WRRC, Albany, CA*
- TP 231 **Cyanobacterial Agar-Based MALDI Mass Spectrometry Imaging;** Humberto Milagre<sup>1</sup>; Beatriz Sandonato<sup>1</sup>; Vanessa Santos<sup>2</sup>; Marcos Eberlin<sup>2</sup>; <sup>1</sup>*UNESP, Araraquara, BRAZIL*; <sup>2</sup>*UNICAMP, Campinas, Brazil*

- TP 232 **Liquid Extraction Surface Analysis Mass Spectrometry of Intact Proteins from Bacterial Colonies;** Elizabeth C. Randall<sup>1</sup>; Josephine Bunch<sup>2</sup>; Iain B. Styles<sup>1</sup>; Helen J. Cooper<sup>1</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>National Physical Laboratory, London, UK
- Antibodies and Antibody: Drug Conjugates, 233 - 252**
- TP 233 **Characterizing Higher Order Structure of Monoclonal Antibodies using Structural Mass Spectrometry;** Parminder Kaur<sup>1,2</sup>; John Schenkel<sup>1</sup>; Janna Kiselar<sup>2</sup>; Wuxian Shi<sup>2</sup>; Mark Chance<sup>1,2</sup>; <sup>1</sup>NeoProteomics, Inc., Cleveland, OH; <sup>2</sup>Case Western Reserve University, Cleveland, OH
- TP 234 **Characterization of Antibody Drug Conjugates Prepared on Magnetic Protein A and G Particles by MS Analysis following IdeS Digestion;** Chris Hosfield<sup>1</sup>; Becky Godat<sup>1</sup>; Nidhi Nath<sup>1</sup>; Archer Smith<sup>2</sup>; Philip Compton<sup>2</sup>; Paul Thomas<sup>2</sup>; Neil L. Kelleher<sup>2</sup>; Michael Rosenblatt<sup>1</sup>; Marjeta Urh<sup>1</sup>; <sup>1</sup>Promega, Madison, WI; <sup>2</sup>Northwestern University, Evanston, IL
- TP 235 **Evaluation of an LC/MS Microfluidic Platform for Quantification of Intact Monoclonal Antibodies;** Catalin Doneanu; Brad Williams; Paul Rainville; Weibin Chen; Waters Corporation, Milford, MA
- TP 236 **Development of Integrated Informatics Workflows for the Automated Assessment of Comparability for Antibody Drug Conjugates (ADCs) using LC/UV and LC/UV/MS;** Robert Birdsall<sup>1</sup>; Henry Shion<sup>1</sup>; Frank Kotch<sup>2</sup>; April Xu<sup>3</sup>; Thomas Porter<sup>4</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Pfizer Bioprocess Research & Development, Pearl River, NY; <sup>3</sup>Pfizer Analytical Research & Development, Pearl River, NY; <sup>4</sup>Pfizer Analytical Research & Development, Andover, MA
- TP 237 **Analysis of C1q Binding by Engineered IgG hexamers and the Initiation of Fluid Phase Complement Activation;** Guanbo Wang<sup>1,2</sup>; Sara Rosati<sup>1,2</sup>; Ewald T. J. van den Bremer<sup>3</sup>; Frank J. Beurskens<sup>3</sup>; Janine Schuurman<sup>3</sup>; Paul W.H.I. Parren<sup>3</sup>; Rob N. de Jong<sup>3</sup>; Albert J.R. Heck<sup>1,2</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Netherlands Proteomics Center, Utrecht, The Netherlands; <sup>3</sup>Genmab, Utrecht, The Netherlands
- TP 238 **The Characterization of Pentameric IgM (MORAb-028) using Enzymatic Digestion and LC-MS/MS: Disulfide Bond Assignment and Glycosylation Site Analysis;** Xin Cheng; Sara Jacob; Andrew Milinichik; Howard Turchin; Young Park; Wolfgang Ebel; Matthew Reeser; Luigi Grasso; Earl Albone; Morphotek Inc., Exton, PA
- TP 239 **Investigation of the Free Heavy Chain-Heavy Chain (HC-HC) Species of a Monoclonal Antibody;** Hyo (Helen) Chung; Lynette Buck; Kristi Daris; Quanzhou Luo; Jette Wypych; *From the Department of Drug Substance Development, Amgen Inc., Thousand Oaks, CA*
- TP 240 **Conformational Difference in IgG2 Disulfide Isoforms Revealed by Hydrogen/Deuterium Exchange Mass Spectrometry;** Zhongqi Zhang; Aming Zhang; Jing Fang; Robert Chou; Pavel Bondarenko; Amgen, Inc., Thousand Oaks, CA
- TP 241 **Improved Sequence Variant Analysis Strategy by Automated False Positive Removal;** Wenzhou Li; Robert Duff; *Department of Analytical Sciences, Amgen Inc, Thousand Oaks, CA*
- TP 242 **Mass Spectrometry Characterization of the Heterogeneity of a Plant-Derived Therapeutic Monoclonal Antibody;** Yanyan Lu; Catherine E. Costello; *Boston University School of Medicine, Boston, MA*
- TP 243 **Improved Identification of Host Cell Proteins in a Mammalian Cell-Derived Antibody Drug Using LCMS in Conjunction with an Enrichment Strategy;** Jenny Heidbrink Thompson; Wai Keen Chung; Min Zhu; Liu Tie; Yali Lu; Nabila Aboulaich; Robert Strouse; Wenjun (David) Mo; *MedImmune, Gaithersburg, MD*
- TP 244 **Identification of Antibody Specificity using Complex Biological Fluids;** Dimitrios Korbakis<sup>1</sup>; Davor Brinc<sup>2</sup>; Ioannis Prassas<sup>1,2</sup>; Ihor Batruch<sup>2</sup>; Bryan Krastins<sup>4</sup>; Mary F. Lopez<sup>4</sup>; Eleftherios P. Diamandis<sup>2,3</sup>; <sup>1</sup>Department of Laboratory Medicine and Pathobiology, University of Toronto, Toronto, Canada; <sup>2</sup>Department of Pathology and Laboratory Medicine, Mount Sinai Hospital, Toronto, Canada; <sup>3</sup>Department of Clinical Biochemistry, University Health Network, Toronto, Canada; <sup>4</sup>Thermo Fisher Scientific BRIMS, Cambridge, Massachusetts, MA
- TP 245 **Novel Sample Treatment and LC/MS Strategies Achieved Highly Accurate and Sensitive Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody;** Ming Zhang<sup>1,2</sup>; Bo An<sup>1,2</sup>; Eslam Nouri-Nigjeh<sup>1,2</sup>; Haoying Yu<sup>1,2</sup>; Samuel Wopperer<sup>2</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY; <sup>2</sup>New York State Center of Excellence, Buffalo, NY
- TP 246 **High Sensitivity Native Antibody Drug Conjugate (ADC) Analysis using LC Mass Spectrometry;** Caroline S. Chu; Andy Gieschen; Ning Tang; *Agilent Technologies, Santa Clara, CA*
- TP 247 **Monoclonal Antibodies Complete Primary Structure and Biosimilarity Assessment in a Single Analysis using Transient Isotachopheresis Sheathless Capillary Electrophoresis-Tandem Mass Spectrometry;** Rabah Gahoual<sup>1</sup>; Jean-Marc Busnel<sup>2</sup>; Johana Chicher<sup>3</sup>; Lauriane Kuhn<sup>3</sup>; Philippe Hamman<sup>3</sup>; Alain Beck<sup>4</sup>; Yannis Francois<sup>1</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>LSMIS, UMR-CNRS 7140, University of Strasbourg, Strasbourg, FRANCE; <sup>2</sup>Beckman Coulter, Brea, CA; <sup>3</sup>Institut de Biologie Moléculaire et Cellulaire, Strasbourg, France; <sup>4</sup>Centre d'immunologie Pierre Fabre, Saint-Julien en Genevois, France
- TP 248 **Accurate Quantitation of Deamidated Peptides to Accelerate Formulation Process Development in Therapeutic Proteins;** Michael Peddicord<sup>1</sup>; Difei Qiu<sup>1</sup>; Ming Gu<sup>2</sup>; Yongdong Wang<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, New Brunswick, NJ; <sup>2</sup>Cerno Bioscience, Norwalk, CT
- TP 249 **Mass Spectrometry Imaging of Therapeutic Antibodies: Distribution of Trastuzumab in CB.17 SCID mice Implanted with the Human Breast BT474 Xenograft;** Aurore Tomezyk<sup>1</sup>; David Bonnel<sup>1</sup>; Chassidy Hall<sup>2</sup>; Robert J. Mullin<sup>2</sup>; Gregory Hamm<sup>1</sup>; Kathryn Simon<sup>2</sup>; Jonathan Stauber<sup>1</sup>; <sup>1</sup>ImaBiotech, MS Imaging Dept., Loos, France; <sup>2</sup>Charles River Discovery Research Services, Morrisville, NC
- TP 250 **Disulfide Bond Analysis on Q Exactive Mass Spectrometry;** Xiaoxi Zhang<sup>1</sup>; Jing Feng<sup>2</sup>; <sup>1</sup>ThermoFisher Scientific, Shanghai, China; <sup>2</sup>Kawin Technology, Beijing, China
- TP 251 **“Minimalistic Sample Preparation Strategies for LCMS Quantification of Protein Therapeutics: A Case Study Highlighting Alpha-1 Antitrypsin”;** Katherine Wright; Dawn Dufield; *Pfizer, Andover, MA*
- TP 252 **Middle-Down MS Characterization of a mAb Reference Material;** Lisa E. Kilpatrick; John Schiel; Trina Formolo; Eric L. Kilpatrick; Karen Phinney; *NIST, Gaithersburg, MD*
- Biosimilars, 253 - 266**
- TP 253 **Mass Spectrometry Characterization of Bioactive Peptide - Synthetic Polymer - Conjugates;** Ahlam Alalwiat; Wen Tang; Matthew Becker; Chrys Wesdemiotis; *The University of Akron, Akron, U.S.A*

- TP 254 **Bottom-up and Top-down LC-MS Approach for Comprehensive Characterization of Low Molecular Weight Heparins (LMWHs);** [Lingyun Li](#); Robert J. Linhardt; *Rensselaer Polytech Institute, Troy, NY*
- TP 255 **Comprehensive Structural Characterization of Biopharmaceuticals by Top-Down Mass Spectrometry and Hydrogen/Deuterium Exchange: Implications for Biosimilars;** Jingxi Pan<sup>1</sup>; [Derek Smith](#)<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*
- TP 256 **Comparison of Hydrogen/Deuterium Exchange Mass Spectrometry and Nuclear Magnetic Resonance Spectroscopy using Granulocyte-Colony Stimulating Factor as a Model Protein;** [Elyssia S. Gallagher](#)<sup>1</sup>; Robert G. Brinson<sup>1</sup>; J. Todd Hoopes<sup>2</sup>; John P. Marino<sup>1</sup>; Jeffrey W. Hudgens<sup>1</sup>; <sup>1</sup>*NIST, Rockville, MD*; <sup>2</sup>*University of Maryland, Rockville, MD*
- TP 257 **Rapid and Structure-Specific LC/MS/MS Screening for Bioactive Glycan Motifs in Therapeutic Glycoproteins;** [Myung Jin Oh](#)<sup>1</sup>; Serenus Hua<sup>1</sup>; Youngsook Seo<sup>1</sup>; Jong Shin Yoo<sup>2</sup>; Rudolf Grimm<sup>3</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*AGRS, Chungnam National University, Daejeon, Korea*; <sup>2</sup>*Korea Basic Science Institute, Ochang, Korea*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- TP 258 **Characterization of Glycoengineered Biopharmaceuticals;** [Andres Guerrero](#)<sup>1</sup>; Yanhong Li<sup>1</sup>; Salem Alkanaimsh<sup>2</sup>; Lucas Arzola<sup>2</sup>; Bryce Hashimoto<sup>2</sup>; Minsook Hwang<sup>3</sup>; Aye Tu<sup>4</sup>; My Phu<sup>4</sup>; Abhaya Dandekar<sup>4</sup>; Bryce Falk<sup>3</sup>; Somen Nandi<sup>3</sup>; Raymond Rodriguez<sup>2</sup>; Karen McDonald<sup>2</sup>; Xi Chen<sup>1</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*UC Davis, Chemistry Department, Davis, CA*; <sup>2</sup>*UC Davis, Chemical Engineering & Materials Science, Davis, CA*; <sup>3</sup>*UC Davis, Plant Pathology, Davis, CA*; <sup>4</sup>*UC Davis, Plant Science, Davis, CA*; <sup>5</sup>*UC Davis, Molecular & Cellular Biology, Davis, CA*
- TP 259 **Rapid and Complete Structural Assignments of Recombinant Monoclonal Antibody Glycans;** [Ting Song](#); Sureyya Ozcan; Alicia Becker; Carlito Lebrilla; *University of California Davis, Davis, California*
- TP 260 **Biosimilar Glyco-analysis Comparison via Procainamide Labeling and Tandem LC-MS;** [Charles Nwosu](#); Natalie Yau; Steven Becht; *Pharmaceutical Product Development, Middleton, WI*
- TP 261 **2D UPLC and Synapt G2 Mass Spectrometry Facilitates mAb Biosimilar Study;** [Suping Zheng](#); Shirley Lin; Steve Becht; *PPD, Inc., Middleton, WI*
- TP 262 **Analysis of Monoclonal Antibody using High Flow HPLC coupled to Time-of-Flight Mass Spectrometry;** [Ravindra Gudihal](#)<sup>1</sup>; Suresh Babu CV<sup>1</sup>; Ning Tang<sup>2</sup>; <sup>1</sup>*Agilent Technologies India Pvt. Ltd, Bangalore, INDIA*; <sup>2</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- TP 263 **Modular Workflow for Biosimilar Antibody Characterization at the Intact and Middle-Down Level;** [Zsolt Gengeliczki](#); Marcell Olajos; Tamás Kiss; János Varga; Krisztián Lenkey; Katalin Baranyáné Ganzler; *Gedeon Richter Plc., Budapest, Hungary*
- TP 264 **Structure Characterization and Differentiation of Biosimilar and Reference Products using Unique Combination of Complementary Fragmentation Mechanisms;** [Zhiqi Hao](#)<sup>1</sup>; Fan Zhang<sup>2</sup>; Shiaw-Lin Wu<sup>2,3</sup>; David Horn<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*BioAnalytix, Cambridge, MA*; <sup>3</sup>*Barnett Institute, Northeastern University, Boston, MA*
- TP 265 **Comprehensive Assessment of the Biosimilarity of Protein Biotherapeutics Based on Ion Signal Statistics in LC/MS Peptide Mapping Data;** [Stephane Houel](#)<sup>1</sup>; Mark Bennett<sup>2</sup>; Ying Qing Yu<sup>1</sup>; Weibin Chen<sup>1</sup>; <sup>1</sup>*Waters Corp, Milford, MA*; <sup>2</sup>*Nonlinear dynamics, Newcastle, UK*
- TP 266 **Absolute Quantification Strategies for Total Protein and Monosaccharide Concentration in a Monoclonal Antibody (IgG) using 'bottom-Up' ID LC-MS/MS Hydrolysis Techniques;** [Mark Lowenthal](#); Eric Kilpatrick; John Schiel; Karen Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
- Food Safety, 267 - 285**
- TP 267 **Rapid Measurement of Food Adulteration with Minimal Sample Preparation and No Chromatography using DSA/TOF;** [Avinash Dalmia](#)<sup>1</sup>; Thomas White<sup>2</sup>; Craig M. Whitehouse<sup>2</sup>; <sup>1</sup>*PerkinElmer, Shelton, CT*; <sup>2</sup>*PerkinElmer, Branford, CT*
- TP 268 **Determination of the Mycotoxin T2 from Oats by Direct Analysis in Real Time - Mass Spectrometry (DART-MS);** Mark Busman; *USDA, ARS, NCAUR, BFP, Peoria, IL*
- TP 269 **Profiling Beer: Solid Phase Micro-Extraction (SPME) Analysis via Direct Analysis in Real Time HRMS;** [Joseph Lapointe](#); Brian Musselman; Robert Goguen; *Insense Inc., Saugus, MA*
- TP 270 **Same Day Analysis of Persistent Organic Pollutants in Food;** [Sevag Palanjian](#); Lawrence Kramer; *Fluid Management Systems, Watertown, MA*
- TP 271 **Total Extractable Fat Using Pressurized Liquid Extraction (PLE);** [Jim Ceven](#); Tom Hall; *Fluid Management Systems, Watertown, MA*
- TP 272 **Simultaneous Positive/Negative Dielectric Barrier Discharge Microplasma Ionization for Multiclass Organic Contaminants' Determination in complex matrices by LC/HRMS;** [Heiko Haven](#)<sup>1,2</sup>; Bienvenida Gilbert-López<sup>3</sup>; Juan F Garcia-Reyes<sup>3</sup>; Antonio Molina-Díaz<sup>3</sup>; Joachim Franzke<sup>4</sup>; <sup>1</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>2</sup>*University of Muenster, Muenster, Germany*; <sup>3</sup>*University of Jaén, Jaén, Spain*; <sup>4</sup>*Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
- TP 273 **Analyses of Chlorinated Contaminants in Food Products by Atmospheric-Pressure Dissociative Electron Attachment Ionization;** Carina Minardi<sup>1</sup>; Paolo Lecchi<sup>2</sup>; [Kaveh Jorabchi](#)<sup>1</sup>; <sup>1</sup>*Georgetown Univ., Washington, DC*; <sup>2</sup>*DSM Nutritional Products, Columbia, MD*
- TP 274 **Development and Validation of a Highly Sensitive LC-MS/MS Method for Quantitation and Confirmation of Oxytocin in Milk;** [Prasanth Joseph](#)<sup>1</sup>; Praveen Kumar Sharma<sup>1</sup>; Manoj Pillai<sup>1</sup>; Sanjivan Bahman<sup>2</sup>; Ajit Dua<sup>2</sup>; S.S. Marwaha<sup>2</sup>; <sup>1</sup>*AB SCIEX, Gurgaon, INDIA*; <sup>2</sup>*Punjab Biotechnology Incubator, Mohali, India*
- TP 275 **High Sensitivity Quantitation Method of Dicyandiamide and Melamine in Milk Powders by Liquid Chromatography Tandem Mass Spectrometry;** [Zhi Wei Ting](#)<sup>1</sup>; Jing Cheng Ng<sup>2</sup>; Jie Xing<sup>1</sup>; Zhaoqi Zhan<sup>1</sup>; <sup>1</sup>*Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore Science Park 1, Singapore*; <sup>2</sup>*Department of Chemistry, National University of Singapore, Singapore*; <sup>\*</sup>*Student*
- TP 276 **Accurate Mass Screening of Nitrogenous Economic Adulterants in Milk Proteins;** Nicholas Cellar<sup>1</sup>; Jonathan Draher<sup>1</sup>; Nicholas Baldauf<sup>2</sup>; [Todime Reddy](#)<sup>1</sup>; <sup>1</sup>*Abbott Laboratories, Columbus, OH*; <sup>2</sup>*Advanced Testing Laboratory, Blue Ash, OH*
- TP 277 **Determination of Emerging Nitrogenous Economic Adulterants in Milk Proteins by HPLC/Compact Mass Spectrometry;** Stefan Ehling<sup>1</sup>; Jonathan Draher<sup>1</sup>; Nick Cellar<sup>1</sup>; Todime Reddy<sup>1</sup>; [Jack Henion](#)<sup>2</sup>; Nigel Sousou<sup>2</sup>; <sup>1</sup>*Abbott Nutrition, Columbus, OH*; <sup>2</sup>*Advion, Inc., Ithaca, NY*
- TP 278 **Enhanced Reduction of Matrix Effects using LC-MS/MS with Online Extraction for the Rapid Quantitation of Antibiotics in Milk;** [Louis Maljers](#); Helen Qingyu Sun; *Bruker Daltonics Inc, Fremont, Ca*



- TP 279 **Simultaneous Determination of Aminoglycoside in Food Products by Ultra-High Performance Liquid Chromatography Tandem Mass Spectrometry with Triggered Multiple Reaction Monitoring;** Wen-Yen Lee; Shan-An Chan; *Agilent Technology, Inc., Taipei, Taiwan*
- TP 280 **Quick and Sensitive Analysis of Multiclass Veterinary Drug Residues in Animal Products using a Novel Benchtop Orbitrap Mass Spectrometry System;** Olaf Scheibner<sup>1</sup>; Maciej Bromirski<sup>1</sup>; Markus Kellmann<sup>1</sup>; Sebastian Westrup<sup>2</sup>; Charles T. Yang<sup>3</sup>; <sup>1</sup>*Thermo Fisher Scientific, Bremen, Germany*; <sup>2</sup>*Thermo Scientific, Dreieich, Germany*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 281 **Determination of Benzimidazole Residues in Animal Tissue by Ultra High Performance Liquid Chromatography/Tandem Mass Spectrometry;** Yin Huo; Changku Li; Qian Sun; Jinting Yao; Song Zhan; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd., Guangzhou, CHINA*
- TP 282 **Rapid Determination of Residues of Beta-Agonists in Animal Tissues using Liquid Chromatography-Tandem Mass Spectrometry including Mass Spectral Library Searching;** Simon Ashton<sup>1</sup>; David Baker<sup>1</sup>; Neil Loftus<sup>1</sup>; Simon Hird<sup>2</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*The Food and Environment Agency, York, UK*
- TP 283 **Detection the Residues of Tetracycline Antibiotics in Pork and Chicken Meat by SPE-LC/MS/MS;** Xuan Su<sup>1</sup>; Guotao Lu<sup>2</sup>; <sup>1</sup>*Bonna Agela Technologies. Ltd, Tianjin, China*; <sup>2</sup>*Bonna Agela Technologies. Inc, Wilmington, DE*
- TP 284 **Analysis of 200+ Pesticides at 500 SRMs/s Using Non-Timed SRMs on a Triple Quadrupole Mass Spectrometer;** Jia Wang; Charles T. Yang; Jonathan Beck; Jennifer Massi; Dipankar Ghosh; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- TP 285 **Quantitative Analysis of Anabolic Steroids in Control Samples from Food-Producing Animals using a Column-Switching LC-HESI-MS/MS Assay;** John Warrander<sup>1</sup>; David Baker<sup>1</sup>; Neil Loftus<sup>1</sup>; Simon Hird<sup>2</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*The Food and Environment Agency, York, UK*
- Lipids: Identification and Structural Analysis, 286 - 299**
- TP 286 **A Combinatorics Approach To Lipid A Structure Identification;** Tao Liang; Michael C. Wilson; Sung Hwan Yoon; Lisa Leung; Robert K. Ernst; David R. Goodlett; *University of Maryland Baltimore, Baltimore, MD*
- TP 287 **Mass Spectrometric Investigation of Rhamnolipids;** Beate Behrens<sup>1,2</sup>; Jeannine Engelen<sup>1</sup>; Heiko Hayen<sup>1,2</sup>; <sup>1</sup>*University of Wuppertal, Wuppertal, Germany*; <sup>2</sup>*University of Muenster, Muenster, Germany*
- TP 288 **Ion Mobility Spectrometry and Tandem Mass Spectrometry for the Characterization of Ganglioside Lipids from Mouse Brain Tissue using Vacuum Ionization;** Corinne Lutomski<sup>1</sup>; Tarick El-Baba<sup>1</sup>; James Wager-Miller<sup>2</sup>; Ken Mackie<sup>2</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*Indiana University, Bloomington, IN*
- TP 289 **Structural Characterization of Phospholipids Using Ultraviolet Photodissociation;** Dustin Klein; Jennifer Brodbelt; *University of Texas at Austin, Austin, TX*
- TP 290 **Method of Coupling Solution-Phase Paterno-Buchi Reaction with on-line MS for Locating C=C Bond in Unsaturated Lipids;** Craig Stinson; Xiaoxiao Ma; Yu Xia; *Purdue University, West Lafayette, IN*
- TP 291 **Influence of Anaerobic Conditions on Activation of CF Specific Modifications to *Pseudomonas aeruginosa* Lipid A by MALDI-TOF MS;** Lauren Hittle; Robert Ernst; *University of Maryland, Baltimore, Baltimore, Maryland*
- TP 292 **Structural Analyses of Lipid A from *Burkholderia pseudomallei* and *Burkholderia thailandensis* by Mass Spectrometry;** Ravi Chandran Reddy Alla<sup>1</sup>; Michael Bechill<sup>2</sup>; Susan Salari<sup>1</sup>; Austen Mance<sup>1</sup>; Kevin Samson<sup>1</sup>; Dragan Isailovic<sup>1</sup>; Mark Wooten<sup>2</sup>; <sup>1</sup>*University of Toledo, Toledo, OH*; <sup>2</sup>*University of Toledo College of Medicine, Toledo, OH*
- TP 293 **Improved Neutral Steroids Detection and Evidence for Their Regiospecific Decompositions using Anion Attachment Mass Spectrometry;** Quentin Dumont<sup>1</sup>; Nalaka Rannulu<sup>2</sup>; Isabelle Bailloux<sup>3</sup>; Corinne Buisson<sup>3</sup>; Nathalie Mechin<sup>3</sup>; Françoise Lasne<sup>3</sup>; Richard B. Cole<sup>1</sup>; <sup>1</sup>*Université Pierre et Marie Curie, Paris, FRANCE*; <sup>2</sup>*Johnson & Johnson, Philadelphia, PA*; <sup>3</sup>*Agence Française de Lutte contre le Dopage, Châtenay-Malabry, France*
- TP 294 **Separation of Lipid Classes, Subclasses and Isobaric/Isomeric Lipids Using a Novel FAIMS Device;** Julie Horner; David A. Peake; Michael Belford; Satendra Prasad; *Thermo Fisher Scientific, San Jose, CA*
- TP 295 **Alkali and Alkaline Earth Metal Anionic Complexes with Unsaturated Fatty Acids: Position of Deprotonation and CID Fragmentation Mechanisms;** Michael Thomas; Geoffrey Nette; *IMBCR, Dunwich, Australia*
- TP 296 **Rapid Identification of Lipids in Human RBC membrane using Direct Infusion MS/MS<sup>all</sup> and Online Information Dependent Analysis Methods;** Chao Zhang; Ting Liu; *AB Sciex Company, Shanghai, China*
- TP 298 **Shotgun Lipidomics with High Analytical Confidence;** Julio Sampaio<sup>1</sup>; Kai Schuhmann<sup>2</sup>; Madalina Oppermann<sup>3</sup>; Kai Simons<sup>1</sup>; Markus Kellmann<sup>3</sup>; Andrej Shevchenko<sup>2</sup>; <sup>1</sup>*Lipotype GmbH, Dresden, Germany*; <sup>2</sup>*MPI-CBG, Dresden, Germany*; <sup>3</sup>*Thermo Fisher Scientific, Bremen, Germany*
- TP 299 **Electron-Induced Dissociation (EID) of Physiologically Relevant Phospholipids and Glycophospholipids;** Jace W. Jones<sup>1</sup>; Christopher Thompson<sup>2</sup>; Claire L. Carter<sup>1</sup>; Gregory Tudor<sup>3</sup>; Catherine Booth<sup>3</sup>; Isabel L. Jackson<sup>1</sup>; Zeljko Vujaskovic<sup>1</sup>; Thomas J. Macvittie<sup>1</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*Bruker Daltonics Inc., Billerica, MA*; <sup>3</sup>*Epistem Ltd., Manchester, UK*
- Toxicology, 300 - 312**
- TP 300 **Doxorubicin-Induced Mitochondrial Toxicity and Metabolomic Lipid Profile;** Ying Zhou<sup>1</sup>; Meredith Crosby<sup>2</sup>; Harriet Kamendi<sup>3</sup>; <sup>1</sup>*AstraZeneca, Infection Chemistry, Analytical Group, Waltham, MA*; <sup>2</sup>*AstraZeneca, Drug Safety and Metabolism, Waltham, MA*; <sup>3</sup>*Kandih Group, LLC, Burtonsville, MD*
- TP 301 **Metabolic Profiling of Gottingen Minipig Plasma Using GC-MS and LC-MS;** Jeffrey Mcquire<sup>1</sup>; Nicholas Vaccaro<sup>2</sup>; <sup>1</sup>*US Army ECBC, Aberdeen Proving Ground, MD*; <sup>2</sup>*The Tome School, North East, MD*
- TP 302 **Formation of Mono- and Di-nitrosopiperazine in Gastric Juices and Their Relationships between Concentrations of Nitrite, Nitrate, Piperazine;** Mehmet Akyüz; Şevket Ata; *Bülent Ecevit University, Zonguldak, Turkey*
- TP 303 **Venom proteome of Malaysian *Bungarus candidus* and *Bungarus fasciatus*;** Iekhsan Othman<sup>1</sup>; Muhamad Rusdi Ahmad Rusmili<sup>1,2</sup>; Ting Yee Tee<sup>1</sup>; Wayne C. Hodgson<sup>2</sup>; <sup>1</sup>*Monash University Malaysia, Jln Lagoon Selatan, Bandar Sunway, MALAYSIA*; <sup>2</sup>*Monash University, Clayton Campus, Melbourne, Vic*
- TP 304 **Quantitation of Pyrethroids in Rat Liver and Muscle Using Gas Chromatography Negative Chemical Ionization Mass Spectrometry;** Darren Gullick; Andrew Popovici; Holly Young; James Bruckner; Brian Cummings; Michael G. Bartlett; *University of Georgia, Athens, GA*

- TP 305 **Identification of Rat Liver Protein Targets of Acrylonitrile *in vivo* using Two-Dimensional Liquid Chromatography and Mass Spectrometry;** Jian Cai; Harrell E. Hurst; Donald E. Nerland; Daniel W. Wilkey; Michael L. Merchant; Frederick W. Benz; *University of Louisville, Louisville, KY*
- TP 306 **Study on the Aconitine-Type Alkaloids of Radix Aconiti Lateralis and Its Stir-Fried Product using HPLC-ESI-MSn;** Beibei wang; Shuang Zhao; Yonggang Liu; Tan Peng; *Beijing, China*
- TP 307 **The Formation of N-nitrosopyrrolidine and N-nitrosopiperidine in Foods;** Sevket Ata; Mehmet Akyüz; *Bülent Ecevit University, Zonguldak, Turkey*
- TP 308 **Analysis of Fluorinated Derivatives of Carcinogenic Aryl Amines Utilizing MRM with a Tandem-Quadrupole;** Matthew Curtis; Rafael Acosta; Fred Feyerherm; *Agilent Technologies, Santa Clara, CA*
- TP 309 **Metabolism of the Two Endocrine Disruptors Benzophenone-2 and Bisphenol-S Studied in Zebrafish and Human Cell Models using LC-HRMS;** Vincent Le Fol<sup>2,4</sup>; Daniel Zalko<sup>2,3</sup>; Selim Ait-Aïssa<sup>4</sup>; François Brion<sup>4</sup>; Laurent Debrauwer<sup>1,3</sup>; <sup>1</sup>INRA UMR 1331 Toxalim - AXIOM Platform, Toulouse, France; <sup>2</sup>INRA UMR 1331 Toxalim - MeX Team, Toulouse, France; <sup>3</sup>Toulouse University, INP, Toxalim, Toulouse, France; <sup>4</sup>INERIS, ECOT Unit, Verneuil-en-Halatte, France
- TP 310 **Rotenone Causes Alterations to Lipid Metabolism in SH-SY5Y Cells;** Andrew J. Worth; Sankha S. Basu; Nathaniel W. Snyder; Ian A. Blair; *University of Pennsylvania, Philadelphia, PA*
- TP 311 **An Aquatic Ecotoxicological Proteomic Study on the Effects of Spirolactone;** Barbara S. Larsen<sup>1</sup>; Robert Hoke<sup>1</sup>; Kimberly Ralson-Hooper<sup>2</sup>; Gary Ankle<sup>3</sup>; Dan Villeneuve<sup>3</sup>; Carlie LaLone<sup>4</sup>; <sup>1</sup>The DuPont Company, Wilmington, DE; <sup>2</sup>Dow AgroSciences LLC, Indianapolis, IN; <sup>3</sup>US EPA, Duluth, Mn; <sup>4</sup>University of Minnesota, Duluth, Mn
- TP 312 **The Metabolic Profiling and Toxicity Study of Maleic Acid in Sprague-Dawley Rats following a Four-Week Oral Gavage Exposure;** Hsin-Chang Chen<sup>1</sup>; Yee-Soon Ling<sup>1</sup>; Charlene Wu<sup>1</sup>; Su-Yin Chiang<sup>2</sup>; Kuen-Yuh Wu<sup>1\*</sup>; <sup>1</sup>National Taiwan University, Taipei, Taiwan; <sup>2</sup>China Medical University, Taichung, Taiwan
- Carbohydrates, 319 - 337**
- TP 319 **Characterization of Carbohydrate-Monophosphoryl Lipid Conjugate Cancer Vaccine Candidates using Matrix Assisted Ionization Vacuum Mass Spectrometry;** Beixi Wang; Guochao Liao; Zhongwu Guo; Sarah Trimpin; *Wayne State University, Detroit, MI*
- TP 320 **Developments towards Full Heparanome Sequence Analysis: Sequencing of a Natural Heparan Sulfate dp4 Library;** Rongrong Huang; Chengli Zong; Andre Venot; Yulun Chiu; Dandan Zhou; Geert-Jan Boons; Joshua S. Sharp; *CCRC, University of Georgia, Athens, GA*
- TP 321 **Reconfirmation of the "Charge-Localization Isomers" of Dibasic Acids using Another GAG Disaccharide;** Yoko Ohashi<sup>1</sup>; Yuya Otsuka<sup>2</sup>; Toshikazu Minamisawa<sup>2</sup>; Takashi Hirano<sup>1</sup>; <sup>1</sup>The University of Electro-Communications, Chofu, Tokyo, Japan; <sup>2</sup>seikagaku Corporation, Higashiyamato-Shi, Tokyo, Japan
- TP 322 **The Effects of Linkage Stereochemistry and Protecting Groups on Glycosidic Bond Stability of Sodium Cationized Glycosyl Phosphates;** Zhihua Yang; Weiwei Chen; David Crich; Mary T. Rodgers<sup>\*</sup>; *Wayne State University, Detroit, MI*
- TP 323 **Deciphering the Glycan Electron Activated Dissociation Processes;** Yiqun Huang<sup>1</sup>; Yi Pu<sup>2</sup>; Xiang Yu<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Cheng Lin<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston University, Boston, MA
- TP 324 **Evidence for Polysialylated N-Glycans in Serum Generated by GlyQ-IQ Software and Long Column Liquid Chromatography-Subambient Pressure Electropray Ionization Mass Spectrometry;** Scott R. Kronewitter; Gordon W. Slys; Ioan Marginean; Jonathan T. Cox; Clay D. Hagler; Brian L. LaMarche; Rui Zhao; Myanna Y. Harris; Matthew E. Monroe; Christina A. Polyukh; Kevin L. Crowell; Anil K. Shukla; Timothy S. Carlson; David G. Camp II; Keqi Tang; Josh N. Adkins; Ronald J. Moore; Gordon A. Anderson; Samuel H. Payne; Karin D. Rodland; Richard D. Smith; *Pacific Northwest National Lab, Richland, WA*
- TP 325 **In-ESI source Hydrogen/Deuterium Exchange of Carbohydrates Ions;** Yury Kostyukevich<sup>1</sup>; Alexey Kononikhin<sup>1,2</sup>; Igor Popov<sup>1,2</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia
- TP 326 **Carbonyl-Reactive Tandem Mass Tag (TMT) Reagents for Mass Spectrometry-Based Quantitative Glycomics: Enabling Quantitative LC-MS Workflows;** Sergei Snovidá<sup>1</sup>; Rosa Viner<sup>2</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- TP 327 **Top-Down Meets Bottom-Up Glycoproteomics of IgG Monoclonal Antibodies;** Arun Everest-Dass<sup>1</sup>; Xiaomin Song<sup>2</sup>; Matthew Fitzhenry<sup>2</sup>; Mark Molloy<sup>1,2</sup>; Nicolle Packer<sup>1</sup>; <sup>1</sup>Macquarie University, Sydney, Australia; <sup>2</sup>Australian Proteome Analysis Facility, Sydney, Australia
- TP 328 **Application of Automated High-Throughput Serum N-Glycan Processing to Ovarian Cancer Biomarker Discovery;** Seunghyup Jeon<sup>1,2</sup>; Jaehan Kim<sup>1</sup>; Serenus Hua<sup>1,2</sup>; Yong-il Kwon<sup>3</sup>; Andrew Kim<sup>4</sup>; Hyun Joo An<sup>1,2</sup>; <sup>1</sup>Chungnam National University, Daejeon, South Korea; <sup>2</sup>Asia Glycomics Reference Site, Daejeon, South Korea; <sup>3</sup>Hallym University College of Medicine, Seoul, South Korea; <sup>4</sup>Beckman Coulter Korea, Seoul, South Korea
- TP 329 **Separation and Structural Characterization of Epimeric Mixtures of Chondroitin and Dermatan Sulfate GAGs using Field Asymmetric Ion Mobility Spectrometry (FAIMS);** Muchena J. Kailemia<sup>1</sup>; Isaac Agyekum<sup>1</sup>; Melvin A. Park<sup>2</sup>; Robert J. Linhardt<sup>3</sup>; Lingyun Li<sup>3</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA; <sup>3</sup>Rensselaer Polytechnic University, Troy, NY
- TP 330 **A Rapid Method to Distinguish 2,3 and 2,6-sialic Acid without Chemical Labeling and Enzyme Treatment;** Chein-Hung Chen; Ya-Ping Lin; Jung-Lee Lin; Chung-Hsuan Chen; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- TP 331 **Separation and Quantitation of N-glycans with Different Sialic Acid Linkages;** Shujuan Tao<sup>1</sup>; Yining Huang<sup>1</sup>; Barry Boyes<sup>1,2</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Advanced Materials Technology Inc, Wilmington, DE
- TP 332 **Human Platelet Function and Stability: Sequential Mass Spectrometry (MSn) and Spectrum-matching Applied to Glycomic Structure Elucidation;** Andrew Hanneman<sup>1,2</sup>; David Ashline<sup>1,2</sup>; Hailong Zhang<sup>1</sup>; Melissa Lee<sup>3</sup>; Joseph Lau<sup>3</sup>; Renata Grozovsky<sup>4</sup>; Karin Hoffmeister<sup>4</sup>; Vernon Reinhold<sup>1</sup>; <sup>1</sup>Glycomics Center, University of New Hampshire, Durham, NH; <sup>2</sup>Glycan Connections, Durham, NH; <sup>3</sup>Roswell Park Cancer Institute, Buffalo, NY; <sup>4</sup>Brigham and Women's Hospital and Harvard Medical, Boston, MA
- TP 333 **Determination of Changes in Cell Surface Glycosylation with Cellular Transformations;** Dayoung Park; Narine Arabyan; Cynthia Williams; Ting Song; Bart Weimer; Carlito Lebrilla; *University of California, Davis, Davis, CA*



- TP 334 **High Sensitivity Analysis of N-glycans by LC-FLD-MRM**; Oscar Potter; Hongfeng Yin; Kevin Killeen; *Agilent Technologies, Santa Clara, CA*
- TP 335 **Human Milk Glycans: Isomeric Mixtures, Novel Structures, and MSn**; David Ashline<sup>1,2</sup>; Hailong Zhang<sup>2</sup>; Vernon Reinhold<sup>2</sup>; <sup>1</sup>*Glycan Connections, Lee, NH*; <sup>2</sup>*University of New Hampshire, Durham, NH*
- TP 336 **A Sensitive On-Line MS/MS Method for Characterizing N-glycans**; Yaping Sun; Dingyi Wen; *biogenidec, Cambridge, MA*
- TP 337 **Deep Sequencing Using an Ultra High Resolution Column and Mass Spectrometer for Isomer Separation and Structural Identification of Glycans**; Julian Saba<sup>1</sup>; Udayanath Aich<sup>2</sup>; Rosa Viner<sup>1</sup>; Xiaodong Liu<sup>2</sup>; Srinivasa Rao<sup>2</sup>; Jeff Rohrer<sup>2</sup>; Andreas Huhmer<sup>1</sup>; Chris Pohl<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Sunnyvale, CA*
- Ion/Molecule, Ion/Ion, Ion/Electron Interactions, 338 - 360**
- TP 338 **Gas-phase Carbopalladation of Olefines with or without Ar/Ph Scrambling: An Investigation of Intermediate Phosphine Aryl Palladium Complex Ions**; Mathias Schaefer; Lukas Fiebig; Nils Schlörner; Hans-Günther Schmalz; *University Cologne, Department of Chemistry, Koeln, Germany*
- TP 339 **Generation of Radical Peptide Cations using Ion/Ion Reactions Coupled with Collisional Activation or 266 nm Photoexcitation**; Joshua D. Gilbert; Jiexun Bu; Boone M. Prentice; Christine M. Fisher; James G. Redwine; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 340 **Exploration of the Energy Surface of a Gas Phase Ion/Ion Reaction between Peptide Cations and sulfo-N-hydroxysuccinimide Ester Anions**; Jiexun Bu; Christine M. Fisher; Joshua D. Gilbert; Boone M. Prentice; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 341 **Selective Removal of Metals from Multiply-Charged Ions via Gas Phase Ion/Ion Reactions Using Weakly Coordinating Anions**; Carl Luongo<sup>1</sup>; Jiexun Bu<sup>1</sup>; Joshua Gilbert<sup>1</sup>; Boone Prentice<sup>1</sup>; Steven Cummings<sup>2</sup>; Christopher Reed<sup>2</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of California Riverside, Riverside, CA*
- TP 342 **Gas Phase Studies Involving Radical Migrations in Tyrosine- and Cysteine-Containing Peptides**; Michael Lesslie; Victor Ryzhov; *Northern Illinois University, DeKalb, IL*
- TP 343 **Hydrogen-Deuterium Exchange Combined with Electron Capture Dissociation to Probe the Conformation of Gaseous Peptide Ions**; Rita Straus<sup>1</sup>; Rebecca A. Jockusch<sup>2</sup>; <sup>1</sup>, *Toronto, Canada*; <sup>2</sup>*University of Toronto, Toronto, ON*
- TP 344 **Structural Effects in Electron Capture Dissociation of High-Valence Metal-Peptide Complexes**; Tao Jiang; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- TP 345 **Reactivity of Carboxylates with N-Hydroxysuccinimide Esters via Ion/Ion Reactions: Observations of New Covalent Chemistry in the Gas Phase**; Zhou Peng; William Mcgee; Nathan Barefoot; Scott McLuckey; *Purdue University, West Lafayette, IN*
- TP 346 **A General Belief Challenged: the Gas Phase m/z 93 Anion Derived from Phenol and Salicylate Does React with CO<sub>2</sub>**; Chongming Liu; Athula B. Attygalle; *Stevens Institute of Technology, Hoboken, NJ*
- TP 347 **Effect of Metal Ion and Neutral Reagent Type on Gas-Phase Adduct Formation**; Mahsan Miladi; Abayomi Olaitan; Behrooz Zekavat; Jackie Lochridge; Touradj Solouki; *Baylor University, Waco, TX*
- TP 348 **Cupric Complexes of Phenolate Siderophores and Superoxide Dismutase Mimicry: an Experimental and Theoretical Study**; Daryl Giblin<sup>1</sup>; Shannon Ohlemacher<sup>2</sup>; Jeffrey P. Henderson<sup>2</sup>; Michael L. Gross<sup>1</sup>; <sup>1</sup>*Washington University, St Louis, MO*; <sup>2</sup>*Washington University School of Medicine, St. Louis, MO*
- TP 349 **Reaction of Ions From Pyrolyzed Cellulose with Adventitious Water in a Quadrupole Ion Trap**; Chelsea Tyler; Sandra Spencer; Gary L. Glish; *Univeristy of North Carolina, Chapel Hill, NC*
- TP 350 **Distinguishing Amorphous and Crystalline Ices by Ultra-Low Energy Collisions of Reactive Ions**; Radha Gobinda Bhuin; Soumabha Bag; T. Pradeep; *Indian Institute of Technology, Madras, Chennai, INDIA*
- TP 351 **GPU Assisted Simulation Study of Ion-Ion Reactions within Quadrupole Ion Traps**; Dan Guo; Muye He; Yuzhuo Wang; Wei Xu; *Beijing Institute of Technology, Beijing, China*
- TP 352 **Intramolecular Halogen Transfer via Halonium Ion Intermediates in the Gas-Phase**; Yuanjiang Pan; Yunfeng Chai; Guofeng Weng; *Zhejiang University, Hangzhou, China*
- TP 353 **Reactions of Biomolecule Ions with Pyrolysis-formed Carbene**; Ziqing Lin<sup>1</sup>; Lei Tan<sup>2</sup>; Yang Yang<sup>2</sup>; Mingji Dai<sup>2</sup>; Frantisek Tureček<sup>3</sup>; Zheng Ouyang<sup>1</sup>; Yu Xia<sup>2</sup>; <sup>1</sup>*Weldon Sch of Biomedical Engr, Purdue University, West Lafayette, IN*; <sup>2</sup>*Department of Chemistry, Purdue University, West Lafayette, IN*; <sup>3</sup>*Department of Chemistry, University of Washington, Seattle, WA*
- TP 354 **Synthesis, Characterization, and Reactivity of Gold (I) Carbene Complexes in the Gas Phase**; Christopher Swift; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- TP 355 **Ligand Tuning for the Selective Oxidation of Methanol by [LFeO]<sup>+</sup>**; Richard A. J. O'Hair<sup>1</sup>; Simon Svane<sup>4</sup>; George N. Khairallah<sup>2</sup>; W. Alex Donald<sup>3</sup>; Christopher Hansen<sup>5</sup>; Christine McKenzie<sup>4</sup>; Fantong Zhang<sup>3</sup>; Gabriel Da Silva<sup>1</sup>; Adam J. Trevitt<sup>5</sup>; <sup>1</sup>*University of Melbourne, Victoria, Australia*; <sup>2</sup>*Bio21 Inst, Uni of Melbourne, Melbourne, Australia*; <sup>3</sup>*University of New South Wales, Sydney, Australia*; <sup>4</sup>*University of Southern Denmark, Odense M, Denmark*; <sup>5</sup>*University of Wollongong, Wollongong, NSW, Australia*
- TP 356 **Experimental Study of Alpha Nucleophile Reactivity**; Jennifer Reece<sup>1</sup>; Charles Nichols<sup>1</sup>; Ditte Thomsen<sup>2</sup>; Veronica M. Bierbaum<sup>1</sup>; <sup>1</sup>*University of Colorado, Boulder, CO*; <sup>2</sup>*University of Copenhagen, Copenhagen, Denmark*
- TP 357 **Collision Cross Sections Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry: Applications to Supramolecular Systems**; Anupriya Anupriya; David V. Dearden; *Brigham Young University, Provo, Utah*
- TP 358 **Gas-Phase Reactivity of a Substituted Charged para-Benzyne, the 6-Cyano-2,5-didehydropyridinium Cation**; Huaming Sheng; Weijuan Tang; Hilikka Kenttämää; *Purdue University, West Lafayette, IN*
- TP 359 **Variable-Temperature Studies of Gas-Phase S<sub>2</sub> and E2 Reactions**; Alexander Wiseman; Nhat Le; Scott Gronert; *Virginia Commonwealth University, Richmond, VA*
- TP 360 **Gas-Phase Studies on the Reactivity of Aromatic Biradicals Towards Amino Acids**; Weijuan Tang; George Pates; Huaming Sheng; Ashley Wittrig; John Nash; Hilikka Kenttämää; *Purdue University, West Lafayette, IN*

## Ion Spectroscopy, 361 - 372

- TP 361 **Laser Spectroscopic Investigations of Heterosubstituted Halogenbenzenes by Means of REMPI and MATI spectroscopy;** Sascha Krüger; Jurgen Grotemeyer; *Christian-Albrechts-Univ, Kiel, Germany*
- TP 362 **A Spectroscopic Investigation of the Hydrogen Bonding Patterns and Mobile Proton Behavior of Leucine Enkephalin;** Nicole Burke; James Redwine; Timothy Zwier; Scott McLuckey; *Purdue University, Lafayette, IN*
- TP 363 **Neutralizing Space Charge: Dual Mode Ion Trapping for Enhanced Trapping and Photodissociation in a 3D Ion Trap;** Corey Stedwell; Nathan Roehr; Nicolas Polfer; *University of Florida, Gainesville, FL*
- TP 364 **IRMPD Spectroscopy Reveals a Novel Rearrangement Reaction for Modified Peptides that involves Elimination of the N-terminal Amino Acid;** Khiry Patterson<sup>1</sup>; John K. Gibson<sup>2</sup>; Giel Berden<sup>3</sup>; Jos Oomens<sup>3</sup>; Michael J. Van Stipdonk<sup>1</sup>; <sup>1</sup>*Duquesne University, Pittsburgh, PA*; <sup>2</sup>*Lawrence Berkeley Laboratory, Berkeley, CA*; <sup>3</sup>*Radboud University Nijmegen, Nijmegen, The Netherlands*
- TP 365 **Fragmentation Chemistry of Asparagine and Glutamine Containing Peptides by IRMPD Spectroscopy;** Josipa Grzetic; Jonathan Martens; Giel Berden; Jos Oomens; *Radboud University Nijmegen, Nijmegen, Netherlands*
- TP 366 **Charge-state Resolved Direct IR Photodissociation Spectra of Protein Ions in the Gas Phase;** Xianglei Kong; Yijie Yang; Guanhua Liao; *Nankai University, Tianjin, China*
- TP 367 **Rearrangements in Tryptophan-Containing Radicals Elucidated by Infrared Laser Spectroscopy;** Ning Zhao; Nicolas Polfer; *University of Florida, Gainesville, FL*
- TP 368 **Gas Phase Structure of Monosaccharide Methyl Glycosides Li<sup>+</sup> Complexes : Gas Phase IR Spectroscopy and Theory;** Oscar Hernandez; Philippe Maitre; *Université Paris Sud, Orsay, France*
- TP 369 **VUV Photoionization Study of Gas-Phase Vitamins A and B1 using Aerosol Thermodesorption and Synchrotron Radiation;** Héloïse Dossmann<sup>1</sup>; Adrian Schwarzenberg<sup>1</sup>; Denis Lesage<sup>1</sup>; Carlos Afonso<sup>2</sup>; Marie Pérot-Taillandier<sup>1,3</sup>; Barbara K. Cunha de Miranda<sup>4,5</sup>; Gustavo A. Garcia<sup>4</sup>; <sup>1</sup>*Université Pierre et Marie Curie, Paris Cedex 05, FRANCE*; <sup>2</sup>*Université de Rouen, Mont-Saint-Aignan Cedex, France*; <sup>3</sup>*Institut de Chimie des Substances Naturelles, CNRS, Gif-sur-Yvette, France*; <sup>4</sup>*Synchrotron SOLEIL, Gif-sur-Yvette Cedex, France*; <sup>5</sup>*Université Paris-Sud, Orsay, France*
- TP 370 **Photodissociation Action Spectroscopy vs. Fluorescence Excitation Spectroscopy: an Experimental Comparison;** Sydney M.J. Wellman; Rebecca A. Jockusch; *University of Toronto, Toronto, Canada*
- TP 371 **Action Spectroscopy of Protonated Pyridines and Diazines: Vibronic Detail and Product Characterization;** Christopher S. Hansen<sup>1</sup>; Stephen J Blanksby<sup>2</sup>; Adam J. Trevitt<sup>1</sup>; <sup>1</sup>*School of Chemistry, University of Wollongong, Australia*; <sup>2</sup>*Central Analytical Research Facility, Queensland University of Technology, Australia*
- TP 372 **Probing Mobility Selected Isomers: Selective Ion-Molecule Reactions and Wavelength-Specific IR Activation;** Oscar Hernandez<sup>1</sup>; Samantha Isenberg<sup>2</sup>; Vincent Steinmetz<sup>1</sup>; Gary L. Glish<sup>2</sup>; Philippe Maitre<sup>1</sup>; <sup>1</sup>*Université Paris Sud, Orsay, France*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*

## Ambient Ionization: Instrumentation, 373 - 379

- TP 373 **Optimization and Exploration of Sampling Methods Affecting Ionization Efficiency for Direct Sample Analysis (DSA);** Suejane Tan; Joshua Wilhide; Gregory Winter; Margaret LaCourse; Ian Shaffer; Rebecca Neubauer; William R. LaCourse; *University of Maryland Baltimore County, Baltimore, MD*
- TP 374 **Understanding the Impact of Space Charge Upon the Sensitivity of Atmospheric Ion Sampling;** Charles Jolliffe; Serguei Savtchenko; Reza Javahery; *IONICS Mass Spec Group, Inc., Bolton, Canada*
- TP 375 **Celebrating DESI – the First 10 Years and Perspectives for the Next Decade: From Automated Histopathology to Understanding Cancer Lipid Biochemistry;** Zoltan Takats; Nicole Strittmatter; Emrys A Jones; Reza Mirnezami; Abigail Speller; Robert D. Goldin; Laura Muirhead; James Kinross; Nima Abbassi-Ghadi; Ottmar Golf; Kirill Veselkov; *Imperial College London, London, UK*
- TP 376 **Multi-Stage Reactive Transmission Mode Desorption Electrospray Ionization;** Richard H. Perry; Kevin C. Peters; Kevin E. Parker; *University of Illinois, Urbana-Champaign, IL*
- TP 377 **Analysis of High Frequency Surface Acoustic Wave Nebulizer for Improved Ion Sensitivity;** Scott Heron; Shivangi Awasthi; Sung Hwan Yoon; David Goodlett; Yue Huang; *University of Maryland, Baltimore, Baltimore, MD*
- TP 378 **Electromigration in Capillary Microsampling Enhances Electrospray Ionization Mass Spectrometry of Volume-limited Samples;** Bindesh Shrestha; Linwen Zhang; Akos Vertes; *the George Washington University, Washington, DC*
- TP 379 **Single-Cell Solid-Phase Microextraction Coupled with Mass Spectrometry for the Detection of Metabolites at Cellular and Subcellular Levels;** Xiaoyun Gong; Xinrong Zhang; *Tsinghua University, Beijing, CHINA*
- Ambient Ionization: Applications, 380 - 409**
- TP 380 **New Method for Surface Sampling Using 3-Nitrobenzonitrile Matrix and Matrix-Assisted Ionization-Inlet;** Khoa Hoang; Charles N. McEwen; *University of the Sciences in Philadelphia, Philadelphia, pa*
- TP 381 **Multi-dimensional Study of Microbial Community Behavior using nanoDESI Mass Spectrometry, SIMS and Fluorescence Microscopy;** Yiqiang Fang; Manfred Auer; James Berleman; Marcin Zemla; Megan Danielewicz; Trent Northen; Musahid Ahmed; *Lawrence Berkeley National Laboratory, Berkeley, California*
- TP 382 **Detection of Trace Ink Compounds in Erased Handwritings Using Electrospray Laser Desorption Ionization Mass Spectrometry;** Yi-Ying Kao<sup>2</sup>; Hsiu-O Ho<sup>2</sup>; Sy Chyi Cheng<sup>1</sup>; Jentaie Shiea<sup>1</sup>; <sup>1</sup>*NSYSU, Kaohsiung, Taiwan*; <sup>2</sup>*Taipei Medical University, Taipei, Taiwan*
- TP 383 **Ionization Characteristics of Amino Acids in Direct Analysis in Real Time-Mass Spectrometry (DART-MS);** Kanako Sekimoto<sup>1</sup>; Motoshi Sakakura<sup>2</sup>; Takatomo Kawamukai<sup>2</sup>; Hiroshi Hike<sup>2</sup>; Teruhisa Shiota<sup>2</sup>; Fumihiko Usui<sup>2</sup>; Yasuhiko Bando<sup>2</sup>; Mitsuo Takayama<sup>1</sup>; <sup>1</sup>*Yokohama City University, Yokohama, Japan*; <sup>2</sup>*AMR, Inc., Tokyo, Japan*
- TP 384 **High-Mass Cluster Ions of Ionic Liquids in Positive-Ion and Negative-Ion DART-MS and their Application for Wide Range Mass Calibrations;** Juergen Gross; *Organisch-Chemisches Institut, Heidelberg, Germany*
- TP 385 **Selective Replacement of Carbon in Aromatics with Nitrogen in an Ambient Discharge;** Zhiping Zhang<sup>1</sup>; Yajun Zheng<sup>1</sup>; Xinrong Zhang<sup>2</sup>; Zheng Ouyang<sup>3</sup>; <sup>1</sup>*Xi'an Shiyou University, Xi'an, China*; <sup>2</sup>*Tsinghua University, Beijing, China*; <sup>3</sup>*Purdue University, West Lafayette, IN*



- TP 386 **Effect of Chemical Matrices on the charged ion peaks produced by ESI and SAWN MS;** Shivanji Awasthi; Yue Huang; Sung Hwan Yoon; Young Ah Goo; David P.A. Kilgour; David Goodlett; *University of Maryland, Baltimore, MD*
- TP 387 **Hantzsch Synthesis of 1,4-dihydropyridines Spray Ionization with On-Line Reaction Monitoring and Off-Line Product Collection;** Ryan Bain; Christopher Pulliam; Xin Yan; Cassandra Moore; R. Graham Cooks; *Purdue University, West Lafayette, IN*
- TP 388 **Extractive Electrospray Ionization Mass Spectrometry of Ionic Liquids;** Yafei Zhou<sup>1</sup>; Konstantin Chingina<sup>1</sup>; Shuiping Yang<sup>1</sup>; Saijin Xiao<sup>1</sup>; Liang Zhu<sup>2</sup>; Eric Handberg<sup>1</sup>; Huanwen Chen<sup>1</sup>; <sup>1</sup>*East China Institute of Technology, Nanchang, China*; <sup>2</sup>*ETH Zurich, Zurich, Switzerland*
- TP 389 **Electrostatic Spray Ionisation for Ambient Mass Spectrometry Imaging;** Liang Qiao<sup>1</sup>; Hubert Girault<sup>1</sup>; Elena Tobolkina<sup>1</sup>; Andreas Lesch<sup>1</sup>; Xiaoqin Zhong<sup>1</sup>; Alexandra Bondarenko<sup>1</sup>; Baohong Liu<sup>2</sup>; Horst Pick<sup>1</sup>; Horst Vogel<sup>1</sup>; <sup>1</sup>*École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*; <sup>2</sup>*Fudan University, Shanghai, China*
- TP 390 **Investigations into the DESI-MS Analysis of Oil Additives Deposited on Metal Surfaces;** Caitlyn Da Costa<sup>1</sup>; Matthew Turner<sup>1</sup>; James Reynolds<sup>1</sup>; Samuel Whitmarsh<sup>2</sup>; Tom Lynch<sup>2</sup>; Colin Creaser<sup>1</sup>; <sup>1</sup>*Loughborough University, Loughborough, UK*; <sup>2</sup>*Castrol, Reading, UK*
- TP 391 **Online and in-situ Release Testing of Erythromycin Ointment by Internal Extractive Electrospray Ionization Mass Spectrometry (iEESI-MS);** Guocan Yao<sup>1,2</sup>; Eric Handberg<sup>2</sup>; Laisheng Li<sup>1</sup>; Huanwen Chen<sup>2</sup>; <sup>1</sup>*Department of Chemistry, Nanchang University, Nanchang, China*; <sup>2</sup>*East China Institute of Technology, Nanchang, China*
- TP 392 **Utilization of Atmospheric Pressure Ionization Coupled to Triple Quadrupole Mass Spectrometry for the Analysis of Mixed-Halo Planar Compounds;** Kari Organtini<sup>1</sup>; Eric Reiner<sup>2</sup>; Karl Jobst<sup>2</sup>; Anne Myers<sup>3</sup>; Adam Ladak<sup>4</sup>; Douglas Stevens<sup>4</sup>; Frank Dorman<sup>1</sup>; <sup>1</sup>*Penn State University, University Park, PA*; <sup>2</sup>*Ontario Ministry of the Environment, Toronto, ON*; <sup>3</sup>*University of Toronto, Toronto, Canada*; <sup>4</sup>*Waters Corporation, Beverly, MA*
- TP 394 **Ambient ionization mass spectrometry: New Directions in Pharmaceutical Analysis;** Lianming Wu; Sonya Kennedy-Gabb; Kevin Facchine; *GlaxoSmithKline, King Of Prussia, PA*
- TP 395 **Electrophoretically-Controlled Solution Mixing in a Borosilicate Theta Glass nESI Emitter;** Christine M. Fisher; Scott A. McLuckey; *Purdue University, West Lafayette, IN*
- TP 396 **Fast Screening of Hazardous Substances in Paper Based Food Packaging Materials using Desorption Corona Beam Ionization (DCBI) Mass Spectrometry;** Chao Gao<sup>1</sup>; Yupeng Cheng<sup>1</sup>; Ding Li<sup>2</sup>; Qiang Li<sup>3</sup>; Yuki Hashi<sup>3</sup>; Wenjian Sun<sup>1</sup>; <sup>1</sup>*Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China*; <sup>2</sup>*SGS (Guangzhou), Guangzhou, China*; <sup>3</sup>*Shimadzu (China) Co., Ltd., Shanghai, China*
- TP 397 **Development of Solvent-Free Ambient Mass Spectrometry for Green Chemistry Applications;** Pengyuan Liu; Amanda Forni; Hao Chen; *Ohio University, Athens, OH*
- TP 398 **Electrospray Ionization of Noble Metals and the Collection of Metal Ions toward the Synthesis of Metallic Nanoparticles and Organometallics;** Anvin Li<sup>1</sup>; Qingjie Luo<sup>2</sup>; Zane Baird<sup>1</sup>; Depanjan Sarkar<sup>3</sup>; Anirban Som<sup>3</sup>; Bootharaju M. S. <sup>3</sup>; Pradeep T. <sup>3</sup>; R. Graham Cooks<sup>1</sup>; <sup>1</sup>*Purdue University, West Lafayette, IN*; <sup>2</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>3</sup>*Department of Chemistry, IIT Madras, Chennai, India*
- TP 399 **Ambient Detection of Chelation Complexes of Metals from Solids using Electrospray Laser Desorption Ionization Mass Spectrometry;** Christopher Shiea<sup>1</sup>; Yi-Lun Chen<sup>2</sup>; Yeou-Lih Huang<sup>1</sup>; Min Zong Huang<sup>2</sup>; <sup>1</sup>*Dept. of Medical Lab Sci. & Biotech., KMU, Kaohsiung, Taiwan*; <sup>2</sup>*Dep. of Chemistry National Sun Yat-Sen University, Kaoshiung, Taiwan*
- TP 400 **Rapid Protein Identification and Quantification using Surface Acoustic Wave Nebulization MS;** Sung Hwan Yoon<sup>1</sup>; Young Ah Goo<sup>1</sup>; John D Chapman<sup>2</sup>; Yue Huang<sup>1</sup>; Scott Heron<sup>1</sup>; Nina Isoherranen<sup>2</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*University of Washington, Seattle, WA*
- TP 401 **Desorption Atmospheric Pressure Photoionization-High Resolution Mass Spectrometry Fingerprinting of Urinary Steroids during Pregnancy;** Anu Vaikkinen<sup>1</sup>; Tiina J Kauppila<sup>1</sup>; Josef Cvacka<sup>2</sup>; Risto Kostianen<sup>1</sup>; <sup>1</sup>*University of Helsinki, Helsinki, FINLAND*; <sup>2</sup>*Institute of Organic Chemistry and Biochemistry, v. Praha, CZECH REPUBLIC*
- TP 402 **On-line Breath Analysis of VOCs in Breath using Atmospheric Pressure Chemical Ionisation with a Compact Quadrupole Mass Spectrometer;** Matthew Turner; Liam Heaney; Kayleigh Arthur; Dorota Ruskiewicz; Colin Creaser; Paul Thomas; James Reynolds; *Loughborough University, Loughborough, UK*
- TP 403 **Development of a Digital Microfluidic-Surface Acoustic Wave Nebulization Affinity Chip for MS Analysis;** Yue Huang<sup>1</sup>; Michael Wilson<sup>1</sup>; Scott Heron<sup>1</sup>; John S. Edgar<sup>2</sup>; Sung Hwan Yoon<sup>1</sup>; Patrick Langridge-Smith<sup>3</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*Deurion, LLC, Seattle, WA*; <sup>3</sup>*University of Edingburgh, edingburgh, UK*
- TP 404 **Development of a Real World Screening Method for Nutraceuticals Using DSA-TOF;** Rebecca Neubauer; Greg Winter; Joshua Wilhide; Suejane Tan; Ian Shaffer; William LaCourse; *University of Maryland Baltimore County, Baltimore, MD*
- TP 405 **A Multifaceted Approach for the Analysis of Electronic Cigarettes using DSA-TOF and Headspace GC-MS;** Ian Shaffer; Margret LaCourse; Suejane Tan; Rebecca Neubauer; Greg Winter; Joshua Wilhide; William LaCourse; *University of Maryland Baltimore County, Baltimore, MD*
- TP 406 **Application of Atmospheric Solid Pressure Analysis Probe with Ion Mobility-Mass Spectrometry for the Characterization of Complex Industrial Mixtures;** Carlos Afonso<sup>1</sup>; Mathilde Farenc<sup>2</sup>; Caroline Barrere<sup>1</sup>; Marie Hubert-Roux<sup>1</sup>; Pierre Giusti<sup>2</sup>; <sup>1</sup>*University of Rouen, Mont Saint Aignan, France*; <sup>2</sup>*TOTAL Refining & Chemicals, Gonfreville, France*
- TP 407 **Internal Energy Deposition for Ultrafast Laser Vaporization and Electrospray Postionization Using Thermometer Ions and Peptides;** Paul Flanigan; Fengjian Shi; Johnny Perez; Santosh Karki; Conrad Pfeiffer; Robert Levis; *Temple University, Philadelphia, PA*
- TP 408 **Metabolite and Lipid Turnover Rates in Live Microalgae by Pulse-Chase Analysis and Laser Ablation Electrospray Ionization Mass Spectrometry;** Tarek Mansour<sup>1</sup>; Sylwia Stopka<sup>1</sup>; Éric Maréchal<sup>2</sup>; Denis Falconet<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, District Of Columbia*; <sup>2</sup>*CEA-CNRS-INRA-Univ. Grenoble Alpes, Grenoble, France*
- TP 409 **Laser Desorption/Ionization (LDI) of Peptides and Steroids from Metal Substrates;** Evgeny Kukaev<sup>1,4</sup>; Alexey Kononikhin<sup>2,4</sup>; Igor Popov<sup>1,4</sup>; Konstantin Mironov<sup>1,3</sup>; Denis Bormotov<sup>2,4</sup>; Natalia Starodubtceva<sup>2,4</sup>; Maria I. Indeykina<sup>1</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>*Emanuel Institute of Biochemical Physics, Moscow, Russian Federation*;

<sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russian Federation; <sup>3</sup>Pirogov Russian National Research Medical Univers., Moscow, Russian Federation; <sup>4</sup>Moscow Institute of Physics and Technology, Moscow, Russian Federation

#### MALDI Sample Preparation, 410 - 420

- TP 410 **A Nanoporous Thin Film Biosensor for Hydrophobic Analyte Enrichment from Complex Mixtures by MALDI-MS;** Roberto Gamez; David H. Russell; *Texas A&M University, College Station, TX*
- TP 411 **Sample Preconcentration in Open Microchannels Combined with MALDI- and nano-ESI-MS;** Saara Mikkonen; Johan Jacksén; Åsa Emmer; *KTH Royal Institute of Technology, Stockholm, Sweden*
- TP 412 **Directed Proteomics of DNA-Binding Proteins;** Linda Nagore; Harry Jarrett; *UT San Antonio, San Antonio, TX*
- TP 413 **Comparative Study of the Efficiency of Different Matrices for the Analysis of Microalgae Intact Cells by MALDI TOF TOF Technique;** Lidiane Maria de Andrade<sup>1</sup>; Maria Anita Mendes<sup>1</sup>; Claudio Augusto Oller do Nascimento<sup>1</sup>; Paul Kowalski<sup>2</sup>; <sup>1</sup>*Chemical Engineering Department of POLI/USP, Sao Paulo, Brazil*; <sup>2</sup>*Bruker Daltonics, Billerica, MA*
- TP 414 **Anthracene-9-carbonitrile Matrix for MALDI-MS of Polyoxoanions;** Jean Boulicault; Sandra Alves; Richard B. Cole; *Univ. P. et M. Curie (Paris 6), Paris Cedex 05, France*
- TP 415 **A Binary Matrix for Improvement of Quantitative Analysis of Microcystins by MALDI-TOF-MS;** Milena Luizete; Beatriz Sandonato; Humberto Milagre; *UNESP, Araraquara, Brasil*
- TP 416 **Increased Survival Yields of Labile Molecules using New Electron Transfer MALDI Matrices;** Laura Castellanos<sup>1</sup>; Brian Castro<sup>2</sup>; Hernando Rosales<sup>1</sup>; Cesar Sierra<sup>2</sup>; Cristian Blanco<sup>1</sup>; Marianny Combariza<sup>1</sup>; <sup>1</sup>*Universidad Industrial de Santander, Bucaramanga, Colombia*; <sup>2</sup>*Universidad Nacional de Colombia, Bogota, Colombia*
- TP 417 **Homogeneous MALDI Sample Spots of Synthetic Polymers using Ionic Liquid Matrices;** Stefan J. Gabriel<sup>1</sup>; Steffen M. Weidner<sup>1</sup>; Clemens Schwarzwinger<sup>2</sup>; Ulrich Panne<sup>1</sup>; <sup>1</sup>*Fed.Inst.f.Mat.Research, Berlin, DE*; <sup>2</sup>*Johannes Kepler University, Linz, AT*
- TP 418 **On the Way to Quantification of Endogenous Lipids by MALDI MSI: a Practical Study of Crucial Sample Preparation Parameters;** Laure Jadoul; Rémi Longuespée; Delphine Debois; Gauthier Epepe; Edwin De Pauw; *Mass Spectrometry Laboratory, University of Liège, Liège, Belgium*
- TP 419 **Deducing Protein Composition from Complex Protein Preparations by MALDI without Peptide Separation;** Kenneth Parker; *SimulTOF/ VIC Instruments, Sudbury, MA*
- TP 420 **Coupling nanoHPLC with Liquid MALDI MS for the Analysis of Complex Protein;** Kanjana Wiangnon; Rainer Cramer; *University of Reading, Reading, UK*
- Biomarkers: Discovery, 421 - 442**
- TP 421 **Characterization of a Distinct 1-D Gel Band from Ultracentrifuge-Enriched Exosomes;** Jeongkwon Kim<sup>1</sup>; Zhijing Tan<sup>2</sup>; Jianhui Zhu<sup>2</sup>; Haidi Yin<sup>2</sup>; Song Nie<sup>2</sup>; David M. Lubman<sup>2</sup>; <sup>1</sup>*Chungnam National University, Daejeon, South Korea*; <sup>2</sup>*University of Michigan, Ann Arbor, U.S.A*
- TP 422 **Probing the Role of APOE in Global Proteomic Changes of Cerebrospinal Fluid in Preclinical Alzheimer's Disease;** Jingxin Wang; Ozioma Okonkwo; Lingjun Li; *UW-Madison, Madison, WI*
- TP 423 **Proteomics Profiling of Pediatric Serum and Discovery of Biomarkers for Differentiation of the Cause of Febrile Illnesses in Madagascar;** Laetitia Cortes<sup>1</sup>; Yiyong Zhou<sup>1</sup>; Melina Messaoudi<sup>4</sup>; Muriel Maeder<sup>2</sup>; Rudolf Guilbaud<sup>1</sup>; Michael Schirm<sup>1</sup>; Jonathan Hoffmann<sup>4</sup>; Bénédicte Contamin<sup>2</sup>; Martin Randriamarotia<sup>3</sup>; Valentina Picot<sup>4</sup>; Glauca Paranhos-Baccalà<sup>4</sup>; Eustache Paramithiotis<sup>1</sup>; <sup>1</sup>*Caprion, Montreal, CANADA*; <sup>2</sup>*Centre d'Infectiologie Charles Mérieux (CICM), Antananarivo, Madagascar*; <sup>3</sup>*Fondation Médicale d'Ampasimanjeva (FMA), Ampasimanjeva, Madagascar*; <sup>4</sup>*Emerging Pathogens Laboratory, Fondation Mérieux, Lyon, France*
- TP 424 **Lipidomic and Transcriptomic Profiling in Mental Disease;** Raissa Lerner; Beat Lutz; Laura Bindila; , Mainz, Germany
- TP 425 **Iron Modified Peptides as Biomarkers of Gynecologic Malignancies;** Meghan Tanner; Lindsay Schambeau; Michael Finan; Rodney Rocconi; Lewis Pannell; *Mitchell Cancer Institute, Mobile, AL*
- TP 426 **Improved Detection and Quantification in Plasma-based Biomarker Discovery;** Michael Burgess<sup>1</sup>; Hasmik Keshishian<sup>1</sup>; D.R. Mani<sup>1</sup>; Philipp Mertins<sup>1</sup>; Karl Clauser<sup>1</sup>; Michael A. Gillette<sup>1,2</sup>; Robert Gerszten<sup>1,2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>*Broad Institute, Cambridge, MA*; <sup>2</sup>*Massachusetts General Hospital, Boston, MA*
- TP 427 **Comparing Ion Thermal Focusing Electrospray and Nanospray LC-MS/MS for Characterizing Human Embryonic Stem Cells and Neural Progenitor Cells;** Raghothama Chaerkady<sup>1</sup>; Vadiraja Bhat<sup>2</sup>; Dawn Stickle<sup>2</sup>; Robert Giuffre<sup>2</sup>; Hyesoo Kim<sup>1</sup>; Robert N Cole<sup>1</sup>; Candace L Kerr<sup>3</sup>; <sup>1</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*; <sup>2</sup>*Agilent Technologies, Wilmington, DE*; <sup>3</sup>*University of Maryland, Baltimore, MD*
- TP 428 **Evaluation of Multiple Search Engines for the Proteomic Analysis of Pap Tests for Biomarker Discovery in Gynecological Malignancies;** Somi Afuni; Kristin Boylan; Timothy Griffin; Amy Skubitz; *University of Minnesota, Minneapolis, MN*
- TP 429 **Proteomic Investigation of Saliva from Children with Autism Spectrum Disorder and Matched Controls by SDS-PAGE and DIGE and LC-MS/MS;** Katherine Beglinger<sup>1</sup>; Kelly Wormwood<sup>1</sup>; Armand Ngounou<sup>1</sup>; Jeanne Ryan<sup>2</sup>; Costel Darie<sup>1</sup>; Alisa G. Woods<sup>1</sup>; <sup>1</sup>*Clarkson University, Potsdam, NY*; <sup>2</sup>*SUNY, Plattsburgh, NY*
- TP 430 **Multiplexed Protein Expression Profiling of Pancreatic Stellate Cells under Nicotine Stress;** Joao Paulo; Steven Gygi; *Harvard Medical School, Boston, MA*
- TP 431 **Application of iTRAQ Proteomics to Study Biotherapeutic mAb Production in CHO Cells;** Deniz Baycin Hizal<sup>1</sup>; David Gold<sup>1</sup>; Huifang Dong<sup>1</sup>; Wei Zhu<sup>1</sup>; Raghothama Chaerkady<sup>2</sup>; Robert Cole<sup>2</sup>; Herren Wu<sup>1</sup>; Michael Bowen<sup>1</sup>; Jie Zhu<sup>1</sup>; <sup>1</sup>*MedImmune, Gaithersburg, MD*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*
- TP 432 **Metabolic Profiling of Transgenic Mouse Model for Polyp-Stage Colorectal Cancer;** Michael Williams<sup>1</sup>; Xing Zhang<sup>1</sup>; Amy Belton<sup>2</sup>; Jeong-Jin Park<sup>1</sup>; William Siems<sup>1</sup>; David Gang<sup>1</sup>; Linda Resar<sup>2</sup>; Raymond Reeves<sup>1</sup>; Herbert Hill<sup>1</sup>; <sup>1</sup>*Washington State University, Pullman, Washington*; <sup>2</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*
- TP 433 **Application of Mass Spectrometry for Tumor Proteogenomic Signature Discovery;** Michael C. Wendl<sup>1</sup>; Song Cao<sup>1</sup>; R. Jay Mash<sup>1</sup>; Kelly Ruggles<sup>4</sup>; Philipp Mertins<sup>5</sup>; Pei Wang<sup>6</sup>; Harsha Gunawardena<sup>7</sup>; John Wrobel<sup>7</sup>; Beifang Niu<sup>1</sup>; Kai Ye<sup>1</sup>; Matthew A. Wyczalkowski<sup>1</sup>; Michael McLellan<sup>1</sup>; Christopher A. Maher<sup>1,2</sup>; Sherri R. Davies<sup>2</sup>; R.

- Reid Townsend<sup>2</sup>; David Fenyó<sup>4</sup>; Steven A. Carr<sup>5</sup>; Xian Chen<sup>7</sup>; Matthew J. Ellis<sup>2,3</sup>; Li Ding<sup>1,2</sup>; <sup>1</sup>The Genome Institute at Washington University, St. Louis, MO; <sup>2</sup>Washington University Dept of Medicine, St. Louis, MO; <sup>3</sup>Siteman Cancer Center, St. Louis, MO; <sup>4</sup>NYU Langone Medical Center, New York, NY; <sup>5</sup>Broad Institute, Cambridge, MA; <sup>6</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>7</sup>UNC School of Medicine, Chapel Hill, NC
- TP 434 **Investigating Post-Transcriptional Modifications of Viral RNA by Affinity Capture and MS Analysis;** W. McIntyre<sup>1</sup>; Rebecca E. Rose<sup>1</sup>; M. Arra<sup>2</sup>; M. Canki<sup>2</sup>; C. Pager<sup>1</sup>; D. Fabris<sup>1</sup>; <sup>1</sup>The RNA Institute, University at Albany, Albany, NY; <sup>2</sup>Albany Medical Center, Albany, NY
- TP 435 **Proteins Regulated by Shear Stress (SS) Intensity and Their Correlation with Atherosclerosis;** Gabriela Venturini<sup>1</sup>; Rafael Dariolli<sup>1</sup>; Jéssica Silva Salgueiro<sup>2</sup>; Karina Helena Morais Cardozo<sup>2</sup>; Valdemir Melechco Carvalho<sup>2</sup>; José Eduardo Krieger<sup>1</sup>; Alexandre da Costa Pereira<sup>1</sup>; <sup>1</sup>Heart Institute - FMUSP, Sao Paulo, SP - Brazil; <sup>2</sup>Fleury Group, São Paulo, SP - Brazil
- TP 436 **Understanding the Effect of Cysteine on Proteomic Profiles in *Saccharomyces cerevisiae* with High Consistency and Accuracy using Data Independent Acquisition;** Ajay Bhat<sup>1,2</sup>; Trayambak Basak<sup>1,2</sup>; Dipankar Malakar<sup>3</sup>; Manoj Pillai<sup>3</sup>; Shantanu Sengupta<sup>1,2</sup>; <sup>1</sup>CSIR-Institute of Genomics and Integrative Biology, New Delhi, India; <sup>2</sup>Academy of Scientific and Innovative Research, New Delhi, India; <sup>3</sup>AB Sciex, India, Gurgaon, India
- TP 437 **Label-free Quantitative Analysis of Radiation-induced Differential Protein Expression in The Mouse Lung Proteome;** Bao Quoc Tran<sup>1</sup>; Young Ah Goo<sup>1</sup>; Catherine Booth<sup>2</sup>; Greg Tudor<sup>2</sup>; Wenjing Li<sup>1</sup>; David R. Goodlett<sup>1</sup>; Thomas J. MacVittie<sup>1</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore, MD; <sup>2</sup>Epistem Ltd, Maschester, UK
- TP 438 **Integrated Phosphoproteogenomic Analyses of Patient-Derived Breast Cancer Xenograft Models Allow Molecular Characterization of Human Disease Biology and Therapeutic Response;** Michael A. Gillette<sup>1,2</sup>; Philipp Mertins<sup>1</sup>; Jana W. Qiao<sup>1</sup>; D. R. Mani<sup>1</sup>; Karl R. Clauser<sup>1</sup>; Sherri R. Davies<sup>5</sup>; Kelly V. Ruggles<sup>3</sup>; Song Cao<sup>5</sup>; Christopher A. Maher<sup>6</sup>; Michael McLellen<sup>5</sup>; David Fenyó<sup>4</sup>; Li Ding<sup>5</sup>; Matthew J. Ellis<sup>5</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>Broad Institute of Harvard and MIT, Cambridge, MA; <sup>2</sup>Massachusetts General Hospital, Boston, MA; <sup>3</sup>NYU Langone Medical Center, New York, NY; <sup>4</sup>New York University, New York, NY; <sup>5</sup>Washington University, St. Louis, Missouri
- TP 439 **Deciphering Systemic Responses to Brain Disorders by Quantitative Proteomics;** Li Cao; Fang Bian; An Zhou; Morehouse school of medicine, Atlanta, GA
- TP 440 **Robotic Preparation of Hundreds of Clinical Samples for Protein Biomarker Verification and Validation;** Tony Tegeler<sup>1</sup>; Matthew Rosenow<sup>1</sup>; Paul Russo<sup>2</sup>; Ruben Magni<sup>2</sup>; Alessandra Luchini<sup>2</sup>; Lance Liotta<sup>2</sup>; Emanuel Petricoin<sup>2</sup>; Patrick Pirrotte<sup>1</sup>; <sup>1</sup>Translational Genomics Research Institute, Phoenix, AZ; <sup>2</sup>Center for Applied Proteomics & Molecular Medicine, Manassas, VA
- TP 441 **Discovery of Tissue Regenerating Biomarkers in the Secretome Released from Human Embryonic Stem Cell-derived Hepatocytes by Using Proteomic Approach;** Hee-Joung Lim<sup>1,2</sup>; Jiyoun Han<sup>1</sup>; Yu Jin Jang<sup>1</sup>; Ae Eun Seok<sup>2</sup>; Jong-Moon Park<sup>3</sup>; Hyun-Jin Jung<sup>4</sup>; Yong-Seung Shin<sup>4</sup>; HooKeun Lee<sup>3</sup>; Jong-Hoon Kim<sup>1</sup>; Hee-Gyoo Kang<sup>2</sup>; <sup>1</sup>Laboratory of Stem Cells, Korea University, Seoul, Republic of Korea; <sup>2</sup>Bio-medical Laboratory, Eulji University, Seongnam, Republic of Korea; <sup>3</sup>Laboratory of Proteomics, Gachon University, Incheon, Republic of Korea; <sup>4</sup>Agilent technologies Ltd, Suwon, Republic of Korea
- TP 442 **Comparative N-glycoproteome of the Secretome of Human Metastatic Hepatocellular Carcinoma Cell Lines;** Wantao Ying; Xianyu Li; Xiaohong Qian; Beijing Institute of Radiation Medicine, Beijing, China
- Disease Biomarkers, 443 - 458**
- TP 443 **Lipidomics Driven Biomarker Identification and Validation Brings Ceramides into Diagnostics for Determining the Lipid Related Risk of Cardiovascular Death;** Kim H Ekroos<sup>1</sup>; Helena Simolin<sup>1</sup>; Matti Suoniemi<sup>1</sup>; Markus Kleber<sup>2</sup>; Reini Hurme<sup>1</sup>; Juha Sinisalo<sup>3</sup>; Winfried März<sup>4</sup>; Reijo Laaksonen<sup>1</sup>; <sup>1</sup>Zora Biosciences Oy, Espoo, Finland; <sup>2</sup>Mannheim Institute of Public Health, Mannheim, Germany; <sup>3</sup>University Hospital of Helsinki, Helsinki, Finland; <sup>4</sup>Synlab Academy, Mannheim, Germany
- TP 444 **PZP as a Novel Biomarker for Early Alzheimer's Disease;** Diana A.T. Nijholt; A. Ikram; J.M. Kros; P.A.E. Sillevis Smitt; P.J. Koudstaal; T.M. Luider; Erasmus Medical Centre, Rotterdam, Netherlands
- TP 445 **Biomarker Discovery in Cerebrospinal Fluid for Schizophrenia and Antipsychotic Drug Treatment-Induced Weight Gain;** Geun-Cheol Gil<sup>1</sup>; Bich Nguyen<sup>1</sup>; Yiyong Zhou<sup>2</sup>; Xiaolei Xie<sup>1</sup>; Rene Allard<sup>2</sup>; Howard Schulman<sup>1</sup>; Daniel Chelsky<sup>1</sup>; Sushmita Mimi Roy<sup>1</sup>; <sup>1</sup>Caprion Proteomics US LLC, Menlo Park, CA; <sup>2</sup>Caprion Proteomics Inc, Montreal, Canada
- TP 446 **Elucidation of Epileptogenic Mechanisms using a Mass Spectrometry-Based Metabolomics Approach;** Svenja Heischmann<sup>1</sup>; Kevin Quinn<sup>2</sup>; Charmion Cruickshank-Quinn<sup>2</sup>; Lindsey B. Gano<sup>1</sup>; Joe Gomez<sup>1</sup>; Nicole Reisdorph<sup>2</sup>; Manisha Patel<sup>1</sup>; <sup>1</sup>University of Colorado Denver, School of Pharmacy, Aurora, CO; <sup>2</sup>National Jewish Health, Denver, CO
- TP 447 **Profiling Urinary Proteome for Stress Induced Female Urinary Incontinence;** Marianne Koch<sup>2</sup>; Rosa Laterza<sup>2</sup>; Wei-Qiang Chen<sup>1</sup>; Miloš Barut<sup>3</sup>; Sonja Seyfert<sup>4</sup>; Heinz Kölbl<sup>2</sup>; Goran Mitulovic<sup>1</sup>; <sup>1</sup>Medical University of Vienna, KIMCL, Vienna, Austria; <sup>2</sup>Medical Univ of Vienna, Dept. of Gyn. and Obst., Vienna, Austria; <sup>3</sup>BIA Separations, Ajdovščina, Slovenia; <sup>4</sup>Medical Univ of Vienna, Proteomics Core Facility, Vienna, Austria
- TP 448 **Immuno-based-LC/SRM as a Diagnostic tool for Measuring Protein Dynamics of Amyloid  $\beta$  Isoforms Instead of ELISA in the Clinical Laboratory;** Kwasi Mawuenyega; Tom Kasten; Vitaliy Ovod; Brendan Lucey; Wendy Sigurdson; Randall Bateman; Washington University School of Medicine, Saint Louis, MO
- TP 449 **Proteome Analysis of Exhaled Breath Condensate for Lung Cancer Biomarker Discovery;** NL Starodubtceva<sup>1,3</sup>; AM Ryabokon<sup>1</sup>; AS Kononikhin<sup>2,3</sup>; EN Kukaev<sup>1,2</sup>; IA Popov<sup>1,2</sup>; VA Bagrov<sup>4</sup>; OV Pikin<sup>4</sup>; VV Barmin<sup>4</sup>; EC Anaev<sup>5</sup>; SD Varfolomeev<sup>1</sup>; EN Nikolaev<sup>1,2</sup>; <sup>1</sup>Emanuel Institute of Biochemical Physics, Moscow, Russia; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>3</sup>Research Center for Obstetrics, Gynecology, Moscow, Russia; <sup>4</sup>Gertsen Institute of Oncology, Moscow, Russia; <sup>5</sup>Research Institute of Pulmonology, Moscow, Russia
- TP 450 **Analysis of Extracellular Matrix Peptides in Chronic Obstructive Pulmonary Disease (COPD) by LC/MS;** Jiangtao He<sup>1,1</sup>; Shuren Ma<sup>1</sup>; Yong Y Lin<sup>1</sup>; Jerome Cantor<sup>2</sup>; Gerard Turino<sup>1</sup>; <sup>1</sup>Icahn School of Medicine at Mount Sinai, New York, NY; <sup>2</sup>St. John's University, New York, NY
- TP 451 **The Mitochondrial Deacetylase SIRT3 is a Host Defense Factor Hijacked during Viral Infection;** Rommel Mathias; Matthew Lefebvre; Ileana M. Cristea; Princeton University, Princeton, NJ

- TP 452 **Investigation on Redox Metabolism and Dopaminergic Cell Death in Response to Neuron Toxins by a MS and NMR Combined Technique;** Shulei Lei; Darrell Marshall; Yuting Huang; Aracely Garcia-Garcia; Renu Nandakumar; Eric Dodds; Rodrigo Franco; Robert powers; *university of nebraska lincoln, lincoln, NE*
- TP 453 **Defining the Exposome: a Critical Quantity to Determine the Causes of Chronic Human Disease;** Anthony Macherone<sup>1,2</sup>; <sup>1</sup>Agilent Technologies, Inc., Wilmington, DE; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- TP 454 **Identification of Potential Metabolite Biomarkers of Lower Urinary Tract Symptoms (LUTS) in Mouse and Human Urines;** Ling Hao<sup>1</sup>; Tyler Greer<sup>2</sup>; Chad Vezina<sup>3</sup>; Will Ricke<sup>4</sup>; Paul Marker<sup>1</sup>; Dale Bjorling<sup>3</sup>; Wade Bushman<sup>4</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>School of Pharmacy, University of Wisconsin-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, UW-Madison, Madison, WI; <sup>3</sup>School of Veterinary Medicine, UW-Madison, madison, WI; <sup>4</sup>Department of Urology, UW-Madison, madison, WI
- TP 455 **A quantitative LC-MS/MS (Qtrap) Method to Profile Sphingolipids in Pancreatic  $\beta$ -cells;** Kumari Ubhayasekera; Bo EK; Jonas Bergquist; *Uppsala University, Uppsala, Sweden*
- TP 456 **Differential Accumulation of Glycosphingolipids in a Tay-Sachs Disease Brain;** Huan He<sup>1</sup>; Yu-Teh Li<sup>2</sup>; Su-Chen Li<sup>2</sup>; Nicolas L. Young<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>Ion Cyclotron Resonance Program, NHMFL, Tallahassee, FL; <sup>2</sup>Tulane University School of Medicine, New Orleans, LA; <sup>3</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- TP 457 **Quantitative Phosphoproteomic Phenotyping of Acquired Resistance to HER2 Kinase Inhibitors in Breast Cancer using Multimodal Phosphopeptide Enrichments;** Erik J. Soderblom<sup>1</sup>; Hongbo Gu<sup>2</sup>; Jeffrey Sliva<sup>2</sup>; J. Will Thompson<sup>1</sup>; Wenle Xia<sup>1</sup>; Neil Spector<sup>1</sup>; M. Arthur Moseley<sup>1</sup>; <sup>1</sup>Duke University School of Medicine, Durham, NC; <sup>2</sup>Cell Signaling Technology, Danvers, MA
- TP 458 **Proteomics Study of SCYL2-Knockdown Effect on the Distribution of Amyloid Precursor Protein and Its Fragments in the APP-Overexpressing N2a Cells;** Ko-Yi Chien; Rong Wang; *Icahn School of Medicine at Mount Sinai, New York, NY*
- Biomarkers: Quantitative Analysis, 459 - 488**
- TP 459 **A Sensitive Isotopic Dilution LC/MS Methodology to Evaluate Asymmetric Dimethyl Arginine Levels as a Plasma Biomarker of Endothelial Function;** Jose Castro-Perez; Paul Miller; Sheng-Ping Wang; Dan Xie; Stephen Previs; Doug Johns; *Merck Research Laboratories, Kenilworth, NJ*
- TP 460 **Quantification of Intact and Truncated Stromal cell-derived factor-1 $\alpha$  (SDF-1 $\alpha$ ) in Circulation by Immunoaffinity Enrichment and Tandem Mass Spectrometry;** Weixun Wang<sup>1</sup>; Bernard Choi<sup>1</sup>; Wenyu Li<sup>1</sup>; Julie Lao<sup>1</sup>; Anita Lee<sup>1</sup>; Sandra Souza<sup>1</sup>; Nathan Yates<sup>2</sup>; Timothy Kowalski<sup>1</sup>; Alessandro Pociari<sup>3</sup>; Lucinda Cohen<sup>1</sup>; <sup>1</sup>Merck Research Labs, Rahway, NJ; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Janssen R&D, Spring House, PA
- TP 461 **Detection of Endothelial Cell Surface Proteins following Irradiation as Potential Targets for Brain Arteriovenous Malformations Molecular Therapy;** Margaret Simonian; *UCLA, Los Angeles, CA*
- TP 462 **Measuring Protein Analyte Panels in Dried Blood Spots (DBS) using an Automated SISCAPA-MS Workflow;** Morteza Razavi<sup>1</sup>; Leigh Anderson<sup>1</sup>; Selena Larkin<sup>1</sup>; Terry Pearson<sup>1,2</sup>; <sup>1</sup>SISCAPA Assay Technologies, Washington, DC; <sup>2</sup>University of Victoria, Victoria, BC Canada
- TP 463 **Quantitative Activity-Based Kinase Profiling in Lung Cancer;** Bin Fang; Jiannong Li; Elizabeth Wood; Y. Ann Chen; Stephen Brantley; Fumi Kinose; Wei Guan; Andrew Myers; Steven Eschrich; Uwe Rix; Eric Haura; John Koomen; *H. Lee Moffitt Cancer Center, Tampa, FL*
- TP 464 **Determination of Urea in Human Serum and Epithelial Lining Fluid Using LCMS; Benchmarking to a Traditional Diagnostic Colorimetric Kit;** Christopher A Evans; Chester L Bowen; Amanda Watkins; Bonnie Orr; *GlaxoSmithKline, King Of Prussia, PA*
- TP 465 **Investigation of Angiotensin Biomarker Dynamics Employing Micro-Flow LC and Microfluidic ESI-MS;** Thomas Mencken; Jonathan Kehler; Matthew Szapacs; Chester Bowen; *GlaxoSmithKline, Collegeville, PA*
- TP 466 **Cross-Validation of a Ligand Binding and Immocapture / LC-MS Assay for the Determination of the Biomarker Periostin;** Jonathan Kehler; Matthew Szapacs; *GlaxoSmithKline, King Of Prussia, PA*
- TP 467 **Targeted MS2 Quantitation of Exon Skipping Restored Dystrophin in a Mouse Model of Duchenne Muscular Dystrophy;** Kristy J. Brown; Kitipong Uaesoontrachoon; Aiping Zhang; Conner Shaughnessy; Ramya Marathi; Sree Rayavarapu; Maria Candida Vila; Eric Hoffman; Kanneboyina Nagaraju; Yetrib Hathout; *Children's National Health System, Washington, DC*
- TP 468 **An Omics study of CSF from HAND patients under cART reveals evidence for macrophage activation and perturbations in glutamate metabolism;** Adriana Bora<sup>1</sup>; Ceereena Ubaida Mohien<sup>1</sup>; Alexey Lyashkov<sup>3</sup>; Anne Blackwell<sup>2</sup>; Linda Chang<sup>4</sup>; Richard IV Moxley<sup>1</sup>; Ned Sacktor<sup>1</sup>; Justin C. McArthur<sup>1</sup>; Norm Haughey<sup>1</sup>; Avindra Nath<sup>3</sup>; David R. Graham<sup>1</sup>; <sup>1</sup>Johns Hopkins Medical School, Baltimore, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>National Institute of Health, Bethesda, MD; <sup>4</sup>Hawaii University, Honolulu, HI
- TP 469 **Simultaneous Quantitation of Neurotransmitters in Dialysates Using LC/MS-MS;** Shiling Jia; Fan Wang; Charles Yang; Wei Tang; Alicia Y Du; *Chempartners, Shanghai, Zhang, Jiang, China*
- TP 470 **Development of a Multiplexed Targeted SRM Assay for NCI's Top Tumor Associated Antigens for Biomarker Screening in Multiple Cancer Types;** Erik J. Soderblom; Lisa St. John - Williams; Wenle Xia; Meredith E. Turner; Matthew W. Foster; Neil Spector; M. Arthur Moseley; *Duke University School of Medicine, Durham, NC*
- TP 471 **Discovery and Verification of Neurotrauma Markers by High Mass Accuracy/High Resolution Mass Spectrometry;** Sean Shen<sup>1</sup>; Ina Wanner<sup>2</sup>; Joseph A. Loo<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Los Angeles, CA; <sup>2</sup>Semel Institute for Neuroscience & Human Behavior, Los Angeles, CA
- TP 472 **Sequence Quantitative Analysis (SEQUANA): targeted-Proteomic Method for Accurate Alzheimer's Disease Diagnostic by CSF Tau Proteoforms Monitoring;** Nicolas Barthélemy<sup>1,2</sup>; Christophe Hirtz<sup>2</sup>; François Fenaille<sup>1</sup>; Susanna Schraen-Maschke<sup>3</sup>; Audrey Gabelle<sup>2</sup>; Christophe Junot<sup>1</sup>; Sylvain Lehmann<sup>2</sup>; François Becher<sup>1</sup>; <sup>1</sup>CEA Saclay, DSV/iBiTec-S/LEMM, Gif s/Yvette, France; <sup>2</sup>CHU Montpellier, Hôpital St Eloi, IRMB/LBPC, Montpellier, France; <sup>3</sup>Inserm, UMR 837, IMPRT, Faculté de Médecine, Lille, France
- TP 473 **ATP7B Analysis by Immuno-SRM-MS for Wilson Disease;** Sunhee Jung; Si Houn Hahn; *Seattle Children's, Seattle, WA*
- TP 474 **Development of a LC-MS/MS Method to Biomonitor 1,3-Butadiene Exposure and Early Biological Effects in Nonsmokers and Smokers;** Xiaotao Zhang<sup>1,2</sup>; Hongwei

- Hou<sup>1</sup>; Longkai Shi<sup>1</sup>; Yong Liu<sup>2</sup>; An Wang<sup>2</sup>; Qingyuan Hu<sup>1</sup>; <sup>1</sup>China National Tobacco Quality Supervision & Test, Zhengzhou, CHINA; <sup>2</sup>Anhui Institute of Optics and Fine Mechanics, Hefei, China
- TP 475 **Simultaneous Determination of N3-methyladenine, N3-ethyladenine and N3-(2-hydroxyethyl)adenine in Human Urine by Liquid Chromatography-Tandem Mass Spectrometry**; Yongfeng Tian<sup>1</sup>; Hongwei Hou<sup>1</sup>; Xiaotao zhang<sup>1</sup>; An Wang<sup>2</sup>; Yong Liu<sup>2</sup>; Qingyuan Hu<sup>1</sup>; <sup>1</sup>China National Tobacco Quality Supervision & Test, Zhengzhou, China; <sup>2</sup>Anhui Institute of Optics and Fine Mechanics, Hefei, China
- TP 476 **Variability of Urinary VOC Metabolites Concentration in Before Bed, First Morning Void, and Spot Urine Samples**; Deepak Bhandari<sup>1</sup>; K. Udeni Alwis<sup>1</sup>; B. Rey deCastro<sup>1</sup>; Connie Sosnoff<sup>1</sup>; Yu Qiu<sup>1</sup>; Marsha Morgan<sup>2</sup>; Jon Sobus<sup>2</sup>; Benjamin Blount<sup>1</sup>; <sup>1</sup>Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>US Environmental Protection Agency, Research Triangle Park, NC
- TP 477 **Identification and Quantitation of N-glycans in Dyssynchronous Heart Failure**; Shuang Yang<sup>1</sup>; Lijun Chen<sup>1</sup>; Punit Shah<sup>1</sup>; Jonathan Kirk<sup>2</sup>; David A. Kass<sup>2</sup>; Jennifer E. van Eyk<sup>3</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>John Hopkins Dept. of Pathology, Baltimore, MD; <sup>2</sup>Johns Hopkins Cellular and Molecular Medicine, Baltimore, MD; <sup>3</sup>Johns Hopkins Institute for Computational Medicine, Baltimore, MD
- TP 478 **Automated Extraction of Glycans and Peptides for Glycomic and Proteomic Analyses**; Jing Chen; Shuang Yang; Hui Zhang; Johns Hopkins University, Baltimore, Maryland
- TP 479 **Utilizing Online Extraction Techniques to Increase Sensitivity and Improve Sample Preparation Efficiency for Quantitative LCMS: A cGMP Biomarker Case Study**; Elisabeth Lonie; Dawn Dufield; Pfizer, Andover, MA
- TP 480 **Accurate Quantitation of Endogenous Compounds by Standard Addition Amended Calibration (SAAC) in Matched Matrix**; Zhenmin Liang; John Hanley; Lisa Borbridge; Allergan, Irvine, CA
- TP 481 **Comparison of Label-Free and Label-Based Strategies for Proteome Analysis of Hepatoma Cell Lines**; Dominik Andre Megger<sup>1</sup>; Leona Louise Pott<sup>1</sup>; Kristin Rosowski<sup>1</sup>; Birgit Korte<sup>1</sup>; Don Marvin Voss<sup>1</sup>; Stephanie Tautges<sup>1</sup>; Thilo Bracht<sup>1</sup>; Maike Ahrens<sup>1</sup>; Juliet Padden<sup>1</sup>; Martin Eisenacher<sup>1</sup>; Katja Kuhlmann<sup>1</sup>; Helmut E. Meyer<sup>1,2</sup>; Barbara Sitek<sup>1</sup>; <sup>1</sup>Ruhr-Universität Bochum, MPC, Bochum, Germany; <sup>2</sup>Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany
- TP 482 **Quantitative Analysis of the PTEN-Induced Kinase (Pink-1) Mutant in C. elegans using Tandem Mass Tags**; Geert Baggerman<sup>1,2</sup>; Dirk Valkenborg<sup>1,2</sup>; Evelyne Maes<sup>1,3</sup>; Karin Schildermans<sup>2</sup>; Inge Mertens<sup>1,2</sup>; <sup>1</sup>VITO, Mol, Belgium; <sup>2</sup>CFP-CeProMa, University of Antwerp, Antwerp, Belgium; <sup>3</sup>Functional Genomics and Proteomics lab, Leuven, Belgium
- TP 483 **Identification of Protein Biomarkers for the Cellular Response to Proteasome Inhibition using a Simple, Robust Platform Enabling Proteome-Wide, Label-Free Quantification**; Aaron Aslanian<sup>1,2</sup>; Xuemei Han<sup>1</sup>; John Yates III<sup>1</sup>; <sup>1</sup>The Scripps Research Institute, La Jolla, CA; <sup>2</sup>Salk Institute for Biological Studies, La Jolla, CA
- TP 484 **Development and Application of a Quantitative Proteomic Method for Verification of Neurodegenerative-related Biomarkers in Human CSF**; Andrew Percy<sup>1</sup>; Juncong Yang<sup>1</sup>; Andrew Chambers<sup>1</sup>; Romain Simon<sup>1</sup>; Darryl Hardie<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- TP 485 **Improving Selectivity and Sensitivity in Clinical Assays using Parallel Reaction Monitoring**; Bruno Doman<sup>1</sup>; Sebastien Gallien<sup>1</sup>; Yeoun-Jin Kim<sup>1</sup>; Guy Berchem<sup>2</sup>; <sup>1</sup>Luxembourg Clinical Proteomics Center, Strassen, Luxembourg; <sup>2</sup>CRP-Sante, Strassen, Luxembourg
- TP 486 **High Sample Throughput SISCAPA-UMRM MS Quantitation of Prostate Specific Antigen in Nondepleted Serum**; Mary Joan Castillo; Adam Mcshane; Min Cai; Alexander Gomes; Xudong Yao; University of Connecticut, Storrs, CT
- TP 487 **An Alternative Computational Solution to Protein Quantitation in Plasma Proteome Analysis using LC-MS/MS with Travelling Wave Ion Mobility**; Charlotte E. Daly; Leong L. Ng; Amirmansoor Hakimi; Richard Willingale; Donald J.L. Jones; University of Leicester, Leicester, UK
- TP 488 **Impaired Regulation of Tyrosine Phosphorylation in Skeletal Muscle in Type 2 Diabetes**; Danjun Ma<sup>1</sup>; Berhane Seyoum<sup>1</sup>; Michael Caruso<sup>1</sup>; Zaher Msallaty<sup>1</sup>; Monique Lewis<sup>1</sup>; Chengjian Tu<sup>2</sup>; Michael Diamond<sup>1</sup>; Abdul Abou-Samra<sup>1</sup>; Xiangmin Zhang<sup>1</sup>; Wissam Al-janabi<sup>1</sup>; Rodney Berry<sup>1</sup>; Kurt Højlund<sup>3</sup>; Jeffrey Horowitz<sup>4</sup>; Rebecca Tagett Tagett<sup>1</sup>; Sorin Draghici<sup>1</sup>; Zhengping Yi<sup>1</sup>; <sup>1</sup>Wayne state university, Detroit, MI; <sup>2</sup>University at Buffalo, Buffalo, NY; <sup>3</sup>Odense University Hospital, Odense, Denmark; <sup>4</sup>University of Michigan, Ann Arbor, MI
- Small Molecule Quantitation, 489 - 523**
- TP 489 **Application of Novel Pre-Charged and Highly Specific Fluorinated Azide for the Trace Analysis of Ethinylestradiol using Copper-Catalyzed Click Reaction**; Priyanka Chitranshi; Lucie Loukotkova; Goncalo Gamboa Da Costa; US-FDA/NCTR, Jefferson, AR
- TP 490 **On-Line Pre-Treatment and Quantification of Trace Estrogens in Serum by Bulk Derivatization and Direct Cation ExchangeTrap-and-Elute LC/MS/MS**; Liangqiao Bian<sup>1,2</sup>; Jana Chalupová<sup>4,5</sup>; Hui Fan<sup>3</sup>; Marek Šebela<sup>4,5</sup>; Maciej Kukula<sup>1,2</sup>; Joe Barrera<sup>2</sup>; Kevin A. Schug<sup>3</sup>; <sup>1</sup>Shimadzu Center for Advanced Analytical Chemistry, The University of Texas at Arlington, Arlington, TX; <sup>2</sup>Shimadzu Institute for Research Technologies, The University of Texas at Arlington, Arlington, TX; <sup>3</sup>Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX; <sup>4</sup>Department of Biochemistry, Palacký University, Olomouc, Czech; <sup>5</sup>Department of Protein Biochemistry and Proteomics, Palacký University, Olomouc, Czech
- TP 491 **Development and Validation of LC/MS/MS Methods to Quantify EC1456 and Tubulysin B Hydrazide in Rat Plasma**; Michael Pugh; Satish Rao; Patrick J. Klein; Christopher P. Leamon; Endocyte, Inc., West Lafayette, IN
- TP 492 **Development and Qualification of a Fast and Sensitive LC-MS/MS Method for the Simultaneous Quantification of Microdosed Statins in Human Plasma**; Cynthia M. Chavez-Eng; Ryan Lutz; Dina Goykhman; Kevin Bateman; Merck & Co., West Point, PA
- TP 493 **Development of an Ultra-Sensitive, High-Throughput Multiplexed LC(HILIC)-MS/MS Method for the Simultaneous Quantitation of Naloxone, Buprenorphine, and Norbuprenorphine**; Xiaodong Zhu; Thomas Horuath; Jingguo Hou; Edward Wells; Steve Unger; Worldwide Clinical Trials Drug Development Solutio, Austin, TX
- TP 494 **Challenges in Quantification of Metal-based Oncology Drugs in Human Plasma Using Triple Quad 5500 System**; Feng Yin; Guangnong Zhang; Urszula Lorent; Emily Epure; Andrew Swenson; Yong-Xi Li; Medpace Bioanalytical Laboratories, Cincinnati, OH

- TP 495 **Simultaneously Sensitive and Accurate Measurements of Seven Steroid Hormones in Post-Menopausal Women Serum by a Robust LC-MS/MS Method;** Yuyong Ke; Renaud Gonthier; Jonathan Bertin; Fernand Labrie; *EndoCeutics Laboratory, Québec, Canada*
- TP 496 **Highly Sensitive Quantitative Estimation of Genotoxic Impurities using LC/MS/MS;** Shruti Raju; Deepti Bhandarkar; Rashi Kochhar; Shailesh Damale; Shailendra Rane; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 497 **Highly sensitive Quantitative Analysis of Felodipine and Hydrochlorothiazide from Plasma using LC/MS/MS;** Shailendra Rane; Rashi Kochhar; Deepti Bhandarkar; Shruti Raju; Shailesh Damale; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 498 **Low level Quantitation of Loratidine from Plasma using LC/MS/MS;** Shailesh Damale; Deepti Bhandarkar; Shruti Raju; Rashi Kochhar; Shailendra Rane; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*
- TP 499 **High Throughput Analysis of Liquiritigenin and Isoliquiritigenin In Rodent Serum Using UPLC-Tandem Mass Spectrometry;** Nathan C. Twaddle<sup>1</sup>; Mona I. Churchwell<sup>1</sup>; Estatira Sepehr<sup>1</sup>; Ashish Sawhney<sup>1</sup>; William G. Helferich<sup>2</sup>; Daniel R. Doerge<sup>1</sup>; <sup>1</sup>*NCTR/FDA, Jefferson, AR*; <sup>2</sup>*University of Illinois at Urbana-Champaign, Urbana, IL*
- TP 500 **An Analytical Method for Automated Analysis of Plasma Dapsone, Trimethoprim, Sulfamethoxazole, Sulfamethazine, Sulfamethizole, and Sulfathiazole for Dose Optimization;** Claudia Meek; Nyokabi Miingi; Erling Beck; Ronald Hall; Richard Leff; *Texas Tech University Health Sciences Center, Dallas, TX*
- TP 501 **LC-MS/MS Bioanalysis of Dapagliflozin and Its Glucuronide Metabolite in Human Blood Using Dried Blood Spot;** Jane Liu<sup>1</sup>; Sophia (Xiaohui) Xu<sup>1</sup>; Guowen Liu<sup>1</sup>; David Boulton<sup>1</sup>; Melanie Pe Benito<sup>1</sup>; Marsha Epstein<sup>1</sup>; Michael Waldron<sup>2</sup>; Pathanjali Kadiyala<sup>1</sup>; Jim Shen<sup>1</sup>; mark arnold<sup>1</sup>; Qin ji<sup>1</sup>; <sup>1</sup>*Bristol-Myers Squibb Co., Princeton, NJ*; <sup>2</sup>*PPD, Richmond, , VA*
- TP 502 **Determination of Pradigastat, a DGAT1 Inhibitor in Human Plasma using Microc-MS/MS;** Tapan Majumdar; Shari Wu; Cindy Chen; Adam Bentley; Jimmy Flarakos; *Novartis Institutes for Biomedical Research, East Hanover, NJ*
- TP 503 **Quantitative Estimation of Potential Genotoxic Impurities in Drug Development without Synthetic Standards by High Resolution Mass Spectrometer and UV Detection;** Chunang (Christine) Gu; Andrew McClory; Sarah Stowers; Jason Gruenhagen; Alan Deese; *Genentech, South San Francisco, CA*
- TP 504 **Overcoming Chiral Method Development Challenges: UPLC-MS/MS Method for Determination of Dextroamphetamine and Levoamphetamine in Human Plasma after Chiral Derivatization;** Yuwen Zhao; Vi Dan; Yuan-Shek Chen; Luca C. Matassa; *QPS, LLC, Newark, DE*
- TP 505 **Ultra-Trace Quantitation of Catechins in Human Blood Plasma to Facilitate Kinesiology Study using Restricted Access Media LC/MS/MS;** Aionna Guerrero<sup>1</sup>; Sarah Hughes<sup>1</sup>; Hui Fan<sup>1</sup>; Michelle Harrison<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>*UT Arlington, Arlington, TX*; <sup>2</sup>*UT Austin, Austin, TX*
- TP 506 **Development and Validation for the Simultaneous Determination of Emtricitabine and Tenofovir in Human Plasma by LC-MS/MS;** Jingguo Hou; Laura Binneboese; Melody Adam; Steven Hoehne; Kevin McManus; Xiaodong Zhu; Edward Wells; *WWCT, Austin, TX*
- TP 507 **Absolute Quantitation of Aminoglycoside Antibiotics in Mouse Plasma by a HILIC-based LC-MS/MS Method;** Ludmila Alexandrova<sup>1</sup>; Allis Chien<sup>1</sup>; Robert Greenhouse<sup>2</sup>; Anthony Ricci<sup>3</sup>; <sup>1</sup>*Stanford University Mass Spectrometry, Stanford, CA*; <sup>2</sup>*SPARK, Stanford University School of Medicine, Stanford, CA*; <sup>3</sup>*Department of Otolaryngology, School of Medicine, Stanford, CA*
- TP 508 **A Simple, Reliable and Rapid LC-MS/MS Method for Simultaneous Determination of Carbamazepine and Carbamazepine-10,11-epoxide in human plasma;** Shuyu Hou; Yuan-Shek Chen; *QPS, LLC, Newark, DE*
- TP 509 **Supercritical Fluid Chromatography-Tandem Mass Spectrometry for Fast Chiral Separation of Cetrizine in Human Plasma;** Han Young Eom; Hyun-Deok Cho; Joon Hyuk Suh; Unyong Kim; Junghyun Kim; Yura Jung; Bong-Joon Kim; Sang Beom Han; *Chung-Ang University, Seoul, South Korea*
- TP 510 **Simultaneous Quantitative Analysis of 20 Amino Acids in Food Samples without Derivatization using LC-MS/MS;** Keiko Matsumoto<sup>1</sup>; Jun Watanabe<sup>1</sup>; Itaru Yazawa<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*Imtakt Corporation, Kyoto, Japan*
- TP 511 **Assay of Human Saliva Steroids by Stable Isotope Coded Derivatization (ICD) and Tandem Mass Spectrometry;** Fabio Mazzotti<sup>1</sup>; Leonardo Di Donna<sup>1</sup>; Domenico Taverna<sup>1</sup>; Anna Napoli<sup>1</sup>; Constantinos M. Athanassopoulos<sup>2</sup>; Giovanni Sindona<sup>1</sup>; <sup>1</sup>*University of Calabria, Arcavacata Di Rende, Italy*; <sup>2</sup>*University of Patras, Patras, Greece*
- TP 512 **A generic LC-MS Cleaning Verification Assay for High Potency Drugs;** Vinayak AK<sup>1</sup>; Syed Lateef<sup>1</sup>; Chunang (Christine) Gu<sup>2</sup>; Michael Dong<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Bangalore, India*; <sup>2</sup>*Genentech, South San Francisco, CA*
- TP 513 **Automated Bioanalytical Method Development for Methotrexate and Sulfasalazine Utilizing Quality-by-Design Approach;** Syed Salman Lateef; Siji Joseph; *Agilent Technologies, Bangalore, INDIA*
- TP 514 **Verification of an LC-MS/MS Method for 14 Antidepressants Utilizing Dried Blood Spots;** Kerry Hassell; Sarah Fair-Wandland; Joseph L. Herman; *ThermoFisher Scientific, Franklin, MA*
- TP 515 **Evaluation and Application of a Non-contact Digital Dispenser, HP D300, in Bioanalysis;** Debra Liao; Susan Chen; Martin Paton; Mark Qian; *Millennium: The Takeda Oncology Company, Cambridge, MA*
- TP 516 **Can DMSO Provide Benefit in Application beyond Proteomic?;** J.C. Yves Leblanc; *AB SCIEX, Concord, On, Canada*
- TP 517 **A Sensitive Method for the Determination of Lithium in Human Plasma Using ICP-MS Detection;** Patrice Lantin; Sylvain Lachance; François Viel; Nadine Boudreau; Ann Levesque; *InVentiv Health Clinical, Québec, Canada*
- TP 518 **Compound Dependence of LC-MS-MS Flow Rate Sensitivity;** Jay Corr; Thomas Covey; *AB SCIEX, Concord, Canada*
- TP 519 **Development of a Highly Sensitive, Efficient, Combo Extraction Method for the Quantitation of Formoterol and Budesonide by UPLC/MS/MS;** Ryan S. Adler; Sherry Liu; Alicia Pietrasiewicz; Spencer J. Carter; Quiying Zhu; Min Meng; *Tandem Labs, Salt Lake City, UT*
- TP 520 **A Simple, Selective and Highly Sensitive UPLC-MS/MS Method for Determination of Mometasone Furoate in Human Plasma;** Hao Li; Huafang Jiang; Ling Zhou; Xiaohang Shen; Jinsong Xing; Wenzhong Liang; *WuXi AppTec (Shanghai) Co. Ltd., Shanghai, China*

- TP 521 **Improving Detection Limits of Prohibited Substances and Therapeutics by Solid Phase Microextraction (SPME) Coupled to LC-MS/MS;** Frenny Ruparella<sup>1</sup>; Lisa Cousins<sup>1</sup>; Nathaly Reyes-Garcés<sup>2</sup>; Germán Augusto Gómez-Ríos<sup>2</sup>; Barbara Bojko<sup>2</sup>; Janusz Pawliszyn<sup>2</sup>; <sup>1</sup>*IONICS Mass Spectrometry, Bolton, Canada*; <sup>2</sup>*Department of Chemistry, University of Waterloo, Waterloo, Canada*
- TP 522 **LC-MS/MS Methods Development for the Analysis of Polymeric Materials and Related Metabolites in Biological Matrices;** Changyu Quang; Brett D. Dunbar; Nichole R. Myers; William C. Nethero; Michael P. Donegan; Elizabeth A. Groeber; *WIL Research, Ashland, OH*
- TP 523 **LC-MS/MS Method of Isradipine: Unsuitability of Isradipine-D3 as Internal Standard Due to Temperature-dependent Transesterification in Ion Source;** Hao Li<sup>1</sup>; Jie Zhang<sup>2</sup>; Yan Fu<sup>1</sup>; Changqing Lin<sup>1</sup>; xiaohang shen<sup>1</sup>; jinsong xing<sup>1</sup>; Wenzhong Liang<sup>1</sup>; <sup>1</sup>*WuXi AppTec (Shanghai) Co. Ltd., Shanghai, CHINA*; <sup>2</sup>*Novartis Institutes for BioMedical Research, East Hanover, NJ*
- Small Molecules: Qualitative Analysis, 524 - 535**
- TP 524 **Isomer Differentiation of Explosives-related Compounds and Clarification of the 30 Da Releases from TNT using Electrospray High-Resolution Multistage Mass Spectrometry;** Adrián Schwarzenberg<sup>1</sup>; Richard B. Cole<sup>1</sup>; Héloïse Dossmann<sup>1</sup>; Xavier Machuron-Mandard<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>*Université Pierre et Marie Curie, IPCM/CSOB, Paris, France*; <sup>2</sup>*CEA, DAM, DIF, F-91297, Arpajon, France*
- TP 525 **Understanding of Fundamental Ion Behavior Leads to Routine Substructure Identification: A Mechanistic Study on Precursor Ions;** Michal Raab; Robert Mistrik; *HighChem, Bratislava, Slovakia*
- TP 526 **Autonomous Orbitrap Platform for Acquisition of MS<sup>n</sup> Spectral Trees Based on intelligent, Real Time Decision Making Logic;** Robert Mistrik<sup>1</sup>; Jakub Mezey<sup>1</sup>; Juraj Lütisan<sup>1</sup>; Tim Stratton<sup>2</sup>; Lukas Najdekr<sup>2,3</sup>; <sup>1</sup>*HighChem, Bratislava, Slovakia*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*IMTM, Palacky University, Olomouc, Czech Republic*
- TP 527 **Parylene-Matrix Target Chip for Small Molecule Analysis using MALDI-TOF Mass Spectrometry;** Jo-Il Kim; Jong-Min Park; Jae-Chul Pyun; *Yonsei University, Seoul, South Korea*
- TP 528 **"nMS<sup>2</sup>" Approach Aids Characterization of Impurities at Sub-ppm Levels – Capecitabine, an Anti-Cancer Drug;** Janani Thyagarajan; Saravanan Subramanian; Rampriya Uthayakumar; Raman Palvannanathan; Govindarajan Chandramohan; Mohan Kasi; Venkat Manohar; *IICMS, Chennai, India*
- TP 529 **Tandem Mass Spectrometry Characterizes the Related Substances of Second Generation FLT3 Inhibitor Quizartinib, Anti-Cancer Compound for Myeloid Leukemia;** Saravanan Subramanian<sup>1</sup>; Arvind Thyagarajan<sup>1</sup>; Rampriya Uthayakumar<sup>1</sup>; Raman Palvannanathan<sup>1</sup>; Govindarajan Chandramohan<sup>1</sup>; Mohan Kasi<sup>1</sup>; Venkat Manohar<sup>1</sup>; Thaminum Ansari Abubacker<sup>2</sup>; <sup>1</sup>*IICMS, Chennai, INDIA*; <sup>2</sup>*Muthurangam Govt. Arts. College,, Vellore, Tamil Nadu,, India*
- TP 530 **Rapid Screening of Adulterated & Counterfeit Products using Bench-Top High Resolution Mass Spectrometer and mzCloud Database Search;** Philippe Lebel<sup>1</sup>; Alexandra Furtos<sup>1</sup>; Karen Waldron<sup>1</sup>; Kate Comstock<sup>2</sup>; Tim Stratton<sup>2</sup>; Maroun El Khoury<sup>2</sup>; <sup>1</sup>*Université de Montréal, Montréal, Qc, Canada*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 531 **Automated Off-Line SPE LC-MS/MS Method Development using Instrumentation with On-Line SPE Functionality;** Roy (TY) Huang; Mike Hastings; Lisa Buchholz; Mingming Ma; *Dow AgroSciences, Indianapolis, IN*
- TP 532 **Degradation Products Analysis of Pantoprazole using High Resolution Mass Spectrometry;** Anoop Kumar<sup>1</sup>; Manoj Pillai<sup>1</sup>; Devkant Shandilya<sup>2</sup>; <sup>1</sup>*AB SCIEX, DHR Holdings India, Gurgaon, India*; <sup>2</sup>*Bhagwant University, Ajmer, India*
- TP 533 **Mass Spectrometry based Combinational Strategy for in vitro and in vivo Metabolite Identification and Confirmation;** Zheng-Xiang Zhang; Tao Bo; *Agilent Technologies (China), Beijing, CHINA*
- TP 534 **Analysis of Additional Impurities in Riboflavin (Vitamin B2) Using a Proposed Alternative USP Method Utilizing LC-MS;** Carmen T. Santasania<sup>1</sup>; Nicolas J. Hauser<sup>2</sup>; <sup>1</sup>*Supelco/Sigma-Aldrich, Bellefonte, PA*; <sup>2</sup>*RTC/Sigma-Aldrich, Laramie, WY*
- TP 535 **Identification of Catechol-Group-Contained Compounds by Chloride Anion Approach using APCI/QTOF Mass Spectrometry;** Emily Lichtenberger; Yufei Chen; Mln Li; Nelson Vinuesa; *NC State University, Raleigh, NC*
- H/D Exchange; Hardware, Software, and Methodology, 536 - 547**
- TP 536 **Small-Molecule Spiking for Deuterium Content Reporting in HDX;** Joey Sheff; David Schriemer; *University of Calgary, Calgary, Canada*
- TP 537 **Enzymatic Characterization of Recombinant Nepenthesin II, as a New Tool for Hydrogen/Deuterium Exchange Mass Spectrometry;** Menglin Yang; Martial Rey; David C. Schriemer; *University of Calgary, Calgary, Canada*
- TP 538 **SWATH-based HX-MS<sup>2</sup> to Investigate Protein Stability of Mitotic Centromere-Associated Kinesin (MCAK) on the Microtubule Lattice;** Kyle Burns; David Schriemer; *University of Calgary, Calgary, Canada*
- TP 539 **Significance of Measured Differences in Comparison Hydrogen Exchange Mass Spectrometry Experiments;** Rane Harrison<sup>1</sup>; Damian Houde<sup>2</sup>; John Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Biogen Idec, Inc., Cambridge, MA*
- TP 540 **Combining Ion Mobility Spectrometry with Hydrogen-Deuterium Exchange and Top-Down MS/MS Structure Determination;** Mahdiar Khakinejad; Hossein Maleki; James Arndt; Greg Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- TP 541 **Probing Site-Specific Interactions between Epidermal Growth Factor Receptor and an Adnectin using HDX-ETD MS Approach;** Jing Fang<sup>1</sup>; Stephane Houel<sup>1</sup>; Ying-Qing Yu<sup>1</sup>; Hui Wei<sup>2</sup>; Jingjie Mo<sup>2</sup>; Daniel Cohen<sup>2</sup>; Dianlin Xie<sup>2</sup>; Zheng Lin<sup>2</sup>; Paul Morin<sup>2</sup>; Michael Doyle<sup>2</sup>; Adrienne Tymiak<sup>2</sup>; Weibin Chen<sup>1</sup>; Guodong Chen<sup>2</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Bristol-Myers Squibb Company, Princeton, NJ*
- TP 542 **Deuteration Effects on the Intrinsic Photophysical Properties of Oxazine Dyes;** Matthew Kusinski; *University of Toronto, Toronto, Canada*
- TP 543 **A two-Site Evaluation of the Repeatability and Precision of an Automated HDX MS Platform;** Alfonso Espada<sup>2</sup>; David Cummins<sup>1</sup>; Scott Novick<sup>3</sup>; Manuel Molina-Martín<sup>2</sup>; Devrishi Goswami<sup>3</sup>; Bruce Pascal<sup>3</sup>; Ryan Stites<sup>1</sup>; Howard Broughton<sup>2</sup>; Michael Chalmers<sup>1</sup>; Patrick Griffin<sup>3</sup>; Jeffrey Dodge<sup>1</sup>; Juan Espinosa<sup>2</sup>; <sup>1</sup>*Eli Lilly and Company, Indianapolis, IN*; <sup>2</sup>*Lilly S.A., Alcobendas, Spain*; <sup>3</sup>*The Scripps Research Institute, Jupiter, FL*

- TP 544 **Subzero Temperature Chromatography Combined with Electron Capture Dissociation for Top-Down Protein Hydrogen Exchange Measurements;** Jingxi Pan<sup>1</sup>; Suping Zhang<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- TP 545 **Purified Protease Type XIII for Enhanced Sequence Coverage in Hydrogen Deuterium Exchange Mass Spectrometry;** Gary Wei; Chengjie Ji; NovaBioAssays, Woburn, MA
- TP 546 **QUDeX-MS: Hydrogen/Deuterium Exchange Calculation for Mass Spectra with Resolved Isotopic Fine Structure;** Joseph Salisbury; Qian Liu; Jeffrey Agar; Northeastern University, Boston, MA
- TP 547 **A Novel Approach to Quantitation of Hydrogen Deuterium Exchanged Peptides to Reveal a Distribution of the Exchange at Various Levels;** Yongdong Wang; Ming Gu; Hongliang (Leo) Xu; Cerno Bioscience, Norwalk, CT
- Environmental Analysis: Pharmaceuticals and Pesticides, 549 - 583**
- TP 549 **Newly Identified Halogenated Organic Compounds in Technical Pesticide Mixtures and Their Occurrence in Southern California Pacific Dolphins;** Susan A. Mackintosh<sup>1</sup>; Eunha Hoh<sup>1</sup>; Nellie J. Shaul<sup>2</sup>; Lihini Aluwihare<sup>2</sup>; Nathan Dodder<sup>3</sup>; <sup>1</sup>San Diego State University, San Diego, CA; <sup>2</sup>Scripps Institution of Oceanography, La Jolla, CA; <sup>3</sup>SCCWRP, Costa Mesa, CA
- TP 550 **Quantitative Determination of Antidepressants and Transformation Products by LC ESI-MS/MS in Terrestrial Environments that Receive Biosolids;** Melissa M. Schultz; Maria Dawaher; Maura Hall; Lydia Niemi; The College of Wooster, Wooster, OH
- TP 551 **High Resolution Mass Spectrometry Detection and Identification of Pharmaceutical Transformation Products and Metabolites in Hospital Effluents and Wastewater;** Damià Barceló<sup>1,2</sup>; Bozo Zonja<sup>1</sup>; Noelia Negreira<sup>1</sup>; Laura Ferrando - Climent<sup>2</sup>; Meritxell Gros<sup>2</sup>; Tina Kosjek<sup>3</sup>; Sandra Pérez<sup>1</sup>; Sara Rodriguez-Mozaz<sup>2</sup>; Ester Heath<sup>3,4</sup>; Miren Lopez de Alda<sup>1</sup>; <sup>1</sup>Water and Soil Quality Research Group, IDAEA-CSIC, Barcelona, SPAIN; <sup>2</sup>Catalan Institute for Water Research (ICRA), Girona, Spain; <sup>3</sup>Jozef Stefan Institute, Ljubljana, Slovenia; <sup>4</sup>Jozef Stefan International Postgraduate School, Ljubljana, Slovenia
- TP 552 **Determination of Emerging Contaminants in Iowa Surface Water at Low PPT Levels Using Direct Injection and SPE LCMSMS;** John Vargo<sup>1</sup>; Michael Schueller<sup>1</sup>; Mary Skopec<sup>2</sup>; <sup>1</sup>State Hygienic Laboratory - University of Iowa, Coralville, IA; <sup>2</sup>Iowa Geological & Water Survey, Iowa City, IA
- TP 553 **Analysis of Trace Organic Pollutants in Wastewater to Assess Biodegradation using Wrong-way-round Ionization in Liquid Chromatography Tandem Mass Spectrometry;** Lijuan Su<sup>1</sup>; Wendell Khunjar<sup>2</sup>; Diana Aga<sup>1</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Hazen and Sawyer P.C., Fairfax, VA
- TP 554 **Analysis of Veterinary Antimicrobials in Stockpiled Feedlot Manure using LC-ESI/MS/MS;** Srinivas Sura<sup>1,2</sup>; Dani Degenhardt<sup>3</sup>; Kerry M. Peru<sup>1</sup>; Jonathan Bailey<sup>1</sup>; Allan Cessna<sup>1,2</sup>; Francis Larney<sup>4</sup>; Tim McAllister<sup>4</sup>; Dena McMartin<sup>5</sup>; John Headley<sup>1</sup>; <sup>1</sup>Environment Canada, Saskatoon, CANADA; <sup>2</sup>Agriculture and Agri-Food Canada, Saskatoon, Canada; <sup>3</sup>Alberta Innovates Technology Futures, Edmonton, Canada; <sup>4</sup>Agriculture and Agri-Food Canada, Lethbridge, Canada; <sup>5</sup>University of Regina, Regina, Canada
- TP 555 **Investigation of the UV degradation of Diclofenac by means of liquid chromatography and mass spectrometry;** Jörg Roscher; Uwe Karst; Münster, Germany
- TP 556 **Rapid and Selective MS/MS Method for Quantification of Light Sensitive Chlortetracycline Drug in Wastewater and Sludge using LTD Ion Source;** Rama Pulicharla<sup>1</sup>; Serge Auger<sup>2</sup>; Satinder Kaur Brar<sup>1</sup>; Patrick Drogui<sup>1</sup>; Rao Y. Surampalli<sup>3</sup>; <sup>1</sup>INRS-ETE, Université du Québec, Québec, Canada; <sup>2</sup>Phytronix Technologies, Quebec, CANADA; <sup>3</sup>US Environmental Protection Agency, Kansas City, KS
- TP 557 **Identification and Quantitation of Pyrethroids using a GC/QTOF in Negative Chemical Ionization Mode;** Ron Honnold<sup>1</sup>; Rafael Acosta<sup>2</sup>; Matthew Curtis<sup>3</sup>; <sup>1</sup>Agilent Technologies, Riverside, CA; <sup>2</sup>Agilent Technologies, Mexico City, Mexico; <sup>3</sup>Agilent Technologies, San Jose, CA
- TP 558 **Sorption Capacities and Interactions of a Mixture of Chemically Diverse Pesticides on Soil using LC-MS/MS;** Heather A. Gamble<sup>1</sup>; Donald S. Gamble<sup>2</sup>; Sha Joshua Ye<sup>1</sup>; Ellie Majidi<sup>1</sup>; <sup>1</sup>IONICS Mass Spectrometry Group, Inc., Bolton, Canada; <sup>2</sup>Department of Chemistry, St. Mary's University, Halifax, Nova Scotia
- TP 560 **Multi-Residue Analysis of Pyrethroids in Soil and Sediment using QuEChERS by LC/MS/MS;** Yuka Fujito<sup>1</sup>; Kiyomi Arakawa<sup>2</sup>; Yoshihiro Hayakawa<sup>2</sup>; <sup>1</sup>Shimadzu Techno Research, Inc., Kyoto, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- TP 561 **Measurement of Multi-Class Herbicides in Dried Environmental Matrices by Paper Spray Ionization Mass Spectrometry;** Steven L. Reeber; Sneha Gadi; Gary L. Glish; University of North Carolina, Chapel Hill, NC
- TP 562 **Application of LC-MS/MS for Monitoring Multiclass Pollutants in Surface and Groundwater;** Zhen Liu<sup>1</sup>; Qinghe Wang<sup>2</sup>; Keyu Zhou<sup>2</sup>; KeFei Wang<sup>2</sup>; <sup>1</sup>Southwest Jiaotong University, Chengdu, China; <sup>2</sup>Bruker Daltonics, Shanghai, China
- TP 563 **Analysis of Pesticides in Foodstuffs by Gas Chromatography Mass Spectrometry: Evaluation of Various Extraction Procedures;** Mohamed S. Muthanna<sup>1</sup>; Esraa Y. Abbas<sup>1</sup>; Siham S. Hersi<sup>1</sup>; Noor M. Bader<sup>1</sup>; Omar Y. Aljarod<sup>1</sup>; Abdullah A. Abdulbaker<sup>1</sup>; Mohammed F Rakib<sup>1</sup>; Shifa M Shaikh<sup>1</sup>; Ahmed A. Ramadan<sup>1</sup>; Basem Shomar<sup>2</sup>; Khalid A. Al-Saad<sup>1</sup>; <sup>1</sup>Qatar University, Doha, Qatar; <sup>2</sup>Qatar Environment and Energy Research Institute, Doha, Qatar
- TP 564 **Evaluation of EN15662:2008 - Determination of Pesticide Residue in Food of Plant Origin, by an Automated QuEChERS Solution;** Tyler Trent<sup>1</sup>; James Barlow<sup>2</sup>; Simon Hird<sup>2</sup>; Sadat Nawaz<sup>2</sup>; Tom Hartlein<sup>1</sup>; <sup>1</sup>Teledyne Tekmar, Mason, Ohio; <sup>2</sup>The Food and Environment Research Agency, York, UK
- TP 565 **Rapid Identification of Environmental Contaminants using High Resolution LC/MS/MS in Combination with Library Search;** Michael P. Schluesener<sup>1</sup>; Jianru Stahl-Zeng<sup>2</sup>; Thomas A. Ternes<sup>1</sup>; Detlev Schleuder<sup>2</sup>; <sup>1</sup>Federal Institute of Hydrology, Department Aquatic, Koblenz, Germany; <sup>2</sup>AB Sciex, Darmstadt, Germany
- TP 566 **Chiral Separation of Three  $\beta$ -blocking Pharmaceuticals and a Major Metabolite using SFC-MS;** Alfred Svan<sup>1</sup>; Mikael Hedeland<sup>2</sup>; Torbjörn Arvidsson<sup>1</sup>; Curt Pettersson<sup>1</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>Nat'l Veterinary Institute, Uppsala, Sweden
- TP 567 **Multiple Elemental Compound Identification by GCxGC-ICP-MS;** Kevin Huncik; National Institute of Standards and Technology, Charleston, SC
- TP 568 **An Enhanced Method for Extraction and Quantification of Highly Lipophilic Pyrethroid Pesticides from Adipose Tissue;** Holly C. Young; Darren R. Gullick; Andrew Popovici;



- James V. Bruckner; Brian S. Cummings; Michael G. Bartlett; *University of Georgia, Athens, GA*
- TP 569 **Unusual Fragmentation of N-Perfluoroacetyl(cycloalkyl)amines; Kirill V. Tretyakov;** Nino G. Todua; Anzor I. Mikaia; *National Institute of Standards and Technology, Gaithersburg, MD*
- TP 570 **Detection of Herbicidal Glyphosate from Environmental Matrices using Matrix-Assisted Inlet Ionization Mass Spectrometry (MAIL-MS); Julie Mercadante;** Sarah Saylor; Catherine Bentzley; *University of the Sciences, Philadelphia, PA*
- TP 571 **Automated Detection of Trace Level Basic and Acidic Pesticides and Herbicides in Drinking Water by Online SPE LC/MS; Edgar Naegele<sup>2</sup>;** Dorothy Yang<sup>1</sup>; <sup>1</sup> Santa Clara, CA; <sup>2</sup>Agilent Technologies, Waldbronn, N/A
- TP 572 **Accurate LCMS Spectral Assignments and Quantification: Methodology and Tools for Pesticides Analyses; Tukiet T. Lam<sup>1</sup>;** Ming Gu<sup>2</sup>; Jean Kanyo<sup>1</sup>; Yongdong Wang<sup>3</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Cerno Bioscience, Yardley, PA; <sup>3</sup>Cerno Bioscience, Norwalk, CT
- TP 573 **Glyphosate and AMPA Analysis in Drinking Water Using Two-Dimensional Liquid Chromatography Mass Spectrometry (2D LC/MS/MS);** Claude Mallet; *Waters Corporation, Milford, MA*
- TP 574 **Quantitative Performance of the Q-Exactive High-Resolution Accurate-Mass (HR/AM) Spectrometer for the Analysis of Tetracyclines in a Complex Environmental Matrix; Morgan Sollicie;** Audrey Roy-Lachapelle; *Université de Montréal, Montréal, Canada*
- TP 575 **Oxidative Removal of Selected PPCPs and Identification of Oxidative Degradates of PPCPs in Drinking Water Using LC-MS/MS; Yinfa Ma<sup>1</sup>;** Ruipu Mu<sup>1</sup>; Honglan Shi<sup>1</sup>; Craig Adams<sup>2</sup>; Todd Eichholz<sup>3</sup>; <sup>1</sup>Missouri S&T, Rolla, MO; <sup>2</sup>Utah State University, Logan, UT; <sup>3</sup>Missouri Department of Natural Resources, Jefferson City, MO
- TP 576 **Pre-concentration, Separation and high-Resolution Tandem Mass Spectrometry Identification of Intermediate Products of Sulfamethazine Antibiotic Formed by Photochemical Degradation in Water;** Tanare Ferreira; Júlia Martins; Amanda Imamura; Leonardo Medinilha; Fernando Lanças; Alvaro Santos-Neto; *University of São Paulo, São Carlos, Brazil*
- TP 577 **High Resolution Mass Spectrometry Based Metabolomics: a New Tool to Detect and Characterize Emerging Pollutants in Water and Food Matrices; Jerome Cotton<sup>1,2</sup>;** Fanny Leroux<sup>2</sup>; Simon Broudin<sup>2</sup>; Bruno Corman<sup>2</sup>; Jean-Claude Tabet<sup>3</sup>; Celine Ducruix<sup>2</sup>; Christophe Junot<sup>1</sup>; <sup>1</sup>CEA, iBiTec-S/SPI/LEMM, Gif-Sur-Yvette, FRANCE; <sup>2</sup>Profilomic, Boulogne-Billancourt, France; <sup>3</sup>UPMC - LCSOB, Paris, France
- TP 578 **Quantitative and Semi-Quantitative Determination of PPCPs and By-products in Wastewater Treatment Plants Samples Using UHPLC-Orbitrap MS and Data Mining Technologies; Paul Yang<sup>3</sup>;** Tung-Vi Nguyen<sup>1</sup>; Ramin Farnood<sup>1</sup>; Dipankar Ghosh<sup>4</sup>; Jonathan Beck<sup>4</sup>; Maciej Bromirski<sup>2</sup>; Charles Yang<sup>4</sup>; <sup>1</sup>University of Toronto, Toronto, Canada; <sup>2</sup>Thermo Fisher Scientific GmbH, Bremen, N/A; <sup>3</sup>Ontario Ministry of the Environment, Etobicoke, Canada; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA
- TP 579 **EPA Draft Method 543 Quantitation of Organic Pesticides in Drinking Water Using Online Pre-concentration/Solid Phase Extraction and Tandem Mass Spectrometry; Jonathan Beck;** Charles Yang; *Thermo Fisher Scientific, San Jose, CA*
- TP 580 **Semi Real Time Screening of PPCP and Pesticide by Field Type Water Sampler with Online SPE-HRAM; Jaewon Choi<sup>1</sup>;** Charles T. Yang<sup>2</sup>; Dipankar Ghosh<sup>2</sup>; <sup>1</sup>Kwater, Daejeon, South Korea; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- TP 581 **Systematic Elucidation of Matrix Effects in liquid Chromatography Hyphenated to Mass Spectrometry; Norbert Wenkel<sup>1</sup>;** Thorsten Teutenberg<sup>2</sup>; Jochen Tuerk<sup>2</sup>; Christoph Portner<sup>2</sup>; Claudia Vom Eyser<sup>2</sup>; Sandy-Dominic Freihoff<sup>2</sup>; <sup>1</sup>Axel Semrau GmbH, Sprockhovel, Germany; <sup>2</sup>Institut für Energie- und Umwelttechnik e.V., Duisburg, Germany
- TP 582 **Gain Productivity and Increase Data Quality with the GC/MS/MS Pesticide Analyzer; Jessica Westland;** Bruce Quimby; Kai Meng; *Agilent Technologies, Wilmington, Delaware*
- TP 583 **Fast and Highly Sensitive Analysis of Multiple Drugs in Ground-, Surface- and Wastewater; Klaus Bollig<sup>1</sup>;** Sven Vedder<sup>2</sup>; Anja Grüning<sup>2</sup>; <sup>1</sup>Shimadzu Deutschland GmbH, Duisburg, Germany; <sup>2</sup>Shimadzu Europe GmbH, Duisburg, Germany
- Energy: Hydrocarbon and Petrochemical, 584 - 610**
- TP 584 **Crude Oil Transformation during Rock Migration via FTICR-MS: From Source Rock to Reservoir; Marcos Pudenzi<sup>1</sup>;** Eduardo Schmidt<sup>1</sup>; Jose Jara<sup>1</sup>; Heliara Nascimento<sup>1</sup>; Elias Tessaro<sup>1</sup>; Vanessa Santos<sup>1</sup>; Pedro Henrique Vendramini<sup>1</sup>; Rosana Pereira<sup>2</sup>; Wagner Bastos<sup>2</sup>; Erica Morais<sup>2</sup>; Alessandro Batezelli<sup>1</sup>; Marcos Eberlin<sup>1</sup>; <sup>1</sup>UNICAMP, Campinas, BRASIL; <sup>2</sup>Petrobras, Rio de Janeiro, Brasil
- TP 585 **Structural Study of Asphaltenes by Laser Desorption Ionization Mass Spectrometry Coupled to Traveling Wave Ion Mobility; Hector Koolen;** Alexandre Gomes; Lyzette Moura; Francina Marcano; Felipe Cardoso; Paulo Rosa; Fabio Gozzo; *UNICAMP, Campinas, Brazil*
- TP 586 **Petroleomics by TWIM-MS: Print Screen of Additives used in Crude Oil Industry; Jandyson Machado Santos<sup>1</sup>;** Heliara D. L. Nascimento<sup>1</sup>; Elias Tessaro<sup>1</sup>; Vanessa Gonçalves Santos<sup>1</sup>; Marcos A. Pudenzi<sup>1</sup>; Eduardo M. Schmidt<sup>1</sup>; Renan de S. Galaverna<sup>1</sup>; Rosana C. L. Pereira<sup>2</sup>; Wagner L. Bastos<sup>2</sup>; Erica T. de Moraes<sup>2</sup>; Gleber Tacio Teixeira<sup>2</sup>; Maira Fasciotti<sup>3</sup>; Alberto Wisniewski Junior<sup>4</sup>; Marcos N. Eberlin<sup>1</sup>; <sup>1</sup>Institute of Chemistry - UNICAMP, Campinas, BRAZIL; <sup>2</sup>PETROBRAS, Rio de Janeiro, Brazil; <sup>3</sup>INMETRO, Rio de Janeiro, Brazil; <sup>4</sup>Chemistry Department - UFS, São Cristóvão, Brazil
- TP 587 **Study of Asphaltene Aggregation by MALDI-TOF-MS; Martha L. Chacón-Patiño<sup>1</sup>;** Andrea Gómez-Escudero<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Instituto Colombiano del Petróleo, Piedecuesta, Colombia
- TP 588 **Phenylenevinylene Derivatives as MALDI Matrices for Electron Transfer Ionization of Asphaltene Model Compounds; Laura J. Castellanos-García<sup>1</sup>;** Martha L. Chacón-Patiño<sup>1</sup>; Brian Castro<sup>2</sup>; Alexander Scherer<sup>3</sup>; Xiaoli Tan<sup>4</sup>; Rik R. Tykwinski<sup>3</sup>; Murray R. Gray<sup>4</sup>; César A. Sierra-Ávila<sup>2</sup>; Cristian Blanco-Tirado<sup>1</sup>; Marianny Y. Combariza<sup>1</sup>; <sup>1</sup>Escuela de Química, Univ Industrial de Santander, Bucaramanga, Colombia; <sup>2</sup>Departamento de Química, Univ Nacional de Colombia, Bogotá, Colombia; <sup>3</sup>University of Erlangen-Nürnberg, Erlangen, Germany; <sup>4</sup>Dept of Chem and Mat Eng, University of Alberta, Edmonton, Canada
- TP 589 **Elucidation of Structural Information for Asphaltenes via Collision-Activated Dissociation of Their Molecular Ions in MS<sup>n</sup> Experiments: A Model Compound Study;**

- TP 590 **Distillate Fraction Composition Estimation Using Crude Oil Petroleomics**; Fan Huang; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- TP 591 **Analysis of Pre-Separated Crude Oil Using an Orbitrap**; Matthew Hurt; Michael Cheng; Chevron, Richmond, CA
- TP 592 **Electrospray Ionization for Determination of Non-Polar Polyaromatic Hydrocarbons and Polyaromatic Heterocycles in Crude Oil Asphaltenes**; Lilla Molnár; Guricza; Wolfgang Schrader; Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany
- TP 593 **High-Resolution Online LC/MS for Characterizing Crude Oils – Grinding the Data**; Alessandro Vetere; Wolfgang Schrader; Max-Planck Inst für Kohlenforschung., Mülheim / Ruhr, Germany
- TP 594 **Evaluation of Polar Composition Changes in Diesel Fuels by FT-ICR MS after Stability Test**; Rosana C. L. Pereira<sup>1</sup>; Helineia O. Gomes<sup>1</sup>; Manoel J.R. Guimarães Neto<sup>1</sup>; Felipe C. Gouveia<sup>1</sup>; Boniek G. Vaz<sup>2</sup>; <sup>1</sup>Petrobras/CENPES, Rio de Janeiro, Brazil; <sup>2</sup>UFG, Goiânia, Brazil
- TP 595 **Dynamic Range Enhancement Stitching of Multiple Ultrahigh Resolution FT-ICR Mass Spectral Segments**; Logan C. Krajewski<sup>1</sup>; Yuri E. Corilo<sup>2,3</sup>; Ryan P. Rodgers<sup>2,3</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>FSU Department of Chemistry and Biochemistry, Tallahassee, FL; <sup>2</sup>Florida State University Future Fuels Institute, Tallahassee, FL; <sup>3</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL
- TP 596 **Targeted Ionization of Oxygen-Containing Compounds in Petroleum Crude Oil by Lithium Cationization Electrospray Ionization FT-ICR Mass Spectrometry**; Rebecca Beasley<sup>1</sup>; Vladislav Lobodin<sup>2,3</sup>; Alan Marshall<sup>1,3</sup>; Ryan Rodgers<sup>1,3</sup>; <sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Tallahassee, FL; <sup>3</sup>National High Magnetic Field Laboratory, Tallahassee, FL
- TP 597 **FT-ICR MS Imaging of Thin Layer Chromatograms of Crude Oil, Field Deposit, and Weathered Oil**; Donald F. Smith<sup>1,4</sup>; Amy M. McKenna<sup>1</sup>; Yuri E. Corilo<sup>1,2</sup>; Ryan P. Rodgers<sup>1,3</sup>; Alan G. Marshall<sup>1,3</sup>; Ron M.A. Heeren<sup>4</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Florida State University, Tallahassee, FL; <sup>3</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL; <sup>4</sup>FOM Institute AMOLF, Amsterdam, The Netherlands
- TP 598 **Modifications to a Novel Method for the Isolation of Interfacial Material from Athabasca Bitumen: Characterization by FT-ICR Mass Spectrometry**; Amy C. Clingenpeel<sup>1</sup>; Jacqueline M. Jarvis<sup>2</sup>; Winston K. Robbins<sup>3</sup>; Alan G. Marshall<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2</sup>; <sup>1</sup>Florida State University, Tallahassee, FL; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Future Fuels Institute, Tallahassee, FL
- TP 599 **Structural Investigation of Interfacially Active Compounds from Petroleum Crude Oil by FT-ICR Mass Spectrometry**; Jacqueline M. Jarvis<sup>1</sup>; Benjamin J. Bythell<sup>2</sup>; Chad R. Weisbrod<sup>1</sup>; Alan G. Marshall<sup>1,3</sup>; Ryan P. Rodgers<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>University of Missouri-St. Louis, St. Louis, MO; <sup>3</sup>Florida State University, Tallahassee, FL
- TP 600 **Characterization, Chromatographic Enrichment, and Trace Metal Analysis of Nickel and Vanadyl Porphyrins from Weathered Natural Seeps by FT-ICR and ICP-MS**; Jonathan Putman<sup>1</sup>; Amy M. McKenna<sup>1</sup>; Jeffrey T. Williams<sup>1</sup>; Ryan P. Rodgers<sup>1,2</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Department of Chemistry and Biochemistry, Tallahassee, FL
- TP 601 **Determination of Isomers in Petroleum by Ion Mobility Mass Spectrometry**; Priscila M. Lalli<sup>1</sup>; Steven M. Rowland<sup>1</sup>; Yuri E. Corilo<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University Future Fuels Institute, Tallahassee, FL; <sup>3</sup>Florida State University, Department of Chemistry, Tallahassee, FL
- TP 602 **Petroleomics: Progress Toward its Full Predictive Power via a Comprehensive Model of the Petroleum Continuum**; Yuri E. Corilo<sup>1,2</sup>; Priscila M. Lalli<sup>1</sup>; Ryan P. Rodgers<sup>1,3</sup>; Alan G. Marshall<sup>1,3</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Future Fuels Institute, Florida State University, Tallahassee, FL; <sup>3</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL
- TP 603 **High Performance Time-of-Flight Mass Spectrometry for Comprehensive Petroleum Analysis**; Clécio Klitzke; David Alonso; Joe Binkley; Jeffrey Patrick; LECO Corporation, St. Joseph, Michigan
- TP 604 **Identification of Organic Compounds in Crude Oils without Catalyst Treatment by Comprehensive Two-Dimensional GC/HRTOFMS**; Morio Ueda<sup>1</sup>; Koji Okuda<sup>2</sup>; Jun Onodera<sup>2</sup>; Akihiko Kusai<sup>2</sup>; Jonathon Bunn<sup>3</sup>; Yoshika Tennichi<sup>1</sup>; Hidehisa Kawamura<sup>1</sup>; Joo-il Park<sup>4</sup>; Seongho YOON<sup>4</sup>; Isao Mochida<sup>4</sup>; <sup>1</sup>Kyushu Environmental Evaluation Association, Fukuoka, Japan; <sup>2</sup>JEOL Ltd., Tokyo, Japan; <sup>3</sup>JEOL USA, Inc., MA; <sup>4</sup>Kyushu University, Fukuoka, Japan
- TP 605 **Genetic Link between Fatty Acids and Hydrocarbons produced During Artificial Maturation of a Type I Kerogen using ESI-FT-ICR-MS and GCxGC-MS**; Albert Kamga<sup>1</sup>; Françoise Behar<sup>2</sup>; Patrick G. Hatcher<sup>1</sup>; <sup>1</sup>ODU Research Foundation, Norfolk, VA; <sup>2</sup>TOTAL SA, Paris, France
- TP 606 **Pressurized Heating for the Rapid Preparation/ Extraction of Coal Samples for Broad Spectrum GC-MS Analysis**; Franco Basile<sup>1</sup>; Rajendra Mahat<sup>1</sup>; Wesley Rodgers<sup>2</sup>; <sup>1</sup>University of Wyoming, Laramie, WY; <sup>2</sup>JR Simplot Co, Boise, ID
- TP 607 **Ultra-Fast Profiling of C20-C60 Alkanes in Waxed Samples using LDTD-MS/MS**; Serge Auger; Gregory Blachon; Pierre Picard; Phytronix Technologies, Quebec, Canada
- TP 608 **Pulsed Flow Modulation GCxGC-MS with Cold EI**; Uri Keshet<sup>1</sup>; Tal Alon<sup>1,2</sup>; Alexander Fialkov<sup>1</sup>; Aviv Amirav<sup>1,2</sup>; <sup>1</sup>Tel-Aviv University, Tel-Aviv, ISRAEL; <sup>2</sup>Aviv Analytical LTD, Tel Aviv, Israel
- TP 609 **Correlation Studies between Chemical Properties of Crude Oils and Mass Spectrometric Analysis on the Molecular Level using LDI and APPI**; Matthias Witt; Gökhan Baykut; Bruker Daltonik GmbH, Bremen, Germany
- TP 610 **Molecular Level Analysis of TLC Fractions of Crude Oil by LDI FT-ICR Mass Spectrometry**; Matthias Witt<sup>1</sup>; Mike Easterling<sup>2</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics Inc., Billerica, MA
- TP 611 **Drug Metabolism: Qualitative Analysis, 611 - 636**
- TP 611 **Rapid Mass Spectrometric Detection of Drug Metabolites Generated in a Microfluidic Electrochemical Cell**; Lars Büter<sup>1</sup>; Floris T.G. van den Brink<sup>2</sup>; Mathieu Odijk<sup>2</sup>; Wouter Olthuis<sup>2</sup>; Albert van den Berg<sup>2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Münster, Münster, Germany; <sup>2</sup>University of Twente, Enschede, The Netherlands

- TP 612 **Simulation of Metabolic Processes of Polycyclic Aromatic Hydrocarbons using Electrochemistry/Mass Spectrometry;** Tina Wigger<sup>1,2</sup>; Lars Bütter<sup>1,2</sup>; Uwe Karst<sup>1</sup>; <sup>1</sup>University of Münster, Münster, Germany; <sup>2</sup>NRW Graduate School of Chemistry, Münster, Germany
- TP 613 **MsXelerator: A Software Platform for Drug Metabolite Detection and Identification using High-Resolution Mass Spectrometry and Post-Acquisition Data Mining;** Marco Ruijken; *MsMetrix, Maarssen, Netherlands*
- TP 614 **Application of LC-MS<sup>n</sup> and NMR Techniques in Identification of *In Vitro* Metabolites;** Regina V. Oliveira<sup>1</sup>; Josiane de O. Cardoso<sup>1</sup>; Bianca F. da Silva<sup>1</sup>; Tiago Venâncio<sup>1</sup>; Rosângela G. Peccinini<sup>2</sup>; Ivan R. Pitta<sup>3</sup>; Maria do Carmo A. de Lima<sup>3</sup>; <sup>1</sup>Chemistry Department, Federal University of São Carlos, São Carlos, SP, Brazil; <sup>2</sup>College of Pharmaceutical Sciences, State University of São Paulo, Araraquara, SP, Brazil; <sup>3</sup>Group of Research in Therapeutic Innovation, Federal University of Pernambuco, Recife, PE, Brazil
- TP 615 **Antitumor Steroidal Lactone Withaferin A in Human Breast Cancer Cells Is Covalently Bound to Cysteine-303 of  $\beta$ -Tubulin;** Guy Uechi; Marie Lue Antony; Eun-Ryeong Hahm; Shivendra Singh; Nathan Yates; *University of Pittsburgh, Pittsburgh, PA*
- TP 616 **Metabolite Profiling Using Human Hepatocyte Co-cultures and UHPLC-Q-TOF-MS with Data Independent MS/MS;** Ronghua Wang<sup>1</sup>; Ragu Ramanathan<sup>1</sup>; Cornelia Smith<sup>2</sup>; Caroline Lee<sup>2</sup>; Helen Shen<sup>1</sup>; Zamas Lam<sup>1</sup>; <sup>1</sup>QPS, LLC, Newark, DE; <sup>2</sup>QPS Hepatic Biosciences, Research Triangle Park, NC
- TP 618 **Characterisation of Metabolites by Utilising Collision Cross Section Measurements in Conjunction with an Integrated Microfluidic Device;** Richard T. Gallagher<sup>1</sup>; Christine Pattison<sup>1</sup>; Kathryn Pickup<sup>1</sup>; Kristin Samuelsson<sup>1</sup>; Mike McCullagh<sup>2</sup>; David S Douce<sup>2</sup>; <sup>1</sup>AstraZeneca, Macclesfield, UK; <sup>2</sup>Waters (MS Technologies), Manchester, UK
- TP 619 **Identification of the Microbial Fermentation Products for Curcumin using Metabolite ID Workflow Based on High Resolution Mass Spectrometry;** Dezhao Lu<sup>1</sup>; Xiaoyan Xu<sup>2</sup>; Ting Liu<sup>2</sup>; Kerong Zhang<sup>2</sup>; Huaifen Liu<sup>2</sup>; Xingde Wo<sup>1</sup>; <sup>1</sup>College of Life Science, Zhejiang Chinese Medical University, Hangzhou, Zhejiang Province, China; <sup>2</sup>AB SCIEX Asia Pacific Application Support Center, Shanghai, China
- TP 620 **Are Low Flow Mass Spectrometry Techniques Reliable Enough to be used for Metabolite Estimation from Human Samples without Standards?;** Jill L. Pirhalla; *GlaxoSmithKline, King Of Prussia, PA*
- TP 621 **Identification of Rilpivirine Metabolites in Human Liver Microsomes and Characterization of Cytochrome P450 Enzymes Involved in the Biotransformation by LC-MS/MS;** Josiane de Oliveira Cardoso<sup>1,2</sup>; Jessica Bo Li Lu<sup>1</sup>; Regina Vincenzi Oliveira<sup>2</sup>; Zeruesenay Desta<sup>1</sup>; <sup>1</sup>Division of Clinical Pharmacology, Indiana University School of Medicine, Indianapolis, IN; <sup>2</sup>Chemistry Department, Federal University of São Carlos, São Carlos, SP, Brazil
- TP 622 **Electrochemistry/MS – a Powerful Tool in Drug Metabolism;** Martin Eysberg; Agnieszka Kraj; Hendrik-Jan Brouwer; Nico Reinhoud; Jean-Pierre Chervet; *Antec (USA), Boston, MA*
- TP 623 **Development of an *in vitro* Platform for Peptide Therapeutic Metabolite Identification;** Joshua L. Johnson; Amin Kamel; *NIBR, Cambridge, MA*
- TP 624 **Investigation of d6-Bisphenol A Diconjugates in Humans Following Oral Administration of d6-BPA on a Cookie;** Mona I. Churchwell; Nathan C. Twaddle; Daniel R. Doerge; *NCTR/FDA, Jefferson, AR*
- TP 625 **Automated Soft-Spot Identification: Success Rate, Limitations, Code Logic and Functionality;** Veronica Zelesky<sup>1</sup>; Nathaniel Woody<sup>1</sup>; Carrie Funk<sup>1</sup>; Hao Sun<sup>1</sup>; John Janiszewski<sup>1</sup>; Christopher Keefer<sup>1</sup>; Ismael Zamora<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain
- TP 626 **Soft-Spot Identification for Drug Discovery: Utilizing Sciex AB 5600 Information Dependent Acquisition Scanning, MassMetasite Software and WebMetabase Browser;** Kerry Fillgrove<sup>1</sup>; Diane Grotz<sup>2</sup>; Somang Kim<sup>1</sup>; Ian Knemeyer<sup>3</sup>; Kevin Bateman<sup>1</sup>; <sup>1</sup>Merck Research Labs, West Point, PA; <sup>2</sup>Merck Research Labs, Kenilworth, NJ; <sup>3</sup>Merck Research Labs, Boston, MA
- TP 627 **Exploiting Variable Swath Techniques to Maximize the Quality of MS/MS Spectra for Metabolite Identification Studies;** Richard Schneider<sup>1</sup>; Veronica Zelesky<sup>2</sup>; Eva Duchoslav<sup>3</sup>; <sup>1</sup>Pfizer Global R&D, Groton, CT; <sup>2</sup>Pfizer Inc., Groton, CT; <sup>3</sup>AB Sciex, Concord, ON
- TP 628 **High Resolution Mass Spectrometric Investigation of the *in vivo* Metabolism of Selective Androgen Receptor Modulators (SARMs) in the Horse;** Mikael Hedeland<sup>4</sup>; Annelie Hansson<sup>1</sup>; Axel Rydevik<sup>1</sup>; Oliver Krug<sup>2</sup>; Mario Thevis<sup>2</sup>; Ulf Bondesson<sup>4</sup>; Heather Knych<sup>3</sup>; Scott Stanley<sup>3</sup>; <sup>1</sup>Uppsala University, Uppsala, Sweden; <sup>2</sup>German Sport University, Cologne, Germany; <sup>3</sup>University of California - Davis, Davis, CA; <sup>4</sup>National Veterinary Institute, Uppsala, Sweden
- TP 629 **Utilizing Ion Mobility Drift Times to Correlate and Track Metabolites across Changing Chromatographic Methods and Modes including SFC and UHPLC;** Hernando Olivos<sup>1</sup>; Adam Ladak<sup>1</sup>; Andrew Baker<sup>3</sup>; Steven Lai<sup>1</sup>; Yun Alelyunas<sup>2</sup>; Paul Rainville<sup>2</sup>; Mark Wrona<sup>2</sup>; <sup>1</sup>Waters, Beverly, MA; <sup>2</sup>Waters, Milford, MA; <sup>3</sup>Waters, Pleasanton, CA
- TP 630 **A Quantitative Determination of Methadone and its Metabolite (EDDP) in Dry Blood Spot by LC-MS/MS;** Hui Qiao; Joshua Sha Ye; Changtong Hao; *IONICS Mass Spectrometry Group Inc, Bolton, Canada*
- TP 631 **Studying Drug Metabolism by Isotope Labeling and High Resolution Tandem Mass Spectrometry;** Leanne Ohlund; Lekha Sleno; *UQAM, Montreal, Canada*
- TP 632 **Application of High Resolution Mass Spectrometry for Unmasking Hidden Genetic Toxicity Structural Alerts from Early Metabolism Studies;** Jackie X. Shang; Qing Chen; Bella Yao; Narciso Alvarez; Kaushik Mitra; *PPDM, Merck Research Lab, Kenilworth, NJ*
- TP 633 ***In vitro* Species Comparison using Long-term Hepatocyte Co-Culture Models and Highly Sensitive UHPLC-Q-TOF-MS with SWATH Analysis;** Jian Yu<sup>1</sup>; Ragu Ramanathan<sup>1</sup>; Cornelia Smith<sup>2</sup>; Caroline Lee<sup>2</sup>; Helen Shen<sup>1</sup>; Zamas Lam<sup>1</sup>; <sup>1</sup>QPS, LLC, Newark, DE; <sup>2</sup>QPS Hepatic Biosciences, Research Triangle Park, NC
- TP 634 **Metabolic Stability Assay Using Human Hepatocyte Co-cultures and Integrated Qualitative/Quantitative High Resolution Mass Spectrometry;** Alex Zang<sup>1</sup>; Ragu Ramanathan<sup>1</sup>; Cornelia Smith<sup>2</sup>; Caroline Lee<sup>2</sup>; Helen Shen<sup>1</sup>; Zamas Lam<sup>1</sup>; <sup>1</sup>QPS, LLC, Newark, DE; <sup>2</sup>QPS Hepatic Biosciences, Research Triangle Park, NC
- TP 635 **Metabolite Identification in Biological Matrices Utilizing High Resolution MS: Comparison of SynaptG2S using MSe and Orbitrap using DDS Methodology;** Amanda Culp; Vishal Shah; David Wagner; *GlaxoSmithKline, Rtp, NC*
- TP 636 **Degradation of B-lactam and Cephalosporin Antibiotics using Chlorine Dioxide and Identification of the Products by ESI and APPI LC/MS/MS;** Robert D. Voyksner<sup>1</sup>; Paul Lorcheim<sup>2</sup>; <sup>1</sup>LCMS Limited, Durham, NC; <sup>2</sup>ClorDiSys Solutions, Inc, Lebanon, NJ

## Metabolomics: Untargeted Metabolite Profiling, 637 - 666

- TP 637 **Mass Spectrometry Fingerprinting of Yeast Metabolome Cultivated under Environmental Stressful Conditions;** Mireia Farres; Benjamí Piña; Romà Tauler; *IDAEA-CSIC, Barcelona, Spain*
- TP 638 **Development of a Biological Internal Reference for Full Scan LC-MS Metabolomics Applied to the Cellular Stress Response;** Amy Caudy; Olga Zaslaver; Julia Hanchard; Christopher Go; Ying Zhang; Adam Rosebrock; *University of Toronto, Toronto, Canada*
- TP 639 **Untargeted Metabolomic Analysis for the Evaluation of Stress Effects on Model Organisms;** Joaquim Jaumot<sup>1</sup>; Meritxell Navarro<sup>1</sup>; Elena Ortiz<sup>1</sup>; Alejandro García-Reiriz<sup>1, 2</sup>; Marta Casado<sup>1</sup>; Benjamín Piña<sup>1</sup>; Romà Tauler<sup>1</sup>; *<sup>1</sup>IDAEA-CSIC, Barcelona, Spain; <sup>2</sup>IQUIR-CONICET, Rosario, Argentina*
- TP 640 **Single-cell Metabolomics and Proteomics by Capillary Electrophoresis ESI MS;** Peter Nemes<sup>1</sup>; Jordan T. Aerts<sup>2</sup>; Rosemary M. Onjiko<sup>1</sup>; Stanislav S. Rubakhin<sup>2</sup>; Jonathan V. Sweedler<sup>2</sup>; *<sup>1</sup>George Washington University, Washington, DC; <sup>2</sup>University of Illinois--Urbana-Champaign, Urbana, IL*
- TP 641 **Direct Tissue Spray Ionization of Living Plants by Mass Spectrometry for Metabolomics;** Dana M. Freund; Amanda C. Martin; Jerry D. Cohen; Adrian D. Hegeman; *University of Minnesota, St. Paul, Minnesota*
- TP 642 **Metabolomics Analysis of Soy Hydrolysate for the Identification of Productivity Markers of Mammalian Cells for Manufacturing Therapeutic Proteins;** Jason L. Richardson; Bhavana Shah; Michele Nicklaus; Pavel Bondarenko; Zhongqi Zhang; *Amgen, Inc., Thousand Oaks, CA*
- TP 643 **Metabolomics Profiling using Atmospheric Pressure Gas Chromatography-MS;** Vladimir Shulaev<sup>2</sup>; Ghaste Manoj<sup>2, 3</sup>; Steven Lai<sup>1</sup>; Carolina Salazar<sup>2</sup>; Nobuhiro Suzuki<sup>2</sup>; Janna Crossley<sup>2</sup>; Ron Mittler<sup>2</sup>; James Langridge<sup>1</sup>; Giuseppe Astarita<sup>1</sup>; Fulvio Mattivi<sup>3</sup>; *<sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>University of North Texas, Denton, TX; <sup>3</sup>Fondazione Edmund Mach, San Michele all'Adige, Italy*
- TP 644 **Differential Metabolomics of Cob Tissues from Maize Genotypes Resistant and Susceptible to Aflatoxin Accumulation;** Olga Pechanova; *MSU, Mississippi State, MS*
- TP 645 **Comparative Metabolomic Studies on Two Chinese Podophyllum Plants;** Xiaoming Jiang<sup>1</sup>; Mingquan Guo<sup>1, 2</sup>; *<sup>1</sup>Wuhan Botany Garden, Chinese Academy of Sciences, Wuhan, China; <sup>2</sup>University of Southern California, Alhambra, CA*
- TP 646 **Profiling of Specialized Metabolites that Accumulate in Trichomes of *Petunia* species;** Xiaoxiao Liu<sup>1</sup>; Cornelius S. Barry<sup>3</sup>; A. Daniel Jones<sup>1, 2</sup>; *<sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI; <sup>3</sup>Department of Horticulture, Michigan State University, East Lansing, MI*
- TP 647 **Comprehensive Untargeted Metabolite Profiling of Alangifolium Salvifolium Bark using LCMS and GCMS Techniques;** Siddaiah Chandranayak<sup>1</sup>; Harischandra Sripathi Prakash<sup>1</sup>; Syed Salman Lateef<sup>2</sup>; Saligrama Adavigowda Deepak<sup>2</sup>; *<sup>1</sup>Department of Studies in Applied Botany/Biotechnol, Mysore, Karnataka, India; <sup>2</sup>Agilent Technologies, Bangalore, INDIA*
- TP 648 **Analysis of Differentially Expressed Metabolites Induced by NPM-ALK in Anaplastic Lymphoma Kinase-Positive Anaplastic Large Cell Lymphoma;** Difei Sun; Kathleen Bone; Raymond Lai; Liang Li; *University of Alberta, Edmonton, Canada*
- TP 649 **Colorectal Cancer, Diet and Lipid Oxidation: towards Non-Targeted LC/HRMS Aldehydomics for Trapping and Analyzing Reactive Aldehydes in the Intestinal Lumen;** Sylvie Chevolleau<sup>1, 3</sup>; Isabelle Jouanin<sup>1, 3</sup>; Françoise Guéraud<sup>2, 3</sup>; Fabrice Pierre<sup>2, 3</sup>; Laurent Debrauwer<sup>1, 3</sup>; *<sup>1</sup>INRA UMR 1331 Toxalim - AXIOM Platform, Toulouse, France; <sup>2</sup>INRA UMR 1331 Toxalim - PPCA Team, Toulouse, France; <sup>3</sup>Toulouse University, INP, Toxalim, Toulouse, France*
- TP 650 **High Performance Isotope Labeling Liquid Chromatography Mass Spectrometry for Investigating the Effect of Drinking Goji Tea on Urine Metabolome Profiling;** Chiao-Li Tseng; Liang Li; *University of Alberta, Edmonton, Canada*
- TP 651 **GC/MS Metabolomics: Metabolic Mapping of the Mouse Gastrointestinal Tract;** Jan Crowley; Chia Hung; Kevin Yarasheski; Jeffrey Henderson; *Washington University, St Louis, MO*
- TP 652 **Assigning Adduct, Charge and Polymer States to High-Resolution Accurate-Mass Spectral Data using Frequency of Assignment in Multiple Difference Networks;** Thomas McClure; Matthew Kump; Michael Athanas; *Thermo Fisher Scientific, San Jose, CA*
- TP 653 **Bioprocess of Yeast Fermentation using IROA Protocol;** Chris Beecher<sup>1</sup>; Felice de Jong<sup>2</sup>; *<sup>1</sup>IROA Technologies, Ann Arbor, Michigan; <sup>2</sup>IROA Technologies LLC, Bolton, MA*
- TP 654 **A New GC Retention Database for Accurate, Reliable Calculation of Retention Times and Tolerance Windows under a Range of Conditions;** Baijie Peng; Mei-Yi Kuo; Josh Hewitt; Daniel Abate; Paul Boswell; *University of Minnesota, Minneapolis, MN*
- TP 655 **Rapid and Accurate Metabolite Identification using a High Resolution MS/MS Human Metabolite Spectral Library for Human Biofluid Metabolomics;** Zhendong Li<sup>1</sup>; Mingguo Xu<sup>1</sup>; Yiman Wu<sup>1</sup>; Chiao-Li Tseng<sup>1</sup>; Tao Huan<sup>1</sup>; Wei Han<sup>1</sup>; Jaspaul Tatlay<sup>1</sup>; Tran Tran<sup>1</sup>; Aiko Barsch<sup>2</sup>; Carsten Baessmann<sup>2</sup>; Liang Li<sup>1</sup>; *<sup>1</sup>UofA, Edmonton, Canada; <sup>2</sup>Bruker Daltonics, Bremen, Germany*
- TP 656 **Hemorrhagic Shock "fingerprint" Based on Global Metabolite Profiling of Porcine Urine Sample;** Monika Tokmina-Lukaszewska<sup>1</sup>; Navid Movahed<sup>1</sup>; Elizabeth Luszczyk<sup>2</sup>; Kristine Mulier<sup>2</sup>; Greg Beilman<sup>2</sup>; Brian Bothner<sup>1</sup>; *<sup>1</sup>Department of Chemistry & Biochemistry, Bozeman, MT; <sup>2</sup>Department of Surgery, University of Minnesota, Minneapolis, MN*
- TP 657 **A Systematic Approach to Untargeted Metabolomics Data Analysis: Comparison of Peak Picking Workflows;** Atefeh Rafiei; Lekha Sleno; *UQAM, Montreal, Canada*
- TP 658 **GCAnalyzer: An Untargeted GC/MS Metabolomics Platform for Quality Control, Accurate Deconvolution and Data Analysis;** Claartje Van Der Kroft; *MsMetrix, Maarsse, Netherlands*
- TP 659 **New Correlation Techniques in the Chemical Assignment and Biomarker Analysis of Metabolomics LC/MS Data;** Stephen L Coy<sup>1</sup>; John B. Tyburski<sup>2</sup>; Frank J. Gonzalez<sup>3</sup>; Albert J. Jr. Fornace<sup>2</sup>; *<sup>1</sup>Northeastern U., Boston, MA; <sup>2</sup>Georgetown U, Washington, DC; <sup>3</sup>National Cancer Institute, Bethesda, MD*
- TP 660 **Using Novel Metabolomics Approaches to Understand Microbial Carbon Cycling in Soil;** Tami Swenson<sup>1</sup>; Stefan Jenkins<sup>1</sup>; Benjamin Bowen<sup>1</sup>; Susan Spaulding<sup>2</sup>; David Burstein<sup>2</sup>; Brian Thomas<sup>2</sup>; Mary Power<sup>2</sup>; Blake Suttle<sup>3</sup>; Jill Banfield<sup>2</sup>; Trent Northen<sup>1</sup>; *<sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>University of California, Berkeley, CA; <sup>3</sup>Imperial College, London, UK*

- TP 661 **Complimentary LC- and GC-Mass Spectrometry Techniques Provide Broader Coverage of the Metabolome;** Baljit Ubhi<sup>1</sup>; Jeff Patrick<sup>2</sup>; Joe Shambaugh<sup>3</sup>; <sup>1</sup>AB SCIEX, Redwood City, CA; <sup>2</sup>Leco Corporation, St. Joseph, MI; <sup>3</sup>Genedata Inc, Lexington, MA
- TP 662 **Incorporating Multiple Chromatographic Methods and High Resolution Accurate Mass Mass Spectrometry into a High Throughput Metabolomics Platform;** Anne Evans<sup>1</sup>; Brandi Bridgewater<sup>1</sup>; Qiang Liu<sup>2</sup>; Matthew Mitchell<sup>1</sup>; Richard Robinson<sup>1</sup>; Hongping Dai<sup>1</sup>; Sandy Steward<sup>1</sup>; Corey DeHaven<sup>1</sup>; Luke Miller<sup>1</sup>; <sup>1</sup>Metabolon, Inc., Durham, NC; <sup>2</sup>Analytical Research Laboratories, Oklahoma City, OK
- TP 663 **Ultrafast Online SPE/MS Work-flow for High Throughput Global Profiling of Human Urine Metabolome;** Michelle Romm; Sumit Shah; *Agilent Technologies, Inc., Wakefield, MA*
- TP 664 **Untargeted Exhaled Breath Condensate Metabolomics by ESI, ESCI, and DART Ion Mobility-Time-of-Flight Mass Spectrometry;** José J. Pérez<sup>1</sup>; María Eugenia Monge<sup>1,2</sup>; Nael A. McCarty<sup>3</sup>; Facundo M. Fernández<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology, Atlanta, GA; <sup>2</sup>CIBION-CONICET, Ciudad de Buenos Aires, Argentina; <sup>3</sup>Emory University School of Medicine, Atlanta, GA
- TP 665 **Search for Chemical Signatures for Aggressive Corrosion in Produced Water Samples Obtained from Oil-Field Systems;** Vincent Bonifay; Whitney Smith; Christopher R. Marks; Eric Kaufman; Brian Harriman; Joseph M. Sufliita; Jan Sunner; *University of Oklahoma, Norman, OK*
- TP 666 **Metabolomics of Anaerobic Hydrocarbon Biodegradation by *Desulfoglaeba alkanexedens* and Its Association with Carbon Steel Biocorrosion;** Egemen Aydin; Vincent Bonifay; Renxing Liang; Jan Sunner; Joseph M. Sufliita; *University of Oklahoma, Norman, OK*
- Plant "omics", 667 - 680**
- TP 667 **Retention 'Projection' Enables Reliable Use of Shared HPLC Metabolite Retention Data Across Labs and Methods;** Daniel Abate-Pella<sup>1</sup>; Dana Freund<sup>1</sup>; Yan Ma<sup>2</sup>; Birgit Beck<sup>3</sup>; Emma Schymanski<sup>3</sup>; Tobias Kind<sup>2</sup>; Adrian Hegeman<sup>1</sup>; Paul Boswell<sup>1</sup>; <sup>1</sup>University of Minnesota, St. Paul, MN; <sup>2</sup>University of California, Davis, CA; <sup>3</sup>Eawag, Dübendorf, Switzerland
- TP 668 **MudPIT Analyses Reveal Auxin Mediated Proteases in Poplar during Storage Protein Remobilization;** Nazrul Islam<sup>1</sup>; Bret Cooper<sup>2</sup>; Wesley M Garrett<sup>2</sup>; Chioma Egekwu<sup>1</sup>; Angus Murphy<sup>1</sup>; Gary D Coleman<sup>1</sup>; <sup>1</sup>University of Maryland, College Park, MD; <sup>2</sup>USDA, Beltsville, MD
- TP 669 **A Protein Expression Atlas of *Medicago truncatula*;** Catherine Minogue; Alicia Richards; Dhileepkumar Jayaraman; Shanmugam Rajasekar; Junko Maeda; Michael Westphall; Michael Sussman; Jean-Michel Ané; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- TP 670 **Developing Highly Sensitive Phosphoproteomics for Signaling in Mature Plants;** Chuan-Chih Hsu<sup>1</sup>; Pengcheng Wang<sup>2</sup>; Liang Xue<sup>1</sup>; Jian-Kang Zhu<sup>2</sup>; Weiguo Andy Tao<sup>1</sup>; <sup>1</sup>Biochemistry, Purdue University, West Lafayette, IN; <sup>2</sup>Horticulture, Purdue University, West Lafayette, IN
- TP 671 **Atmospheric Pressure Photoionization Combined with a UV Femtosecond Laser for Plant Metabolite Imaging;** Katherine-Jo Galayda; Timothy Anderson; Patrick McVey; R.S. Houk; *Iowa State University, Ames, IA*
- TP 672 **The Steady State N-terminal Proteome of Chloroplasts; Determinants of Protein Maturation and Stability;** Elden Rowland<sup>1,2</sup>; Klaas van Wijk<sup>1,2</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Cornell University, Ithaca, NY
- TP 673 **Mass Spectrometry as a Tool for the Detection of Emerald Ash Borer Attack;** Naomi Stock<sup>1</sup>; Michael Doran<sup>1</sup>; Ron Bonner<sup>2</sup>; Raymond March<sup>1</sup>; <sup>1</sup>Trent University, Peterborough, Canada; <sup>2</sup>AB SCIEX, Concord, ON
- TP 674 **iTRAQ Analysis Reveals Mechanisms of Enantioselective of Imazethapyr on Root Growth in *Arabidopsis thaliana*;** Haifeng Qian<sup>1</sup>; Haiyan Ding<sup>1</sup>; Zhongyi Cheng<sup>2</sup>; Zhengwei Fu<sup>1</sup>; <sup>1</sup>Zhejiang University of Technology, Hangzhou, CN; <sup>2</sup>PTM Biolabs, Inc, Hangzhou, China
- TP 675 **Capturing the Dynamics of Crassulacean Acid Metabolism (CAM): Transcriptome and Proteome Analysis of Diel Cycle Gene Expression in *Agave americana*;** Paul Abraham; Hengfu Yin; Gerald Tuskan; Xiaohan Yang; Robert Hettich; *Oak Ridge National Laboratory, Oak Ridge, TN*
- TP 676 **Multi-OMICs Evaluation of Arogenate Dehydrates Knock-Out and Over Expression Mutants in *Arabidopsis thaliana*;** Kim K. Hixson<sup>1</sup>; Oliver Corea<sup>2</sup>; Alan Budgeon<sup>1</sup>; Sarah Brewer<sup>1</sup>; Karl Weitz<sup>3</sup>; Rosey Chu<sup>3</sup>; Matthew Monroe<sup>3</sup>; Ljiljana Pasa-Tolic<sup>3</sup>; Mary Lipton<sup>3</sup>; Laurence Davin<sup>1</sup>; Norman Lewis<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Sirman Fraser University, Vancouver, British Columbia, Canada; <sup>3</sup>Pacific Northwest National Laboratory, Richland, WA
- TP 677 **Proteomic Analysis of Wastewater Cultured *Chlamydomonas reinhardtii*: Comparing protein Expression for Enhanced Phycoremediation and Biomass Production;** Anil Patel; Eric Huang; Mark Lefsrud; *Bioresource Engineering, McGill University, Ste-Anne-de-Bellevue, Canada*
- TP 678 **Molecular and Genomic Mechanisms for Plant Defense Revealed by Improved Proteomics Method;** Yixiang Zhang<sup>2</sup>; Joshua Yuan<sup>2</sup>; Susie Dai<sup>1</sup>; <sup>1</sup>Office of the Texas State Chemist, Department of V, College Station, TX; <sup>2</sup>Department of Plant Pathology and Microbiology, College Station, TX
- TP 679 **Combination of Different Extraction, Separation and Mass-Spectrometric Approaches for Identification of Complex Mixtures of Volatile Compounds Emanated from Tropical Flowers;** Elena Stashenko; Silvia Cardenas; Corina Bernal; Jairo Rene Martinez; *Universidad Industrial de Santander, Bucaramanga, Colombia*
- TP 680 **Overcoming the Challenges in Proteome Analysis of *Populus tremuloides* using High-Throughput RNA Sequencing;** Landon Wilson<sup>1</sup>; Avinash Sreedasyam<sup>2</sup>; Geetika Trivedi<sup>2</sup>; Leland Cseke<sup>2</sup>; Helen Kim<sup>1</sup>; Stephen Barnes<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>University of Alabama-Huntsville, Huntsville, AL
- Approaches to Quantitation, 681 - 694**
- TP 681 **A LC/MS/CAD Method of Comparison of DMSO Stock Solution Concentrations after Storage under Various Conditions;** Yutao Jiang; Deven Wang; Baiwei Lin; Joe Pease; Michael Shieh; *Genentech, South San Francisco, CA*
- TP 682 **Separation and Quantitation of three surfactants in a formulation using LC/ESI/MS;** Teresa E. Peterson; *Kimberly-Clark, Roswell, GA*
- TP 683 **Intensity-based Label-Free Quantification of the Kinome across 64 colorectal Cancer Cell Lines;** Martin Frejno<sup>1</sup>; Susan Klaeger<sup>2</sup>; Mathias Wilhelm<sup>2</sup>; Guillaume Médard<sup>2</sup>; Bernhard Kuster<sup>2</sup>; Stephan Feller<sup>1</sup>; <sup>1</sup>Oxford University, Oxford, UK; <sup>2</sup>Technical University Munich, Freising, Germany
- TP 684 **Dwell Time, a Critical Factor on Precision in N-in-One Assays Utilizing UPLC-MS/MS;** Lan Li; Tracey Wilson; Yuan-Shek Chen; Luca Matassa; *QPS, LLC, Newark, DE*

- TP 685 **Quantitative analysis of sodium arsenite-induced kinome perturbation in human skin fibroblasts with ATP-affinity probes;** Lei Guo; Yongsheng Xiao; Yinsheng Wang; *University of California, Riverside, Riverside, CA*
- TP 686 **Cross-Species Quantification of Snake Venoms using iTRAQ;** Erika Velásquez<sup>1</sup>; Rafael D Melani<sup>1</sup>; Paulo Costa Carvalho<sup>2</sup>; Diogo B Lima<sup>2</sup>; Magno Junqueira<sup>1</sup>; Fabio CS Nogueira<sup>1</sup>; Gilberto Domont<sup>1</sup>; <sup>1</sup>Univ Federal Do Rio De Janeiro, Rio De Janeiro, Brazil; <sup>2</sup>Carlos Chagas Institute, Curitiba, Pr
- TP 687 **Improved Identification and Extended Quantitative Mass Range of Peptide Tagged TMT by Combined N-Terminal Enzyme and Triple-Stage Mass Spectrometry;** Ya-Ping Lin; Chein-Hung Chen; Jung-Lee Lin; Chung-Hsuan Chen; *Genomics Research Center, Academia sinica, Taipei, Taiwan*
- TP 688 **Application of Multistage Tandem Mass Spectrometry for Quantification of Endogenous Metabolites In Lung Tissue;** Keely Pierzchalski<sup>1</sup>; Jace W. Jones<sup>1</sup>; Catherine Booth<sup>2</sup>; Gregory Tudor<sup>2</sup>; Alexander Bennett<sup>3</sup>; Ann Farese<sup>3</sup>; Thomas MacVittie<sup>3</sup>; Pu-Ting Xu<sup>3</sup>; Isabel Jackson<sup>3</sup>; Zeljko Vujaskovic<sup>3</sup>; Maureen Kane<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Baltimore, MD; <sup>2</sup>Episteme Ltd, Manchester, UK; <sup>3</sup>University of Maryland, School of Medicine, Baltimore, MD
- TP 689 **Stable Isotope Labeled Internal Standards in Quantification of Biomolecules using LC MS/MS;** Meiyao Wang; Illarion Turko; *NIST, IBBR, Rockville, MD*
- TP 690 **Improved Uncertainty in the Analysis of PETN in APCI- LCMS Determinations using Ammonium Nitrate as an Ionization Additive;** William Maccrehan; *NIST, Gaithersburg, MD*
- TP 691 **Examination of Imported Children's Toys for the Presence of Toxic Elements using Digestion and Migration Testing Methods;** Patricia Atkins; *Spex Certiprep, Metuchen, NJ*
- TP 692 **Understanding Protein Expression Levels and Quantitation in Single Cell Analyses Using ICP-QQQ;** Jonathan Wanagat<sup>1</sup>; Amir Liba<sup>2</sup>; <sup>1</sup>UCLA, Dept. of Medicine, Los Angeles, CA; <sup>2</sup>Agilent Tech., Wilmington, DE
- TP 693 **Achieving Maximal Sensitivity Gain When Scaling a Protein Immunocapture Assay from Traditional to Low Micro-Flow LC-MS/MS;** Eugene F. Ciccimaro<sup>1</sup>; Bogdan Sleczyka<sup>1</sup>; John T. Mehl<sup>1</sup>; Lorell Disenza<sup>1</sup>; Asoka Ranasinghe<sup>1</sup>; Celia D'Arienzo<sup>1</sup>; Jim Murphy<sup>3</sup>; Brad Coopersmith<sup>2</sup>; Paul Rainville<sup>3</sup>; Catalin Doneanu<sup>3</sup>; Timothy Olah<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>2</sup>Waters, Richboro, PA; <sup>3</sup>Waters, Milford, MA
- TP 694 **Trypsin as the Ligase for N-terminal Labeling of Tryptic Peptides for Proteomics Analysis;** Mingliang Ye; Yanbo Pan; Hanfa Zou; *Dalian Institute of Chemical physics, CAS, Dalian, China*
- Instrumentation: New Concepts, 709 - 724**
- TP 709 **Development of a Liquid Phase Quadrupole Filter;** Yeon Jae Ko; Alessandra Ferzoco; *Rowland Institute at Harvard, Cambridge, MA*
- TP 710 **Ion Enhancement and MS/MS for Analysis of Organics in Complex Mars Analog Matrices with the MOMA Ion Trap Mass Spectrometer;** Ryan M. Danell<sup>1</sup>; Friso H.W. van Amerom<sup>2</sup>; Veronica Pinnick<sup>3</sup>; Xiang Li<sup>3</sup>; Stephanie Getty<sup>3</sup>; Ricardo Arevalo<sup>3</sup>; William Brinckerhoff<sup>3</sup>; Paul Mahaffy<sup>3</sup>; <sup>1</sup>Danell Consulting, Inc., Winterville, NC; <sup>2</sup>Mini-Mass Consulting, Inc., Hyattsville, MD; <sup>3</sup>NASA GSFC, Greenbelt, MD
- TP 711 **High Speed and Accurate Pressure Measurement with a micro Pirani Pressure Gauge for Pressures from 100 mTorr to sub 1mTorr.;** Adrian Southard<sup>1</sup>; Tomoko Adachi<sup>2</sup>; Ricardo Arevalo<sup>3</sup>; Gary Brown<sup>3</sup>; Christopher Johnson<sup>3</sup>; Zachary Gonnsen<sup>4</sup>; Stephen Meyer<sup>3</sup>; William Brinckerhoff<sup>3</sup>; Paul Mahaffy<sup>3</sup>; <sup>1</sup>University Space Research Agency, Greenbelt, Maryland; <sup>2</sup>Catholic University, Washington, DC; <sup>3</sup>NASA GSFC, Greenbelt, MD; <sup>4</sup>Microtell LLC, Greenbelt, MD - Maryland
- TP 712 **Micro Mass Analyzer for the Investigation of Cometary Bodies;** Ashish Chaudhary<sup>1</sup>; Tim Short<sup>1</sup>; Michelle Cardenas<sup>1</sup>; Emily Barrentine<sup>2</sup>; Danny Glavin<sup>2</sup>; Paul Mahaffy<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Yun Zheng<sup>2</sup>; Friso H.W. Van Amerom<sup>1</sup>; <sup>1</sup>SRI International, St. Petersburg, FL; <sup>2</sup>NASA GSFC, Greenbelt, MD
- TP 713 **A multi-stage Image-Charge Detector Made from Printed Circuit Boards;** Brandon L Barney; Daniel E Austin; *Brigham Young University, Provo, UT*
- TP 714 **Development of a Hybrid Ion Mobility Spectrometry/ Time-of-Flight Mass Spectrometer with Printed Circuit Board Technology;** Ian K. Webb; Tsung-Chi Chen; Xinyu Zhang; Sandilya V. B. Garimella; Randolph V. Norheim; Gordon A. Anderson; Yehia M. Ibrahim; Keqi Tang; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 715 **Improving Mass Spectrometric Sensitivity and Ionization Efficiency Using a nanoESI Emitter Array at Subambient Pressures;** Jonathan T. Cox; Ioan Marginean; Ryan Kelly; Richard D. Smith; Keqi Tang; *Pacific Northwest National Laboratory, Richland, WA*
- TP 716 **Simulation Driven Design and Development of Structures for Lossless Ion Manipulations;** Sandilya V.B. Garimella; Ian K. Webb; Yehia M. Ibrahim; Aleksey V. Tolmachev; Keqi Tang; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 717 **Fundamental Aspects of Ion Confinement in SLIM Devices;** Aleksey V. Tolmachev; Xinyu Zhang; Sandilya V.B. Garimella; Ian K. Webb; Yehia M. Ibrahim; Gordon A. Anderson; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- TP 718 **A Novel Linear Ion Trap Mass Analyzer built with Triangular Electrodes;** Chuan-fan Ding; Yu Xiao; *Fudan University, Shanghai, China*
- TP 719 **Accelerating 2D FT-ICR by non-Uniform Sampling and Maximum Entropy Reconstruction for Increased Resolution and/or Decreased Acquisition Time;** Fabrice Bray<sup>1</sup>; Lionel Chiron<sup>2</sup>; Marie-Aude Coutouly<sup>2</sup>; Caroline Tokarski<sup>1</sup>; Marc-André Delsuc<sup>3</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Univ. de Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France; <sup>2</sup>NMRTEC, Illkirch-Graffenstaden, France; <sup>3</sup>IGBMC, Illkirch-Graffenstaden, France
- TP 720 **Toward Determination of Ion Collision Cross Sections for Biomolecules within FT-ICR Cells;** Lu Mao<sup>1</sup>; Yu Chen<sup>1</sup>; Yu Chen<sup>2</sup>; Nathan K. Kaiser<sup>2</sup>; Alan G. Marshall<sup>2, 3</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology, Beijing, CHINA; <sup>2</sup>ICR Program, National High Magnetic Field Lab, Tallahassee, FL; <sup>3</sup>Department of Chemistry & Biochemistry, FSU, Tallahassee, FL
- TP 721 **Kinetic Study of Novel Precursors for the Hot-Wire Chemical Vapor Deposition;** Ismail Badran; Yujun Shi; *University of Calgary, Calgary, Canada*
- TP 722 **Novel Operating Modes of an Ion Mobility Quadrupole Time of Flight Hybrid Instrument;** Jason L Wildgoose; Kevin Giles; Steven Pringle; Keith Richardson; *Waters Corporation, Manchester, UK*

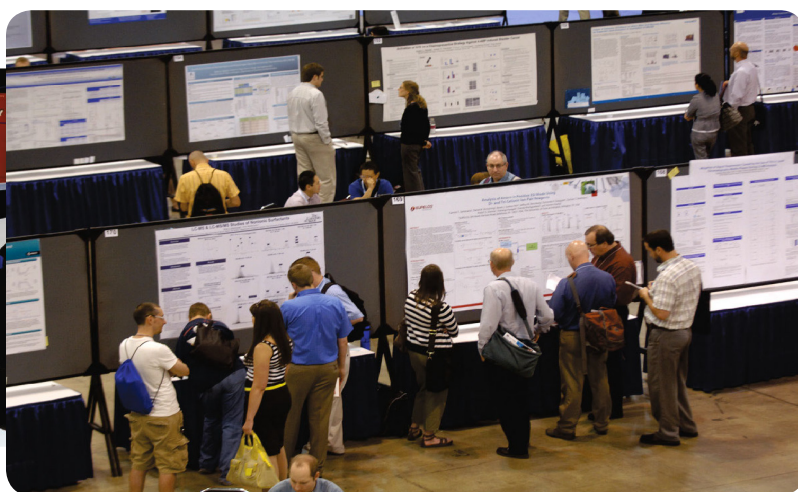
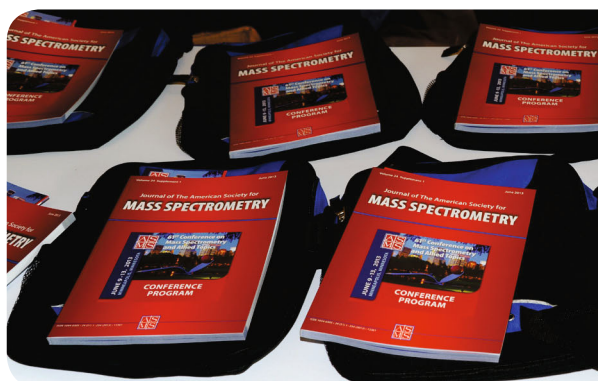
- TP 723 **Design and Utility of a Multi-Pass Cyclic Ion Mobility Separator;** [Kevin Giles](#); Jason L Wildgoose; Steven Pringle; John Garside; Peter Carney; Peter Nixon; David Langridge; *Waters Corporation, Wilmslow, UK*
- TP 724 **The Extraction of Maximum Information from Individual Ion Arrivals and Its Application to Extending the Dynamic Range of IMS-ooToF-MS Data;** [Martin Green](#); Garry Scott; Darrell Williams; Tony Gilbert; Keith Richardson; Martin Palmer; Nick Tomczyk; *Waters Corporation, Manchester, UK*
- Instrumentation: New Developments in Ionization and Sampling, 725 - 745**
- TP 725 **Alternating Current Corona Discharge APCI Ion Source for the Detection of Explosives;** [Dilshadbek Usmanov](#)<sup>1,2</sup>; Lee Chuin Chen<sup>1</sup>; Kenzo Hiraoka<sup>1</sup>; <sup>1</sup>*University of Yamanashi, Kofu, Japan*; <sup>2</sup>*Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*
- TP 726 **Analysis of Non-Volatile Samples by Flash Desorption/Mass Spectrometry;** [Kenzo Hiraoka](#)<sup>1</sup>; Dilshadbek Usmanov<sup>1,2</sup>; Satoshi Ninomiya<sup>1</sup>; <sup>1</sup>*University of Yamanashi, Kofu, Japan*; <sup>2</sup>*Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*
- TP 727 **Applications of Super-Atmospheric Pressure ESI in Superheated ESI-MS and Nano-ESI using Disposable Pipet Tip;** [Lee Chuin Chen](#); Md. Matiur Rahman; Kenzo Hiraoka; *University of Yamanashi, Kofu, Japan*
- TP 728 **Plasma Induced Secondary Ionization - Ion Mobility Spectrometry (PISI-IMS) for Real Time Drug Quality Assessment;** [Prabha Dwivedi](#)<sup>1</sup>; Paula Holmes<sup>2</sup>; Adam Kaylor<sup>1</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Photonis USA Inc., Sturbridge, MA*
- TP 729 **Microplasma Ion Source for Rapid Air/Water Volatile Organic Contaminant Analysis on board the International Space Station;** [Rosana M. Alberici](#)<sup>2</sup>; Joel D. Keelor<sup>1</sup>; Josh M. Symonds<sup>1</sup>; Thomas M. Orlando<sup>1</sup>; Ariel Macatangay<sup>3</sup>; Prabha Dwivedi<sup>1</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*ThermoFisher Mass Spectrometry Laboratory, UNICAMP, Campinas, Brazil*; <sup>3</sup>*NASA Johnson Space Center, Houston, TX*
- TP 730 **Liquid Chromatography Plasma-Spray Ionization-Mass spectrometry (LC-PLASI-MS): Overcoming ESI Limitations;** [Adam Kaylor](#)<sup>1</sup>; Prabha Dwivedi<sup>1</sup>; Guilong Cheng<sup>2</sup>; Jian Wang<sup>2</sup>; Shelly Li<sup>2</sup>; Jennifer L. Belsky<sup>3</sup>; Facundo M. Fernandez<sup>1</sup>; <sup>1</sup>*Georgia Institute of Technology, Atlanta, GA*; <sup>2</sup>*Pfizer Analytical R&D, Eastern Point Road, CT*; <sup>3</sup>*U.S. Pharmacopeial Convention, Rockville, MD*
- TP 731 **Validation of Computational Fluid dynamic Simulations (CFD) with Background Oriented Schlieren technique (BOS);** [Sebastian Klopotoski](#); Alexander Haack; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 732 **Investigation of Gas- and Ion-Dynamics in Heated Glass and Metal Inlet Capillaries: Work in progress ...;** [David Mueller](#); Yessica Brachthaeuser; Valerie Derpmann; Sebastian Klopotoski; Markus Langner; Christine Polaczek; Hendrik Kersten; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 733 **Fundamental Ion-Molecule Reaction Studies at Elevated Ion Temperatures and Analytical Application of an Ion Activation Stage ("ion tunnel");** [Sonja Klee](#); Albrecht Brockhaus; Marco Thinius; Walter Wissdorf; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 734 **Development of a Compact Multiple-Ionization-Stage TOF Mass Analyzer System for Trace Component Monitoring within Chemically Challenging Process Gas Matrices;** [Yessica Brachthaeuser](#); David Mueller; Hendrik Kersten; Klaus J. Brockmann; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 735 **Integrated Ion Trajectory Simulations in OpenFOAM, an Open Source Framework for Complex Numerical Simulations;** [Walter Wissdorf](#); Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 736 **An Efficient Ion Funnel Operated at 100 mbar Background Pressure;** [Sascha Albrecht](#)<sup>1</sup>; Jochen Barthel<sup>1</sup>; Armin Afchine<sup>1</sup>; Fred Stroh<sup>1</sup>; Thorsten Benter<sup>2</sup>; <sup>1</sup>*Forschungszentrum Jülich GmbH, Jülich, Germany*; <sup>2</sup>*University of Wuppertal, Wuppertal, Germany*
- TP 737 **Kinetic Measurements of Electronically Excited Noble Gas Species Radiating in the Far VUV;** [Ian Barnes](#); Sebastian Klopotoski; Kai Kroll; Hendrik Kersten; Thorsten Benter; *University of Wuppertal, Wuppertal, Germany*
- TP 738 **A Microfabricated Ionizer for High Pressure Mass Spectrometry;** [Craig Cavanaugh](#)<sup>1</sup>; Kenion Blakeman<sup>1</sup>; Tina Stacy<sup>1</sup>; Stanley Pau<sup>2</sup>; J Michael Ramsey<sup>1</sup>; <sup>1</sup>*University of North Carolina, Chapel Hill, NC*; <sup>2</sup>*University of Arizona, Tuscon, AZ*
- TP 739 **Coupling Electrospray Ionization with High Pressure Mass Spectrometry;** [William M. Gilliland, Jr.](#); J. Scott Mellors; J. Michael Ramsey; *UNC-Chapel Hill, Chapel Hill, NC*
- TP 740 **Evaluation of Monolithic Silicon-Chip-Based Multinozzle Emitter Arrays for Nano- and Micro-Electrospray Mass Spectrometry;** [Eloy R. Wouters](#)<sup>1</sup>; Pan Mao<sup>2</sup>; Jean-Jacques Dunyach<sup>1</sup>; Daojing Wang<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Newomics Inc., Emeryville, CA*
- TP 741 **Preparation and Reactions of Metal Cluster Ions;** [Soumabha Bag](#); Michael Wlekinski; R. Graham Cooks; *Purdue University, West Lafayette, Indiana*
- TP 742 **Characterization and Application of Nanoliter Sample Infusion Into a Miniaturized Liquid Bridge using a Capillary Gap Sampler;** [Volker Neu](#)<sup>1</sup>; Pablo Dörig<sup>1</sup>; Müller Stephan<sup>2</sup>; Christof Fattinger<sup>2</sup>; Renato Zenobi<sup>1</sup>; <sup>1</sup>*ETH Zurich, Zurich, Switzerland*; <sup>2</sup>*Hoffmann-La Roche AG, Basel, Switzerland*
- TP 743 **Slurry Flow Injection Analysis Coupled with Atmospheric Pressure Chemical Ionization Mass Spectrometry for Quantitative Real-Time Monitoring of Batch Slurry Reactions;** [Zhengqian Zhu](#)<sup>1</sup>; David S. Cho<sup>2</sup>; John E. Bartmess<sup>1</sup>; Mary Ellen McNally<sup>3</sup>; Ron M. Hoffman<sup>3</sup>; Kelsey D. Cook<sup>1</sup>; Ligu Song<sup>1</sup>; <sup>1</sup>*Department of Chemistry, University of Tennessee, Knoxville, TN*; <sup>2</sup>*Oak Ridge Institute for Science and Education, FBI, Quantico, VA*; <sup>3</sup>*Analytical Sciences, DuPont Crop Protection, Newark, DE*
- TP 744 **Detection of Explosives by using a Low Pressure Dielectric Barrier Discharge Ion Source;** [Masuyuki Sugiyama](#); Shun Kumano; Hideki Hasegawa; Kazuki Tanaka; Yuichiro Hashimoto; *Hitachi, Ltd., Tokyo, Japan*
- TP 745 **IR Laser Ablation with Plume Capture by a Continuous Flow Solvent Probe;** [Jeremy T. O'Brien](#)<sup>1,2</sup>; Evan R. Williams<sup>1,2</sup>; Hoi-Ying Holman<sup>1</sup>; <sup>1</sup>*Lawrence Berkeley National Laboratory, Berkeley, CA*; <sup>2</sup>*University of California, Berkeley, Berkeley, CA*
- GCMS: Instrumentation and Applications, 746 - 770**
- TP 746 **Smart Sampling Enables a Fully Automated Workflow for Liquid Injection and Headspace GC and GC/MS;** [Douglas Doster](#)<sup>1</sup>; Roger Pearson<sup>1</sup>; Tom Flug<sup>2</sup>; Guenter Boehm<sup>2</sup>; Brian Peat<sup>2</sup>; <sup>1</sup>*Aspen Research Corp, Maple Grove, MN*; <sup>2</sup>*CTC Analytics, Zwingen, Switzerland*

- TP 747 **A Microfluidic Derivatization Device for GC/MS in Chromatographic Column Chips;** Sanggoo Kim; Sungmin Lim; *Korea Basic Sci. Institute, Seoul, South Korea*
- TP 748 **Laser Ablation Sample Transfer Coupled to Gas Chromatography Mass Spectrometry;** Chinthaka A. Seneviratne; Suman Ghorai; Kermit K. Murray; *Louisiana State University, Baton Rouge, LA*
- TP 749 **Development of a Standard Gas Generating Vial for Performing Quality Control and Evaluation of Portable GC-MS Instrumentation with Solid-Phase Microextraction;** Jonathan Grandy; German Augusto Gómez-Ríos; Janusz Pawliszyn; *University of Waterloo: Pawliszyn Research Group, Waterloo, Canada*
- TP 750 **Improvements in Quantitative and Qualitative Metabolic Profiling using a Novel Atmospheric Pressure GC Source Coupled to High Resolution TOF-MS Analysis;** Christian Wachsmuth<sup>1</sup>; Katja Dettmer-Wilde<sup>1</sup>; Peter J. Oefner<sup>1</sup>; Christoph Gebhardt<sup>2</sup>; Verena Tellström<sup>2</sup>; Aiko Barsch<sup>2</sup>; Thomas Arthen-Engeland<sup>2</sup>; <sup>1</sup>*University of Regensburg, Regensburg, Germany*; <sup>2</sup>*Bruker Daltonik, Bremen, Germany*
- TP 751 **Methods for Improving the Reproducibility of an Atmospheric Pressure Chemical Ionisation Source for Gas Chromatography Analysis;** Gareth Rhys Jones<sup>1</sup>; David S Douce<sup>2</sup>; <sup>1</sup>*Waters UK Ltd, Wilmslow, UK*; <sup>2</sup>*Waters (MS Technologies), Manchester, UK*
- TP 752 **Identification of Polycyclic Aromatic Sulfur Heterocycles in Petroleum Using Soft-Ionization GC-QTOFMS;** Viorica Lopez-Avila; Patrick J. Roach; Randall Urdahl; *Agilent Technologies, Santa Clara, CA*
- TP 753 **Exploring the Ionization Space in Traditional EI with high-resolution ToF-MS for Thermally Labile Compounds;** Jonathan Byer; Charles Lyle; Joe Binkley; Jeffrey Patrick; *Leco Corporation, St Joseph, MI*
- TP 754 **Innovative Approach to Helium Carrier Gas Conservation in Analytical Gas Chromatography – Mass Spectrometry;** Alexander Semyonov<sup>1</sup>; Massimo Santoro<sup>2</sup>; Sergio Guazzotti<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, Austin, TX*; <sup>2</sup>*Thermo Fisher Scientific, Milan, Italy*
- TP 755 **Identification of Co-Eluted Components by High Mass Accuracy and Spectral Accuracy with Quadrupole GC-MS Systems;** Alexander Semyonov<sup>1</sup>; Mark Belmont<sup>2</sup>; Massimo Santoro<sup>3</sup>; Sergio Guazzotti<sup>1</sup>; Ming Gu<sup>4</sup>; Yongdon Wang<sup>4</sup>; <sup>1</sup>*Thermo Fisher Scientific, Austin, TX*; <sup>2</sup>*Thermo Fisher Scientific, Schaumburg, IL*; <sup>3</sup>*Thermo Fisher Scientific, Milan, Italy*; <sup>4</sup>*Cerno Bioscience, Norwalk, CT*
- TP 756 **Metabolomic Analysis of Human Plasma by GC-MS;** Yue Luo; Cristina Di Poto; Mohammad R Nezami Ranjbar; Rency Varghese; Chi Zhang; Mahlet Tadesse; Habtom Resson; *Georgetown University, Washington, DC*
- TP 757 **Simultaneous Determination of 20 Kinds of Common Drugs and Pesticides in Human Blood by GPC-GC-MS/MS;** Qian Sun; Changkun Li; Jun Fan; Taohong Huang; Shin-ichi Kawano; Yuki Hashi; *Shimadzu Global COE, Shimadzu (China) Co., Ltd, Shanghai, China*
- TP 758 **Quechers Sample Preparation and Gas Chromatography-Tandem Mass Spectrometry Analysis of Multi-Pesticide Residues in Tea and Grain;** Zeying He<sup>1</sup>; Shanshan Chen<sup>1</sup>; Xiaowei Liu<sup>1</sup>; Wenwen Wang<sup>2</sup>; Chang Liu<sup>2</sup>; <sup>1</sup>*Agro-Environmental Quality Supervision & Testing, Tianjin, CHINA*; <sup>2</sup>*Agilent Technologies Co. Ltd, Beijing, China*
- TP 759 **Headspace GC/MS Analysis of Hydrogen Cyanide in Mainstream Cigarette Smoke;** Megan Mcguigan; LaQuasha Gaddis; Dana Chafin; Sydney Holmberg; Yan Ding; Clifford Watson; *Centers for Disease Control and Prevention, Atlanta, GA*
- TP 760 **Identification of Oxygenate Compounds In Gas-to-Olefin Products by Comprehensive Two-Dimensional Gas Chromatography Coupled with Time of Flight Mass Spectrometer;** Junyan Liu; Zhenlei Peng; Jiwen Li; *Sinopec SH. Research Inst. of Petrochemical Tech., Shanghai, China*
- TP 761 **Analysis of Allergens found in Cosmetics using MDGC-GCMS (Multi-dimensional gas chromatography mass spectrometer);** Sanket Chiplunkar; Prashant Hase; Dheeraj Handique; Ankush Bhone; Durvesh Sawant; Ajit Datar; Jitendra Kelkar; Pratap Rasam; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India*
- TP 762 **Multi pesticide Residue Analysis in Tobacco by GCMS/MS using QuEChERS as an Extraction Method;** Durvesh Sawant<sup>1</sup>; Ankush Bhone<sup>1</sup>; Dheeraj Handique<sup>1</sup>; Prashant Hase<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Ajit Datar<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Kaushik Banerjee<sup>2</sup>; Zareen Khan<sup>2</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*; <sup>2</sup>*National Referral Laboratory, NRCG, Pune-412307, Maharashtra, India*
- TP 763 **Analysis of Styrene Leached from Polystyrene Cups using GCMS Coupled with Headspace (HS) Sampler;** Ankush Bhone<sup>1</sup>; Dheeraj Handique<sup>1</sup>; Prashant Hase<sup>1</sup>; Sanket Chiplunkar<sup>1</sup>; Durvesh Sawant<sup>1</sup>; Ajit Datar<sup>1</sup>; Jitendra Kelkar<sup>1</sup>; Pratap Rasam<sup>1</sup>; Nivedita Subhedar<sup>2</sup>; <sup>1</sup>*Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai-400059, Maharashtra, India*; <sup>2</sup>*Ramnarain Ruia College, Matunga (E), Mumbai-400019, Maharashtra, India*
- TP 764 **GC-MSMS Characterization of EDCS in Human Tissues for Environmental Risk Factors Assessment in the Sudden Infant and Sudden Intrauterine Death Syndromes;** Pierangela Palma; Veronica Termopoli; Giorgio Famigliani; Fabiana Capriotti; Achille Cappiello; *University of Urbino, Urbino, Italy*
- TP 765 **Simultaneous Determination of Polybrominated Diphenyl Ethers (PBDEs) and Their Hydroxylated Metabolites in Bovine Milk;** Yan-Ping Lin; Katherine Dang; Birgit Puschner; *University of California, Davis, CA*
- TP 767 **Flavor and Aroma Profiles of Truffle Oils by Thermal Desorption GC/MS;** Ronald Shomo; Robert Frey; Christopher Baker; John Manura; *Scientific Instrument Services, Ringoes, NJ*
- TP 768 **Profiling Organic Composition of Art Samples Through HPLC-MS, GC-MS, and Multi-Dimensional Analysis;** Ching Ying Lin<sup>1</sup>; Keely Glass<sup>1</sup>; Amy Huang<sup>1</sup>; Carol Jiang<sup>1</sup>; Jen Skerritt<sup>1</sup>; George Dubay<sup>1</sup>; John Simon<sup>2</sup>; <sup>1</sup>*Duke University, Durham, NC*; <sup>2</sup>*University of Virginia, Charlottesville, VA*
- TP 769 **Analyzing Archaeological Sample Composition through HPLC-MS, GC-MS and Principle Component Analysis;** Amy Huang<sup>1</sup>; Keely Glass<sup>2</sup>; Michael Wei<sup>2</sup>; Roman Lin<sup>2</sup>; Carol Jiang<sup>2</sup>; Jen Skerritt<sup>2</sup>; Carla Antonaccio<sup>2</sup>; George Dubay<sup>2</sup>; <sup>1</sup>*Coral Springs, FL*; <sup>2</sup>*Duke University, Durham, NC*
- TP 770 **GCMS as the Ion Chromatograph of the 21st Century: Determination of Inorganic Anions in Matrices of Environmental and Biomedical Interest;** Enea Pagliano<sup>1</sup>; Juris Meija<sup>1</sup>; Massimo Onor<sup>2</sup>; Sara Ammazzini<sup>2</sup>; Emanuela Pitzalis<sup>2</sup>; Emilia Bramanti<sup>2</sup>; Alessandro D'Ulivo<sup>2</sup>; Zoltán Mester<sup>1</sup>; <sup>1</sup>*National Research Council Canada, Ottawa, Canada*; <sup>2</sup>*Consiglio Nazionale delle Ricerche, Pisa, Italy*
- Polymers, 773 - 792**
- TP 773 **In-line RP-LC-ESI-MS of Gen3 PAMAM Dendrimers;** John R. Lloyd; M. P. Suresh Jayasekara; Kenneth A. Jacobson; *NIH/NIDDK, Bethesda, MD*





- TP 774 **Detecting Peptide and Protein Biomarkers in Serum using Polymeric Reverse Micelles and MALDI-MS Analysis;** [Mahalia Serrano](#); Huan He; Rajasekhar Ramireddy; Sankaran Thayumanavan; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- TP 775 **Evaluation of ASAP-IM/MS(MS) Technique for the Characterization of PEEK;** [Emilie Cossoul](#)<sup>1</sup>; [Marie Hubert-Roux](#)<sup>1</sup>; Muriel Sebban<sup>1</sup>; Florence Churlaud<sup>2</sup>; Hassan Oulyadi<sup>1</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>*University of Rouen - UMR CNRS 6014 Cobra, Mont-Saint-Aignan, FRANCE*; <sup>2</sup>*Arkema - CERDATO, Serquigny, France*
- TP 776 **Composition and Architecture of Hyperbranched, Highly Fluorinated Polymers;** [Lydia Cool](#)<sup>1</sup>; Matthew Quast<sup>2</sup>; Anja Mueller<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*The University of Akron, Akron, Ohio*; <sup>2</sup>*Central Michigan University, Mount Pleasant, MI*
- TP 777 **Rapid, Simplified Analysis and Data Interpretation of Biodegradable Polymer Mixtures using MALDI-IMMS;** Kirsten Craven; *Waters, Manchester, UK*
- TP 778 **Gas-phase Chemistry of Lithiated Synthetic Polymers: Folding, Charge Solvation and Fragmentation;** Benjamin Bythell; *Univ. of Missouri-St. Louis, St. Louis, MO*
- TP 779 **Negative Ion Electrospray Ionization Mass Spectrometry of Polyglycerol;** [Xiaodong Huang](#); Xiaojin Li; *Ecolab Inc., Naperville, IL*
- TP 780 **Combined Developments in MALDI Mass Spectrometry, Size Exclusion Chromatography and Diffusion NMR for a Successful Characterization of poly(4-vinylpyridine) Molecular Weight;** Christophe Chendo; Marion Rollet; Trang Phan; Stephane Viel; Esra Altuntas; Didier Gigmes; [Laurence Charles](#); *Aix-Marseille University, Marseille Cedex 20, France*
- TP 781 **ESI-MS/MS Structural Characterization of a New Impurity during the Synthesis of PAMAM Dendrimers;** [Aura Tintaru](#); Rémi Ungaro; Xiaoxuan Liu; Laurent Giordano; Ling Peng; [Laurence Charles](#); *Aix-Marseille University, Marseille, France*
- TP 782 **Rapid Analysis of Carbon Fiber Reinforced Plastic using DART-MS;** [Hideaki Kusano](#)<sup>1</sup>; Jun Watanabe<sup>1</sup>; Yuki Kudou<sup>3</sup>; Teruhisa Shiota<sup>2</sup>; <sup>1</sup>*Shimadzu Corporation, Kyoto, Japan*; <sup>2</sup>*AMR, Inc., Tokyo, JAPAN*; <sup>3</sup>*BioChromato, Fujisawa, Japan*
- TP 783 **Rapid Qualitative and Semi-Quantitative Analysis of PAEs in PVC Samples by Direct Injection Probe APCI High Resolution TOF Mass Spectrometry;** Zhaoyang Liu; *Bruker Daltonics, Inc, Shanghai, China*
- TP 784 **Glycopolymers – Separating Oligomers and Identifying Structural Isomers;** [Sarah Robinson](#); Lydia Cool; Cesar Lopez Gonzalez; Coleen Pugh; Chrys Wesdemiotis; *The University of Akron, Akron, Ohio*
- TP 785 **Characterization of Poly-L-Lysine and Its Noncovalent Complexes by Ion-Mobility- Mass Spectrometry;** [Mehmet Atakay](#)<sup>1,2</sup>; Bekir Salih<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; <sup>1</sup>*Department of Chemistry, The University of Akron, Akron, OH*; <sup>2</sup>*Department of Chemistry, Hacettepe University, Ankara, Turkey*
- TP 786 **MALDI-TOF Characterization of  $\alpha,\omega$ -Difunctionalized Poly(ethylene glycol) for Bioconjugate Synthesis;** C. Adrian Figg; [Maria Cristina A. Dancel](#); Bryan S. Tucker; Brent S. Sumerlin; *University of Florida, Gainesville, FL*
- TP 787 **Quantitative Analysis of Bulk and Extractable PVP incorporated in Silicone Hydrogel Contact Lenses using APCI HR/AM-SIM Mass Spectrometry;** [William Nichols](#)<sup>1</sup>; Andrew J. Hoteling<sup>2</sup>; Lawrence Salvati III<sup>2,2</sup>; Patricia Harmon<sup>2</sup>; <sup>1</sup>*Mass2Charge Consulting LLC, Newark, NY*; <sup>2</sup>*Bausch+Lomb, Rochester, NY*
- TP 788 **Structural and Mixture Characterization of Polysorbate 60 using GPC-Spray Deposition and MALDI-ToF MS;** Mark Arnould; *Xerox, Webster, NY*
- TP 789 **Direct Analysis in Real Time (DART) Ion Trap Mass Spectrometry for Detection and Identification of poly(dimethylsiloxane) Polymers on Surfaces;** [Curtis Mowry](#); Michael Brumbach; Adam Pimentel; Alex Mirabal; *Sandia National Laboratories, Albuquerque, NM*
- TP 790 **Characterization of Homo-arm and Mikto-arm Poly(ethylene Glycol) Stars using Vacuum Ionization-Ion Mobility Spectrometry-Mass Spectrometry;** [Casey Foley](#)<sup>1</sup>; Tarick El-Baba<sup>1</sup>; Boyu Zhang<sup>2</sup>; Scott Grayson<sup>2</sup>; Sarah Trimpin<sup>1</sup>; <sup>1</sup>*Wayne State University, Detroit, MI*; <sup>2</sup>*Tulane University, New Orleans, LA*
- TP 791 **Comprehensive Analysis of Extractable from Rubber Stopper used in Medical Devices and Pharmaceutical Products;** [Andrew Feilden](#)<sup>1</sup>; Amalendu Sarkar<sup>2</sup>; Kate Comstock<sup>3</sup>; <sup>1</sup>*Smithers Rapra, Shrewsbury, UK*; <sup>2</sup>*Qure Medical, Rock Hill, SC*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- TP 792 **Comparing Additives and other Extractables from Primary and After-Market Cell Phone Cases by Gas Chromatography-Time of Flight Mass Spectrometry;** [Christina Nieh](#)<sup>1</sup>; Joe Binkley<sup>2</sup>; <sup>1</sup>*LECO Corporation, Saint Joseph, MI*; <sup>2</sup>*LECO Corporation, St. Joseph, MI*



7:30 – 8:00 am..... Set up all Wednesday posters  
 10:30 am – 1:00 pm..... Odd-numbered posters present  
 12:00 – 2:30 pm..... Even-numbered posters present  
 7:30 – 8:00 pm..... Remove all Wednesday posters

Imaging MS: Sample Preparation.....	001-013
Informatics: Profile Analysis.....	014-023
Informatics: General.....	024-037
Informatics: Peptide Identification and Characterization II.....	038-054
Intact Proteins: PTM Discovery.....	055-059
Glycoproteins.....	060-089
Phosphopeptides: Enrichment Methods.....	090-098
Peptides: Quantitative Analysis (Applications to Peptide and Protein Targets).....	099-121
Peptides: Quantitative Analysis (Advances in Sample Preparation and Workflow.....	122-133
Proteomics: Clinical Applications.....	134-157
Proteomics: New Approaches.....	158-178
Protein Therapeutics: Quantitative Analysis.....	179-200
Protein Therapeutics: Structural Characterization.....	201-216
H/D Exchange: Protein Structure Function.....	217-231
Proteomics: Tissue.....	232-241
Systems Biology / Quantitative Proteomics.....	242-259
Antibodies and Antibody: Drug Conjugates.....	260-278
Lipids: Profile Analysis.....	279-290
Forensics.....	291-311

Natural Products.....	319-339
Elemental Analysis.....	340-346
Food Safety: Pesticides.....	347-362
Nucleic Acids.....	363-374
Ambient Ionization: Fundamentals.....	375-388
Ambient Ionization: Applications.....	389-418
Diagnostics Clinical Chemistry.....	421-453
Biomarker Discovery.....	454-478
Biomarkers: Quantitative Analysis.....	479-505
Biomarkers: Quantitative Analysis.....	509-518
Small Molecule Quantitation.....	519-553
Environmental Analysis: General.....	554-580
Metabolomics: General II.....	581-594
Metabolomics: Quantitative Analysis.....	595-615
Drug Metabolism: High Throughput Analysis.....	616-627
Drug Metabolism: Quantitative Analysis.....	628-639
Drug and Metabolite Analysis: Dried Biological Samples.....	640-656
Ion Mobility: Applications.....	657-685
Ion Mobility: Fundamentals.....	686-700
Nanomaterials.....	701-707
Challenges in Identification.....	709-723
High Mass Accuracy / High Performance MS: Applications.....	724-739
Instrumentation: New Developments in Ionization and Sampling.....	740-759
FAIMS and DMS.....	760-779

**Imaging MS: Sample Preparation, 001 - 013**

- WP 001 **Highly Robust Sample Preparation with 2,5-dihydroxyacetophenone for MALDI Imaging of Proteins (2-70 kDa) at High Spatial Resolution (5 µm);** Junhai Yang; Andre Zavalin; Richard Caprioli; Vanderbilt University, Nashville, TN
- WP 002 **Digging Deeper: Using Acid-Cleavable Detergents to Uncover More of the MSI Proteome;** Peggi Angel; Erin H. Seeley; Gregory Boyce; Greg W. Kilby; Protea Biosciences, Inc., Morgantown, WV
- WP 003 **Photo-Thermal Decomposition/Digestion (Photo-TDD) of Proteins and Its Application in MALDI-MS Imaging;** Rong Zhou; Franco Basile; University of Wyoming, Laramie, WY
- WP 004 **Infrared Laser Ablation Sample Transfer with On-Target Digestion for MALDI Imaging;** Fan Cao; Kermit K. Murray; Louisiana State University, Baton Rouge, LA
- WP 005 **Imaging MALDI MS of Dosed Mouse Brain Utilizing Novel Sample Preparation Technique;** Cristine Quiason; Sheerin K. Shahidi-Latham; Justin Q. Ly; Edna F. Choo; Genentech Inc., South San Francisco, CA
- WP 006 **In-Depth Characterization of the Neuropeptidome in Crustacean Stomatogastric Nervous System by Imaging Mass Spectrometry on an Orbitrap Platform;** Chuanzi Ouyang<sup>1</sup>; Bingming Chen<sup>2</sup>; Albert Kim<sup>3</sup>; Lingjun Li<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, UW-Madison, Madison, WI; <sup>2</sup>School of Pharmacy, UW-Madison, Madison, WI; <sup>3</sup>Department of Biochemistry, UW-Madison, Madison, WI
- WP 007 **A High Throughput Method for Mass Spectrometric Profiling of Glycomics and Proteomics from Tissue Microarrays;** Chun Shao; Lilla Turiák; Le Meng; Qi Wang; Nancy Leymarie; Cheng Lin; Joseph Zaia; School of Medicine, Boston University, Boston, MA
- WP 008 **Simultaneous Proteomics and Glycomics Profiling from Histological Tissue;** Lilla Turiák; Le Meng; Chun Shao; Kshitij Khatri; Nancy Leymarie; Qi Wang; Joseph Zaia; Boston University School of Medicine, Boston, MA
- WP 009 **High-resolution Ambient Mass Spectrometry Imaging of Mouse Tissues by Surface Micro-Extraction using the Single-probe;** Wei Rao; Ning Pan; Renmeng Liu; Zhibo Yang; University of Oklahoma, Norman, OK

- WP 010 **Heat Fixation Inactivates Viral and Bacterial Pathogens and is Compatible with Downstream MALDI Mass Spectrometry Tissue Imaging;** Lisa H. Cazares<sup>1,2</sup>; Sean Vantongeren<sup>3</sup>; Tara Kenny<sup>3</sup>; Douglas Lane<sup>3</sup>; Rekha Panchal<sup>3</sup>; Sina Bavari<sup>3</sup>; <sup>1</sup>Henry M. Jackson Foundation, Frederick, MD; <sup>2</sup>DoD, BHSI, Fredrick, MD; <sup>3</sup>USAMRIID/ Molecular and Translational Sciences, Frederick, MD
- WP 011 **Investigating the Use of Heat Stabilization during Sample Preparation of Tissues for Mass Spectrometry Imaging;** Suzanne Robertson<sup>1</sup>; Jeremy Barry<sup>1</sup>; Guillaume Robichaud<sup>1</sup>; Nagendran Muthusamy<sup>1</sup>; Craig Sykes<sup>2</sup>; Corbin Thompson<sup>2</sup>; Troy Ghashghaei<sup>1</sup>; Angela Kashuba<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>North Carolina State University, Raleigh, NC; <sup>2</sup>University of North Carolina at Chapel Hill, Chapel Hill, NC
- WP 012 **High Quality Sections and Molecular Distribution Images of Neuropeptides From Heat Stabilized Tissue;** Mats Borén<sup>1</sup>; Olof Sköld<sup>1</sup>; Anna Nilsson<sup>2</sup>; Richard Goodwin<sup>2,3</sup>; Per E. Andren<sup>2</sup>; <sup>1</sup>Denator AB, Uppsala, Sweden; <sup>2</sup>Uppsala University, Uppsala, Sweden; <sup>3</sup>AstraZeneca, Macclesfield, UK
- WP 013 **Measuring MALDI: Investigating MALDI Fundamentals with ToF-SIMS;** Melissa K. Passarelli<sup>1</sup>; Ian S. Gilmore<sup>1</sup>; Josephine Bunch<sup>1</sup>; Peter Marshall<sup>2</sup>; Sophie Myhill<sup>2</sup>; Andy West<sup>2</sup>; <sup>1</sup>National Physical Laboratory, Teddington, U.K.; <sup>2</sup>GlaxoSmithKline, Stevenage, U.K.

**Informatics: Profile Analysis, 014 - 023**

- WP 014 **Comprehensive Characterization of the Secretome of CNS Cell Lines using High-Resolution LC-MS/MS;** Jongmin Woo<sup>1</sup>; Dohyun Han<sup>2</sup>; Youngsoo Kim<sup>2</sup>; <sup>1</sup>Department of Biomedical Sciences, SNU, Seoul, Korea; <sup>2</sup>Department of Biomedical Engineering, SNU, Seoul, Korea
- WP 015 **An Extensive and Reproducible Ion-Current-based Proteomic Profiling Provided New Insights into the Understanding the Mechanism of Myogenic Differentiation;** Jun Qu<sup>1</sup>; Chengjian Tu<sup>1</sup>; Jun Li<sup>1</sup>; Shichen Shen<sup>1</sup>; James Clements<sup>2</sup>; yahao Bu<sup>2</sup>; David Hangauer<sup>2</sup>; <sup>1</sup>University at Buffalo, Buffalo, NY; <sup>2</sup>Kinex Pharmaceuticals LLC, Buffalo, NY
- WP 016 **The Omics Evidences: Single Nucleotide Variants Transmissions on Chromosome 20 in Liver Cancer Cell Lines;** Quanhui Wang<sup>1,2</sup>; Bo Wen<sup>2</sup>; Shaohang Xu<sup>2</sup>;

- Zhe Ren<sup>2</sup>; Guixue Hou<sup>1,2</sup>; Ruo Zhou<sup>2,2</sup>; Jin Zi<sup>2</sup>; Xiaomin Lou<sup>1</sup>; Haidan Sun<sup>1</sup>; Fan Zhong<sup>3</sup>; Qingyu He<sup>4</sup>; Ping Xu<sup>5</sup>; Liang Lin<sup>2</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>Beijing Institute of Genomics, CAS, Beijing, China; <sup>2</sup>BGI-Shenzhen, Shenzhen, China; <sup>3</sup>Fudan University, Shanghai, China; <sup>4</sup>Jinan University, Guangzhou, China; <sup>5</sup>Beijing Proteome Research Center, Beijing, China
- WP 017 **A Cloud Computing Implementation of Differential Mass Spectrometry: A Label Free Method for Proteomic Profiling;** Nathan Yates<sup>1</sup>; Christine Wu<sup>2</sup>; Michael J. Maccoss<sup>3</sup>; Andrey Bondarenko<sup>4</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>University of Pittsburgh School of Medicine, Pittsburgh, PA; <sup>3</sup>Univ of Washington, Seattle, WA; <sup>4</sup>InfoClinika, Bellevue, WA
- WP 018 **mTMT-visHTS: A Novel Method for Multiplexing TMT Datasets with a Tunable Visualization High Throughput Screening Software for Easy Protein Profiling;** Piero Ricchiuto<sup>1</sup>; Katsumi Yabusaki<sup>1,2</sup>; Hiroshi Iwata<sup>1</sup>; Iwao Yamada<sup>1,2</sup>; Masanori Aikawa<sup>1</sup>; Sasha Singh<sup>1</sup>; <sup>1</sup>Harvard Medical School & BWH, Boston, MA; <sup>2</sup>Kowa Company, Ltd., Tokyo, Japan
- WP 019 **The Modelling and Poisson Harvesting of LC-MS Spectra;** Edmond Breen; *APAF, Sydney, AUSTRALIA*
- WP 020 **Automated Classification and Visualization of Histological Features by Mass Spectrometry Imaging;** Ottmar Golf<sup>1,2</sup>; Nazanin Zounemat Kermani<sup>1</sup>; Sabine Guenther<sup>1,2</sup>; Robert D. Goldin<sup>1</sup>; James Kinross<sup>1</sup>; Abigail V. M. Speller<sup>1</sup>; Zoltan Takats<sup>1</sup>; Kirill Veselkov<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Justus Liebig University, Giessen, Germany
- WP 021 **An Informatics Approach for Evaluating and Guiding Method Development for Biomarker;** Y. Melodie Du<sup>1</sup>; R. Graham Cooks<sup>1</sup>; Yu Xia<sup>1</sup>; Ye Hu<sup>2</sup>; Zheng Ouyang<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>The Methodist Hospital Research Institute, Houston, TX
- WP 022 **The Use of Fragment Ion and Collision Cross Section for Confident Identification from LC-Ion Mobility-MS Metabolomics Data;** Giorgis Isaac<sup>1</sup>; Giuseppe Astarita<sup>1</sup>; Steven Lai<sup>1</sup>; Adam Ladak<sup>1</sup>; James Langridge<sup>3</sup>; John Shockcor<sup>1</sup>; Andy Borthwick<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Nonlinear Dynamics, Newcastle, UK; <sup>3</sup>Waters Corporation, Manchester, UK
- WP 023 **Automated Glycan Assignment using Accurate Mass Measurement with a Calibrated Retention Time in Glucose Units;** Ying-Qing Yu<sup>1</sup>; Weibin chen<sup>1</sup>; Mark Hilliard<sup>2</sup>; Niaobh McLoughlin<sup>2</sup>; Pauline Rudd<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>NIBRT, Dublin, Ireland
- Informatics: General, 024 - 037**
- WP 024 **Application of Performance Metrics Software for Optimization of Proteomics Data Acquisition;** David Mccaskill; Yaw Nti-Addae; Suresh Babu Annangudi Palani; Tao Xu; Jeffrey Gilbert; *Dow AgroSciences, Indianapolis, IN*
- WP 025 **An Innovative Software Platform for the Visualization of Routine GC and LC-MS Data;** David Hardy<sup>1</sup>; Vitaly Lashin<sup>2</sup>; Pranas Japertas<sup>3</sup>; <sup>1</sup>ACD/Labs, Bracknell, UK; <sup>2</sup>ACD/Labs, Moscow, Russia; <sup>3</sup>ACD/Labs, Vilnius, Lithuania
- WP 026 **Reconstruction of Mass Spectra Using Fuzzy Optimal Associative Memories (FOAMs);** Zhengfang Wang; Mengliang Zhang; Peter Harrington; *Ohio University, Athens, Ohio*
- WP 027 **Carbocationic Mass Tags for Information Encoding and Multiplex Bioanalytical Applications;** Artyom Topolyan<sup>1</sup>; Vladimir Bylev<sup>1</sup>; Alexey Ustinov<sup>2</sup>; Andrey Formanovsky<sup>1</sup>; Vladimir Korshun<sup>1</sup>; <sup>1</sup>Institute of Bioorganic Chemistry RAS, Moscow, Russia; <sup>2</sup>Lumiprobe Corporation, Hallandale Beach, FL
- WP 028 **Analysis of Longitudinal Serum Proteomics Profiles from Studies of a T1D-risk Cohort;** Robert Moulder<sup>1</sup>; Santosh Bhosale<sup>1</sup>; Heikki Hyöty<sup>2,3</sup>; Riitta Veijola<sup>4</sup>; Mikael Knip<sup>5,6</sup>; Jorma Ilonen<sup>7,8</sup>; Tuula Simell<sup>10</sup>; Jorma Toppari<sup>1,12</sup>; Harri Lähdesmäki<sup>11</sup>; Olli Simell<sup>10</sup>; Riitta Lahesmaa<sup>1</sup>; David Goodlett<sup>1,9</sup>; <sup>1</sup>Turku Centre for Biotechnology, Turku, Finland; <sup>2</sup>School of Medicine, University of Tampere, Tampere, Finland; <sup>3</sup>Fimlab Laboratories, Pirkanmaa Hospital District, Tampere, Finland; <sup>4</sup>Dept. of Pediatrics, Uni.of Oulu & Central Hospital, Oulu, Finland; <sup>5</sup>Dept. Pediatrics, Helsinki Uni. Central Hospital, Helsinki, Finland; <sup>6</sup>Dept. of Pediatrics, Tampere University Hospital, Tampere, Finland; <sup>7</sup>Dept. of Clinical Microbiology, Uni.Eastern Finland, Kuopio, Finland; <sup>8</sup>Immunogenetics Laboratory, University of Turku, Turku, Finland; <sup>9</sup>University of Maryland, Baltimore, MD; <sup>10</sup>Department of Pediatrics, University of Turku, Turku, Finland; <sup>11</sup>Aalto University School of Science, Espoo, Finland; <sup>12</sup>Department of Physiology, University of Turku, Turku, Finland
- WP 029 **PEFF: A Common Sequence Database Format in Proteomics;** Pierre-Alain Binz<sup>1</sup>; Eugene Kapp<sup>2</sup>; Jim Shofstahl<sup>3</sup>; David Creasy<sup>4</sup>; Lydie Lane<sup>5</sup>; Robert Chalkley<sup>6</sup>; Matt Chambers<sup>7</sup>; Harald Barsnes<sup>8</sup>; Sean L. Seymour<sup>9</sup>; <sup>1</sup>CHUV, Lausanne, Switzerland; <sup>2</sup>Ludwig Institute for Cancer Research, Melbourne, Australia; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Matrix Science Ltd, London, United-Kingdom; <sup>5</sup>Swiss Institute of Bioinformatics, Geneva 4, Switzerland; <sup>6</sup>UCSF, San Francisco, CA; <sup>7</sup>Vanderbilt University, Nashville, TN; <sup>8</sup>University of Bergen, Bergen, Norway; <sup>9</sup>AB Sciex, Foster City, CA
- WP 030 **Automated Mass Shift Detection, Accurate Peak Area Integration, Identification and Relative Quantification of INLIGHT™ Derivatized N-Glycans for LC-MS Comparative Glycomics;** Kenneth Garrard; Amber Cook; Guillaume Robichaud; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- WP 031 **Critical Assessment of the Elemental Isotope Definition in Mass-Spectrometry-Based Proteomics;** Jürgen Claesen<sup>1</sup>; Frank Sobott<sup>3</sup>; Tomasz Burzykowski<sup>1</sup>; Dirk Valkenborg<sup>2</sup>; <sup>1</sup>Hasselt University, Diepenbeek, Belgium; <sup>2</sup>VITO, Mol, Belgium; <sup>3</sup>CFP-CeProMa, University of Antwerp, Antwerp, Belgium
- WP 032 **Identification of Non-Synonymous SNP Products to Search High Resolution Tandem Mass Spectra Against a Novel Protein Database;** Carol Nilsson<sup>1</sup>; Cheryl Lichti<sup>1</sup>; Ekaterina Mostovenko<sup>1</sup>; Fabrizio Donnarumma<sup>2</sup>; Melinda Rezel<sup>3</sup>; György Marko-Varga<sup>3</sup>; Akos Vegvari<sup>3</sup>; <sup>1</sup>UTMB, Galveston, TX; <sup>2</sup>Louisiana State University, Baton Rouge, LA; <sup>3</sup>Lund University, Lund, Sweden
- WP 033 **The Probabilistic Convolution Tree: A Dynamic Programming Algorithm for Sub-Quadratic Inference with Generic Causal Graphical Models;** Oliver Serang; *Thermo Fisher Scientific, Bremen, Germany*
- WP 034 **GradientOptimizer: An Open-Source Graphical Environment for Calculating Optimized Gradients in Reversed-Phase Liquid Chromatography;** Luminita Moruz<sup>1</sup>; Lukas Käll<sup>2</sup>; <sup>1</sup>Stockholm University, Stockholm, Sweden; <sup>2</sup>Royal Institute of Technology, Stockholm, Sweden
- WP 035 **McFine - An Algorithm to Approximate the Isotope Fine Structure of Peptides and Proteins;** Piotr Dittwald<sup>1</sup>; Dirk Valkenborg<sup>2,3</sup>; Alan L. Rockwood<sup>4,5</sup>; Anna Gambin<sup>1</sup>; <sup>1</sup>University of Warsaw, Warsaw, Poland; <sup>2</sup>VITO, Mol, Belgium; <sup>3</sup>I-Biostat, Hasselt University, Diepenbeek, Belgium; <sup>4</sup>ARUP Laboratories, Salt Lake City, UT; <sup>5</sup>Department of Pathology, University of Utah, School of Medicine, Salt Lake City, UT

- WP 036 **Persistent Myths and Uncomfortable Truths: Taking MS-omics Data Processing from the Emperor's New Clothes to a Rigorous Science**; Rob Smith; Dan Ventura; John Prince; *Brigham Young University, Provo, UT*
- WP 037 **CHORUS: A Community Based Solution for the Storage, Analysis, and Exchange of Mass Spectrometry Data and Information**; Andrey Bondarenko<sup>1</sup>; Michael J. Maccoss<sup>2</sup>; Christine Wu<sup>4</sup>; Nathan Yates<sup>3</sup>; <sup>1</sup>*InfoClinika, Bellevue, WA*; <sup>2</sup>*Univ of Washington, Seattle, WA*; <sup>3</sup>*University of Pittsburgh, Pittsburgh, PA*; <sup>4</sup>*University of Pittsburgh School of Medicine, Pittsburgh, PA*
- Informatics: Peptide Identification and Characterization, 038 - 054**
- WP 038 **Altered Fragmentation Patterns in Amidinated Tryptic Peptides Enhance Peptide Identification**; Sujun Li; Suraj Saraswat; James P. Reilly; Haixu Tang; Predrag Radivojac; *Indiana University, Bloomington, IN*
- WP 039 **Cleaved and Missed Sites for Trypsin, Lys-C, Lys-N can be Predicted with High Confidence on the Basis of Sequence Context**; Andrew J Alpert<sup>2</sup>; Paul Gershon<sup>1</sup>; <sup>1</sup>*UC-Irvine, Irvine, CA*; <sup>2</sup>*PolyLC Inc., Columbia, MD*
- WP 040 **Improving the Accuracy of Peptide Retention Time Prediction by Machine Learning Techniques**; Bob Xiong; Susan Deupree; Brian Nofsinger; Mike Allen; *Tandem Labs - RTP, Durham, NC*
- WP 041 **Rapid Characterization, Annotation and Comparison of Peptide Maps**; Michael Kim<sup>1</sup>; Yong Kil<sup>2</sup>; Marshall Bern<sup>2</sup>; Chris Becker<sup>2</sup>; Richard Seipert<sup>1</sup>; <sup>1</sup>*Genentech, South San Francisco, CA*; <sup>2</sup>*Protein Metrics, San Carlos, CA*
- WP 042 **Pattern Detection in Associated Artifact Peaks in Mass Spectra with Frequent Itemset Mining**; Trung Nghia Vu<sup>1,4</sup>; Dirk Valkenborg<sup>2,3</sup>; Evelyne Maes<sup>2,3</sup>; Filip Lemièr<sup>1,3</sup>; Bart Goethals<sup>1</sup>; Kris Laukens<sup>1,4</sup>; <sup>1</sup>*University of Antwerp, Antwerp, Belgium*; <sup>2</sup>*VITO, Mol, Belgium*; <sup>3</sup>*Centre for Proteomics, University of Antwerp, Antwerp, Belgium*; <sup>4</sup>*biomina, Antwerpen, Belgium*
- WP 043 **Rule Based Peak Filtering of High Mass Accuracy MS/MS-spectra Improves Peptide Identification Rates**; Jakob Bunkenborg<sup>1</sup>; Per Hågglund<sup>2</sup>; Henrik Molina<sup>3</sup>; <sup>1</sup>*Copenhagen University Hospital, Hvidovre, Denmark*; <sup>2</sup>*Technical University of Denmark, Kgs. Lyngby, Denmark*; <sup>3</sup>*The Rockefeller University, New York, NY*
- WP 044 **Removing Isobaric-Related Ions Significantly Improves the Peptide/Protein Identification Sensitivity of High Resolution MS/MS Data**; Quanhu Sheng<sup>1</sup>; Rongxia Li<sup>2</sup>; Jie Dai<sup>3</sup>; Qingrun Li<sup>2</sup>; Chen Li<sup>2</sup>; Zhiduan Su<sup>2</sup>; Yu Shyr<sup>1</sup>; Rong Zeng<sup>2</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Shanghai Institutes for Biological Sciences, Shanghai, China*; <sup>3</sup>*University of Southern Denmark, Odense, Denmark*
- WP 045 **Improving Protein and Peptide Identification in Tandem Mass Spectrometry by Peptide Search Space Reduction**; Avinash Shanmugam; Chih-Chiang Tsou; Dmitry Avtonomov; Anastasia Yocum; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- WP 046 **A Fast Filtering Method for Peptide Identification by Blocked Pattern Matching**; Fei Deng<sup>1</sup>; Xiaowen Liu<sup>2</sup>; Lusheng Wang<sup>1</sup>; <sup>1</sup>*Dept. of Computer Science, City Univ. of Hong Kong, Hong Kong, China*; <sup>2</sup>*IUPUI, Indianapolis, IN*
- WP 047 **A Chromatography Independent 2-Phase Algorithm for Increasing DDA Protein Identifications by up to 80% and Peptide Identifications by 200%**; David Scigocki<sup>1</sup>; Christian Claude<sup>1</sup>; Patrick Vayn<sup>1</sup>; Elie Abenmoha<sup>1,2</sup>; John Lindsay<sup>1,3</sup>; David Znaty<sup>1</sup>; John Asara<sup>4,5</sup>; <sup>1</sup>*Physikron, Inc., Paris, FR*; <sup>2</sup>*Me Conseil, Paris, FR*; <sup>3</sup>*SciPartners, Inc., Westford, MA*; <sup>4</sup>*Beth Israel Deaconess Medical Center, Boston, MA*; <sup>5</sup>*Harvard Medical School, Boston, MA*
- WP 048 **fishTones.js: Interactive Peptide MSMS Characterization in Non-Traditional Proteomic Workflows**; Alexandre Masselot; Victoria Pham; Lilian Phu; Tobias Maile; Wendy Sandoval; Donald Kirkpatrick; David Arnott; *Genentech, South San Francisco, CA*
- WP 049 **PeptideAnalyzer: An Integrated Platform for Efficient In-Depth Characterization of Therapeutic Proteins**; Vincent Larrailet<sup>1</sup>; Georg Drabner<sup>1</sup>; Amy Hilderbrand<sup>2</sup>; Maximiliane Hilger<sup>1</sup>; Tobias Kailich<sup>3</sup>; Michael Kim<sup>2</sup>; Hans Koll<sup>1</sup>; Wilma Lau<sup>1</sup>; Ingo Lindner<sup>3</sup>; Michael Molhoj<sup>1</sup>; Richard Seipert<sup>2</sup>; X. Christopher Yu<sup>2</sup>; Hans Rainer Voelger<sup>1</sup>; <sup>1</sup>*Pharma Research, Roche Diagnostics GmbH, Penzberg, Germany*; <sup>2</sup>*Protein Analytical Chemistry, Genentech, South San Francisco, United States*; <sup>3</sup>*Pharma Biotech Development, Roche Diagnostics GmbH, Penzberg, Germany*
- WP 050 **Software Tools to Accelerate Peptide Mapping and Related Analysis for Characterizing Biotherapeutics**; Joe Shambaugh<sup>1</sup>; Peter Haberl<sup>2</sup>; Alessio Ceroni<sup>2</sup>; Arnd Brandenburg<sup>3</sup>; Jens Hoefkens<sup>1</sup>; <sup>1</sup>*Genedata Inc., Lexington, MA*; <sup>2</sup>*Genedata GmbH, Martinsried, Germany*; <sup>3</sup>*Genedata AG, Basel, Switzerland*
- WP 051 **Creation of a Tandem MS HCD Spectral Library for Identification of Peptides and Modifications of a Therapeutic Monoclonal Antibody**; Qian Dong; Xinjian Yan; Yuri Mirokhin; Yuexue Liang; Stephen Stein; *NIST, Gaithersburg, MD*
- WP 052 **Scrambling and Enumeration Modules Developed for the Structure Elucidation of MS<sup>n</sup> Data Utilizing the MASSPEC Algorithm**; Marshall M. Siegel; Gary Walker; *MS Mass Spec Consultants, Fair Lawn, NJ*
- WP 053 **pParse 2.0: A Faster and More Sensitive Algorithm for Detection of Monoisotopic Peaks**; Long Wu<sup>1</sup>; Wen-Feng Zeng<sup>1</sup>; Zuo-Fei Yuan<sup>1</sup>; Kun Zhang<sup>1</sup>; Jia-Ming Meng<sup>1</sup>; Sheng-Bo Fan<sup>1</sup>; Chao Liu<sup>1</sup>; Hao Chi<sup>1</sup>; Lai-Yun Qing<sup>2</sup>; Rui-Xiang Sun<sup>1</sup>; Si-Min He<sup>1</sup>; <sup>1</sup>*Institute of Computing Technology, CAS, Beijing, China*; <sup>2</sup>*School of Computer and Control Engineering, UCAS, Beijing, China*
- WP 054 **pFind: Fast and Comprehensive Analysis of High Resolution MS Data**; Hao Chi; Wen-Feng Zeng; Long Wu; Kun He; Chao Liu; Rui-Xiang Sun; Si-Min He; *Institute of Computing Technology, CAS, Beijing, China*
- Intact Proteins: PTM Discovery, 055 - 059**
- WP 055 **LC-MS Analysis of Intact Enzymes using the Synapt G2 Mass Spectrometer**; Ioana Barbu; Nicolas Abello; Jort Gerritsma; Marcel van Tilborg; Maurien Olsthoorn; *DSM Biotechnology Center, Analysis department, Delft, Netherlands*
- WP 056 **Structural Determination of Different Protein Phosphoforms**; Matthias Vonderach<sup>1</sup>; Francesco Lanucara<sup>1</sup>; Ben Cossins<sup>2</sup>; Claire Eyers<sup>1</sup>; <sup>1</sup>*Institute of Integrative Biology, Liverpool, UK*; <sup>2</sup>*UCB, Slough, UK*
- WP 057 **Comprehensive Characterization of Molecular Heterogeneities in  $\alpha$ -actins from Cardiac Tissues by Top-Down Mass Spectrometry**; Serife Ayaz Guner<sup>2</sup>; Ying Peng<sup>2</sup>; Ivy Chen<sup>2</sup>; Ying Ge<sup>1,2</sup>; <sup>1</sup>*Cell and Regenerative Biology, Madison, WI*; <sup>2</sup>*University of Wisconsin - Madison, Madison, WI*
- WP 058 **Targeted Protein Enrichment by Intact Protein SRM and Fraction Collection to Enable PTM-Based Biomarker Discovery from CSF of Individual Patients**; Junmei Zhang; Daniel Plymire; John Corbett; Steven Patrie; *UT Southwestern, Dallas, TX*
- WP 059 **Complete Post-Translational Modification Mapping of Pilins from Clinical Strains of Pathogenic *Neisseria meningitidis* Requires Top-Down Mass Spectrometry**; Joseph Gault<sup>1</sup>; Christian Malosse<sup>1,2</sup>; Marie-Cécile Ploy<sup>6</sup>;

Catherine E. Costello<sup>3</sup>; Guillaume Dumenil<sup>4,5</sup>; Julia Chamot-Rooke<sup>1,2</sup>; <sup>1</sup>Institut Pasteur, Paris, France; <sup>2</sup>CNRS UMR3528, Paris, France; <sup>3</sup>Boston University School of Medicine, Boston, MA; <sup>4</sup>INSERM U970, Paris, France; <sup>5</sup>Université Paris Descartes, Paris, France; <sup>6</sup>INSERM UMR1092, Limoges University Hospital, Limoges, France

### Glycoproteins, 060 - 089

- WP 060 **Analysis of Serum Haptoglobin Fucosylation in Hepatocellular Carcinoma and Liver Cirrhosis of Different Etiologies;** Jianhui Zhu<sup>1</sup>; Zhenxin Lin<sup>1</sup>; Jing Wu<sup>1</sup>; Haidi Yin<sup>1</sup>; Jianliang Dai<sup>2</sup>; Ziding Feng<sup>2</sup>; Jorge Marrero<sup>3</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>University of Michigan Medical Center, Ann Arbor, MI; <sup>2</sup>University of Texas MD Anderson Cancer Center, Houston, TX; <sup>3</sup>UT Southwestern Medical Center, Dallas, TX
- WP 061 **Ultracentrifugation-based Glycoproteomic: Approach for Discovery of Plasma Glycoprotein Markers;** Esther Cheow; NTU, Singapore, Singapore
- WP 062 **A Comparative Glycoproteome Study of Developing Endosperm in the Hexose-Deficient *miniature1* Seed Mutant and Its Wild Type Mn1 in maize;** Cecilia Silva-Sanchez<sup>1</sup>; Jinxi Li<sup>1</sup>; Sixue Chen<sup>1,2</sup>; Prem Chourey<sup>3</sup>; <sup>4</sup>ICBR-Proteomics UF, Gainesville, FL; <sup>2</sup>University of Florida, Gainesville, FL; <sup>3</sup>USDA-Agricultural Research Service, CMAVE, Gainesville, FL; <sup>4</sup>Department of Agronomy, UF, Gainesville, FL
- WP 063 **Improved Glycopeptide Analysis using Acetonitrile Enriched Sheath Gas and Oxonium Ion Dependent ETD;** Kristina Marx; Andrea Kiehne; Markus Meyer; Bruker Daltonik GmbH, Bremen, Germany
- WP 064 **Identification of Complex Glycopeptides using Tandem Mass Spectra;** Yanlin Zhang<sup>1</sup>; Chuan-Yih Yu<sup>2</sup>; Shuaicheng Li<sup>3</sup>; Haixu Tang<sup>2</sup>; Xiaowen Liu<sup>1</sup>; <sup>1</sup>IUPUI, Indianapolis, IN; <sup>2</sup>Indiana University, Bloomington, IN; <sup>3</sup>City University of Hong Kong, Hong Kong, China
- WP 065 **Comprehensive Analysis of Recombinant Human Erythropoietin Glycoforms by Capillary Electrophoresis and Nanoflow Liquid Chromatography Coupled with Middle-Down Mass Spectrometry;** Rosa Viner<sup>1</sup>; Anthonius A.M. Heemskerk<sup>2</sup>; David M Horn<sup>1</sup>; Julian Saba<sup>1</sup>; Marshall W. Bern<sup>2</sup>; David R Bush<sup>4</sup>; Marcia R Santos<sup>5</sup>; Hans Dewald<sup>6</sup>; Alexander R. Ivanov<sup>4</sup>; Barry L. Karger<sup>4</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Leiden University Medical Center, Leiden, Netherlands; <sup>3</sup>Protein Metrics, Palo Alto, CA; <sup>4</sup>Barnett Inst., Northeastern University, Boston, MA; <sup>5</sup>AB Sciex LLC, Brea, CA
- WP 066 **Online Enrichment and Decoupled LC Separation of Sialylated/Phosphorylated Glycans and Glycopeptides;** Serenus Hua<sup>1</sup>; Gregory Staples<sup>2</sup>; Youngsuk Seo<sup>1</sup>; Myung Jin Oh<sup>1</sup>; Rudolf Grimm<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>AGRS, Chungnam National University, Daejeon, Korea; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 067 **Dynamics of Residue-Specific Chromatin O-GlcNAcylation *in vivo*;** Xiaoshi Wang; Benjamin A Garcia; University of Pennsylvania, Philadelphia, PA
- WP 068 **A Seamless Workflow for Comprehensive Analysis of the Mucin-Type O-linked Glycoproteome;** Jun Zhu<sup>1</sup>; Kai Cheng<sup>1</sup>; Jin Wenhai<sup>2</sup>; Fangjun Wang<sup>1</sup>; Mingming Dong<sup>1</sup>; Mingliang Ye<sup>1</sup>; Christie Hunter<sup>3</sup>; Hanfa Zou<sup>1</sup>; <sup>1</sup>Dalian Institute of Physical Chemistry, Dalian, China; <sup>2</sup>AB SCIEX China, Shanghai, China; <sup>3</sup>AB SCIEX, USA, Foster City, CA
- WP 069 **The Identification and Characterization of a General Protein O-glycosylation System within the Burkholderia cepacia Complex;** Nichollas Scott<sup>1</sup>; Julian Saba<sup>2</sup>; Helene Cardasis<sup>3</sup>; Leonard Foster<sup>1</sup>; Jon Dennis<sup>4</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada; <sup>2</sup>Thermo Fisher Scientific, Montreal, QC; <sup>3</sup>Thermo Scientific, New York, NY; <sup>4</sup>University of Alberta, Edmonton, Canada
- WP 070 **A Data-Independent Acquisition Strategy on the Q Exactive for Monitoring GALNT2-mediated APOCIII Glycosylation in Cell Culture;** Iwao Yamada<sup>1,2</sup>; Hideo Yoshida<sup>1,2</sup>; Sasha A. Singh<sup>1</sup>; Masanori Aikawa<sup>1</sup>; <sup>1</sup>Brigham and Women's Hospital, Boston, MA; <sup>2</sup>Kowa Company, Ltd., Tokyo, Japan
- WP 071 **Characterization of O-GlcNAc Modified Sites on the RUNX2 Osteogenic Transcription Factor;** Alexis Nagel; Lauren Ball; MUSC, Charleston, SC
- WP 072 **A Multiple Reaction Monitoring Method to Specifically Characterize and Relatively Quantify the O-glycans of the Potential Biologic Lubricin;** Sarah Flowers<sup>1</sup>; Catherine Lane<sup>2</sup>; Liaqat Ali<sup>1</sup>; Tannin Schmidt<sup>3</sup>; Niclas Karlsson<sup>1</sup>; <sup>1</sup>Gothenburg University, Gothenburg, Sweden; <sup>2</sup>AB Sciex, Warrington, UK; <sup>3</sup>University of Calgary, Calgary, Canada
- WP 073 **Characterization of O-glycosyltransferase Reactions at the Molecular Level using nanoLCMS;** Tyler Stewart<sup>1</sup>; Kazuo Takahashi<sup>2</sup>; Milan Raska<sup>3</sup>; Milada Stuchlova Horynova<sup>3</sup>; Jan Novak<sup>1</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham, Birmingham, AL; <sup>2</sup>Fujita Health Univ., Toyoake, Japan; <sup>3</sup>Palacky University, Olomouc, Czech Republic
- WP 074 **Identification and Profiling of O-Glycans in Human Factor Xa by Advanced LC-MS/MS Techniques;** Jeremy Woods; Song Klapoetke; Michael Xie; KBI Biopharma, Durham, NC - North Carolina
- WP 075 **Glycopeptide CID MS/MS Analysis for Elucidation of the Impact of a Single Nucleotide Polymorphism on O-Glycan Microheterogeneity in Glycoprotein ITIH4;** Kevin B Chandler<sup>1</sup>; Miloslav Sanda<sup>2</sup>; Zuzana Brnakova<sup>2</sup>; Nathan Edwards<sup>3</sup>; Radoslav Goldman<sup>2</sup>; <sup>1</sup>Boston University, Boston, MA; <sup>2</sup>Georgetown University, Lombardi Cancer Center, Washington, DC; <sup>3</sup>Georgetown University, Department of Biochemistry, Washington, DC
- WP 076 **Applying improved ionization Procedures for O-glycopeptide Characterization of Arabinogalactan Protein 31 (AGP31) by Combined CID and ETD Fragmentation;** Kristina Marx<sup>1</sup>; Cecile Albenne<sup>2</sup>; Guillaume Tremintin<sup>3</sup>; Ulrike Schweiger-Hufnagel<sup>1</sup>; Pierre-Olivier Schmit<sup>4</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Université de Toulouse, Castanet-Tolosan, France; <sup>3</sup>Bruker Daltonics, Fremont, CA; <sup>4</sup>Bruker Daltonique S.A, Wissembourg, France
- WP 077 **Comprehensive N-glycomic Analysis of Clear Cell Renal Cell Carcinoma Plasma using Lectin Affinity HPLC Fractionation and Porous Graphitized Carbon LC-ESI-MS/MS;** Francisca Gbormittah<sup>1</sup>; William Hancock<sup>1</sup>; Othon Iliopoulos<sup>2</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA
- WP 078 **Sequential Ion Mobility Resolved Electron Transfer Dissociation and Collision Induced Dissociation of N-Glycopeptides;** Venkata Kollu<sup>1</sup>; Eric D. Dodds<sup>2</sup>; <sup>1</sup>Univ of Nebraska Lincoln, Lincoln, NE; <sup>2</sup>University of Nebraska - Lincoln, Lincoln, NE
- WP 079 **N-glycome Characterization of Secreted N-glycoproteins from a Panel of Eight Breast Cell Lines using Porous Graphitized (PGC) Carbon LC-MS/MS Analysis;** Ling Y. Lee<sup>1</sup>; Morten Thaysen-Andersen<sup>1</sup>; Mark S. Baker<sup>1</sup>; Nicolle H. Packer<sup>1</sup>; William S. Hancock<sup>1,2</sup>; Fanayan Susan<sup>1</sup>; <sup>1</sup>Macquarie University, Sydney, Australia; <sup>2</sup>Northeastern University, Boston, MA

- WP 080 **Targeting the N-Linked Glycome;** Ron Orlando<sup>1</sup>; Shujuan Tao<sup>1</sup>; Yining Huang<sup>1</sup>; Alex Harvey<sup>2</sup>; Barry Boyes<sup>3</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>GlycoScientific, LLC, Athens, Georgia; <sup>3</sup>Advanced Materials Technology Inc., Wilmington, DE
- WP 081 **The Effect of Antibody N-Glycosylation on FcRn Binding;** Jake Pawlowski<sup>1</sup>; Tyler Carlage<sup>2</sup>; Adriana Bajardi-Taccioli<sup>2</sup>; Damian Houde<sup>2</sup>; Marina Feschenko<sup>2</sup>; Li Zang<sup>2</sup>; Yelena Lyubarskaya<sup>2</sup>; <sup>1</sup>UMASS Amherst, Amherst, Massachusetts; <sup>2</sup>Biogen Idec, Cambridge, MA
- WP 082 **N-glycosylation Analysis in Human Scavenger Receptor CD36 by HCD Product Ion-Triggered ETD Mass Spectrometry;** Cleidiane G. Zamprônio<sup>1</sup>; David J. Sanders<sup>2</sup>; Kenneth J. Linton<sup>2</sup>; Andrew J. Creese<sup>1</sup>; Helen J. Cooper<sup>1</sup>; <sup>1</sup>School of Biosciences, University of Birmingham, Birmingham, UK; <sup>2</sup>Blizard Institute, Queen Mary University, London, UK
- WP 083 **High Speed HILIC HPLC for Glycan Analysis;** James Martosella<sup>1</sup>; Chris Rogers<sup>2</sup>; Oscar Potter<sup>3</sup>; Jia Liu<sup>1</sup>; <sup>1</sup>Agilent Technologies, Wilmington, de; <sup>2</sup>Agilent Technologies, Shropshire, UK; <sup>3</sup>Agilent Technologies, Santa Clara, CA
- WP 084 **Displacement Phenomena in Serial Lectin Affinity Chromatography;** Wonryeon Cho; *Wonkwang University, Iksan, Republic of Korea*
- WP 085 **Comparative Glycoproteomics Analysis of Influenza Virus Hemagglutinin using a Multidimensional LC-MS/MS Based Workflow;** Kshiti Khatri; Nancy Leymarie; Joseph Zaia; *Boston University, Boston, MA*
- WP 086 **Comprehensive Site-Specific Characterization of Glycoproteins using Enzymes of Varying Cleavage Specificities;** Carlito Lebrilla; Evan Parker; Michael Xin Sun; Jincui Huang; Andres Guerrero; *UC Davis, Davis, CA*
- WP 087 **Absolute Quantitation of Human Milk Proteins and Their Glycoforms using Multiple Reaction Monitoring (MRM);** Jincui Huang; Qiuting Hong; Rocchina Sabia; Carlito Lebrilla; *UC Davis, Davis, CA*
- WP 088 **An Integrated Top-Down and Bottom-Up Approach for Intact Glycoprotein Analysis of Aspergillus niger Secretome;** Yi Qu<sup>1</sup>; Li Cao<sup>2</sup>; Ju Feng<sup>1</sup>; Zhaorui Zhang<sup>1</sup>; Erika Zink<sup>1</sup>; Rui Zhao<sup>1</sup>; Shuang Deng<sup>1</sup>; Yuxuan Jiang<sup>1</sup>; Nikola Tolic<sup>1</sup>; Da Meng<sup>1</sup>; Uma Aryal<sup>3</sup>; Ljiljana Paša-Tolić<sup>1</sup>; Weijun Qian<sup>1</sup>; Marshall W. Bern<sup>4</sup>; Qibin Zhang<sup>1</sup>; Mary Lipton<sup>1</sup>; Jian-Zhi Hu<sup>1</sup>; Scott Baker<sup>1</sup>; Si Wu<sup>1</sup>; <sup>1</sup>PNNL, Richland, WA; <sup>2</sup>Morehouse school of medicine, Atlanta, GA; <sup>3</sup>Department of Biochemistry and Agronomy, West Lafayette, IN; <sup>4</sup>Protein Metrics, Palo Alto, CA
- WP 089 **Characterization of Hemopexin Glycosylation Associated with Liver Disease;** Miloslav Sanda; Julius Benicky; Radoslav Goldman; *Georgetown University, Lombardi Cancer Center, Washington, DC*
- Phosphopeptides: Enrichment Methods, 090 - 098**
- WP 090 **Fractionation Scheme Comparison for In-depth Phosphoproteome;** Qing-Run Li; Hong-Wen Zhu; Rong Zeng; *Shanghai Institutes for Biological Sciences, Shanghai, China*
- WP 091 **Anion-Exchange Chromatography of Tryptic Acidic Peptides and Phosphopeptides: WAX vs. SAX and AEX vs. ERLIC;** Andrew J Alpert<sup>1</sup>; Nikolai Mischerikow<sup>2</sup>; Karl Mechtler<sup>2</sup>; <sup>1</sup>PolyLC Inc., Columbia, MD; <sup>2</sup>IMP, Vienna, Austria
- WP 092 **Head-to-Head Comparison of Magnetic Beads for Phosphopeptide Enrichment;** Alex Campos; Laurence Brill; *Sanford-Burnham Medical Research Institute, La Jolla, CA*
- WP 093 **In-depth Characterization and Optimization of High pH Reversed-Phase Off-Line Fractionation for Phosphoproteomics;** Tanveer Bath; Chiara Francavilla; Jesper V Olsen; *University of Copenhagen, Copenhagen, Denmark*
- WP 094 **In vitro Evolution of DNA Aptamers Specific for the pTyr- and pSer-modified Polypeptides;** Yeva Mirzakhanyan; Jiri Misek; Andrej Luptak; Paul Gershon; *UC-Irvine, Irvine, CA*
- WP 095 **Everything All the Time: Comprehensive and Reproducible Phosphopeptide Enrichment using Fe<sup>3+</sup> - IMAC Columns;** Benjamin Ruprecht<sup>1</sup>; Heiner Koch<sup>1</sup>; Max Mundt<sup>1</sup>; Guillaume Medard<sup>1</sup>; Bernhard Kuster<sup>1</sup>; Simone Lemeer<sup>1,2</sup>; <sup>1</sup>Chair of Proteomics and Bioanalytics TUM, Freising, Germany; <sup>2</sup>Biomolecular Mass Spectrometry and Proteomics, Utrecht, Netherlands
- WP 096 **Characterization of Automated Sample Preparation Workflows Featuring Phosphopeptide Enrichment using TiO<sub>2</sub> Microchromatography Cartridges on a Precision Liquid Handler;** Jason Russell; Steve Murphy; *Agilent Technologies, Inc., Madison, WI*
- WP 097 **Thiol-phosphorylation for Monitoring Signaling to Chromatin;** Yumiao Han; Rosalynn Molden; Zuofei Yuan; Benjamin Garcia; *University of Pennsylvania, Philadelphia, PA*
- WP 098 **Development of a Multidimensional ERLIC/IMAC/TiO<sub>2</sub> Phosphoproteomic Method and Its Application to Kinase Pathway Analysis of PDGF-stimulated NIH 3T3 Cells;** Laura E. Edwards; Kevin Blackburn; Kyle G. Grant; Jason M. Haugh; Michael B. Goshe; *North Carolina State University, Raleigh, NC*
- Peptides: Quantitative Analysis (Applications to Peptide and Protein Targets), 099 - 121**
- WP 099 **LC-MS<sup>3</sup> Quantitation Methods for Synthetic Glycosylated PACAP Analogs;** Nicholas Laude; Bobbi Anglin; Robin Polt; Michael Heien; *University of Arizona, Tucson, AZ*
- WP 100 **Quantification of Linaclotide and its Bioactive Metabolite in Human Breast Milk using LC-MS/MS;** Qingguo Tian; Andreas Grill; Daksha Desai-Krieger; *Forest Laboratories, Inc., Farmingdale, NY*
- WP 101 **Development of an LC-MS/MS Method for pharmacokinetic Studies of the Anticoagulant Peptide Variegins;** Norrapat Shih<sup>1,2</sup>; R. Manjunatha Kini<sup>1</sup>; <sup>1</sup>Dept. of Biological Sciences, National University of Singapore, Singapore; <sup>2</sup>NUS graduate school for Integrative Sciences and, Engineering (NGS), Singapore
- WP 102 **Simultaneous Quantification of Active and Inactive Intracellular and Secreted GLP-1 Peptides from Cultured Cells by Selected Reaction Monitoring;** Michiko Amao; Yoshiro Kitahara; Ayaka Tokunaga; Kazutaka Shimbo; Yuzuru Eto; Naoyuki Yamada; *Ajinomoto Co., Inc, Kawasaki-Shi, Japan*
- WP 103 **A Sub-picogram (0.5 pg/ml) Level Quantification Method for Desmopressin in Human Plasma using Liquid Chromatography Electrospray Mass Spectrometry;** Rahul Baghla<sup>1</sup>; Swati Guttikar<sup>2</sup>; Dharmesh Patel<sup>2</sup>; Abhishek Gandhi<sup>2</sup>; Anoop Kumar<sup>1</sup>; Manoj Pillai<sup>1</sup>; <sup>1</sup>AB SCIEX, Gurgaon, India; <sup>2</sup>Veeda Clinical Research, Ahmadabad, India
- WP 104 **Quantification of Polypeptide MB56142 in Pig Lithium Heparin Plasma Using API-4000 LC-MS/MS Systems;** Guangchun Zhou; Nicole Roenker; Yong-Xi Li; *Medpace, Cincinnati, OH*

- WP 105 **LC/MS/MS Analysis of Active Ghrelin and the Inactive Isoform des-octanoyl-ghrelin;** David Broadwell; Derek Parks; Greg Waitt; Jon D. Williams; *GlaxoSmithKline, Research Triangle Park, NC*
- WP 106 **A Rapid and Sensitive Method for the Quantification of Goserelin in Human Plasma Using HPLC-MS/MS;** Meng Fang; Yinghe Li; Yifan Shi; *Alliance Pharma, Inc, Malvern, PA*
- WP 107 **Validation of a Quantitative LC/MS/MS Method to Measure SNAP 25 Cleavage by Botulinum A Toxin;** Kathleen Housman; Joshua Emory; Nizamettin Gul; Matthew Levit; Michael Adler; Jonathan Oyler; *USA Medical Research Institute of Chemical Defense, Aberdeen Proving Ground, MD*
- WP 108 **Quantification of Glargine and Its Metabolites in Human Plasma using a Hybrid Immunoaffinity Purification and LC-MS/MS Methodology;** Li Sun; Yang Xu; Melanie Anderson; Sheila Breidinger; Kevin Bateman; Eric Woolf; *PPDM, Merck Research Laboratories, West Point, PA*
- WP 109 **Deciphering the Temporal Proteome Response to PARP Inhibitor Treatment by Quantitative Proteomics;** Sara Charlotte Larsen; Rita Martello; Stephanie Jungmichel; Michael Lund Nielsen; *NNF Center for Protein Research, Copenhagen N, Denmark*
- WP 110 **Multiplexed LC-MS/MS Quantitation of Endogenous Allergens from Soybean Varieties;** Trent Oman; Ryan Hill; Barry Schafer; Guomin Shan; *Dow AgroSciences, Indianapolis, IN*
- WP 111 **Towards the Development of Novel Mycobacterium Tuberculosis Treatments: Determining the Mechanism of Secretion System Esx-3;** Jessica R. Chapman<sup>1</sup>; Joann Tufariello<sup>2</sup>; Laura E. Cole<sup>2</sup>; Emir Tinaztepe<sup>1</sup>; Jennifer Phillips<sup>1</sup>; William R. Jacobs<sup>2,3</sup>; Beatrix Ueberheide<sup>4</sup>; <sup>1</sup>NYULMC, New York, NY; <sup>2</sup>Albert Einstein College of Medicine, New York, NY; <sup>3</sup>Howard Hughes Medical Institute, Chevy Chase, MD; <sup>4</sup>New York University, New York, NY
- WP 112 **Metallomic Analysis of Metalloproteins within the Lyme Disease Pathogen *Borrelia burgdorferi*;** Matthew McIlvin<sup>1</sup>; J. Dafne Aguirre<sup>2</sup>; Hillary Clark<sup>2</sup>; Valeria Culotta<sup>2</sup>; Mak Saito<sup>1</sup>; <sup>1</sup>Woods Hole Oceanographic Inst., Woods Hole, MA; <sup>2</sup>Johns Hopkins University, Baltimore, MD
- WP 113 **Quantification of Lysine Malonylation in SIRT5 Knockout Animals using MS1 Filtering in Skyline;** Matthew Rardin<sup>2</sup>; Yuya Nishida<sup>1</sup>; Alexandria Sahu<sup>2</sup>; Eric Verdin<sup>2</sup>; Bradford W. Gibson<sup>2</sup>; <sup>1</sup>Gladstone Institute of Virology and Immunology, San Francisco, CA; <sup>2</sup>Buck Institute for Research on Aging, Novato, CA
- WP 114 **Proteomic Analysis Defines p53 and c-myc Activities as Effective Determinants of Chronic Myeloid Leukaemia Primitive Cell Survival;** Andrew Williamson<sup>1</sup>; Andrew Pierce<sup>1</sup>; Lisa Hopcroft<sup>2</sup>; Sheela Abraham<sup>2</sup>; Mark Aspinall-O'Dea<sup>1</sup>; Emma Carrick<sup>1</sup>; Tessa Holyoake<sup>2</sup>; Anthony Whetton<sup>1</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>University of Glasgow, Glasgow, UK
- WP 115 **Regulation of Protein Expression by Transcription Factors in *Saccharomyces cerevisiae*;** Gennifer Merrihew; Ying Sonia Ting; Michael J. Maccoss; *University of Washington, Seattle, WA*
- WP 116 **Two-dimensional LC/MS Analysis of CXCL12 in Plasma and Spleens of Patients with Myelofibrosis;** Sool Yeon Cho; Xiaoli Wang; Ronald Hoffman; John Roboz; *Ichan School of Medicine at Mount Sinai, New York, NY*
- WP 117 **Proteomic Analysis of Aged *C. elegans* Infected with *P. aeruginosa*;** Christina King<sup>1</sup>; Daljeet Singh<sup>1</sup>; Kyle Holden<sup>2</sup>; Annie Bea Govan<sup>1</sup>; Arjumand Ghazi<sup>2</sup>; Rena A.S. Robinson<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>Department of Pediatrics, Children's Hospital, Pittsburgh, PA
- WP 118 **Isolated Synaptosomes from Cortex and Striatum of Huntington Disease Mice Show Selective Loss of Synaptosome-Specific Proteins but No Bioenergetics Deficit;** Birgit Schilling; Ryan Ng; Jennifer Holcomb; Sung W. Choi; Anna Picca; Shana Katzman; Dylan J. Sorensen; Steven R. Danielson; Lisa M. Ellerby; Akos A. Gerencser; Martin D. Brand; Bradford W. Gibson; *Buck Institute for Research on Aging, Novato, CA*
- WP 119 **Kinetic Evaluation of Trypsin Digests of Apolipoprotein-A1: Implications for Quantitative Mass Spectrometry;** Scott Walmsley<sup>1</sup>; Yuxue Liang<sup>2</sup>; Xinjian Yan<sup>2</sup>; Stephen Stein<sup>2</sup>; Alexey Nesvizhskii<sup>1</sup>; <sup>1</sup>University of Michigan Department of Pathology, Ann Arbor, MI; <sup>2</sup>NIST, Gaithersburg, MD
- WP 120 **Method Development and Validation for Multiplexing Quantitation of Proteins in Soybean Tissues Using Tandem Mass Spectrometry (LC-MS/MS);** Ryan Hill; Trent Oman; Guomin Shan; Barry Schafer; *Dow AgroSciences, Indianapolis, IN*
- WP 121 **Quantitative Peptide Assays for Mass Spectrometry Applications;** Sijian Hou; Erum Raja; Paul Haney; Chris Etienne; Ramesh Ganapathy; Nikki Jarrett; Kay Opperman; Sergei Snovida; Bhavin Patel; John C. Rogers; *Thermo Fisher Scientific, Rockford, IL*
- Peptides: Quantitative Analysis (Advances in Sample Preparation and Workflow), 122 - 133**
- WP 122 **Optimization of Solid Phase Extraction Procedure for Leuprolide in Human Plasma;** Mei Li; Helen Deng Deng; Nicola Hughes; *Bioanalysis Laboratory Services (LifeLabs), Toronto, Canada*
- WP 123 **A High Sensitivity SPE LC/MS/MS Method for the Quantitation of Bradykinin in Human Plasma using Novel Integrated Microscale LC/MS Technology;** Mary Lame; Erin Chambers; Kenneth Fountain; *Waters Technologies Corporation, Milford, MA*
- WP 124 **A Highly Robust SPE-LC-MS/MS Workflow for Quantitation of Endogenous Amyloid Beta in Human Cerebrospinal Fluid;** Lei Xiong; Sahana Mollah; Kelli Jonakin; John McNamara; *AB SCIEX, Redwood City, CA*
- WP 125 **Novel Integrated Microfluidics Increase Sensitivity and Reduce Sample Volume in a Quantitative LC/MS Assay for rhPTH (Teriparatide) in Human Plasma;** Erin E. Chambers<sup>1,2</sup>; Mary Lame<sup>1</sup>; Kenneth Fountain<sup>1</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>King's College London, London, England
- WP 126 **Performance Investigation of a Novel Integrated Microfluidics Platform in High-Throughput LC-MS MRM Disease Protein Marker Verification;** Chris Hughes; Johannes Pc Vissers; Lee A Gethings; James Langridge; *Waters Corporation, Manchester, UK*
- WP 127 **The Evaluation of Micro Flow LC/MS/MS in Regulated Bioanalysis for the Quantitation of Peptide/Protein: Sensitivity, Precision, Accuracy and Ruggedness/robustness;** Moucun Yuan<sup>1</sup>; Morse Faria<sup>2</sup>; Dongliang Zhan<sup>1</sup>; Diego Cortes<sup>1</sup>; William R. Mylott<sup>1</sup>; Bruce Hidy<sup>1</sup>; Rand Jenkins<sup>1</sup>; <sup>1</sup>PPD, Richmond, VA; <sup>2</sup>Virginia Commonwealth University, Richmond, VA
- WP 128 **Ultra-Sensitive Quantitation of Exenatide with Micro-Flow LC Trap-and-Elute and High Resolution and Triple Quadrupole Mass Spectrometry Workflow;** Jinyuan Wang<sup>1</sup>; Daniel Warren<sup>2</sup>; Anthony Romanelli<sup>2</sup>; <sup>1</sup>AB SCIEX, Redwood City, CA; <sup>2</sup>AB SCIEX, Framingham, MA
- WP 129 **Boosting the Limits of SRM by Asn<sub>3</sub>;** An Staes<sup>1,2</sup>; Bart Ruttens<sup>1,2</sup>; Luminita Moruz<sup>3</sup>; Kris Gevaert<sup>1,2</sup>; <sup>1</sup>Department of Medical Protein Research, VIB, Gent, Belgium; <sup>2</sup>Department of Biochemistry, Ghent University, Gent, Belgium;

- <sup>3</sup>Department of Biochemistry and Biophysics, Stockh, Stockholm, Sweden
- WP 130 **Development of a nanoLC-MRM-based Quantitative Platform for Multiple Enzymes Associated with the Central Metabolic Pathway by using Ultra-Fast Mass Spectrometry;** Fumio Matsuda<sup>1</sup>; Tairo Ogura<sup>2</sup>; Nobuyuki Okahashi<sup>1</sup>; Atsumi Tomita<sup>1</sup>; Ichiro Hirano<sup>2</sup>; Hiroshi Shimizu<sup>1</sup>; <sup>1</sup>Osaka University, Suita, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan
- WP 131 **Functionalized Edman-type Reagents: Applications to Absolute Protein Quantification;** Ryo Satoh<sup>1</sup>; Masamitsu Maekawa<sup>2</sup>; Takaaki Goto<sup>1</sup>; Seon Hwa Lee<sup>1</sup>; Tomoyuki Oe<sup>1</sup>; <sup>1</sup>Tohoku University, Sendai, Japan; <sup>2</sup>Tohoku University Hospital, Sendai, Japan
- WP 132 **Strategies to Eliminate Anti-Drug Antibody (ADA) Interference due to Immunogenicity on Large Molecule Quantification by LC-MS/MS;** Daniel Villeneuve; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 133 **Absolute Targeted Quantitation of Proteins and Therapeutic Biologics using Integrated LC-MS Workflow;** Xin Zhu<sup>1</sup>; Vadi Bhat<sup>1</sup>; Nalini Sadagopan<sup>1</sup>; Ning Tang<sup>2</sup>; <sup>1</sup>Agilent Technologies, Wilmington, DE; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- Proteomics: Clinical Applications, 134 - 157**
- WP 134 **Variables Affecting the Quality of Digestion-based Protein Quantification: Implications of Enzyme Kinetics on Clinical Measurements;** Christopher Shuford; Martin Green; Russell Grant; *Laboratory Corporation of America, Burlington, NC*
- WP 135 **Immobilized Monolithic Enzymatic Reactors for Online Digestion of Proteins Secreted by Developing Human Embryos;** Wei-Qiang Chen<sup>1</sup>; Philipp Obermayr<sup>1</sup>; Urh Černigoj<sup>3</sup>; Jana Vidič<sup>3</sup>; Miloš Barut<sup>3</sup>; Tanja Panić-Janković<sup>1</sup>; Mikhail Gorshkov<sup>4</sup>; Goran Mitulović<sup>1,2</sup>; <sup>1</sup>Medical University of Vienna, Vienna, Austria; <sup>2</sup>Proteomics Core Facility, Medical University of Vienna, Vienna, Austria; <sup>3</sup>BIA Separations, Ajdovščina, Slovenia; <sup>4</sup>Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia
- WP 136 **Improving Prediction of IVF Success: Looking for Putative Biomarkers in IVF-Media upon Embryo Cultivation;** Tanja Panic-Jankovic<sup>3</sup>; Detlef Pietrowski<sup>1</sup>; Weiqiang Chen<sup>3</sup>; Rainer Schmid<sup>3</sup>; Mikhail V. Gorshkov<sup>2</sup>; Anna Lobas<sup>2</sup>; Goran Mitulovic<sup>3</sup>; <sup>1</sup>Medizinische Universitaet Wien, Wien, Austria; <sup>2</sup>INEPCP RAS, Moscow, Russian Federation; <sup>3</sup>Medical University of Vienna, KIMCL, Vienna
- WP 137 **Impact of Human Blood Specimen Collection Processing, and Storage on Protein Integrity and Implications for Use in Clinical Research;** Geun-Cheol Gil; Bich Nguyen; Yiyong Zhou; Julie Lamontagne; Xiaolei Xie; Michael Schirm; Rene Allard; Daniel Chelsky; Sushmita Mimi Roy; *Caprion Proteomics US LLC, Menlo Park, CA*
- WP 138 **A Comprehensive Proteomic Study on the Effect of General Anesthesia on Human Peripheral Blood Mononuclear Cells from Colon Cancer Patients;** Xiaolei Xie; Bich Nguyen; Geun-Cheol Gil; Aude Tartiere; Louiza Mahrouche; Yiyong Zhou; Rene Allard; Daniel Chelsky; Sushmita Mimi Roy; *Caprion Proteomics US LLC, Menlo Park, CA*
- WP 139 **Integrated Approaches for Analyzing U1-70K Cleavage in Alzheimer's disease;** Bing Bai<sup>1</sup>; Junmin Peng<sup>2</sup>; <sup>1</sup>Emory University, Atlanta, GA; <sup>2</sup>St.Jude Children's Research Hospital, Memphis, TN
- WP 140 **Identification and Validation of Platelet Low Biological Variation Proteins, Superior to GAPDH, Actin and Tubulin, as Tools in Clinical Proteomics;** Marianne Koch<sup>1</sup>; Ellen Umlauf<sup>2</sup>; Michael Veitinger<sup>2</sup>; Sheila Guterres<sup>2</sup>; Eduard Rappold<sup>4</sup>; Rita Babeluk<sup>2</sup>; Goran Mitulovic<sup>1</sup>; Rudolf Oehler<sup>3</sup>; Maria Zellner<sup>2</sup>; Roland Baumgartner<sup>2</sup>; <sup>1</sup>Medical University of Vienna, KIMCL, Vienna, Austria; <sup>2</sup>Med. Univ. Wien. Inst. of Physiology, Vienna, Austria; <sup>3</sup>Med. Univ. Wien, Surgical Res. Laboratories, Vienna, Austria; <sup>4</sup>Gerontology-2. Department, Otto Wagner Spital, Vienna, Austria
- WP 141 **Development and Clinical Validation of a Quantitative Mass Spectrometric Assay for PD-L1 Protein in FFPE NSCLC Samples;** Eunkyung An<sup>1</sup>; Wei-Li Liao<sup>1</sup>; Sheeno Thyparambil<sup>1</sup>; Adele Blackler<sup>1</sup>; Jaime Rodriguez<sup>2</sup>; Ravi Salgia<sup>3</sup>; Ignacio Wistuba<sup>2</sup>; Jon Burrows<sup>1</sup>; Todd Hembrough<sup>1</sup>; <sup>1</sup>OncoPlex Diagnostics, Rockville, MD; <sup>2</sup>MD Anderson Cancer Center, Houston, TX; <sup>3</sup>The University of Chicago, Chicago, IL
- WP 142 **Validation of Putative Proteomic Biomarkers of Clinically Significant Ureteropelvic Junction Obstruction (UPJO) via Mass Spectrometry;** John Froehlich; Richard Lee; *Children's Hospital Boston, Boston, MA*
- WP 143 **Proteomic Analysis of Biopsy Specimen Revealed the Profiles of Adenoma-Carcinoma Sequence of Colorectal Cancer;** Masaya Ono<sup>1</sup>; Masahiro Kamita<sup>1</sup>; Kumiko Kawasaki<sup>3</sup>; Masahiro Gomi<sup>3</sup>; Tomohiro Sakuma<sup>3</sup>; Yosuke Otake<sup>2</sup>; Taku Sakamoto<sup>2</sup>; Takeshi Nakajima<sup>2</sup>; Takahisa Matsuda<sup>2</sup>; Yutaka Saito<sup>2</sup>; Tesshi Yamada<sup>1</sup>; <sup>1</sup>Natl Cancer Ctr Research Institute, Tokyo, Japan; <sup>2</sup>Natl Cancer Ctr Hospital, Tokyo, Japan; <sup>3</sup>Mitsui Knowledge Industry Co.,Ltd., Tokyo, Japan
- WP 144 **Designing Targeted Quantitation Methods on a Nano HPLC Q Exactive System for Proteomic Analysis of Human Pancreatic Juice;** Jenny Chen<sup>1</sup>; Lewis Pannell<sup>2</sup>; Lindsay Schambeau<sup>2</sup>; Jana Rocker<sup>2</sup>; Gerald Koncar<sup>1</sup>; Reiko Kiyonami<sup>1</sup>; Keith Waddell<sup>1</sup>; <sup>1</sup>Thermo Scientific, San Jose, CA; <sup>2</sup>Mitchell Cancer Institute, Mobile, AL
- WP 145 **Proteomics Analysis of Urinary Exosomes for Sensitive Detection of Tubular Injury Markers in Cystinuria;** Ida Chiara Guerrera<sup>1</sup>; Matthieu Bourderioux<sup>1</sup>; Cerina Chhuon<sup>1</sup>; Thao Nguyen-khoa<sup>2</sup>; Bertrand Knebelmann<sup>2</sup>; Estelle Escudier<sup>3</sup>; Bernard Escudier<sup>4</sup>; Aleksander Edelman<sup>1</sup>; <sup>1</sup>INSERM, Paris, France; <sup>2</sup>APHP Necker, Paris, FR; <sup>3</sup>APHP Trousseau, Paris, FR; <sup>4</sup>Institut Gustave Roussy, Paris, FR
- WP 146 **Expression Analysis and Mass Spectrometric Structure Characterization Reveals Unknown Ezrin Truncations in Lymph Node Metastases of Breast Cancer Patients;** Claudia Röwer<sup>1</sup>; Christian George<sup>2</sup>; Toralf Reimer<sup>2</sup>; Bernd Gerber<sup>2</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>Proteome Center Rostock, Rostock, Germany; <sup>2</sup>Department of Obstetrics and Gynecology, Rostock, Germany
- WP 147 **iTRAQ-based Profiling and Label-Free Quantification Revealed a Panel of Regulated Proteins in Cervical Intraepithelial Neoplasia and Cervical Cancer Serum;** Alexander Boychenko<sup>1</sup>; Natalia Govorukhina<sup>1</sup>; Ate van der Zee<sup>2</sup>; Rainer Bischoff<sup>1</sup>; <sup>1</sup>Analytical Biochemistry, University of Groningen, Groningen, The Netherlands; <sup>2</sup>University Medical Centre, Groningen, The Netherlands
- WP 148 **Molecular Mechanisms of Synaptic Dysfunction in a Female Monkey Model of Depression;** Stephanie L. Willard<sup>1</sup>; Karin E. Borgmann-Winter<sup>1,2</sup>; Hoau-Yan Wang<sup>3</sup>; Matthew L. MacDonald<sup>4</sup>; Carol A. Shively<sup>5</sup>; Chang-Gyu Hahn<sup>1</sup>; <sup>1</sup>University of Pennsylvania Dept of Psychiatry, Philadelphia, PA; <sup>2</sup>Children's Hospital of Philadelphia, Philadelphia, PA; <sup>3</sup>CUNY Medical School, Pharmacology & Neuroscience, New York, NY; <sup>4</sup>University of Pittsburgh,



- Dept of Psychiatry, Pittsburgh, PA; <sup>5</sup>Wake Forest School of Med, Dept of Comparative Med, Winston-Salem, NC
- WP 149 **Proteomic Analysis Reveals Defects in Energy Metabolism in Asthenozoospermia**; Guo Yueshuai; Xin Niu; Tao Zhou; Zuomin Zhou; Xuejiang Guo; Jiahao Sha; Nanjing Medical University, Nanjing, China
- WP 150 **N-terminal Proteomics using TAILS on B-lymphocytes of a Patient with Combined Immunodeficiency**; Theo Klein<sup>1</sup>; Shan-Yu Fung<sup>1,2</sup>; Michael A. Blank<sup>3</sup>; Rosa Viner<sup>3</sup>; Stuart Turvey<sup>1,2</sup>; Christopher M. Overall<sup>1</sup>; <sup>1</sup>UBC, Vancouver, Canada; <sup>2</sup>Children and Family Research Institute, Vancouver, Canada; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA
- WP 151 **A Novel LC-MS Method for the Detection of Mutations Related to Antibiotic Resistance in Gyrase of Salmonella Isolates**; Lennard Dekker; Robbert-Jan Hassing; Lona Zeneyedpour; Theo Luidier; Wil Goessens; Erasmus Medical Center, Rotterdam, The Netherlands
- WP 152 **Integration of SWATH and MRM for Biomarker Discovery of Esophageal Squamous Cell Carcinoma**; Guixue Hou<sup>1,2</sup>; Liang Lin<sup>2</sup>; Xiaomin Lou<sup>1</sup>; Jin Zi<sup>2</sup>; Quanhui Wang<sup>1,2</sup>; Yulin Sun<sup>3</sup>; Xiaohang Zhao<sup>3</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>Beijing Institute of Genomics, CAS, Beijing, China; <sup>2</sup>BGI-Shenzhen, Shenzhen, China; <sup>3</sup>Cancer Institute, CAMS, Beijing, China
- WP 153 **Analysis of Surface Charge Influences in Interactions of Nanoparticles with Human-Bronchoalveolar-Lavage-Fluid using HPLC - MS/MS**; Theresa Kristl<sup>1</sup>; Matthew Boyles<sup>1</sup>; Martin Himly<sup>1</sup>; Romana Mikes<sup>2</sup>; Michael Studnicka<sup>2</sup>; Albert Duschl<sup>1</sup>; Christian Huber<sup>1</sup>; <sup>1</sup>University of Salzburg, Salzburg, Austria; <sup>2</sup>Paracelsus Medical University, Salzburg, Austria
- WP 154 **Evaluation of Targeted Proteomics Approaches for Optimal Quantification Strategies Applied to Drug Toxicity Profiling in 3D Tissue Models**; Asa Wahlander<sup>1</sup>; Nathalie Selevsek<sup>1</sup>; Jonas Grossmann<sup>1</sup>; Christian Panse<sup>1</sup>; Patrina Gunness<sup>2</sup>; Jens Kelm<sup>2</sup>; Ralph Schlapbach<sup>1</sup>; <sup>1</sup>Functional Genomics Center Zurich (FGCZ), Zurich, Switzerland; <sup>2</sup>InSphero AG, Schlieren, Switzerland
- WP 155 **A Rapid, Data Independent Acquisition Method for Population-Scale Proteome Barcoding using PCT-SWATH**; Tiannan Guo; Ruedi Aebersold; ETH Zurich, Zurich, Switzerland
- WP 156 **Automated Top-Down Mass Spectrometry of Hemoglobin for a Clinical Application**; Didia Coelho Graça<sup>1</sup>; Adelina E Acosta-Martin<sup>1,2</sup>; Wolfgang Jabs<sup>3</sup>; Ralf Hartmer<sup>3</sup>; Lorella Clerici<sup>2</sup>; Markus Meyer<sup>3</sup>; Kaveh Samii<sup>4</sup>; Yury O Tsybin<sup>5</sup>; Denis Hochstrasser<sup>1,2</sup>; Pierre Lescuyer<sup>1,2</sup>; Alexander Scherl<sup>1,2</sup>; <sup>1</sup>DHPS, Faculty of Medicine, Geneva University, Geneva, Switzerland; <sup>2</sup>DGLM, Geneva University Hospitals, Geneva, Switzerland; <sup>3</sup>Bruker Daltonics, Bremen, Germany; <sup>4</sup>Division of Hematology, Geneva University Hospital, Geneva, Switzerland; <sup>5</sup>BMSL, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- WP 157 **Label-Free Quantitation of Proteoforms by High-Throughput Top Down Proteomics for Biomarker Discovery**; Ioanna Ntai<sup>1</sup>; Kyung-Kon Kim<sup>1</sup>; Ryan Fellers<sup>1</sup>; Owen Skinner<sup>1</sup>; Bryan Early<sup>1</sup>; Richard Leduc<sup>2</sup>; Paul Thomas<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>Northwestern University, Evanston, IL; <sup>2</sup>Indiana University, Bloomington, IN
- Proteomics: New Approaches, 158 - 178**
- WP 158 **Description of a Novel Multi-Column / Multi-Dimensional nanoLC-MS/MS Platform for Automated Proteomic Analysis**; Steven Mullett<sup>1</sup>; Gary Valaskovic<sup>2</sup>; Mike Lee<sup>3</sup>; Nathan Yates<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, PA; <sup>2</sup>New Objective, Inc., Woburn, MA; <sup>3</sup>Milestone Development Services, Newtown, PA
- WP 159 **The Integration of Nano Scale Separation and Ionization for the Analysis of Complex Proteomes**; Peter Wang<sup>1</sup>; Zhou Hu<sup>2</sup>; Yang Yi-Ming<sup>2</sup>; Amanda Berg<sup>3</sup>; Gary A. Valaskovic<sup>3</sup>; <sup>1</sup>New Objective, Inc., Shanghai, China; <sup>2</sup>Shanghai Institute of Materia Medica, CAS, Shanghai, China; <sup>3</sup>New Objective, Inc., Woburn, MA
- WP 160 **Comparison of Shotgun Proteomic Methods For Small Scale Analysis of Complex Proteomes**; Lu Yu; Jyoti Choudhary; Wellcome Trust Sanger Institute, Cambridge, UK
- WP 161 **Online Affinity and Digestion: A Flexible and Robust Tool for the Characterization and Quantification of Proteins**; David Colquhoun<sup>1</sup>; Mohamed Nazim Boutaghou<sup>1</sup>; Rachel Lieberman<sup>1</sup>; Brian Feild<sup>1</sup>; Kevin W. Meyer<sup>2</sup>; Scott Kuzdzal<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Perfinity Biosciences, West Lafayette, IN
- WP 162 **Investigation of Fractionation Strategies for Intact Proteins Compatible with Top-down Mass Spectrometry**; Santosh G. Valeja<sup>1</sup>; Lichen Xiu<sup>2</sup>; Andrew J. Alpert<sup>3</sup>; Song Jin<sup>2</sup>; Ying Ge<sup>1,2</sup>; <sup>1</sup>Dept. of Cell & Regenerative Biology, UW-Madison, Madison, WI; <sup>2</sup>Department of Chemistry, UW-Madison, Madison, WI; <sup>3</sup>PolyLC Inc., Columbia, MD
- WP 163 **Fluorescence Complementation - Mass Spectrometry (FC-MS) for Identifying Direct Upstream Kinases**; Lingfei Zeng<sup>1</sup>; Chang-Deng Hu<sup>1</sup>; Weiguo Tao<sup>2</sup>; <sup>1</sup>Department of MCMP, Purdue University, West Lafayette, IN; <sup>2</sup>Department of Biochemistry, Purdue University, West Lafayette, IN
- WP 164 **Applicability of Partial Edman Degradation for MS/MS-free Protein Identifications in Shotgun Proteomics**; Anna A. Lobas<sup>1</sup>; Mark V. Ivanov<sup>1</sup>; Lev I. Levitsky<sup>1</sup>; Marina L. Pridatchenko<sup>1</sup>; Irina A. Tarasova<sup>1</sup>; Alexander V. Gorshkov<sup>2</sup>; Anatoly N. Verenchikov<sup>3</sup>; Mikhail V. Gorshkov<sup>1</sup>; <sup>1</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia; <sup>2</sup>N.N. Semenov's Institute of Chemical Physics, Moscow, Russia; <sup>3</sup>Mass Spectrometry Consulting Ltd., Bar, Montenegro
- WP 165 **Isolation of N-terminal Fragments from Cyanogen Bromide Cleaved Proteins after Combined Micro Liquid- and Solid Phase Derivatization**; Heinz Nika<sup>1</sup>; David Hawke<sup>2</sup>; Ruth Hogue Angeletti<sup>1</sup>; <sup>1</sup>Albert Einstein College of Medicine, Bronx, NY; <sup>2</sup>UT- M.D. Anderson Cancer Center, Houston, TX
- WP 166 **Dual Matrix-Based Immobilized Trypsin Combined magnetic Separation for Fast Proteolytic Digestion and In-depth Proteomics Analysis**; Wanjun Zhang; Chao Fan; Duan Feng; Weijie Qin; Xiaohong Qian; Beijing Proteome Reserach Center, Beijing, China
- WP 167 **A New Protease for Bottom Up and Middle-Down Proteomics**; Martial Rey<sup>1</sup>; Hynek Mrazek<sup>2</sup>; Petr Halada<sup>2</sup>; Petr Man<sup>2</sup>; David Schriemer<sup>1</sup>; <sup>1</sup>University of Calgary, Calgary, Canada; <sup>2</sup>Institute of Microbiology, Prague, Czech Republic
- WP 168 **Amino Acid Labeling With Tryptic Digestion: An Approach for Middle-Down Proteomics**; Nathanael F. Zinne; William K. Russell; David H. Russell; Texas A&M University, College Station, TX
- WP 169 **Introducing a Highly Selective Cleavage into Proteins in a Pseudo-Top Down Proteomics Approach to Produce Simplified and Predictable Fragmentation Spectra**; William Mcgee<sup>1</sup>; Zhen Wu<sup>1</sup>; Victoria Hedrick<sup>2</sup>; Lake Paul<sup>2</sup>; Mary Wirth<sup>1</sup>; Scott McLuckey<sup>1</sup>; <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Purdue Proteomics Facility, West Lafayette, IN

- WP 170 **A Thermostable, N-terminal Arginine and Lysine Specific Protease for  $\leq 1$  hr Digestion, Simplified Peptide Fragmentation and Increased MS/MS Sensitivity**; John P. Wilson<sup>1</sup>; Jonathan J. Ipsaro<sup>1</sup>; Samantha N. Peacock<sup>1</sup>; Keith D. Rivera<sup>1</sup>; Katharine H. Dusenbury<sup>2</sup>; Darryl J.C. Pappin<sup>1</sup>; <sup>1</sup>Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; <sup>2</sup>Dana Farber Cancer Institute, Boston, MA
- WP 171 **Chemical Cleavage for Middle-Down Analysis by Electron Transfer Dissociation**; Jan Fish; Jasparl Cheema; Elzbieta Piatkowska; Sarah R Hart; Keele University, Newcastle-Under-Lyme, UK
- WP 172 **Chemical Hydrolysis-Based Middle-Down Proteomics**; Kristina Srzentić<sup>1</sup>; Grigory Karateev<sup>1</sup>; Luca Fornelli<sup>1</sup>; Lev I. Levitsky<sup>2</sup>; Anna A. Lobas<sup>2</sup>; Elena Dubikovskaya<sup>1</sup>; Mikhail V. Gorskhov<sup>2</sup>; Unige A. Laskay<sup>1</sup>; Daniel Ayoub<sup>1</sup>; Yury O. Tsybin<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland; <sup>2</sup>Institute for Energy Problems of Chemical Physics, Moscow, Russia
- WP 173 **N-terminal Positional Proteomics using SPITC (4-sulfophenyl isothiocyanate) for Enrichment and Identification**; Yanjie Jiang<sup>1,2</sup>; James Madsen<sup>1</sup>; Victor Farutin<sup>1</sup>; Jonathan Lansing<sup>1</sup>; Richard Cole<sup>2,3</sup>; <sup>1</sup>Momenta pharmaceuticals, Cambridge, MA; <sup>2</sup>Department of Chemistry; University of New Orleans, New Orleans, LA; <sup>3</sup>Université Pierre et Marie Curie, Paris, France
- WP 174 **Automated Protein Digestion Workflows for MS-based Proteomics Applications**; Gunnar Dittmar<sup>1</sup>; Oliver Popp<sup>1</sup>; Guenter Boehm<sup>2</sup>; Andreas Bruchmann<sup>3</sup>; <sup>1</sup>MDC, Berlin, Germany; <sup>2</sup>CTC Analytics, Zwingen, Switzerland; <sup>3</sup>Axel Semrau GmbH, Sprockhovel, Germany
- WP 175 **Optimization of Dual Polarity Ultraviolet Photodissociation Proteomics**; Sylvester Greer; Jennifer Brodbelt; The University of Texas, Austin, TX
- WP 176 **Higher Confidence Analysis of E. coli Lysate by Reducing Spectral Complexity Using 351 nm UVPD**; Scott Robotham; Joe Cannon; Jennifer Brodbelt; University of Texas at Austin, Austin, TX
- WP 177 **Specific Detection of Proteins in Biological Matrices by Targeting Cysteine-Containing Peptides with Visible Photodissociation in an Q-Exactive Mass Spectrometer**; Marion Girod; Jordane Biarc; Rodolphe Antoine; Philippe Dugourd; Jérôme Lemoine; University of Lyon, Villeurbanne, France
- WP 178 **Towards Cell-Type Specific Nuclear Proteomes from Human Neurodegenerative Disease Brain**; Eric Dammer; Duc Duong; Ian Diner; James Lah; Allan Levey; Nicholas Seyfried; Emory University, Atlanta, GA
- Protein Therapeutics: Quantitative Analysis, 179 - 200**
- WP 179 **Internal Standardization Approaches for Quantification of 25k Da Fusion Protein to Support Early Stage Drug Development by LC-MS**; Jean-Nicholas Mess<sup>1</sup>; Karl-Rudolf Erlemann<sup>2</sup>; Jerzy Pieczykolan<sup>3</sup>; Sebastian Pawlak<sup>3</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma Inc., Laval, QC, Canada; <sup>2</sup>InSymbiosis, Montreal, QC, Canada; <sup>3</sup>Adamed Group, Czosnów, Poland
- WP 180 **Impact of Oxidative Modifications on the Quantification of Intact Therapeutic Proteins by High Resolution Mass Spectrometry**; Louis-Philippe Morin; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 181 **Quantification of Growth Hormone Receptor Antagonist Pegvisomant by LC-MS/MS in Rat Plasma: Method Development Considerations for PEGylated Proteins**; Jonathan R. St-Germain; Jean-Nicholas Mess; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 182 **Analysis of Polysorbates in Biotherapeutic Products using Two-Dimensional HPLC Coupled with Mass Spectrometer**; William Hedgpeath; Kenichiro Tanaka; Shimadzu Scientific Instruments, Inc., Columbia, MD
- WP 183 **A Versatile Method using Immunoaffinity LC-MS/MS to Quantify Antigen Protein in Animal Studies of Monoclonal Antibody Therapeutics**; Ichio Onami; Miho Ayabe; Naoaki Murao; Masaki Ishigai; Chugai Pharmaceutical Company, Ltd., Gotemba, Japan
- WP 184 **LC-MS Method Development for Therapeutic Antibody Quantitation in Animal Plasma**; Qian Zhang<sup>1</sup>; Zhenlian Ke<sup>1</sup>; Daniel Spellman<sup>1</sup>; Nathan Hatcher<sup>1</sup>; Daniela Tomazela<sup>2</sup>; Maribel Beaumont<sup>2</sup>; Bernard Choi<sup>3</sup>; Jane Harrelson<sup>1</sup>; Kevin Bateman<sup>1</sup>; <sup>1</sup>Merck & Co., Inc., West Point, PA; <sup>2</sup>Merck & Co., Inc., Palo Alto, CA; <sup>3</sup>Merck & Co., Inc., Rahway, NJ
- WP 185 **The Optimization of Host-cell Protein Detection using Data-Independent SWATH-MS**; Randy J. Arnold; Eric Johansen; Justin Blethrow; AB Sciex, Redwood City, CA
- WP 186 **Automated High Throughput Peptide and Protein MRM Optimization for Pharmaceutical Method Development**; Ian Moore; Suma Ramagiri; AB SCIEX, Concord, Canada
- WP 187 **Quantitative Proteomic Analysis of Outer Membrane Vesicles (OMV) from Neisseria meningitidis**; Alessandro Vadi; Novartis Vaccines and Diagnostics, Siena, IT
- WP 188 **Method Validation and Sample Analysis of a Protein Drug Candidate in Monkey Serum Using LC-MS/MS**; yue zhao; Guowen Liu; aida angeles; Lora Hamuro; mark arnold; jim shen; Bristol-Myers Squibb Co., Princeton, NJ
- WP 189 **Relative Quantification of MABS Glycosylation Changes during Stability and Accelerated Degradation Studies using Stable-Isotope Labeling and UPLC-ESI-QTOF**; Silvia Millan Martin<sup>1</sup>; Cedric Delporte<sup>1</sup>; Natalia Navas<sup>2</sup>; Niaobh McLoughlin<sup>1</sup>; Jonathan Bones<sup>1</sup>; <sup>1</sup>NIBRT, Dublin, Ireland; <sup>2</sup>UGR (University of Granada), Granada, Spain
- WP 190 **Development of a High Resolution LC-MS Method for Absolute Quantitation of Hemagglutinin and Neuraminidase Proteins in Influenza Virus-Like Particle Vaccines**; Jingzhong (Tim) Guo; Yali Lu; Jingning Li; Ziping Wei; Erica Shane; Oleg Borisov; NovaVax, Rockville, Md
- WP 191 **A Streamlined Workflow for Characterizing Low Abundance Glycans on Therapeutic Proteins**; Michael Kimzey; Shiva Pourkaveh; Samngan Tep; Sybil Lockhart; Justin Hyché; Ted Haxo; Jo Wegstein; ProZyme, Hayward, CA
- WP 192 **A Simple and Robust Targeted Quantitative Method for Insulin and its Therapeutic Analogs**; Eric Niederkofler<sup>1</sup>; Scott Peterman<sup>2</sup>; Amanda Leber<sup>1</sup>; Kwasi Antwi<sup>1</sup>; Tara Schroeder<sup>2</sup>; Urban Kiernan<sup>1</sup>; Kemmons Tubbs<sup>1</sup>; Bryan Krastins<sup>2</sup>; Amol Prakash<sup>2</sup>; Jennifer L. Frahm<sup>3</sup>; Mary F Lopez<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Tempe, AZ; <sup>2</sup>Thermo Fisher Scientific, BRIMS, Cambridge, MA; <sup>3</sup>Thermo Fisher Scientific, San Diego, CA
- WP 193 **Surfactant-aided Precipitation/On-Pellet-Digestion (SOD) for Straightforward, Efficient and Reproducible Sample Preparation for Targeted Quantification of mAb in Plasma and Tissues**; Bo An<sup>1,2</sup>; Ming Zhang<sup>1,2</sup>; Jun Qu<sup>1,2</sup>; <sup>1</sup>SUNY at Buffalo, Buffalo, NY; <sup>2</sup>New York State Center of Excellence, Buffalo, NY, Buffalo, NY
- WP 194 **Direct Analysis of Cell Culture Media using Targeted Peptide Mapping to Analyze the Post-Translational Modifications of Recombinant Proteins**; Chris Barton; Jeong Lee; Xiaojun Lu; David Spencer; Mark Schenerman; Jihong Wang; MedImmune, Gaithersburg, MD
- WP 195 **Multiplex Quantitation of Reversible Cysteine Oxidation in Mouse Heart: Effects of Catalase Overexpression and Type-2 Diabetogenic Diet**; Chunxiang Yao; Jessica

- Behring; Deborah Siwik; Stephen Whelan; Catherine E. Costello; Wilson Colucci; Richard Cohen; Mark E. McComb; Markus Bachschmid; *Boston University School of Medicine, Boston, Ma*
- WP 196 **MS in QC: A Fully Compliant Multi-Attribute Quantitative Method for Quality Control and Release Testing of Biologics;** Sabrina Benchaar<sup>1</sup>; Richard Rogers<sup>2</sup>; Nancy Nightlinger<sup>2</sup>; Quanzhou Luo<sup>1</sup>; Amanda Miller<sup>2</sup>; Wenzhou Li<sup>1</sup>; Brittny Livingston<sup>2</sup>; Gang Huang<sup>1</sup>; Robert Bailey<sup>2</sup>; Ryo Komatsuzaki<sup>3</sup>; Jennifer Sutton<sup>3</sup>; Christoph Nickel<sup>3</sup>; Alain Balland<sup>2</sup>; <sup>1</sup>Amgen, Thousand Oaks, CA; <sup>2</sup>Amgen, Seattle, WA; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- WP 197 **Release Testing of Biotherapeutics by Mass Spectrometry with Automated Detection of Unexpected Features;** Richard Rogers<sup>1</sup>; Nancy Nightlinger<sup>1</sup>; Jennifer Sutton<sup>2</sup>; Sabrina Benchaar<sup>3</sup>; Alain Balland<sup>1</sup>; Robert Bailey<sup>1</sup>; <sup>1</sup>Amgen, Seattle, WA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA; <sup>3</sup>Amgen, Thousand Oaks, CA
- WP 198 **The Effects of Alternative Carbon Sources on CHO Cell Metabolism and Product Quality;** Peter Slade<sup>1</sup>; Guy Caspary<sup>1</sup>; Shilpa Nargund<sup>2</sup>; Arvia Morris<sup>1</sup>; <sup>1</sup>Amgen, Seattle, WA; <sup>2</sup>Amgen, Thousand Oaks, CA
- WP 199 **Evaluation of Label-free MS-based Relative Quantitation of Post-translational Modifications of Therapeutic proteins;** Hongji Liu; Qing Paula Lei; Michael Washabaugh; *MedImmune, Gaithersburg, MD*
- WP 200 **High Throughput Screening of Deubiquitylase Activity, Specificity and Inhibition by MALDI-TOF Mass Spectrometry;** Maria Stella Ritorto<sup>1</sup>; Richard Ewan<sup>1</sup>; Ana Perez-Oliva<sup>1</sup>; Axel Knebel<sup>1</sup>; Nicholas Morrice<sup>2</sup>; Dario Alessi<sup>1</sup>; Matthias Trost<sup>1</sup>; <sup>1</sup>MRC Protein Phosphorylation and Ubiquitylation Uni, Dundee, UK; <sup>2</sup>The Beatson Institute for Cancer Research, Glasgow, UK
- Protein Therapeutics: Structural Characterization, 201 - 216**
- WP 201 **Characterising and Mapping Regions of Self-Interaction and Oligomerisation of Monoclonal Antibodies using ESI-IMS-MS;** Paul W.A. Devine<sup>1</sup>; Daniel Higazi<sup>2</sup>; David Lowe<sup>2</sup>; Alison E. Ashcroft<sup>1</sup>; Sheena E Radford<sup>1</sup>; <sup>1</sup>University of Leeds, Leeds, UK; <sup>2</sup>MedImmune, Cambridge, UK
- WP 202 **Comprehensive Sequence and Post-translational Modifications Analysis of Monoclonal Antibody by Flash Digest and LC-High Resolution MS;** Hongxia (Jessica) Wang<sup>1</sup>; John O'Grady<sup>2</sup>; David Horn<sup>1</sup>; Zhiqi Hao<sup>1</sup>; Kevin Meyer<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Perfinity Biosciences, Inc, West Lafayette, IN
- WP 203 **Degradation Profiling of a Monoclonal Antibody using Multiple Fragmentation Techniques and a Novel Peptide Mapping Software;** Jie Qian; Mark Sanders; *Thermo Fisher Scientific, Somerset, NJ*
- WP 204 **Orthogonal Solutions for Determination of Charge Heterogeneity in Monoclonal Antibody;** M Sundaram Palaniswamy<sup>1</sup>; Suresh Babu<sup>1</sup>; Ravindra Gudihal<sup>1</sup>; Ning Tang<sup>2</sup>; <sup>1</sup>Agilent Technologies, Bangalore, India; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 205 **Reducing Time-to-Measurement of Monoclonal Antibodies Using Microfluidic LC/MS Approaches;** Gregory Staples; Hongfeng Yin; Kevin Killeen; *Agilent Laboratories, Santa Clara, CA*
- WP 206 **Variant Identification from Human Recombinant Erythropoietin by LC-MS/MS;** Jung-Keun Suh<sup>1</sup>; Hyong-Ha Kim<sup>2</sup>; <sup>1</sup>Korean German Institute of Technology, Seoul, South Korea; <sup>2</sup>Korea Research Institute of Standards and Science, Daejeon, Korea
- WP 207 **Novel Protein Targets of Indomethacin in BT474 Human Breast Cancer Cells using Proteomics;** Valeriy Shevchenko; Sergei Kovalev; Marat Taipov; Natalia Arnotskaya; Igor Kudryavtsev; *N. N. Blokhin Russian Cancer Research Center, Moscow, Russian Federation*
- WP 208 **Structural Elucidation of a Reference IgG1 Monoclonal Antibody by Ultrahigh-Resolution QTOF Mass Spectrometry;** Melissa Ly; Himakshi Patel; Keith Johnson; Heather DeGruttola; Daniel Haq; Andrew Saati; Lisa Marzilli; Jason Rouse; *Pfizer, Inc, Andover, MA*
- WP 209 **Comprehensive Disulfide Bond Characterization through Differential MS Analysis by LC-ESI QTOF MS;** Song Klapoetke; Hongwei Xie; *KBI, Durham, NC*
- WP 210 **Mass Spectrometric Characterization of Photo-induced Degradation of a Maytansinoid Antibody-Drug Conjugate (AMC);** Lintao Wang; Xuan Chen; Megan Ellis; Alexandru Lazar; *ImmunoGen Inc., Waltham, MA*
- WP 211 **Determination of Heroin Hapten Densities in Protein Conjugates: Comparison of MALDI-TOF MS, TNBS and Indirect Ellman Assay;** Mohamed Nazim Boutaghoul<sup>1</sup>; Oscar B. Torres<sup>2,3</sup>; Rashmi Jalah<sup>2,3</sup>; Brian J. Feild<sup>1</sup>; Scott A. Kuzdzal<sup>1</sup>; Gary R. Matyas<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instrument, Columbia, MD; <sup>2</sup>Lab. Adjuvant and Antigen Res. US Mil. HIV Res., Silver Spring, MD; <sup>3</sup>U.S. Military HIV Res. Prog, H. M. Jackson Found., Bethesda, MD
- WP 212 **Mapping Disulfide Bridges in Chemokines using ETD and CID;** Michael Pereckas; Kathleen R. Noon; Brian F. Volkman; Rebekah L. Gundry; *Medical College of Wisconsin, Milwaukee, WI*
- WP 213 **Detection of Trace Protein Impurities in a Commercial Recombinant Protein Therapeutic Using LC-MS/MS Label-free Quantitative Proteomics Techniques;** Thomas A. Shaler; Sophia Chen; Hua Lin; *SRI International, Menlo Park, CA*
- WP 214 **Stability Analysis of the NIST Monoclonal Antibody Candidate Reference Material;** Trina Formolo; John Schiel; Lisa Kilpatrick; Karen Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
- WP 215 **H/D Exchange Links Changes in Conformational Dynamics to Improved Pharmacokinetic Properties and Decreased Stability in an IgG1 mAb Triple Mutant;** Ranajoy Majumdar<sup>1</sup>; Reza Esfandiary<sup>3</sup>; Steven Bishop<sup>3</sup>; C Middaugh<sup>1</sup>; David Volkin<sup>1</sup>; David Weis<sup>2</sup>; <sup>1</sup>Department of Pharm. Chem., University of Kansas, Lawrence, KS; <sup>2</sup>Department of Chemistry, University of Kansas, Lawrence, KS; <sup>3</sup>Department of Formulation Sciences, MedImmune, Gaithersburg, MD
- WP 216 **Development of an On-Line Ion Exchange Chromatography/Mass Spectrometry Method for Characterization of Heterogeneity in Protein-Drug Conjugates;** Khaja Muneeruddin; Igor Kaltashov; *University of Massachusetts, Amherst, MA*
- H/D Exchange: Protein Structure Function, 217 - 231**
- WP 217 **Self-association Behavior Studies of Chaperone CsgE and Its Interaction with Major Curli Protein CsgA;** Hanliu Wang<sup>1</sup>; Qin Shu<sup>2</sup>; Carl Frieden<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>Mass Spectrometry Center, Chemistry Dept, Washington University in St. Louis, MO; <sup>2</sup>Biochemistry and Molecular Biophysics Dept., Washington University in St. Louis, MO
- WP 218 **The Combination of Molecular Dynamics, Amide Hydrogen Exchange, and Mass Spectrometry to Understand mAb Conformational Dynamics;** Benjamin Walters<sup>1</sup>; Thomas Patapoff<sup>1</sup>; Jennifer Zhang<sup>1</sup>; <sup>1</sup>Protein Analytical Chemistry, Genentech Inc., South San Francisco, CA; <sup>2</sup>Early Stage Pharmaceutical Dev., Genentech Inc., South San Francisco, CA
- WP 219 **Investigation of the Dynamics of the Translocase Motor SecA by Hydrogen Deuterium-Exchange Mass Spectrometry;** Malvina Papanastasiou<sup>1</sup>; Morten B. Trelle<sup>3</sup>;

- Alexandra Tsirigotaki<sup>2,4</sup>; Spyridoula Karamanou<sup>1,4</sup>; Thomas J.D. Jorgensen<sup>3</sup>; Anastassios Economou<sup>2,4</sup>; <sup>1</sup>IMBB, FoRTH, Iraklio, Crete, Greece; <sup>2</sup>IMBB, FoRTH, Dpt of Biology, UoC, Iraklio, Crete, Greece; <sup>3</sup>Dpt of Biochemistry & Molecular Biology, USD, Odense, Denmark; <sup>4</sup>Dpt of Microbiology and Immunology, KU Leuven, Leuven, Belgium
- WP 220 **Dynamics of the SH3 Domains of Tec Family Tyrosine Kinases by Hydrogen Exchange Mass Spectrometry;** Justin Roberts<sup>1</sup>; Sreya Tarafdar<sup>2</sup>; Thomas Wales<sup>1</sup>; Thomas Smithgall<sup>2</sup>; John Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA
- WP 221 **Probing Regulatory Domain Interactions in the Tec-family Tyrosine Kinase Btk using HXMS;** Thomas E. Wales<sup>1</sup>; Raji E. Joseph<sup>2</sup>; Amy H. Andreotti<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Iowa State University, Ames, IA
- WP 222 **Effects of 9cUAB30 Methyl Derivatives and Coactivator on the Structure of RXR by Hydrogen Deuterium Exchange Mass Spectrometry;** Emily Cowart; *University of Alabama at Birmingham, Birmingham, Alabama*
- WP 223 **Conformational Dynamics of Y-family DNA Polymerases are Related to Nucleotide Selection as Revealed by Hydrogen-Deuterium Exchange Mass Spectrometry;** Philip Nevin; John R. Engen; Penny J. Beuning; *Northeastern University, Boston, MA*
- WP 224 **HDX-MS for Calcium Binding Protein Secretagogin; Structural and Functional Studies of Secretagogin in Insulin Secretion;** Jae Jin Lee; Seo-Yun Yang; Kong-Joo Lee; *College of Pharmacy, Ewha womans univ., Seoul, South Korea*
- WP 225 **Structural and Functional Insights of Small Molecule Disruptors of the Glucokinase-Glucokinase Regulatory Protein Interaction by Hydrogen/Deuterium Exchange Mass Spectrometry;** Min Shen; Klaus Michelsen; Paul Schnier; *Amgen Inc., Thousand Oaks, CA*
- WP 226 **Probing the Conformational Dynamics of a Novel Kinase Induced by ATP and Substrate Binding by HDX-MS;** Jianzhong Wen<sup>1</sup>; Sheng Li<sup>2</sup>; Jeffrey Esko<sup>1</sup>; Jack E. Dixon<sup>1</sup>; <sup>1</sup>UC San Diego, San Diego, CA; <sup>2</sup>UCSD, La Jolla, CA
- WP 227 **Congo Red Induced Unfolding of Human Insulin by Pulsed Labeling Hydrogen-Deuterium Exchange Coupled with ESI and Mass Spectrometry;** Teerapat Rojsajakul; Fred King; *Department of Chemistry, West Virginia University, Morgantown, WV*
- WP 228 **Structural Characterization of Hsp70 Protein Complexes using Hydrogen Deuterium Exchange Mass Spectrometry;** Victoria A. Assimon<sup>1</sup>; Jennifer N. Rauch<sup>1</sup>; Terry Zhang<sup>2</sup>; Shenheng Guan<sup>2</sup>; Jason E. Gestwicki<sup>1</sup>; <sup>1</sup>Institute for Neurodegenerative Diseases, San Francisco, CA; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 229 **The Non-Native Code of Secreted Preproteins Investigated by HDX-MS and Native IM/MS;** Alexandra Tsirigotaki<sup>1,2</sup>; M. Papanastasiou<sup>3</sup>; A. Konijnenberg<sup>4</sup>; K. Chatzi<sup>1</sup>; M.B. Trelle<sup>5</sup>; T.J.D. Jørgensen<sup>5</sup>; F. Sobott<sup>4</sup>; S. Karamanou<sup>1,3</sup>; A. Economou<sup>1,2</sup>; <sup>1</sup>Dpt of Microbiology and Immunology, KU Leuven, Leuven, Belgium; <sup>2</sup>IMBB, FoRTH, Dpt of Biology, UoC, Iraklio, Crete, Greece; <sup>3</sup>IMBB, Forth, Iraklio, Crete, Greece; <sup>4</sup>Chemistry Department, U. Antwerpen, Antwerp, Belgium; <sup>5</sup>Dpt of Biochemistry and Molecular Biology, SDU, Odense, Denmark
- WP 230 **Allosteric Conformational Destabilization of CFTR Nucleotide Binding Domain 1 (NBD1) by the Cystic Fibrosis Mutation  $\Delta F508$ ;** Naoto Soya<sup>1,2</sup>; Ariel Roldan<sup>1</sup>; Miklos Bagdany<sup>1</sup>; Gergely Lukacs<sup>1,2</sup>; <sup>1</sup>Department of Physiology, McGill University, Montreal, Canada; <sup>2</sup>GRASP, McGill University, Montreal, Canada
- WP 231 **HDX and MS Reveals pH-dependent Conformational Changes of Monomeric and Dimeric Diphtheria Toxin T Domain;** Jing Li<sup>1</sup>; Mykola Rodnin<sup>2</sup>; Alexey Ladokhin<sup>2</sup>; Michael Gross<sup>1</sup>; <sup>1</sup>Washington University in St. Louis, St. Louis, MO; <sup>2</sup>University of Kansas Medical Center, Kansas City, KS
- Proteomics: Tissue, 232 - 241**
- WP 232 **A Highly Reproducible Ion-Current-Based Method Enabled a 44-plex, Large-Scale Investigation of Protein Expression Time Courses Induced by influenza A Infection;** Shichen Shen<sup>1</sup>; Jun Li<sup>1</sup>; Xiaomeng Shen<sup>1</sup>; Andrew Ng<sup>1</sup>; Eslam Nouri<sup>2</sup>; Sina Ghaemmaghami<sup>3</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>University at Buffalo, SUNY, Buffalo, NY; <sup>2</sup>University of California Los Angeles, Los Angeles, CA; <sup>3</sup>University of Rochester, Rochester, NY
- WP 233 **Quantitative Proteomics of Estrogenic Effects in the Rat Uterus *in vivo*;** Fatima Sahyouni; Szabolcs Szarka; Vien Nguyen; Katalin Prokai-Tatrai; Laszlo Prokai; *University of North Texas Health Science Center, Fort Worth, TX*
- WP 234 **Quantitative Proteomic Analysis of Rat Adrenal Medulla in Response to 2-deoxy-D-glucose;** Mehdi Mirzaei<sup>1</sup>; Masoud Zabet Moghaddam<sup>2</sup>; Lindsay Parker<sup>1</sup>; Phill Bokinieci<sup>1</sup>; Yunqi Wu<sup>1</sup>; Paul Haynes<sup>1</sup>; Ann Goodchild<sup>1</sup>; <sup>1</sup>Macquarie University, Sydney, Australia; <sup>2</sup>Texas Tech University, Lubbock, TX
- WP 235 **Quantitative Proteomic Analysis of Various Grades of Glioma Tissues Across Indian Patient Population;** Kishore Gollapalli<sup>2</sup>; Ravi Kumar Krovvidi<sup>1</sup>; Leo Bonilla<sup>1</sup>; sanjeeva Srivastava<sup>2</sup>; <sup>1</sup>Agilent Tech, Richland, WA; <sup>2</sup>Dept of Biosciences and Bioengineering, Mumbai, India
- WP 236 **High Pressure-Assisted Extraction for the Improved Proteomic Analysis of FFPE Tissue;** Carol B. Fowler<sup>1</sup>; Timothy J. Waybright<sup>2</sup>; Timothy D. Veenstra<sup>2</sup>; Timothy J. O'Leary<sup>3</sup>; Jeffrey T. Mason<sup>1</sup>; <sup>1</sup>Baltimore VA Medical Center, Baltimore, MD; <sup>2</sup>National Cancer Institute, Frederick, MD; <sup>3</sup>BLR&D Service, Veterans Health Administration, Washington, DC
- WP 237 **Evaluating the Effect of Formalin Fixation on Mass Spectrometry Based Proteomic Profiling;** Drexel Neumann<sup>1</sup>; Eric Dammer<sup>2</sup>; Duc Duong<sup>2</sup>; Nicholas Seyfried<sup>2</sup>; James A Atwood<sup>1</sup>; <sup>1</sup>Omni International, Inc., Kennesaw, GA; <sup>2</sup>Emory University, Atlanta, GA
- WP 238 **A Novel Approach for the Analysis of Membrane Proteins Applied to Glioma Stem Cell Xenografts;** Norelle Wildburger<sup>1</sup>; Cheryl Lichti<sup>1</sup>; Ekaterina Mostovenko<sup>1</sup>; Frederick Lang<sup>2</sup>; Joy Gumin<sup>2</sup>; Carol Nilsson<sup>1</sup>; <sup>1</sup>UTMB, Galveston, TX; <sup>2</sup>MD Anderson Cancer Center, Houston, TX
- WP 239 **Proteomics Analysis of Decellularized Biological Scaffolds for Tissue Engineering;** Qiyao Li<sup>1</sup>; Changying Ling<sup>2</sup>; Sinan Ozer<sup>3,4</sup>; Brian Frey<sup>1</sup>; Zhen Chang<sup>2</sup>; Basak Uygun<sup>3,4</sup>; Nathan Welham<sup>2</sup>; Lloyd Smith<sup>1</sup>; <sup>1</sup>Dept. of Chemistry, UW-Madison, Madison, WI; <sup>2</sup>Dept. of Surgery, UW-Madison, Madison, WI; <sup>3</sup>Center for Engineering in Medicine, Boston, MA; <sup>4</sup>Massachusetts General Hospital, Boston, MA
- WP 240 **A Proteomic Profiling Strategy for the Non-Human Primate Animal Model, Rhesus Monkey;** Jin-Gyun Lee<sup>1</sup>; Kimberly McKinney<sup>1</sup>; Yong-Yook Lee<sup>1</sup>; Haena Chung<sup>1</sup>; Antonis Pavlopoulos<sup>1</sup>; Kook Jung<sup>1</sup>; Woong-Ki Kim<sup>2</sup>; Marcelo Kuroda<sup>3</sup>; Sunil Hwang<sup>1</sup>; <sup>1</sup>Carolinas Healthcare System, Charlotte, NC; <sup>2</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>3</sup>Tulane University, Covington, LA
- WP 241 **Large Scale Kinome Analysis of Human Skeletal Muscle using ATP Probes and HPLC-ESI-MS/MS;** Yue Qi; Danjun Ma; Michael Caruso; Monique Lewis; Xiangmin Zhang; Wissam Al-Janabi; Divyasri Damacharla; Zhao Yang;

Rodney Berry; Abdullah Mallisho; Zaher Msallaty; Sorin Draghici; Assia Shisheva; Berhane Seyoum; Zhengping Yi; *Wayne State University, Detroit, MI*

#### Systems Biology: Quantitative Proteomics, 242 - 259

- WP 242 **Absolute Protein Quantitation of Bacterial Proteome using Super-SILAC and iBAQ Approaches;** Boumediene Soufi; Andreas Harst; Karsten Krug; Boris Macek; *Proteome Center Tuebingen, Tuebingen, Germany*
- WP 243 **Quantitative Proteomic and Systems Analysis of Cells in Response to External Stimuli;** Allison Galassie<sup>1</sup>; Parimal Samir<sup>2</sup>; Kristen Hoek<sup>2</sup>; Xinnan Niu<sup>2</sup>; Andrew Link<sup>2</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*Vanderbilt University School of Medicine, Nashville, TN*
- WP 244 **Tracking the Impact of Viral Infection on Cellular Organelle Remodeling using Quantitative Organelle Proteomics;** Pierre Jean Beltran; Rommel Mathias; Todd M. Greco; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- WP 245 **Uncovering Cytomegalovirus-Targeted Host Cellular Processes by Quantifying Changes in the Nuclear Proteome;** Dominique Carter<sup>1,2</sup>; Justin Reitsma<sup>1,2</sup>; Kathleen Noon<sup>1,3</sup>; Scott Terhune<sup>1,2</sup>; <sup>1</sup>*Medical College of Wisconsin, Milwaukee, Wisconsin*; <sup>2</sup>*Microbiology & Molecular Genetics, Milwaukee, WI* <sup>3</sup>*Biotechnology & Bioengineering Center, Milwaukee, WI*
- WP 246 **Quantitative Proteomics of MAOA-knockdown Prostate Cancer Cells;** Sheng-Ta Tsai<sup>1</sup>; Shok-Li Ng<sup>1</sup>; Kai-Yun Chen<sup>1</sup>; Ting-Jen Cheng<sup>1</sup>; Jason Boyang Wu<sup>2</sup>; Jean Chen Shih<sup>3</sup>; Chung-Hsuan Chen<sup>1</sup>; <sup>1</sup>*Genomics Research Center, Taipei, Taiwan*; <sup>2</sup>*Cedars-Sinai Medical Center, Los Angeles, CA*; <sup>3</sup>*University of Southern California, Los Angeles, CA*
- WP 247 **Quantitative Profiling of Differentially Regulated Proteins in Niemann-Pick Type C Disease;** Navin Raunivay; Kanagaraj Subramanian; John R. Yates; *The Scripps Research Institute, La Jolla, CA*
- WP 248 **Skin Aging – Identification of Proteins Related to *in situ* Aging of Human Dermal Fibroblasts using a Quantitative Proteomic Approach;** Daniel M. Waldera-Lupa<sup>1</sup>; Faiza Khalfallah<sup>2</sup>; Fritz Boege<sup>2</sup>; Kai Stühler<sup>1</sup>; <sup>1</sup>*Molecular Proteomics Laboratory, Düsseldorf, Germany*; <sup>2</sup>*Zentralinstitut für Klinische Chemie, Düsseldorf, Germany*
- WP 249 **Proteomic Analysis of Adipocytes in Response to Fructose and Glucose Treatment;** Yuan Gao; Vijayalakshmi Varma; Greg T. Nolen; Zhijun Cao; Li-Rong Yu; *National Center for Toxicological Research, FDA, Jefferson, AR*
- WP 250 **Elucidating Global Proteomic Changes Induced by the Epstein-Barr Virus Oncoproteins LMP1 and LMP2A;** Robert M. DeKroon<sup>1</sup>; Harsha P. Gunawardena<sup>2</sup>; Nancy Raab-Traub<sup>1</sup>; <sup>1</sup>*Lineberger Comprehensive Cancer Center, UNC-Chapel Hill, NC*; <sup>2</sup>*Program in Molecular Biology & Biotechnology, UNC-Chapel Hill, NC*
- WP 251 **Insights into Kinome Perturbation during NLRP3 Inflammasome Activation using an Isotope-Coded ATP-affinity Probe and Targeted Mass Spectrometry;** Preston Williams; Lei Guo; Yinsheng Wang; *University of California - Riverside, Riverside, CA*
- WP 252 **Label-free Quantitative Proteomics Study of the Synergistic Effect of Oxacillin and a Novel Erythromycin Derivative against Methicillin-Resistant *Staphylococcus aureus*;** Xiaofen Liu<sup>1</sup>; Pei-Jing Pai<sup>1</sup>; Yingwei Hu<sup>1</sup>; Daijie Chen<sup>2</sup>; Henry Lam<sup>1</sup>; <sup>1</sup>*Hong Kong University of Science and Technology, Hong Kong, China*; <sup>2</sup>*China State Institute of Pharmaceutical Industry, Shanghai, China*
- WP 253 **Interactome of a Jumping Gene;** Martin S. Taylor<sup>1</sup>; John LaCava<sup>2</sup>; Paolo Mita<sup>1</sup>; Kelly R. Molloy<sup>2</sup>; Donghui Li<sup>1</sup>; Emily M. Adney<sup>1</sup>; Hua Jiang<sup>2</sup>; Brian T. Chait<sup>2</sup>; Michael P. Rout<sup>2</sup>; Jef D. Boeke<sup>3</sup>; Lixin Dai<sup>1</sup>; <sup>1</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*; <sup>2</sup>*The Rockefeller University, New York, NY*; <sup>3</sup>*NYU Langone University School of Medicine, New York, NY*
- WP 254 **Proteomics Methods for Chinese Hamster Ovary (CHO) Cell Culture Optimization;** Gang Xiao; Sohye Kang; Pavel Bondarenko; Da Ren; *Amgen Inc., Thousand Oaks, CA*
- WP 255 **Proteomic Investigation of the Osmoregulatory Protein Interactome using the Mass Spectrometry-Cleavable Chemical Crosslinker DC4;** Kevin R. Ramkissoon<sup>1</sup>; Jenna F. Dumond<sup>1</sup>; Guanghui Wang<sup>2</sup>; Marjan Gucek<sup>2</sup>; Maurice B. Burg<sup>1</sup>; Joan D. Ferraris<sup>1</sup>; <sup>1</sup>*Systems Biology Center, NHLBI, NIH, Bethesda, MD*; <sup>2</sup>*Proteomics Core, NHLBI, NIH, Bethesda, MD*
- WP 256 **Proteomic Profiling of the Secretome upon Toll-like Receptor Stimulation;** Marijke Koppenol-Raab; Virginie Sjoelund; Aleksandra Nita-Lazar; *NIH/NIAID/LSB, Bethesda, MD*
- WP 257 **In-depth and Time-Resolved Dissection of Early Phosphoproteome and Ensuing Proteome Changes in Response to TGF- $\beta$ ;** Kirti Sharma<sup>1</sup>; Rochelle CJ D'souza<sup>1</sup>; Anna Korhonen<sup>2,4</sup>; Nagarajuna Nagaraj<sup>1</sup>; Chunaram Choudhary<sup>3</sup>; Peter ten Dijke<sup>2</sup>; Matthias Mann<sup>1,3</sup>; <sup>1</sup>*Max Planck Institute for Biochemistry, Martinsried (Near Munich), Germany*; <sup>2</sup>*Leiden University Medical Center, Leiden, The Netherlands*; <sup>3</sup>*University of Copenhagen, Copenhagen, Denmark*; <sup>4</sup>*University of Turku, Turku, Finland*
- WP 258 **Filamentous Growth Response of Yeast by Quantitative Phosphoproteomics;** Hye Kyong Kweon; Christian Shively; Anuj Kumar; Philip Andrews; *The University of Michigan, Ann Arbor, MI*
- WP 259 **Quantitative Analysis of HDAC6-regulated Proteome and Lys Acetylome;** Yue Chen<sup>1</sup>; Zhongyi Cheng<sup>1</sup>; Rui Hao<sup>2</sup>; Sangkyu Lee<sup>1</sup>; Tso-Pang Yao<sup>2</sup>; Yingming Zhao<sup>1</sup>; <sup>1</sup>*University of Chicago, Chicago, IL*; <sup>2</sup>*Duke University, Durham, NC*

#### Antibodies and Antibody: Drug Conjugates, 260 - 278

- WP 260 **Simultaneous Verification of Correct and Alternative Disulfide Connectivity in IgG3 Monoclonal Antibody using Extracted Ion Chromatograms of ETD Spectra;** Jude Lakubub; Daniel Clark; Zhikai Zhu; Eden Go; Heather Desaire; *University of Kansas, Lawrence, KS*
- WP 261 **Characterization of Monoclonal Antibodies by Middle-Down 193 nm Ultraviolet Photodissociation;** Victoria C. Cotham; Jennifer S. Brodbelt; *University of Texas at Austin, Austin, TX*
- WP 262 **Analysis of Monoclonal Antibodies, Aggregates, and their Fragments by Size Exclusion Chromatography Coupled with an Orbitrap Mass Spectrometer;** Shanhua Lin; Hongxia Wang; Zhiqi Hao; David Horn; Mark Tracy; Xiaodong Liu; *Thermo Fisher Scientific, Sunnyvale, CA*
- WP 263 **Structure Characterization of Intact Monoclonal Antibody using Orbitrap Tribrid Mass Spectrometer;** Terry Zhang; David Horn; Jenny Chen; Zhiqi Hao; *ThermoFisher, San Jose, CA*
- WP 264 **Middle-down Analysis of Monoclonal Antibody using Nano-flow Liquid Chromatography and a Novel Tribrid Orbitrap Mass Spectrometer;** Jie Qian<sup>1</sup>; Keith A. Waddell<sup>2</sup>; Zhiqi Hao<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Somerset, NJ*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*

- WP 265 **Monoclonal Antibody and Related Product Characterization under Native Conditions using a Benchtop Exactive Plus EMR Mass Spectrometer;** Yue Xuan<sup>1</sup>; Francois Debaene<sup>2</sup>; Johann Stojko<sup>2</sup>; Alain Beck<sup>3</sup>; Alain Van Dorsselaer<sup>2</sup>; Sarah Cianferani<sup>2</sup>; Maciej Bromirski<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific GmbH, Bremen, Germany; <sup>2</sup>University of Strasbourg, Strasbourg, France; <sup>3</sup>Pierr-Fabre, Strasbourg, France
- WP 266 **Highly Sensitive and Robust LC-MS Method for Therapeutic Monoclonal Antibody Analysis from Complex Matrices;** Joshua Nicklay<sup>1</sup>; Eric Niederkofler<sup>2</sup>; Urban Kiernan<sup>2</sup>; Kemmons Tubbs<sup>2</sup>; Scott Peterman<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific, Tempe, AZ; <sup>3</sup>Thermo Fisher Scientific BRIMS, Cambridge, MA
- WP 267 **Application and Advantages of HRMS in the Quantification of Therapeutic Monoclonal Antibodies: "The Rituximab Case Study";** Kevorik Mekhssian; Jean-Nicholas Mess; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*
- WP 268 **Liquid Chromatography-High Resolution Mass Spectrometry Bioanalytical Approach for the Quantification of Total Antibody-Drug Conjugate (ADC, DAR $\geq$ 0) in Rat Plasma;** Jean-Nicholas Mess<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Gary Impey<sup>2</sup>; Fabio Garofolo<sup>1</sup>; *Algorithme Pharma Inc., Laval, Quebec, Canada; <sup>2</sup>AB Sciex, Concord, Ontario, Canada*
- WP 269 **Intact Protein Separation by CE-UV/MALDI-MS for Top-Down Proteomics;** Michael Biacchi<sup>1</sup>; Alain Beck<sup>2</sup>; Yannis Francois<sup>1</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>LSMIS UMR-CNRS7140, University of Strasbourg, Strasbourg, France; <sup>2</sup>Centre d'immunologie Pierre Fabre, Saint-Julien en Genevois, Francois
- WP 270 **Accurate Identification of Drug Conjugation Sites on Antibody-Drug Conjugates using MS/MS;** Kelli Jonakin; Eric Johansen; St John Skilton; Justin Blethrow; *AB SCIEX, Redwood Shores, CA*
- WP 271 **Optimizing Chromatography and High Resolution Time-of-Flight Mass Spectrometry for Antibody-Drug Conjugate DAR Characterization;** Katherine Wright<sup>1</sup>; Shakey Quazi<sup>1</sup>; Brigitte Simons<sup>2</sup>; Dawn Dufield<sup>1</sup>; <sup>1</sup>Pfizer, Andover, MA; <sup>2</sup>AB SCIEX, Concord, ON
- WP 272 **Direct Measurement of Conjugated Drug on ADC with Cleavable Linker via Enzymatic Cleavage and LC/MS Analysis;** Brian Rago<sup>1</sup>; Sean Han<sup>1</sup>; Frank Barletta<sup>2</sup>; <sup>1</sup>Pfizer, Groton, CT; <sup>2</sup>Pfizer, Pearl River, NY
- WP 273 **Overcoming Challenges in Heightened Characterization for Antibody Drug Conjugates with Unique Approaches, New Methodologies and Ultrahigh-Resolution Mass Spectrometry;** Olga Friese<sup>1</sup>; Jacquelyn Smith<sup>1</sup>; James Carroll<sup>1</sup>; Jason Rouse<sup>2</sup>; <sup>1</sup>Pfizer, Inc., St. Louis, MO; <sup>2</sup>Pfizer, Inc, Andover, MA
- WP 274 **Characterization of Isoforms of Cysteine-Conjugated Antibody Drug Conjugates (ADCs) using On-line 2D-LC/MS;** Frank Kotch<sup>1</sup>; Robert Birdsall<sup>2</sup>; Henry Shion<sup>2</sup>; April Xu<sup>1</sup>; Thomas Porter<sup>3</sup>; Weibin Chen<sup>2</sup>; <sup>1</sup>Pfizer, Pearl River, NY; <sup>2</sup>Waters Corporation, Milford, MA; <sup>3</sup>Pfizer, Andover, MA
- WP 275 **Rapid Mass Analysis of the Minor Variants in IgG1 Antibodies by 2D-LC/Q Exactive System;** Jin Li; *Genentech, South San Francisco, CA*
- WP 276 **Rapidly Quantify Tryptophan Oxidation of an IgG1 Antibody Fragment by Parallel-Reaction-Monitoring Based HR/AM Approach on an UHPLC/Q Exactive System;** Weitao Jia; Jennifer Zhang; *Genentech Inc., South San Francisco, CA*
- WP 277 **Understanding of Stability and Structural Changes of Antibody-Drug-Conjugates (ADCs) *in vivo* by Affinity Capture LC-MS;** Dian Su; Carl Ng; Surinder Kaur; Keyang Xu; *Genentech Inc, South San Francisco, CA*
- WP 278 **Mass Spectrometric Characterization of Transglutaminase Based Site-Specific Antibody-Drug Conjugates;** Santiago Farias; Pavel Strop; Kathy Delaria; Magdalena Dorywalska Dorywalska; Meritxell Galindo Casas; David Shelton Shelton; Jaume Pons; Arvind Rajpal Rajpal; *Pfizer Rinat, San Francisco, CA*
- Lipids: Profile Analysis, 279 - 290**
- WP 279 **Development of an Ultrafast 15-sec Online SPE/MS Method for high Throughput Lipidomics Profiling of Human Serum Samples;** Sumit Shah; Michelle Romm; *Agilent Technologies, Inc., Wakefield, MA*
- WP 280 **Analysis of Lipids in Serum Using Continuous Tandem Spectra Acquisition and Customized Instrument Control Software;** Joseph A. Hankin<sup>1</sup>; Robert M. Barkley<sup>1</sup>; Jeff Brown<sup>2</sup>; Mike Morris<sup>2</sup>; Emmy Hoyes<sup>2</sup>; Richard Chapman<sup>2</sup>; Robert Murphy<sup>1</sup>; <sup>1</sup>University of Colorado Denver, Aurora, CO; <sup>2</sup>Waters Corporation, Manchester, UK
- WP 281 **Plasma Lipid Profiling using high Resolution Mass Spectrometry and Complementary Fragmentation Strategies;** Claire Daully<sup>1</sup>; Alexandre Seyer<sup>2</sup>; Samia Boudah<sup>3</sup>; Simon Broudin<sup>2</sup>; Christophe Junot<sup>3</sup>; Benoit Colsch<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, Courtaboeuf, France; <sup>2</sup>Profilomic SA, Boulogne-Billancourt, France; <sup>3</sup>CEA-Centre d'Etude de Saclay, Laboratoire d'étud, Gif-sur-Yvette, France
- WP 282 **Systematic Characterization of Experimental Conditions for High-Throughput Yeast Lipid Profiling by MALDI-MS;** Junya Nakamura<sup>1</sup>; Daichi Yukihira<sup>1</sup>; Hiroyuki Wariishi<sup>2</sup>; Yoshinori Fujimura<sup>2</sup>; Daisuke Miura<sup>2</sup>; <sup>1</sup>Grad. Sch. Biores. Bioenviron. Sci., Kyushu Univ., Fukuoka, Japan; <sup>2</sup>ICMRN, Kyushu Univ., Fukuoka, Japan; <sup>3</sup>Fac. Arts and Sci., Kyushu Univ., Fukuoka, Japan
- WP 283 **Profiling of Regioisomeric Triacylglycerols in Edible Oils by Supercritical Fluid Chromatography/Tandem Mass Spectrometry;** Takeshi Bamba<sup>1</sup>; Jae Won Lee<sup>2</sup>; Toshiharu Nagai<sup>2</sup>; Naohiro Gotoh<sup>3</sup>; Eiichiro Fukusaki<sup>1</sup>; <sup>1</sup>Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, Japan; <sup>2</sup>Tsukishima Foods Industry Co., Ltd, Tokyo, Japan; <sup>3</sup>Dept. Food Sci. Tech., Tokyo University of Marine, Tokyo, Japan
- WP 284 **Influence of the Silica Gel Layer Thickness on the Quality of TLC / MALDI Mass Spectra of Lipids;** Egidijus Machtejevas<sup>1</sup>; Michael Schulz<sup>1</sup>; Katerina Matheis<sup>2</sup>; Juergen Schiller<sup>3</sup>; <sup>1</sup>Merck Millipore, Merck KGaA, Darmstadt, Germany; <sup>2</sup>Merck KGaA, Department of Bioanalytical Chemistry, Darmstadt, Germany; <sup>3</sup>University of Leipzig, Faculty of Medicine, Leipzig, Germany
- WP 285 **Chromatography Couples through On-Line Liquid-Liquid Extraction with Electrospray Mass Spectrometry (CLL-MS) and Its Application to Lipoprotein Analysis;** Albert Koulman; Michael Osei; Julian L. Griffin; *Medical Research Council, Cambridge, UK*
- WP 286 **Pitfalls in Long-Term and Large-Scale LC-MS-based Lipidomics Studies of Human Plasma;** Tomas Cajka<sup>1</sup>; Brian DeFelice<sup>1</sup>; Carlos Leon<sup>1</sup>; William Wikoff<sup>1</sup>; Stanley Hazen<sup>2</sup>; Oliver Fiehn<sup>1</sup>; <sup>1</sup>UC Davis Genome Center, Davis, CA; <sup>2</sup>Cleveland Clinic Lerner Research Institute, Cleveland, OH
- WP 287 **Higher Resolution LC-MS and MS-MS Analysis of Lipid Extracts using Benchtop Orbitrap-based Mass Spectrometers and LipidSearch Software;** David Peake<sup>1</sup>; Junhua Wang<sup>1</sup>; Yasuto Yokoi<sup>2</sup>; Yingying Huang<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>MKI, Tokyo, Japan

- WP 288 **Characterization of Lipopolysaccharide Modifications in Select Antibiotic-Resistant Gram-negative Bacteria using Surface Acoustic Wave Nebulization Mass Spectrometry;** Lisa M. Leung; David R. Goodlett; Robert K. Ernst; *University of Maryland, Baltimore, Maryland*
- WP 289 **Comprehensive Analysis of Gangliosides by MALDI MS;** Sangwon Cha; Dongkun Lee; *HUFS, Yongin, South Korea*
- WP 290 **A Data-Independent LC-MS/MS Workflow for Eicosanoid Identification and Quantification;** Mark J. Sartain<sup>1</sup>; Anne E. Blackwell<sup>2</sup>; Yanan Yang<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Inc, Santa Clara, CA*; <sup>2</sup>*Agilent Technologies, Wilmington, DE*
- Forensics, 291 - 311**
- WP 291 **Chemical Imaging and Trace Detection of Explosives, Illicit Narcotics, and Inorganic Radionuclides by Desorption Electro-Flow Focusing Ionization Mass Spectrometry;** Thomas Forbes<sup>1</sup>; Edward Sisco<sup>2</sup>; Tim Brewer<sup>1</sup>; Greg Gillen<sup>1</sup>; <sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD*; <sup>2</sup>*University of Maryland, College Park, MD*
- WP 292 **Direct Analysis in Real Time Mass Spectrometric Analysis of the "Legal" Drug Alternative Kratom (*Mitragyna speciosa*);** Ashton Lesiak<sup>1</sup>; Robert Cody<sup>2</sup>; John Dane<sup>2</sup>; Rabi Musah<sup>1</sup>; <sup>1</sup>*University at Albany, Albany, New York*; <sup>2</sup>*JEOL USA, Inc., Peabody, MA*
- WP 293 **Sample Preparation in Coated 96 Deep Well Plates for Clinical and Forensic Applications;** Susanne Nussbaumer<sup>1</sup>; Wolfgang Weinmann<sup>1</sup>; Michal Svoboda<sup>2</sup>; Roland Geyer<sup>2</sup>; Stefan König<sup>1</sup>; <sup>1</sup>*Institut für Rechtsmedizin, Universität Bern, Bern, Switzerland*; <sup>2</sup>*Tecan Schweiz AG, Männedorf, Switzerland*
- WP 294 **Species Identification from Hair by Means of Spectral Library Searches;** Katleen Van Steendam; Ellen Scheerlinck; Maarten Dhaenens; Dieter Deforce; *Laboratory of Pharmaceutical Biotechnology, University Ghent, Belgium*
- WP 295 **Impact of Novel MS/MS<sup>ALL</sup> Acquisition and Processing Techniques on Forensic Toxicological Screening with a Q-TOF Tandem Mass Spectrometer;** David Cox; Michael J. Y. Jarvis; Evelyn McClure; Adrian Taylor; *AB SCIEX, Concord, Canada*
- WP 296 **Ultra-fast LDTD-APCI-MS/MS Analysis of Gamma-Hydroxybutyric Acid and Its Precursors in Beverages and Biological Samples;** Paul Fayad<sup>1</sup>; Sung Vo Duy<sup>1</sup>; André Lajeunesse<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>*Université de Montréal, Montreal, QC, Canada*; <sup>2</sup>*Université du Québec à Trois-Rivières, Trois-Rivières, QC, Canada*
- WP 297 **Identifying Common Spices in Concentrated Hydrogen Peroxide (CHP) Explosive Mixtures with GC/MS;** Lisa Lang; *ATF, Ammendale, U.S.A.*
- WP 298 **Automatic Screening of Major Impurities in Methamphetamine Samples Synthesized by Emde Method Using Accurate Mass Spectrometry;** Zhendong Hua<sup>1</sup>; Wei Jia<sup>1</sup>; Fengyun Pan<sup>2</sup>; <sup>1</sup>*Drug Intelligence and Forensic Center, Beijing, China*; <sup>2</sup>*AB SCIEX, Beijing, China*
- WP 299 **Useful Yield Determination for Nuclear Materials via Non-Contact Volume Analyses of Craters Generated by Ion Bombardment;** David Willingham; Benjamin E. Naes; Albert J. Fahey; *Pacific Northwest National Laboratory, Richland, WA*
- WP 300 **Dating of Fingerprints by GC-MS;** Stefanie Pleik<sup>1,2</sup>; Bernhard Spengler<sup>2</sup>; Steven Luhn<sup>1</sup>; Dieter Urbach<sup>1</sup>; Dieter Kirsch<sup>1</sup>; <sup>1</sup>*Bundeskriminalamt, Wiesbaden, Germany*; <sup>2</sup>*Justus Liebig University, Giessen, Germany*
- WP 301 **Issues of Sports Drug Testing - New Substances and Fake Doping Agents Characterized by Mass Spectrometry;** Mario Thevis<sup>1</sup>; Katja Walpurgis<sup>1</sup>; Andreas Thomas<sup>1</sup>; Andreas Lagojda<sup>2</sup>; Catharina Crone<sup>3</sup>; Martin Zeller<sup>3</sup>; Markus Kellmann<sup>3</sup>; Wilhelm Schänzer<sup>1</sup>; <sup>1</sup>*German Sport University, Cologne, Germany*; <sup>2</sup>*Bayer CropScience, Monheim, DE*; <sup>3</sup>*Thermo Fisher, Bremen, DE*
- WP 302 **Comparison of Mass Spectral Imaging Techniques for the Analysis of Latent Fingerprints;** Edward Sisco<sup>1</sup>; Thomas Forbes<sup>2</sup>; Shin Muramoto<sup>2</sup>; Greg Gillen<sup>2</sup>; <sup>1</sup>*University of Maryland, College Park, MD*; <sup>2</sup>*National Institute of Standards and Technology, Gaithersburg, MD*
- WP 303 **Proteomics Applications in Forensic Science;** Heyi Yang<sup>1</sup>; Kaylee Hershfeld<sup>2</sup>; Matthew Goldstein<sup>3</sup>; Bo Zhou<sup>1</sup>; Donald Siegel<sup>1</sup>; <sup>1</sup>*Office of Chief Med Exam, New York, NY*; <sup>2</sup>*Towson University, Towson, MD*; <sup>3</sup>*Virginia Commonwealth University, Richmond, VA*
- WP 304 **Is Synchrotron X-ray Analysis Really Non-destructive?;** Christopher Rollman<sup>1</sup>; Mehdi Moini<sup>2</sup>; <sup>1</sup>*Towson University, Baltimore, MD*; <sup>2</sup>*George Washington University, Washington, DC*
- WP 305 **Identification of Artificial Aging and Possible Forgery in Archaeological Silk;** Mehdi Moini<sup>1</sup>; Christopher Rollman<sup>2</sup>; Esther Methe<sup>3</sup>; Sumru Belger Krody<sup>3</sup>; <sup>1</sup>*George Washington University, Washington, DC*; <sup>2</sup>*Towson University, Baltimore, MD*; <sup>3</sup>*Textile Museum, Washington, DC*
- WP 306 **Analysis of Sulfonated Anthraquinone Dyes by ESI QTOF Tandem Mass Spectrometry;** Min Li; Nelson Vinueza; David Hinks; *North Carolina State University, Raleigh, North Carolina*
- WP 307 **Characterization of Complex Forensic Samples by Gas Chromatography – High Resolution Time-of-Flight Mass Spectrometry;** John Rorabeck<sup>2</sup>; David Alonso<sup>1</sup>; Joe Binkley<sup>1</sup>; <sup>1</sup>*Leco Corporation, St. Joseph, MI*; <sup>2</sup>*Berrien County Forensic Laboratory, Berrien Springs, MI*
- WP 308 **Sheathless Capillary Electrophoresis-Mass Spectrometry for the Forensic Analysis of Cathinone Drugs and Metabolites;** Adrian Taylor<sup>1</sup>; Michael J. Y. Jarvis<sup>1</sup>; John Hudson<sup>2</sup>; <sup>1</sup>*AB SCIEX, Concord, Canada*; <sup>2</sup>*SCIEX Separations, Brea, CA*
- WP 309 **Towards Fieldable Technologies for Comprehensive Forensic Analysis: Laser Ablation-Microwave Plasma Torch and Multimode Ambient Ionization Mass Spectrometry;** Kenyon Evans-Nguyen<sup>1</sup>; Hilary Brown<sup>1</sup>; Jennifer Speer<sup>1</sup>; John Gerling<sup>2</sup>; <sup>1</sup>*University of Tampa, Tampa, FL*; <sup>2</sup>*Gerling Applied Engineering, Modesto, CA*
- WP 310 **Portable MS Systems for Rapid Screening of Forensic Evidence at Clandestine Drug Operations;** Christopher Mulligan; Adam O'Leary; Seth Hall; Jamie Wieland; Michael Gizzi; *Illinois State University, Normal, IL*
- WP 311 **Calculation of Biogeographic Background and Identity Measurements Based on Identification of Non-Synonymous Single Nucleotide Polymorphism-Bearing Peptides in Archaeological Hair Samples;** Jonathan Hilmer<sup>1</sup>; Katherine Giddings<sup>1</sup>; Andrew Wilson<sup>2</sup>; Brian Bothner<sup>1</sup>; Glendon Parker<sup>3</sup>; <sup>1</sup>*Montana State University, Bozeman, MT*; <sup>2</sup>*University of Bradford, Bradford, England*; <sup>3</sup>*Utah Valley University, Orem, UT*

**Natural Products, 319 - 339**

- WP 319 **Metabolite Fingerprinting and Profiling of an Endophyte *Bartalinia pondoensis* Marinc of *Citrus aurantium* L. by using LC-MS;** Ahmed M. Zaher<sup>1</sup>; Makboul A. Makboul<sup>2</sup>; Ahmed M. Moharrum<sup>3</sup>; Angela I. Calderón<sup>1</sup>; <sup>1</sup>*Department of Pharmacal Science, Auburn University, Auburn, Alabama*; <sup>2</sup>*Department of Pharmacognosy, Assiut University, Assiut, Egypt*; <sup>3</sup>*Mycology Center, Assiut University, Assiut, Egypt*

- WP 320 **Mass Spectrometric Method for Rapid Dereplication of Natural Product Platensimycin and Its Congeners in Producer Extracts**; Kithsiri Herath<sup>1</sup>; Stephen Previs<sup>1</sup>; Thomas Roddy<sup>1</sup>; Athula Attygalle<sup>2</sup>; Sheo Singh<sup>1</sup>; <sup>1</sup>Merck & Co., Kenilworth, NJ; <sup>2</sup>Stevens Institute of Technology, Hoboken, NJ
- WP 321 **Techniques for DESI-MS Imaging of Fungal Cultures to Explore Chemical Interactions *in situ***; Vincent Sica; Huzefa Raja; Tamam El-Elimat; Nicholas Oberlies; UNCG, Greensboro, NC
- WP 322 **ESI Mass Spectral Study of (-)  $\Delta^9$ -tetrahydrocannabinol (THC) and Cannabidiol (CBD) Photochemical Reactions Initiated During On-Line Diode Array UV Measurements**; David Hasman<sup>1,2</sup>; Richard Smith<sup>3</sup>; <sup>1</sup>British Columbia Institute of Technology, Burnaby, British Columbia, Canada; <sup>2</sup>Procyon Research, Vancouver, British Columbia, Canada; <sup>3</sup>University of Waterloo, Waterloo, Ontario, Canada
- WP 323 **Characterization of Condensed Tannin Oligomers using MALDI-TOF MS and MALDI-TOF-TOF MS**; Patricia M. Peacock; E. I. DuPont de Nemours & Co., Wilmington, DE
- WP 324 **Evaluation of the Inhibitory Activity of Marine Natural Compounds against *Mycobacterium tuberculosis* Shikimate Kinase (MtSK) by LC-MS**; Johayra Simithy<sup>1</sup>; Douglas Goodwin<sup>1</sup>; Mark T. Hamann<sup>2</sup>; Angela I. Calderón<sup>1</sup>; <sup>1</sup>Auburn University, Auburn, AL; <sup>2</sup>The University of Mississippi, University, MS
- WP 325 **Further Characterization of the Nitrogenous Metabolome of Black Cohosh (*Actaea racemosa*)**; Dejan Nikolic; Tamara Cisowska; David C. Lankin; Shao-Nong Chen; Guido F. Pauli; Richard B. van Breemen; University of Illinois College of Pharmacy, Chicago, IL
- WP 326 **Determination of Betulin Purity and Impurity Profiling of Birch Bark Extracts**; Mikael Fridén; Uppsala University, Uppsala, Sweden
- WP 327 **Analysis of Nutraceuticals for Pesticides by Time of Flight Mass Spectrometry with Fragment Ion Confirmation**; Sue Dantonio<sup>1</sup>; Dawn Stickle<sup>2</sup>; <sup>1</sup>Agilent Technologies, Flatonia, TX; <sup>2</sup>Agilent Technologies, Wilmington, DE
- WP 328 **Tandem Mass Spectrometry Enables Characterization of the Major Phytoconstituents of "Sivakarantai" – *Sphaeranthus Amaranthoides* – An Indian Rejuvenator Herb**; S. Suhitha<sup>1</sup>; Mohan Kasi<sup>2</sup>; Rampriya Uthayakumar<sup>2</sup>; Venkat Manohar<sup>2</sup>; Kesavan Muthu<sup>1</sup>; K Rangasamy Siddhar<sup>3</sup>; Devadasan Velmurugan<sup>1</sup>; <sup>1</sup>CAS in Crystallography & Biophysics, University of Madras, Guindy campus, Chennai, India; <sup>2</sup>IICMS, Chennai, India; <sup>3</sup>Kongaran Herbal Vedic Academy, Palani, Tamil Nadu, India
- WP 329 **Improving Molecular Structural Determination of a Pantetheine Analogue by Combining the Results of Alkali Metal Adduction Assisted EID & CAD**; Samantha L. Benson<sup>1</sup>; David P. A. Kilgour<sup>2</sup>; Juan Wei<sup>1</sup>; Mark Barrow<sup>1</sup>; Manuela Tosin<sup>1</sup>; Peter B. O'Connor<sup>1</sup>; <sup>1</sup>University of Warwick, Coventry, UK; <sup>2</sup>University of Maryland, Baltimore, Baltimore, MD
- WP 330 **Investigation of an Unprecedented Natural Non-Enzymatic Reaction with Laser Ablation Electrospray Ionization (LAESI) Mass Spectrometry Technology**; Lin Du<sup>1</sup>; Haddon Goodman<sup>2</sup>; Robert Cichewicz<sup>1</sup>; <sup>1</sup>University of Oklahoma, Norman, OK; <sup>2</sup>Protea Biosciences, Inc., Morgantown, WV
- WP 331 **Development of a High-Throughput Ultrafiltration MS-based Assay for Ligands to Retinoid X Receptor**; Elisabeth Hersman; Michael Rush; Dejan Nikolic; Richard B. van Breemen; University of Illinois College of Pharmacy, Chicago, IL
- WP 332 **High Throughput Screening for 15-Lipoxygenase Ligands Utilizing Pulsed Ultrafiltration and UHPLC-MS/MS**; Michael Rush; Elizabeth Hersman; Dejan Nikolic; Richard van Breemen; UIC Dept of Medicinal Chemistry and Pharmacognosy, Chicago, IL
- WP 333 **Characterization of Biologically Active Compounds Produced by Isolated Strains of *Paenibacillus* with Multiple MS Platforms**; Ann M. Knolhoff; Jie Zheng; Melinda A. McFarland; John H. Callahan; Eric W. Brown; Timothy R. Croley; FDA/CFSSAN, College Park, MD
- WP 334 **Multi-detector Approach for Comparison and Differentiation of Similar Botanicals. UHPLC/UV/CAD/HRMS Analysis of *Ginkgo biloba* Extracts**; Kady Krivos; Procter & Gamble, Cincinnati, OH
- WP 335 **Improved LC/FT-ICR MS for Interrogation of Natural Product Biosynthetic Enzymes "In Action"**; Wendi Hale; Doug A. Hansen; Alison R. Narayan; David H. Sherman; Kristina Hakansson; University of Michigan, Ann Arbor, MI
- WP 336 **Identification and Differentiation of *Datura* Seed Species by Direct Analysis in Real Time Mass Spectrometry**; Rabi Musah<sup>1</sup>; Ashton Lesiak<sup>1</sup>; Robert B. Cody<sup>2</sup>; A. John Dane<sup>2</sup>; <sup>1</sup>University at Albany-SUNY, Albany, NY; <sup>2</sup>JEOL USA, Inc., Peabody, MA
- WP 337 **Characterization of Anthocyanins and Non-anthocyanin Polyphenols Using the Mass Spectrometric Behaviors of Anthocyanins in Negative Ionization Mode**; Jianghao Sun; Longze Lin; Pei Chen; USDA-ARS FCMDL, Beltsville, US
- WP 338 **Flow Injection Mass Spectrometric Fingerprinting (FIMS) Analysis for Differentiation of Three Black Cohosh Species**; Pei Chen<sup>1</sup>; Huihui Huang<sup>1</sup>; Jianghao Sun<sup>1</sup>; Joe-Ann McCoy<sup>2</sup>; James Harnly<sup>1</sup>; <sup>1</sup>USDA-ARS, Beltsville, MD; <sup>2</sup>3The NC Arboretum Germplasm Repository, Asheville, NC
- WP 339 **Characterizing Compositional Differences in Isolated Populations of Little-Devil Frog Using LC-MS and GC-MS Analysis of Alkaloids**; Gary Byrd<sup>1</sup>; Lauren O'Connell<sup>2</sup>; Sunia Trauger<sup>1</sup>; Luis Coloma<sup>3</sup>; <sup>1</sup>FAS Small Molecule MS Core Facility, Harvard Univ., Cambridge, MA; <sup>2</sup>FAS Center for Systems Biology, Harvard University, Cambridge, MA; <sup>3</sup>Centro Jambatu de Investigación y Con. de Anfibios, Quito, Ecuador

## Elemental Analysis, 340 - 346

- WP 340 **An Element-Specific Examination of the Presence, Formation, and Transformation of Volatile Halogenated Organic Species in Wastewater Extracts using GC-ICPMS**; Armando Durazo; Shane A. Snyder; University of Arizona, Tucson, AZ
- WP 341 **Simultaneous Analysis of Trace Elements in Carious Teeth by Laser Ablation Inductively Coupled Plasma Mass Spectrometry: Implications for Tooth Decay**; Khalid A. Al-Saad<sup>1</sup>; Mohamed A. Amr<sup>1</sup>; Elham Fawzi<sup>2</sup>; Saeed Almeer<sup>1</sup>; <sup>1</sup>Qatar University, Doha, Qatar; <sup>2</sup>Queen Medical Center, Doha, Qatar
- WP 342 **Speciation without Chromatography Using Hydride Generation for the Selective Determination of Inorganic Arsenic**; Ásta Pétursdóttir<sup>1,3</sup>; Stanislav Musil<sup>1,2</sup>; Nils Friedrich<sup>1</sup>; Andrea Raab<sup>1</sup>; Helga Gunnlaugsdóttir<sup>3</sup>; Eva Krupp<sup>1</sup>; Jorg Feldmann<sup>1</sup>; Jenny Nelson<sup>4</sup>; <sup>1</sup>TESLA-Trace Element Speciation Laboratory, Aberdeen, UK; <sup>2</sup>Institute of Analytical Chemistry of the ASCR, Brno, Czech Republic; <sup>3</sup>Matis, Environment and Genetics Department, Reykjavik, Iceland; <sup>4</sup>Agilent, Berkley, CA
- WP 343 **Differentiating Rice Varieties by Inductively Coupled Plasma/Mass Spectrometry Chemical Profiling**; Xinyi Wang; Peter B. Harrington; Ohio University, Athens, OH





- WP 345 **Digital Ion Trap Mass Spectrometry for Radiological Debris Analysis;** [Theresa Evans-Nguyen](#)<sup>1</sup>; Di Wang<sup>2</sup>; Friso H.W. Van Amerom<sup>3</sup>; <sup>1</sup>*Draper Laboratory, Tampa, FL*; <sup>2</sup>*Johns Hopkins School of Medicine, Baltimore, MD*; <sup>3</sup>*Mini-Mass Consulting, Inc., St. Pete Beach, FL*
- WP 346 **Use of Azo Dyes as Matrices and Chelators for the Detection of Metal Chelation Complexes using Matrix-Assisted Time-Of-Flight Mass Spectrometry;** Christopher Shiea<sup>1</sup>; Yi-Lun Chen<sup>2</sup>; Min Zong Huang<sup>2</sup>; [Yeou-Lih Huang](#)<sup>1</sup>; <sup>1</sup>*Dept. of Medical Lab Sci. & Biotech., KMU, Kaohsiung, Taiwan*; <sup>2</sup>*Dep. of Chemistry National Sun Yat-Sen University, Kaohsiung, Taiwan*
- Food Safety: Pesticides, 347 - 362**
- WP 347 **Rapid Detection of Pesticide Residues in Okra using Ultra Performance Liquid Chromatography and Tandem Mass Spectrometry;** Dimple Shah<sup>1</sup>; Mark Benvenuti<sup>1</sup>; [Kendon Graham](#)<sup>1</sup>; PMN Rajesh<sup>2</sup>; Antonietta Gledhill<sup>3</sup>; Jennifer Burgess<sup>1</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters India, Bangalore, India*; <sup>3</sup>*Waters Corporation, Manchester, UK*
- WP 348 **Quantitative Analysis of Pesticides in QuEChERS Extracts using APGC/MS/MS;** [Douglas Stevens](#)<sup>1</sup>; Dominic P T Roberts<sup>2</sup>; Ramesh Rao<sup>2</sup>; <sup>1</sup>*Waters Corporation, Milford, MA*; <sup>2</sup>*Waters Corporation, Wimslow, UK*
- WP 349 **Pesticide Screening of Food Samples using a Prototype Microfluidic Device;** [Gregory Roman](#); Lauren Mullin; Gareth Cleland; Dimple Shah; Jennifer Burgess; *Waters Corporation, Milford, MA*
- WP 350 **Multiresidue Pesticide Analysis from Dried Chili Powder using LC/MS/MS;** [Deepti Bhandarkar](#); Shrutu Raju; Rashi Kochhar; Shailesh Damale; Shailendra Rane; Ajit Datar; Pratap Rasam; Jitendra Kelkar; *Shimadzu Analytical (India) Pvt. Ltd., Andheri (E), Mumbai, Maharashtra, India*
- WP 351 **Highly Polar Pesticide Analysis in Food Samples by LC- MS/MS;** [David Baker](#)<sup>1</sup>; Mikaël Levi<sup>2</sup>; Eric Capodanno<sup>3</sup>; <sup>1</sup>*Shimadzu, Manchester, UK*; <sup>2</sup>*Shimadzu Corporation, Marnes-La-Vallée, France*; <sup>3</sup>*Phytocontrol, Nimes, France*
- WP 352 **Design of a Software Prototype for High Resolution MS Screening of Food Products;** [Hongliang \(Leo\) Xu](#); Ming Gu; Yongdong Wang; *Cerno Bioscience, Norwalk, CT*
- WP 353 **An Ultra-High Performance LC-QToF workflow for Multi-Residue Pesticide Screening Using Enhanced Confirmation Criteria;** Tony Drury; *Bruker Daltonics, Coventry, UK*
- WP 354 **New High-Throughput GC/MS Unknowns Analysis Workflow for Pesticide Screening in Food;** Lei Tao; Vadim Kalmeyer; Yoshimasa Tsunoi; [Marc Tischler](#); Harry Prest; *Agilent Technologies, Santa Clara, CA*
- WP 355 **Eliminating Matrix Effects during multi-Residue Pesticide Analysis by Extensive Dilution using a New Triple Quadrupole MS with Enhanced Sensitivity;** Thomas Glauner<sup>2</sup>; Dorothy Yang<sup>1</sup>; Bernhard Wuest<sup>3</sup>; Anabel Fandino<sup>1</sup>; [Na Pi](#)<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Santa Clara, CA*; <sup>2</sup>*Agilent Technologies GmbH, Waldbronn, N/A*; <sup>3</sup>*Agilent Technologies GmbH, Waldbronn, Germany*
- WP 356 **Development of a Multi-Targets for Pesticides in Tea Extracts using Liquid Chromatography-Tandem Mass Spectrometry with Dynamic MRM and Triggered MRM;** [Man-Yu Zhang](#)<sup>1</sup>; Yue Song<sup>1</sup>; Jin-Lan Sun<sup>1</sup>; Shao-Zhen Wang<sup>1</sup>; Wen-Yen Lee<sup>2</sup>; Shan-An Chan<sup>2</sup>; <sup>1</sup>*Agilent, Shanghai, China*; <sup>2</sup>*Agilent, Taipei, Taiwan*
- WP 357 **Screening for Known and Unknown Food Residues and Contaminants using Accurate Mass LC-MS/MS and Automatic data Processing;** [Andre Schreiber](#)<sup>1</sup>; David Cox<sup>1</sup>; Nick Zhu<sup>2</sup>; Cheng Yuan Cai<sup>2</sup>; <sup>1</sup>*AB SCIEX, Concord, Canada*; <sup>2</sup>*AB SCIEX, Shanghai, China*
- WP 358 **Simultaneous Analysis of Mycotoxins and Pesticides in Crude Extracts of Fruits and Grains by Micro Flow LC-MS/MS;** Takeo Sakuma; [Matthew Noestheden](#); Andre Schreiber; *AB SCIEX, Concord, ON*
- WP 359 **Using GC Triple Quadrupole MS for High Sensitivity, High Capacity and Selective Multi-Residue Pesticide Methods;** Paul Silcock<sup>1</sup>; Dwain Cardona<sup>2</sup>; Cristian Cojocariu<sup>2</sup>; [Jason Cole](#)<sup>2</sup>; Alexander Semyonov<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, Runcorn, UK*; <sup>2</sup>*Thermo Fisher Scientific, Austin, TX*
- WP 360 **Development of Retention Time Locked Accurate Mass EI Mass Spectral Database and Workflow for Pesticide Residue Screening Using GC/Q-TOF;** Samanta Uclés Duque<sup>1</sup>; Noelia Belmonte Valles<sup>1</sup>; Milagros Mezcua Peral<sup>1</sup>; Amadeo Fernández-Alba<sup>1</sup>; Klaus Wilmers<sup>2</sup>; Peter Fuerst<sup>2</sup>; [Sofia Aronova](#)<sup>3</sup>; Kai Meng<sup>3</sup>; Hong Chen<sup>3</sup>; Jennifer Gushue<sup>3</sup>; Maithilee Samant<sup>3</sup>; <sup>1</sup>*University of Almeria, Almeria, Spain*; <sup>2</sup>*Chemical and Veterinary Analytical Institute, Muenster, Germany*; <sup>3</sup>*Agilent Technologies, Inc., Santa Clara, CA*
- WP 361 **High-Throughput Determination of 5 Neonicotinoids in Honey using Differential Ion Mobility and LDTD-MS/MS;** [Sylvain Letarte](#); Gregory Blachon; Alex Birsan; Pierre Picard; Serge Auger; *Phytronix Technologies Inc., Quebec, QC*
- WP 362 **Evaluation of Different HILIC and Normal-Phase Approaches for the Liquid Chromatography/Mass Spectrometry-based Determination of Challenging Highly Polar Pesticides;** [Juan F Garcia-Reyes](#)<sup>1</sup>; Andrea Vass<sup>2</sup>; Patricia Pérez-Ortega<sup>1</sup>; Mihaly Dernovics<sup>2</sup>; Antonio Molina-Díaz<sup>1</sup>; <sup>1</sup>*University of Jaen, Jaen, Spain*; <sup>2</sup>*Corvinus University of Budapest, Budapest, Hungary*
- Nucleic Acids, 363 - 374**
- WP 363 **Inductive Based Fluidics Mass Spectrometry for the Analysis of RNAs Containing Modified Nucleosides;** [Robert Ross](#)<sup>1</sup>; Drew Sauter<sup>2</sup>; Patrick Limbach<sup>1</sup>; <sup>1</sup>*University of Cincinnati, Cincinnati, OH*; <sup>2</sup>*Nanoliter, LLC, Henderson, NV*
- WP 364 **Improving Mass Spectral Analysis of Oligoribonucleotides Obtained from Ribonuclease U2 Digests;** [Whitney Houser](#); Patrick Limbach; *University of Cincinnati, Cincinnati, Ohio*
- WP 365 **Improving the Detection of Thionucleosides by Derivatization With Benzylhalogenides;** Jef Rozenski; *Rega Institute, Leuven, Belgium*
- WP 366 **Identification and Quantification of Oxidatively Generated  $\alpha$ -2'-deoxynucleosides by Liquid Chromatography-Tandem Mass Spectrometry Coupled with the Stable Isotope-Dilution Method;** Nicholas J. Amato; Candace R. Guerrero; [Yinsheng Wang](#); *University of California, Riverside, CA*
- WP 367 **LC-MS/MS Detection of Oxidatively Induced 5-Methyl-2'-eoxycytidine Derivatives in Isolated DNA;** [Candace Guerrero](#); Yinsheng Wang; *UC Riverside, Riverside, CA*
- WP 368 **Characterization of DNA Adducts using Ultraviolet Photodissociation;** [Julia Aponete](#); Jennifer Brodbelt; *University of Texas Austin, Austin, TX*
- WP 369 **Gas-Phase Structural Characterization of Anionic RNA Oligonucleotides;** [Kevin Ilikea](#); Jessica Rabuck; Brandon Ruotolo; Kristina Hakansson; *University of Michigan, Ann Arbor, MI*
- WP 370 **Assessing Accuracy and Precision of DNA Composition Determination Based on Digestion to Deoxynucleotide Monophosphates and Mass Spectrometry Analysis;** [John-Emmett Mahon](#); Deepali Rathore; Eric D. Dodds; *University of Nebraska, Lincoln, NE*

- WP 371 **Determination of Antisense Oligonucleotide Purity after Correction LC-MS Analysis;** Jiongwei Pan; *PPD, Middleton, WI*
- WP 372 **Comprehensive Mass Spectrometry-Based Structural Determination of Small Subunit Ribosomal RNA: Characterization of N<sup>4</sup>-acetylcytidine and Identification of the Responsible Enzyme;** Masato Taoka<sup>1</sup>; Daisuke Ishikawa<sup>1</sup>; Yuko Nobe<sup>1</sup>; Hideaki Ishikawa<sup>2</sup>; Hiroshi Nakayama<sup>3,4</sup>; Yoshio Yamauchi<sup>1</sup>; Nobuhiro Takahashi<sup>2,4</sup>; Toshiaki Isobe<sup>1,4</sup>; <sup>1</sup>Department of Chemistry, Tokyo Metropolitan Univ., Tokyo, Japan; <sup>2</sup>Department of Applied Biological Science, Tokyo Un, Tokyo, Japan; <sup>3</sup>RIKEN, Wako, Japan; <sup>4</sup>CREST, JST, Tokyo, Japan
- WP 373 **Steps toward Understanding the Molecular Basis of Bladder Carcinogenesis. Validation of a nanoLC-ESI-MS/MS platform and Application to 4-aminobiphenyl Dosing Studies;** Joshua Klaene<sup>1</sup>; Arup Bhattacharya<sup>2</sup>; Yueheng Zhang<sup>2</sup>; James Glick<sup>1</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Roswell Park Cancer Institute, Buffalo, NY
- WP 374 **Comprehensive Ribonucleotide Modification Maps as Possible Tracking Tools for the Multistage Processes Involved in Cell Transformation from Normalcy to Malignancy;** Rebecca E. Rose; Jennifer Giza; D. Fabris; *The RNA Institute, University at Albany, Albany, NY*
- Ambient Ionization: Fundamentals, 375 - 388**
- WP 375 **Molecular Motion in Porous Substrates under Electrospray Ionization Conditions;** Bin Hu; Zhongping Yao; *Department of Applied Biology and Chemical Technol, The Hong Kong Polytechnic University, Hong Kong, P. R. China*
- WP 376 **A Comparative Study of Ionization Efficiency of Solvent Assisted Inlet Ionization (SAIL) versus Electrospray Ionization (ESI);** Madeline Fenner; Charles McEwen; *University of the Sciences, Philadelphia, PA*
- WP 377 **Ionization Mechanism of Positive-Ion Nitrogen Direct Analysis in Real Time;** Liguo Song; Zhenqian Zhu; John Bartmess; *Department of Chemistry, University of Tennessee, Knoxville, Tennessee*
- WP 378 **Comparison of desorption Atmospheric Pressure Photoionization and Direct Analysis in Real Time;** Riikka Räsänen<sup>1</sup>; Prabha Dwivedi<sup>2,3</sup>; Facundo M. Fernández<sup>2,3</sup>; Tiina J. Kauppila<sup>1</sup>; <sup>1</sup>University of Helsinki, Helsinki, Finland; <sup>2</sup>Georgia Inst. of Technology, Atlanta, GA; <sup>3</sup>Center for Chemical Evolution, Atlanta, GA
- WP 379 **Investigation of the Chemical Interactions of the Triad: Sample, Solvent and Surface and Their Effects in DESI-MS Imaging Analysis;** Elaine Cristina Cabral; Wagner Polcelli; Demian Iffa; *York University, Toronto, Canada*
- WP 380 **Characterization of Ion Transport in Desorption Electrospray Ionization using Time-of-Flight Secondary Ion Mass Spectrometry;** Shin Muramoto; Thomas Forbes; Matthew Staymates; Greg Gillen; *National Institute of Standards and Technology, Gaithersburg, MD*
- WP 381 **Development of Solid Probe Assisted Electrospray Ionization Mass Spectrometry;** Mridul Kanti Mandal<sup>1</sup>; Kenzo Hiraoka<sup>2</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, IN; <sup>2</sup>University of Yamanashi, Kofu, Yamanashi, Japan
- WP 382 **Relative Humidity Control for Reproducible Atmospheric Pressure Chemical Ionization Mass Spectrometry;** G. Asher Newsome<sup>1</sup>; Kevin J. Johnson<sup>2</sup>; <sup>1</sup>Nova Research, Alexandria, VA; <sup>2</sup>U.S. Naval Research Laboratory, Washington, DC
- WP 383 **Controlled *in situ* Formation of Molecular Ions, or Protonated Molecules, under Atmospheric Pressure Helium Plasma Ionization Mass Spectrometry (HePI-MS);** Athula B. Attygalle; Rekha Gangam; Julius Pavlov Julius Pavlov; Freneil Jariwala; *Stevens Institute of Technology, Hoboken, NJ*
- WP 384 **The Importance of Sample form and Surface Temperature in Plasma Assisted Desorption Ionisation Mass Spectrometry (PADI-MS);** Tara La Roche Salter; Ian Gilmore; Josephine Bunch; *National Physical Laboratory, Teddington, UK*
- WP 385 **First-Principle Transport Modeling of Protonated Peptides and Water Clusters in Ion Funnel and Nozzle-Skimmer Interfaces;** Sergey Gimelshein<sup>1</sup>; Natalia Gimelshein<sup>2</sup>; Taylor Lilly<sup>3</sup>; Rebecca Webb<sup>3</sup>; Eugene Moskovets<sup>4</sup>; <sup>1</sup>University of Southern California, Los Angeles, CA; <sup>2</sup>Gimel Inc., Montrose, CA; <sup>3</sup>University of Colorado Colorado Springs, Colorado Springs, CO; <sup>4</sup>MassTech Inc., Columbia, MD
- WP 386 **A VAMAS Interlaboratory Study for Desorption Electrospray Ionisation (DESI) Intensity Repeatability and Constancy;** Elzbieta Gurdak; Felicia M. Green; Martin P. Seah; Paulina D. Rakowska; Tara La Roche Salter; Ian S. Gilmore; Josephine Bunch; *National Physical Laboratory, Teddington, UK*
- WP 387 **Improved Analyte Sensitivity using Additives with Matrix-Assisted Inlet Ionization Mass Spectrometry;** Nicholas Chubaty; Charles McEwen; *University of the Sciences, Philadelphia, PA*
- WP 388 **Direct Profiling of Unsaturated Lipids in Tissue Using Extraction Spray Mass Spectrometry with Paternò-Büchi Reaction;** Yuan Su; Xiaoxiao Ma; Yu Xia; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- Ambient Ionization: Applications, 389 - 418**
- WP 389 **Evaluation of ASAP- and DART-MS for the Analysis of Sulfur-Containing Coal-Related Model Compounds;** Xing Fan<sup>1</sup>; Ai-Li Zheng<sup>1</sup>; Hao Li<sup>2</sup>; Xian-Yong Wei<sup>1</sup>; Zhong-Hai Ni<sup>1</sup>; Shou-Ze Wang<sup>1</sup>; Yun-Peng Zhao<sup>1</sup>; Zhi-Min Zong<sup>1</sup>; <sup>1</sup>China University of Mining & Technology, Xuzhou, China; <sup>2</sup>Los Alamos National Laboratory, Los Alamos, NM
- WP 390 **Paper Spray Mass Spectrometry (PS-MS) for the Quantification of Small Molecules Drugs in Plasma;** John Takyi-Williams<sup>1</sup>; Haiqing Gong<sup>1</sup>; Yang Wang<sup>2</sup>; Wenyang Jian<sup>2</sup>; Kai Tang<sup>1</sup>; <sup>1</sup>Nanyang Technological University, Singapore, Singapore; <sup>2</sup>Janssen, a division of Johnson & Johnson, Shanghai, China
- WP 391 **Forensic Application of Solvent Assisted Ionization Inlet Mass Spectrometry (SAIL-MS);** Lyla Hassan; *USciences, Philadelphia, PA*
- WP 392 **The Analysis of Omega-3 Fatty Acid Oxidation by DESI and ESI-MS;** Raymond West<sup>1</sup>; Rachel Marvin<sup>1</sup>; Dragan Isailovic<sup>1</sup>; Kenneth Hensley<sup>2</sup>; <sup>1</sup>University of Toledo, Toledo, OH; <sup>2</sup>University of Toledo Medical Center, Toledo, OH
- WP 393 **Applications of Desorption Corona Beam Ionization-Mass Spectrometry;** Yuki Hashi<sup>1</sup>; Shin-ichi Kawano<sup>1</sup>; Changkun Li<sup>1</sup>; Qian Sun<sup>1</sup>; Taohong Huang<sup>1</sup>; Tomoomi Hoshi<sup>2</sup>; Wenjian Sun<sup>3</sup>; <sup>1</sup>Shimadzu (China) Co., Ltd., Shanghai, China; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China
- WP 394 **Rapid Detection and Quantification with Novel Sorbent-Coated Mesh Substrate Using DART Mass Spectrometry;** Douglas B. Henderson; Johnny K. Ho; Yvette R. Hudson; William A. Harris; Danielle N. Dickinson; *Northrop Grumman, Linthicum Heights, MD*

- WP 395 **Single-probe Ionization Device: Development and Application to the Detection of Sulfated Post-Translationally Modified Proteins;** Rachel Vowcicefski; Ning Pan; Zhibo Yang; *University of Oklahoma, Norman, OK*
- WP 396 **Quantitative Analysis of Phosphoric Acid Esters in Aqueous Samples by Stir Bar Sorptive Extraction Combined with Isotope Dilution DART-HRMS;** Maxime Bridoux; Françoise Leprince; Frédéric Progent; Xavier Machuron-Mandard; *CEA, DAM, DIF, Arpajon, France*
- WP 397 **Exploration of Ambient Ionization Methods for Identification and Characterization of Biomarkers for Melanoma;** Michael T. Costanzo<sup>1</sup>; Candice Ulmer<sup>1</sup>; Shekher Mohan<sup>2</sup>; Nikolaus Gravenstein<sup>3</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>*Dept. of Chemistry, University of Florida, Gainesville, FL;* <sup>2</sup>*CTRND, College of Medicine, University of Florida, Gainesville, FL;* <sup>3</sup>*Dept of Anesthesiology, University of Florida, Gainesville, FL*
- WP 398 **Characterizing High-Valent Iron Porphyrin C-H Hydroxylation Reactions by Reactive Transmission Mode Desorption Electrospray Ionization Mass Spectrometry;** Kevin Peters; Kevin Parker; Richard Perry; *University of Illinois, Champaign, Illinois*
- WP 399 **Lipidomic Classification of Human Mammary Cancer Cells According to Metastatic Potential and Oncogene Expression by Desorption Electrospray Ionization Mass Spectrometry;** Heather Robison; Troy Comi; Seung Ryu; Richard Perry; *University of Illinois at Urbana-Champaign, Champaign, IL*
- WP 400 **Comparison of Paper Spray -MS/MS and Current Techniques for Screening Drugs of Abuse in Urine;** Joseph H Kennedy<sup>1</sup>; Justin Wiseman<sup>1</sup>; Brian C. Laughlin<sup>1</sup>; Greg Lyons<sup>1</sup>; Nicholas E Manicke<sup>2</sup>; Dianne Rampersaud<sup>3</sup>; Howard Lee<sup>3</sup>; <sup>1</sup>*Prosolia, Inc., Indianapolis, IN;* <sup>2</sup>*IUPUI, Indianapolis, IN;* <sup>3</sup>*Clinitox Diagnostix, Mississauga, Ontario*
- WP 401 **Characterization of Ammonium Nitrate Vapor with Flowing Atmospheric-Pressure Afterglow Mass Spectrometry;** G. Asher Newsome<sup>1</sup>; F. Lucus Steinkamp<sup>2</sup>; Braden C. Giordano<sup>3</sup>; <sup>1</sup>*Nova Research, Alexandria, VA;* <sup>2</sup>*National Research Council, Washington, DC;* <sup>3</sup>*U.S. Naval Research Laboratory, Washington, DC*
- WP 402 **Applications of Confined DART (Direct Analysis in Real Time) Ion Source for Online *in vivo* Analysis of Human Breath;** Yue Li; *The University of Maryland, College Park, MD*
- WP 403 **Effective Use of Direct Ionization Mass Spectrometry for Screening Food, Packaging & Cosmetics;** Luke Ackerman<sup>1</sup>; Karim Bentayeb<sup>2</sup>; Timothy Begley<sup>1</sup>; <sup>1</sup>*FDA Center for Food Safety, College Park, MD;* <sup>2</sup>*Analytical Chem., Univ. Zaragoza, Zaragoza, Spain*
- WP 404 **Rapid Determination of Clenbuterol in Pig's Urine by Direct Analysis in Real Time Tandem Mass Spectrometry;** Zong Yang<sup>1</sup>; Xiaokun Duan<sup>1</sup>; Charles C. Liu<sup>1</sup>; Qinghe Zhang<sup>2</sup>; Xiuqin Li<sup>2</sup>; Dazhou Chen<sup>2</sup>; <sup>1</sup>*ASPEC Technologies Limited, Beijing, China;* <sup>2</sup>*National Institute of Metrology, Beijing, China*
- WP 405 **Mass Spectrometry Imaging of Skin Wound Healing Biomarkers Using Laser Ablation Electrospray Ionization Mass Spectrometry (LAESI-MS);** Pamela Cantrell<sup>1</sup>; Callee Walsh<sup>1</sup>; Greg Kilby<sup>1</sup>; Tanya Shaw<sup>2</sup>; <sup>1</sup>*Protea Biosciences Group, Inc., Morgantown, WV;* <sup>2</sup>*St. George's, University of London, London, UK*
- WP 406 **Fingerprint of Anthocyanins from Two Varieties of Beans using ESI-MS and Direct Infusion;** Carlos Fidelis<sup>1</sup>; Renata Sancho<sup>2</sup>; Marcos N Eberlin<sup>1</sup>; Glauca Pastore<sup>2</sup>; <sup>1</sup>*Institute of Chemistry - University of Campinas, Campinas, Brazil;* <sup>2</sup>*Faculty of Food Eng. University of Campinas, Campinas, Brazil*
- WP 407 **Rapid Determination and Semi-Quantitative Analysis of Dicyandiamide in Milk by Direct Analysis in Real Time (DART) Time-Of-Flight Mass Spectrometry;** Liya Zhang<sup>1</sup>; Wei Yong<sup>2</sup>; Xiaogang Chu<sup>2</sup>; Tianyang Guo<sup>1</sup>; Yiyang Dong<sup>1</sup>; Xiaokun Duan<sup>3</sup>; Zong Yang<sup>3</sup>; Charles C. Liu<sup>3</sup>; <sup>1</sup>*Beijing University of Chemical Technology, Beijing, China;* <sup>2</sup>*Chinese Academy of Inspection and Quarantine, Beijing, China;* <sup>3</sup>*ASPEC Technologies Limited, Beijing, China*
- WP 408 **Rapid Screening of the SAMHSA (NIDA) Panel in Urine using DSA/TOF;** Avinash Dalmia<sup>1</sup>; Leslie Sullivan<sup>1</sup>; George Perkins<sup>1</sup>; Craig M. Whitehouse<sup>2</sup>; <sup>1</sup>*PerkinElmer, Shelton, CT;* <sup>2</sup>*PerkinElmer, Branford, CT*
- WP 409 ***In situ* Detection of Pnictogen Elements in Minerals by Ambient-Pressure Helium Plasma Ionization Mass Spectrometry;** Julius Pavlov; Athula Attygalle; *Stevens Institute of Tech, Hoboken, NJ*
- WP 410 **Detection and Quantification of Naturally Occurring Ions in Ethylene Flames and the Effect of Ethanol Addition on Polyaromatic Hydrocarbon Formation;** Thomas Bierkandt<sup>1</sup>; Denis A. Knyazkov<sup>2</sup>; Erdal Akyildiz<sup>1</sup>; Tina Kasper<sup>1</sup>; <sup>1</sup>*University of Duisburg-Essen, Duisburg, Germany;* <sup>2</sup>*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*
- WP 411 **Quantitative Assessment of Amino Acid Profiles in Foodstuffs with Microwave Hydrolysis and Desorption Electrospray Ionization Mass Spectrometry;** Jonathan Person; Christopher Mulligan; *Illinois State University, Normal, IL*
- WP 412 **Molecular Ionization from Carbon Nanotube Paper;** Rahul Narayanan<sup>1</sup>; Depanjan Sarkar<sup>1</sup>; R. Graham Cooks<sup>2</sup>; Pradeep T. I.; <sup>1</sup>*IIT Madras, Chennai, India;* <sup>2</sup>*Purdue University, West Lafayette, IN*
- WP 413 **A Novel Approach to Determine Tyrosine, 3-Chlorotyrosine and 3-Nitrotyrosine in Human Plasma by DART-MS/MS;** Yu-Qiao Song<sup>1</sup>; Jie Liao<sup>1</sup>; Cheng Zha<sup>1</sup>; Bin Wang<sup>1</sup>; Zong Yang<sup>2</sup>; Charles C. Liu<sup>2</sup>; <sup>1</sup>*Medical Exp & Anal Ctr PLA General Hospital, Beijing, China;* <sup>2</sup>*ASPEC Technologies Limited, Beijing, China*
- WP 414 **A Rapid Procedure Using Direct Analysis in Real Time-Mass Spectrometry to Screen for Adulterants in Herbal Dietary Supplements;** Xiaokun Duan<sup>1</sup>; Yu Zhao<sup>2</sup>; Lihui Yin<sup>2</sup>; Changqin Hu<sup>2</sup>; Zong Yang<sup>1</sup>; Charles C. Liu<sup>1</sup>; <sup>1</sup>*ASPEC Technologies Limited, Beijing, China;* <sup>2</sup>*National Institutes for Food and Drug Control, Beijing, China*
- WP 415 **Rapid Quantification of Drugs in Blood Using Solid Phase Microextraction Coupled to Thermal Desorption Electrospray Ionization Mass Spectrometry;** Chin-Hsiung Wang<sup>1</sup>; Min Zong Huang<sup>2</sup>; Jo-Han Chou<sup>2</sup>; Jentaie Shiea<sup>2</sup>; <sup>1</sup>*Protech Pharmaservices Co., Taipei, Taiwan;* <sup>2</sup>*National Sun Yat-Sen Univ., Kaohsiung, Taiwan*
- WP 416 **Authenticity Assessment of Imported Olive Oil using Direct Analysis in Real Time Mass Spectrometry;** Fengqi Wu<sup>1</sup>; Zhenfeng Yue<sup>1</sup>; Xiaokun Duan<sup>2</sup>; Zong Yang<sup>2</sup>; Honghui Hua<sup>1</sup>; Weidong Wu<sup>1</sup>; Charles C. Liu<sup>2</sup>; <sup>1</sup>*Entry-Exit Inspection and Quarantine Bureau, Shenzhen, China;* <sup>2</sup>*ASPEC Technologies Limited, Beijing, China*
- WP 418 **Atmospheric Pressure Photoionization: Establishing the Ionization Limits for Synthetic Organic and Organometallic Complexes;** Konstantin O. Zhurov; Laure Menin; Yury O. Tsybin; *Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*
- Diagnostic Clinical Chemistry, 421 - 453**
- WP 421 **Targeted Exposomics: Profiling Urinary Organic Acids;** Anthony Macherone<sup>1,2</sup>; Timothy Conielko<sup>1</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE;* <sup>2</sup>*Johns Hopkins University, Baltimore, MD*

- WP 422 **Using Fine Needle Aspiration Combined with Matrix-Assisted Laser Desorption Ionization/Time-of-Flight Mass Spectrometry to Diagnose Breast Cancer;** Hung Su<sup>1</sup>; Ya-Fei Bao<sup>1</sup>; Yi-Tzu Cho<sup>2</sup>; Jentaie Shiea<sup>1</sup>; Pei-Yung Nien<sup>3</sup>; Ya-Hui Chang<sup>3</sup>; Ming-Feng Hou<sup>3</sup>; <sup>1</sup>National Sun Yat-Sen Univ., Kaohsiung, Taiwan; <sup>2</sup>Yuh-Ing Junior College of Health Care & Management, Kaohsiung, Taiwan; <sup>3</sup>Cancer Research Center, Kaohsiung Medical Univ., Kaohsiung, Taiwan
- WP 423 **A Validated LC-MS/MS Method for Rapid Methotrexate Determination in Human Saliva and Its Application to an Excretion Evaluation Study;** Igor Rodin; Arkady Braun; Andrey Stavrianidi; Irina Ananieva; Oleg Shpigun; *MSU, Moscow, RU*
- WP 424 **Detecting Lymph Node Metastases *in-vivo* with Rapid Evaporative Ionization Mass Spectrometry;** Julia Balog<sup>1,2</sup>; Attila Enyedi<sup>3</sup>; Orsolya Nagyhazi<sup>3</sup>; Laszlo Toth<sup>3</sup>; Peter Varga<sup>2</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Medimass Ltd, Budapest, Hungary; <sup>3</sup>Debrecen University, Debrecen, Hungary
- WP 425 **Using MRM<sup>3</sup> for Removing Interferences in Plasma Metanephrines Analysis: The Quest for an Improved Clinical Service;** Michael Wright<sup>1</sup>; Rebecca Thomas<sup>1</sup>; Chris Hodgkins<sup>2</sup>; <sup>1</sup>SEALS, Prince of Wales Health Pathology, Sydney, Australia; <sup>2</sup>ABSciex, Sydney, Australia
- WP 426 **A HILIC-ESI-MS/MS Method for the Quantification of Free and Total Carnitine for Patient Care;** Tiffany Thomas; Jorge Sepulveda; Michael Pesce; *Columbia University Medical Center, New York, NY*
- WP 427 **An Improved Internal Standard Ratio Quantitation Technique for Clinical Diagnostics;** Brian Rappold; *Essential Testing, Collinsville, IL*
- WP 428 **Burden of Proof: Providing Clinical Confidence in the Face of Analytical Fallacies;** Martin Green; Christopher Shuford; Patricia Holland; Russell Grant; *Laboratory Corporation of America, Burlington, nc*
- WP 429 **Measurement of Low Level Endogenous Biomarkers for Use in Clinical Diagnostics;** Stacy Dee; Christopher Shuford; Matthew Crawford; Patricia Holland; Yvonne Wright; Martin Green; Russell Grant; *LabCorp, Burlington, NC*
- WP 430 **A Novel Approach for the Diagnosis of Gaucher Disease using Flow Injection Tandem Mass Spectrometry;** Jie Chen<sup>1</sup>; Michael Bennett<sup>1,2</sup>; <sup>1</sup>Children's Hospital of Philadelphia, Philadelphia, PA; <sup>2</sup>University of Pennsylvania, Philadelphia, PA
- WP 431 **An LC-ESI-MS/MS Method for Plasma Oxysterols Derivatized as Dimethylaminobutyrate Esters;** David W. Johnson<sup>1</sup>; Sara Boenzi<sup>2</sup>; <sup>1</sup>SA Pathology/Women's and Children's Hospital, North Adelaide, Australia; <sup>2</sup>Ospedale Pediatrico Bambino Gesù, Rome, Italy
- WP 432 **Simultaneous Measurement of 6 $\alpha$ -Hydroxy-Melatonin Sulfate and Cortisol in Human Urine by LC/MS/MS;** Bhasin Shalender; Xiaohong Chen; Gordon Harold Williams; Liming Peng; *Brigham and Women's Hospital, Boston, Massachusetts*
- WP 433 **A Fast and Effective Approach for the Analysis of Urinary Cortisol, Cortisone, Prednisolone and Prednisone using SPE and LC-MS/MS;** Xianrong (Jenny) Wei; Sean Orłowicz; *Torrance, ca*
- WP 434 **Development of a Sensitive Ultrapressure Liquid Chromatography Tandem Mass Spectrometry Method for Quantification of Dihydrotestosterone in Human Serum;** Karina Helena Morais Cardozo; Jessica Silva Salgueiro; Valdemir Melechco Carvalho; *Fleury Group, São Paulo, Brazil*
- WP 435 **Enhanced Application Stability utilizing SPLC-MS/MS;** Christopher L. Esposito<sup>1</sup>; Francois A. Espourteille<sup>2</sup>; <sup>1</sup>Thermo Scientific, Franklin, MA; <sup>2</sup>Thermo Fisher Scientific, Franklin, MA
- WP 436 **Quantitation of Reduced and Oxidized Glutathione and Cysteine in Acid-Preserved Samples by Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry;** Alan W. Taylor; Deborah Hobbs; Debbie J. Mustacich; Balz Frei; *Oregon State University, Corvallis, OR*
- WP 437 **Ultrafast Antiretroviral Drug Analysis in Human Serum;** Kari Schlicht; Vaughn Miller; William A. Lamarr; *Agilent Technologies, Wakefield, MA*
- WP 438 **Plasma Citric Acid Cycle Intermediates Levels by LC-MS/MS - A Prospective Application in Diagnosis of Mitochondrial Disorders;** Yana Sandler<sup>1,2</sup>; Richard Kelley<sup>1,2</sup>; <sup>1</sup>Kennedy Krieger Institute, Division of Metabolism, Baltimore, MD; <sup>2</sup>Johns Hopkins University, Department of Pediatrics, Baltimore, MD
- WP 439 **Direct Measurement of Pancreatic Polypeptide in Human Serum and plasma by Immuncapture-Liquid-Chromatography-Tandem Mass Spectrometry;** Hernando Escobar; Mark M. Kushnir; Alan L. Rockwood; A. Wayne Meikle; *ARUP Laboratories-University of Utah, Salt Lake City, UT*
- WP 440 **Fast and Robust LC-MS/MS Method for Determination of the Alcohol Biomarker Phosphatidylethanol (PEth) in Whole Blood using Automated Extraction;** Anders Blomgren; *Clinical Chemistry, Lund, Sweden*
- WP 441 **UPLC-MS/MS Multiplex Analysis for Mass or High-Risk Screening of Creatine Synthesis and Transport Disorders, Triple H Syndrome and OTC Deficiency;** Pamela Lavoie; Bruno Maranda; Christiane Auray-Blais; *Université de Sherbrooke/CRC-CHUS, Sherbrooke, Canada*
- WP 442 **Mass Spectrometry-Based Elemental Bioimaging and Speciation Analysis as Diagnostic Tools for Nephrogenic Systemic Fibrosis;** Uwe Karst; Kristina Wentker; Marvin Birka; Christoph Wehe; Michael Holtkamp; Michael Sperling; *University of Münster, Münster, Germany*
- WP 443 **Multiplex Newborn Screening of Lysosomal Storage Disorders using Flow Injection Tandem Mass Spectrometry;** Mariana Barcenás<sup>1</sup>; Martin Sadilek<sup>1</sup>; C. Ronald Scott<sup>3</sup>; Frantisek Turecek<sup>1</sup>; Michael Gelb<sup>1,2</sup>; <sup>1</sup>University of Washington, Department of Chemistry, Seattle, WA; <sup>2</sup>University of Washington, Dept. of Biochemistry, Seattle, WA; <sup>3</sup>University of Washington, Dept. of Pediatrics, Seattle, WA
- WP 444 **Clinical Screening of Hemoglobinopathies using Top Down Mass Spectrometry;** James Scrivens<sup>1</sup>; Smith Julia<sup>3</sup>; Sarah Nicolle<sup>4</sup>; Jane Newbold<sup>4</sup>; Krisztina Radi<sup>2</sup>; <sup>1</sup>Univ of Warwick, Coventry, UK; <sup>2</sup>University of Warwick - Life Sciences, Coventry, UK; <sup>3</sup>Bruker, Coventry, UK; <sup>4</sup>Coventry and Warwickshire Hospital, Coventry, UK
- WP 445 **Top-down MS/MS Hemoglobinopathy Screening of Neonatal Samples;** Roger Theberge<sup>1</sup>; Carolyn Hoppe<sup>2</sup>; Christian Heckendorf<sup>1</sup>; David H. K. Chui<sup>1</sup>; Catherine E. Costello<sup>1</sup>; Mark E. McComb<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Children's Hospital & Research Center Oakland, Oakland, CA
- WP 446 **Towards the Development of Saliva-Based Malaria Diagnostics: Mass Spectrometry Based Identification of Gametocyte Proteins in Human Saliva;** Dingyin Tao<sup>1</sup>; Isabelle Morlais<sup>2</sup>; Tamaki Kobayashi<sup>1</sup>; William John Moss<sup>1</sup>; Rhoel R Dinglasan<sup>1</sup>; <sup>1</sup>Johns Hopkins Bloomberg School of Public Health, Baltimore, MD; <sup>2</sup>Laboratoire de Recherche sur le Paludisme, Yaoundé, Cameroun

- WP 447 **Apolipoprotein E  $\epsilon$ 2,  $\epsilon$ 3 and  $\epsilon$ 4 Isoform Specific Quantification in Human Sera using LC-MRM;** Christophe Hirtz<sup>1</sup>; Jérôme Vialaret<sup>1</sup>; Susanna Schraen<sup>2</sup>; Benlian Pascale<sup>3</sup>; Sandrine Mary<sup>3</sup>; Laurent Tiers<sup>1</sup>; Baptiste Gor<sup>1</sup>; Pauline Bros<sup>1</sup>; Constance Delaby<sup>1</sup>; Audrey Gabelle<sup>1,4</sup>; Sylvain Lehmann<sup>1</sup>; <sup>1</sup>CHU de Montpellier and UM1, Montpellier, France; <sup>2</sup>Inserm U837, Lille, France; <sup>3</sup>U4M, Lille, France; <sup>4</sup>Centre Mémoire Ressources Recherche LR, Montpellier, France
- WP 448 **Sample Treatment and Stability of Urine Samples from Patients with APRT Deficiency Used in Mass Spectrometry Based Clinical Diagnostics;** Margret Thorsteinsdottir<sup>1,2</sup>; Finnur F Eiriksson<sup>1,2</sup>; Hrafnhildur L Runolfsdottir<sup>1</sup>; Vidar O Edvardsson<sup>3</sup>; Runolfur Palsson<sup>1,3</sup>; <sup>1</sup>University of Iceland, Reykjavik, Iceland; <sup>2</sup>ArcticMass, Reykjavik, Iceland; <sup>3</sup>Landspítali – The National University Hospital, Reykjavik, Iceland
- WP 449 **Development and Validation of 2D-LC/MS/MS Method for Quantitative Analysis of 1 $\alpha$ ,25-Dihydroxyvitamin D3 in Human Serum;** Daryl Kim Hor Hee<sup>1</sup>; Lawrence Soon-U Lee<sup>1</sup>; Edwin Zhi Wei Ting<sup>2</sup>; Jie Xing<sup>2</sup>; Sandhya Nargund<sup>2</sup>; Miho Kawashima<sup>3</sup>; Zhaoqi Zhan<sup>2</sup>; <sup>1</sup>Department of Medicine Research Laboratories, National University of Singapore, 6 Science Drive, 2, Singapore 117546; <sup>2</sup>Customer Support Centre, Shimadzu (Asia Pacific), Pte Ltd, 79 Science Park Drive, #02-01/08, Singapore 118264; <sup>3</sup>Global Application Development Centre, Shimadzu, Corporation, 1-3 Kanda Nishihiki-cho, Chiyoda-ku., Tokyo 101-8448, Japan
- WP 450 **The Analysis of Vitamin D Metabolites in Serum by LC-MS/MS;** Shun-Hsin Liang; Sharon Lupo; Restek, Bellefonte, PA
- WP 451 **Stability of 25-Hydroxyvitamin D Metabolites in Calibration Solutions used for LC-MS Assays;** Mary Bedner; Katrice Lipka; NIST, Gaithersburg, MD
- WP 452 **Systematic Investigation of Isobaric Interferences in Vitamin D Analysis by Differential Ion Mobility Spectrometry and FTICR Mass Spectrometry;** Florian Meier<sup>1</sup>; Timon Geib<sup>1</sup>; Pascal Schorr<sup>1</sup>; Yulin Qi<sup>1</sup>; Mark Bokhart<sup>2</sup>; Elias Rosen<sup>2</sup>; David Muddiman<sup>2</sup>; Dietrich Volmer<sup>1</sup>; <sup>1</sup>Saarland University, Saarbrücken, Germany; <sup>2</sup>North Carolina State University, Raleigh, NC
- WP 453 **Value Assignment of Vitamin D Metabolites in Vitamin D Standardization Program (VDSP) Serum Samples;** Karen Phinney<sup>1</sup>; Johanna Camara<sup>2</sup>; Susan Tai<sup>2</sup>; Linda Thienpont<sup>3</sup>; Blaza Toman<sup>2</sup>; Antonio Possolo<sup>2</sup>; Christopher Sempos<sup>4</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>2</sup>NIST, Gaithersburg, MD; <sup>3</sup>Ghent University, Ghent, Belgium; <sup>4</sup>NIH Office of Dietary Supplements, Bethesda, MD
- Biomarker Discovery, 454 - 478**
- WP 454 **Shotgun Proteomics of Human Sputum Identifies Potential Cancer and Metabolic Biomarkers from Exposures to Diesel and Biodiesel Exhaust;** Aaron Mehus<sup>1,2</sup>; Sally Littau<sup>2</sup>; Eric Lutz<sup>2</sup>; Jeffrey Burgess<sup>2</sup>; <sup>1</sup>University of Arizona College of Medicine, Tucson, AZ; <sup>2</sup>University of Arizona College of Public Health, Tucson, AZ
- WP 455 **Deconvolution of Chemical Signals from Endangered African Wild Dogs;** Peter Apps<sup>1</sup>; John Moncur<sup>2</sup>; <sup>1</sup>Botswana Predator Conservation Trust, Maun, Botswana; <sup>2</sup>SpectralWorks Ltd, Runcorn, UK
- WP 456 **An LC/MS/MS Screening Approach to Discover Unknown Hemoglobin Adducts;** Henrik Carlsson; Hans von Stedingk; Ulrika Nilsson; Margareta Törnqvist; Stockholm University, Stockholm, Sweden
- WP 457 **Proteomic Investigation of Sera and Saliva Samples from Children with Autism Spectrum Disorder (ASD) and Matched Controls;** Kelly Wormwood<sup>1</sup>; Armand G. Ngounou Wetie<sup>1</sup>; Izabela Sokolowska<sup>1</sup>; Katherine Beglinger<sup>1</sup>; Jeanne Ryan<sup>2</sup>; Alisa Woods<sup>1</sup>; Costel Darie<sup>1</sup>; <sup>1</sup>Clarkson University, Potsdam, NY; <sup>2</sup>SUNY Plattsburgh, Plattsburgh, NY
- WP 458 **Mass Selected Site-Specific Core-Fucosylation of Ceruloplasmin in Alcohol-Related Hepatocellular Carcinoma;** Haidi Yin<sup>1</sup>; Zhenxin Lin<sup>1</sup>; Song Nie<sup>1</sup>; Jing Wu<sup>1</sup>; Zhijing Tan<sup>1</sup>; Jianhui Zhu<sup>1</sup>; Jianliang Dai<sup>2</sup>; Ziding Feng<sup>2</sup>; Jorge Marrero<sup>3</sup>; David Lubman<sup>1</sup>; <sup>1</sup>University of Michigan Medical Center, Ann Arbor, MI; <sup>2</sup>University of Texas MD Anderson Cancer Center, Houston, TX; <sup>3</sup>University of Texas Southwestern Medical Center, Dallas, TX
- WP 459 **Mass Spectrometric Investigation of Potential Biomarkers of Cold Stress in Saliva;** Rachel Marvin; Brooke Saepoo; Jonathan Tomko; Dr. Kenneth Hensley; Dr. David Giovannucci; Dr. Dragan Isailovic; University of Toledo, Toledo, Ohio
- WP 460 **Discovery-to-Targeted Biomarkers and Therapeutic Targeted Pipeline;** Rebeca Kawahara<sup>1</sup>; Gabriela Meirelles<sup>1</sup>; Henry Herbele<sup>2</sup>; Daniela Granato<sup>1</sup>; Sami Yokoo<sup>1</sup>; Rafael Canevarolo<sup>1</sup>; Romênia Domingues<sup>1</sup>; Flavia Winck<sup>1</sup>; Ana Carolina Prado<sup>8</sup>; Paulo Filgueiras<sup>5</sup>; Karen Cruz<sup>9</sup>; Alexandre Barbuto<sup>9</sup>; Ronei Poppi<sup>5</sup>; Rosane Minghim<sup>2</sup>; Guilherme Telles<sup>7</sup>; Felipe Paiva<sup>3</sup>; Jay Fox<sup>6</sup>; Alan Santos-Silva<sup>3</sup>; Ricardo Coletta<sup>3</sup>; Nicholas Sherman<sup>6</sup>; Adriana Paes Leme<sup>1</sup>; <sup>1</sup>Laboratório Nacional de Biotecnologia, Campinas, Brazil; <sup>2</sup>Instituto de Ciências Matemáticas e de Computação, São Carlos, SP; <sup>3</sup>Faculdade de Odontologia de Piracicaba, UNICAMP, Piracicaba, SP; <sup>4</sup>Centro Infantil Boldrini, Campinas, SP; <sup>5</sup>Instituto de Química, UNICAMP, Campinas, SP; <sup>6</sup>W. M. Keck Biomedical Mass Spectrometry Lab, Charlottesville, VA; <sup>7</sup>Instituto de Computação, UNICAMP, Campinas, SP; <sup>8</sup>Instituto do Câncer do Estado de São Paulo, São Paulo, SP; <sup>9</sup>Instituto de Ciências Biomédicas, USP, São Paulo, SP
- WP 461 **Use of Mass Spectrometry for Identification of Biomarkers of Exposure to Flame Retardants;** Manori Silva<sup>1</sup>; Donald Hilton<sup>1</sup>; Jonathan Furr<sup>2</sup>; L Earl Gray<sup>2</sup>; James Preau<sup>1</sup>; Antonia Calafat<sup>1</sup>; Xiaoyun Ye<sup>1</sup>; <sup>1</sup>CDC, Atlanta, GA; <sup>2</sup>FDA, Research Triangle Park, NC
- WP 462 **Mass Spectrometry in Clinical Diagnosis: A Preliminary Application in Tumor Cellular Proteomics for Biomarker Discovery;** Ming-Hui Yang<sup>1</sup>; Yung-Yu Chang<sup>2</sup>; Tsung-Min Wang<sup>2</sup>; Yu-Chang Tyan<sup>2</sup>; <sup>1</sup>National Applied Research Laboratories, Hsinchu, Taiwan; <sup>2</sup>Kaohsiung Medical University, Kaohsiung, Taiwan
- WP 463 **Comparative Label-Free Proteomics of Pericytes, Circulatory Fibrocytes, in contact with Vascular Endothelium (huVEC);** Harsha P. Gunawardena<sup>2</sup>; Jingjing Li<sup>1</sup>; <sup>1</sup>Department of Surgery, School of Medicine, UNC-Chapel Hill, NC; <sup>2</sup>Program in Molecular Biology & Biotechnology, UNC-Chapel Hill, NC
- WP 464 **Lipids Regulators in B-cell Chronic Lymphocytic Leukemia;** Huan Kang; David Bearss; John Prince; Brigham Young University, Provo, Utah
- WP 465 **Identification of New Toxicity Biomarkers for Microbicides;** Benben Song<sup>1</sup>; Scott Fields<sup>2</sup>; Bazeza Rasoul<sup>1</sup>; Carsten Alt<sup>2</sup>; Mary J. Tanga<sup>2</sup>; Jon Mirsalis<sup>2</sup>; Annalisa D'Andrea<sup>2</sup>; <sup>1</sup>SRI International, Harrisonburg, VA; <sup>2</sup>SRI International, Menlo Park, CA
- WP 466 **Correction of Precursor and Product Ion Abundances in Order to Standardize CID Spectra and Improve Ecom50 Accuracy for Non-Targeted Metabolomics;** Ritvik Dubey<sup>1</sup>; David Grant<sup>1</sup>; Dennis Hill<sup>1</sup>; Steven Lai<sup>2</sup>; Chen

- Ming Hui<sup>3</sup>; <sup>1</sup>University of Connecticut School of Pharmacy, Storrs, CT; <sup>2</sup>Waters Corporation, Boston, MA; <sup>3</sup>University of Connecticut, Dept. of Statistics, Storrs, CT
- WP 467 **Proteomic Analysis of Extracellular Vesicles from Patients with Systemic Sclerosis; Ole Østergaard<sup>1</sup>**; Line V. Iversen<sup>2</sup>; Søren Jacobsen<sup>3</sup>; Niels HH Heegaard<sup>1</sup>; <sup>1</sup>Statens Serum Institut, Copenhagen, Denmark; <sup>2</sup>Department of Dermatology, Bispebjerg Hospital, Copenhagen, Denmark; <sup>3</sup>Department of Rheumatology, Rigshospitalet, Copenhagen, Denmark
- WP 468 **Proteomic and Informatic Approaches in the U-BIOPRED Severe Asthma Project: Large-Scale MS<sup>E</sup>, Data Mining, Machine Learning, and Topological Data Analysis; Dominic Burg<sup>1,2</sup>**; Doroteya Staykova<sup>1</sup>; Xian Yang<sup>3</sup>; Yike Guo<sup>3</sup>; Ratko Djukanović<sup>2</sup>; Paul Skipp<sup>1</sup>; U-BIOPRED Consortium<sup>4,5</sup>; <sup>1</sup>Centre for Proteomic Research, Uni of Southampton, Southampton, UK; <sup>2</sup>NIHR Respiratory Biomedical Research Unit, Southampton General Hospital, UK; <sup>3</sup>Imperial College, London, UK; <sup>4</sup>European Lung Foundation, Sheffield, UK; <sup>5</sup>Innovative Medicines Initiative, Bruxelles, Belgium
- WP 469 **A Quantitative Proteomic Approach to Study the Interplay between Colorectal Cancer and the Immune System; Evelynne Maes<sup>1,2</sup>**; Geert Baggerman<sup>2,3</sup>; Dirk Valkenborg<sup>2,3</sup>; Bart Landuyt<sup>1</sup>; Liliame Schoofs<sup>1</sup>; Hans Prenen<sup>4</sup>; Inge Mertens<sup>2,3</sup>; <sup>1</sup>KU Leuven, Functional Genomics and Proteomics lab, Leuven, Belgium; <sup>2</sup>Flemish Institute for Technological Research (VITO), Mol, Belgium; <sup>3</sup>Center for Proteomics, Antwerp, Belgium; <sup>4</sup>Digestive oncology unit, UZ Leuven, Leuven, Belgium
- WP 470 **Proteomic Analysis of Doxorubicin-induced Cardiotoxicity in Mice; Zhijun Cao; Yuan Gao; Varsha G. Desai; James C. Fuscoe; Li-Rong Yu; National Center for Toxicological Research, FDA, Jefferson, AR**
- WP 471 **Targeted and Untargeted Mass Spectrometry for Identification of Metabolomic Changes in a Human Epigenetic Model of Chronic Stress; Constance Sobsev<sup>1</sup>**; Jun Han<sup>1</sup>; Clemens Kirschbaum<sup>2</sup>; Karl Radtke<sup>3</sup>; Thomas Elbert<sup>3</sup>; Christoph Borchers<sup>1,4</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Dresden University of Technology, Psychology Dept, Dresden, Germany; <sup>3</sup>Universität Konstanz, Clinical Psychol. & Neurol., Konstanz, Germany; <sup>4</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 472 **Mass Spectrometric Identification of Lipids Associated with Pulmonary Aspergillus Infections; Rita Semis; Gabriel B. Gugiu; Teresa B. Hong; Markus Kalkum; City of Hope, Duarte, CA**
- WP 473 **High Sensitivity Enrichment of Glycopeptides from Complex Biological Samples using Metal Organic Frameworks; Hongqiang Qin<sup>1</sup>**; Chunli Fang<sup>1</sup>; Zhichao Xiong<sup>1</sup>; Guang Huang<sup>1</sup>; Junfeng Huang<sup>1</sup>; Xiuping Yan<sup>2</sup>; Shun Feng<sup>1</sup>; Mingliang Ye<sup>1</sup>; Hanfa Zou<sup>1</sup>; <sup>1</sup>Key Laboratory of Separation Science for Analytica, Dalian, China; <sup>2</sup>Nankai University, Tianjin, China
- WP 474 **Proteome and Glycoproteome Analyses for Breast Cancer Biomarker Discovery with Nipple Discharge Using Two-Dimensional Nano LC/Nano-ESI-MS; Sadamu Kurono<sup>1,2</sup>**; Norifumi Kobayashi<sup>1,2</sup>; Tomoyuki Nakajima<sup>3</sup>; Shuji Matsuura<sup>1</sup>; Nariaki Matsuura<sup>1</sup>; Haruki Oishi<sup>1</sup>; <sup>1</sup>Osaka University Graduate School of Medicine, Suita, Osaka, Japan; <sup>2</sup>Wako Pure Chemical Industries, Ltd., Osaka, Osaka, Japan; <sup>3</sup>Shinshu University Hospital, Matsumoto, Nagano, Japan
- WP 475 **Laser Capture Microdissection for Advanced LC-MS Discovery of Specific Cell Populations within Tissue Samples; Lisa Staunton<sup>1</sup>**; Marie Reidy<sup>2</sup>; Rosina Lis<sup>3</sup>; Kieran Wynne<sup>1</sup>; Belinda Hernandez<sup>1</sup>; Steve Finn<sup>2</sup>; William Watson<sup>1</sup>; Massimo Loda<sup>3</sup>; Michaela Bowden<sup>3</sup>; Stephen Pennington<sup>1</sup>; <sup>1</sup>Conway Institute, Dublin 4, Ireland; <sup>2</sup>St. James' Hospital, Dublin, Ireland; <sup>3</sup>Dana Faber Cancer Institute, Boston, MA
- WP 476 **Identification of New Quorum Sensing Molecules in Complex Media using High resolution Mass Spectrometry and MS-MS Fragmentation; Daniel Todd<sup>1</sup>**; David Zich<sup>1</sup>; Keivan Etefagh<sup>1</sup>; Alexander Horswill<sup>2</sup>; Nadja Cech<sup>1</sup>; <sup>1</sup>Univ. of N. Carolina Greensboro, Greensboro, NC; <sup>2</sup>University of Iowa, Iowa City, IA
- WP 477 **Profiling of Proteins and Polar Metabolites in Rat Tears by High Resolution Mass Spectrometry; Toshiyuki Mikami; Takafumi Matsumoto; Tsuyoshi Noguchi; Dainippon Sumitomo Pharma, Osaka, Japan**
- WP 478 **Human Eye Peptidomics for More Efficient Screening of Donor Corneal Tissue; Bharath Kumar Raghuraman<sup>1</sup>**; Martijn Pinkse<sup>1</sup>; Mervin Pieterse<sup>1</sup>; Valerie Bentivegna<sup>1</sup>; Marieke Bruinsma<sup>2</sup>; Hans Frank<sup>2</sup>; Gerrit Melles<sup>2</sup>; Peter D. Verhaert<sup>1</sup>; <sup>1</sup>Delft University of Technology, Delft, Netherlands; <sup>2</sup>NIIOS, Rotterdam, Netherlands
- Biomarkers: Quantitative Analysis, 479 - 508**
- WP 479 **Ultra-Sensitive Stable Isotope Dilution Liquid Chromatography-Tandem Mass Spectrometry Method for Quantification of Estrogens and Estrogen Metabolites in Human Serum; Qingqing Wang<sup>1,2</sup>**; Clementina Mesaros<sup>1</sup>; Lisa Bottalico<sup>1</sup>; Kannan Rangiah<sup>3</sup>; Ian A. Blair<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Beijing Institute of Radiation Medicine, Beijing, China; <sup>3</sup>Center for Cellular and Molecular Platforms, Bangalore, India
- WP 480 **Development and Validation of LC-MS/MS Methods for Quantitative Determination of Key Kynurenine Pathway Metabolites in Human Plasma and Cerebrospinal Fluid; Mike Allen<sup>1</sup>; Ben Begley<sup>1</sup>; Kelvin Chan<sup>2</sup>; David Delinsky<sup>1</sup>; Roger Demers<sup>3</sup>; Valerie Kempf<sup>1</sup>; Kathryn Lyons<sup>4</sup>; Brian Nofsinger<sup>1</sup>; Kendall Powell<sup>1</sup>; Daren Stephens<sup>1</sup>; Weslyn Ward<sup>1</sup>; Daria Wentzel<sup>3</sup>; Patricia Wheelan<sup>1</sup>; Ignacio Munoz<sup>2</sup>; Ladislav Mrzljak<sup>2</sup>; Leticia Toledo-Sherman<sup>2</sup>; Celia Dominguez<sup>2</sup>; <sup>1</sup>Tandem Labs, Durham, NC; <sup>2</sup>CHDI Foundation, Princeton, NJ; <sup>3</sup>Tandem Labs, West Trenton, NJ; <sup>4</sup>PK Consultant, Holland, NY**
- WP 481 **Profiling EGFR Kinase Inhibitor Resistance Pathways in Non-Small Lung Cancer Cells; Ryan Bomgarden<sup>1</sup>**; Gregory Botting<sup>2</sup>; Ryan Jacobs<sup>2</sup>; Rosa Viner<sup>3</sup>; Neelu Puri<sup>2</sup>; John C. Rogers<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Rockford, IL; <sup>2</sup>University of Illinois at Chicago, Rockford, IL; <sup>3</sup>ThermoFisher Scientific, San Jose, CA
- WP 482 **Determining the Functional Role of Keratin Filament in Apoptosis via the PI3K/Akt Signaling Pathway using LTQ Orbitrap MS/MS Analysis; Nancy Fernandes; Nicole Morin Jaskiewicz; Feixia Chu; Dave Townson; University of New Hampshire, Durham, NH**
- WP 483 **Development and Qualification of a Method for Quantitative Determination of Multiple Bile Acids with microLC/MS/MS; Michael Johnson; Takeda Pharmaceuticals, Cambridge, MA**
- WP 484 **Quantitative Analysis of the Biomarkers Dopamine, DOPAC (3,4-Dihydroxyphenylacetic Acid), and HVA (Homovanillic Acid) in Rat Brain Tissue Homogenate; Angela Qi Shen; Wenlin Yuan; Ritika Kurian; Steven Wiltshire; Agilux Laboratories, Worcester, MA**
- WP 485 **Measuring the Cooked Meat Carcinogen 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in Dyed Hair; Jingshu Guo<sup>1</sup>**; Kim Yonemori<sup>2</sup>; Kami K. White<sup>2</sup>; Lynne R. Wilkens<sup>2</sup>; Loic Le Marchand<sup>2</sup>; Robert Turesky<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of Hawaii, Honolulu, HI

- WP 486  **$\gamma$ -Aminobutyric Acid and Glutamic Acid as Biomarkers of Neuropathic Pain Caused by Palictaxel;** Pei Li; Benjamin Albrecht; Hanrong Weng; Michael Bartlett; *University of Georgia, Athens, GA*
- WP 487 **Analyte Stability, Selectivity, and Importance of Sample Preparation for the Accurate Determination of LPA, a Potential Stratification Biomarker, in Biofluids;** Joelle Onorato; Petia Shipkova; Anne Minnich; Anne Aubry; John Easter; Adrienne Tymiak; *Bristol-Myers Squibb, Princeton, NJ*
- WP 488 **A Novel LC-MS/MS Method for Quantitation of Three Free Form Fatty Acids in Human Plasma;** Dawei Zhou<sup>1</sup>; Du-Shieng Chien<sup>2</sup>; Xiping Fang<sup>1</sup>; Xingye Yang<sup>1</sup>; Jinn Wu<sup>1</sup>; <sup>1</sup>*XenoBiotic Laboratories, Inc., Plainsboro, NJ*; <sup>2</sup>*Efficient Pharma Management Corporation, Taipei, Taiwan*
- WP 489 **Membrane Protein Enrichment Strategy to Identify Biomarker Candidates in Alzheimer's Disease using Quantitative Mass Spectrometry;**  Sravani Musunuri; Kim Kultima; Martin Ingelsson; Lars Lannfelt; Jonas Bergquist; Ganna Shevchenko; *Uppsala University, Uppsala, Sweden*
- WP 490 **Biomonitoring of Methylene Diphenyl Diisocyanate Adducted to Lysine Amino Acids (K-MDA) in Rat Urine;**  Leah Luna; Michael Bartels; Dan Markham; Kathy Brzak; *The Dow Chemical Company, Midland, MI*
- WP 491 **Multiple Biomarker Analysis of Breast Cancer Clinical Biopsies using MRM MS;** Chris Sutton<sup>1</sup>; Sadr-ul Shaheed<sup>1</sup>; Andreas Hadjisavvas<sup>2</sup>; Kyriacos Kyriacou<sup>2</sup>; Paul Loadman<sup>1</sup>; <sup>1</sup>*Institute of Cancer Therapeutics, Bradford, UK*; <sup>2</sup>*Cyprus Institute of Neurology and Genetics, Nicosia, Cyprus*
- WP 492 **Nanoprobe-Based Affinity Multiple Reaction Monitoring (MRM) Approach for Verification of Hepatocellular Carcinoma (HCC) Biomarkers;** Mira Anne C. Dela Rosa<sup>1,2</sup>; Kai-Yi Wang<sup>1,2</sup>; Rofeamor P. Obena<sup>3</sup>; Rey Y. Capangpangan<sup>2,3</sup>; Pei-Yi Lin<sup>3</sup>; Yu-Ju Chen<sup>3</sup>; <sup>1</sup>*Department of Chemistry, National Taiwan University, Taipei, Taiwan*; <sup>2</sup>*Taiwan International Graduate Program, Taipei, Taiwan*; <sup>3</sup>*Institute of Chemistry, Academia Sinica, Taipei, Taiwan*
- WP 493 **A Strategy for MRM-based Verification of Bladder Cancer Protein Biomarkers;** Cheng-Han Tsai<sup>1</sup>; Ting Chung<sup>1</sup>; Chien-Lun Chen<sup>2</sup>; Jau-Song Yu<sup>1</sup>; Yi-Ting Chen<sup>1</sup>; <sup>1</sup>*Chang Gung University, Tao-Yuan, Taiwan*; <sup>2</sup>*Chang Gung Memorial Hospital, Tao-Yuan, Taiwan*
- WP 494 **Development of MRM Methods for Clinical Analysis of Urinary Myoglobin;** James Hribar<sup>1</sup>; Jon Klein<sup>1,2</sup>; Daniel Wilkey<sup>1</sup>; Kenneth McLeish<sup>1,2</sup>; Michael Merchant<sup>1</sup>; <sup>1</sup>*Department of Medicine-Nephrology, Louisville, KY*; <sup>2</sup>*Veterans Administration Medical Center, Louisville, KY*
- WP 495 **SRM-based Kinetic Measurements of Biomarkers for Cardiovascular Disease, Utilizing Isotope Enrichment Studies in Non-Human Primates and Human Subjects;** Fang Xie; Brooke Rock; Maurice Emery; Dan Rock; *Amgen, Seattle, WA*
- WP 496 **Method Development for the Quantitation of a Urine Biomarker for Acute Kidney Injury using a QTRAP® Mass Spectrometer;** Dietrich Merkel; Christian Baumann; Jörg Dojahn; *AB SCIEX, Darmstadt, Germany*
- WP 497 **An Integrated High-Throughput Protein Quantification Workflow by Robotic Sample Preparation and Selected Reaction Monitoring in Large-Scale Biomarker Study;** Xiaoqian Liu<sup>1,2</sup>; Qin Fu<sup>1,2</sup>; Michael P Kowalski<sup>3</sup>; Graham J Threadgill<sup>4</sup>; Christie Hunter<sup>6</sup>; Weihua Ji<sup>6</sup>; Joan M Bathon<sup>7</sup>; Jennifer E Van Eyk<sup>1,2</sup>; <sup>1</sup>*Johns Hopkins University, Baltimore, MD*; <sup>2</sup>*Cedars Sinai Medical Systems, Los Angeles, CA*; <sup>3</sup>*Beckman Coulter Life Science, Indianapolis, IN*; <sup>4</sup>*Beckman Coulter, Brea, CA*; <sup>5</sup>*AB SCIEX, Foster City, CA*; <sup>6</sup>*National Institute of Standards and Technology, Gaithersburg, MD*; <sup>7</sup>*Columbia University, New York, NY*
- WP 498 **Secretome Analysis using Label-Free Quantitative Proteomics to Discover Potential Cancer Biomarkers of Benzo(a)Pyrene Exposure;** Marianne Ibrahim<sup>1</sup>; Lauriane Kuhn<sup>2</sup>; Zeina Dagher<sup>3</sup>; Johana Chicher<sup>2</sup>; Ramez Chahine<sup>4</sup>; Philippe Hamman<sup>2</sup>; Emmanuelle Leize-Wagner<sup>1</sup>; <sup>1</sup>*LSMIS, CNRS-UMR 7140, University of Strasbourg, Strasbourg, France*; <sup>2</sup>*Plateforme Protéomique Strasbourg Esplanade (IBMC), Strasbourg, France*; <sup>3</sup>*Equipe Molécules Bioactives, Lebanese University, Beirut, Lebanon*; <sup>4</sup>*Laboratoire Stress Oxydatif, Lebanese University, Beirut, Lebanon*
- WP 499 **Validation Studies for Serum Biomarkers of Pancreatic Cancer;** Clementina Mesaros<sup>1,2</sup>; Nathaniel Snyder<sup>1,2</sup>; Kenneth Yu<sup>1,3</sup>; Ian A. Blair<sup>1,2</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Center for Excellence in Environmental Toxicology, Philadelphia, PA*; <sup>3</sup>*Memorial Sloan-Kettering Cancer Center, New York, NY*
- WP 500 **iTRAQ-Based Quantitative Proteomic Analysis of Core-Fucosylated Glycopeptides in Serum of Pancreatic Cancer;** Zhijing Tan; Zhenxin Lin; Song Nie; Haidi Yin; David M. Lubman; *University of Michigan, Ann Arbor, U.S.A*
- WP 501 **High-throughput Analysis of Glycan Variation on Glycoproteins from Serum by the Reverse Lectin-based ELISA Assay and MRM Analysis;** Jing Wu; Jianhui Zhu; Haidi Yin; Ronald Buckanovich; David M. Lubman; *University of Michigan, Ann Arbor, MI*
- WP 502 **Mass Spectrometry Quantitation of sPLA2 Alteration in Human Serum Samples to Investigate Its Proinflammatory Activity;** Vahid Farrokhi<sup>1</sup>; Reza Nemat<sup>1</sup>; Emily Anstadt<sup>2</sup>; Frank C. Nichols<sup>3</sup>; Robert B. Clark<sup>2</sup>; Xudong Yao<sup>1</sup>; <sup>1</sup>*University of Connecticut, Storrs, CT*; <sup>2</sup>*University of Connecticut School of Medicine, Farmington, CT*; <sup>3</sup>*University of Connecticut School Dental Medicine, Farmington, CT*
- WP 503 **Western Blotting for Post Translational Modifications vs. Quantitative Mass Spectrometry: Study of 3-Nitrotyrosine;** Nadya Galeva; Elena Dremina; Maria Feeney; Christian Schöneich; *University of Kansas, Lawrence, KS*
- WP 504 **Mass Spectrometry (MS) Based Serum Protein Profiling of Depleted and Undepleted Serum;** Santosh Bhosale<sup>1</sup>; Robert Moulder<sup>1</sup>; Olli Raitakari<sup>2</sup>; David Goodlett<sup>2</sup>; Riitta Laheesmaa<sup>1</sup>; <sup>1</sup>*University of turku, Turku, Finland*; <sup>2</sup>*University of Maryland, Baltimore, MD*; <sup>3</sup>*Department of Clinical Physiology and Nuclear Medi, Turku, Finland*
- WP 505 **Rapid Quantitation of Substance P in Plasma using Differential Mobility Spectrometry and Microflow Chromatography;** Daniel Warren; Sushmit Maitra; *AB SCIEX, Framingham, MA*
- WP 506 **Comparison of Different Methods and Informatics Tools for Protein Quantification;** Martha Stapels; Petra Olivova; Monica Lane; Kate Zhang; *Genzyme Corporation, Framingham, MA*
- WP 507 **Quantitative Analysis of Creatinine in Rodent Plasma by Laser Diode Thermal Desorption Coupled to Tandem Mass Spectrometry;** Kristina Gueneva-Boucheva<sup>1</sup>; Roger Dinallo<sup>1</sup>; Pierre Picard<sup>2</sup>; <sup>1</sup>*Boehringer Ingelheim, Ridgefield, CT*; <sup>2</sup>*Phytronix Technologies Inc., Quebec, Canada*
- WP 508 **Enhanced Laser Ionization Methodology for the Quantitative Analysis of a Biomedically Relevant Analyte;** Logan Miller<sup>1</sup>; Steve Shuttleworth<sup>2</sup>; Matt Pamukcu<sup>3</sup>; H.M "Skip" Kingston<sup>1</sup>; <sup>1</sup>*Duquesne University, Pittsburgh, PA*; <sup>2</sup>*Photon Machines Inc., Bozeman, MT*; <sup>3</sup>*Applied Isotope Technologies, Pittsburgh, PA*

## Biomarkers: Quantitative Analysis, 509 -518

WP 509 **LC-MS/MS: A Tool to Mitigate Interferences in Complex Matrices;** Carolyn Burdette; Benjamin Place; Johanna Camara; NIST, Gaithersburg, MD

WP 510 **Liver Mitochondria Proteomics: Protein and PTM Quantitation;** Jenny T.C. Ho<sup>1</sup>; Loic Dayon<sup>2</sup>; John Corthesy<sup>2</sup>; Umberto De Marchi<sup>2</sup>; Antonio Nunez<sup>2</sup>; Rosa Viner<sup>3</sup>; Michael Blank<sup>3</sup>; Steven Danielson<sup>3</sup>; Madalina Oppermann<sup>1</sup>; Martin Hornshaw<sup>1</sup>; Andreas Wiederkehr<sup>2,4</sup>; Martin Kussmann<sup>2,5</sup>; <sup>1</sup>Thermo Fisher Scientific, Hemel Hempstead, UK; <sup>2</sup>NIH, Lausanne, Switzerland; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Ecole Polytechnique Federale Lausanne, Lausanne, Switzerland; <sup>5</sup>Aarhus University, Aarhus, Denmark

WP 511 **Targeted Quantitative Proteomics of Protein Biomarkers for Plasma Nutrient Status using Heavy Stable Isotope Labeled Recombinant Proteins;** Raghothama Chaerkady<sup>1</sup>; Robert O'Meally<sup>1</sup>; Lauren Devine<sup>1</sup>; Hee-Sool Rho<sup>1</sup>; Jamie L Johnson<sup>2</sup>; Kerry Schulze<sup>2</sup>; John D Groopman<sup>2</sup>; Keith P West<sup>2</sup>; Robert N Cole<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>Johns Hopkins School of Public Health, Baltimore, MD

WP 512 **Targeted Proteomics to monitor Pharmacological Induction of Embryonic Beta Globins in Adult Mice;** Michelle Salemi<sup>1</sup>; Hugh Rienhoff<sup>2</sup>; Brett Phinney<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Children s Hospital of Oakland, Oakland, CA

WP 513 **Exploring the Detection Limits of ERG Oncoprotein in Prostate Cancer using Different Sample Types Simulating Clinical Specimens;** Jintang He<sup>1</sup>; Tujin Shi<sup>1</sup>; Athena A. Schepmoes<sup>1</sup>; Thomas L. Fillmore<sup>1</sup>; Chaochao Wu<sup>1</sup>; Albert Dobi<sup>2</sup>; Shiv Srivastava<sup>2</sup>; Shyh-Han Tan<sup>2</sup>; Ahmed A. Mohamed<sup>2</sup>; Anshu Rastogi<sup>2</sup>; Jacob Kagan<sup>3</sup>; Sudhir Srivastava<sup>3</sup>; Wei-Jun Qian<sup>1</sup>; Richard D. Smith<sup>1</sup>; Karin D. Rodland<sup>1</sup>; Tao Liu<sup>1</sup>; David G. Camp<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory, Richland, WA; <sup>2</sup>Center for Prostate Disease Research, Rockville, MD; <sup>3</sup>National Cancer Institute, Rockville, MD

WP 514 **Enrichment of EGFR/PI3K/AKT/PTEN Proteins using Immunoprecipitation and Analysis with Mass Spectrometry-based Proteomics;** Bhavin Patel; Scott Meier; Kay Opperman; Paul Haney; Barb Kaboord; John C. Rogers; Thermo Fisher Scientific, Rockford, IL

WP 515 **Real-Time Qualitative and Quantitative Analysis of Differentially Expressed Proteins Using a Modified DIA Method;** Tara Schroeder<sup>1</sup>; Scott Peterman<sup>2</sup>; Amol Prakash<sup>2</sup>; Shadab Ahmad<sup>2</sup>; Barbara Frewen<sup>2</sup>; Mary Lopez<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Somerset, NJ; <sup>2</sup>Thermo Fisher Scientific, Cambridge, MA

WP 516 **A High-Throughput, Semi-Automated, Sample Handling Platform for Quantitative Proteomics: A Test-Case Study of Gene Regulation in Mouse Hippocampus;** Paul Piehowski<sup>1</sup>; Vladislav Petyuk<sup>1</sup>; Arshad Khan<sup>2</sup>; Anil Shukla<sup>1</sup>; Desmond Smith<sup>2</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Lab, Richland, WA; <sup>2</sup>UCLA Molecular and Medical Pharmacology Department, Los Angeles, CA

WP 517 **A SISCAPA Immuno-Mass Spectrometric Assay for Quantification of Soluble Transferrin Receptor (sTfR) in Human Serum;** Oliver Drews<sup>1</sup>; Rainer Paape<sup>1</sup>; Waltraud Evers<sup>1</sup>; Morteza Razavi<sup>2</sup>; Matt Pope<sup>2</sup>; Leigh Anderson<sup>2</sup>; Detlev Suckau<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Bremen, Germany; <sup>2</sup>SISCAPA Assay Technologies, Victoria, Canada

WP 518 **Development of a SISCAPA-MALDI Assay for Multiplexed Analysis of Apolipoprotein A1, Apolipoprotein B and Apolipoprotein E in Human Serum;** Irene van den Broek<sup>3</sup>; Jan Nouta<sup>3</sup>; Oliver Drews<sup>4</sup>; Detlev Suckau<sup>4</sup>; Rainer Paape<sup>4</sup>; Yuri E.M. van der Burg<sup>3</sup>; Christa M. Cobbaert<sup>3</sup>; N. Leigh Anderson<sup>1</sup>; Terry W. Pearson<sup>1,2</sup>; <sup>1</sup>SISCAPA Assay Technologies,

Washington, DC; <sup>2</sup>University of Victoria, Victoria, BC; <sup>3</sup>Leiden University Medical Center (LUMC), Leiden, The Netherlands; <sup>4</sup>Bruker Daltonik GmbH, Bremen, Germany

## Small Molecule Quantitation, 519 - 553

WP 519 **Development of a Fast, Sensitive chiral-LC/MS/MS Method for Quantitation of Empagliflozin, a SGLT-2 Inhibitor, and Its Epimer in Human Plasma;** Lin-Zhi Chen<sup>1</sup>; Shirin Pagels<sup>1</sup>; Steffen Penk<sup>2</sup>; Michael Wedel<sup>2</sup>; <sup>1</sup>Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT; <sup>2</sup>Boehringer Ingelheim Pharma GmbH & Co. KG, Biberach, Germany

WP 520 **A Robust and Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Quantification of 24(S)-Hydroxycholesterol in Human Plasma and Cerebrospinal Fluid;** Xuntian Jiang; Rohini Sidhu; Hui Jiang; Jean E. Schaffer; Daniel S. Ory; *Diabetic Cardiovascular Disease Center, Washington, St. Louis, MO*

WP 521 **Comparison of Gas Chromatography and Ultra-performance Liquid Chromatography Coupled with Tandem Mass Spectrometry for Determining Perfluorinated Chemicals;** Yi-Chieh Lai; Chia-Yang Chen; *National Taiwan University, Taipei, Taiwan*

WP 522 **Troubleshooting and Real Time Monitoring of Matrix Effect Generated by Consumable Labware during Ivermectin Quantification by LC-MS/MS;** Mathieu Lahaie; Kevork Mekhssian; Romain Beauvois; Georges Koudssi; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 523 **Post-Column Addition of High pH Solution to Improve Analyte Sensitivity and Avoid On-Column Degradation of Unstable Metabolites in LC-MS/MS;** Julien Nantel; Laurence Mayrand-Provencher; Milton Furtado; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 524 **Bioanalytical Method for Quantification of Total Apomorphine in Human Plasma by LC-MS/MS;** Melvin Tan; Francesca Ekpo; Erica Hutton; Venetra DeLeon; Edward Wells; Steve Unger; *Worldwide Clinical Trials, Austin, TX*

WP 525 **In Depth Bioanalytical Investigation and Root Cause Analysis of Lamotrigine Severe Degradation in Hemolyzed Plasma Samples by LC-MS/MS;** Nicolaos Soilis; Richard Lavallée; Milton Furtado; Josée Michon; Fabio Garofolo; *Algorithme Pharma Inc., Laval, Canada*

WP 526 **Evaluation of Stability of Acyl Glucuronides using LC-MS/MS;** Qingguo Tian; Andreas Grill; Daksha Desai-Krieger; *Forest Laboratories, Inc., Farmingdale, NY*

WP 527 **PPM Level Quantitative Analysis of Genotoxic Impurities in a Pharmaceutical Starting Material;** Meng Xu<sup>1</sup>; Catherine Brookes<sup>2</sup>; Alison Bretnall<sup>2</sup>; Hongfei Yue<sup>1</sup>; John Castoro<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb, New Brunswick, NJ; <sup>2</sup>Bristol-Myers Squibb Company, moreton, UK

WP 528 **LC-MS/MS Bioanalysis of Loratadine in DBS Samples Collected by Subjects in a Clinical Study for Assessment of Remote PK Sampling;** Wenkui Li; John Doherty; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*

WP 529 **An Extremely Sensitive LC-MS/MS Method for Quantitation of Fluticasone Propionate (0.4 pg/mL) in Human Plasma;** Xinping Fang; Dawei Zhou; Jinn Wu; *XenoBiotic Laboratories, Inc., Plainsboro, NJ*

WP 530 **Determination of Gangliosides in Human Plasma by a Novel UHPLC/MS/MS Assay;** Qianyang Huang<sup>1</sup>; Xiang Zhou<sup>1</sup>; Danting Liu<sup>1</sup>; Baozhong Xin<sup>2</sup>; Karen Cechner<sup>2</sup>; Heng Wang<sup>2</sup>; Aimin Zhou<sup>1</sup>; <sup>1</sup>Cleveland State University, Cleveland, Ohio; <sup>2</sup>DDC Clinic, Middlefield, OH



- WP 531 **A Sensitive LC-MS/MS Method for the Quantification of Ethinyl Estradiol and Drospirenone in Human Plasma;** Siddhartha Khurana<sup>1</sup>; Naveen Dubey<sup>1</sup>; Dhananjay Sharma<sup>1</sup>; Sandeep Sharma<sup>1</sup>; Anoop Kumar<sup>2</sup>; Manoj Pillai<sup>2</sup>; <sup>1</sup>Jubilant Clinsys, Noida, India; <sup>2</sup>AB SCIEX DHR holdings India, Gurgaon, India
- WP 532 **In Depth Evaluation of a Novel On-line HybridSPE Technology for Removal of Phospholipids from Protein Precipitation Plasma Samples by LC-MS/MS;** Laurence Mayrand-Provencher<sup>1</sup>; Richard Lavallée<sup>1</sup>; Milton Furtado<sup>1</sup>; David Bell<sup>2</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma Inc., Laval, Canada; <sup>2</sup>Sigma-Aldrich, Bellefonte, PA
- WP 533 **Development and Validation of of an Ultra Sensitive UPLC-MS/MS Method for the Determination of Naloxone in Human Plasma;** Xiaohan Cai; Lina Tang; Lan Li; Yuan-Shek Chen; Luca Matassa; QPS, LLC, Newark, DE
- WP 534 **Selecting the Right Weighting Factors for Linear and Quadratic Calibration Curves in Bioanalytical LC-MS/MS Assays;** Huidong Gu; Guowen Liu; Jian Wang; Anne Aubry; Mark Arnold; Bristol-Myers Squibb, Princeton, NJ
- WP 535 **Impact of Plasma Hemolysis on the Recovery of Phenprocoumon LC-MS/MS Chiral Assay;** Nikolay Youhnovski; Romain Beauvois; Mathieu Lahaie; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 536 **Oral Fluid Testing for Buprenorphine and THC by “Dilute and Shoot” LC-MS/MS;** Jeffrey Enders; Ayodele Morris; Gregory Mcintire; Ameritox, Ltd, Greensboro, NC
- WP 537 **Development and Qualification of an UPLC-MS/MS Method for Simultaneous Determination of Five Isomeric Analytes (potential metabolites) in Human Plasma;** Yu-Luan Chen<sup>1</sup>; Shoko Ochiai<sup>2</sup>; Estela Skende<sup>1</sup>; Julie Tollefson<sup>3</sup>; Amber LaFayette<sup>3</sup>; <sup>1</sup>Sunovion, Inc., Marlborough, MA; <sup>2</sup>Dainippon Sumitomo Pharma, Osaka, Japan; <sup>3</sup>Covance, Madison, WI
- WP 538 **Parallelism Comparison between Surrogate and Biological Matrix for the Quantification of Endogenous Levels using Surrogate Matrix Calibration Curve by LC-MS/MS;** Richard Lavallée; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 539 **A Fast and Simple LCMSMS Derivatization Approach towards Quantification of Low Molecular Weight Compounds of Molecular Weight Less than 100Da;** Mohan Kasi<sup>1</sup>; Arvind Thyagarajan<sup>2</sup>; Saravanan Subramaniyan<sup>2</sup>; Rampriya Uthayakumar<sup>2</sup>; Raman Palvannanathan<sup>2</sup>; Govindarajan Chandramohan<sup>2</sup>; Venkat Manohar<sup>2</sup>; Devadasan Velmurugan<sup>1</sup>; <sup>1</sup>Dept. of CAS in Crystallography & Biophysics., University of Madras, Chennai., India; <sup>2</sup>IICMS, Chennai, India
- WP 540 **Simultaneous Quantitation of Nebivolol and Valsartan in Human Plasma;** Mei Li; Hongzhi Liu; Helen Deng; Anita Dalko; Surya Kandukuri; Nicola Hughes; Bioanalytical Laboratory Services (LifeLabs), Toronto, Canada
- WP 541 **Quantitative Measurement of Ultra-low Level of Tiotropium Bromide in Human Plasma using Two-Dimensional Liquid Chromatography (2D-LC) and Tandem Mass Spectrometry;** Jingdian Chi; Melissa Meyer; Fumin Li; PPD Inc, Madison, WI
- WP 542 **A Study of the Electrospray/Mass Spectral Characteristics of De-Protonated Molecular and Chloride Adduct Ions of Phenicols: Implications in Quantitative Analysis;** Kwenga Sichilongo; University of Botswana, Gaborone, Botswana
- WP 543 **The Bioanalysis of Propylparaben, a Suspected Environmental Estrogenic Agent, by LC-MS/MS;** Yue Zhao; Guowen Liu; Hongwu Shen; lakshmi Sivaraman; Anne-Francoise Aubry; Mark Arnold; Jim Shen; Bristol-Myers Squibb Co., Princeton, NJ
- WP 544 **Evaluation of the Budesonide 22R and 22S Epimers Fragmentation in LC-MS/MS and its Impact in Quantitative Bioanalysis;** Eugénie-Raphaëlle Bérubé; Sylvain Latour; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval, Canada
- WP 545 **How to Prevent Changes in Plasma Integrity and its Impact on LC-MS/MS Bioanalysis Due to Organic Solvent and Storage Conditions;** Romain Beauvois<sup>1</sup>; Silvana Olivieri<sup>2</sup>; Milton Furtado<sup>1</sup>; Fabio Garofolo<sup>1</sup>; <sup>1</sup>Algorithme Pharma Inc., Laval, Canada; <sup>2</sup>ACRAF – Angelini Research Center, S. Palomba, Pomezia, Rome, Italy
- WP 546 **Quantitation of Budesonide in Human Plasma: Improved Sensitivity Using Acetate Adduct Ion;** HongZhi Liu; Mei Li; Rizwan Muhammad; Jenny Shen; Surya Kandukuri; Anita Dalko; Nicola Hughes; Bioanalysis Laboratory Services (LifeLabs), Toronto, Canada
- WP 547 **Challenges in Developing a Ten Analyte Statin HPLC-MS/MS Assay in Multiple Rat Matrices;** Ryan Lutz; Cynthia M. Chavez-Eng; Dina Goykhman; Kevin Bateman; Merck & Co., West Point, PA
- WP 548 **A Highly Specific Pre-Charged Triphenylphosphine-Based Derivatization Agent for Trace-Level Detection of Ethinylestradiol;** Lucie Loukotkova<sup>1</sup>; Priyanka Chitranshi<sup>1</sup>; Gordon Surratt<sup>2</sup>; Goncalo Gamboa da Costa<sup>1</sup>; <sup>1</sup>FDA/NCTR, Jefferson, AR; <sup>2</sup>Waters Corp., Milford, MA
- WP 549 **Large-Scale Retrospective Evaluation of Regulated LC-MS Bioanalysis Projects Using Different Total Error Approaches;** Aimin Tan<sup>1</sup>; Taoufiq Saffaj<sup>2</sup>; Adrien Musuku<sup>3</sup>; Kayode Awaiye<sup>1</sup>; Bouchaib Hssane<sup>2</sup>; Fayçal Jhila<sup>2</sup>; Saad. Alaoui Sosse<sup>2</sup>; Fethi Trabelsi<sup>1</sup>; <sup>1</sup>BioPharma Services Inc., Toronto, Canada; <sup>2</sup>Université Sidi Mohamed Ben Abdallah, Fès, Morocco; <sup>3</sup>Pharmascience Inc., Montreal, Canada
- WP 550 **A Novel Microflow UPLC-MS/MS Multiplexed Assay for the Absolute Quantitation of Thyroid Hormones in Serum;** Hend Ibrahim; Lisa Wolfe; Corey Broeckling; Jessica Prenni; Jessica Prenni; Colorado State University, Fort Collins, CO
- WP 551 **Evaluation of Integrated Microfluidic Device device for targeted small molecule bioanalysis;** Aaron Ledvina; Covance Laboratories Inc., Madison, WI
- WP 552 **Quantitation of Aminoglycosides in Pharmaceutical Preparations by ESI-MS without the Need of Chromatographic Separation or Derivatization;** Freneil B. Jariwala; John A. Hibbs; Iryna Zhuk; Svetlana A. Sukhishvili; Athula B. Attygalle; Stevens Institute of Technology, Hoboken, NJ
- WP 553 **Using HPLC-MS to Assess Host-Mediated Conversion of Pyrazinamide to Pyrazinoic Acid Across Species;** Matthew Zimmerman; Xiaohua Li; Brendan Prideaux; Jansy Sarathy; Veronique Dartois; Public Health Research Institute, Rutgers, Newark, NJ
- Environmental Analysis: General, 554 - 580**
- WP 554 **Study of Cyanobacterial Microcystins using High Performance Tandem Mass Spectrometry;** Yulin Qi; Stella Bortoli; Dietrich Volmer; Saarland University, Saarbrücken, Germany
- WP 555 **Stercobilin Detection and Quantification in Public Swimming Facilities: Method Development for Low and High Resolution Mass Spectrometry;** Heather L. Rudolph; Troy Wood; SUNY University at Buffalo, Buffalo, NY

- WP 556 **Screening of Polymer Additives in Drinking Water Stored in PET Bottles by UHPLC-ESI-IT-TOF MS;** Mustafa Yilmaz; Hamdi TEMEL; DUBTAM, Dicle University, Diyarbakir, Turkey
- WP 557 **Environmental Forensic Investigation of PAHs: Determination and Apportionment of Possible Sources;** Ashley Gates<sup>1</sup>; Jack Cochran<sup>2</sup>; Melinda Pham<sup>1</sup>; Frank Dorman<sup>1</sup>; <sup>1</sup>Penn State University, State College, PA; <sup>2</sup>Restek, Bellefonte, PA
- WP 558 **Sensitive and Accurate LC-MS/MS Assay of Perfluorinated Compounds in Water;** Hui Qiao; Joshua Sha Ye; Changtong Hao; IONICS Mass Spectrometry Group Inc, Bolton, Canada
- WP 559 **Non-targeted Analysis Phase II Metabolites in Surface water using Full Scan Tandem Quadrupole Mass Spectrometry;** Matthew Reichert; Piotr Krolkowski; M. Paul Chiarelli; Loyola University, Chicago, IL
- WP 560 **Determination of Endocrine Disrupting Chemicals in Drinking Water at Sub ng/L Levels Using Direct Injection and Triple Quadrupole Mass Spectrometry;** Dorothy Yang<sup>1</sup>; László Tölgyesi<sup>2</sup>; Bernhard Wuest<sup>3</sup>; Anabel Fandino<sup>4</sup>; <sup>1</sup>, Santa Clara, CA; <sup>2</sup>Agilent Technologies Sales & Services GmbH & Co. K, Waldbronn, Germany; <sup>3</sup>Agilent Technologies GmbH, Waldbronn, Germany; <sup>4</sup>Agilent Technologies, Santa Clara, CA
- WP 561 **Direct Injection LC-MS/MS Determination of Acesulfame and Sucralose for Monitoring of Water Quality;** Minghuo Wu; Yichao Qian; Xing-Fang Li; University of Alberta, Edmonton, Canada
- WP 562 **Occurrence and Toxicity of Haloacetaldehydes in Drinking Waters: Discovery of Iodo-Acetaldehyde as a Drinking Water Disinfection By-Product;** Susan Richardson<sup>1</sup>; Cristina Postigo<sup>2,4</sup>; Clara Jeong<sup>3</sup>; Elizabeth Wagner<sup>3</sup>; Jane Ellen Simmons<sup>2</sup>; Michael Plewa<sup>3</sup>; Damia Barcelo<sup>4</sup>; <sup>1</sup>University of South Carolina, Columbia, SC; <sup>2</sup>U.S. EPA, NHEERL, RTP, NC; <sup>3</sup>University of Illinois, Urbana, IL; <sup>4</sup>Spanish National Research Council, Barcelona, Spain
- WP 563 **Determination of Unknown Chlorinated Water Pollutants in the Chicago River;** Qian Wang<sup>1</sup>; Kathryn M. Renyer<sup>2</sup>; M. Paul Chiarelli<sup>1</sup>; <sup>1</sup>Loyola University, Chicago, IL; <sup>2</sup>Morehead St. University, Morehead, KY
- WP 564 **High Resolution/Accurate Mass (HR/AM) Detection of Anatoxin-a in Lake Water Using LDTD-APCI Coupled to a Q-Exactive Mass Spectrometer;** Audrey Roy-Lachapelle<sup>1</sup>; Morgan Sollicet<sup>1</sup>; Christian Deblois<sup>2</sup>; Marc Sinotte<sup>3</sup>; <sup>1</sup>Université de Montréal, Montréal, Canada; <sup>2</sup>MDDEFP, CEAEQ, Québec, Canada; <sup>3</sup>MDDEFP, DSEE, Québec, Canada
- WP 565 **Ultra-fast LDTD-APCI-MS/MS Analysis of Estrogens in Chlorinated Drinking Water and the Impact of Bromide on the Oxidation Kinetics;** Sung Vo Duy<sup>1</sup>; Paul Fayad<sup>1</sup>; Michèle Prévost<sup>2</sup>; Sébastien Sauvé<sup>1</sup>; <sup>1</sup>Université de Montréal, Montreal, QC, Canada; <sup>2</sup>École Polytechnique de Montréal, Montreal, QC, Canada
- WP 566 **The Use of Chemometrics and High Resolution Accurate Mass GC/Q-TOF in the Identification of Environmental Pollutants in Wastewater Effluents;** Anthony Gravell<sup>1</sup>; Praveen Kutty<sup>1</sup>; Sofia Aronova<sup>2</sup>; Jennifer Gushue<sup>2</sup>; Terry Sheehan<sup>2</sup>; <sup>1</sup>Natural Resources Wales, Wales, UK; <sup>2</sup>Agilent Technologies, Inc., Santa Clara, CA
- WP 567 **HPLC-MS/MS Investigation of Halo-hydroxylbenzoquinones as Stable Haloquinone Disinfection By-Products in Treated Water;** Wei Wang; Yichao Qian; Steve Hruddy; Xing-Fang Li; University of Alberta, Edmonton, Canada
- WP 568 **Investigation of Suspected and Unknown Micropollutants and Transformation Products from a Waste Water Treatment Plant with Full Scale Ozonation;** Christoph Portner<sup>1</sup>; Olaf Scheibner<sup>2</sup>; Sebastian Westrup<sup>3</sup>; Jochen Tuerk<sup>1</sup>; <sup>1</sup>Institute of Energy and Environmental Technology, Duisburg, Germany; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>3</sup>Thermo Scientific, Dreieich, Germany
- WP 569 **Determination and Removal of N-Nitrosamine Precursors in Drinking Water System;** Honglan Shi<sup>1</sup>; Qihua Wu<sup>1</sup>; Yinfa Ma<sup>1</sup>; Craig Adams<sup>2</sup>; Hua Jiang<sup>3</sup>; <sup>1</sup>Missouri S&T, Rolla, MO; <sup>2</sup>Utah State University, Logan, UT; <sup>3</sup>City of Tulsa Water and Sewer Department, Tulsa, OK
- WP 570 **Environmental Forensics of Wastewater Samples for Determination of Emerging Contaminants;** Adrienne Brockman<sup>1</sup>; Dr. Frank Dorman<sup>1</sup>; Jack Cochran<sup>2</sup>; Michelle Misselwitz<sup>2</sup>; <sup>1</sup>, University Park, PA; <sup>2</sup>Restek, Bellefonte, PA
- WP 571 **Dioxin in Drinking Water by One-Step Solid Phase Extraction;** Hamid Shirkhan; Tom Hall; Fluid Management Systems, Watertown, MA
- WP 572 **EPA 625: Base, Neutral, Acid Semi-Volatiles in Municipal and Industrial Waste Water by SPE;** Philip Germansderfer; Lawrence Kramer; Fluid Management Systems, Watertown, MA
- WP 573 **Automated Low Background Solid Phase Extraction System for Perfluorinated Compounds from Water;** Phil Bassignani; Fluid Management Systems, Inc., Watertown, MA
- WP 574 **Organic Extract Analysis by in-Line Dilution Reversed-Phase LC-MS/MS;** Brent McKay Allred<sup>1</sup>; Mathew Perkins<sup>1</sup>; Johnsie Lang<sup>2</sup>; Morton Barlaz<sup>2</sup>; Jennifer Field<sup>1</sup>; <sup>1</sup>Oregon State University, Corvallis, Oregon; <sup>2</sup>North Carolina State University, Raleigh, NC
- WP 575 **Strategies and Techniques for Identifying Unknown Compounds in Environmental Samples;** Eric J. Reiner<sup>1</sup>; Karl J. Jobst<sup>1</sup>; Miren Pena-Abaurrea<sup>2</sup>; Anne L. Myers<sup>2</sup>; Li Shen<sup>1</sup>; Alina Muscalu<sup>1</sup>; Ralph Ruffolo<sup>1</sup>; Vince Y. Taguchi<sup>1</sup>; Paul A. Helm<sup>1</sup>; <sup>1</sup>Ontario Ministry of the Environment, Toronto, Canada; <sup>2</sup>University of Toronto, Toronto, Canada
- WP 576 **Analysis of Electronics Waste by 2D-GC Combined with High-Resolution Mass Spectrometry: Using Exact Mass Information to Explore the Data;** Masaaki Ubukata<sup>1</sup>; Karl J. Jobst<sup>2</sup>; Eric J. Reiner<sup>2</sup>; Stephen Reichenbach<sup>3</sup>; Qingping Tao<sup>4</sup>; Jiliang Hang<sup>4</sup>; Zhanpin Wu<sup>5</sup>; A. John Dane<sup>1</sup>; Robert B. Cody<sup>1</sup>; <sup>1</sup>JEOL USA, INC., Peabody, MA; <sup>2</sup>Ontario Ministry of the Environment, Toronto, Canada; <sup>3</sup>University of Nebraska-Lincoln, Lincoln, NE; <sup>4</sup>GC Image LLC, Lincoln, NE; <sup>5</sup>Zoex Corporation, Houston, TX
- WP 577 **Non-Targeted Analysis of Environmental Contaminants in Northern Fur Seals Using Comprehensive Two-Dimensional Gas Chromatography Time-of-Flight Mass Spectrometry;** Jacolin Murray<sup>1</sup>; Benjamin Place<sup>1</sup>; Natalie Rosenfelder<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>2</sup>Chemical and Veterinary Investigations Office, Stuttgart, Germany
- WP 578 **Persistent Organic Pollutants in Serum using Pressurized Liquid Extraction, Multi-Column Clean Up and Concentration;** Tom Hall; Rudolf Addink; Fluid Management Systems, Watertown, MA
- WP 579 **Oklahoma Fish Kill Study: Looking for a Toxic Needle in an Environmental Haystack;** Tammy Jones-Lepp<sup>1</sup>; Wayne Sovocool<sup>2</sup>; Don Betowski<sup>1</sup>; Patrick DeArmond<sup>3</sup>; Vince Taguchi<sup>4</sup>; Charlita Rosal<sup>1</sup>; <sup>1</sup>USEPA/ORD/NERL-ESD, Las Vegas, NV; <sup>2</sup>retired USEPA, Henderson, NV; <sup>3</sup>former USEPA post-doctoral Fellow, Las Vegas, NV; <sup>4</sup>Ministry of the Environment-Ontario, Toronto, Canada

- WP 580 **Determination of Alkylphenol Ethoxylate in Textiles and Leathers by NPLC and Quadrupole Orbitrap MS; Nam-Yong Cheong<sup>1</sup>; Bruce Lee<sup>1</sup>; Su-Jin Eo<sup>1</sup>; Yoon-Suk Lee<sup>2</sup>; Seoung-Woon Myung<sup>3</sup>; <sup>1</sup>KATRI, An-Yang, Korea; <sup>2</sup>Euro Science, Seong-Nam, Korea; <sup>3</sup>Kyonggi University, Su-Woon, Korea**
- Metabolomics: General, 581 - 594**
- WP 581 **Metabolomic Analysis of Estradiol-Induced Effects in the Human Breast Cancer Lines MCF-7 and T47D; Liang Zhao<sup>1</sup>; Shelly Odwin-DaCosta<sup>1</sup>; Marguerite Vantangoli<sup>2</sup>; Mounir Bouhifd<sup>1</sup>; Andre Kleensang<sup>1</sup>; Lena Smirnova<sup>1</sup>; Helena Hogberg<sup>1</sup>; Kim Boekelheide<sup>2</sup>; James D. Yager<sup>1</sup>; Thomas Hartung<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Brown University, Providence, RI**
- WP 582 **A Steroidomics Approach to Detect the Misuse of Oral Anabolic Steroids in Equine Sports by Biomarkers Profiling; George H.M. Chan; Emmie N.M. Ho; Terence S.M. Wan; *Racing Laboratory, The Hong Kong Jockey Club, Sha Tin, N. T., Hong Kong, China***
- WP 583 **Metabolomics Investigation of Spiked Compound Differences in Human Plasma; Amrita Cheema<sup>1</sup>; John M Asara<sup>2</sup>; Thomas Neubert<sup>3</sup>; Chris Turck<sup>4</sup>; <sup>1</sup>Georgetown University, Washington, DC; <sup>2</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>3</sup>Skirball Institute, NYUMC, New York, NY; <sup>4</sup>Max Planck Institute of Psychiatry, Munich, Germany**
- WP 584 **Development, Quantitative Evaluation and Application of a High Resolution Metabolomics Technology using HILIC Chromatography Coupled to a Q-Exactive Mass Spectrometer; Xiaojing Liu; Alexander Shestov; Jason Locasale; *Cornell University, Ithaca, NY***
- WP 585 **Gas Chromatography-Mass Spectrometry Analysis of Human Mesenchymal Stem Cell Metabolism during Proliferation and Osteogenic Differentiation under Different Oxygen Tensions; Nathalie Munoz; Yijun Liu; Timothy Logan; *FSU, Tallahassee, Florida***
- WP 586 **Ion Mobility-derived Collision Cross-Sections Databases for Metabolomics and Lipidomics; Giuseppe Paglia<sup>1</sup>; Jonathan P. Williams<sup>2</sup>; Lochana Menikarachchi<sup>3</sup>; J. Will Thompson<sup>4</sup>; Hernando Olivos<sup>5</sup>; Steven Lai<sup>6</sup>; Richard Tyldesley-Worster<sup>9</sup>; Arthur Moseley<sup>6</sup>; David Grant<sup>3</sup>; James Langridge<sup>5</sup>; Bernhard O. Palsson<sup>7</sup>; Giuseppe Astarita<sup>5</sup>; <sup>1</sup>Center for Systems Biology, University of Iceland, Reykjavik, Iceland; <sup>2</sup>Waters, Manchester, N/A; <sup>3</sup>University of Connecticut, Storrs, CT; <sup>4</sup>Duke University School of Medicine, Durham, NC; <sup>5</sup>Waters, Milford, MA; <sup>6</sup>Duke University School of Medicine, Durham, NC; <sup>7</sup>Systems Biology Research Group, UCSD, San Diego, CA**
- WP 587 **Comparative Bovine and Human Milk Metabolomics: Generating a Reference Metabolome for Human Breast Function Diagnosis; Robert Trengove<sup>1</sup>; Erin Fee<sup>2</sup>; Joel Gummer<sup>1</sup>; Kristin Piper<sup>3</sup>; James Lui<sup>3</sup>; Catherine Rawlinson<sup>1</sup>; Ching Lai<sup>3</sup>; Naomi Trengove<sup>2</sup>; Donna Geddes<sup>3</sup>; Peter Hartmann<sup>3</sup>; <sup>1</sup>Murdoch University, Murdoch, Australia; <sup>2</sup>The University of Notre Dame Australia, Fremantle, WA; <sup>3</sup>The University of Western Australia, Perth, Australia**
- WP 588 **Myth Busters: The Truth About Metabolomics And Gas Chromatography-High Resolution Time-of-Flight Mass Spectrometry; David Alonso<sup>1</sup>; Joe Binkley<sup>1</sup>; Lorne Fell<sup>2</sup>; <sup>1</sup>Leco Corporation, St. Joseph, MI; <sup>2</sup>Leco, St Joseph, MI**
- WP 589 **Development of a Plant, Algae, and Microbial Metabolomics Research Coordination Network and US Chapter of the Metabolomics Society; Lloyd W. Sumner<sup>1</sup>; Oliver Fiehn<sup>2</sup>; Georg Jander<sup>3</sup>; James C. Liao<sup>4</sup>; Basil Nikolau<sup>5</sup>; <sup>1</sup>The Samuel Roberts Noble Foundation, Ardmore, OK; <sup>2</sup>University of California, Davis, Davis, CA;**
- <sup>3</sup>Boyce Thompson Institute for Plant Research, Ithaca, NY; <sup>4</sup>University of California, Los Angeles, Los Angeles, CA; <sup>5</sup>Iowa State University, Ames, IA
- WP 590 **A Novel Batch Automated Multi-Recursive Data Processing Workflow for Rigorous Metabolite Profiling of Human Urine Analyzed by LC/MS; Benjamin Owen; Sumit Shah; *Agilent Technologies, Wakefield, MA***
- WP 591 **High Quality Batch Feature Extraction of Mass Spectrometry Data to Improve Statistical Analysis Results; Yugin Dai; Steven M. Fischer; Norton Kitagawa; Theodore R. Sana; *Agilent Technologies, Santa Clara, CA***
- WP 592 **Metabolomics Technology Validated Quality Markers for Biobank Plasma Samples; Michael Herold<sup>1</sup>; Beate Kamlage<sup>1</sup>; Oliver Schmitz<sup>1</sup>; Philipp Schatz<sup>2</sup>; <sup>1</sup>metanomics GmbH, Berlin, Germany; <sup>2</sup>Metanomics Health GmbH, Berlin, Germany**
- WP 593 **Metabolomics Profiling Workflow of Combining MS and NMR Datasets for a Single Sample; Darrell Marshall<sup>1</sup>; Shulei Lei<sup>1</sup>; Yuting Huang<sup>1</sup>; Aracely Garcia-Garcia<sup>2</sup>; Rodrigo Franco<sup>2</sup>; Eric D. Dodds<sup>1</sup>; Robert Powers<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Nebraska-L, Lincoln, Nebraska; <sup>2</sup>School of Veterinary Medicine and Biomedical Scie, Lincoln, NE**
- WP 594 **Direct Mitochondrial Metabolites Detection in a HepG2 Cell by Live Single-cell Mass Spectrometry; Tsuyoshi Esaki; Sachiko Date; Hajime Mizuno; Ai Fujita; Tsutomu Masujima; *Quantitative Biology Center (QBiC), RIKEN, Suita, Osaka, Japan***
- Metabolomics: Quantitative Analysis, 595 - 615**
- WP 595 **Comprehensive, Accurate, and Precise Quantification of Acylcarnitines and Acyl-CoAs in Tissues using On-Line Ion-Exchange Trapping and UHPLC-MS/MS; Charles L. Hoppel; Paul E. Minkler; Maria S.K. Stoll; Stephen T. Ingalls; *Case Western Reserve Univ., Cleveland, OH***
- WP 596 **A Validated High-throughput Assay for the Quantification of Amino Acids in Metabolic Phenotyping Studies; Nicola Gray<sup>1</sup>; Robert Plumb<sup>2</sup>; Ian Wilson<sup>1</sup>; Jeremy Nicholson<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Waters, Milford, MA**
- WP 597 **Characterization of HILIC Columns with Zwitterionic Functional Groups: Correlation between Retention, Selectivity, Stationary Phase and Water Layer Thickness; David Lentz<sup>2</sup>; Tobias Jonsson<sup>1</sup>; Phuoc Dinh<sup>3</sup>; Patrik Appelblad<sup>1</sup>; Wen Jiang<sup>1</sup>; <sup>1</sup>Merck Millipore, Darmstadt, Germany; <sup>2</sup>EMD Millipore, Billerica, MA; <sup>3</sup>Umea University, Umea, Sweden**
- WP 598 **Trapping micro-LC/MS/MS Isotope Dilution Mass Spectrometry in the High Throughput and Ultra-Sensitive Quantification of Serum Vitamin D Metabolites; Eslam Nouri; ming zhang; Haoying Yu; Jun Qu; *University at Buffalo, Buffalo, NY***
- WP 599 **Development of a Chromatography-less Quantification Method for Plant Secondary Metabolites by Solvent-compensated System Tandem Electrospray Mass Spectrometry; Che-I Liao; Kuo-Lung Ku; *National Chiayi University, Chiayi City, Taiwan***
- WP 600 **Omics Tools for the Biological Evaluation of Olive-Derived Bioactive Substances; Nikolaos Lemonakis<sup>1</sup>; Maria Halabalaki<sup>1</sup>; Vassilios Mougios<sup>2</sup>; Lindsay Brown<sup>3</sup>; Hemant Poudyal<sup>3</sup>; Alexios Leandros Skaltsounis<sup>1</sup>; Anthony Tsarbopoulos<sup>4</sup>; Evangelos Gikas<sup>1</sup>; <sup>1</sup>University of Athens, Department of Pharmacy, Athens, Greece; <sup>2</sup>Aristotle University of Thessaloniki, Thessaloniki, Greece; <sup>3</sup>University of Southern Queensland, Australia; <sup>4</sup>University of Athens Medical School, Athens, Greece**

- WP 601 **Disruption of Amino Acid Metabolism in Radiation-Induced Lung Injury;** Fei Li<sup>1</sup>; Jace Jones<sup>1</sup>; Gregory Tudor<sup>2</sup>; Catherine Booth<sup>2</sup>; Thomas MacVittie<sup>3</sup>; Maureen Kane<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Baltimore, MD; <sup>2</sup>Epistem Ltd, Manchester, UK; <sup>3</sup>University of Maryland, School of Medicine, Baltimore, MD
- WP 602 **Multioomic Profiling of Acute Immune Response in an SIV Macaque Model of HIV-AIDS;** Ravi Tharakan<sup>1</sup>; Anne Blackwell<sup>2</sup>; Ceereena Ubaida Mohien<sup>1</sup>; David Colquhoun<sup>3</sup>; Brigitte Simons<sup>4</sup>; David Graham<sup>1</sup>; <sup>1</sup>JHU, Baltimore, MD; <sup>2</sup>Agilent Technologies, Wilmington, DE; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>4</sup>AB SCIEX, Montreal, QC
- WP 603 **Metabolomic and Lipidomic Analyses of Diet-Induced Inhibition of Hepatic De Novo Lipogenesis with Carbohydrate Restriction;** Daniela M Schlatter<sup>1</sup>; Michelle A Puchowicz<sup>1</sup>; Giovanni Pallante<sup>2</sup>; Tim Stratton<sup>2</sup>; Mark R Chance<sup>1</sup>; Junhua Wang<sup>2</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- WP 604 **MRMPROBS Suite: Metabolomics Software for Large-Scale Multiple Reaction Monitoring Assays;** Hiroshi Tsugawa<sup>1,2</sup>; Mitsuhiro Kanazawa<sup>3</sup>; Atsushi Ogiwara<sup>3</sup>; Masanori Arita<sup>1,4</sup>; <sup>1</sup>RIKEN, Yokohama, Japan; <sup>2</sup>Osaka Univ., Osaka, Japan; <sup>3</sup>Reifycs, Inc., Minato-ku, Japan; <sup>4</sup>NIG, Mishima, Japan
- WP 605 **Development of Peak Reconstruction Program for Isotope Labeling LC-MS-based Quantitative Metabolomics;** Tao Huan; Liang Li; University of Alberta, Edmonton, Canada
- WP 606 **Quantitation of Amino Acids and Vitamins in Culture Media and Mammalian Cells by Liquid Chromatography-Tandem Mass Spectrometry;** Jinshu Qiu; Pik Kay Chan; Pavel V. Bondarenko; Amgen, Thousand Oaks, CA
- WP 607 **An LC-MS-MS-based Targeted Metabolomics Platform and Its Use to Define a Metabolomic Signature of Glutamine-Dependent Reductive Carboxylation in Cancer Cells;** Zeping Hu; UT Southwestern Medical Center, Dallas, TX
- WP 608 **In vivo Stable Isotope Labeling of <sup>13</sup>C and <sup>15</sup>N Labeled Metabolites and Lipids;** Susanne Breitkopf<sup>1</sup>; Min Yuan<sup>1</sup>; Costas Lyssiotis<sup>3</sup>; John M Asara<sup>1,2</sup>; <sup>1</sup>Beth Israel Deaconess Medical Center, Boston, MA; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Weill Cornell Medical College, New York, NY
- WP 609 **Protocol for Determination of Redox and Bioenergetics Molecules in Tissue Samples using Tandem Mass Spectrometry and Zwitterionic HILIC Columns;** Hardik Shah; Albert Einstein College of Medicine, Bronx, NY
- WP 610 **Development and Application of a UPLC/MRM-MS Method for the Comprehensive Analysis of >50 Bile Acids in Human and Mouse Samples;** Jun Han<sup>1</sup>; Yang Liu<sup>1</sup>; Renxue Wang<sup>2</sup>; Victor Ling<sup>2</sup>; Christoph Borchers<sup>1,3</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>BC Cancer Agency, University of British Columbia, Vancouver, Canada; <sup>3</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 611 **3-Nitrophenylhydrazine as an Efficient Chemical Derivatization Reagent in LC/MS-Based Quantitative Metabolomics;** Jun Han<sup>1</sup>; Karen Lin<sup>1</sup>; Carita Sequeria<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- WP 612 **LC/MS Response Factor Dependence on Mobile Phase Composition using newly Authenticated Acylsugar Metabolites;** Banibrata Ghosh; Zhenzhen Wang; A. Daniel Jones; Michigan State University, East Lansing, MI
- WP 613 **Simultaneous Analysis of Primary Metabolites by Triple Quadrupole LC/MS/MS using Pentafluorophenylpropyl Column;** Tsuyoshi Nakanishi; Shimadzu Corporation, Kyoto, Japan
- WP 614 **Parallel UHPLC-MS/MS System for High-Speed SRM Quantification using Fast Electrospray Polarity Switching;** Kyoko Watanabe<sup>1,2</sup>; Emmanuel Varesio<sup>1</sup>; Neil Loftus<sup>3</sup>; Gerard Hopfgartner<sup>1</sup>; <sup>1</sup>University of Geneva, University of Lausanne, Geneva, Switzerland; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Shimadzu Corporation, Manchester, UK
- WP 615 **MALDI-TOF as a New Tool for Quantification of Polyamines;** Masoud Zabet Moghaddam<sup>1</sup>; Ruchi Hooda<sup>1</sup>; Mohamed Fokar<sup>2</sup>; Susan San Francisco<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>Oklahoma State University, Ardmore, OK
- Drug Metabolism: High Throughput Analysis, 616 - 627**
- WP 616 **A Comparison of Scheduled and Non-Scheduled Multiple Reaction Monitoring (MRM) for Increased Throughput of Targeted Metabolomics in Early Discovery;** Carrie Funk; Hui Zhang; Richard Schneider; Pfizer, Groton, CT
- WP 617 **High-throughput Quantification of Low Molecular Weight Biomarkers using Liquid Chromatography Coupled with High Resolution Accurate Mass Spectrometry;** Mary Piotrowski; David Pirman; John Janiszewski; Pfizer, Groton, ct
- WP 618 **Human rCYP Phenotyping as a Model Experiment for Combination of Qualitative and Quantitative HRMS Data in Drug Discovery;** JianHua Liu<sup>1</sup>; Veronica Zelesky<sup>1</sup>; Carrie Funk<sup>2</sup>; Nathaniel Woody<sup>2</sup>; John Janiszewski<sup>1</sup>; Ismael Zamora<sup>3</sup>; Eva Duchoslav<sup>4</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>Pfizer, Groton, CT; <sup>3</sup>Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; <sup>4</sup>AB Sciex, Concord, ON
- WP 619 **Simultaneous Metabolic Stability Determination and Metabolite Identification Using Q Exactive System;** Ruiqing Qiu; Gang Luo; Covance, Madison, WI
- WP 620 **High Resolution Mass Spectrometry Quan/Qual-applications in high Throughput Hepatocyte Stability Assay;** Yongmin Li<sup>1</sup>; Sam Sperry<sup>1</sup>; Keeley Murphy<sup>2</sup>; John Fink<sup>2</sup>; Juntyma Engrakul<sup>1</sup>; Niresh Hariparsad<sup>1</sup>; Jean-Francois Levesque<sup>1</sup>; Peter Littlewood<sup>1</sup>; Alice Tsai<sup>1</sup>; Weichao Chen<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals Inc., San Diego, CA; <sup>2</sup>ThermoFisher Scientific, San Jose, CA
- WP 621 **Development of a Quantitative LCMS Method for the Novel Antifungal Compound Occidiofungin using TraceFinder 3.1 with Intelligent Sequencing;** Jamie K Humphries; Thermo Electron, Keller, TX
- WP 622 **An Integrated Process for Metabolite Based in vitro Reaction Phenotyping in Early Discovery using LC/HRMS;** Jonathan L. Josephs<sup>1</sup>; Emily Luk<sup>1</sup>; Mary Grubb<sup>1</sup>; Yanou Yang<sup>1</sup>; William Humphreys<sup>2</sup>; <sup>1</sup>Bristol-Myers Squibb, Pennington, NJ; <sup>2</sup>Bristol-Myers Squibb, Lawrenceville, NJ
- WP 623 **Rapid LC-MS/MS Determination of Digoxin and Digitoxin with Minimal Matrix Effects;** Xiaoning Lu; David S. Bell; Sigma-Aldrich, Bellefonte, PA
- WP 624 **Determination of  $\beta$ -blockers from Human Plasma with SPE 96-well Plate Format and LC-MS/MS;** Ruyi Wang<sup>1</sup>; Guotao Lu<sup>2</sup>; <sup>1</sup>Bonna Agela Technologies Ltd., Tianjin, China; <sup>2</sup>Bonna Agela Technologies Inc, Wilmington, DE
- WP 625 **The Application of UHPLC and Ultrafast-LCMSMS to the Analysis of Small Volume Biological Samples for Drug Residues;** Paul Wynne<sup>1</sup>; Bruce Fraser<sup>2</sup>; John Hewetson<sup>3</sup>; Nigel Gieves<sup>3</sup>; <sup>1</sup>Shimadzu, Park Orchards, Australia;

<sup>2</sup>Shimadzu Scientific Instruments (Oceania), Palmerston North, New Zealand; <sup>3</sup>Shimadzu Australasia, Sydney, Australia

WP 626 **Strategy for Predicting Molecular Coverage and Enhancing Successful Analysis for CACO2 Studies in High-Throughput LDTD-MS/MS;** Pierre Picard; Serge Auger; Alex Birsan; Sylvain Letarte; Jean Lacoursiere; *Phytronix Technologies, Inc., Quebec, Canada*

WP 627 **The ADME-Hub: Formalizing and Automating Information Flow in the Preparation and Measurement of Lead Optimization Assays;** Wayne Lootsma<sup>1</sup>; Steven Ainley<sup>1</sup>; Nick Levitt<sup>2</sup>; Brendon Kapinos<sup>3</sup>; Veronica Zelesky<sup>3</sup>; John Janiszewski<sup>3</sup>; <sup>1</sup>Sound Analytics, LLC, Niantic, CT; <sup>2</sup>TwoCenter Technologies, Cambridge, MA; <sup>3</sup>Pfizer Inc., Groton, CT

#### Drug Metabolism: Quantitative Analysis, 628 - 639

WP 628 **Accelerated and Robust Monitoring for Immunosuppressants using Triple Quadrupole Mass Spectrometry;** Natsuyo Asano; Tairo Ogura; Kiyomi Arakawa; *Shimadzu Corporation, Kyoto, Japan*

WP 629 **Development of a Sensitive Liquid Chromatography-Tandem Mass Spectrometric Method for Pharmacokinetic Study of Telbivudine in Human Plasma;** Bicui Chen<sup>1</sup>; Bin Wang<sup>1</sup>; Xiaojin Shi<sup>1</sup>; Yuling Song<sup>2</sup>; Changkun Li<sup>2</sup>; Qian Sun<sup>2</sup>; Jinting Yao<sup>2</sup>; Taohong Huang<sup>2</sup>; Kawano Shin-ichi<sup>2</sup>; Hashi Yuki<sup>2</sup>; <sup>1</sup>Pharmacy Department, Huashan Hospital, Shanghai, China; <sup>2</sup>Shimadzu (China) Co., Ltd, Shanghai, China

WP 630 **Application of In-Source Fragmentation in More Accurate Metabolite Semi-quantification by Peak Area from High-Resolution Mass Spectrometry;** Lin Chen; Xiping Fang; Jinn Wu; Li-Quan Wang; *XenoBiotic Laboratories, Inc, Plainsboro, NJ*

WP 631 **UPLC Coupled with High Resolution Mass Spectrometry for Un-biased MS Scanning and Data Banking for Metabolite Exposure Comparison across Species;** Hongying Gao; R. Scott Obach; *Pfizer, Inc, Groton, CT*

WP 632 **Mass Spectrometric Pharmacokinetics and Pharmacodynamics Analysis of Drugs on Three-Dimensional (3-D) Cell Cultures in a 3-D Printed Microfluidic Device;** Xin Liu<sup>1</sup>; Sarah Y. Lockwood<sup>2</sup>; Amanda B. Hummon<sup>1</sup>; Dana M. Spence<sup>2</sup>; <sup>1</sup>University of Notre Dame, Notre Dame, Indiana; <sup>2</sup>Michigan State University, East Lansing, MI

WP 633 **Quantitation of Insulin Analogue Glargine and Its Two Metabolites M1 and M2 with LC-MS/MS for Dog Toxicokinetics Study;** Yong-Xi Li<sup>1</sup>; Yan Ke<sup>1</sup>; Junyu Li<sup>1</sup>; Run Li<sup>2</sup>; Xiaofeng Chen<sup>2</sup>; Sahana Mollah<sup>3</sup>; Xu Wang<sup>3</sup>; <sup>1</sup>Medpace, Cincinnati, OH; <sup>2</sup>HEC Pharma Co. Ltd, Guangdong, China; <sup>3</sup>AB SCIEX, Framingham, MA

WP 634 **Acyl Glucuronides Separation Method for Plasma Analysis by LDTD-MS/MS in Less than 9 Seconds per Sample;** Jean Lacoursiere; Alex Birsan; Serge Auger; Sylvain Letarte; Pierre Picard; *Phytronix Technologies Inc., Quebec, Canada*

WP 635 **Investigating Biological Variation in Human Hepatocytes of Phase I and II drug Metabolism Enzymes;** Xu Wang<sup>1</sup>; Hui Zhang<sup>2</sup>; Christie Hunter<sup>3</sup>; <sup>1</sup>AB SCIEX, Framingham, MA; <sup>2</sup>Pfizer, Groton, CT; <sup>3</sup>AB SCIEX, Redwood City, CA

WP 636 **Overcoming Metabolite Interferences in Measuring Absolute Oral Bioavailability using Intravenous Microdosing of <sup>14</sup>C-Labeled Drug and Accelerator Mass Spectrometry (AMS);** Naiyu Zheng<sup>1</sup>; Jianing Zeng<sup>1</sup>; Michael Furlong<sup>1</sup>; Xiaolu Tao<sup>1</sup>; Stephen Dueker<sup>2</sup>; Van Ly<sup>1</sup>;

Daisie Chiuu<sup>2</sup>; Wesley Turley<sup>1</sup>; John Easter<sup>1</sup>; Ishani Savant<sup>1</sup>; Anne-Françoise Aubry<sup>1</sup>; Mark E. Arnold<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company, Princeton, NJ; <sup>2</sup>Eckert & Ziegler Vitalea Science, Davis, CA

WP 637 **Achieving Maximum Sensitivity for Drug Metabolism and Bioanalytical Workflows: Investigating Time-Of-Flight and Ion Mobility Modes of Acquisition;** Mark Wrona; Craig Dorschel; Yun Aleyunas; Kevin Cook; Stephen McDonald; Paul Rainville; *Waters, Milford, MA*

WP 638 **Capillary Microsampling (CMS) of Whole Blood for Drug Discovery Studies in Mice: An Alternative to DBS Sampling in Bioanalysis;** Walter Korfmacher<sup>1</sup>; Maria Fitzgerald<sup>1</sup>; Yongyi Luo<sup>2</sup>; Stacy Ho<sup>1</sup>; Jie Wang<sup>2</sup>; Zhongtao Wu<sup>2</sup>; Richard Knapp<sup>2</sup>; Gregory Snow<sup>3</sup>; Tom O'Shea<sup>1</sup>; <sup>1</sup>Genzyme, Waltham, MA; <sup>2</sup>Sanofi, Waltham, MA; <sup>3</sup>Agilux Laboratories, Worcester, MA

WP 639 **Fast and Sensitive Quantitation of Substrates of Hepatic Uptake Transporters in Cells: Paradim Shift from Radioactivity Detection to LC/MS Analysis;** Ming Yao; Hong Shen; Weiping Zhao; Yong-Hae Han; Praveen Balimane; W. Griff Humphreys; Mingshe Zhu; *Bristol-Myers Squibb, Princeton, NJ*

#### Drug and Metabolite Analysis: Dried Biological Samples, 640 - 656

WP 640 **A Novel Dried Matrix Microsampling Device that Eliminates the Volume Based Hematocrit Bias Associated with DBS Sub-Punch Workflows;** Stuart Kushon<sup>1</sup>; Allen Bischofberger<sup>1</sup>; Anna Carpenter<sup>1</sup>; Phillip Denniff<sup>2</sup>; Yibo Guo<sup>1</sup>; Peter Rahn<sup>1</sup>; James Rudge<sup>1</sup>; Neil Spooner<sup>2</sup>; Emmet Welch<sup>1</sup>; <sup>1</sup>Phenomenex, Torrance, CA; <sup>2</sup>GSK, Ware, UK

WP 641 **Next Generation Plasma Collection Technology for the Clinical Analysis of Temozolomide by HILIC/MS/MS;** Alan J Barnes<sup>1</sup>; Adam McMahon<sup>2</sup>; Neil J Loftus<sup>1</sup>; <sup>1</sup>Shimadzu, Manchester, UK; <sup>2</sup>WMIC, University of Manchester, Manchester, UK

WP 642 **Investigation of Solid Phase Micro Extraction as an Alternative to Dried Blood Spot;** Craig Aurand; David Bell; Robert Shirey; Emily Barrey; *Sigma Aldrich, Bellefonte, PA*

WP 643 **Determination of Drugs in Blood Samples by Automatic SPE Apparatus Coupled with Gas Chromatography-Mass Spectrometry;** Xiaoyan Cao; Guotao Lu; *Bonna-Agela, Tianjin, China*

WP 644 **Dried Plasma Spots Derived from Filtered Whole Blood. Hemato-compatible?;** Robert Sturm<sup>1</sup>; Jack Henion<sup>1</sup>; Richard Abbott<sup>2</sup>; Phillip Wang<sup>3</sup>; <sup>1</sup>Quintiles, Ithaca, NY; <sup>2</sup>Shire, Hampshire, UK; <sup>3</sup>Shire, Wayne, PA

WP 645 **Evaluation of Plasma Microsampling for Dried Plasma Spots (DPS) in Quantitative LC-MS/MS Bioanalysis using Ritonavir as a Model Compound;** Wenkui Li; John Doherty; Sarah Favara; Christopher Breen; Jimmy Flarakos; Francis Tse; *Novartis Institutes for Biomedical Research, East Hanover, NJ*

WP 646 **A Sensitive Liquid Chromatography-Tandem Mass Spectrometry Method for Quantitative Analysis of Efavirenz, Emtricitabine and Tenofovir in Human Dried Blood Spots;** Praveen Srivastava; Jeffrey Barrett; Athena Zuppa; Ganesh Moorthy; *CHOP, Philadelphia, PA*

WP 647 **Optimization of the Quantitation of Drugs in Dried Whole Blood and Plasma Spots by Wide-Isolation MALDI-MS<sup>n</sup>;** Elizabeth Dhumakupt; Richard A. Yost; *University of Florida, Gainesville, FL*

- WP 648 **Quantitation of Underivatized Tetrahydrocannabinol (THC) in Dry Blood Spots by a Highly Sensitive LC-MS/MS Instrument**; Sha Joshua Ye; Mitesh Patel; Hui Qiao; Ellie Majidi; *IONICS Mass Spectrometry Grp, Bolton, Canada*
- WP 649 **Biomonitoring Platform for Measuring Pesticide Levels in Tissue - Capillary LC-MS Analysis of Pesticides in Plasma from Noviplex Cards**; Jeremy Post; Christopher Gilles; Scott Kuzdzal; *Shimadzu Scientific Instruments, Columbia, MD*
- WP 650 **High Resolution, Accurate Mass Screening of Anesthetic Compounds and Their Metabolites in Urine by Paper-Spray Q Exactive Mass Spectrometry**; Maria C. Prieto Conaway<sup>1</sup>; Tim Stratton<sup>1</sup>; Hans Grensemann<sup>2</sup>; Caroline Ding<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- WP 651 **Automated Analysis of Dried Blood, Plasma and Urine Samples by Flow-Through Desorption Coupled to Online SPE and Mass Spectrometry**; Lena Knecht; Emile Koster; Cornelis Tump; *Spark Holland, Emmen, Netherlands*
- WP 652 **Application of Dried Blood Spot Technology for Quantitation of the Glucan Synthesis Inhibitor MK-3118 (SCY-078) in Human Blood by LC-MS/MS**; Huizhi Xie; Yang Xu; Lingling Xue; Sheng Bi; Michael Schwartz; Cindy Miller-Stein; Wei Xie; Wendy Comisar; Evan Friedman; Michele Trucksis; Sheila Breidinger; Eric Woolf; *Merck & Co., West Point, PA*
- WP 653 **Identification of Metabolites of Harmine in Rat Plasma using HPLC-Trap-MS-MS**; Shuang Zhao; Beibei wang; Peng Tan; Liu Yonggang; *Beijing, China*
- WP 654 **Multiplexed MRM-based Protein Quantification in Dried Blood Spot Samples**; Andrew Chambers<sup>1</sup>; Andrew Percy<sup>1</sup>; Juncong Yang<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>*University of Victoria-Genome BC Proteomics Centre, Victoria, Canada*; <sup>2</sup>*UVic Dept of Biochemistry and Microbiology, Victoria, Canada*
- WP 655 **Determination of Psychosine and Glucopsychosine in Dried Blood Spots by LC-MS/MS for Krabbe and Gaucher Diseases**; Coleman Turgeon<sup>1</sup>; Joseph Orsini<sup>2</sup>; Mark J. Magera<sup>1</sup>; Dimitar Gavrilov<sup>1</sup>; Devin Oglesbee<sup>1</sup>; Kimiyo Raymond<sup>1</sup>; Silvia Tortorelli<sup>1</sup>; Piero Rinaldo<sup>1</sup>; Dietrich Matern<sup>1</sup>; <sup>1</sup>*Biochemical Genetics Laboratory, Mayo Clinic, Rochester, MN*; <sup>2</sup>*New York State Dept of Health, Wadsworth Center, Albany, NY*
- WP 656 **Clinical Diagnostics of Neuronal Ceroid Lipofuscinoses on Dry Blood Spots by Fluorimetry and MRM-MS using New Coumarin-based Substrates**; Michael Przybylski<sup>1</sup>; Claudia Cozma<sup>1</sup>; Marius Iurascu<sup>1</sup>; Thomas Braulke<sup>2</sup>; Angela Schulz<sup>2</sup>; <sup>1</sup>*Universität Konstanz, Konstanz, Germany*; <sup>2</sup>*University Medical Center Hamburg-Eppendorf, Hamburg, Germany*
- Ion Mobility Applications, 657 - 685**
- WP 657 **Use of Multivariate Curve Resolution and Ion Mobility-Mass Spectrometry for Isomer Differentiation**; Behrooz Zekavat<sup>1</sup>; Brett Harper<sup>1</sup>; Matthew Brantley<sup>2</sup>; Michael E. Pettit<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*; <sup>2</sup>*University of Texas at Tyler, Tyler, TX*
- WP 658 **Energy Resolved Ion Mobility Deconvolution of Isobaric Mixtures**; Brett Harper<sup>1</sup>; Behrooz Zekavat<sup>1</sup>; Matthew Brantley<sup>2</sup>; Michael Pettit<sup>1</sup>; Touradj Solouki<sup>1</sup>; <sup>1</sup>*Baylor University, Waco, TX*; <sup>2</sup>*University of Texas at Tyler, Tyler, TX*
- WP 659 **Development of Relative Ion Mobility and Molecular Modeling (RIM3) as a Novel Approach to Metabolite Structural Identification**; Sean Yu; Ian Mcintosh; Deping Wang; Dan Cui; *Merck & Co, West Point, PA*
- WP 660 **Elucidation of Gramicidin A Conformational Preferences Utilizing Ion Mobility Mass Spectrometry**; John Patrick<sup>1</sup>; David H. Russell<sup>2</sup>; <sup>1</sup>*Texas A&M, College Station, TX*; <sup>2</sup>*Texas A&M University, College Station, TX*
- WP 661 **Evolution of Hydrogen Bond Networks in Protonated Water Clusters H<sup>+</sup> (H<sub>2</sub>O)<sub>n</sub> (n = 1-150) Studied by Cryogenic Ion Mobility-Mass Spectrometry**; Kelly A. Servage; Joshua A. Silveira; Kyle L. Fort; David H. Russell; *Texas A&M University, College Station, TX*
- WP 662 **Displacement of Metal Ions from Metallothionein using N-ethylmaleimide: Kinetics and Effect of Covalent Labeling on Conformation**; Shu-Hua Chen; Liuxi Chen; David H. Russell; *Texas A&M University, College Station, TX*
- WP 663 **Analysis of Ions Generated From Native Spray Conditions with Trapped Ion Mobility Spectrometry (TIMS)**; Mark Ridgeway; Joshua Silveira; Jacob Meier; Melvin A. Park; *Bruker Daltonics, Inc., Billerica, MA*
- WP 664 **Temperature-Dependent Conformer State Distributions of Model Peptides in Trapped Ion Mobility Spectrometry**; Joshua Silveira; Mark Ridgeway; Jacob Meier; Melvin Park; *Bruker Daltonics, Billerica, MA*
- WP 665 **UPLC Ion Mobility Mass Spectrometry: A New Approach to Authentication and Routine Screening of Ginsenocide Isomers in Functional Food Products**; McCullagh Mike; David Douce; Robert Lewis; *Waters (MS Technologies), Wilmslow, UK*
- WP 666 **Discovery of Pesticide Protomers Using Routine Ion Mobility Screening**; Michael McCullagh<sup>1</sup>; Jeff Goshawk<sup>1</sup>; Severine Goscinny<sup>2</sup>; Vincent Hanot<sup>2</sup>; Kieran Neeson<sup>1</sup>; David Eatough<sup>1</sup>; Chris Carver<sup>1</sup>; <sup>1</sup>*Waters, Manchester, UK*; <sup>2</sup>*Institut Scientifique de Santé Publique, Brussels, Belgium*
- WP 667 **Combining an Integrated Microfluidic Device with CCS Ion Mobility Screening for the Analysis of Pesticide Residues in Food**; Michael McCullagh<sup>1</sup>; Séverine Goscinny<sup>2</sup>; Vincent Hanot<sup>2</sup>; David Douce<sup>1</sup>; <sup>1</sup>*Waters (MS Technologies), Wilmslow, UK*; <sup>2</sup>*Scientific Institute of Public Health, Brussels, Belgium*
- WP 668 **Using the Routine Separation Dimension and Identification Criteria of UPLC Ion Mobility to Enhance Specificity in Profiling Complex Samples**; Michael McCullagh<sup>1</sup>; Kieran J. Neeson<sup>1</sup>; C. A. M. Pereira<sup>2</sup>; J. H. Yariwake<sup>2</sup>; Chris Carver<sup>1</sup>; David Douce<sup>1</sup>; <sup>1</sup>*Waters Corporation, Manchester, UK*; <sup>2</sup>*Universidade de Sao Paulo, Sao Paulo, Brasil*
- WP 669 **Supercharging of Native-Like Proteins and Protein Complexes: Effects of m-Nitrobenzyl Alcohol versus Sulfolane**; Christiane N. Stachl; Samuel J. Allen; Matthew F. Bush; *University of Washington, Seattle, WA*
- WP 670 **Analysis of Motor Oil by Selected Accumulation Ion Mobility Spectrometry**; Kyle Fort<sup>1</sup>; William K. Russell<sup>1</sup>; Do Yong Kim<sup>1</sup>; Desmond Kaplan<sup>2</sup>; Melvin A. Park<sup>3</sup>; David H. Russell<sup>1</sup>; Mark Ridgeway<sup>3</sup>; <sup>1</sup>*Texas A&M University, College Station, TX*; <sup>2</sup>*Bruker Daltonics, inc., Fremont, CA*; <sup>3</sup>*Bruker Daltonics, Inc., Billerica, MA*
- WP 671 **Steroid and Lipid Analysis by High Resolution Ion Mobility-TOF MS**; Michael Groessl<sup>1</sup>; Bernhard Dick<sup>2</sup>; Bruno Vogt<sup>2</sup>; Richard Knochenmuss<sup>1</sup>; <sup>1</sup>*Tofwerk, Thun, Switzerland*; <sup>2</sup>*Bern University Hospital, Bern, Switzerland*
- WP 672 **Ion Mobility Spectrometry Tandem Mass Spectrometry (IMS-MS<sup>n</sup>) and Parallel Dissociation of Plasma Metabolites and Fragments**; Gregory Donohoe; Stephen Valentine; *West Virginia University, Morgantown, WV*
- WP 673 **Metabolomics of Plasma Fluids from Apolipoprotein A-V Knockout Mice by Hadamard Transform Ion Mobility Time-of-Flight Mass Spectrometry (HT-IMtofMS)**; Xing Zhang<sup>1</sup>; Min Xu<sup>2</sup>; Patrick Tso<sup>2</sup>; William Siems<sup>1</sup>; Herbert Hill<sup>1</sup>;



- <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>University of Cincinnati, Cincinnati, OH
- WP 674 **Database to Predict the Collision Cross Section of Glycopeptides by IMS-MS;** Rebecca S. Glaskin<sup>1</sup>; Kshiti Khatri<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Alex Mordehai<sup>2</sup>; Joseph Zaia<sup>1</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 675 **Ion Mobility-Mass Spectrometry Reveals Significant Structural Rearrangements During the Collision Induced Dissociation of Charge Reduced Protein Complexes;** Russell Bornschein; Shuai Niu; Brandon Ruotolo; *University of Michigan, Ann Arbor, MI*
- WP 676 **A Study of the Effects of Calibrant Choice in Determination of Ion-Neutral Collision Cross Sections via Traveling Wave Ion Mobility;** Rebecca E. Jarratt; Abby S. Gelb; Yuting Huang; Eric D. Dodds; *University of Nebraska-Lincoln, Lincoln, NE*
- WP 677 **An Ion Mobility Spectrometry-Mass Spectrometry Study of Metalated Isomeric Carbohydrates and their Electron Transfer Products;** Yuting Huang<sup>1</sup>; Eric D. Dodds<sup>2</sup>; <sup>1</sup>University of Nebraska-Lincoln, Lincoln, NE; <sup>2</sup>University of Nebraska - Lincoln, Lincoln, NE
- WP 678 **Collision Cross Section Dependence upon Glycan Size, Charge State, and Peptide Sequence of High Mannose N-Linked Glycopeptides;** Abby S. Gelb; Yuting Huang; Rebecca E. Jarratt; Eric D. Dodds; *University of Nebraska-Lincoln, Lincoln, NE*
- WP 679 **Ion Mobility-Mass Spectrometry Monitoring of isoxazolidin-5-one Organocatalyzed Synthesis;** Corinne Loutelier-Bourhis; Clisy Maganga; Marie Hubert-Roux; Vincent Levacher; Jean-François Brière; Carlos Afonso; *University of Rouen, Mont Saint Aignan, France*
- WP 680 **Improved Separation Methods for Rapid Analysis of Targeted Small Molecules on IMS/Q-TOF Platform;** Christopher Beekman<sup>1</sup>; David L. Wong<sup>2</sup>; Christian Klein<sup>2</sup>; Ruwan Kurulugama<sup>2</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- WP 681 **An Artificial Intelligence Technique is used in Optimization of Dual Separation System, IM-QTOF;** Huy Bui; Christian Klein; William Moore; Dung Le; Sandra Tang; William Frazer; Bruce Wang; Gregor Overney; Ruwan Kurulugama; Alex Mordehai; George Stafford; *Agilent Technologies, Santa Clara, CA*
- WP 682 **Structural and Conformational Studies of Non-Covalent Complexes Formed upon Ion Pairing;** Christophe Chendo<sup>1</sup>; Momar Touré<sup>1</sup>; Olivier Chuzel<sup>1</sup>; Stéphane Viel<sup>1</sup>; Erik Laurini<sup>2</sup>; Paola Posocco<sup>2</sup>; Sabrina Pricl<sup>2</sup>; Jean-Luc Parrain<sup>1</sup>; Laurence Charles<sup>1</sup>; <sup>1</sup>Aix-Marseille University, Marseille, France; <sup>2</sup>University of Trieste, Trieste, Italy
- WP 683 **Evidence for Unknown Structure Changes in Strained PAH Macrocyces by Fragmentation Ion Mobility Mass Spectrometry;** Wen Zhang; Martin Quernheim; Hans Joachim Räder; Klaus Müllen; *MPI for Polymer Research, Mainz, Germany*
- WP 684 **Discrimination of Large Maltooligosaccharides from Isobaric Dextran and Pullulan using Ion Mobility Mass Spectrometry;** Abdul M Rashid; Gerhard Saalbach; Stephen Bornemann; *John Innes Centre, Norwich, UK*
- WP 685 **Ion Mobility Mass Spectrometry Applied to the Mechanistic Elucidation of Asymmetric Morita-Baylis-Hillman Reaction;** Renan Galaverna; Marla Godoi; Giovana Bataglion; Fernando Coelho; Marcos Eberlin; *State university of campinas, Campinas, Brasil*
- Ion Mobility: Fundamentals, 686 - 700**
- WP 686 **Experimental Validation of an Analytical Model for Trapped Ion Mobility Spectrometry;** Melvin A. Park<sup>1</sup>; Karsten Michelmann<sup>2</sup>; Joshua Silveira<sup>1</sup>; Mark Ridgeway<sup>1</sup>; <sup>1</sup>Bruker Daltonics, Inc., Billerica, MA; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany
- WP 687 **Predictive Mathematical Descriptors of Biological Class Trends in Ion Mobility-Mass Spectrometry Analysis;** Caleb B. Morris; Jody C. May; John A. McLean; *Vanderbilt University, Nashville, TN*
- WP 688 **Technical Advances and Theoretical Performance Assessment of a Spatially Multiplexed Ion Mobility-Mass Spectrometer;** Katrina L. Leaptrot; Jody C. May; John A. Mclean; *Vanderbilt University, Nashville, TN*
- WP 689 **A New Solver to Calculate Ion Density Distribution and Electric Field in Dense Gas;** Roger Giles<sup>1</sup>; Vadim Sizykh<sup>2</sup>; Alina Andreyeva<sup>3</sup>; <sup>1</sup>Shimadzu Research Laboratory, Manchester, UK; <sup>2</sup>Moscow State University of Inst Eng & Informatics, Moscow, Russia; <sup>3</sup>(3)Advanced Numerical Simulations, Huddersfield, UK
- WP 690 **Derivation of an Analytical Model for Trapped Ion Mobility Spectrometry;** Karsten Michelmann; Joshua Silveira; Mark Ridgeway; Melvin Park; *Bruker Daltonics, Billerica, MA*
- WP 691 **Theoretical and Experimental Study of Fast Ion Separation and Detection in Liquid;** Yi-Hong Cai; Jia-Der Lin; Yi-Sheng Wang; *GRC, Academia Sinica, Taipei, Taiwan*
- WP 692 **Maximizing the Multiplexing Advantage: Mobility-Specific Sources of Transform Error and Means of Correction;** Brian H. Clowers; Xing Zhang; Zhihau Yu; William F. Siems; *Washington State University, Pullman, WA*
- WP 693 **Accurate Ion Mobility Spectrometer;** Brian Hauck<sup>1</sup>; Bill Siems<sup>1</sup>; Charles Harden<sup>2</sup>; Vince McHugh<sup>3</sup>; Herbert Hill, Jr.<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>LEIDOS - US Army ECBC Operations, Gunpowder, MD; <sup>3</sup>U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD
- WP 694 **Effects of MALDI Matrix Ions in Traveling Wave Ion Mobility Mass Spectrometry;** Joseph Mwangi; Norman Chiu; *University of North Carolina at Greensboro, Greensboro, NC*
- WP 695 **The Effect of Charge Location in Ion Mobility Mass Spectrometry for Small Molecule Analytes;** Cris Laphorn<sup>1</sup>; Frank Pullen<sup>1</sup>; Babur Chowdhry<sup>1</sup>; George Perkins<sup>2</sup>; Trevor Dines<sup>3</sup>; Michael McCullagh<sup>4</sup>; <sup>1</sup>University of Greenwich, Chatham Maritime, UK; <sup>2</sup>PerkinElmer Inc, Branford, CT; <sup>3</sup>University of Dundee, Dundee, UK; <sup>4</sup>Waters Corporation, Manchester, UK
- WP 696 **Correlating DMS Simulations with Experiment;** Frank Londry; Brad Schneider; Thomas Covey; *AB SCIEX, Concord, Canada*
- WP 697 **Characterization of Gas Phase Ion/Neutral Interactions in DMS;** David Gode; Dietrich Volmer; *Saarland University, Saarbrücken, Germany*
- WP 698 **Improving Ion Mobility Measurement Sensitivity by Utilizing Helium in an Ion Funnel Trap;** Yehia Ibrahim; Sandilya Garimella; Aleksey Tolmachev; Erin Baker; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 699 **Cytochrome c Conformations Studied by Ion Mobility Spectrometry with Hydrogen-Deuterium Exchange and MS/MS Techniques;** Samaneh Ghassabi Kondalaji; Mahdiar Khakinejad; Stephen Valentine; *Morgantown, WV*

WP 700 **Conformational Preferences of Peptide – Alkali Metal Ion Adducts: The Effects of Polar Side Chain – Alkali Metal Ion Interactions;** [Chunying Xiao](#); Lisa M. Pérez; David H. Russell; *Texas A&M University, College Station, Texas*

#### Nanomaterials, 701 - 707

WP 701 **Inkjet Printed Gold Nanoparticle Surfaces for the Detection of Biomolecules by Laser Desorption/Ionization Mass Spectrometry;** [Alyssa Marsico](#); Brian Creran; Bradley Duncan; S. Gokhan Elci; Vincent Rotello; Richard Vachet; *University of Massachusetts Amherst, Amherst, Massachusetts*

WP 702 **Characterization of Monolayer Films of Asymmetric Metallosurfactants by Matrix Assisted Ionization Vacuum Mass Spectrometry;** [Tarick El-Baba](#); Lanka Wickramasinghe; Claudio Verani; Sarah Trimpin; *Wayne State University, Detroit, MI*

WP 703 **Combined Mass Spectrometric Imaging for Obtaining Site-Specific Information about Nanoparticle Stability in Tissues;** [Sukru Gokhan Elci](#); Bo Yan; Sung Tae Kim; Chang Soo Kim; Krishnendu Saha; Daniel F. Moyano; Vincent M. Rotello; Richard W. Vachet; *University of Massachusetts, Amherst, MA*

WP 704 **Investigation of Protein Corona on CpG Oligodeoxynucleotides Conjugated Nanotube with Mass Spectrometry;** [Shang Zeng](#); Wenwan Zhong; *University of California, Riverside, Riverside, CA*

WP 705 **Cluster Ion Source Coupled to a 9.4 T FT-ICR Mass Spectrometer for Experimental Study of Fullerene Formation and Gas-Phase Chemistry;** [Paul W. Dunk](#)<sup>1</sup>; Ryan A. Barrett<sup>2</sup>; Nathan K. Kaiser<sup>1</sup>; Alan G. Marshall<sup>3</sup>; Harold W. Kroto<sup>2</sup>; <sup>1</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Florida State University, Tallahassee, FL; <sup>3</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL

WP 706 **Mass Spectrometry-Based Analysis of Graphene Oxide Degradation Products;** [Wentao Jiang](#)<sup>1</sup>; Hao Bai<sup>1</sup>; Gregg P. Kotchey<sup>1</sup>; Wissam A. Saidi<sup>1</sup>; Benjamin J. Bythell<sup>2</sup>; Jacqueline M. Jarvis<sup>3</sup>; Alan G. Marshall<sup>2,3</sup>; Rena A.S. Robinson<sup>1</sup>; Alexander Star<sup>1</sup>; <sup>1</sup>University of Pittsburgh, Pittsburgh, Pennsylvania; <sup>2</sup>National High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Florida State University, Tallahassee, FL

WP 707 **Investigating Engineered Nanomaterial Induced Damage to Genomic DNA via Tandem Mass Spectrometry;** Elijah J. Petersen; Pawel Jaruga; Miral Dizdaroglu; [Bryant C. Nelson](#); *National Institute of Standards and Technology, Gaithersburg, MD*

#### Challenges in Identification, 709 -723

WP 709 **The Secret of Stradivarius: Is it Possible to Clue It?;** [Olga Polyakova](#)<sup>1</sup>; Savva Girshenko<sup>1</sup>; Slava. Artav<sup>3</sup>; Alessandra Tata<sup>2</sup>; Andreia Porcari<sup>2</sup>; Eduardo Schmidt<sup>2</sup>; Marcos Eberlin<sup>2</sup>; Albert T. Lebedev<sup>1</sup>; <sup>1</sup>Moscow State University, Moscow, Russian Federation; <sup>2</sup>ThoMSon Mass Spectrometry Laboratory, Campinas, Brazil; <sup>3</sup>LECO Corporation, St Joseph, MI

WP 710 **Isolation, Structure Elucidation and Reference Synthesis of Impurities in LX1606 by Mass Directed Fraction Collection, MS/MS, TOF/MS and NMR Spectroscopy;** [Leonard O. Hargiss](#); Philip Keyes; Matthew M. Zhao; Weiguo Liu; *Lexicon Pharmaceuticals, Princeton, NJ*

WP 711 **Comparison of Electrospray Ionization(ESI) and Atmospheric Pressure Chemical Ionization(APCI) of Labile Anti-Malarial Compounds to Monitor Pharmacokinetics of Transdermal Patches;** [Almas Taj Awan](#)<sup>1</sup>; Ilza M. O. Sousa<sup>2</sup>; Fabricio F. Favero<sup>2</sup>; Nubia C. A. Queiroz<sup>2</sup>; Marcos N. Eberlin<sup>1</sup>; Mary Ann Foglio<sup>2</sup>; <sup>1</sup>ThoMSon

*Mass spectrometry Laboratory, UNICAMP, Campinas, SP; <sup>2</sup>CPQBA, UNICAMP, Campinas, SP*

WP 712 **Characterization of Novel Methylindole-Glutathione-related Conjugates by LC-High Resolution Mass Spectrometry;** [Chenghong Zhang](#); Shuguang Ma; Cornelius Hop; Cyrus Khojasteh; *Genentech, South San Francisco, CA*

WP 713 **The Use of Linear Ion Trap for HPLC Profiling of Ginsenosides in Plant Extracts and Ginseng Based Products;** [Andrey Stavriani](#); Igor Rodin; Irina Ananieva; Oleg Shpigun; *MSU, Moscow, RU*

WP 714 **Characterization of Glycosylated Flavonoids in Plant Extracts : A “Same Masses” Nightmare;** [Claude-Paul Lafrance](#); Maxim Maheux; *TransBIOTech, Levis,*

WP 715 **Proteolytic Activity Elicited during Work-Up Of Human Serum Samples – Obstacle for Biomarker Analysis: Mass Spectrometric Characterization of Cleavage Products;** [Jingzhi Yang](#)<sup>1</sup>; Claudia Roewer<sup>1</sup>; Cornelia Koy<sup>1</sup>; Manuela Russ<sup>1</sup>; Martin Sklorz<sup>2,3</sup>; Ralf Zimmermann<sup>2,3</sup>; Uwe Fritschen<sup>4</sup>; Juliane C. Finke<sup>4</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>Proteome Center Rostock, University of Rostock, Rostock, Germany; <sup>2</sup>Institute of Chemistry, University of Rostock, Rostock, Germany; <sup>3</sup>Helmholtz Zentrum München, Munich, Germany; <sup>4</sup>HELIOS Clinic Emil von Behring, Berlin, Germany

WP 716 **Elevated Pressure Improves the Extraction and Identification of Proteins Recovered from Formalin-Fixed, Paraffin-Embedded Tissue Surrogates;** Carol Fowler<sup>1</sup>; Cedric Moore<sup>3</sup>; Timothy O’Leary<sup>2</sup>; [Jeffrey Mason](#)<sup>1</sup>; <sup>1</sup>Baltimore VA Medical Center, Baltimore, MD; <sup>2</sup>Veterans Health Administration, Washington, DC; <sup>3</sup>Johns Hopkins University, Baltimore, MD

WP 717 **LC-MS/MS Impurity Profiling and Quantitation for an Improved Bioprocess for the Production of a Fab Fragment in *E. coli*;** [Anita Krishnan](#); Shirishkumar Patel; Shalvi Shah; Sudheer Babu; Shardul Salunkhe; Sachin Rewanwar; Naidu Mookala; Archana Verma; Nagnath Mandi; Praveen Muneshwar; Sandeep Somani; Ashok Mishra; Brajesh Varshney; Rustom Mody; *Lupin limited, Biotech, Pune, India*

WP 718 **Discovery and Characterization of a Novel Photo-Oxidative Histidine-Histidine Crosslink in IgG1 Antibody Utilizing <sup>18</sup>O-labeling and Mass Spectrometry;** [Min Liu](#)<sup>1,2</sup>; Zhongqi Zhang<sup>1</sup>; Janet Cheetham<sup>1</sup>; Da Ren<sup>1</sup>; Zhaohui Sunny Zhou<sup>2</sup>; <sup>1</sup>Amgen, Inc., Thousand Oaks, CA; <sup>2</sup>Northeastern University, Boston, MA

WP 719 **Comparative Identification Methods of MS Data: Profile Versus Centroid Acquisition and the Advantage of Preliminary Multivariate Curve Resolution (MCR-ALS) Analysis;** [Eva Gorrochategui](#)<sup>1</sup>; Yongdong Wang<sup>2</sup>; Silvia Lacorte<sup>1</sup>; Cinta Porte<sup>1</sup>; Romà Tauler<sup>1</sup>; <sup>1</sup>Institute of Environ. Assessment & Water Research, Barcelona, Spain; <sup>2</sup>Cerno Bioscience, Norwalk, VA

WP 720 **A New GC “Retention Projection” Database Enables Calculation of Appropriate Retention Time Tolerance Windows without Having Standards Physically on Hand;** Brian Barnes<sup>1</sup>; Michael Wilson<sup>2</sup>; Peter Carr<sup>1</sup>; Mark Vitha<sup>3</sup>; Corey Broeckling<sup>4</sup>; Adam Heuberger<sup>4</sup>; Jessica Prenni<sup>4</sup>; Gregory Janis<sup>5</sup>; Henry Corcoran<sup>5</sup>; Nicholas Snow<sup>6</sup>; Shilpi Chopra<sup>6</sup>; Ramkumar Dhandapani<sup>6</sup>; Amanda Tawfall<sup>7</sup>; Lloyd Sumner<sup>7</sup>; [Paul Boswell](#)<sup>2</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>University of Minnesota, Saint Paul, MN; <sup>3</sup>Drake University, Des Moines, IA; <sup>4</sup>Colorado State University, Fort Collins, CO; <sup>5</sup>MedTox Laboratories, Saint Paul, MN; <sup>6</sup>Seton Hall University, South Orange, NJ; <sup>7</sup>The Samuel Roberts Noble Foundation, Ardmore, OK



- WP 721 **Accurate Prediction of Retention in Hydrophilic Interaction Chromatography (HILIC) by Back-Calculation of HPLC Gradient Profiles;** Nu Wang; Paul G. Boswell; *University of Minnesota, Saint Paul, MN*
- WP 722 **Validation of Decoy Models for HRM/SWATH Acquisition as Used in Spectronaut;** Oliver M. Bernhardt; Roland M. Bruderer; Tejas Gandhi; Saša M. Miladinović; Oliver Rinner; Lukas Reiter; *BiognoSYS AG, Zurich, Switzerland*
- WP 723 **Differentiating Gold Nanoparticle Cell Surface Adhesion from Cellular Internalization using Laser Desorption Ionization Mass Spectrometry;** Singyuk Hou; Ying Jiang; Sung Tae Kim; Ziwen Jiang; Vincent Rotello; Richard Vachet; *University of Massachusetts, Amherst, Massachusetts*
- High Mass Accuracy / High Performance MS: Applications, 724 - 739**
- WP 724 **Isotopic Exchange Mass Spectrometry Reveals Molecular Structure of Natural Organic Matter;** Yury Kostyukevich<sup>1</sup>; Alexey Kononikhin<sup>1</sup>; Igor Popov<sup>2</sup>; Eugene Nikolaev<sup>1</sup>; <sup>1</sup>*Institute for Energy Problems of Chemical Physics, Moscow, RUSSIA*; <sup>2</sup>*IBCP RAS, Moscow, Russian Federation*
- WP 725 **Qual/Quan Discovery Bioanalytical Strategies for Macromolecular Peptides using High Resolution Mass Spectrometry;** Asoka Ranasinghe; Eugene F. Ciccimaro; Celia D'Arienzo; Timothy Olah; *Bristol-Myers Squibb, Princeton, NJ*
- WP 726 **Eliminating Interferences in Serum Extracts using High Resolution Accurate Mass Spectrometry;** Jolaine Hines; Amy Gorsh; Kendall Cradic; Ravinder Singh; Stefan Grebe; *Mayo Clinic, Rochester, MN*
- WP 727 **Characterization of an Improved Ultra-High Resolution Quadrupole Time of Flight (UHR-TOF) Instrument for Proteomics Applications;** Markus Lubeck; Stephanie Kaspar; Annette Michalski; Oliver Raether; Christoph Gebhardt; Carsten Baessmann; *Bruker Daltonik GmbH, Bremen, Germany*
- WP 728 **Utilizing Very High Resolution Fine Isotopic Fragmentation Data to Refine Elemental Composition Determination;** Tim Stratton; *Thermo Fisher Scientific, San Jose, CA*
- WP 729 **High-resolution Two-Dimensional FT-ICR Mass Spectrometry and Applications to Top-Down and Bottom-up Proteomics and Environmental Samples;** Maria van Agthoven<sup>1</sup>; Christopher Wootton<sup>1</sup>; Andrew Soulby<sup>1</sup>; Juan Wei<sup>1</sup>; Mark Barrow<sup>1</sup>; Lionel Chiron<sup>2</sup>; Marie-Aude Coutouly<sup>2</sup>; Marc-André Delsuc<sup>3</sup>; Christian Rolando<sup>4</sup>; Peter O'Connor<sup>1</sup>; <sup>1</sup>*University of Warwick, Coventry, UK*; <sup>2</sup>*NMRTEC, Illkirch-Graffenstaden, France*; <sup>3</sup>*IGBMC, Illkirch-Graffenstaden, France*; <sup>4</sup>*Université Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France*
- WP 730 **Faster is Better? A Look at Speed vs Complexity in the Orbitrap Fusion;** Jolene K. Diedrich<sup>1</sup>; Antonio F. M. Pinto<sup>2</sup>; John R. Yates III<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, La Jolla, CA*; <sup>2</sup>*CAPES Foundation, Brasilia, Brazil*
- WP 731 **Rapid Accurate Mass Strategy for Photodegradation Study of Machite Green under Natural Sunlight Irritation;** Yanchun Sun<sup>1</sup>; Jiehui Hu<sup>2</sup>; Xiaoyan Xu<sup>2</sup>; Ting Liu<sup>2</sup>; Chengyuan Cai<sup>2</sup>; <sup>1</sup>*Heilongjiang River Fishery Research Institute, Harbin, China*; <sup>2</sup>*AB SCIEX, Shanghai, China*
- WP 732 **Utility of High Resolution ESI CID, HCD and ETD MS<sup>n</sup> for Complete Structural Elucidation of Large Cyclic Peptides and Metabolites;** Eugene F. Ciccimaro<sup>1</sup>; Qian Ruan<sup>1</sup>; Serhiy Hnatyshyn<sup>1</sup>; Timothy Olah<sup>1</sup>; Hongxia (Jessica) Wang<sup>3</sup>; Gary Walker<sup>2</sup>; Marshall M. Siegel<sup>2</sup>; <sup>1</sup>*Bristol-Myers Squibb, Princeton, NJ*; <sup>2</sup>*MS Mass Spec Consultants, Fair Lawn, NJ*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- WP 733 **High Resolution Mass Spectrometry (GC-APCI-/LDI-/ESI-FTICRMS) of Heavy Fuel Oil and Particulate Matter Emitted by a Ship Diesel Engine;** Martin Sklorz<sup>1,2</sup>; Christopher Rieger<sup>1,2</sup>; Theo Schwemer<sup>1,2</sup>; Ralf Zimmermann<sup>1,2</sup>; <sup>1</sup>*University of Rostock, Rostock, Germany*; <sup>2</sup>*Helmholtz Zentrum München, Munich, Germany*
- WP 734 **Resolution Requirement for Isotopic Fine Structure Determination of Peptide Fragment with Introduced mDa Stable Isotope Encoding;** Greg T. Blakney<sup>1</sup>; Chad Weisbrod<sup>1</sup>; Nathan Kaiser<sup>1</sup>; Chris L. Hendrickson<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*Dept. of Chemistry, Florida State University, Tallahassee, FL*
- WP 735 **Determination of Site-Specific Protein Disulfide Bond Redox Potentials by Top-Down FT-ICR Mass Spectrometry;** Xiaoyan Guan<sup>1</sup>; Nicolas L. Young<sup>1</sup>; Alan G. Marshall<sup>1,2</sup>; <sup>1</sup>*National High Magnetic Field Laboratory, Tallahassee, FL*; <sup>2</sup>*Florida State University, Tallahassee, FL*
- WP 736 **Developing an MS-based Platform for High-throughput and Quantitative Assessment of Protein-ligand Interaction: Application in Drug Candidate Screening;** Xin Chen<sup>1</sup>; Shanshan Qin<sup>1</sup>; Lixin Li<sup>2</sup>; Cheng Yang<sup>2</sup>; Wenqin Shui<sup>3</sup>; <sup>1</sup>*College of Life Sciences, Nankai University, Tianjin, China*; <sup>2</sup>*High-throughput Molecular Drug Discovery Center, Tianjin, China*; <sup>3</sup>*Tianjin Institute of Industrial Biotechnology, CAS, Tianjin, China*
- WP 737 **Large Scale Targeted Protein Quantification using WISIM-DIA workflow on a Orbitrap Fusion Tribrid Mass Spectrometer;** Reiko Kiyonami<sup>1</sup>; Bhavin Patel<sup>2</sup>; Michael W. Senko<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Jarrett Egertson<sup>3</sup>; Ying Sonia Ting<sup>3</sup>; Michael J. Maccoss<sup>3</sup>; John C. Rogers<sup>2</sup>; Andreas FR Hühmer<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*Thermo Fisher Scientific, Rockford, IL*; <sup>3</sup>*Univ of Washington, Seattle, WA*
- WP 738 **TMT 10-plex Quantification with Synchronous Precursor selection-MS<sup>3</sup> Enables Robust Global Classification of Protein Subcellular Localization in Pluripotent Embryonic Stem Cells;** Andy Christoforou<sup>1,2</sup>; Claire Mulvey<sup>1,2</sup>; Lisa M. Breckels<sup>1</sup>; Penny Hayward<sup>2</sup>; Laurent Gatto<sup>1</sup>; Rosa Viner<sup>3</sup>; Alfonso Martinez Arias<sup>2</sup>; Kathryn S. Lilley<sup>1</sup>; <sup>1</sup>*Dept. of Biochemistry, University of Cambridge, Cambridge, UK*; <sup>2</sup>*Dept. of Genetics, University of Cambridge, Cambridge, UK*; <sup>3</sup>*ThermoFisher Scientific, San Jose, CA*
- WP 739 **Characterization of Metabolites Inmicrosomal Metabolism of aconitineby High-Performance Liquid Chromatography/Quadrupole Ion Trap/Time-Of-Flight Mass Spectrometry;** Cuiping Yang<sup>1</sup>; Changkun Li<sup>2</sup>; Tianhong Zhang<sup>1</sup>; Qian Sun<sup>2</sup>; Yueqi Li<sup>2</sup>; Guixiang Yang<sup>2</sup>; Taohong Huang<sup>2</sup>; Shin-ichi Kawano<sup>2</sup>; Yuki Hashi<sup>2</sup>; Zhenqing Zhang<sup>1</sup>; <sup>1</sup>*Beijing Institute of Pharmacology and Toxicology, Beijing, China*; <sup>2</sup>*Shimadzu (China) Co., Ltd., Shanghai, China*
- Instrumentation: New Developments in Ionization and Sampling, 740 - 759**
- WP 740 **Remote Laser Ablation Electrospray Ionization Mass Spectrometry for Non-Proximate Analysis;** Laine Compton<sup>1</sup>; Brent Reschke<sup>2</sup>; Jordan Friend<sup>2</sup>; Matthew Powell<sup>2</sup>; Akos Vertes<sup>1</sup>; <sup>1</sup>*George Washington University, Washington, District of Columbia*; <sup>2</sup>*Protea Biosciences, Inc., Morgantown, WV*

- WP 741 **Single-probe: A Novel Sampling and Ionization Device for Mass Spectrometry Studies of Single Cells, Biological Tissues, and Protein PTMs;** Zhibo Yang; Ning Pan; Wei Rao; Rachel Vowcicefski; Chuanbin Mao; Xuewei Qu; *University of Oklahoma, Norman, OK*
- WP 742 **A Comparison of Ion Suppression Across Flow Regimes and the Implications of Reduced Suppression on Sensitivity and Assay Precision;** Jay S. Johnson; James Murphy; Paul Rainville; *Waters Corporation, Milford, MA*
- WP 743 **Conical Duct (ConDUCT) ESI Inlet Electrodes Produce Intense Laser-Like Focused Ion Beams with Close to 100% Ion Transmission Efficiency;** Andrew N. Krutchinsky; Julio C. Padovan; Herbert Cohen; Brian T. Chait; *Rockefeller University, New York, NY*
- WP 744 **Comprehensive Mass Spectrometric Analysis of Ablated Proteins in Ultrafast Desorption by Vibrational Excitation (DIVE);** Marcel Kwiatkowski<sup>1</sup>; Marcus Wurlitzer<sup>1</sup>; Ling Ren<sup>2</sup>; Yinfei Lu<sup>2</sup>; Wesley Robertson<sup>2</sup>; R.J. Dwayne Miller<sup>2</sup>; Hartmut Schlüter<sup>1</sup>; <sup>1</sup>*University Medical Centre Hamburg-Eppendorf, Hamburg, Germany*; <sup>2</sup>*MPSD for Structural Dynamics, Hamburg, Germany*
- WP 745 **Sub-ambient Pressure Ionization Nanoelectrospray (SPIN): High Sensitivity Detection and Extended Structural Characterization of Labile Compounds Unattainable by Conventional ESI;** Jonathan T. Cox; Scott R. Kronewitter; Anil Shukla; Ronald J. Moore; Keqi Tang; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 746 **Novel Quantitative Strategies for Condensed Phase Membrane Introduction Mass Spectrometry: Mitigating Ion Suppression and Extending Linear Dynamic Range;** Kyle D. Duncan<sup>1,2</sup>; Gregory W. Vandergrift<sup>1</sup>; Mathias Baltes<sup>1</sup>; Erik T. Krogh<sup>1,2</sup>; Christopher G. Gill<sup>1,2</sup>; <sup>1</sup>*Applied Environmental Research Laboratories (AERL), Vancouver Island University, Nanaimo, Canada*; <sup>2</sup>*Chem. Dept, University of Victoria, Victoria, BC, Canada*
- WP 747 **Slug Flow Microextraction NanoESI with Real-Time Derivatization for Rapid Analysis of Biofluid Samples;** Yue Ren; Morgan McLuckey; Jiangjiang Liu; Zheng Ouyang; *Purdue University, West Lafayette, IN*
- WP 748 **Persistent Multiply Charged Ion Signals Generated by Liquid MALDI Enables Sensitive ETD and Ion Mobility MS Analysis;** Jeff Brown<sup>1,2</sup>; Michael Morris<sup>2</sup>; Pavel Ryumin<sup>1</sup>; Rainer Cramer<sup>1</sup>; <sup>1</sup>*University of Reading, Reading, UK*; <sup>2</sup>*Waters Corporation, Wilmslow, UK*
- WP 749 **Controlling Ionization Chemistry in Plasma-Assisted Reaction Chemical Ionization;** Haopeng Wang<sup>1</sup>; Ninghang Lin<sup>1</sup>; Kaveh Kahen<sup>2</sup>; Hamid Badiei<sup>2</sup>; Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>*Georgetown University, Washington, DC*; <sup>2</sup>*PerkinElmer Inc., Woodbridge, Canada*
- WP 750 **Optimization of Thin Film Solid Phase Microextraction (SPME) Devices for Direct Analysis in Real Time (DART) Coupled with Tandem MS;** Germán Augusto Gómez-Ríos; Nathaly Reyes-Garcés; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*
- WP 751 **Characterising Linear and Radial Surface Acoustic Wave Nebulisation Devices for Optimising Protein Ionisation by Design;** Andrew Dennison<sup>1</sup>; Yifan Li<sup>1</sup>; Scott Heron<sup>2</sup>; C. Logan Mackay<sup>1</sup>; David Goodlet<sup>2</sup>; Patrick Langridge-Smith<sup>1</sup>; Anthony Walton<sup>1</sup>; Andrew Mount<sup>1</sup>; <sup>1</sup>*The University of Edinburgh, Edinburgh, UK*; <sup>2</sup>*University of Maryland, Baltimore, MD*
- WP 752 **Signal and Signal-to-noise Enhancement Mediated by Helium with Coanda Effect Electrospray Ionization (CEESI) Source;** Yixin Zhu<sup>2</sup>; Tingting Lv<sup>2</sup>; Peiming Song<sup>2</sup>; Rong Wang<sup>1</sup>; <sup>1</sup>*Icahn School of Medicine at Mount Sinai, New York, NY*; <sup>2</sup>*Zhejiang Haochuang, Hangzhou, China*
- WP 753 **Development of a Vacuum Ultraviolet Photoionization Source for Gas Chromatography used with a High Resolution Time of Flight Mass Spectrometer;** Lloyd Allen; Roza Wojcik; Viatcheslav Artaev; *LECO Corp., Saint Joseph, MI*
- WP 754 **Development of a Chip-Based Nanobore Column Platform with Universal Connectivity, Column Heating and Sheath Gas Capability;** Helena Svobodova<sup>1</sup>; Peter Wang<sup>2</sup>; Amanda Berg<sup>1</sup>; Gary A. Valaskovic<sup>1</sup>; <sup>1</sup>*New Objective, Inc., Woburn, MA*; <sup>2</sup>*New Objective, Inc., Shanghai, China*
- WP 755 **Matrix Assisted Ionization Vacuum (MAIV) Using FT-ICR;** Evgenia Tisdale<sup>1</sup>; Beixi Wang<sup>2</sup>; Sarah Trimpin<sup>2</sup>; Charles L. Wilkins<sup>1</sup>; <sup>1</sup>*University of Arkansas, Fayetteville, AR*; <sup>2</sup>*Wayne State University, Detroit, MI*
- WP 756 **Flow Dynamics Technique for Sampling and Separation of Neutrals from Analytes Based on Their Axial Momentum Density Differences;** Gary Salazar<sup>1,2</sup>; Soenke Szidat<sup>1,2</sup>; <sup>1</sup>*Depart. of Chem. and Biochem., Univ. of Bern, Bern, Switzerland*; <sup>2</sup>*Oeschger Centre for Climate Change Research, Bern, Switzerland*
- WP 757 **Development of a Novel TRESI-MS Capillary Mixing Device and Proof of Concept via Characterization of Known Protein Interactions;** Nicholas Zinck<sup>1</sup>; Ann-Katherine Stark Stark<sup>1</sup>; Michal Sharon<sup>2</sup>; Derek Wilson<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*; <sup>2</sup>*Weizmann Institute of Science, Rehovot, Israel*
- WP 758 **Further Developments Interfacing a High Performance Ion Mobility Spectrometer to LTQ Series Mass Spectrometers;** Robert Jackson; Adam Graichen; Mark Osgood; Ching Wu; *Excellims Corporation, Acton, MA*
- WP 759 **Development of an Inline Microfluidic Electrochemical Cell to Study Carbon Dioxide Reduction Mechanisms;** Luke Wooster; Yeon Jae Ko; Alessandra Ferzoco; *Rowland Institute at Harvard, Cambridge, MA*

## FAIMS and DMS, 760 - 779

- WP 760 **Optimization and Performance Characterization of a Microscale FAIMS Chip Coupled to an Orbitrap Mass Spectrometer;** Lauren Brown<sup>1</sup>; Robert Smith<sup>1</sup>; Alastair Taylor<sup>1</sup>; Michael Winter<sup>1</sup>; Danielle Toutoungi<sup>1</sup>; Dirk Nolting<sup>2</sup>; Alexander Makarov<sup>2</sup>; <sup>1</sup>*Owlstone Ltd, Cambridge, UK*; <sup>2</sup>*ThermoFisher Scientific, Bremen, Germany*
- WP 761 **On a Novel Interface for Electrospray Ionization (ESI)-Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) and Significant Improvement in Sensitivity;** Satendra Prasad; Michael W. Belford; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- WP 762 **Effect of Electrode Geometry on FAIMS Gas Flow Focusing and Lateral Diffusion;** Jean-Jacques Dunyach; Satendra Prasad; Michael Belford; *Thermo Fisher Scientific, San Jose, CA*
- WP 763 **Effect of FAIMS Gas Velocity on Resolution, Sensitivity, and Nanospray Formation;** Michael Belford; Satendra Prasad; Jean-Jacques Dunyach; *Thermo Fisher Scientific, San Jose, CA*
- WP 764 **Development and Application of FAIMS for the Investigation of FGF Signaling;** Hongyan Zhao; Debbie L. Cunningham; Andrew J. Creese; John K. Heath; Helen J. Cooper; *School of Biosciences, University of Birmingham, Birmingham, UK*
- WP 765 **FAIMS Coupled with HCD Product Ion-Triggered ETD Mass Spectrometry for the Analysis of N-glycosylation in Proteins;** Gloria N. Ulasi; Andrew Creese; Cleidiane G. Zampronio; Helen J. Cooper; *School of Biosciences, University of Birmingham, Edgbaston, UK*



- WP 766 **FAIMS Fractionation Improves Protein Identification for Low-Abundance Samples;** Kristian E. Swearingen; Jason M. Winget; Michael R. Hoopmann; Robert L. Moritz; *Institute for Systems Biology, Seattle, WA*
- WP 767 **Differential Ion Mobility Separations in Pure Helium and He Mixtures using Microchips;** Alexandre A. Shvartsburg; Yehia Ibrahim; Richard D. Smith; *Pacific Northwest National Laboratory, Richland, WA*
- WP 768 **Determination of Solvent Effects from Ionization Source on Differential Ion Mobility Spectrometry Separations;** Brandon Santiago; Gary Glish; *University of North Carolina at Chapel Hill, Chapel Hill, NC*
- WP 769 **Differential Mobility Separation Pre-filtration on a Portable, Compact Mass Spectrometer;** Spiros Manolakos; Theresa Evans-Nguyen; Francy Sinatra; James Alberti; *The Charles Stark Draper Laboratory, Tampa, FL*
- WP 770 **Linked Scanning of Helium and Compensation Voltage to Improve the Resolving Power of Differential Ion Mobility Spectrometry Separations;** Rachel Harris; Samantha Isenberg; Brandon Santiago; Gary L. Glish; *University of North Carolina, Chapel Hill, NC*
- WP 771 **Improved DMS Performance with a Jet Injector Inlet;** Brad Schneider<sup>1</sup>; Erkinjon Nazarov<sup>2</sup>; Thomas Covey<sup>1</sup>; <sup>1</sup>AB SCIEX, Concord, Canada; <sup>2</sup>Draper Laboratories Bioengineering Center, Tampa, FL
- WP 772 **Improved Mass Spectrometer Robustness with DMS Pre-Filtering;** Yang Kang; Bradly Schneider; Thomas R. Covey; *AB Sciex, Concord, Canada*
- WP 773 **Discovery of Abundant, Ubiquitous and Intriguing Contaminants in Drinking Water using Differential Ion Mobility and Soft Mass Spectrometry;** Wojciech Gabryelski<sup>1</sup>; Jadwiga Lyczko<sup>1</sup>; Daniel Beach<sup>2</sup>; <sup>1</sup>University of Guelph, Guelph, Canada; <sup>2</sup>National Research Council Canada, Halifax, Canada
- WP 774 **Feasibility Study on the Detection of Volatile Organic Compounds (VOCs) from Potato Tuber Soft Rot by Differential Mobility Spectrometry (DMS);** Lav R. Khot<sup>1</sup>; Jessica Tufariello<sup>2</sup>; Ashley Almaguer<sup>1</sup>; Eric J. Lynch<sup>3</sup>; Paul J. Rauch<sup>3</sup>; Dennis A. Johnson<sup>4</sup>; Nora Olsen<sup>5</sup>; William Siems<sup>2</sup>; Herbert H. Hill<sup>2</sup>; <sup>1</sup>Biological Systems Engineering WSU, Pullman, WA; <sup>2</sup>Chemistry WSU, Pullman, WA; <sup>3</sup>Chemring Sensors and Electronic Systems, Charlotte, NC; <sup>4</sup>Plant Pathology WSU, Pullman, WA; <sup>5</sup>Plant, Soil, and Entomological Sciences UI, Moscow, ID
- WP 775 **Rapid Identification of  $\beta$ -carboline Hallucinogens: Harmine and Harmaline, by Pressure Cycling Technology (PCT) and DMS-MS;** Adam B. Hall<sup>1</sup>; Amol Kafle<sup>1</sup>; Alex Thompson<sup>3</sup>; Frederick Li<sup>2</sup>; Kaitlyn Duffy<sup>1</sup>; James Glick<sup>1</sup>; Stephen L. Coy<sup>1</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Boston University School of Medicine, Boston, MA; <sup>3</sup>Vermont Forensic Laboratory, Waterbury, VT
- WP 776 **Targeted Analysis of Polar Analytes by DMS-MS for Radiation Biodosimetry;** Amol Kafle<sup>1</sup>; Stephen Coy<sup>1</sup>; Fred Li<sup>1</sup>; Evagelia Laiakis<sup>2</sup>; Albert Fornace<sup>2</sup>; Paul Vouros<sup>1</sup>; <sup>1</sup>Northeastern University, Boston, MA; <sup>2</sup>Georgetown University, Washington, DC
- WP 777 **The Application of Differential Mobility Spectrometry(DMS) to the Characterization of the Lipid Profile of Commercially Available Olive Oils;** Paul C. Winkler<sup>1</sup>; Paul Baker<sup>2</sup>; Christopher Borton<sup>1</sup>; <sup>1</sup>AB Sciex, Golden, CO; <sup>2</sup>AB Sciex, Framingham, MA
- WP 778 **Trimethylation and Chemical Modifiers in IMS/MS Peptide Analysis: Performance Enhancement Through Solution- And Gas-Phase Chemistry;** Voislav Blagojevic; Amanda De Filippis; Diethard K. Bohme; *York University, Toronto, Canada*
- WP 779 **Conformer Isolation in Intrinsically Disordered Protein Ensembles using DMS-MS;** Shaolong Zhu<sup>1</sup>; Larry Campbell<sup>2</sup>; Yves LeBlanc<sup>2</sup>; Derek J. Wilson<sup>1</sup>; <sup>1</sup>York University, Toronto, Canada; <sup>2</sup>AB SCIEX, Toronto, Canada



7:30 - 8:00 am ..... Set up all Thursday posters  
 10:30 am - 1:00 pm ..... Odd-numbered posters present  
 12:00 - 2:30 pm ..... Even-numbered posters present  
 2:30 - 3:00 pm ..... Remove all Thursday posters

Imaging MS: Instrumentation.....001-012  
 Informatics: Quantitation/Validation .....013-036  
 Informatics: Pathway Analysis .....037-040  
 Informatics: Systems Biology .....041-046  
 Informatics: Crosslinking and Structure Analysis.....048-056  
 Informatics: Intact Proteins .....057-064  
 Intact Proteins: quantitative Analysis .....065-069  
 Proteins Phosphoproteins .....070-083  
 Proteins: Non-covalent Interactions.....084-104  
 Proteins: Aggregation .....105-106  
 Proteins: Conformation Analysis.....107-113  
 H/D Exchange: Protein Structure and Function.....114-138  
 Glycoproteins.....139-168  
 Peptides: Quantitative Analysis (New Methods and Applications of Labels) .....169-179  
 Peptides: Ion Activation/Dissociation Strategies.....180  
 Peptides: Fragmentation Mechanisms .....181-196  
 Phosphopeptides Quantitative Analysis .....197-218  
 Peptides: PTM Identification.....219-249  
 Proteomics: Plasma.....250-261  
 Proteomics: Clinical Applications.....262-288  
 Proteomics: Tissue .....289-314

Proteomics: New Approaches .....315-336  
 Immunology .....337-349  
 Biomolecular Structure Analysis: Covalent Labeling .....350-363  
 Astrobiology and Atmospheric Chemistry .....364-370  
 Lipids: Profile Analysis.....375-394  
 Lipids: Quantitative Analysis.....395-412  
 Ambient Ionization: Applications .....413-417  
 Biomarkers: Quantitative Analysis .....421-451  
 Biomolecular Structure Analysis: Chemical Crosslinking .....452-468  
 Ion Mobility: Fundamentals.....469-482  
 Ion Mobility: Applications .....483-512  
 Nucleic Acids .....513-526  
 Traditional Chinese Medicine .....527-530  
 High Mass Accuracy / High Performance MS: Applications .....531-547  
 Environmental Analysis: General.....549-574  
 Forensics .....575-604  
 Food"omics": MS Characterization of Food and Nutritional Supplements .....605-633  
 Metabolomics: General.....634-653  
 Metabolomics: Clinical Applications.....654-664  
 Drug Metabolism: Quantitative Analysis .....665-684  
 Ion Activation / Dissociation .....685-702  
 Carbohydrates .....709-734  
 Agriculture .....735-737  
 Instrumentation: General .....738-764  
 LCMS Sample Preparation.....765-784

**Imaging MS: Instrumentation, 001 - 012**

- ThP 001 **Optimization of the MALDI Imaging Laser Repetition Rates using an Orthogonal MALDI Mass Spectrometer;** Emmanuelle Claude; Mark Towers; James Langridge; *Waters corporation, Manchester, UK*
- ThP 002 **Modifications to a Linear Time-of-Flight Mass Spectrometer for Mass Resolved Microscopy with the PimMS Camera;** Edward Halford<sup>1</sup>; Benjamin Winter<sup>1</sup>; Simon King<sup>1</sup>; Mark Mills<sup>2</sup>; Steve Thompson<sup>2</sup>; Vic Parr<sup>2</sup>; Jaya John John<sup>1</sup>; Andrei Nomerotski<sup>3</sup>; Claire Vallance<sup>1</sup>; Renato Turchetta<sup>4</sup>; Mark Brouard<sup>1</sup>; <sup>1</sup>*University of Oxford, Oxford, UK*; <sup>2</sup>*SAI Ltd., Manchester, UK*; <sup>3</sup>*Brookhaven National Laboratory, Upton, NY*; <sup>4</sup>*Rutherford Appleton Laboratory, Oxford, UK*
- ThP 003 **Toward Subcellular MALDI-MS Imaging of Plant Tissues by Modification of MALDI-LTQ-Orbitrap Optics;** Andrew Korte<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; <sup>1</sup>*Iowa State University, Ames, IA*; <sup>2</sup>*Ames Laboratory - US DoE, Ames, IA*
- ThP 004 **Vertically Aligned Transmission Geometry Laser Ablation into a Non-Contact Liquid Vortex Capture Probe for Mass Spectrometry Imaging;** Gary J. Van Berkel; Olga Ovchinnikova; Deepak Bhandari; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 005 **Multimodal Chemical and Physical Surface Characterization on a Combined AFM-MS Platform;** Olga S. Ovchinnikova; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 006 **Comparison of UV-MALDI and IR-MALDESI Mass Spectrometry Imaging of Biological Tissue Sections;** Milad Nazari<sup>1</sup>; Elias Rosen<sup>1</sup>; Mark T. Bokhart<sup>1</sup>; Corbin Thompson<sup>2</sup>; Craig Sykes<sup>2</sup>; Angela D. M. Kashuba<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*The University of North Carolina, Chapel Hill, NC*
- ThP 007 **Toward High Spectral and Spatial Resolution Mass Spectrometry Imaging of Biological Tissue Sections by IR-MALDESI Coupled to the Q Exactive;** Eli Rosen; Guillaume Robichaud; Jeremy Barry; David C. Muddiman; *NC State University, Raleigh, NC*

- ThP 008 **Multiple MS/MS Transition Monitoring in a Single Laser Shot on a MALDI TOF/TOF Mass Spectrometer;** Boone Prentice; Richard Caprioli; *Vanderbilt University, Nashville, TN*
- ThP 009 **Tissue Protein Imaging at 2.5µm Spatial Resolution and High Speed using Transmission Geometry MALDI Source Integrated into a TOFMS Instrument;** Andre Zavalin<sup>1</sup>; Junhai Yang<sup>1</sup>; Kevin Hayden<sup>2</sup>; Marvin Vestal<sup>2</sup>; Richard Caprioli<sup>1</sup>; <sup>1</sup>*Vanderbilt University, Nashville, TN*; <sup>2</sup>*SimulTOF Systems, Sudbury, MA*
- ThP 010 **Mass Spectrometry Imaging of Biological Systems using Laser Ablation Plume Capture in Aerosol (LAPCA);** Jonathan Brauer; Jan Sunner; Iwona Beech; Eric Kaufman; *University of Oklahoma, Norman, OK*
- ThP 011 **Improved Biological Imaging with Gas Cluster Ion Beams;** John Fletcher<sup>1</sup>; Tina Angerer<sup>1</sup>; Paul Blenkinsopp<sup>2</sup>; Andrew Ewing<sup>1,3</sup>; <sup>1</sup>*University of Gothenburg, Gothenburg, Sweden*; <sup>2</sup>*Ionoptika Ltd, Southampton, UK*; <sup>3</sup>*Chalmers University of Technology, Gothenburg, Sweden*
- ThP 012 **Development of New Stigmatic Imaging Mass Spectrometer and its Application to surface Analysis of High Functional Organic Materials;** Jun Aoki; Hisanao Hazama; Kunio Awazu; Michisato Toyoda; *Osaka University, Toyonaka-Shi, Japan*

**Informatics: Quantitation/Validation, 013 - 036**

- ThP 013 **A Novel and Straightforward Experimental Null Strategy Enables Accurate Evaluation and Control of False-Discovery of Significantly-Altered-Proteins in Label-Free Quantitative Proteomics;** Xiaomeng Shen; Jun Qu; Jun Li; *University at Buffalo, Buffalo, New York*
- ThP 014 **Systematic Assessment of Survey Scan- and MS2-Based Strategies for Label-Free Quantitative Proteomics using High-Resolution MS Data;** Chengjian Tu<sup>1</sup>; Jun Li<sup>1</sup>; Quanhu Sheng<sup>2</sup>; Ming Zhang<sup>1</sup>; Jun Qu<sup>1</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*Vanderbilt University, Nashville, TN*

- ThP 015 **Comparison of High-End Software for label Free Quantitative Proteomics**; Alon Savidor<sup>1</sup>; Stefan Tenzer<sup>2</sup>; Joerg Kuharev<sup>2</sup>; Yishai Levin<sup>1</sup>; <sup>1</sup>Weizmann Institute of Science, Rehovot, Israel; <sup>2</sup>University Medical Center of the Johannes Gutenbe, Mainz, Germany
- ThP 016 **Comparison of Label Free Quantification Tools**; Lei Xin<sup>1</sup>; Baozhen Shan<sup>1</sup>; Hao Lin<sup>1</sup>; Weiwu Chen<sup>1</sup>; Mohammad Rahman<sup>1</sup>; Bin Ma<sup>2</sup>; <sup>1</sup>Bioinformatics Solutions Inc., Waterloo, CANADA; <sup>2</sup>University of Waterloo, Waterloo, ON
- ThP 017 **Protein Identification and Quantitative Analysis with N-Terminal Sequencing by Mass Spectrometry**; Baozhen Shan; Hao Lin; *Bioinformatics Solutions Inc., Waterloo, Canada*
- ThP 018 **False Quantification in SILAC Proteomic Experiments**; Chris McKennan; Hua Ding; Lynn Spruce; Steven H. Seeholzer; *Children's Hospital of Philadelphia, Philadelphia, PA*
- ThP 019 **Systematic Comparison of Super-SILAC and Label-Free Quantification for Single-Shot Proteome Analysis**; Andreas Tebbe; Martin Klammer; Stefanie Sighart; Christoph Schaab; Felix Oppermann; Henrik Daub; *Evotec München, Munich, Germany*
- ThP 020 **Estimating Effects of Peptide Co-Fragmentation on iTRAQ Quantification by Simulating Multiplexed Spectra for Reliable Identification of Differentially Expressed Peptides**; Honglan Li<sup>1</sup>; Kyu-Baek Hwang<sup>1</sup>; Dong-Gi Mun<sup>2</sup>; Hokeun Kim<sup>2</sup>; Hangyeore Lee<sup>2</sup>; Sang-Won Lee<sup>2</sup>; Eunok Paek<sup>3</sup>; <sup>1</sup>Soongsil University, Seoul, Republic of Korea; <sup>2</sup>Korea University, Seoul, Republic of Korea; <sup>3</sup>Hanyang University, Seoul, Republic of Korea
- ThP 021 **Census 2: Isobaric Labeling Data Analysis in an Automated Way**; Robin Park; Aaron Aslanian; Daniel B. McClatchy; Harshil Shah; Xuemei Han; John Yates; *The Scripps Research Institute, San Diego, CA*
- ThP 022 **Logical Bayesian Networks for Proteomics**; Kurt De Grave; Jan Ramon; *KU Leuven, Leuven, Belgium*
- ThP 023 **Statistical Analysis of Bayesian Hierarchical Inversion for MRM Protein Quantification and QDA Serum Sample Classification**; Laurent Gerfault<sup>1</sup>; Amna Klich<sup>2</sup>; Catherine Mercier<sup>2</sup>; Pascal Roy<sup>2</sup>; Jean François Giovannelli<sup>3</sup>; Audrey Giremus<sup>3</sup>; Pierre Mahe<sup>4</sup>; Jean Philippe Charrier<sup>5</sup>; Bruno Lacroix<sup>5</sup>; Pierre Grangeat<sup>1</sup>; <sup>1</sup>CEA, Leti, Minatec Campus, Grenoble, France; <sup>2</sup>HCL, Univ. Lyon 1, CNRS UMR 5558, Lyon, France; <sup>3</sup>Univ. Bordeaux, IMS, UMR 5218, Bordeaux, France; <sup>4</sup>bioMérieux, Grenoble, France; <sup>5</sup>bioMérieux, Marcy L'etoile, France
- ThP 024 **Identification and Verification of the Missing Proteins for the C-HPP by Using the Mass Spectral Library and MRM Technique**; Jin-Young Cho; Hyoung-Joo Lee; Seul-Ki Jeong; Kwang-Youl Kim; Young-Ki Paik; *YPRC, Seoul, Korea, Republic*
- ThP 025 **CPTAC Assay Portal: a community Web-Based Repository for Well-Characterized Quantitative Targeted Proteomics Assays**; Jeff Whiteaker<sup>1</sup>; Goran Halusa<sup>2</sup>; Andrew Hoofnagle<sup>3</sup>; Vagisha Sharma<sup>3</sup>; Brendan MacLean<sup>3</sup>; Ping Yan<sup>1</sup>; John Wrobel<sup>4</sup>; Jacob Kennedy<sup>1</sup>; DR Mani<sup>5</sup>; Lisa Zimmerman<sup>6</sup>; Matthew Meyer<sup>7</sup>; Mehdi Mesri<sup>8</sup>; Henry Rodriguez<sup>8</sup>; Amanda Paulovich<sup>1</sup>; <sup>1</sup>Fred Hutchinson Cancer Research Center, Seattle, WA; <sup>2</sup>Leidos Biomedical Research Inc, Frederick, MD; <sup>3</sup>University of Washington, Seattle, WA; <sup>4</sup>University of North Carolina, Chapel Hill, NC; <sup>5</sup>Broad Institute, Cambridge, MA; <sup>6</sup>Vanderbilt University School of Medicine, Nashville, TN; <sup>7</sup>Washington University School of Medicine, St. Louis, MO; <sup>8</sup>National Cancer Institute, Bethesda, MD
- ThP 026 **A Scientific Workflow for Automatic Peptide Selection for Targeted Proteomics Experiments**; Yassene Mohammed<sup>1,2</sup>; Dominik Domanski<sup>3</sup>; Angela Jackson<sup>1</sup>; Derek Smith<sup>1</sup>; Andre Deelder<sup>2</sup>; Magnus Palmblad<sup>2</sup>; Christoph Borchers<sup>1,4</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>Center for Proteomics and Metabolomics, Leiden Univ, Leiden, The Netherlands; <sup>3</sup>Polish Academy of Sciences, Warsaw, Poland; <sup>4</sup>UVIC Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 027 **Protein Prospector as a Component in a Label Free/ SRM Pipeline**; Peter R Baker<sup>1</sup>; Anatoly Urisman<sup>2</sup>; Robert Chalkley<sup>2</sup>; <sup>1</sup>UCSF, Rokitnica, POLAND; <sup>2</sup>UCSF, San Francisco, CA
- ThP 028 **MS-Umpire: Java Open-Source MS<sup>1</sup> Quantitation Software Based on Untargeted Feature Detection Algorithm for Proteomics and Metabolomics Data**; Chih-Chiang Tsou; Alexey Nesvizhskii; *University of Michigan, Ann Arbor, MI*
- ThP 029 **Unprecedented Quantitative Evaluation of LC-MS Isotope Trace Feature Detection Using Ground Truth Data**; Rob Smith; Ryan Money; John Prince; Dan Ventura; *Brigham Young University, Provo, UT*
- ThP 030 **Novel Proteomics Mass Spectrometry Simulation in Java: JAMSS**; Rob Smith; John Prince; *Brigham Young University, Provo, UT*
- ThP 031 **New Functionality for the Trans-Proteomic Pipeline: Tools for the Analysis of Proteomics Data**; Luis Mendoza<sup>1</sup>; David D. Shteynberg<sup>1</sup>; Joseph Slagel<sup>1</sup>; Michael R. Hoopmann<sup>1</sup>; Henry Lam<sup>2</sup>; Jimmy Eng<sup>3</sup>; Eric W Deutsch<sup>1</sup>; Robert L Moritz<sup>1</sup>; <sup>1</sup>Institute For Systems Biology, Seattle, WA; <sup>2</sup>Hong Kong University of Science and Technology, Hong Kong, China; <sup>3</sup>University of Washington, Seattle, WA
- ThP 032 **A GPU-Powered, Massively Parallel Nonparametric Statistics Server for Analysis and Exploration of Large-Scale Quantitative Data between and across Quantitative Experiments**; John P. Wilson<sup>1</sup>; Eric Paniagua<sup>1</sup>; Robert M. Farber<sup>2</sup>; Darryl J.C. Pappin<sup>1</sup>; <sup>1</sup>Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; <sup>2</sup>Blackdog Endeavors LLC, Gig Harbor, WA
- ThP 033 **PeptideDepot Plugin: Using Statistical Tool to Improve Quality of Quantitative Proteomics Data Generated by Mass Spectrometry**; Qinglin Ji<sup>1</sup>; Samantha Beik<sup>2</sup>; Arthur Salomon<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Brown University, Providence, RI; <sup>2</sup>Department of Molecular Biology, Cell Biology, and, Providence, RI
- ThP 034 **ProteoSuite v1.0 – An Open Source Framework for Quantitative Proteomics Analysis Based on PSI Data Standards**; Faviel Gonzalez<sup>1</sup>; Andrew Collins<sup>1</sup>; Jun Fan<sup>2</sup>; Huaizhong Zhang<sup>3</sup>; Andrew Dowsey<sup>3</sup>; Henning Hermjakob<sup>4</sup>; Conrad Bessant<sup>2</sup>; Simon Hubbard<sup>3</sup>; Andrew Jones<sup>1</sup>; <sup>1</sup>University of Liverpool, Liverpool, UK; <sup>2</sup>Queen Mary University of London, London, UK; <sup>3</sup>University of Manchester, Manchester, UK; <sup>4</sup>European Bioinformatics Institute, Cambridge, UK
- ThP 035 **Multi-Instrument, Skyline-Based Comparison of DIA Peptide Identification and Statistical Confidence Tools Enables Improved, Novel Peak Scoring Strategy**; Dario Amodè<sup>1</sup>; Don Marsh<sup>2</sup>; Hannes Rost<sup>3</sup>; Lucia Espona Pernas<sup>3</sup>; George Rosenberger<sup>3</sup>; Ruedi Aebersold<sup>3</sup>; Parag Mallick<sup>1</sup>; Michael J. Maccoss<sup>2</sup>; Brendan Maclean<sup>2</sup>; <sup>1</sup>Stanford University, Palo Alto, California; <sup>2</sup>Univ of Washington, Seattle, WA; <sup>3</sup>ETH Zurich, Zurich, Switzerland
- ThP 036 **Evaluation of Progenesis QI for Proteomics and Progenesis Post-Processor (PPP) as a Simplified Workflow for Ion-Mobility Enabled Data-Independent SILAC Studies**; Joanne B. Connolly<sup>1</sup>; Lee A Gethings<sup>1</sup>; Kelly McMahon<sup>1</sup>; Robert Tonge<sup>1</sup>; Johannes Pc Vissers<sup>1</sup>;

Anthony D Whetton<sup>2</sup>; Andrew R Jones<sup>3</sup>; James Langridge<sup>1</sup>;  
<sup>1</sup>Waters Corporation, Manchester, UK; <sup>2</sup>University of  
Manchester, Manchester, UK; <sup>3</sup>University of Liverpool,  
Liverpool, UK

**Informatics: Pathway Analysis, 037 - 040**

ThP 037 **Improved Peak Detection and Deconvolution of Native Protein Complex Electrospray Mass Spectra**; Jonathan Lu; Michael Trnka; Shenheng Guan; Alma Burlingame; University of California, San Francisco, San Francisco, CA

ThP 038 **Quantitative Proteomics to Unravel the Expression and Translocation of MET Proto-Oncoprotein to Mitochondria**; Kae Hwan Sim; Siu Kwan SZE; School of Biological Sciences, Nanyang Technological University, Singapore 637551, SINGAPORE

ThP 039 **Using Causal Discovery Techniques to Infer Signaling Pathways from Mass Spectrometry Data**; Jennifer Teubl<sup>1</sup>; Kelly Ruggles<sup>1</sup>; Himanshu Grover<sup>1</sup>; Philipp Mertins<sup>2</sup>; Karl Clauser<sup>2</sup>; Sherri R. Davies<sup>3</sup>; R. Reid Townsend<sup>3</sup>; Matthew J. Ellis<sup>3</sup>; Steven A. Carr<sup>2</sup>; David Fenyo<sup>1</sup>; <sup>1</sup>NYU Langone Medical Ctr, Ny, NY; <sup>2</sup>Broad Institute, Cambridge, MA; <sup>3</sup>Washington University, St. Louis, MO

ThP 040 **Pathway Enrichment Analysis for Multi-omic Data using netSVM**; Li Chen; Yuan Tian; Caitlin Choi; Shisheng Sun; Jianying Zhou; Hui Zhang; Daniel Chan; Zhen Zhang; Johns Hopkins School of Medicine, Baltimore, MD

**Informatics: Systems Biology, 041 - 046**

ThP 041 **A Novel Method for Integration of Proteomic and Transcriptomic Data**; Ekaterina Mostovenko<sup>1</sup>; Cheryl Lichti<sup>1</sup>; Qianghu Wang<sup>2</sup>; Erik Sulman<sup>2</sup>; Carol Nilsson<sup>1</sup>; <sup>1</sup>UTMB Galveston, Galveston, TX; <sup>2</sup>University of Texas M.D. Anderson Cancer Center, Houston, TX

ThP 042 **Co-Expression Network Analysis of Quantitative Proteomics Data: A New Approach for Studying Neuropsychiatric Disease**; Matthew L MacDonald<sup>1</sup>; Ying Ding<sup>2</sup>; Jason Newman<sup>1</sup>; David A Lewis<sup>1</sup>; Robert A Sweet<sup>1</sup>; Nathan Yates<sup>2</sup>; <sup>1</sup>University of Pittsburgh, Dept of Psychiatry, Pittsburgh, Pennsylvania; <sup>2</sup>University of Pittsburgh, Biomedical Mass Spectr, Pittsburgh, Pennsylvania

ThP 043 **Construction and Assessment of Individualized Proteogenomic Databases for Large-Scale Analysis of Non-Synonymous Single Nucleotide Variants**; Karsten Krug; Sasa Popic; Alejandro Carpy; Katarina Matic; Christoph Taumer; Boris Macek; Proteome Center Tuebingen, University of Tuebingen, Tuebingen, Germany

ThP 044 **Flexible, Accessible and Reproducible Workflows for Tandem Proteogenomic and Metaproteomic Analysis using the Galaxy-P Platform**; Pratik Jagtap<sup>1,2</sup>; Julie Yang<sup>2</sup>; Getiria Onsongo<sup>4</sup>; Joel Kooren<sup>2</sup>; Sricharan Bandhakavi<sup>3</sup>; James Johnson<sup>4</sup>; Joel Rudney<sup>2</sup>; Tim Griffin<sup>2</sup>; <sup>1</sup>Center for Mass Spectrometry and Proteomics, UMN, St.Paul, MN; <sup>2</sup>University of Minnesota, Minneapolis, MN; <sup>3</sup>Bio-Rad Laboratories, Hercules, CA; <sup>4</sup>Minnesota Supercomputing Institute, Minneapolis, MN

ThP 045 **Proteogenomics as a Crucial Tool in the Search for Short Secreted Proteins**; Ira Cooke<sup>1,2</sup>; Dan Jones<sup>3</sup>; Cecilia Deng<sup>5</sup>; Pierre Faou<sup>1</sup>; Nathan Hall<sup>2</sup>; Vignesh Jayachandran<sup>1</sup>; Michael Liem<sup>1</sup>; Adam Taranto<sup>3</sup>; Kim Plummer<sup>3</sup>; Suresh Mathivanan<sup>1</sup>; <sup>1</sup>Department of Biochemistry, La Trobe University, Melbourne, Australia; <sup>2</sup>Life Sciences Computation Centre (VLSCI), Melbourne, Australia; <sup>3</sup>Department of Botany, La Trobe University, Melbourne, Australia; <sup>4</sup>Plant Biosecurity CRC, Canberra, Australia; <sup>5</sup>Institute for Plant and Food Research, Auckland, New Zealand

ThP 046 **Mass Spectrometry based Draft of the Human Proteome**; Mathias Wilhelm<sup>1</sup>; Judith Schlegel<sup>2</sup>; Hannes Hahne<sup>1</sup>; Amin Moghaddas Gholami<sup>1</sup>; Marcus Lieberenz<sup>2</sup>; Emanuel Ziegler<sup>2</sup>; Lars Butzmann<sup>2</sup>; Siegfried Gessulat<sup>2</sup>; Harald Marx<sup>1</sup>; Mikhail Savitski<sup>3</sup>; Karsten Schnatbaum<sup>4</sup>; Ulf Reimer<sup>4</sup>; Holger Wenschuh<sup>4</sup>; Marcus Bantscheff<sup>3</sup>; Anja Gerstmaier<sup>2</sup>; Franz Faerber<sup>2</sup>; Bernhard Kuster<sup>1</sup>; <sup>1</sup>Technical University Munich, Freising, Germany; <sup>2</sup>SAP AG, Walldorf, DE; <sup>3</sup>Cellzome, Heidelberg, DE; <sup>4</sup>JPT Peptide Technologies, Berlin, DE

**Informatics: Crosslinking and Structure Analysis, 048 - 056**

ThP 048 **Identifying Cross-linked Peptides using Protein Prospector**; Robert Chalkley<sup>1</sup>; Michael Trnka<sup>1</sup>; Nicholas Michael<sup>2</sup>; Peter R Baker<sup>1</sup>; <sup>1</sup>UCSF, San Francisco, CA; <sup>2</sup>Reading Scientific Services Ltd, Reading, UK

ThP 049 **Comprehensive Identification of Disulfide Bonds Using Proteinase K Digestion and Second-Order Crosslinking Analysis**; Karl Makepeace<sup>1</sup>; Jason Serpa<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada

ThP 050 **Application of a Fast Sorting Algorithm to the Assignment of Mass Spectrometric Crosslinking Data**; Evgeniy Petrotchenko<sup>1</sup>; Carol Parker<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada

ThP 051 **Optimizing pLink for Disulfide-bond Analysis**; Sheng-Bo Fan<sup>1</sup>; Shan Lu<sup>2</sup>; Bing Yang<sup>2</sup>; Jia-Ming Meng<sup>1</sup>; Chi Hao<sup>1</sup>; Long Wu<sup>1</sup>; Kun Zhang<sup>1</sup>; Rui-Xiang Sun<sup>1</sup>; Meng-Qiu Dong<sup>2</sup>; Si-Min He<sup>1</sup>; <sup>1</sup>ICT, Chinese Academy of Sciences, Beijing, China; <sup>2</sup>National Institute of Biological Sciences, Beijing, China

ThP 052 **Software Tools for Improved Efficiency and Automated Interpretation of Mass Spectrometric Analysis of Chemically Crosslinked Proteins**; Guanghai Wang<sup>1</sup>; Kevin Ramkissoon<sup>2</sup>; Jenna Dumond<sup>2</sup>; Joan Ferraris<sup>2</sup>; Maurice Burg<sup>2</sup>; Marjan Gucek<sup>1</sup>; <sup>1</sup>Proteomics Core, NHLBI, NIH, Bethesda, MD; <sup>2</sup>LKEM, NHLBI, NIH, Bethesda, MD

ThP 053 **Application of Non-selective Photoreactive Cross-linking in Mass Spectrometry-based Structural Proteomics**; Kuan-Chieh Peng; Pang-Hung Hsu; National Taiwan Ocean University, Keelung, Taiwan

ThP 054 **Analysis of Protein-Protein Interactions using Chemical Cross-Linking Mass Spectrometry (CXMS): Novel Computational Approaches**; Mihir Jaiswal<sup>1,2</sup>; Nathaniel Crabtree<sup>1,2</sup>; Michael Bauer<sup>2</sup>; Roger Hall<sup>2</sup>; Kevin Raney<sup>2</sup>; Boris Zybailov<sup>1,2</sup>; <sup>1</sup>University of Arkansas at Little Rock, Little Rock, AR; <sup>2</sup>University of Arkansas for Medical Sciences, Little Rock, AR

ThP 055 **Metaproteomic Protein Identification Based on a Species-Level Similarity Correction**; Anke Penzlin; Martin Lindner; Joerg Doellinger; Wojtek Dabrowski; Andreas Nitsche; Bernhard Renard; Robert Koch Institute, Berlin, Germany

ThP 056 **<sup>14</sup>N<sup>15</sup>N DXMSMS Match Program for the Automated Analysis of LC/ESI-MS/MS Crosslinking Data from Experiments Using <sup>15</sup>N Metabolically Labeled Proteins**; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada

## Informatics: Intact Proteins, 057 - 064

- ThP 057 **Automated Protein Identification and Sequencing Using Top-Down MS Data**; Christian Heckendorf; Roger Theberge; Jean Spencer; Catherine E. Costello; Mark E. Mccomb; *Boston University School of Medicine, Boston, MA*
- ThP 058 **ProSight Lite: Freeware for Targeted Top Down Protein Mass Spectrometry and PTM Localization**; Ryan Fellers<sup>1</sup>; Richard Leduc<sup>2</sup>; Xiang Yu<sup>1</sup>; Bryan Early<sup>1</sup>; Paul Thomas<sup>1</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Indiana University, Bloomington, IN*
- ThP 059 **Improvements upon the C-Score: a Bayesian Framework for Proteoform Characterization in Top Down Proteomics**; Paul Thomas<sup>1</sup>; Ryan Fellers<sup>1</sup>; Bryan Early<sup>1</sup>; Joseph Greer<sup>1</sup>; Richard Leduc<sup>2</sup>; Neil L. Kelleher<sup>1</sup>; <sup>1</sup>*Northwestern University, Evanston, IL*; <sup>2</sup>*Indiana University, Bloomington, IN*
- ThP 060 **A Framework for Error-Tolerant Identification and Characterization of Protein Complexes by Database Searching and Top Down Tandem Mass Spectrometry**; Pierre C. Havugimana; Owen S. Skinner; Philip D. Compton; Bryan P. Early; Joseph B. Greer; Ryan T. Fellers; Neil L. Kelleher; *Northwestern University, Evanston, IL*
- ThP 061 **Differential Profiling of Intact Proteins Using a Novel Two-Pass Approach**; Norton Kitagawa; Christine Miller; Steven M. Fischer; Yinghang Yang; Stephen Madden; *Agilent Technologies, Inc., Santa Clara, CA*
- ThP 062 **A Top-Down Driven Approach To De Novo Protein Sequencing**; Kira Vyatkina<sup>1</sup>; Lennard Dekker<sup>2</sup>; Si Wu<sup>3</sup>; Vitalii Demyanyuk<sup>4</sup>; Xiaowen Liu<sup>5</sup>; Mikhail Dvorkin<sup>1</sup>; Sonya Alexandrova<sup>1</sup>; Martijn M. Vanduijn<sup>2</sup>; Theo M. Luider<sup>2</sup>; Nikola Tolic<sup>3</sup>; Ljiljana Pasa-Tolic<sup>3</sup>; Pavel A. Pevzner<sup>1,6</sup>; <sup>1</sup>*SPb Academic University, St Petersburg, Russian Federation*; <sup>2</sup>*Erasmus Medical Center, Rotterdam, Netherlands*; <sup>3</sup>*PNNL, Richland, WA*; <sup>4</sup>*SPb National Research University IFMO, St Petersburg, Russian Federation*; <sup>5</sup>*IUPUI, Indianapolis, IN*; <sup>6</sup>*UCSD, La Jolla, CA*
- ThP 063 **Complete and Confident Protein Characterization Using Top-down Mass Spectrometry and Isotopic Envelope Fingerprinting**; Zhixin Tian; kaijie Xiao; *Department of Chemistry, Tongji University, Shanghai, China*
- ThP 064 **De novo protein sequencing by combining top-down and bottom-up tandem mass spectra**; Xiaowen Liu<sup>1</sup>; Lennard Dekker<sup>2</sup>; Si Wu<sup>3</sup>; Martijn Vanduijn<sup>2</sup>; Theo Luider<sup>2</sup>; Nikola Tolic<sup>3</sup>; Mikhail Dvorkin<sup>4</sup>; Sonya Alexandrova<sup>4</sup>; Kira Vyatkina<sup>4</sup>; Ljiljana Pasa-Tolic<sup>3</sup>; Pavel Pevzner<sup>5</sup>; <sup>1</sup>*IUPUI, Indianapolis, IN*; <sup>2</sup>*Erasmus Medical Center, Rotterdam, Netherlands*; <sup>3</sup>*PNNL, Richmond, WA*; <sup>4</sup>*St. Peterburg Academic University, St. Peterburg, Russia*; <sup>5</sup>*UCSD, La Jolla, CA*
- Intact Proteins: Quantitative Analysis, 065 - 069**
- ThP 065 **Top-down Quantitative Proteomics Reveals Concerted Changes in Myofilaments in Ischemic Heart**; Ying Peng<sup>1</sup>; Zachery Gregorich<sup>2</sup>; Santosh G Valeja<sup>3</sup>; Huseyin Guner<sup>1</sup>; Yi-Chen (Ivy) Chen<sup>4</sup>; Timothy Hacker<sup>1</sup>; Xiaowen Liu<sup>5</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>*University of Wisconsin - Madison, Madison, WI*; <sup>2</sup>*UW Madison, Madison, WI*; <sup>3</sup>*University of Wisconsin- Madison, MADISON, WI*; <sup>4</sup>*University of Wisconsin-Madison, Madison, WI*; <sup>5</sup>*IUPUI, Indianapolis, IN*
- ThP 066 **Investigation of Instrumental Variables Effect on Intact Protein Multiple Reaction Monitoring Reproducibility in a Next Generation Triple Quadrupole Mass Spectrometer**; Evelyn Wang<sup>1</sup>; Peter Combe<sup>2</sup>; Erin McAllister<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>*University of Texas at Arlington, Arlington, TX*; <sup>2</sup>*Shimadzu Scientific Instruments, Columbia, MD*
- ThP 067 **Characterization of Intact and Reduced Therapeutic Monoclonal Antibodies using Microflow Size Exclusion Chromatography Coupled with Mass Spectroscopy**; Khaled Mriziq<sup>1</sup>; Xiang Zhu<sup>1</sup>; Remco Van Soest<sup>1</sup>; Eric Johansen<sup>2</sup>; Subodh Nimkar<sup>1</sup>; <sup>1</sup>*SCIEX Separations, Division of AB SCIEX, Redwood City, CA*; <sup>2</sup>*AB SCIEX, Redwood City, CA*
- ThP 068 **NeuCode SILAC Enables Multiplexed Protein Quantitation From the Top Down**; Timothy W. Rhoads; Christopher M. Rose; Nicholas M. Riley; Derek J. Bailey; Anna E. Merrill; Alexander S. Hebert; Michael S. Westphall; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- ThP 069 **Generalized Top-down Proteomics and Proteoform Analysis Platform with Wide and Narrow pI IEF-SPLC-MS**; Steven Patrie; *UT Southwestern Med. Center, Dallas, TX*
- Proteins: Phosphoproteins, 070 - 083**
- ThP 070 **Differential Phosphoproteomic Profiling of Human Myogenesis using Stable Isotope Labeling by Amino acids (SILAC)**; Natarajan V Bhanu<sup>1</sup>; Rosalynn Molden<sup>2</sup>; Zuofei Yuan<sup>1</sup>; Benjamin A Garcia<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*Princeton University, Princeton, NJ*
- ThP 071 **Hidden quantification – Obvious Modifications: Combining Metabolic Labeling with Top- Down Phospho- Proteomics using 2D Gel Electrophoresis (2D GE)**; Andreas Otto; Carolin Dewald; Christian Henschker; Michael Hecker; Dörte Becher; *University Greifswald, Greifswald, Germany*
- ThP 072 **Identification of Potential Downstream Targets of a Histidine Phosphatase Domain of the General Transcription Factor IIIC**; Marco L. Hennrich<sup>1</sup>; Nicholas M. I. Taylor<sup>2</sup>; Sebastian Glatt<sup>1</sup>; Helga Groetsch<sup>1</sup>; Anne-Claude Gavin<sup>1</sup>; Christoph W. Mueller<sup>1</sup>; <sup>1</sup>*EMBL Heidelberg, Heidelberg, Germany*; <sup>2</sup>*Centro de Investigaciones Biológicas, Madrid, Spain*
- ThP 073 **Demonstration of Orthogonal Complementary Enrichment Methods for Enhanced Phosphopeptide Profiling of Drug-Treated Gastric Carcinoma Cells**; Charles L. Farnsworth; Hongbo Gu; Xiaoying Jia; Kimberly Lee; Jian Min Ren; Jeffrey C. Silva; *Cell Signaling Technology, Danvers, MA*
- ThP 074 **Dimethyl Labeling Approach to the Study of the TLR Response Pathway**; Art Nuccio; Nathan Manes; Virginie Sjoelund; Aleksandra Nita-Lazar; *NIH, Bethesda, MD*
- ThP 075 **Meta-analysis of Arabidopsis Phospho-proteomics**; Klaas J. van Wijk<sup>1</sup>; Giulia Friso<sup>1</sup>; Dirk Walther<sup>2</sup>; Waltraud X. Schulze<sup>3</sup>; <sup>1</sup>*Cornell University, Ithaca, NY*; <sup>2</sup>*Max Planck Institute for Plant Physiology, Golm, Germany*; <sup>3</sup>*Department of Plant Systems Biology, Stuttgart, Germany*
- ThP 076 **Quantitative Analysis of Phosphoproteins During *Candida albicans* Hyphal Formation**; Susan T. Weintraub<sup>1</sup>; Kevin Hakala<sup>1</sup>; Sammy Pardo<sup>1</sup>; Brian C. Searle<sup>2</sup>; Derek Thomas<sup>3</sup>; <sup>1</sup>*UT Health Science Center at San Antonio, San Antonio, TX*; <sup>2</sup>*Proteome Software Inc., Portland, OR*; <sup>3</sup>*Grand Valley State University, Allendale, MI*
- ThP 077 **Global Phosphoproteome Profiling For the Characterization of Escherichia Coli Strains**; Rabih Jabbour<sup>1</sup>; Raja Sekhar Nirujogi<sup>3</sup>; Samir Deshpande<sup>2,2</sup>; Mary Wade<sup>1</sup>; A. Peter Snyder<sup>4</sup>; Akhilesh Pandey<sup>3</sup>; <sup>1</sup>*ECBC, Apg, MD*; <sup>2</sup>*Science and Technology Corp., Edgewood, MD*; <sup>3</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*; <sup>4</sup>*US Army/ECBC, Bel Air, MD*
- ThP 078 **Development of Antibody-like Nanomaterials to Enrich Phosphoproteins for Proteome Analysis**; Leekyoung Hwang; Zachery R. Gregorich; Santosh G. Valeja; Serife A. Gunner; Wenxuan Cai; Song Jin; Ying Ge; *University of Wisconsin-Madison, Madison, WI*

- ThP 079 **A Sensitive Assay to Estimate Total Protein Phosphorylation Level in Complex Samples;** Li Pan; Jiazhen Zhang; Chuan-Chih Hsu; Linna Wang; Anton Iliuk; Weiguo Andy Tao; *Purdue University, West Lafayette, IN*
- ThP 080 **SILAC-based Quantitative Phosphoproteomics Identifies Substrates of Ser/Thr/Tyr Kinases and Phosphatases in *Bacillus Subtilis*;** Vaishnavi Ravikumar<sup>1</sup>; Lei Shi<sup>2</sup>; Karsten Krug<sup>1</sup>; Ivan Mijakovic<sup>2,3</sup>; Boris Macek<sup>1</sup>; <sup>1</sup>*Proteome Center Tuebingen, Tuebingen, Germany*; <sup>2</sup>*AgroParisTech, Grignon, France*; <sup>3</sup>*Chalmers University of Technology, Gothenburg, Sweden*
- ThP 081 **Quantitative Phosphoproteomics of STEK Cell Lines Implicates Novel Pathways in Pathogenesis of Fragile X Syndrome and Autism Spectrum Disorders;** Katarina Matic<sup>1</sup>; Timo Eninger<sup>1</sup>; Barbara Bardoni<sup>2,3</sup>; Laetitia Davidovic<sup>2,3</sup>; Boris Macek<sup>1</sup>; <sup>1</sup>*Proteome Center Tuebingen, Tuebingen, Germany*; <sup>2</sup>*Institut de Pharmacologie Moléculaire et Cellulaire, Valbonne, France*; <sup>3</sup>*Université de Nice-Sophia Antipolis, Nice, France*
- ThP 082 **Quantitative Analysis of the Phosphoproteome Demonstrates Novel Roles of the O-GlcNAc Transferase in Modulating Cellular Signaling;** Jun Zhong; Marissa Martinez; Srna Sengupta; Albert Lee; Xinyan Wu; Raghothama Chaerkady; Robert O'Meally; Karen Reddy; Robert Cole; Akhilesh Pandey; Natasha Zachara; *Johns Hopkins University, Baltimore, MD*
- ThP 083 **-Omics Investigation of *Sulfolobus solfataricus* in Response to Different Carbon Sources;** Wen Qiu; Trong Khoa Pham; Phillip C. Wright; *Chelsi Institute, The University of Sheffield, Sheffield, UK*
- Proteins: Non-Covalent Interactions, 084 - 104**
- ThP 084 **Characterization of Drug Mode-of-Action using Protein Stability Measurements;** M. Ariel Geer<sup>1</sup>; Douglas H. Weitzel<sup>2</sup>; Do Yeon Kwon<sup>1</sup>; Tesia N. Stephenson<sup>1</sup>; Mark W. Dewhurst<sup>2</sup>; Jiyong Hong<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>*Duke University, Durham, NC*; <sup>2</sup>*Duke University Medical Center, Durham, NC*
- ThP 085 **SILAC-Based Strategy for Proteome-Wide Thermodynamic Analysis of Protein-Ligand Binding Interactions;** Jagat Adhikari<sup>1</sup>; Michael C. Fitzgerald<sup>1,2</sup>; <sup>1</sup>*Duke Medical Center, Durham, NC*; <sup>2</sup>*Duke University, Durham, NC*
- ThP 086 **The Effect of Mutations in beta-Amyloid on Zinc Ion Coordination;** Igor Popov<sup>1,2</sup>; Maria Indeykina<sup>2,4</sup>; Alexey Kononikhin<sup>1,2</sup>; Sergey Kozin<sup>3</sup>; Eugene Nikolaev<sup>1,2</sup>; <sup>1</sup>*Moscow Institute of Physics and Technology, Dolgoprudny, Russia*; <sup>2</sup>*Emanuel Institute of Biochemical Physics, Moscow, Russia*; <sup>3</sup>*Engelhardt Institute of Molecular Biology, Moscow, Russia*; <sup>4</sup>*Institute for Energy Problems of Chemical Physics, Moscow, Russia*
- ThP 087 **Natural Products: A Promising Source for Potential  $\beta$ -Amyloid Inhibitors;** Anthony Tsarbopoulos<sup>1</sup>; Nikolaos Stavros Koulakiotis<sup>2</sup>; Dimitrios Anagnostopoulos<sup>3</sup>; Ioannis Kostakis<sup>4</sup>; <sup>1</sup>*University of Athens Medical School, Athens 115 27, Greece*; <sup>2</sup>*University of Patras, Pharmacy Department, Patras 26504, Greece*; <sup>3</sup>*The Goulandris Natural History Museum, Kifissia 145 62, Greece*; <sup>4</sup>*University of Athens, Pharmacy Dpt., Athens 157 71, Greece*
- ThP 088 **Folding of Gaseous Protein Ions;** Fred W. McLafferty<sup>1</sup>; Sergio Castro<sup>1</sup>; Owen Skinner<sup>1</sup>; Kathrin Breuker<sup>2</sup>; <sup>1</sup>*Cornell University, Ithaca, NY*; <sup>2</sup>*University of Innsbruck, Innsbruck, Austria*
- ThP 089 **Unbiased Proteome-wide Interaction Analysis using Intracellular Protein Crosslinking;** Mark Larance; Kathryn Kirkwood; Thomas Crozier; Yasmeen Ahmad; Gareth Agius; Angus Lamond; *University of Dundee, Dundee, UK*
- ThP 090 **Evaluation of Gallium as a Tracer of Hemoglobin-Haptoglobin Complexes in Drug Delivery;** Shengsheng Xu; Rinat R. Abzalimov; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- ThP 091 **Proteomics Profiling of Target Complexes of Vorinostat using Chemical Probe and Mass Spectrometry Analysis;** Congcong Lu<sup>1</sup>; Kai Zhang<sup>1,2</sup>; Yi Zhang<sup>3</sup>; Minjia Tan<sup>3</sup>; <sup>1</sup>*Nankai University, department of chemistry, Tianjin, China*; <sup>2</sup>*Tianjin Medical University, Tianjin, China*; <sup>3</sup>*Shanghai Institute of Materia Medica, Shanghai, China*
- ThP 092 **Native Mass Spectrometry Analysis of the Novel Lipid-Binding Protein Mdm12;** Jiang Zhang; Andrew Young; Pascal Egea; Joseph A. Loo; *UCLA, Los Angeles, CA*
- ThP 093 **Probing Protein-Protein and Protein-DNA Interactions by Native Mass Spectrometry and Global Hydrogen Deuterium Exchange using Surface Acoustic Wave Nebulization (SAWN);** Lucas Monkkonen<sup>1</sup>; Scott Heron<sup>2</sup>; Matthew Bush<sup>1</sup>; Carlos Catalano<sup>1</sup>; David Goodlett<sup>2</sup>; <sup>1</sup>*University of Washington, Seattle, WA*; <sup>2</sup>*University of Maryland, Baltimore, MD*
- ThP 094 **Fast Online Solid-phase Extraction Frontend to Characterize Covalent and Non-covalent Interactions in Early Drug Discovery with Mass Spectrometry;** Pascal Bernet; Reto Brunner; Johannes Ottl; Christian Bergsdorf; *Novartis Institutes for BioMedical Research, Basel, Switzerland*
- ThP 095 **Real-time Native MS to Monitor the Effect of Point Mutations, Inhibitor or tRNA Binding on Tgt Subunitexchange and Dimer Stability;** Francois Debaene<sup>1</sup>; Tran Xuan Phong Nguyen<sup>2</sup>; Frederick Ehrmann<sup>2</sup>; Alain Van Dorsseleer<sup>1</sup>; Klaus Reuter<sup>2</sup>; Gerhard Klebe<sup>2</sup>; Sarah Cianferani<sup>1</sup>; <sup>1</sup>*LSMBO, IPHC-DNA, Uds, CNRS, Strasbourg, France*; <sup>2</sup>*Philipps-Universität Marburg, Marburg, Germany*
- ThP 096 **Improving the Reliability of Binding Constants Determined with Mass Spectrometry for Peptide-Zinc (II) Complexes;** Whitney A. Parrish; Allison S. Danell; *East Carolina University, Greenville, NC*
- ThP 097 **Semi-quantitative ESI-MS Assay for Screening Complex Oligosaccharides Mixtures against Proteins;** Elena Kitova; Amr El-Hawiet; John Klassen; *University of Alberta, Edmonton, Canada*
- ThP 098 **Novel Ligands for Human Noroviruses;** Ling Han<sup>1</sup>; Elena Kitova<sup>1</sup>; Ming Tan<sup>2</sup>; Xi Jiang<sup>2</sup>; John Klassen<sup>1</sup>; <sup>1</sup>*University of Alberta, Edmonton, Canada*; <sup>2</sup>*Cincinnati Children's Hospital Medical Center, Cincinnati, OH*
- ThP 099 **Quantifying Protein-Carbohydrate Interactions Using Liquid Sample Desorption Electrospray Ionization Mass Spectrometry;** Yuyu Yao; Km Shams-Ud-Doha; Rambod Daneshfar; Elena Kitova; John Klassen; *University of Alberta, Edmonton, Canada*
- ThP 100 **Enter Titleidentification of Novel E. coli Ribosome-Associated Proteins;** Suraj Saraswat; James P. Reilly; *Indiana University, Bloomington, IN*
- ThP 101 **AP-SWATH Dynamic Interactome of DJ-1 Under Oxidative Stress: Implications for Parkinson's Disease;** Bruno Manadas<sup>1</sup>; Sandra Anjo<sup>1</sup>; Matilde Melo<sup>1</sup>; Liliana Loureiro<sup>1</sup>; Lucia Sabala<sup>1</sup>; José Carvalho<sup>1,2</sup>; Vera Mendes<sup>1</sup>; Tiago Faria<sup>2</sup>; Pedro Castanheira<sup>3</sup>; Rui Brito<sup>2</sup>; Mário Grãos<sup>3</sup>; <sup>1</sup>*Center for Neuroscience and Cell Biology, Cantanhede, Portugal*; <sup>2</sup>*University of Coimbra, Coimbra, Coimbra, Portugal*; <sup>3</sup>*Biocant - Innovation Center, Cantanhede, Portugal*
- ThP 102 **50 Ways to Leave Your Ligand: Finding Weak Interactions in a Fragment-Based Drug Discovery Screen;** Harry Sterling; Gavin Dollinger; *Novartis, San Francisco, CA*



- ThP 103 **An Improved AP/MS Platform for Identification of Extracellular Receptor-Ligand Interactions;** [Xiaoting Tang](#)<sup>1</sup>; Sufen Shang<sup>1</sup>; Mark Heipel<sup>1</sup>; Joseph Kuijper<sup>1</sup>; Cameron Brandt<sup>1</sup>; Collin Hauskins<sup>1</sup>; Asha Yabannavar<sup>1</sup>; Vibeke Stennicke<sup>2</sup>; Wenfeng Xu<sup>1</sup>; <sup>1</sup>*Novo Nordisk Research Center, Seattle, WA*; <sup>2</sup>*Novo Nordisk A/S, Måløv, Denmark*
- ThP 104 **New method: Differential Enzymatic <sup>16</sup>O/<sup>18</sup>O Labelling for the Identification of Cross-Linked DNA-protein Heteroconjugates;** [Fiona Flett](#); C Logan Mackay; Heidrun Interthal; *University of Edinburgh, Edinburgh, UK*
- Proteins: Aggregation, 105 - 106**
- ThP 105 **Importance of Lysine Residues in Huntington Exon 1 Aggregation: Analysis by HDX-MS-MS and Covalent Labeling LC-MS;** [James Arndt](#); Maxmore Chaibva; Robert Brown; Kathleen Burke; Justin Legleiter; Stephen J. Valentine; *West Virginia University, Morgantown, WV*
- ThP 106 **Determining the Mode of Small Molecule Inhibition of Amyloid Formation from the Type-II Diabetes Related Peptide hIAPP using ESI-IMS-MS;** [Lydia M. Young](#); Sheena E. Radford; Alison E. Ashcroft; *University of Leeds, Leeds, UK*
- Proteins: Conformation Analysis, 107 - 113**
- ThP 107 **Mass Spectrometry Reveals Chemically Induced Structural Changes of Protein G' by Which Intact Immune Complexes are Released from Affinity Columns;** [Yelena Yefremova](#)<sup>1</sup>; Mahmoud Al-Majdoub<sup>1</sup>; Kwabena F.M. Opuni<sup>1</sup>; Cornelia Koy<sup>1</sup>; Yuetian Yan<sup>2</sup>; Michael Gross<sup>2</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, University of Rostock, Rostock, Germany*; <sup>2</sup>*Washington University in St. Louis, St. Louis, MO*
- ThP 108 **Monitoring Dynamic Solvent-Induced Protein Unfolding by ESI-MS;** [Michael Cammarata](#); [Ryan Parker](#); Jennifer Brodbelt; *University of Texas, Austin, TX*
- ThP 109 **Determination of Structural and Dynamic Changes in Different Misfolded Forms of Superoxide Dismutase (SOD1) by Hydrogen Deuterium Exchange Mass Spectrometry;** [Xiaobin Xu](#); [Sheng Gu](#); Fang Qian; Paul Weinreb; Dingyi Wen; *Biogen Idec, Cambridge, MA*
- ThP 110 **Analysis of Intact Native Proteins by UVPD and ETD to Reveal Structural Information in the Gas Phase;** [Michael Cammarata](#); Jennifer Brodbelt; *University of Texas, Austin, TX*
- ThP 111 **Dynamics Analysis of Ribosome Structure using 1 mg Cell Revealed by H/D Exchange;** [Tatsuya Yamamoto](#)<sup>1,2</sup>; Yasuaki Kabe<sup>1,2</sup>; Makoto Suematsu<sup>1,2</sup>; <sup>1</sup>*Keio University, Tokyo, Japan*; <sup>2</sup>*ERATO, JST, Tokyo, Japan*
- ThP 112 **Tandem-Mass-Tags as Sensors for Local Conformational Change during Activation of Coagulation Factor IX;** [Eduard Ebberink](#)<sup>1</sup>; Mariëtte Boon-Spijker<sup>1</sup>; Esther Bloem<sup>1</sup>; Alexander Meijer<sup>1,2</sup>; Koen Mertens<sup>1,2</sup>; <sup>1</sup>*Department of Plasma Proteins, Sanquin, Amsterdam, The Netherlands*; <sup>2</sup>*Pharmaceutical Sciences, Utrecht University, Utrecht, The Netherlands*
- ThP 113 **Covalent Fragments from SID Fragmentation of the Helical Protein ROP Correlate with Precursor Secondary Structure;** [Lindsay Morrison](#); Thomas Magliery; Vicki Wysocki; *Ohio State University, Columbus, OH*
- H/D Exchange: Protein Structure and Function, 114 - 138**
- ThP 114 **Identifying Metal-bound Histidine Residues Using Hydrogen Deuterium Exchange and Mass Spectrometry;** [Katie Love](#); Jia Dong; Nicholas Borotto; Richard Vachet; *University of Massachusetts Amherst, Amherst, MA*
- ThP 115 **Examining the Complementary Nature of Hydrogen/Deuterium Exchange and Covalent Labeling through the Structural Analysis of  $\beta$ 2-Microglobulin;** [Nicholas Borotto](#)<sup>1</sup>; Vanessa Mendoza<sup>2</sup>; Richard Vachet<sup>1</sup>; <sup>1</sup>*University of Massachusetts, Amherst, MA*; <sup>2</sup>*Boston University, Boston, MA*
- ThP 116 **Characterization of Transferrin Receptor Binding Mechanism throughout Endocytosis by Hydrogen Exchange and Electron Capture Dissociation;** [Hanwei Zhao](#); Cedric E. Bobst; Igor A. Kaltashov; *University of Massachusetts, Amherst, MA*
- ThP 117 **High Sensitivity HX-MS<sup>2</sup> for Structure Function Studies of the Non-Homologous End Joining Complex;** [Morgan Hoepfner](#); Yaping Yu; Martial Rey; Susan Lees-Miller; David Schriemer; *University of Calgary, Calgary, CANADA*
- ThP 118 **HDXMS Study of the Interaction between ASB9 and Creatine Kinase;** [Deepa Balasubramaniam](#); Jamie Schiffer; Jonathan Parnell; Elizabeth Komives; *UCSD, La Jolla, California*
- ThP 119 **HDX-MS Epitope Mapping of Hemagglutinin in Complex with Influenza Neutralizing Biomolecules;** Cristina Puchades; Otto Diefenbach; Eveline Sneekes-Vriese; Els Brinkman-Van der Linden; Başak Kükrer; [Adrian Apetri](#); *Crucell Vaccine Institute, Leiden, The Netherlands*
- ThP 120 **Rationalizing Differences in Thermodynamic Stability of Immunoglobulins using shape Selective Mass Spectrometry and Hydrogen/Deuterium-Exchange;** [Matthew Edgeworth](#)<sup>1</sup>; Jonathan Phillips<sup>2</sup>; David Lowe<sup>2</sup>; Daniel Higazi<sup>2</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>*University of Warwick, Coventry, UK*; <sup>2</sup>*MedImmune, Cambridge, UK*
- ThP 121 **Dynamic Signatures of Thermal Adaptation in DNA Polymerases Observed by Hydrogen Exchange;** [Daniel Deredge](#)<sup>1</sup>; Chin-Chi Liu<sup>2</sup>; Vince LiCata<sup>2</sup>; Patrick Wintrode<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*Louisiana State University, Baton Rouge, LA*
- ThP 122 **Comparing the Structure and Dynamics of Phosphatidylinositol-Specific Phospholipase C from *Bacillus thuringiensis* and *Staphylococcus aureus*;** [Bhavna Jois](#)<sup>2</sup>; Anne Gershenson<sup>3</sup>; Mary Roberts<sup>4</sup>; [Patrick Wintrode](#)<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*University of Maryland Baltimore County, Baltimore, MD*; <sup>3</sup>*University of Massachusetts at Amherst, Amherst, MA*; <sup>4</sup>*Boston College, Chestnut Hill, MA*
- ThP 123 **Beyond Structure Characterization: Structure Dynamics (Hydrogen Deuterium Exchange) Guided Biocatalyst Improvement;** Rui Zhang<sup>1</sup>; Ugur Uzuner<sup>2</sup>; Su Sun<sup>1</sup>; Joshua Yuan<sup>2</sup>; [Susie Dai](#)<sup>1</sup>; <sup>1</sup>*Office of the Texas State Chemist, Department of V, College Station, TX*; <sup>2</sup>*Department of Plant Pathology and Microbiology, College Station, TX*
- ThP 124 **Does Protein-Ligand Binding Generally Induce Reduced Deuteration Rates? Globin Oxygenation Studies Provide Insights Into HDX Fundamentals;** [Modupeola Sowole](#); Lars Konermann; *Univ. of Western Ontario, London, ON*
- ThP 125 **Epitope mapping and Interrogation of Allosteric Changes in Protein-Ligand Interactions Enabled by Site-Specific, Sub-Second-Timescale HDX on an Integrated Microfluidic Device;** [Diana Resetca](#)<sup>1</sup>; Sina Haftchenary<sup>2</sup>; Patrick Gunning<sup>2</sup>; Derek Wilson<sup>1</sup>; <sup>1</sup>*York University, Toronto, Canada*; <sup>2</sup>*University of Toronto Mississauga, Mississauga, Canada*
- ThP 126 **HDX MS Depicts Intrinsic Structural Rearrangements of RIG-I upon Sensing Viral RNA and ATP Hydrolysis;** [Jie Zheng](#); Huiyee Yong; Nantika Panutdaporn; Chun Loong Ho; Xueming Dong; Xiaobao Bi; Chuanfa Liu; Dahai Luo; Kai Tang; *Nanyang Technological University, Singapore*

- ThP 127 **Estimation of Protein Folding Rates of Staphylococcal Nucleases and Ubiquitin using PEPS(Protein Equilibrium Population Snapshot)-HDX-ESI-MS; Rohana Livanage**; Reece Ritter; Wesley Stites; Jennifer Gidden; Jackson O. Lay Jr; *University of Arkansas, Fayetteville, AR*
- ThP 128 **An Autoantibody Binding Epitope in ADAMTS13 Protease Identified by Hydrogen/Deuterium Exchange Mass Spectrometry**; Wenbing Hu<sup>1</sup>; Veronica C. Casina<sup>2</sup>; Zhong-yuan Kan<sup>1</sup>; Leland Mayne<sup>1</sup>; X. Long Zheng<sup>2</sup>; S. Walter Englander<sup>1</sup>; <sup>1</sup>*University of Pennsylvania, Philadelphia, PA*; <sup>2</sup>*The Children's Hospital of Philadelphia, Philadelphia, PA*
- ThP 129 **Lysyl-tRNA Synthetase (KRS)-induced Conformational Changes to the 37-kDa Laminin Receptor Precursor (37LRP)-Nanodisc Complex Revealed by H/D Exchange FT-ICR MS**; Yeqing Tao<sup>1</sup>; Pengfei Fang<sup>3</sup>; Nicolas L. Young<sup>2</sup>; Min Guo<sup>3</sup>; Alan G. Marshall<sup>2</sup>; <sup>1</sup>*Florida State University, Tallahassee, FL*; <sup>2</sup>*NHMFL / FSU, Tallahassee, FL*; <sup>3</sup>*The Scripps Research Institute, Jupiter, FL*
- ThP 130 **Insights into the Conformational Dynamics of Oxidized Cu, Zn Superoxide Dismutase (SOD1), an ALS-Associated Post-Translational Modification**; Jared R. Auclair<sup>1,2</sup>; Roxana E. Iacob<sup>1</sup>; Qian Liu<sup>2</sup>; Dagmar Ringe<sup>2</sup>; Gregory A. Petsko<sup>2</sup>; John R. Engen<sup>1</sup>; Jeffrey N. Agar<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*Brandeis University, Waltham, MA*
- ThP 131 **Investigating Fatty Acid Amide Hydrolase Membrane Association by Hydrogen Deuterium Exchange Mass Spectrometry**; Brent Kochert; Michael Johnson; Alexandros Makriyannis; John Engen; *Northeastern University, Boston, MA*
- ThP 132 **Conformational Dynamics of the Src-family kinase Hck following HIV-1 Nef and Small Molecule Inhibitor Binding**; Jamie A. Moroco<sup>1</sup>; Thomas E. Wales<sup>1</sup>; Lori A. Emert-Sedlak<sup>2</sup>; Thomas E. Smithgall<sup>2</sup>; John R. Engen<sup>1</sup>; <sup>1</sup>*Northeastern University, Boston, MA*; <sup>2</sup>*University of Pittsburgh School of Medicine, Pittsburgh, PA*
- ThP 133 **Structural Basis of  $\beta$ -arrestin-mediated GPCR Signaling --- Structural Information of  $\beta$ 2AR- $\beta$ -arr1 Complexes Revealed by Mass Spectrometry**; Kunhong Xiao<sup>1</sup>; Arun Shukla<sup>1</sup>; Sheng Li<sup>2</sup>; Xiao Jie Yao<sup>1</sup>; Minjung Choi<sup>1</sup>; Jiang Qian<sup>1</sup>; Adi Blanc<sup>1</sup>; Robert Lefkowitz<sup>3</sup>; <sup>1</sup>*Duke University Medical Center, Durham, NC*; <sup>2</sup>*University of California at San Diego, La Jolla, CA*; <sup>3</sup>*HHMI, Duke University Medical Center, Durham, NC*
- ThP 134 **Characterization of the Binding Interface between rFVIIIc Fusion Protein and the von Willebrand Factor by Hydrogen/Deuterium Exchange Mass Spectrometry**; George Bou-Assaf; Ekta Seth Chhabra; John Kulman; *Biogen Idec, Cambridge, MA*
- ThP 135 **Detecting Differences in Structure and Dynamics between Wild Type hGH and a Variant by Hydrogen/Deuterium Exchange Mass Spectrometry and ETD**; Signe Teuber Seger<sup>1,2</sup>; Mette Dahl Andersen<sup>1</sup>; Jens Breinholt<sup>1</sup>; Johan Faber<sup>1</sup>; Christine Bruun Schjødt<sup>1</sup>; Kasper D. Rand<sup>2</sup>; <sup>1</sup>*Novo Nordisk, Måløv, Denmark*; <sup>2</sup>*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*
- ThP 136 **Probing the Conformational Dynamics and Regulation of Dynamin Function using HDX Mass Spectrometry**; Venkat Dharmarajan<sup>1</sup>; Saipraveen Srinivasan<sup>2</sup>; Sandra Schmid<sup>2</sup>; Patrick Griffin<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, Jupiter, FL*; <sup>2</sup>*UT Southwestern Medical Center, Dallas, TX*
- ThP 137 **Characterization of PPAR $\gamma$  Mutations on Protein Dynamics With HDX**; David Marciano<sup>1</sup>; Scott Novick<sup>1</sup>; Bruce Pascal<sup>1</sup>; John Bruning<sup>2</sup>; Patrick Griffin<sup>1</sup>; <sup>1</sup>*The Scripps Research Institute, Jupiter, FL*; <sup>2</sup>*The University of Adelaide, Adelaide, Australia*
- ThP 138 **Hydrogen/deuterium Exchange Mass Spectrometry Study of a New PPAR Ligand**; Luana Oliveira dos Santos<sup>1</sup>; Aline Villanova Bridi<sup>2</sup>; Ana Carolina Migliorini Figueira<sup>2</sup>; Fabio C Gozzo<sup>1</sup>; <sup>1</sup>*Institute of Chemistry - University of Campinas, Campinas, SP*; <sup>2</sup>*Brazilian Biosciences National Laboratory, Campinas, SP*
- Glycoproteins, 139 - 168**
- ThP 139 **Alternation of Glycans Site Specificity in Patients with Liver Diseases**; Petr Pompach<sup>1,2</sup>; Petra Darebna<sup>2</sup>; Petr Novak<sup>1,2</sup>; Ondrej Topolcan<sup>3</sup>; Julius Benicky<sup>4</sup>; Miloslav Sanda<sup>4</sup>; David Ashline<sup>5</sup>; Radoslav Goldman<sup>4</sup>; <sup>1</sup>*Institute of Microbiology ASCR, Prague, Czech Republic*; <sup>2</sup>*Faculty of Science, Charles University, Prague, Czech Republic*; <sup>3</sup>*Faculty Hospital in Pilsen, Pilsen, Czech Republic*; <sup>4</sup>*Georgetown University, Washington, DC, DC*; <sup>5</sup>*University of New Hampshire, Durham, NH*
- ThP 140 **A Combined Glycomics and Glycoproteomics Approach to Study the N-glycoproteome of Human Cerebrospinal Fluid**; Arnaud Goyallon; Sophie Cholet; Christophe Junot; Francois Fenaille; *CEA, iBiTec-S, SPI, Gif Sur Yvette, FRANCE*
- ThP 141 **Characterization of Pronase Digestion for biopharmaceutical glycosylation analysis**; Marion Baeumlisberger<sup>1</sup>; Dominic Baeumlisberger<sup>2</sup>; Michael Karas<sup>1</sup>; <sup>1</sup>*Goethe University, Frankfurt Am Main, Germany*; <sup>2</sup>*SunChrom GmbH, Friedrichsdorf, Germany*
- ThP 142 **Separation and Analysis of the Individual Components in Glycopeptide Isomeric Mixtures via HILIC-MS**; Yining Huang<sup>1</sup>; Yongxin Nie<sup>2</sup>; Barry Boyes<sup>1,3</sup>; Ron Orlando<sup>1</sup>; <sup>1</sup>*University of Georgia, Athens, GA*; <sup>2</sup>*ShanDong Agricultural University, Taian, SD*; <sup>3</sup>*Advanced Materials Technology Inc., Wilmington, DE*
- ThP 143 **Direct Site-Specific Glycoform Identification and Quantitative Comparison of Glycoprotein therapeutics: Cerezyme® and Velaglucerase**; Hongping Ye<sup>1</sup>; John Hill<sup>2</sup>; Ashley Gucinski<sup>1</sup>; Michael Boyne<sup>1</sup>; Lucinda Buhse<sup>1</sup>; <sup>1</sup>*Food and Drug Administration, St. Louis, MO*; <sup>2</sup>*Retired, Carrollton, TX*
- ThP 144 **Optimized Digestion and Isolation of HIV-related Immunoglobulins for Glycoanalysis by FTICR Mass Spectrometry**; Tyler A Zimmerman; Xiang Yu; Archer D. Smith; Neil L. Kelleher; *Northwestern University, Evanston, IL*
- ThP 145 **Electrochemical Enrichment of Glycopeptides using Polyaniline Boronic Acid**; Edward Bodnar; Hélène Perreault; *University of Manitoba, Winnipeg, Canada*
- ThP 146 **Glycoproteomic Analysis of Breast Cancer Cell Lines**; Majlinda Kullolli; Maria Arampatzidou; Sharon Pitteri; *Stanford University School of Medicine, Palo Alto, CA*
- ThP 147 **Glycoproteomic Study of the Mycobacterium Tuberculosis Cell Wall and Cell Membrane**; Roxana Eggleston-Rangel; Michael Sweredoski; Geoffrey T Smith; Sonja Hess; *Caltech, Pasadena, CA*
- ThP 148 **LC-MS Analysis of Permethylated Sulfated Glycans Released from Bovine Thyroid-Stimulating Hormone (bTSH)**; Tianjiao Yang; Shiyue Zhou; Yehia Mechref; *Texas Tech University, Lubbock, Texas*
- ThP 149 **Impact of Glycosylation Patterns of HIV-1 Envelope Glycoprotein on Virus Infectivity**; Audra H. Laube<sup>1</sup>; Milan Raska<sup>1,2</sup>; Qing Wei<sup>1</sup>; Barbora Knoppova<sup>2</sup>; Stacy Hall<sup>1</sup>; Katerina Zachova<sup>2</sup>; Zhi-Qiang Huang<sup>1</sup>; Lydie Czernekova<sup>1,2</sup>; Zina Moldoveanu<sup>1</sup>; Jan Novak<sup>1</sup>; Matthew B. Renfrow<sup>1</sup>; <sup>1</sup>*University of Alabama at Birmingham, Birmingham, AL*; <sup>2</sup>*Palacky University in Olomouc, Olomouc, Czech Republic*

- ThP 150 **The Analysis of *Helicobacter pylori*'s Glycoproteins: Mass Spectral Fragmentation of azido-Sugars Labelled with Phosphine-FLAG Peptide Variants;** Sunnie Kuna; Danielle Dube; Elizabeth A. Stemmler; *Bowdoin College, Brunswick, ME*
- ThP 151 **Evaluation and Comparison of Electron Capture Dissociation and Collision Induced Dissociation for Intact Glycoprotein Analysis;** Ze Wang; Tak Wah Dominic Chan; *the Chinese University of Hong Kong, Hong Kong, PR China*
- ThP 152 **Global Comparative Characterization of Hemoglobin Glycation in Normal and Diabetic Bloods by LC-MSMS;** Shu-Hui Chen<sup>1</sup>; Shih-Hao Wang<sup>1</sup>; Tzu-Fan Wang<sup>1</sup>; Chih-Hsing Wu<sup>2</sup>; <sup>1</sup>*Chem. Dept. Natl. Cheng Kung Univ., Tainan, Taiwan*; <sup>2</sup>*Medicine College, Natl. Cheng Kung Univ., Tainan, Taiwan*
- ThP 153 **Monitoring Responses of Antibody Glycosylation to HIV Infection;** Cynthia Williams; Anne Fenton; Lauren Nagy; Qiuting Hong; L. Renee Ruhaak; Satya Dandekar; Carlito Lebrilla; *UC Davis, Davis, CA*
- ThP 154 **An Integrated Pipeline for Analysis of LC-MS based Glycomic Data;** Minkun Wang<sup>1</sup>; Tsung-Heng Tsai<sup>1</sup>; Yunli Hu<sup>2</sup>; Shiyue Zhou<sup>2</sup>; Yehia Mechref<sup>2</sup>; Habtom Resson<sup>1</sup>; <sup>1</sup>*Georgetown University, Washington, DC*; <sup>2</sup>*Texas Tech University, Lubbock, TX*
- ThP 155 **A Systems Approach to Protein-Specific Glycosylation Analyses of Serum Glycoproteins for Cancer Diagnosis;** Renee Ruhaak<sup>1</sup>; Carol Stroble<sup>1,2</sup>; Qiuting Hong<sup>1</sup>; Suzanne Miyamoto<sup>2</sup>; Kyoungmi Kim<sup>1</sup>; Gary Leiserowitz<sup>2</sup>; Carlito Lebrilla<sup>1</sup>; <sup>1</sup>*UC Davis, Davis, CA*; <sup>2</sup>*UC Davis Medical Center, Sacramento, CA*
- ThP 156 **MMP-9 Associated Extracellular Proteins Identified in the Left Ventricle Infarct using Glycoproteomics;** Yuan Tian<sup>1,2</sup>; Kristine DeLeon-Pennell<sup>1,3</sup>; Bai Zhang<sup>2</sup>; Presley Cannon<sup>1,3</sup>; Punit Shah<sup>2</sup>; Paul Aiyetan<sup>2</sup>; Ganesh Halade<sup>3,4</sup>; Yonggang Ma<sup>1,3</sup>; Zhen Zhang<sup>2</sup>; Hui Zhang<sup>2</sup>; Merry Lindsey<sup>5</sup>; <sup>1</sup>*University of Mississippi Medical Center, Jackson, MS*; <sup>2</sup>*Johns Hopkins University, Baltimore, MD*; <sup>3</sup>*San Antonio Cardiovascular Proteomics Center, San Antonio, TX*; <sup>4</sup>*The University of Alabama at Birmingham, Birmingham, AL*; <sup>5</sup>*GV (Sonny) Montgomery Veterans Affairs Medical Cen, Jackson, MS*
- ThP 157 **Hypoxia-induced Changes to Integrin Alpha 3 Glycosylation Facilitate Migration in A431;** Yan Ren; Piliang Hao; Alex Law; Siu Kwan Sze; *Nanyang Technological University, Singapore, Singapore*
- ThP 159 **De novo Glycomics of the Parasite *Cryptosporidium parvum*;** John Haserick<sup>1</sup>; John Samuelson<sup>2</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Boston University School of Dental Medicine, Boston, MA*
- ThP 160 **A Novel LC-MS<sup>2</sup> Product Dependent Parallel Data Acquisition Function and Data Analysis Workflow for Sequencing and Identification of intact Glycopeptides;** Sz-Wei Wu<sup>1,2</sup>; Tsung-Hsien Pu<sup>1</sup>; Rosa Viner<sup>3</sup>; Kay-Hooi Khoo<sup>1</sup>; <sup>1</sup>*Academia Sinica, Taipei, Taiwan*; <sup>2</sup>*Thermo Fischer Scientific Taiwan, Taipei, Taiwan*; <sup>3</sup>*Thermo Fischer Scientific, San Jose, CA*
- ThP 161 **Characterization of Novel, Polyfucosyl-LacdiNAc Epitope Containing Glycans from Hydra using Ultra Sensitive MALDI-TOF/TOF Mass Spectrometry;** Sonu Sahadevan<sup>1</sup>; Antonopolous Aristotelus<sup>2</sup>; Stuart Haslam<sup>2</sup>; Anne Dell<sup>2</sup>; Subramanian Ramaswamy<sup>1</sup>; Babu Ponnusamy<sup>3</sup>; <sup>1</sup>*InStem, NCBS-TIFR, Bangalore, India*; <sup>2</sup>*Imperial College London, London, U.K.*; <sup>3</sup>*Centre for Cellular and Molecular Platforms, Bangalore, India*
- ThP 162 **Quantitative Glycoform Analysis of Human IgG using a Novel Stable Isotope-Labeling and MALDI-TOF Mass Spectrometry;** Masaki Kuroguchi; Junko Amano; *the noguchi institute, Tokyo, Japan*
- ThP 163 **Unique Glyco-peptides as Biomarkers and for Detection of Exogenous Biosimilar Administration;** Hui-Chung Liang<sup>1</sup>; Claire Russell<sup>1</sup>; Ray Chung<sup>2</sup>; Chantal Bazenet<sup>2</sup>; Abdul Hye<sup>2</sup>; Simon Lovestone<sup>2</sup>; David Cowan<sup>2</sup>; Ian Pike<sup>1</sup>; Malcolm Ward<sup>1</sup>; <sup>1</sup>*Proteome Sciences plc, London, UK*; <sup>2</sup>*Kings College London, London, UK*
- ThP 164 **Glycosylation Analysis of an Engineered Influenza Hemagglutinin (H3N2) Series with an Increasing Number of Sequentially Added Historically relevant Glycosylation Sites;** Yanming An<sup>1</sup>; Jonathan McCullers<sup>2</sup>; John Cipollo<sup>1</sup>; <sup>1</sup>*FDA, Bethesda, MD*; <sup>2</sup>*St. Jude Children's Research Hospital, Memphis, TN*
- ThP 165 **Glycan Elution Time Predictor for Glycan Profiling by Liquid Chromatography Coupled Mass Spectrometry;** Chuan-Yih Yu<sup>1</sup>; Ryutaro Ichise<sup>2</sup>; Kiyoko F Aoki-Kinoshita<sup>3</sup>; Haixu Tang<sup>1</sup>; <sup>1</sup>*Indiana University, Bloomington, IN*; <sup>2</sup>*National Institute of Informatics, Tokyo, Japan*; <sup>3</sup>*Soka University, Tokyo, Japan*
- ThP 166 **Efficient Isolation and Identification of Exosomal Glycoproteins following Sugar-azide Metabolic Labeling and Alkyne-bead Capture;** Stephen M. Roper<sup>1</sup>; Peng Gao<sup>1</sup>; Benjamin A. Neely<sup>1</sup>; Robert Gemmill<sup>2</sup>; Lauren Ball<sup>1</sup>; Richard Drake<sup>1</sup>; <sup>1</sup>*Department of Cell and Molecular Pharmacology MUSC, Charleston, SC*; <sup>2</sup>*Department of Medicine, MUSC, Charleston, SC*
- ThP 167 **An Integrated Platform of LC-MS, HPAEC-PAD, and Bioinformatics for the Carbohydrate Profiling of Therapeutic Glycoproteins;** Andrea Gray; Joshua Wilhite; Shaunak Uplekar; Govind Rao; William LaCourse; *University of Maryland Baltimore County, Baltimore, MD*
- ThP 168 **Targeted Glycoproteomic Analysis of Serum Haptoglobin Reveals Glycosite-Specific Biomarkers for Gastric Cancer;** Serenus Hua<sup>1</sup>; Sung-Hyeon Lee<sup>2</sup>; Myung Jin Oh<sup>1</sup>; Rudolf Grimm<sup>3</sup>; Jung Hoe Kim<sup>2</sup>; Hyun Joo An<sup>1</sup>; <sup>1</sup>*AGRS, Chungnam National University, Daejeon, Korea*; <sup>2</sup>*Korea Advanced Institute of Science and Technology, Daejeon, Korea*; <sup>3</sup>*Agilent Technologies, Santa Clara, CA*
- Peptides: Quantitative Analysis (New Methods and Applications of Labels), 169 - 179**
- ThP 169 **High-Resolution Enabled 12-plex DiLeu Isobaric Labels for Quantitative Proteomics;** Dustin Frost; Tyler Greer; Lingjun Li; *University of Wisconsin-Madison, Madison, WI*
- ThP 170 **Higher Isobaric Multiplexing for Discovery Proteomics of Genomically-Characterized Patient-Derived Breast Cancer Xenografts;** Petra Erdmann-Gilmore<sup>1</sup>; Alan E. Davis<sup>1</sup>; Henry W. Rohrs<sup>1</sup>; Shunqiang Li<sup>1</sup>; Sherri R. Davies<sup>1</sup>; Xuya Wang<sup>2</sup>; David Fenyo<sup>3</sup>; Matthew J. Ellis<sup>1</sup>; Ryan Bomgarden<sup>4</sup>; Rosa Viner<sup>2</sup>; John C. Rogers<sup>4</sup>; Jason M. Held<sup>1</sup>; R. Reid Townsend<sup>1</sup>; <sup>1</sup>*Washington University, St Louis, MO*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>3</sup>*New York University, New York, NY*; <sup>4</sup>*Thermo Fisher Scientific, Rockford, IL*
- ThP 171 **Development of Isotope-Labeled Viral Protein Concatemers for Targeted, Absolute Quantification of all Herpes Simplex Virus Structural Proteins during Infection;** Todd M. Greco<sup>1</sup>; Beatriz Oliveira<sup>1</sup>; Aaron Lin<sup>1</sup>; Kay Grunewald<sup>2</sup>; Ileana M. Cristea<sup>1</sup>; <sup>1</sup>*Princeton University, Princeton, NJ*; <sup>2</sup>*Oxford University, Oxford, UK*
- ThP 172 **Quantitative Mass Spectrometry of Protein Complexes in the Chromatophores of *Rhodobacter sphaeroides* using <sup>15</sup>N-labelled Artificial (QconCAT) Proteins as Internal Standards;** Philip Jackson; Amanda Brindley;

- Michael Cartron; Pu Qian; Mark Dickman; Neil Hunter; *University of Sheffield, Sheffield, UK*
- ThP 173 **MS<sup>E</sup> as a Means of Determining Label Incorporation Efficiency and Determining Empirical Normalization Constants for iTRAQ/TMT-based Experiments;** Yong Yang<sup>1</sup>; Kevin Howe<sup>1</sup>; Sheng Zhang<sup>2</sup>; Theodore W Thannhauser<sup>1</sup>; <sup>1</sup>USDA-ARS, Cornell University, Ithaca, NY; <sup>2</sup>Cornell University, Ithaca, NY
- ThP 174 **Direct Comparison of TMT Labeling vs. Spectral Counting for Relative Peptide Quantification using a Two-proteome Model;** Rachel Rodrigues; David Nusinow; Steven Gygi; *Harvard Medical School, Boston, MA*
- ThP 175 **Ratio Contamination in TMT-based Quantitation on Q Exactive Instruments: In-Depth Characterization and Alternative Methods for Improved Accuracy;** Neha Goswami; Hisham Ben Hamidane; Johannes Graumann; *Weill Cornell Medical College in Qatar, Doha, QATAR*
- ThP 176 **Comparison of Peptide Isotope Ratio and Protein Calibration Curve Back-Calculation for Absolute Protein Quantification by LC-MS/MS;** Carmen Fernandez-Metzler; Bonnie Baker; Richard King; *PharmaCadence Analytical Services, LLC, Hatfield, PA*
- ThP 177 **The Nuts and Bolts of NeuCode Quantification;** Anna Merrill; Nicholas Kwieciec; Christopher Rose; Alex Hebert; Michael Westphall; Joshua J. Coon; *University of Wisconsin-Madison, Madison, WI*
- ThP 178 **NeuCode Labeling for Multiplexed, Global Protein Quantification;** Anna E. Merrill<sup>1</sup>; Alexander S. Hebert<sup>1</sup>; Matthew E. MacGilvray<sup>1</sup>; Christopher M. Rose<sup>1</sup>; Derek J. Bailey<sup>1</sup>; Joel C. Bradley<sup>2</sup>; William W. Wood<sup>2</sup>; Marwan ElMasri<sup>2</sup>; Michael S. Westphall<sup>1</sup>; Audrey P. Gasch<sup>1</sup>; Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Cambridge Isotope Laboratories, Andover, MA
- ThP 179 **NeuCode SILAC for Ultra-Plexed, Targeted Quantification of Vesicular Stomatitis Virus Proteins and Host Cell Phosphorylation;** Gregory K. Potts; Emily A. Voigt; Michael S. Westphall; Alexander S. Hebert; John Yin; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- Peptides: Ion Activation/Dissociation Strategies, 180**
- ThP 180 **Sequencing Acidic Peptides with Negative Ion Mode In-Source Decay MALDI/TOF MS;** Chelsea L. McMillen; Carolyn J. Cassidy; *The University of Alabama, Tuscaloosa, AL*
- Peptides: Fragmentation Mechanisms, 181 - 196**
- ThP 181 **Electron Transfer Dissociation (ETD) on Acidic Peptides;** Changgen Feng; Carolyn Cassidy; *The University of Alabama, Tuscaloosa, AL*
- ThP 182 **The Effect of Peptide Size on Multiple Charging and Electron Transfer Dissociation Fragmentation of Acidic Peptides;** Juliette J Commodore; Carolyn J Cassidy; *The University of Alabama, Tuscaloosa, AL*
- ThP 183 **Electron Transfer Dissociation (ETD) of Conformationally Restricted Peptides;** Huong (Ivy) Nguyen; *University of Washington, Seattle, WA*
- ThP 184 **Fragmentation Patterns and Mechanisms of Protonated Peptoids under CID Conditions;** Jianhua Ren<sup>1</sup>; Yuan Tian<sup>1</sup>; Michael Connolly<sup>2</sup>; Ronald Zuckermann<sup>2</sup>; <sup>1</sup>University of the Pacific, Stockton, CA; <sup>2</sup>Lawrence Berkeley National Laboratory, Berkeley, CA
- ThP 185 **The Fragmentation Reactions Mechanism of Proline-Containing Heptapeptides;** Cagdas Tasoglu<sup>1</sup>; Alex G. Harrison<sup>2</sup>; Talat Yalcin<sup>1</sup>; <sup>1</sup>IYTE, Urla-Izmir, Turkey; <sup>2</sup>University of Toronto, Toronto, ON
- ThP 186 **Fundamental Predictions of Ion Intensities in Tandem Mass Spectra of Three Pentapeptides;** Tibor Pechan; *Mississippi State University, Mississippi State, MS*
- ThP 187 **The Effect of Charge Carrier on the Fragmentation Behavior of Small Peptide Sulfinyl Radical Ions in the Gas Phase;** Hanfeng Hu; Lei Tan; Yu Xia; *Department of Chemistry Purdue University, West Lafayette, Indiana*
- ThP 188 **Thermodynamics and Mechanisms of Protonated TriGlycine Decomposition – Guided Ion Beam and Theoretical Approach;** Abhigya Mookherjee; Peter Armentrout; *University of Utah, Salt Lake City, UT*
- ThP 189 **Immonium Ions from Singly Charged Peptides;** Nick DeGraan-Weber; James P. Reilly; *Indiana University, Bloomington, IN*
- ThP 190 **Winning the Last Battle against Edman Degradation: Reliable Leucine/Iso-Leucine Differentiation in Peptide Sequencing using Orbitrap Fusion Mass Spectrometer;** Albert T. Lebedev<sup>1</sup>; Eugen Damoc<sup>2</sup>; Alexander Makarov<sup>2</sup>; Tatiana Samgina<sup>1</sup>; <sup>1</sup>Moscow State University, Moscow, Russian Federation; <sup>2</sup>ThermoFisher Scientific, Bremen, Germany
- ThP 191 **MassTodon: An Automated Method to Quantify the Extent of ETD, ETnD, and PTR Reactions in Native Top-Down Proteomics;** Mateusz Lacki<sup>1</sup>; Frederik Lermite<sup>2,3</sup>; Frank Sobott<sup>2,5</sup>; Anna Gambin<sup>1</sup>; Dirk Valkenburg<sup>3,4</sup>; <sup>1</sup>Institute of Informatics, University of Warsaw, Poland; <sup>2</sup>Biomolecular and Analytical Mass Spectrometry, University of Antwerp, Belgium; <sup>3</sup>Applied Bio & Molecular Systems, VITO, Antwerp, Belgium; <sup>4</sup>I-BioStat, Hasselt University, Belgium; <sup>5</sup>Center for Proteomics, University of Antwerp, Belgium
- ThP 192 **Tuning the Reactive Duality of Sulfinyl Radical in Peptides – Radical vs. Base;** Lei Tan; Joseph S. Francisco; Yu Xia; *Purdue University, West Lafayette, IN*
- ThP 193 **Simpson's Paradox: Basic Residues Inhibit Neutral Loss of H<sub>3</sub>PO<sub>4</sub> from Phosphopeptides, Yet Increase the Amount of Neutral Loss we Observe;** Robert Brown; Scott Stuart; Natalie Ahn; William Old; *University of Colorado, Boulder, CO*
- ThP 194 **Peptide Dimethylation: Fragmentation Control via Distancing the Dimethylamino Group;** Adam McShane; Yuanyuan Shen; Mary Joan Castillo; Xudong Yao; *University of Connecticut, Storrs, CT*
- ThP 195 **Fragmentation Energetics of Doubly Protonated Tryptic Hexapeptides;** Oleg Obolensky; Yi-Kuo Yu; *National Center for Biotechnology Information, NLM, Bethesda, MD*
- ThP 196 **Peptide Fragmentation by High-Energy Collision-Induced Dissociation in MALDI-TOF/TOF Mass Spectrometer;** Fang Qian; Rong Wang; *Icahn School of Medicine at Mount Sinai, New York, NY*
- Phosphopeptides: Quantitative Analysis, 197 - 218**
- ThP 197 **A Workflow for Quantitating Low Abundant Phosphorylation Events;** Alon Savidor; Alexandra Gabashvili; Maya Maor; Avraham Yaron; Yishai Levin; *Weizmann Institute of Science, Rehovot, Israel*
- ThP 198 **Accurate Determination of Peptide Phosphorylation Extent via Immobilized Alkaline Phosphatase-based Automated Diagonal Capillary Electrophoresis Coupled with Mass Spectrometry;** Si Mou; Liangliang Sun; Norman Dovichi; *University of Notre Dame, Notre Dame, IN*
- ThP 199 **Quantitative Phosphoproteomic Analysis of Glucose-Stimulated Human Islets;** Haowei Song; Min Tan; Mary Wholtman; Connie Marshall; Nidhi Rohatgi; Michael McDaniel; John Turk; *Washington University in St. Louis, School of Medi, St. Louis, MO*



- ThP 200 **Proteomic and Phosphoproteomic Analysis of Differential Protein Expression and Phosphorylation Patterns in 2D and 3D Cultured Colorectal Cancer Cells;** Xiaoshan Yue; Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*
- ThP 201 **Radio-sensitization of Human Leukemic Cells HL-60 by ATR-kinase Inhibitor (VE-821): Phosphoproteomic Analysis;** Barbora Salovska; Ales Tichy; Ivo Fabrik; Marek Link; Jirina Vavrova; Jiri Stulik; *University of Defence, Hradec Kralove, Czech Republic*
- ThP 202 **Quantitative Analysis of Deubiquitinating Enzyme Activation in Response to DNA Damage;** Lisa A. Vasicek<sup>1</sup>; Kelly A. Conrads<sup>1</sup>; Pang-Ning Teng<sup>1</sup>; Guisong Wang<sup>1</sup>; Brian L. Hood<sup>1</sup>; Chad A. Hamilton<sup>1,4</sup>; G. Larry Maxwell<sup>1,2</sup>; Martin R. Larsen<sup>3</sup>; Thomas P. Conrads<sup>1</sup>; <sup>1</sup>Women's Health Integrated Research Center at Inova, Annandale, VA; <sup>2</sup>Inova Fairfax Hospital, Falls Church, VA; <sup>3</sup>Univ. Southern Denmark, Odense, N/A; <sup>4</sup>Walter Reed National Military Medical Center, Bethesda, MD
- ThP 203 **Label-free Quantitative Phosphoproteomics on B Cell Antigen Receptor Signaling using Data-Independent Acquisition;** Kuan-Ting Pan<sup>1</sup>; Thomas Oellerich<sup>2</sup>; Jasmin Corso<sup>1</sup>; Christof Lenz<sup>1,3</sup>; Henning Urlaub<sup>1,3</sup>; <sup>1</sup>Bioanal. MS Group, Max Plank Inst for Biophys Chem, Goettingen, Germany; <sup>2</sup>Department of Medicine II, Goethe University, Frankfurt, Germany; <sup>3</sup>Dept. of Clin. Chem., Univ. Med. Center Goettingen, Goettingen, Germany
- ThP 204 **A Quantitative Phosphoproteomic Analysis to Study the Dynamics of Tyrosine Phosphorylation in EGFR Signaling Abrogated by TKIs;** Xu Zhang<sup>1</sup>; Tapan Maity<sup>1</sup>; Manoj Kashyap<sup>2</sup>; Arivusudar Marimuthu<sup>2</sup>; Harrys K. C. Jacob<sup>2</sup>; Natalia Belkina<sup>1</sup>; Abhilash Venugopalan<sup>1</sup>; Raghothama Chaerkady<sup>2</sup>; Akhilesh Pandey<sup>2</sup>; Udayan Guha<sup>1</sup>; <sup>1</sup>Thoracic and GI Oncology Branch, NCI, NIH, Bethesda, MD; <sup>2</sup>Johns Hopkins University School of Medicine, Baltimore, MD
- ThP 205 **Comparison of Multiplexed Chemical Labeling Strategies for Quantitative Global Proteomic, Phosphorylation, and Lysine-Acetylation Profiling of Xenograft Breast Cancer Tumors;** Jana W. Qiao<sup>1</sup>; Philipp Mertins<sup>1</sup>; Tanya Svinkina<sup>1</sup>; Namrata Udeshi<sup>1</sup>; Caitlin Feeney<sup>1</sup>; Jacob Jaffe<sup>1</sup>; Karl R. Clauser<sup>1</sup>; D. R. Mani<sup>1</sup>; Michael A. Gillette<sup>1</sup>; Sherri R. Davies<sup>2</sup>; Matthew J. Ellis<sup>2</sup>; Reid Townsend<sup>2</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Washington University, St. Louis, Missouri
- ThP 206 **Quantitative Proteomics Study of MyD88-Dependent Phosphorylation of Endotoxin-Tolerant Macrophages;** Xin Wei; Cui Liu; Li Wang; Xian Chen; *Biochemistry & Biophysics, School of Medicine, UNC-Chapel Hill, NC*
- ThP 207 **Quantitative Phosphoproteomics Discovers Metastasis Biomarkers in Patient-matched Colon Cancer Cell Line Pair SW480/SW620;** Alissa Schunter; Xiaoshan Yue; Amanda B. Hummon; *University of Notre Dame, Notre Dame, IN*
- ThP 208 **Phosphoproteomic Analysis of the Interleukin-33 Signal Transduction Pathway;** Sneha M. Pinto<sup>1,2</sup>; Pamela Leal Rojas<sup>1</sup>; Raja Sekhar Nirujogi<sup>1,2</sup>; Rajesh Raju<sup>2</sup>; Yashwanth Subbannayya<sup>2</sup>; T.S. Keshava Prasad<sup>2</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Institute of Bioinformatics, Bangalore, India
- ThP 209 **Development of a Mass Spectrometry-Based Kinase Activity Assay for Glioma;** Lona Zenevedpour<sup>1</sup>; Marcel Stoop<sup>1</sup>; Lennard Dekker<sup>1</sup>; Elmar vanHooorn<sup>1</sup>; Jan-Willem Jachtenberg<sup>1</sup>; Sieger Leenstra<sup>1</sup>; Jos Joore<sup>2</sup>; Theo Luider<sup>1</sup>; <sup>1</sup>Erasmus Medical Center, Rotterdam, Netherlands; <sup>2</sup>Pepscope B.V, Utrecht, Netherlands
- ThP 210 **Connecting the Fibroblast Growth Factor 2-Mediated Cardioprotection mechanism through Threonine 17 of Phospholamban by Global and Targeted Phosphoproteomics;** Aruna Wijeratne<sup>1</sup>; Janet Manning<sup>3</sup>; Jo El Schultz<sup>2</sup>; Ken Greis<sup>1</sup>; <sup>1</sup>Department of Cancer Biology, Cincinnati, OH; <sup>2</sup>University of Cincinnati, Cincinnati, OH; <sup>3</sup>University of Kentucky, Lexington, KY
- ThP 211 **Qualitative and Quantitative Phosphoproteomic Analysis of the Host Response to Brucella infection;** William K. Russell<sup>1</sup>; Scott Peterman<sup>2</sup>; Julian Saba<sup>3</sup>; Sergei Snovida<sup>4</sup>; Ryan Bomgardner<sup>5</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>Thermo Fisher Scientific, Grimes, IA; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Thermo Fisher Scientific, Rockford, IL; <sup>5</sup>ThermoFisher Scientific, Rockford, IL
- ThP 212 **Towards a Comprehensive Quantitative Characterization of Phosphorylation Dynamics;** Piero Giansanti<sup>1,2</sup>; Erik L. de Graaf<sup>1,2</sup>; Arjen Scholten<sup>1,2</sup>; A.F. Maarten Altelaar<sup>1,2</sup>; Albert J.R. Heck<sup>1,2</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Netherlands Proteomics Centre, Utrecht, The Netherlands
- ThP 213 **Purification and Characterization of Human Synaptosomes Derived from human Neural Stem Cells using Advanced MS Analysis;** Marcella Melo-Braga; Morten Meyer; Martin R. Larsen; *University of Southern Denmark, Odense, Denmark*
- ThP 214 **Evaluating and Optimizing TMT-Based Quantitative Phosphoproteomics on a Next Generation Tribrid Orbitrap;** Brian K Erickson; Graeme C McAlister; Robert A Everley; Mark P Jedrychowski; Steven P Gygi; *Harvard Medical School, Boston, MA*
- ThP 215 **Solid Phase Amino-Labeling with TMTs on Complex Digests for Subsequent Phosphopeptide Enrichment;** Gitte Boehm; Petra Préfot; Stephan Jung; Vikram Mitra; David Britton; Karsten Kuhn; Andrew Thompson; *Proteome Sciences Plc, Cobham, UK*
- ThP 216 **Quantitative Phosphoproteomics Reveals Novel Aspects of the FGF Pathway in FGFR Addicted Breast Cancer Cell Lines;** Debbie L. Cunningham; Andrew J. Creese; Katherine P.B. Larkins; John K. Heath; *University of Birmingham, Birmingham, UK*
- ThP 217 **New Challenges in Targeted Peptide Quantitation: Phosphopeptides;** Lindsay Pino<sup>1</sup>; Susan E. Abbatiello<sup>1</sup>; Lola Fagbami<sup>1</sup>; Heidi Greulich<sup>1,2</sup>; Eric Kuhn<sup>1</sup>; Jacob D. Jaffe<sup>1</sup>; Steven A. Carr<sup>1</sup>; <sup>1</sup>The Broad Institute of MIT and Harvard, Cambridge, MA; <sup>2</sup>Dana-Farber Cancer Institute, Boston, MA
- ThP 218 **Measuring Phosphorylation Signaling Dynamics using Peptide Immunoaffinity Enrichment Coupled to Quantitative Mass Spectrometry;** Jeff Whiteaker; Lei Zhao; Richard Ivey; Julia Voytovich; Regine Schoenherr; Jacob Kennedy; Chenwei Lin; Ping Yan; Amanda Paulovich; *Fred Hutchinson Cancer Research Center, Seattle, WA*
- Peptides: PTM Identification, 219 - 249**
- ThP 219 **Quantitative Multiple PTM Analyses Discovered Novel Modules in Cytokine Signaling Pathways;** Jun Zhong<sup>1</sup>; Min-Sik Kim<sup>1</sup>; Raghothama Chaerkady<sup>1</sup>; Xinyan Wu<sup>1</sup>; Tai-Chung Huang<sup>1</sup>; Derese Getnet<sup>1</sup>; Robert O'meally<sup>1</sup>; Robert Cole<sup>1</sup>; Akinori Yoda<sup>2</sup>; Diederik van Bodegom<sup>2</sup>; Albrecht Moritz<sup>2</sup>; John Rush<sup>3</sup>; Jeffrey Tyner<sup>4</sup>; Steven Ziegler<sup>5</sup>; David Weinstock<sup>2</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>Cell Signaling Technology Inc., Danvers, MA; <sup>4</sup>Oregon Health and Science University, Portland, OR; <sup>5</sup>Benaroya Research Institute at Virginia Mason, Seattle, WA

- ThP 220 **A Novel Metabolic Labeling-Based Workflow for *in silico* Validation of Unrestricted Identifications of PTMs;** Salvatore Cappadona; Francesco Mattia Mancuso; Cristina Chiva; Eduard Sabidó; *CRG - Centre for Genomic Regulation, Barcelona, Spain*
- ThP 221 **Global Identification of Protein Post-translational Modifications in a Single-Pass Database Search;** Michael R. Shortreed<sup>1</sup>; Craig D. Wenger<sup>2</sup>; Brian L. Frey<sup>1</sup>; Mark Scalf<sup>1</sup>; Gloria M. Sheynkman<sup>1</sup>; Lloyd M. Smith<sup>1</sup>; <sup>1</sup>*University of Wisconsin, Madison, WI*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- ThP 222 **TMT10-Tails Workflow for Identification and Quantification of neo N-terminal Proteolytic Peptides;** Michael A. Blank<sup>1</sup>; Theo Klein<sup>2</sup>; Shane Fung<sup>2,3</sup>; Rosa Viner<sup>1</sup>; Wilfred Tang<sup>4</sup>; Marshall Bern<sup>4</sup>; Bernard Delanghe<sup>5</sup>; Torsten Uecker<sup>5</sup>; Andreas Huhmer<sup>1</sup>; Stuart Turvey<sup>2,3</sup>; Christopher M. Overall<sup>2</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*University of British Columbia, Vancouver, BC*; <sup>3</sup>*Children and Family Research Institute, Vancouver, BC*; <sup>4</sup>*Protein Metrics, San Carlos, CA*; <sup>5</sup>*Thermo Fisher Scientific, Bremen, DE*
- ThP 223 **Enrichment and Identification of N-terminal Peptides by a Solid-Phase Acid-Cleavable Reagent and Mass Spectrometry;** Jonathan Yang<sup>1</sup>; Gerhard Munske<sup>2</sup>; Daria Zhukova<sup>1</sup>; James Bruce<sup>3</sup>; Saiful Chowdhury<sup>1</sup>; <sup>1</sup>*University of Texas at Arlington, Arlington, TX*; <sup>2</sup>*Washington State University, Pullman, WA*; <sup>3</sup>*University of Washington, Seattle, WA*
- ThP 224 **ChaFRADIC – A Novel Multifunctional Tool for PTM-Specific Proteomics;** Saskia Venne; Albert Sickmann; René Zahedi; *Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*
- ThP 225 **Strategies for Improving PTM Identification;** Clarissa Dickhut<sup>1</sup>; Christian Hedberg<sup>2</sup>; René Zahedi<sup>1</sup>; <sup>1</sup>*Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany*; <sup>2</sup>*Max-Planck-Institut für Molekulare Physiologie, Dortmund, Germany*
- ThP 226 **Qualitative and Quantitative Analysis of Post-Translational Modifications using CESI-MS;** Herbert H. Lindner; Klaus Faserl; Leopold Kremser; Bettina Sarg; *Biocenter, Division of Clinical Biochemistry, Innsbruck, AUSTRIA*
- ThP 227 **Differentiating Isobaric Compounds by Infrared ion Spectroscopy: Peptides and PTMs;** Amanda Patrick; Corey Stedwell; Nicolas Polfer; *University of Florida, Gainesville, FL*
- ThP 228 **189 High-Confidence Static and Dynamic Phosphorylation Sites Identified within a Virus Particle;** Jacob Matson<sup>2</sup>; Tuan Ngo<sup>1</sup>; Wayne Chou<sup>1</sup>; Paul Gershon<sup>1</sup>; <sup>1</sup>*UC-Irvine, Irvine, CA*; <sup>2</sup>*University of North Carolina, Chapel Hill, NC*
- ThP 229 **Identification of Viral Phosphorylation in Human Immunodeficiency Viruses;** Hung Trinh<sup>1,2</sup>; David Colquhoun<sup>1</sup>; David Graham<sup>1</sup>; Mangala Rao<sup>3</sup>; <sup>1</sup>*School of Medicine, Johns Hopkins University, Baltimore, MD*; <sup>2</sup>*USMHRP, Henry M Jackson Foundation, Bethesda, MD*; <sup>3</sup>*USMHRP, Walter Reed Army Institute of Research, Silver Spring, MD*
- ThP 230 **A Universal Chemical Enrichment Method for Mapping Protein N-glycosylation;** Weixuan Chen; Johanna Smeeckens; Ronghu Wu; *Georgia Institute of Technology, Atlanta, GA*
- ThP 231 **Factors that Contribute to the Complexity of Glycopeptide Analysis – besides Site-Specific Heterogeneity;** Zsuzsa Darula<sup>1</sup>; Katalin F. Medzihradzsky<sup>1,2</sup>; <sup>1</sup>*Biological Research Centre HAS, Szeged, Hungary*; <sup>2</sup>*UCSF, San Francisco, CA*
- ThP 232 **Site-specific N-linked Glycoproteomics Analysis by Nano-LC Tandem Mass Spectrometry and Spectral Library Searching;** Pei-Jing Pai; Yingwei Hu; Henry Lam; *The Hong Kong University of Science & Technology, Clear Water Bay, Hong Kong*
- ThP 233 **Developing Online LWAC-IM-MS Method for Rapid Screening and Characterization of Glycopeptides;** Feifei Zhu; Jonathan Trinidad; David Clemmer; *Indiana University, Bloomington, IN*
- ThP 234 **Targeted LC-MS/MS Analysis of a Mycobacterial O-Glycopeptide by Low-Energy CID and ETD Fragmentation;** Lisa M. Wolfe<sup>1,2</sup>; Helene Cardasis<sup>3</sup>; Karen Dobos<sup>1</sup>; Jessica Prenni<sup>1,2</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*Proteomics & Metabolomics Facility, Fort Collins, CO*; <sup>3</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 235 **Characterization of Polyubiquitin Chains: Building a Foundation for Reading the Ubiquitin Code;** Amanda Lee<sup>1</sup>; Carlos Castaneda<sup>1</sup>; Rajesh Singh<sup>1</sup>; Yan Wang<sup>1</sup>; Nathan J. Edwards<sup>2</sup>; David Fushman<sup>1</sup>; Catherine Fenselau<sup>1</sup>; <sup>1</sup>*University of Maryland, College Park, MD*; <sup>2</sup>*Georgetown University Medical Center, Washington, DC*
- ThP 236 **Defining the Yeast E2 Enzyme Specific Ubiquitin Landscape;** Danielle Swaney; Judit Villen; *University of Washington, Seattle, WA*
- ThP 237 **A Heavy Labelled Synthetic Ubiquitinated Histone Peptide Library for Epigenetic Investigations;** Samuel Wein; Kelly Karch; Benjamin A Garcia; *University of Pennsylvania, Philadelphia, PA*
- ThP 238 **Unraveling the Ubiquitome of the Mouse Testis;** Xuejiang Guo; Yueshuai Guo; Tao Zhou; Zuomin Zhou; Jiahao Sha; *Nanjing Medical University, Nanjing, China*
- ThP 239 **A Quantitative Proteomics and Ubiquitinomics Investigation into Proteasome Malfunctioning;** Karen Sap; Karel Bezstarosti; Dick Dekkers; Olaf Voets; Erikjan Rijkers; Peter Verrijzer; Jeroen Demmers; *Erasmus University Medical Center, Rotterdam, Netherlands*
- ThP 240 **Methods for the Comprehensive Analysis of Ubiquitin-Modified Proteins in Yeast;** Tanya Porras-Yakushi; Michael J Sweredoski; Sonja Hess; *Caltech, Pasadena, CA*
- ThP 241 **Proteome-wide Identification of Sites of SUMO Modification;** Triin Tammsalu<sup>1</sup>; Ivan Matic<sup>2</sup>; Ellis G. Jaffray<sup>1</sup>; Adel Ibrahim<sup>1</sup>; Michael H. Tatham<sup>1</sup>; Ronald T. Hay<sup>1</sup>; <sup>1</sup>*University of Dundee, Dundee, UK*; <sup>2</sup>*Max Planck Institute for Biology of Ageing, Cologne, Germany*
- ThP 242 **CESI-MS for Monitoring Histone H4 Citrullination;** Bettina Sarg<sup>1</sup>; Klaus Faserl<sup>1</sup>; Verena Maurer<sup>2</sup>; Nicolas Singewald<sup>2</sup>; Herbert H. Lindner<sup>1</sup>; <sup>1</sup>*Div. of Clin. Biochemistry, Biocenter Innsbruck, Innsbruck, Austria*; <sup>2</sup>*Department of Pharmacology and Toxicology, Insttit, Innsbruck, Austria*
- ThP 243 **Proteomic Analysis of Arginine Methylation Sites in Human Cells Reveals Dynamic Regulation during Transcriptional Arrest and DNA Damage;** Kathrine Sylvestersen; Heiko Horn; Stephanie Jungmichel; Lars Juhl Jensen; Michael Lund Nielsen; *NNF Center for Protein Research, Copenhagen N, Denmark*
- ThP 244 **Identification of Functional Arginine Residues of Proteins by Selective Chemical Labeling and Mass Spectrometry;** Maheshika Wanigasekara; Ruchika Bhawal; Saiful Chowdhury; *University of Texas at Arlington, Arlington, TX*
- ThP 245 **A Novel Method for Large-Scale Profiling of Prenylated Peptides by Tandem Mass Spectrometry;** Ruchika Bhawal; Saiful Chowdhury; *University of Texas at Arlington, Arlington, TX*

- ThP 246 **High Resolution MS Confirms the Presence of a Hydroxyproline (Hyp) PTM in a G4P linker of an Fc-Fusion Protein**; Christopher S. Spahr; John O. Hui; John H. Robinson; Brian D. Soriano; Gunasekaran Kannan; Stone D. H. Shi; Amgen, Thousand Oaks, CA
- ThP 247 **Variable Carboxylation of Osteocalcin in Human Bone**; Timothy P. Cleland<sup>1</sup>; Corinne Thomas<sup>1</sup>; Caren M. Gundberg<sup>2</sup>; Deepak Vashishth<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute, Troy, NY; <sup>2</sup>Yale University, New Haven, CT
- ThP 248 **Methionine to Homoserine Conversion in the Heat Shock Cognate 71 kDa Protein in Human Cancer Cell Lines**; Alexey Chernobrovkin<sup>1</sup>; Arthur Kopylov<sup>2</sup>; Mikhail Pyatnitsky<sup>2</sup>; Ksenia Kuznetsova<sup>2</sup>; Victor Zgodina<sup>2</sup>; Andrey Lisitsa<sup>2</sup>; Sergei Moshkovskii<sup>2,3</sup>; <sup>1</sup>Karolinska Institute, Stockholm, Sweden; <sup>2</sup>Orekhovich Institute of Biomedical Chemistry, Moscow, Russia; <sup>3</sup>Pirogov Russian National Research Medical University, Moscow, Russia
- ThP 249 **Proteomics Studies of Allergic Contact Dermatitis: Qualitative and Quantitative Analysis of Skin Protein Haptension**; Erika Parkinson<sup>1,2</sup>; Maja Aleksic<sup>3</sup>; Richard Cubberley<sup>3</sup>; Paul Skipp<sup>1,2</sup>; <sup>1</sup>Centre for Proteomic Research, Uni of Southampton, Southampton, UK; <sup>2</sup>Centre for Biological Sciences, Uni of Southampton, Southampton, UK; <sup>3</sup>Safety & Environmental Assurance Centre, Unilever, Colworth Science Park, Sharnbrook, UK
- Proteomics: Plasma, 250 - 261**
- ThP 250 **Comparative Analysis of Protein Profiles of Major Human Biofluids**; Elke Hammer; Nico Jehmlich; Vishnu Dhople; Martin Feig; Claudia Schurmann; Julia Bischof; Manuela Gesell Salazar; Annette Murr; Uwe Völker; *University Medicine Greifswald, Greifswald, GERMANY*
- ThP 251 **Intact Stable Isotope Labeled Plasma Proteins from the SILAC-labeled HepG2 Secretome**; Adam Hawkridge; John Mangrum; *Virginia Commonwealth University, Richmond, VA*
- ThP 252 **MRM-based Quantitation of a Broad Panel of Disease-linked Proteins in Mouse Plasma**; Andrew Percy<sup>1</sup>; Jessica Tamura-Wells<sup>1</sup>; Juncong Yang<sup>1</sup>; Joel Nyberg<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 253 **High Quantification Efficiency in Plasma Targeted Proteomics with a Full-Capability Discovery Q-TOF Platform**; Stephanie Kaspar<sup>1</sup>; Pierre-Olivier Schmit<sup>2</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik, Bremen, Germany; <sup>2</sup>Bruker Daltonique S.A., Wissembourg, France
- ThP 254 **Targeted Proteomics Applied to Biomarker Verification for Lung Cancer Diagnostics**; Yeoun Jin Kim<sup>1</sup>; Katriina Sertamo<sup>1</sup>; Marie-Aline Pierrard<sup>1</sup>; Sebastien Gallien<sup>1</sup>; Sang-Yoon Kim<sup>1</sup>; Suruchi Gutgutia<sup>1</sup>; Guy Berchem<sup>2</sup>; Bruno Domon<sup>1</sup>; <sup>1</sup>Luxembourg Clinical Proteomics Center, Strassen, Luxembourg; <sup>2</sup>CRP-Santé, Strassen, Luxembourg
- ThP 255 **A Comprehensive and Scalable Automated Proteomic Workflow: When Large Human Clinical Discovery Study Meets Throughput and Robustness**; Loïc Davon<sup>1</sup>; Antonio Núñez Galindo<sup>1</sup>; John Corthésy<sup>1</sup>; Ornella Cominetti<sup>1</sup>; Martin Kussmann<sup>1,2</sup>; <sup>1</sup>Nestlé Institute of Health Sciences, Lausanne, Switzerland; <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
- ThP 256 **Data dependent Versus Data independent acquisition applied to samples of different protein dynamic range**; Nicolas Smargiasso<sup>1</sup>; Gabriel Mazzucchelli<sup>1</sup>; Dominique Baiwir<sup>1</sup>; Edouard Louis<sup>2</sup>; Florence Quesada-Calvo<sup>1</sup>; Marie-Alice Meuwis<sup>2</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>Univeristy of Liege, MS Lab - GIGA, Liege, Belgium; <sup>2</sup>Department of Gastroenterology, CHU, GIGA-R, Liege, Belgium
- ThP 257 **Establishing the Heritability Dimension of Human Plasma Proteome via SWATH Mass Spectrometry and a Twin Strategy**; Yansheng Liu<sup>1</sup>; Alfonso Buil<sup>2</sup>; Ben Collins<sup>1</sup>; Ludovic CJ Gillet<sup>1</sup>; Lorenz Blum<sup>1</sup>; Tim D Spector<sup>3</sup>; Lin-Yang Cheng<sup>4</sup>; Olga Vitek<sup>4</sup>; Ruedi Aebersold<sup>1,5</sup>; <sup>1</sup>Institute of Molecular Systems Biology ETH Zurich, Zurich, Switzerland; <sup>2</sup>University of Geneva Medical School, Geneva, Switzerland; <sup>3</sup>King's College London, London, UK; <sup>4</sup>Purdue University, West Lafayette IN; <sup>5</sup>Faculty of Science University of Zurich, Zurich, Switzerland
- ThP 258 **Depletion of Abundant Plasma Proteins by Hydrogel Particles for Detection of Low Abundance Proteins by LC-MS/MS**; Estela Ventura-Espejo; Gerard Such-Sanmartin; Ole Jensen; *University of Southern Denmark, Odense, Denmark*
- ThP 259 **Evaluation of Protein Levels in Serum after Combinatorial Peptide Ligand Library (CPLL) Treatment**; Jin Ren<sup>1</sup>; Ran An<sup>2</sup>; Chengsi Huang<sup>2</sup>; Yun Zhang<sup>2</sup>; Vicki Wysocki<sup>2</sup>; <sup>1</sup>Thomas Jefferson University, Philly, PA; <sup>2</sup>The Ohio State University, Columbus, OH
- ThP 260 **Comparison of Column and High-Throughput 96 Well Filter Plate Formats for Plasma Immunodepletion**; Henry Duewel; Kevin Ray; Tom Juehne; Gordon Nicol; Lillian Vickery; David Rhee; *Sigma-Aldrich Corp., St. Louis, MO*
- ThP 261 **Electrophoretic Enrichment and Prefractionation of Low Molecular Weight Proteins Derived from Plasma through Precipitation, SDS Solubilization and GELFREE Separation**; Andrew Crowell; Alan Doucette; *Department of Chemistry, Dalhousie University, Halifax, Canada*
- Proteomics: Clinical Applications, 262 - 288**
- ThP 262 **Development of an Immuno-MALDI (iMALDI) Assay for Brain Natriuretic Peptide (BNP) in Human Plasma**; David Lin<sup>1</sup>; Robert Popp<sup>1</sup>; Andrew Chambers<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 263 **Optimization of Protein Identification from Schirmer's Tear Test Strips Using Different Extraction, Digestion and Fractionation Methods**; Liwen Zhang; Jeremy Keirse; Kari Green; *Ohio State University, Columbus, OH*
- ThP 264 **Proteomic Analysis of formalin-Fixed, Paraffin-Embedded Liver Tissues using LC-MS/MS**; Xianyin Lai; *Indiana University School of Medicine, Indianapolis, IN*
- ThP 265 **A Novel Method of Immunoglobulin Alpha Isolation by HPLC Affinity Purification**; Joseph J. Otto; Jana D. Rocker; Lewis K. Pannell; *U. of South Alabama Mitchell Cancer Institute, Mobile, AL*
- ThP 266 **Development of an LC-MRM based Assay of prostate Specific Antigen (PSA) in Human Blood**; Maurizio Splendore; Paul Shei; Milady Ninonuevo; Robert Maxwell; Desmond Kaplan; *Bruker Daltonics, inc., Fremont, CA*
- ThP 267 **Development and Translation of a Targeted Assay to Detect Aspiration Across a Clinical Cohort**; Laura Dubois<sup>1</sup>; J. Will Thompson<sup>1</sup>; William Parke<sup>2</sup>; Shu Lin<sup>2</sup>; R. Duane Davis<sup>2</sup>; Sassan Azad<sup>3</sup>; Shaf Keshavjee<sup>3</sup>; Arthur Moseley<sup>1</sup>; <sup>1</sup>Duke University School of Medicine, Durham, NC; <sup>2</sup>Duke Department of Surgery, Durham, NC; <sup>3</sup>Toronto Lung Transplant Program, Toronto, Canada
- ThP 268 **Development of a Reference Measurement System for Urinary Albumin**; Ashley Beasley-Green; David Bunk; Karen Phinney; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 269 **Adductomics Analysis of Human Serum Albumin by Mass spectrometry**; Lu Deng<sup>1,2</sup>; Rupasri Mandal<sup>1,2</sup>; David Wishart<sup>1,2</sup>; <sup>1</sup>The Metabolomics Innovation Centre, Edmonton, AB; <sup>2</sup>University of Alberta, Edmonton, Canada

- ThP 270 **Quantification of Mucins in Sputum by Targeted Mass Spectrometry and Stable Isotope Dilution;** Rui Cao; Amina Ford; Giorgia Radicioni; Tiffany Wang; Yuanli Li; Mehmet Kesimer; *University of North Carolina, Chapel Hill, NC*
- ThP 271 **Normal Prion Protein in *Drosophila* Enhances the Toxicity of Pathogenic Polyglutamine Proteins;** Jong Bok Seo<sup>1</sup>; Eunjung Bang<sup>1</sup>; Young Ho Koh<sup>2</sup>; <sup>1</sup>*Korea Basic Science Institute, Seoul, South Korea*; <sup>2</sup>*Ilsong Institute of Life Science, Hallym University, Anyang, South Korea*
- ThP 272 **QC Metrics Fulfill Regulatory Need for Clinical Laboratory;** Surendra Dasari; Jason D Theis; Roman Zenka; Julie A Vrana; Paul J Kurtin; *Mayo Clinic, Rochester, MN*
- ThP 273 **Mass Spectrometry Approaches to Investigating HIV-1 Sequence Variance;** Ceereena Ubaida Mohien; Ravi Tharakan; David Graham; *Johns Hopkins University, Baltimore, MD*
- ThP 274 **Exploring Resistance to Targeted Therapies Through Pathway-Level Proteomics;** Lauren C. Keilich<sup>1</sup>; Andrew J. Phillips<sup>1</sup>; Katerina Politi<sup>2</sup>; Xiaoling Song<sup>2</sup>; Brad J. Williams<sup>3</sup>; Scott J. Geromanos<sup>3</sup>; Dustin Yaworsky<sup>3</sup>; Stuart Welling<sup>3</sup>; <sup>1</sup>*Department of Chemistry, Yale University, New Haven, CT*; <sup>2</sup>*Department of Pathology, Yale Medical School, New Haven, CT*; <sup>3</sup>*Waters Corporation, Milford, CT*
- ThP 275 **Temporal Phosphoproteomic Study on Estrogen Receptor-Dependent Cytotoxicity in Renal Cell Carcinoma;** Wei-Chi Ku<sup>1</sup>; Zhi-Yu Liu<sup>1,2</sup>; Chi-Jung Huang<sup>1,3</sup>; Kuo-Chiang Chen<sup>3</sup>; Yen-Chieh Wang<sup>3</sup>; Shao-Kuan Chen<sup>3</sup>; Chih-Ming Lin<sup>3</sup>; <sup>1</sup>*Fu Jen Catholic University, New Taipei, Taiwan*; <sup>2</sup>*National Taiwan University, Taipei, Taiwan*; <sup>3</sup>*Cathay General Hospital, Taipei, Taiwan*
- ThP 276 **Comprehensive Proteomic Analysis of Cisplatin Sensitive and Resistant Epithelial Ovarian Cancer Tumor Cells Guided by Transcriptomics;** Elizabeth Nguyen<sup>1</sup>; Kaisa Huhtinen<sup>1</sup>; Youngah Goo<sup>2</sup>; Jussi Salmi<sup>1</sup>; Riika Lund<sup>1</sup>; Robert Moulder<sup>1</sup>; Olli Carpen<sup>1</sup>; Riita Lahesmaa<sup>1</sup>; David Goodlett<sup>2</sup>; <sup>1</sup>*Turku Centre for Biotechnology, Turku, Finland*; <sup>2</sup>*University of Maryland, Baltimore, MD*
- ThP 277 **Towards Mass Spectrometric Profiling of Urinary Bladder Cancer—Optimization of sample Preparation, Protein Extract Generation, In-Solution Digestion, and nanoESI-IMS-MSe Analysis;** Cornelia Kov<sup>1</sup>; Gargee Mukherjee<sup>1</sup>; Claudia Roewer<sup>1</sup>; Samantha Wickramasekara<sup>2</sup>; Claudia S. Maier<sup>2</sup>; Chris Protzel<sup>3</sup>; Oliver Hakenberg<sup>3</sup>; Michael O. Glocker<sup>1</sup>; <sup>1</sup>*Proteome Center Rostock, Rostock, Germany*; <sup>2</sup>*Department of Chemistry, Oregon State University, Corvallis, OR*; <sup>3</sup>*Urology Clinic and Polyclinic, University Medicine, Rostock, Germany*
- ThP 278 **Proteomic Analysis of Plasmodium Berghei Hepatic Stage Merosomes;** Raja Sekhar Nirujogi<sup>1,4</sup>; Satish Mishra<sup>2</sup>; Photini Sinnis<sup>3</sup>; Akhilesh Pandey<sup>4</sup>; <sup>1</sup>*Institute of Bioinformatics, Bangalore, India*; <sup>2</sup>*Central Drug Research Institute, Lucknow, UP, India*; <sup>3</sup>*JHMRI, Johns Hopkins University, Baltimore, MD*; <sup>4</sup>*Johns Hopkins University School of Medicine, Baltimore, MD*
- ThP 279 **Effect of Statins on the Proteome of Human Pancreatic Stellate Cells;** Nerea Cuevas Polo<sup>1</sup>; Kevin Broadbelt<sup>1</sup>; Darwin Conwell<sup>2</sup>; Hanno Steen<sup>1</sup>; <sup>1</sup>*Harvard Medical School/Children's Hospital Boston, Boston, MA*; <sup>2</sup>*Ohio State University Wexner Medical Center, Ohio, OH*
- ThP 280 **A Comprehensive Tumor Tissue Analysis in Glioblastoma: Towards Understanding the Pathophysiology of Tumor Progression;** Vadhiraja B. Bhat<sup>1</sup>; Maxime S. Heroux<sup>2</sup>; Marla A. Chesnik<sup>2</sup>; Mona Al-Gizawi<sup>2</sup>; Shama P. Mirza<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Wilmington, DE*; <sup>2</sup>*Medical College of Wisconsin, Milwaukee, WI*
- ThP 281 **Quantitative Profiling of protein Tyrosine Kinases In Human Cancer Cell Lines by Multiplexed Parallel Reaction Monitoring Assays;** Hye-Jung Kim<sup>1,2</sup>; Ming Li<sup>3</sup>; Daniel C. Liebler<sup>1,2</sup>; <sup>1</sup>*Department of Biochemistry, Vanderbilt University, Nashville, TN*; <sup>2</sup>*Jim Ayers Institute, Vanderbilt-Ingram Center, Nashville, TN*; <sup>3</sup>*Department of Biostatistics, Vanderbilt University, Nashville, TN*
- ThP 282 **Quantitative Analysis of the Synaptic Proteome in the Nucleus Accumbens in Schizophrenia;** Suhong Zhang<sup>1</sup>; Stephanie Willard<sup>1</sup>; Warren Bilker<sup>2</sup>; Karin Borgmann-Winter<sup>1,3</sup>; Chang-Gyu Hahn<sup>1</sup>; <sup>1</sup>*Univ of Pennsylvania Dept of Psychiatry, Philadelphia, PA*; <sup>2</sup>*Univ of Penn Dept of Biostatistics and Epidemiology, Philadelphia, PA*; <sup>3</sup>*Children's Hospital of Philadelphia, Philadelphia, PA*
- ThP 283 **96FASP is a High Throughput Approach for Quantitative Clinical Proteomics;** Yanbao Yu; Moo-Jin Suh; Patricia Sikorski; Keehwan Kwon; Karen Nelson; Rembert Pieper; *J. Craig Venter Institute, Rockville, MD*
- ThP 284 **Urinary Proteomics in the Discovery of Candidate Protein Biomarkers in Type 1 Diabetes Cohort;** Moo-Jin Suh; Yanbao Yu; Karen Nelson; Ramana Madupu; Rembert Pieper; *J. Craig Venter Institute, Rockville, MD*
- ThP 285 **Development and Validation of an Analytical Method for Discovery of Biomarkers of Preterm Birth;** Tracey C. Fleischer; Chad L. Bradford; Ashoka D. Polpitiya; Jeff S. Flick; Trina Pugmire; Robert D. Severinsen; Ilia Ichetovkin; Durlin Hickok; J. Jay Boniface; *Sera Prognostics, Salt Lake City, UT*
- ThP 286 **Development of Multiplex Biomarker Analysis Approach for the Diagnosis of Transitional Cell Carcinoma from Canine Urine Proteome;** Samanthi I Wickramasekara<sup>1</sup>; Shay Bracha<sup>1</sup>; Michael McNamara<sup>2</sup>; Ian Hilgart<sup>1</sup>; Marcus Weinman<sup>1</sup>; Milan Milavancev<sup>1</sup>; Jan Medlock<sup>1</sup>; Claudia Maier<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*Providence Portland Medical Center, Portland, OR*
- ThP 287 **Evaluation of SWATH™ as a Diagnostic Tool for Bacterial Identification Using a Strain's Specific Library;** Sylvie Bourassa<sup>1</sup>; Isabelle Kelly<sup>1</sup>; Frederic Fournier<sup>1</sup>; Benjamin Nehme<sup>1</sup>; Daniel Defoy<sup>1</sup>; Brigitte Simons<sup>2</sup>; Maurice Boissinot<sup>3</sup>; Michel Bergeron<sup>3</sup>; Arnaud Droit<sup>1,4</sup>; <sup>1</sup>*Proteomics, CHU de Quebec Research Center, Quebec, Canada*; <sup>2</sup>*AB SCIEX, Concord, ON*; <sup>3</sup>*Infectiology, CHU de Quebec Research Center, Quebec, Qc*; <sup>4</sup>*Molecular Medicine, Laval University, Quebec, Qc*
- ThP 288 **Multivariate Statistical Procedures Implemented within the Framework of Statistical Process Control to Evaluate Data Quality in LC MS/MS;** Michael Bereman; Gina Hilton; Emily Griffith; *North Carolina State University, Raleigh, NC*

## Proteomics: Tissue, 289 - 314

- ThP 289 **Proteomic Comparison among CD133+ and CD133- Population in Colorectal Cancer and Normal Colon Epithelium;** Smathorn Thakolwiboon<sup>1,2</sup>; Jianhui Zhu<sup>1</sup>; David M. Lubman<sup>1</sup>; <sup>1</sup>*University of Michigan Medical Center, Ann Arbor, MI*; <sup>2</sup>*Faculty of Medicine Siriraj Hospital, Mahidol Univ, Bangkok, Thailand*
- ThP 290 **Classification of Breast Cancer Sub-types with Site-Specific Phosphorylation Changes;** Harsha P. Gunawardena<sup>1</sup>; Jonathon O'Brien<sup>2</sup>; John A. Wrobel<sup>1</sup>; Ling Xie<sup>1</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>*Biochemistry & Biophysics, School of Medicine, UNC-Chapel Hill, NC*; <sup>2</sup>*Biostatistics, Gillings School of Public Health, UNC-Chapel Hill, NC*
- ThP 291 **Comparative Tissue Proteomics of Microdissected Specimens for Biomarker Discover of Bladder Cancer;** Yi-Ting Chen<sup>1</sup>; Chien-Lun Chen<sup>2</sup>; Ting Chung<sup>1</sup>; Chih-Ching Wu<sup>1</sup>; Jau-Song Yu<sup>1</sup>; Yu-Sun Chang<sup>1</sup>; *Chang Gung*



- University, Taoyuan, Taiwan; <sup>2</sup>Department of Urology, Chang Gung Memorial Hospital, Taoyuan, Taiwan
- ThP 292 **Retrospective Label-Free Characterization of Androgen-Regulated Prostate Cancer Associated Proteins from Murine Formalin Fixed Paraffin Embedded Tissue Sections;** Owen E. Branson<sup>1,2</sup>; Jennifer M. Thomas-Ahner<sup>2</sup>; Steven K. Clinton<sup>2</sup>; Michael A. Freitas<sup>1,2</sup>; <sup>1</sup>The Ohio State Biochemistry Program, Columbus, OH; <sup>2</sup>The Ohio State University Wexner Medical Center, Columbus, OH
- ThP 293 **Extracellular Matrix Proteome in Colorectal Cancer;** Cinzia Magagnotti<sup>1</sup>; Luca Genovese<sup>1</sup>; Manuela Nebuloni<sup>2</sup>; Massimo Alfano<sup>1</sup>; Annapaola Andolfo<sup>1</sup>; <sup>1</sup>San Raffaele Scientific Institute, Milan, Italy; <sup>2</sup>University of Milan, Milan, Italy
- ThP 294 **Proteomics Profiling of Pancreatic Patient Tumors and Their Xenografts: a Case Study;** Bingwen Lu<sup>1</sup>; Camino Menendez<sup>3</sup>; Pedro P. Lopez-Casas<sup>3</sup>; Peter Olson<sup>1</sup>; David Shields<sup>2</sup>; Manuel Hidalgo<sup>3</sup>; Jeremy Myers<sup>1</sup>; Kim Arndt<sup>1</sup>; <sup>1</sup>Pfizer, Pearl River, NY; <sup>2</sup>Pfizer, La Jolla, CA; <sup>3</sup>Spanish National Cancer Research Center, Madrid, SP
- ThP 295 **Toward the Elucidation of Changes in Protein Ubiquitylation Correlating with Ovarian Cancer BRCA1 Clinical Subtypes;** Stefani Thomas<sup>1</sup>; Ie-Ming Shih<sup>1</sup>; Douglas Levine<sup>2</sup>; Zhen Zhang<sup>1</sup>; Daniel Chan<sup>1</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Memorial Sloan Kettering Cancer Center, New York, NY
- ThP 296 **Two-Dimensional Liquid Chromatography Coupled to Mass Spectrometry for Proteomic Profiling of Paraffin Embedded Lung Tumor Tissues;** Nilini Ranbaduge; Ferdinando Cerciello; Joseph Amann; David Carbone; Vicki Wysocki; *The Ohio State University, Columbus, OH*
- ThP 297 **Stretch-Induced Proteomic Changes in Vascular Smooth Muscle Cells of Rat Portal Vein in Vivo;** Rui Zhu<sup>1</sup>; Amani Al Outa<sup>2</sup>; Zein Farhat<sup>2</sup>; Firas Kobeissy<sup>2</sup>; Ramzi Sabra<sup>2</sup>; Asad Zeidan<sup>2</sup>; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX; <sup>2</sup>American University of Beirut, Beirut, Lebanon
- ThP 298 **Age-Dependent Changes of Protein Expressions in Caenorhabditis elegans;** Krishna Vukoti; Masaru Miyagi; *Case Western Reserve University, Cleveland, OH*
- ThP 300 **Proteomic Analyses of Aortas Reveal Conserved Protein Abundance Changes Associated with Aging in Monkeys and Rats;** Zongming Fu<sup>1</sup>; Mingyi Wang<sup>2</sup>; Eric Grote<sup>1</sup>; Jing Zhang<sup>2</sup>; Vidya Venkatraman<sup>1</sup>; Xiaoqian Liu<sup>1</sup>; Pingbo Zhang<sup>1</sup>; Allen Everett<sup>1</sup>; Edward Lakatta<sup>2</sup>; Jennifer Van Eyk<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Laboratory of Cardiovascular Science, NIA, NIH, Baltimore, MD
- ThP 301 **Direct Monitoring of Cerebellar Phosphorylation Dynamics in a Kinase Knockout Mouse;** Eleonora Corradini<sup>1,2</sup>; Raghavan Vallur<sup>3,4</sup>; Linsey M. Raaijmakers<sup>1,2</sup>; Susanne Feil<sup>3</sup>; Robert Feil<sup>3</sup>; Albert J. R. Heck<sup>1,2</sup>; Arjen Scholten<sup>1,2</sup>; <sup>1</sup>Utrecht University, Utrecht, The Netherlands; <sup>2</sup>Netherlands Proteomics Centre, Utrecht, The Netherlands; <sup>3</sup>University of Tübingen, Tübingen, Germany; <sup>4</sup>German Center for Neurodegenerative diseases, Tübingen, Germany
- ThP 302 **DiART Tandem Mass Spectrometric Analysis Reveals Anti-Oxidant Signaling of Elderberry and Sutherlandia against Transient Cerebral Ischemia in Mice;** Hui Zhou<sup>1,2</sup>; Zhe Qu<sup>1,2</sup>; Jiankun Cui<sup>1,2</sup>; Agnes Simonyi<sup>2,3</sup>; Jilong Li<sup>4</sup>; Shuwei Li<sup>8</sup>; Victoria A. Engel<sup>1,2</sup>; Shanyan Chen<sup>1,2</sup>; Jianlin Cheng<sup>4</sup>; C. Michael Greenleaf<sup>6</sup>; Andrew L. Thomas<sup>6</sup>; Kevin L. Fritsche<sup>7</sup>; William R. Folk<sup>3</sup>; Dennis B. Lubahn<sup>3,7</sup>; Grace Y. Sun<sup>2,3</sup>; Zezong Gu<sup>1,2</sup>; <sup>1</sup>University of Missouri School of Medicine Pathology, Columbia, MO; <sup>2</sup>MU SOM Center for Translational Neuroscience, Columbia, MO; <sup>3</sup>University of Missouri School of Medicine Biochem, Columbia, MO; <sup>4</sup>University of Missouri Computer Sci., Informatics, Columbia, MO; <sup>5</sup>University of Missouri Department of Chemistry, Columbia, MO; <sup>6</sup>University of Missouri Southwest Res. Center, Columbia, MO; <sup>7</sup>University of Missouri Division of Animal Sciences, Columbia, MO; <sup>8</sup>University of Maryland Chemistry and Biochemistry, College Park, MD
- ThP 303 **Proteomic Profiling of Pig Colon Mucosa to Study the Effect of Consuming Anthocyanin-Rich Purple-fleshed Potatoes;** Sridhar Radhakrishnan<sup>1,2</sup>; Vadiraja Bhat<sup>3</sup>; Sungwoo Kim<sup>4</sup>; Andrey Ptitsyn<sup>5</sup>; Lavanya Reddivari<sup>6</sup>; Jairam Vanamala<sup>2</sup>; <sup>1</sup>Colorado State University, Fort Collins, Colorado; <sup>2</sup>Food Science, Penn State University, University Park, PA; <sup>3</sup>Agilent Technologies, Wilmington, DE; <sup>4</sup>Animal Science, North Carolina State University, Raleigh, North Carolina; <sup>5</sup>Sidra Medical and Research Center, Doha, Qatar; <sup>6</sup>Plant Science, Penn State University, State College, PA
- ThP 304 **Comparative Proteomic Analysis of Carbonylated Proteins from the Striatum and Cortex of Pesticide Treated Mice;** Christina Coughlan<sup>1</sup>; Douglas Walker<sup>2</sup>; Kelly Lohr<sup>3</sup>; Michael Caudle<sup>3</sup>; Kristofer Fritz<sup>1</sup>; James Roede<sup>1</sup>; <sup>1</sup>University of Colorado Anschutz Medical Campus, Aurora, CO; <sup>2</sup>Tufts University, Medford, MA; <sup>3</sup>Emory University, Atlanta, GA
- ThP 305 **Liver Proteome Analysis Suggests Altered Lipid Metabolism in Alzheimer's Disease;** Adam Evans; Renā Robinson; *University of Pittsburgh, Department of Chemistry, Pittsburgh, Pa*
- ThP 306 **Multi-platform Data Integration of the Cerebral Cortex Proteome in Rodent Models of Fear Conditioning and Repetitive Blast;** Angela M. Boutte<sup>1</sup>; Joy Guingab-Cagmat<sup>2</sup>; Eric Mauldin-Jeronimo<sup>3</sup>; Larry P. Simmons<sup>1</sup>; Stephen T. Ahlers<sup>3</sup>; Raymond F. Genovese<sup>1</sup>; Frank C. Tortella<sup>1</sup>; Kara E. Schmid<sup>1</sup>; Jitendra R. Dave<sup>1</sup>; <sup>1</sup>Walter Reed Army Institute of Research, Silver Spring, MD; <sup>2</sup>Banyan Biomarkers, Inc., Alachua, FL; <sup>3</sup>Naval Medical Research Center, Silver Spring, MD
- ThP 307 **Proteomic Analysis of Liver in Rats with lead Exposure and Iron-Supplemented;** Mileni Silva Fernandes<sup>2</sup>; Aline Lima Leite<sup>2</sup>; Fernanda Zucki<sup>1</sup>; Lucas Ferreira Almeida<sup>1</sup>; Marília Afonso Rabelo Buzalaf<sup>1</sup>; <sup>1</sup>USP-FOB, Bauru, BRAZIL; <sup>2</sup>Federal University of São Carlos, São Carlos, SP
- ThP 308 **Proteomic MS analysis of FASP-Processed FFPE Leptomeningeal Amyloid Brain Tissue Identifies Transthyretin Where Immunohistochemical Staining Fails;** Anna Okumu<sup>1</sup>; Michael Greicius<sup>2</sup>; Edward Plowey<sup>3</sup>; Yuxi Wu<sup>1</sup>; Allis Chien<sup>1</sup>; Chris Adams<sup>1</sup>; <sup>1</sup>Stanford University Mass Spectrometry, Stanford, CA; <sup>2</sup>Dept of Neurology, Stanford Univ. Sch. of Medicine, Stanford, CA; <sup>3</sup>Dept of Pathology, Stanford Univ. Sch. of Medicine, Stanford, CA
- ThP 309 **Identification of Toluene Diisocyanate-Conjugated Murine Protein Targets following Dermal Exposures;** Justin M. Hettick; Ajay P. Nayak; Carrie M. Long; Stacey E. Anderson; Paul D. Siegel; *NIOSH, Morgantown, WV*
- ThP 310 **Novel Proteogenomic Analysis Establishes the Sea Star *Patiria miniata* as a New Systems Biology Model for Neuronal Regeneration;** Catarina Franco<sup>1,2</sup>; Michael Sweredoski<sup>2</sup>; Parul Kudtarkar<sup>3</sup>; R. Andrew Cameron<sup>3</sup>; Sonja Hess<sup>2</sup>; <sup>1</sup>Instituto de Tecnologia Química e Biológica, Oeiras, Portugal; <sup>2</sup>Proteome Exploration Laboratory, Caltech, Pasadena, CA; <sup>3</sup>Center for Computational Regulatory Genomics, Caltech, CA
- ThP 311 **In-Depth Proteomic Analysis of Human Substantia Nigra;** Chan-Hyun Na; *Johns Hopkins University School of Medicine, Baltimore, MD*

- ThP 312 **Comparative Proteome Analysis of Porcine Placenta between Small and Large Litter Size Groups;** Dong-Gi Lee<sup>1</sup>; Young-Moon Kang<sup>1,4</sup>; Sang-Je Park<sup>2</sup>; Hwa Chun Park<sup>3</sup>; Chul Wook Kim<sup>2</sup>; Jong-Soon Choi<sup>1,4</sup>; <sup>1</sup>*Korea Basic Science Institute, Daejeon, South Korea*; <sup>2</sup>*Gyeongnam National University of Science and Techn, Jinju, South Korea*; <sup>3</sup>*Dasan Genetics, Namwon, South Korea*; <sup>4</sup>*GRAS, Chungnam National University, Daejeon, South Korea*
- ThP 313 **Mass Spectrometry-based Proteomics of Human Induced Pluripotent Stem Cells (hiPSC) Cultured in Suboptimal Culture Conditions;** Melkamu Getie-Kebltie<sup>1</sup>; Natalia Pripuzova<sup>1</sup>; Christopher Grunseich<sup>2</sup>; Colin Sweeney<sup>3</sup>; Harry Malech<sup>3</sup>; Michail Alterman<sup>1</sup>; <sup>1</sup>*Division of Cell and Gene Therapy, CBER, FDA, Bethesda, MD*; <sup>2</sup>*Neurogenetics Branch, NINDS, NIH, Bethesda, MD*; <sup>3</sup>*Laboratory of Host Defenses, NIAID, NIH, Bethesda, MD*
- ThP 314 **Phosphoproteomic Analysis Reveals Regulatory Mechanisms at the Kidney Filtration Barrier;** Markus Rinschen<sup>1</sup>; Xiongwu Wu<sup>2</sup>; Tim König<sup>3</sup>; Trairak Pisitkun<sup>4</sup>; Bernard Brooks<sup>2</sup>; Pedro Beltrao<sup>5</sup>; Marcus Krüger<sup>6</sup>; Paul Brinkkötter<sup>1</sup>; Thomas Benzinger<sup>1</sup>; <sup>1</sup>*Internal Medicine II, University Hospital Cologne, Koeln, Germany*; <sup>2</sup>*NIH, NHLBI, Bethesda, MD*; <sup>3</sup>*CECAD, Cologne, Germany*; <sup>4</sup>*Chulalongkorn University, Bangkok, Thailand*; <sup>5</sup>*EMBL, EBI, Hinxton, Cambridge, UK*; <sup>6</sup>*MPI Bad Nauheim, Bad Nauheim, Germany*
- Proteomics: New Approaches, 315 - 336**
- ThP 315 **Short GeLC-SWATH: a Fast and reliable Quantitative Approach for Proteomic Screenings - Special Focus on Membrane Proteins;** Sandra Anjo<sup>1,2</sup>; Cátia Santa<sup>1</sup>; Bruno Manadas<sup>1,3</sup>; <sup>1</sup>*CNC - Center for Neuroscience and Cell Biology, Cantanhede, Portugal*; <sup>2</sup>*University of Coimbra, Coimbra, Portugal*; <sup>3</sup>*Biocant - Biotechnology Innovation Center, Cantanhede, Portugal*
- ThP 316 **Exploring Impact of Dynamic Accumulation for Improving MS/MS Quality of QqTOF Data;** Aaron Hudson<sup>1</sup>; Christie Hunter<sup>2</sup>; Sean L. Seymour<sup>3</sup>; Nic Bloomfield<sup>1</sup>; <sup>1</sup>*AB SCIEX, Framingham, MA*; <sup>2</sup>*AB SCIEX, Foster City, CA*; <sup>3</sup>*AB SCIEX, Redwood City, CA*
- ThP 317 **In-Depth Proteome Coverage by Iterative Data Dependent Acquisition on a Benchtop Orbitrap Mass Spectrometer;** Mathias Mueller; Tabiwang N. Arrey; Thomas Rietpietsch; Florian Grosse-Coosmann; Andreas Kuehn; Catharina Crone; Torsten Ueckert; Markus Kellmann; *Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*
- ThP 318 **Comparison of Data-Dependent Acquisition (DDA) and Data-Independent Acquisition (DIA) Strategies in Discovery and Label-Free Quantitation of a Complex Proteome;** Suresh Annangudi; David McCaskill; Jeffrey Gilbert; *Dow Agrosciences, Indianapolis, IN*
- ThP 319 **Examining the Proteomic Consequences of Aneuploidy in Yeast using a Multi-Notch MS3-method for Accurate Multiplexed Quantification with Isobaric Tags;** Noah E. Dephoure<sup>1</sup>; Eduardo Torres<sup>2</sup>; Steven Gygi<sup>3</sup>; <sup>1</sup>*Weill Cornell Medical College, New York, NY*; <sup>2</sup>*University of Massachusetts Medical School, Worcester, MA*; <sup>3</sup>*Harvard Medical School, Boston, MA*
- ThP 320 **MS<sup>3</sup>-based Quantitative Proteomics using Pulsed-Q Dissociation (PQD);** Zhiyun Cao; Adam R. Evans; Renā A. S. Robinson; *University of Pittsburgh, Pittsburgh, PA*
- ThP 321 **Performance Evaluation of a Fast Sequencing Quadrupole Orbitrap MS for Shotgun Proteomics;** Christian D. Kelstrup<sup>1</sup>; Tabiwang N. Array<sup>2</sup>; Rosa R. Jersie-Christensen<sup>1</sup>; Andreas Kuehn<sup>2</sup>; Markus Kellmann<sup>2</sup>; Jesper V. Olsen<sup>1</sup>; <sup>1</sup>*NNF Center for Protein Research, Copenhagen, Denmark*; <sup>2</sup>*Thermo Fisher Scientific, Bremen, Germany*
- ThP 322 **High Resolution Large-Scale Targeted Proteomics Using Intelligent Parallel Reaction Monitoring;** Sebastien Gallien; Sang-Yoon Kim; Bruno Doman; *Luxembourg Clinical Proteomics Center, Strassen, Luxembourg*
- ThP 323 **Expansion of Ion Library for Mining SWATH Data through Fractionation Proteomics;** Jin Zi<sup>1</sup>; Shenyang Zhang<sup>1</sup>; Ruo Zhou<sup>1</sup>; Baojin Zhou<sup>1</sup>; Guixue Hou<sup>1,2</sup>; Fengji Tan<sup>1</sup>; Bo Wen<sup>1</sup>; Quanhui Wang<sup>1,2</sup>; Liang Lin<sup>1</sup>; Siqi Liu<sup>1,2</sup>; <sup>1</sup>*Proteomics Division, BGI-Shenzhen, Shenzhen, China*; <sup>2</sup>*Beijing Institutes of Genomics, CAS, Beijing, China*
- ThP 324 **Evaluation of Data-Independent Acquisition (DIA) Approaches for Spiked Peptides in HeLa Digest on Q-OT-qIT Mass Spectrometer;** Wei Zhang<sup>1</sup>; Reiko Kiyonami<sup>2</sup>; Zheng Jiang<sup>1</sup>; Wei Chen<sup>1</sup>; <sup>1</sup>*ThermoFisher Scientific, Shanghai, CHINA*; <sup>2</sup>*ThermoFisher Scientific, San Jose, CA*
- ThP 325 **Captive Spray Ionization Facilitates Data Independent Acquisition - PACIFIC for Proteomics;** Young Ah Goo<sup>1</sup>; John Chapman<sup>2</sup>; Scott Edgar<sup>2</sup>; Bao Tran<sup>1</sup>; David Goodlett<sup>1</sup>; <sup>1</sup>*University of Maryland, Baltimore, MD*; <sup>2</sup>*University of Washington, Seattle, WA*
- ThP 326 **An Approach for Peptide Identification Combining DDA and DIA on a Q Exactive Plus Prototype with a High-Field Orbitrap;** Han-Yin Yang; Jarrett Egertson; Gennifer Merrihew; Michael J. Maccoss; *Univ of Washington, Seattle, WA*
- ThP 327 **NeuCode + SWATH = a Good Combination;** Alicia Richards; Catherine E. Minogue; Alex Hebert; Jarred W. Rensvold; Anna Merrill; Allison Balloon; Michael S. Westphall; Audrey P. Gasch; David J. Pagliarini; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- ThP 328 **Training Wheels and (Data) Independence for Top-Down Proteomics;** Aaron O. Bailey; David M. Horn; *Thermo Fisher Scientific, San Jose, CA*
- ThP 329 **Combination of DDA, DIA and Targeted Approaches for the Analysis of Protein-Metabolite Interactions using Proteolytic Probes and an Orbitrap Fusion;** Paolo Nanni<sup>1</sup>; Paul Boersema<sup>2</sup>; Yuehan Feng<sup>2</sup>; Christian Trachsel<sup>1</sup>; Nathalie Selevsek<sup>1</sup>; Paola Picotti<sup>2</sup>; Ralph Schlapbach<sup>1</sup>; <sup>1</sup>*University/ETH Zurich - FGCZ, Zurich, Switzerland*; <sup>2</sup>*ETH Zurich, Dept Biology, Institute of Biochemistry, Zurich, Switzerland*
- ThP 330 **Differential Mobility Separation (DMS) to Improve Spectral Correlation in SWATH™ Acquisition;** Nic Bloomfield; J.C. Yves Leblanc; Stephen A Tate; *AB SCIEX, Concord, On, Canada*
- ThP 331 **Proteomic Analysis of Cuticular Proteins from Anopheles Gambiae using LC-MS/MS;** Majors Badgett; Ron Orlando; Judith Willis; Tyler Reed; Yihong Zhou; *University of Georgia, Athens, GA*
- ThP 332 **Implementation of an Optimized Metaproteomic Approach for Comprehensively Characterizing the Microbial Functionality in the Human Infant Gut;** Weili Xiong<sup>1</sup>; Rachel Adams<sup>1</sup>; Michael Morowitz<sup>2</sup>; Jill Banfield<sup>3</sup>; Robert Hettich<sup>4</sup>; <sup>1</sup>*University of Tennessee, Knoxville, TN*; <sup>2</sup>*School of Medicine, University of Pittsburgh, Pittsburgh, PA*; <sup>3</sup>*Department of Earth and Planetary Science, UC, Berkeley, CA*; <sup>4</sup>*Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 333 **Mass Spectrometry-based Proteomics for the Identification and Characterization of Double-Blind Microorganism Mixtures;** A. Peter Snyder<sup>1</sup>; Rabi Jabbour<sup>1</sup>; Mary Margaret Wade<sup>1</sup>; Samir Deshpande<sup>2</sup>; Patrick McCubbin<sup>3</sup>; <sup>1</sup>*US Army /ECBC, Bel Air, MD*; <sup>2</sup>*Science and Technology Corporation, Abingdon, MD*; <sup>3</sup>*Optimetrics, Abingdon, MD*

- ThP 334 **Temporal Analysis of Pathogen-Induced Gastrointestinal Inflammatory States via Host-Centric Proteomic Analysis of Stool**; Joshua S. Lichtman; Katharine Ng; Angela Marcobal; Justin S. Sonnenburg; Joshua E. Elias; *Stanford University, Stanford, CA*
- ThP 335 **Identifying Novel Coregulators and Post-Translational Modifications that Control LRH1 Function using Proteomic Approaches**; Yelenis Mari; Graham M. West; Bruce D. Pascal; Patrick R. Griffin; *Scripps Florida, Jupiter, FL*
- ThP 336 **Novel Insights into the Dynamic Deep Redox Proteome**; Aleksandra Binek; Inmaculada Jorge Cerrudo; Emilio Camafeita; Elena Bonzón-Kulichenko; Juan Antonio López; Borja Ibáñez; Mario Nuño Ayala; Jesús Vázquez; *CNIC, Madrid, Spain*
- Immunology, 337 - 349**
- ThP 337 **Francisella Infection Alters Phosphatidylinositol in White Pulp Splenic Macrophages**; Alison Scott; Robert Ernst; *University of Maryland, Baltimore, Baltimore, MD*
- ThP 338 **Systems Biology Analysis of Temporally-Resolved Phagosome Proteomes following Uptake via Key Phagocytic Receptors**; Brian Dill<sup>1</sup>; Marek Gierliński<sup>2</sup>; Alba Gonzales Arandilla<sup>1</sup>; Manman Guo<sup>1</sup>; Matthias Trost<sup>1</sup>; <sup>1</sup>MRC PPU, *University of Dundee, Dundee, UK*; <sup>2</sup>Data analysis group, *University of Dundee, Dundee, UK*
- ThP 339 **Development of IP-MS Method for Discovery of Downstream Mediators of mTOR Signaling that Regulate T-helper Cell Differentiation**; Olesya Chornoguz; Stefani Thomas; Robert O'Meally; Jonathan Powell; *Johns Hopkins School of Medicine, Baltimore, MD*
- ThP 340 **The Protein Interactome of Critical Viral DNA Sensors Reveals New Insights into Innate Immunity**; Benjamin Diner; Tuo Li; John Fuesler; Marni Crow; Ileana M. Cristea; *Princeton University, Princeton, NJ*
- ThP 341 **Identification of Naturally Processed MHC Class I-restricted HIV Epitopes Presented by Human HIV-Infected Cells**; Marijana Rucevic; *Ragon Institute of MGH, MIT & Harvard, Boston, MA*
- ThP 342 **Defining the Peptidome of HIV-1 Infected Cells using an Optimized LC-MS/MS Analysis Workflow**; Nicola Ternette; Hongbing Yang<sup>1</sup>; Philip Charles<sup>1</sup>; Roman Fischer<sup>1</sup>; Nadine Dudek<sup>2</sup>; Anthony Purcell<sup>2</sup>; Lucy Dorrell<sup>1</sup>; Benedikt Kessler<sup>1</sup>; Tomas Hanke<sup>1</sup>; <sup>1</sup>University of Oxford, *Oxford, UK*; <sup>2</sup>Monash University, *Melbourne, Australia*
- ThP 343 **A nano-UPLC-ESI-MS<sup>3</sup> Method To Directly Identify Low Abundant HPV T Cell Epitopes on the Cell Surface**; Renata Blatnik; Stephanie Hoppe<sup>1</sup>; Marius Kuepper<sup>1</sup>; Agnieszka K. Grabowska<sup>1</sup>; Annette Scharf<sup>2</sup>; Uwe Warnken<sup>1</sup>; Martina Schnoelzer<sup>1</sup>; Thomas Ruppert<sup>2</sup>; Christoph Roesli<sup>1</sup>; Angelika B. Riemer<sup>1</sup>; <sup>1</sup>German Cancer Research Center (DKFZ), *Heidelberg, Germany*; <sup>2</sup>ZMBH, *Heidelberg, Germany*
- ThP 344 **The CD90+ T-cell Proteome during the Progression of Alzheimer's Disease**; Zhiyun Cao; Renā Robinson; *University of Pittsburgh, Pittsburgh, PA*
- ThP 345 **Immunoglobulin Light Chain Repertoire Profiling using microLC-ESI-Q-TOF MS**; David Barnidge<sup>1</sup>; Surendra Dasari<sup>2</sup>; Melissa Snyder<sup>1</sup>; Jerry Katzmann<sup>1</sup>; David Murray<sup>1</sup>; <sup>1</sup>Mayo Clinic / DLMP, *Rochester, MN*; <sup>2</sup>Mayo Clinic, *Rochester, MN*
- ThP 346 **Investigation of Macrophage Polarization States by LC/ESI/MS and LC/MALDI/MS**; Matthias Knust; Rohana Lyianage; Jackson, Jr. Lay; Julie A. Stenken; *University of Arkansas, Fayetteville, AR*
- ThP 347 **Characterization of CD200R-Mediated Signaling in Human Macrophages by Comprehensive Quantitative PTMomics Strategies**; Ane Landt Larsen<sup>2</sup>; Torben Barington<sup>2</sup>; Martin Røssel Larsen<sup>1</sup>; <sup>1</sup>Department of Biochemistry and Molecular Biology, *University of Southern Denmark, Odense, Denmark*; <sup>2</sup>Department of Clinical Immunology, *Odense University Hospital, Denmark*
- ThP 348 **Comparative Proteomics of Eosinophils and Neutrophils**; Emily M. Wilkerson; Nicholas W. Kwicien; Mats W. Johansson; Nicholas M. Riley; Michael S. Westphall; Deane Mosher; Joshua J. Coon; *University of Wisconsin, Madison, WI*
- ThP 349 **Monitoring IgM and IgA Monoclonal Immunoglobulins in Patients with a Monoclonal Gammopathy using microLC-ESI-Q-TOF MS**; Paula Ladwig<sup>1</sup>; David Barnidge<sup>2</sup>; David Murray<sup>2</sup>; <sup>1</sup>Mayo Clinic, *Rochester, MN*; <sup>2</sup>Mayo Clinic / DLMP, *Rochester, MN*
- Biomolecular Structure Analysis: Covalent Labeling, 350 - 363**
- ThP 350 **Probing Conformational Changes of Eukaryotic Elongation Factor 2 Kinase by Covalent Labeling**; Christopher M. Crittenden; John P. O'Brien; William R. Parker; Clint Tavares; David Giles; Kevin Dalby; Jennifer S. Brodbelt; *University of Texas at Austin, Austin, TX*
- ThP 351 **A New Method for Detecting and Identifying Carbonylated Biomolecules: Application to *in vitro* Oxidized Tau Protein by MALDI-Mass Spectrometry**; Lyna Sellami<sup>1</sup>; Claude Villard<sup>1</sup>; Passale Barbier<sup>1</sup>; Jean-Michel Brunel<sup>1</sup>; Matthew Openshaw<sup>2</sup>; Omar Belgacem<sup>2</sup>; Daniel Lafitte<sup>1</sup>; <sup>1</sup>Aix-Marseille Université, *Marseille, FR*; <sup>2</sup>Shimadzu, *Kratos, Manchester, UK*
- ThP 352 **High Resolution Characterization of Antithrombin III-Arixtra Binding Interface by Sub-Microsecond Hydroxyl Radical Protein Footprinting**; Qi Gao; *Complex Carbohydrate Research Center, UGA, Athens, GA*
- ThP 353 **Profiling Yeast Cell Surface Proteins of *S. cerevisiae* by Magnetic Nanoparticles Based Covalent Labeling of Amine Groups**; Ujwal Patil<sup>1</sup>; Parisa Pirani<sup>1</sup>; Yang Cai<sup>2</sup>; Matthew Tarr<sup>1</sup>; <sup>1</sup>University of New Orleans, *New Orleans, LA*; <sup>2</sup>The Research Institute for Children, *New Orleans, LA*
- ThP 354 **Membrane Interactions of Cytochrome P450 2B4 and Cytochrome b<sub>5</sub> Studied by Photoactivable Protein Nanoprobes and High Resolution Mass Spectrometry**; Tomas Jecmen<sup>1,2</sup>; Renata Ptackova<sup>1,2</sup>; Vera Cerna<sup>2</sup>; Petr Novak<sup>1,2</sup>; Petr Hodek<sup>2</sup>; Miroslav Sulc<sup>1,2</sup>; <sup>1</sup>Institute of Microbiology, *ASCR, Prague, Czech Republic*; <sup>2</sup>Department of Biochemistry, *Charles University, Prague, Czech Republic*
- ThP 355 **Uncovering Biomolecular Structure at Single Residue Resolution using Mass Spectrometry Based Covalent Labeling**; Parminder Kaur<sup>1,2</sup>; Janna Kiselar<sup>1</sup>; Giridharan Gokulrangan<sup>1</sup>; Mark Chance<sup>1,2</sup>; <sup>1</sup>Case Western Reserve University, *Cleveland, OH*; <sup>2</sup>NeoProteomics, *Inc., Cleveland, OH*
- ThP 356 **Time-Resolved OH-Footprinting Reveals Mechanism of Proton-Coupled Zinc Transport in YiiP**; Mark Chance<sup>1</sup>; Sayan Gupta<sup>1</sup>; Jie Cheng<sup>2</sup>; Dax Fu<sup>2</sup>; <sup>1</sup>Case Western Reserve University, *Cleveland, OH*; <sup>2</sup>Johns Hopkins University, *Baltimore, MD*
- ThP 357 **Characterization of the Modification of Bruton's Tyrosine Kinase (BTK) by Small Molecule Covalent Inhibitor Using LC-MS**; Keerthi Jayasundera<sup>2</sup>; Wilson Phung<sup>1</sup>; Wendy Sandoval<sup>1</sup>; Ryan Takahashi<sup>1</sup>; James Crawford<sup>1</sup>; Adam Johnson<sup>1</sup>; Cyrus Khojasteh<sup>1</sup>; Cornelis Hop<sup>1</sup>; Shuguang Ma<sup>1</sup>; <sup>1</sup>Genentech Inc, *South San Francisco, CA*; <sup>2</sup>Purdue University, *West Lafayette, IN*
- ThP 358 **Promoting Ozonolysis for Protein Footprinting by Radical Probe Mass Spectrometry**; Simin D. Maleknia<sup>1</sup>; Keith Fisher<sup>2</sup>; <sup>1</sup>University of New South Wales, *Sydney, Australia*; <sup>2</sup>University of Sydney, *Sydney, Australia*

- ThP 359 **Covalent-labeling Strategy for the Thermodynamic Analysis of Protein Folding and Ligand Binding in Complex Mixtures;** Yingrong Xu<sup>1</sup>; Erin C. Strickland<sup>1,2</sup>; Emily R. Derbyshire<sup>1</sup>; Michael C. Fitzgerald<sup>1</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>Current Address: Ameritox, Greensboro, NC
- ThP 360 **Differential Surface Modification under Denaturing And Native Conditions for the Identification of Surface-Exposed Amino Acid Residues in Alpha-Synuclein;** Nicole Sessler<sup>1</sup>; Nicholas Brodie<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 361 **Structural Proteomic Analysis of SOD1 Aggregation;** Nicholas Brodie<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; <sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada
- ThP 362 **Conformational Analysis of Intrinsically Disordered Proteins by Fast Photochemical Oxidation of Proteins;** Mohammed Al-Naqshabandi<sup>1,2</sup>; Hao Zhang<sup>3</sup>; Ben Niu<sup>3</sup>; Michael L. Gross<sup>3</sup>; David Weis<sup>1</sup>; <sup>1</sup>University of Kansas, Lawrence, KS; <sup>2</sup>University of Soran, Erbil, Iraq; <sup>3</sup>Washington University, St Louis, MO
- ThP 363 **Probing Conformational Changes in Amyloid Beta Aggregation by Fast Photochemical Oxidation of Proteins (FPOP);** Ke Sherry Li; Ying Zhang; Don L. Rempel; Michael L. Gross; *Department of Chemistry, Washington University, St. Louis, MO*
- Astrobiology and Atmospheric Chemistry, 364 - 370**
- ThP 364 **A Laser Desorption Mass Spectroscopy Study of Titan Aerosol Analogs Formed from Aromatic Precursors;** Melissa Trainer<sup>1</sup>; Joshua Sebree<sup>2</sup>; Xiang Li<sup>1</sup>; Veronica Pinnick<sup>1</sup>; Stephanie Getty<sup>1</sup>; William Brinckerhoff<sup>1</sup>; <sup>1</sup>NASA, Greenbelt, MD; <sup>2</sup>University of Northern Iowa, Cedar Falls, IA
- ThP 365 **In Situ Analysis of Organics on Planetary Surfaces by Miniature Two-Step Laser Time-of-Flight Mass Spectrometer;** Xiang Li<sup>1</sup>; Stephanie Getty<sup>2</sup>; William Brinckerhoff<sup>2</sup>; Timothy Cornish<sup>3</sup>; Scott Ecelberger<sup>3</sup>; Melissa Floyd<sup>2</sup>; Qinghao Wu<sup>4</sup>; Richard Zare<sup>4</sup>; Jamie Elsilá Cook<sup>2</sup>; <sup>1</sup>University of Maryland, Baltimore County, Baltimore, MD; <sup>2</sup>NASA GSFC, Greenbelt, MD; <sup>3</sup>C&E Research, Inc., Columbia, MD; <sup>4</sup>Stanford University, Stanford, CA
- ThP 366 **The Identification of Biosignatures on Planetary Surfaces from in situ Techniques, Including Miniaturized Mass Spectroscopy;** Kyle Uckert<sup>1</sup>; Nancy J. Chanover<sup>1</sup>; Stephanie Getty<sup>2</sup>; William B. Brinckerhoff<sup>2</sup>; David G. Voelz<sup>1</sup>; Nancy McMillan<sup>1</sup>; Xifeng Xiao<sup>1</sup>; Xiang Li<sup>3</sup>; Mellisa Floyd<sup>2</sup>; Penelope J. Boston<sup>4</sup>; <sup>1</sup>New Mexico State University, Las Cruces, NM; <sup>2</sup>NASA GSFC, Greenbelt, MD; <sup>3</sup>University of Maryland, Baltimore County, Greenbelt, MD; <sup>4</sup>New Mexico Institute of Mining and Technology, Socorro, NM
- ThP 367 **Molecular Composition and Optical Properties of Organo-Nitrogen Species in Organic Aerosol;** Chris Stangl; Murray Johnston; *University of Delaware, Newark, DE*
- ThP 368 **Reaction of Gas-Phase Dimethylamine with Ammonium Sulfate Aerosol Particles;** Justin Krasnomowitz; Bryan Bzdek; Murray Johnston; *University of Delaware, Newark, Delaware*
- ThP 369 **Gas Chromatography-Mass Spectrometry Performance Demonstration of the Mars Organic Molecule Analyzer;** Veronica Pinnick<sup>1</sup>; Arnaud Buch<sup>2</sup>; Noël Grand<sup>4</sup>; Cyril Szopa<sup>3</sup>; Friso H.W. Van Amerom<sup>5</sup>; Ryan M. Danell<sup>6</sup>; Caroline Freissinet<sup>1</sup>; Ricardo Arevalo<sup>1</sup>; Stephanie Getty<sup>1</sup>; William Brinckerhoff<sup>1</sup>; Paul Mahaffy<sup>1</sup>; Fred Goesmann<sup>7</sup>; <sup>1</sup>NASA GSFC, Greenbelt, MD; <sup>2</sup>Ecole Centrale Paris, Châtenay-Malabry, France; <sup>3</sup>LATMOS, Paris, France; <sup>4</sup>LISA, Paris, France; <sup>5</sup>MiniMass, Hyattsville, MD; <sup>6</sup>Danell Consulting, Inc., Winterville, NC; <sup>7</sup>Max Planck Institut für Sonnensystemforschung, Lindau, Germany
- ThP 370 **Survivability of Electrosprayed Bacterial Spores upon High-Velocity Surface Impact;** Brandon L Barney; Kit Anderson; Daniel E Austin; *Brigham Young University, Provo, UT*
- Lipids: Profile Analysis, 375 - 394**
- ThP 375 **Lipidome Analysis of Plasma, Livers, And Adipose Tissues in High-Fat-Diet-Fed Mice Using Supercritical Fluid Chromatography Coupled to High-Resolution Mass Spectrometry;** Takayuki Yamada<sup>1</sup>; Yoshihiro Izumi<sup>1</sup>; Shin Nishiumi<sup>2</sup>; Masaru Yoshida<sup>2</sup>; Eiichiro Fukusaki<sup>1</sup>; Takeshi Bamba<sup>1</sup>; <sup>1</sup>Dept. Biotech., Grad. Sch. Eng., Osaka Univ., Suita, Japan; <sup>2</sup>Div. Gastro., Kobe Univ. Grad. Sch. Med., Kobe, Japan
- ThP 376 **Alterations of Lipid Metabolism in Preeclampsia: Lipid Characterization in the Maternal Circulation and Placenta;** Simon Brown<sup>1</sup>; Samuel Eather<sup>1</sup>; Dilys Freeman<sup>2</sup>; Barbara Meyer<sup>1</sup>; Todd W Mitchell<sup>1</sup>; <sup>1</sup>University of Wollongong, Wollongong, Australia; <sup>2</sup>University of Glasgow, Glasgow, UK
- ThP 377 **Understanding the Role of Lipids during the Embryonic Development of the American Alligator (Alligator mississippiensis) using a Lipidomics Approach;** Stephen Somerville<sup>1</sup>; John Bowden<sup>2</sup>; Theresa Cantu<sup>1</sup>; Louis J. Guillette, Jr. <sup>1</sup>; <sup>1</sup>Medical University of South Carolina, Charleston, SC; <sup>2</sup>NIST, Charleston, SC
- ThP 378 **Supercritical Fluid Chromatography Coupled to Mass Spectrometry for Comprehensive Bile Acid Profiling;** Kaori Taguchi; Eiichiro Fukusaki; Takeshi Bamba; *Graduate school of engineering, Osaka university, Suita, Japan*
- ThP 379 **Characterization of Human Cancer Cell Lines Using Rapid Evaporative Ionization Mass Spectrometry;** Nicole Strittmatter<sup>1</sup>; Anna Lovrics<sup>2</sup>; Emrys A Jones<sup>1</sup>; Ottmar Golf<sup>1</sup>; Kirill Veselkov<sup>1</sup>; Gergely Szakacs<sup>2</sup>; Zoltan Takats<sup>1</sup>; <sup>1</sup>Imperial College London, London, UK; <sup>2</sup>Hungarian Academy of Sciences, Budapest, Hungary
- ThP 380 **Lipogenesis in Adipocyte using Isotope Tracer Mass Spectrometry;** Fereshteh Zandkarimi; Claudia S. Maier; *Chemistry Department of Oregon State University, Corvallis, OR*
- ThP 381 **Lipidomics by Infusion-Based MS/MS<sup>ALL</sup> Reveals Novel Aspects of Fatty Liver Disease;** Jeff McDonald; *UT Southwestern Medical Center, Dallas, TX*
- ThP 382 **Quantitative Characterization of Protein and Lipid Content of Lipoprotein Particle Size Fractions by AF4, Dynamic Light Scattering and LC-MS/MS;** John R. Barr; Zsuzsanna Kuklenyik; Michael Gardner; Jon Rees; David M. Schieltz; Lisa McWilliams; James Pirkle; *CDC, Atlanta, GA*
- ThP 383 **Direct Identification of Omega-3/6 Fatty Acid Incorporated Phosphatidylcholine in Mouse Serum and Tissue by MALDI-MS and LC-MS Based Metabolic Profiling;** Lin Tan; Patrea Rhea; Peiyang Yang; *MD Anderson Cancer Center, Houston, TX*
- ThP 384 **Analysis of Polyunsaturated Fatty Acid Metabolites in Brain After Traumatic Brain Injury by High Resolution LC-MS/MS;** Karl R Kevala; Abhishek Desai; Hee-Yong Kim; *National Institutes of Health, Bethesda, MD*
- ThP 385 **Lipidomic Analysis of Differentiating Osteoblastic Cells;** Xiaoli Gao; Lee-Chuan Caroline Yeh; Sammy Pardo; Martin L. Adamo; John C. Lee; Susan T. Weintraub; *UT Health Science Center at San Antonio, San Antonio, TX*

- ThP 386 **Angiotensin Converting Enzyme Regulates the Lipid Composition of Macrophages**; Bogdan-Gabriel Gugu<sup>1</sup>; Teresa Hong<sup>1</sup>; Kenneth Bernstein<sup>2</sup>; Markus Kalkum<sup>1</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>Cedars-Sinai Medical Center, Los Angeles, CA
- ThP 387 **Ethanol Induced Quantitative Brain Lipid Changes in Mice**; Aurelie Roux<sup>1</sup>; Shelley N Jackson<sup>1</sup>; Ludovic Muller<sup>1,2</sup>; Joseph R. O'Rourke<sup>3</sup>; Panayotis K. Thanos<sup>3</sup>; Nora D. Volkow<sup>1</sup>; Amina S. Woods<sup>1</sup>; <sup>1</sup>NIDA-IRP, NIH, Baltimore, MD; <sup>2</sup>University of Pittsburgh, Pittsburgh, PA; <sup>3</sup>Stony Brook University, Stony Brook, NY
- ThP 388 **Multivariate Analyses of Phospholipids in Normal and Ischemic Rat Brain Parenchyma**; Hay-Yan J. Wang<sup>1</sup>; Hsuan-Wen Wu<sup>1</sup>; Zhi-Fu Zheng<sup>1</sup>; Ping-Ju Tsai<sup>2</sup>; Cheng Bin Liu<sup>1,3</sup>; <sup>1</sup>National Sun Yat-Sen University, Kaohsiung, TAIWAN; <sup>2</sup>Yuan's General Hospital, Kaohsiung, Taiwan; <sup>3</sup>Veterans General Hospital-Kaohsiung, Kaohsiung, Taiwan
- ThP 389 **State-of-the-art LC-MS Based Lipidomics Applied to the Study of Lung Diseases**; Koen Sandra<sup>1</sup>; Ruben t'Kindt<sup>1</sup>; Eef Telenga<sup>2</sup>; Roland Hoffmann<sup>2</sup>; Lucie Jorge<sup>1</sup>; Antoon van Oosterhout<sup>2</sup>; Nick ten Hacken<sup>2</sup>; Pat Sandra<sup>1</sup>; <sup>1</sup>RIC, Kortrijk, Belgium; <sup>2</sup>UMCG, Groningen, The Netherlands
- ThP 390 **Identification of Lipid Biomarkers from Mouse Lung Tissue via the Use of UPC<sup>2</sup> Tandem Mass Spectrometry**; Jace W. Jones; Fei Li; Claire L. Carter; Keely Pierzchalski; Pu-Ting Xu; Isabel L. Jackson; Zeljko Vujaskovic; Maureen A. Kane; *University of Maryland, Baltimore, MD*
- ThP 391 **Cerebrospinal Fluid and Plasma Lipid Profiling using High Resolution Mass Spectrometry and Integrated Data Processing Tools**; Benoit Colsch<sup>1</sup>; Alexandre Seyer<sup>2</sup>; Samia Boudah<sup>1</sup>; Simon Broudin<sup>2</sup>; Christophe Junot<sup>1</sup>; <sup>1</sup>CEA de SACLAY, Gif Sur Yvette Cedex, France; <sup>2</sup>Profilomic SA, Boulogne-Billancourt, France
- ThP 392 **Comparative Metabolomics Analysis of Prostate Cancer Cells with Different Ethnic Backgrounds**; Julius Nyalwidhe<sup>1</sup>; Tanya Burch<sup>1</sup>; John Rhim<sup>2</sup>; James Langridge<sup>4</sup>; Andy Baker<sup>3</sup>; Giorgis Isaac<sup>3</sup>; <sup>1</sup>Eastern Virginia Medical School, Norfolk, VA; <sup>2</sup>Center for Prostate Disease Research, Bethesda, MD; <sup>3</sup>Waters Corporation, Milford, MA; <sup>4</sup>Waters Corporation, Manchester, UK
- ThP 393 **Lipidomic Analysis of Different Cotton Seed Oil Genotypes Using Novel Analytical and Informatics Tools**; Vladimir Shulaev<sup>1</sup>; Michael Jones<sup>2</sup>; Drew Sturtevant<sup>1</sup>; Patrick Horn<sup>1</sup>; Janna Crossley<sup>1</sup>; Kent Chapman<sup>1</sup>; James Langridge<sup>3</sup>; Giorgis Isaac<sup>2</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>Waters Corporations, Milford, MA; <sup>3</sup>Waters Corporations, Manchester, UK
- ThP 394 **Rejuvenation of Negative Ion Chemical Ionization Mass Spectrometry for the Lipid Biomarker Detection of Tuberculosis and Leprosy in Archaeological Material**; Houdini Wu<sup>1</sup>; Oona Lee<sup>1</sup>; David Minnikin<sup>1</sup>; Gurdyal Besra<sup>1</sup>; Helen Donoghue<sup>2</sup>; Ildiko Pap<sup>3</sup>; Christos Economou<sup>4</sup>; Anna Kjellström<sup>4</sup>; Gareth Llewellyn<sup>5</sup>; Christopher Williams<sup>5</sup>; <sup>1</sup>University of Birmingham, Birmingham, UK; <sup>2</sup>University College London, London, UK; <sup>3</sup>Hungarian Natural Science Museum, Budapest, HUNGARY; <sup>4</sup>Stockholm University, Stockholm, Sweden; <sup>5</sup>Swansea University, Swansea, UK
- Lipids: Quantitative Analysis, 395 - 412**
- ThP 395 **Tandem Mass Spectrometric Quantification of Oxidized Products of Polyunsaturated Fatty Acids in biofluids and tissue**; Jaeman Byun; Lixia Zeng; Subramaniam Pennathur; *University of Michigan, Ann Arbor, MI*
- ThP 396 **Lipidomic Differentiation of Breast Cancer Tissues and Surrounding Normal Tissues using HILIC-HPLC/ESI-MS**; Eva Cifková<sup>1</sup>; Michal Holčapek<sup>1</sup>; Miroslav Lisa<sup>1</sup>; Vitaliy Chagovets<sup>1</sup>; David Vrána<sup>2</sup>; Jiří Gatěk<sup>3</sup>; Bohuslav Melichar<sup>2</sup>; <sup>1</sup>University of Pardubice, Pardubice, Czech Republic; <sup>2</sup>Palacký University, Olomouc, Czech Republic; <sup>3</sup>Tomáš Bata University, Zlín, Czech Republic
- ThP 397 **Isometric Separation of Brain Glucosylated Lipids by Hydrophilic Interaction Liquid Chromatography –ESI-MS using Zwitterionic Columns**; Kazuki Nakajima; Hisako Akiyama; Kaori Tanaka; Yoshio Hirabayashi; *RIKEN Brain Science Institute, Wako-Shi, Japan*
- ThP 398 **A Comprehensive Monitoring Method for lipid Mediators using a High-Speed LC/MS with Continuous Ionization Polarity Switching**; Masaki Yamada<sup>1,2</sup>; Yoshihiro Kita<sup>1</sup>; Takahiro Kohira<sup>1,3</sup>; Suzumi Tokuko<sup>1</sup>; Takao Shimizu<sup>1,4</sup>; <sup>1</sup>The University of Tokyo, Tokyo, JAPAN; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>Japanese Red Cross Society, Tokyo, Japan; <sup>4</sup>National Center for Global Health and Medicine, Tokyo, Japan
- ThP 399 **Shotgun Fatty Acidomics Analysis of Eicosanoids in Biological Samples by Charge-Remote Fragmentation Approaches**; Miao Wang; Chunyan Wang; Xianlin Han; *Sanford-Burnham Medical Research Institute, Orlando, FL*
- ThP 400 **Micro-LC-MS/MS Analysis of Endocannabinoids in Brain Tissues**; Ming Qi; Matthew Hill; David Schriemer; *University of Calgary, Calgary, CANADA*
- ThP 401 **Evaluation of Anti-Proliferative and Lipoygenase-Inhibitory Effects of Protolichesterinic Acid**; Finnur F. Eiriksson<sup>1,2</sup>; Margrét Bessadóttir<sup>1</sup>; Stefan Becker<sup>1</sup>; Margrét H. Ögmundsdóttir<sup>1</sup>; Sesselja S. Ómarsdóttir<sup>1</sup>; Helga Ögmundsdóttir<sup>1</sup>; Margrét Thorsteinsdóttir<sup>1,2</sup>; <sup>1</sup>University of Iceland, Reykjavik, IS; <sup>2</sup>ArcticMass, Reykjavik, IS
- ThP 402 **Quantitative Analysis of Bile Acids and Taurine Conjugates in Mouse Plasma Using a High Resolution Accurate Mass Approach**; Shunyan Mo; Karin Green; Timothy P. Fitzgibbons; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*
- ThP 403 **High Throughput and High Sensitivity LC-MS/MS Analysis of GM1 and GM2 Gangliosides in Brain**; Karin Green; Cara M. Weismann; Miguel Sena Esteves; Scott A. Shaffer; *University of Massachusetts Medical School, Worcester, MA*
- ThP 404 **LC-MS Analysis of Cholesteins Acid from Microliter Volumes of Plasma**; Fred Bjorn Lih; Michael Fessler; Kenneth B. Tomer; Leesa Deterding; *NIEHS/NIH, Research Triangle Park, NC*
- ThP 405 **Application of LC-MS/MS based Lipid Profiling/ Biochemical Assays and Affinity Proteomics for MAGL Target Validation**; Timothy He; Scott Britain; Tatiana Tolstykh; Heike Arlt; Ronaldo Tomlinson; Frank Sun; Hong Cheng; Dmitri Wiederschain; Bailin Zhang; *Sanofi Oncology, Cambridge, MA*
- ThP 406 **Improving Lipid Profiling Performance using MicroFlow Liquid Chromatography and High Resolution Mass Spectrometry**; Jinyuan Wang<sup>1</sup>; Baljit Ubhi<sup>1</sup>; Christie Hunter<sup>1</sup>; Anthony Romanelli<sup>2</sup>; Alexander Chassy<sup>3</sup>; Tomas Cajka<sup>3</sup>; Oliver Fiehn<sup>3</sup>; <sup>1</sup>AB SCIEX, Redwood City, CA; <sup>2</sup>AB SCIEX, Framingham, MA; <sup>3</sup>UC Davis, Davis, CA
- ThP 407 **Qualitative and Quantitative Analysis of Oxidized Fatty Acids by Information Dependent and Data Independent Strategies on a QTOF Instrument**; Xu Wang<sup>1</sup>; Priscilla BMC Derogis<sup>2</sup>; Sayuri Miyamoto<sup>2</sup>; Sahana Mollah<sup>3</sup>; Christie Hunter<sup>3</sup>; <sup>1</sup>AB SCIEX, Framingham, MA; <sup>2</sup>Instituto de Química - Universidade de São Paulo, São Paulo, Brazil; <sup>3</sup>AB SCIEX, Redwood City, CA
- ThP 408 **Application of SPME in Plasma Lipid Analysis: Quantification of Polyunsaturated Fatty Acids in Fish Plasma, and Patients Undergoing Cardiac Surgery**; Afsoon Pajand Birjandi; Barbara Bojko; Janusz Pawliszyn; *University of Waterloo, Waterloo, Canada*

- ThP 409 **Multiplexed Lipid Quantification via Isobaric Mass Tagging and Targeted MS/MS**; Shuai Nie<sup>1</sup>; Cassie J. Fhaner<sup>1</sup>; Gavin E. Reid<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Michigan State University, East Lansing, MI; <sup>2</sup>Department of BMB, Michigan State University, East Lansing, MI
- ThP 410 **Supercritical Fluid Chromatography - Electrospray Ionization Mass Spectrometry as a Novel Approach for Fast and Complex Lipidomic Characterization**; Michal Holcapek; Miroslav Lisa; University of Pardubice, Pardubice, Czech Republic
- ThP 411 **Total Cholesterol Analysis in Plasma at 7 Seconds Per Sample using LDTD-MS/MS**; Sarah Demers<sup>1</sup>; Pierre Picard<sup>2</sup>; Serge Auger<sup>2</sup>; Gregory Blachon<sup>2</sup>; <sup>1</sup>Université Laval, Québec, QC; <sup>2</sup>Phytrox Technologies, Inc., Quebec, QC
- ThP 412 **Quadruple Parallel Mass Spectrometry (LC1/MS4) 'extract-Filter-Shoot' Method for Lipid and Vitamin D Analysis**; William C Byrdwell; USDA, ARS, BHNRC, FCMDL, Beltsville, MD  
**Ambient Ionization: Applications, 413 - 417**
- ThP 413 **Herbal Supplement Screening: HPTLC Ambient Mass Spectrometry for Rapid Separation and Screening from Complex Mixtures**; Elizabeth Crawford<sup>1</sup>; Robert Goguen<sup>1</sup>; Brian Musselman<sup>1</sup>; Jason Shepard<sup>2</sup>; <sup>1</sup>IonSense, Inc., Saugus, MA; <sup>2</sup>University at Albany, Albany, NY
- ThP 414 **Rapid Screening of Antibacterials in a Wide Variety of Consumer Products using Ambient Ionization Mass Spectrometry**; Sharanya Reddy; Craig Whitehouse; PerkinElmer, Shelton, CT
- ThP 415 **Statistical Analysis and Forensics Determination of Designer Drugs via Direct Analysis in Real Time Mass Spectrometry (DART-MS)**; Jason Shepard<sup>1</sup>; Joseph Lapointe<sup>2</sup>; Brian D. Musselman<sup>2</sup>; Rabi Musah<sup>1</sup>; Robert B. Cody<sup>3</sup>; A. John Dane<sup>3</sup>; <sup>1</sup>University at Albany, Albany, NY; <sup>2</sup>IonSense, Inc., Saugus, MA; <sup>3</sup>JEOL USA, Inc., Peabody, MA
- ThP 416 **Rapid Analysis and Differentiation of Smokeless Powders using DSA/TOF**; Avinash Dalmia<sup>1</sup>; Jeff Jagmin<sup>2</sup>; Sergey Rakov<sup>3</sup>; Craig M. Whitehouse<sup>3</sup>; <sup>1</sup>PerkinElmer, Shelton, CT; <sup>2</sup>Washington State Patrol, Seattle, WA; <sup>3</sup>PerkinElmer, Branford, CT
- ThP 417 **Metabolomics Study of Arabidopsis Mutants Using Atmospheric Pressure GC-MS<sup>E</sup> Approach and Multivariate Statistical Analysis**; Carolina Salazar<sup>1</sup>; Giorgis Isaac<sup>2</sup>; Steven Lai<sup>2</sup>; Nobuhiro Suzuki<sup>1</sup>; Janna Crossley<sup>1</sup>; James Langridge<sup>2</sup>; Ron Mittler<sup>1</sup>; Giuseppe Astarita<sup>2</sup>; Vladimir Shulaev<sup>1</sup>; <sup>1</sup>University of North Texas, Denton, TX; <sup>2</sup>Waters Corporation, Milford, MA  
**Biomarkers: Quantitative Analysis, 421 - 451**
- ThP 421 **SILAC-Based LC-MS Assay to Measure Microtubule Dynamics in Neuronal Cell Cultures**; Cong Wei; Craig Polson; Joseph L. Cantone; Jere E. Meredith; Dieter M. Drexler; Bristol-Myers Squibb, Wallingford, CT
- ThP 422 **A Simplified LC-MS/MS-MRM Method for Quantitation of Risperidone and 9-Hydroxyrisperidone in Human Plasma**; Rachelle Jacoby; Farbod Fazlollahi; Kym Francis Fauli; UCLA, Los Angeles, CA
- ThP 423 **Altered Steroid Profiles in Metastatic Bone Prostate Cancer Models using LC/MSMS**; Sumankalai Ramachandran; Zahi Mitri; Sankar Maity; John Araujo; Eleni Efstathiou; Christopher Logothetis; Mark Titus; , Houston, TX
- ThP 424 **Differential Mobility Spectrometry: Investigating Instrument Parameters That Influence Sensitivity in Quantitative LC/MS/MS Bioanalysis**; Jefry Shields<sup>1</sup>; Brendon Kapinos<sup>1</sup>; John Janiszewski<sup>1</sup>; Richard Kibbey<sup>3</sup>; Anthony Romanelli<sup>2</sup>; <sup>1</sup>Pfizer Inc., Groton, CT; <sup>2</sup>AB SCIEX, Framingham, MA; <sup>3</sup>Yale University, New Haven, CT
- ThP 425 **Exploring microLC/MS/MS for Accelerating Peptide Quantitation Assays**; Xiang Zhu<sup>1</sup>; Christie Hunter<sup>2</sup>; Khaled Mriziq<sup>1</sup>; Remco Van Soest<sup>1</sup>; Subodh Nimkar<sup>1</sup>; <sup>1</sup>SCIEX Separations, Division of AB SCIEX, Redwood City, CA; <sup>2</sup>AB SCIEX, Redwood City, CA
- ThP 426 **New LC-MS/MS Method to Quantify Biotin and Biotinylated Biotin in Urine**; Olga Malysheva<sup>1</sup>; Cydne Perry<sup>1,2</sup>; Larry Walker<sup>1</sup>; Marie Caudill<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>Shephard University, Shepherdstown, WV
- ThP 427 **Low Picomole Quantification of Metanephrine and Normetanephrine in Plasma by SPE-LC-MS/MS**; Sha Joshua Ye; Mitesh Patel; Hui Qiao; Ellie Majidi; *Ionics Mass Spectrometry Gro, Bolton, Canada*
- ThP 428 **Quantification of 17 $\beta$ -Estradiol as A Biomarker in Mouse Plasma: A Microsampling Approach Coupled with LC-MS/MS Analysis**; Jianshuang Wang; Brian Dean; Xiao Ding; Genentech, South San Francisco, CA
- ThP 429 **Development of a Quantitative High-Throughput Immunomagnetic-UHPLC-MS/MS Method for Detecting Human Exposure to Tricresyl Phosphate**; Darryl Johnson<sup>1</sup>; Melissa Carter<sup>2</sup>; Brian Crow<sup>2</sup>; Thomas Blake<sup>2</sup>; Rudolph Johnson<sup>2</sup>; <sup>1</sup>ORISE Centers for Disease Control and Prevention, Atlanta, GA; <sup>2</sup>CDC, Atlanta, GA
- ThP 430 **An Integrated LC-MS System for Simultaneous Preparation, Separation, Detection, and Quantification of Proteins and Small Molecules from Biological Fluids**; Evelyn Wang<sup>1</sup>; Danajava Kalu appulage<sup>1</sup>; Benjamin Figard<sup>2</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>The University of Texas at Arlington, Arlington, TX; <sup>2</sup>Shimadzu Scientific Instruments, Inc., Houston, TX
- ThP 431 **Nanospray HPLC-Chip/MS System for Detection of F<sub>2</sub>-Isoprostanes in Urine and Plasma**; Paul E. Minkler; Stephen T. Ingalls; Lori Hezel; Charles L. Hoppel; Case Western Reserve Univ., Cleveland, OH
- ThP 432 **LC-MS/MS Method Development and Stability Assessment for the Analysis of Norepinephrine in Pig Kidney Tissues**; Ling Morgan; Agilux Laboratories, Worcester, MA
- ThP 433 **Comparison of Nano-Flow and Standard Flow-Rate LC-QQQ Platforms using Putative Prostate Cancer Protein Biomarkers**; Brian Flatley<sup>1</sup>; Cathy Rooney<sup>1</sup>; Stella Ademowo<sup>1</sup>; Xiao Zhang<sup>2</sup>; Christine Miller<sup>3</sup>; Trevor Clancy<sup>4</sup>; Moyez Dharsee<sup>2</sup>; Kristin Austlid Taskén<sup>4</sup>; Lorelei Mucci<sup>5</sup>; William Watson<sup>1</sup>; Kenneth Evans<sup>2</sup>; Stephen Pennington<sup>1</sup>; <sup>1</sup>University College Dublin, Dublin, IRELAND; <sup>2</sup>Ontario Cancer Biomarker Network, Toronto, Canada; <sup>3</sup>Agilent Technologies, Santa Clara, CA; <sup>4</sup>Oslo University Hospital, Oslo, Norway; <sup>5</sup>Harvard School of Public Health, Boston, MA
- ThP 434 **LC-MS/MS Analysis of urinary Multiple Biomarkers : Stability Study and Artificial Formation of 8-OHdG, Biomarker for Oxidative Stress**; Shu-Ting Chen; Kuen-Yuh Wu; Institute of Occupational Medicine and Industrial, Taipei, Taiwan
- ThP 435 **A Rapid LC-MS/MS Measurement of Urea as a Biomarker in Human Bronchoalveolar Lavage Fluid and Plasma**; Tian-Sheng Lu; Aiping Zhu; Elise Snider; Jon Bruss; Yong-Xi Li; Medpac, Cincinnati, OH
- ThP 436 **Determination of Homocysteine, Cysteine, Cystathionine, S-Adenosylmethionine and S-Adenosylhomocysteine in Biological Samples Using Ultra Performance Liquid Chromatography with Tandem Mass Spectrometry**; Yi Tao; Lizhi Guo; Hongmei Wang; Weimin Hu; Fangfang Chen; Xin Zhang; WuXi AppTec Co., Shanghai, China

- ThP 437 **Method to Detect Blood Doping Practices in Sport Through the Measurement of Reticulocytes in Dried Blood Spots by LC-MS/MS;** Holly Cox; Cole Hughes; Daniel Eichner; *Sports Medicine Research and Testing Laboratory, Salt Lake City, UT*
- ThP 438 **Improved Sensitivity for the Selective Quantitation of LTB4 in Human Plasma and Sputum via UPLC-MS/MS;** Chad Moore; Dan Li; Aihua Liu; Laixin Wang; Min Meng; *Tandem Labs, Salt Lake City, UT*
- ThP 439 **A Quantitative Proteomic Approach (UPLC-HDMS<sup>F</sup>) to Identify Biomarkers of Myofibroblast Formation in Idiopathic Pulmonary Fibrosis;** Leanne Wickens<sup>1,2</sup>; Akul Singhania<sup>3</sup>; Franco Conforti<sup>3</sup>; Katherine O'Reilly<sup>2,4</sup>; Donna Davies<sup>2,3</sup>; Paul J. Skipp<sup>1,2</sup>; <sup>1</sup>Centre for Proteomic Research, Uni of Southampton, Southampton, UK; <sup>2</sup>NIHR Respiratory Biomedical Research Unit, Southampton, UK; <sup>3</sup>Faculty of Medicine, University of Southampton, Southampton, UK; <sup>4</sup>Respiratory Medicine, MMUH, Dublin, Ireland
- ThP 440 **Quantitative Analysis of cAMP and cGMP in Microwave Fixed Brain Tissue by HPLC/MS/MS: Adenosine is Key in Determining Sample Quality;** Forrest Helfrich; Marieke Van Der Hart; Arash Rassoulpour; *Brains On-Line, South San Francisco, CA*
- ThP 441 **Immunoaffinity LC-MS/MS for the Quantitation of IL-6R in Mouse Colon Tissue Samples for Preclinical Study;** Yongxin Zhu; Celia D'Arienzo; John Mehl; Guodong Chen; Huadong Sun; Qihong Zhao; Adrienne Tymiak; Timothy Olah; *Bristol-Myers Squibb Company, Princeton, NJ*
- ThP 442 **Combining Immuno Affinity Purification and Fast LC-MS to Characterize Peptide Isoforms of Diagnostic Cancer Markers;** Antoine Lesur; Lina Ancheva; Sebastien Gallien; Jan van Oostrum; Bruno Doman; *Luxembourg Clinical Proteomics Center, Strassen, Luxembourg*
- ThP 443 **Determination of Acetylcholine in Microdialysis Samples using HILIC coupled with High Resolution Mass Spectrometry;** Emily Miller; Hongying Gao; Christopher Holliman; *Pfizer, Groton, CT*
- ThP 444 **Analysis of Multiple DNA Adducts in Cancer Patients by Stable Isotope Dilution Nanoflow LC-Nanospray Ionization Tandem Mass Spectrometry;** Hsueh-Chun Wang; Hauh-Jyun Candy Chen; *National Chung Cheng Univ., Ming-Hsiung, Chia-Yi, Taiwan*
- ThP 445 **Development of a Robust, Accurate and Reproducible Procedure for Quantitative Analysis of Cardiac Troponin T using a Chip-Based Nanospray Source;** Mariola Olkowicz<sup>1</sup>; Iwona Rybakowska<sup>1</sup>; Stefan Chłopicki<sup>2</sup>; Helena Svobodova<sup>3</sup>; Gary Valaskovic<sup>3</sup>; Ryszard Smolenski<sup>1</sup>; <sup>1</sup>Medical University of Gdansk, Gdansk, Poland; <sup>2</sup>Jagiellonian Centre for Experimental Therapeutics, Krakow, Poland; <sup>3</sup>New Objective Inc., Woburn, MA
- ThP 446 **Analysis of Pteridines by CE-MS;** Nicolas Drouin<sup>2</sup>; Julie Schappler<sup>2</sup>; Serge Rudaz<sup>2</sup>; Martin Greiner<sup>1</sup>; *Agilent Technologies, Waldbronn, Germany; <sup>2</sup>University of Geneva, Geneva, Switzerland*
- ThP 447 **Quantitation of Glutathione and Its Redox Species in Blood and Saliva using Speciated Isotope Dilution Mass Spectrometry (EPA Method 6800);** Mesay Mulugeta Wolle<sup>1</sup>; Logan Miller<sup>1</sup>; Timothy Fahrenholz<sup>2</sup>; H. M. Skip Kingston<sup>1</sup>; Matt Pamuku<sup>2</sup>; Scott Faber<sup>3</sup>; *<sup>1</sup>Duquesne University, Pittsburgh, PA; <sup>2</sup>Applied Isotope Technologies, Pittsburgh, PA; <sup>3</sup>The Children's Institute of Pittsburgh, Pittsburgh, PA*
- ThP 448 **An Effective Biomarker in Chronic Obstructive Pulmonary Disease (COPD);** Shuren Ma<sup>1</sup>; Jiangtao He<sup>1</sup>; Yong Y Lin<sup>1</sup>; Jerome Cantor<sup>2</sup>; Toyonobu Usuki<sup>3</sup>; Gerard Turino<sup>1</sup>; *<sup>1</sup>Roosevelt Hospital, Mount Sinai School of Medicine, New York, NY; <sup>2</sup>St John's University - Queens, New York, NY; <sup>3</sup>Sophia University, Tokyo, Japan*
- ThP 449 **Mass Spectrometry-Based Proteomics: Discovery and Absolute Quantification of Neuroinjury Biomarkers;** Ahmed Moghieb; Nancy Denslow; Richard A. Yost; Kevin K.W. Wang; *University of Florida, Gainesville, Florida*
- ThP 450 **Characterizing Qualitative and Quantitative Global Changes in Mesenchymal Stem Cells using a Novel Real-Time Modified DIA Method;** Maryann S. Vogelsang<sup>1</sup>; Amol Prakash<sup>1</sup>; David Sarracino<sup>1</sup>; Scott Peterman<sup>1</sup>; Barbara Frewen<sup>1</sup>; Victoria V Lunyak<sup>2</sup>; Benny Blackwell<sup>2</sup>; James R. Tollervey<sup>2</sup>; Gouri Vadali<sup>1</sup>; Shadab Ahmad<sup>1</sup>; Gregory Byram<sup>1</sup>; Bryan Krastins<sup>1</sup>; Mary F. Lopez<sup>2</sup>; *<sup>1</sup>BRIMS, Thermo Fisher Scientific, Cambridge, MA; <sup>2</sup>Buck Institute for Age Research, Novato, CA*
- ThP 451 **Scheduled Collision Energy Improves the Proteome Coverage and Quantification Accuracy by iTRAQ;** Jian-Ying Zhou; Lijun Chen; Daniel W. Chan; Hui Zhang; *Johns Hopkins School of Medicine, Baltimore, MD*

#### Biomolecular Structure Analysis: Chemical Crosslinking, 452 - 468

- ThP 452 **New Chemical Cross-Linking Methodology for Acidic Side Chain Residues;** Mariana Fioramonte<sup>1</sup>; Fabio C Gozzo<sup>2</sup>; *<sup>1</sup>University of Campinas, Campinas, Brazil; <sup>2</sup>IQ - University of Campinas, Campinas, Brazil*
- ThP 453 **Use of Cross-Linking/Mass Spectrometry to Predict Tertiary Structure of a Polyketide Synthase;** Hugo César Ramos De Jesus<sup>1</sup>; Gabriela Desireé Tormet González<sup>1</sup>; Luciana Gonzaga de Oliveira<sup>1</sup>; Tiago S. Balbuena<sup>2</sup>; Fabio C. Gozzo<sup>1</sup>; *<sup>1</sup>State University of Campinas - UNICAMP, Campinas, Brazil; <sup>2</sup>São Paulo State University - UNESP, Jaboticabal, Brazil*
- ThP 454 **Applications of New Reagents for *in vitro* and *in vivo* Chemical Crosslinking of Protein Complexes by Mass Spectrometry (CXL-MS);** Angela Walker; Lolita Piersimoni; Chunchao Zhang; Hye Kyong Kweon; Eric Tse; Billy Samulak; Janine Maddock; Daniel Southworth; Hollis Showalter; Philip Andrews; *University of Michigan, Ann Arbor, MI*
- ThP 455 **Using Isotopically-Coded N-terminal Modification and Non-Specific Proteinase K Digestion for the Identification of Zero-Length Crosslinks;** Jason Serpa<sup>1</sup>; Evgeniy Petrotchenko<sup>1</sup>; Christoph Borchers<sup>1,2</sup>; *<sup>1</sup>University of Victoria-Genome BC Proteomics Centre, Victoria, Canada; <sup>2</sup>UVic Dept of Biochemistry and Microbiology, Victoria, Canada*
- ThP 456 **Improving Cross-Linked Peptide Identification in Megadalton Complexes across Different High Resolution Instrument Platforms;** Romina Hofele<sup>1</sup>; Chung-Tien Lee<sup>1</sup>; Olexandr Dybkov<sup>1</sup>; Christof Lenz<sup>1,2</sup>; Henning Urlaub<sup>1,2</sup>; *<sup>1</sup>Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; <sup>2</sup>Inst. for Clin. Chem., Univ. Med. Center Göttingen, Göttingen, Germany*
- ThP 457 **Mass-spectrometry-Based Quantitative Protein-RNA Cross-Linking Study;** Saadia Qamar<sup>1</sup>; Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Oliver Kohlbacher<sup>2</sup>; Henning Urlaub<sup>1,3</sup>; *<sup>1</sup>Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; <sup>2</sup>University of Tübingen, Tübingen, Germany; <sup>3</sup>University Medical Center Göttingen, Göttingen, Germany*
- ThP 458 **Protein-RNA Contacts in CRISPR-Cas Protein Complexes of the Prokaryotic Adaptive Immune Systems;** Kundan Sharma<sup>1</sup>; Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Oliver Kohlbacher<sup>2</sup>; Raymond Staals<sup>3</sup>; Tim Künne<sup>3</sup>; Stan J. J. Brouns<sup>3</sup>; John Van der Oost<sup>3</sup>; Henning Urlaub<sup>1,4</sup>; *<sup>1</sup>Max Planck Institute for Biophysical Chemistry, Göttingen, Germany; <sup>2</sup>University of Tübingen, Tübingen,*

- Germany; <sup>3</sup>Wageningen University, Wageningen, The Netherlands; <sup>4</sup>University Medical Center Göttingen, Göttingen, Germany
- ThP 459 **DTT Mediates Site-Specific Protein/RNA Crosslinking upon UV Irradiation;** Uzma Zaman<sup>1</sup>; Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Oliver Kohlbacher<sup>2</sup>; Christof Lenz<sup>1,3</sup>; Henning Urlaub<sup>1,3</sup>; <sup>1</sup>Max Planck Institute for biophysical Chemistry, Goettingen, Germany; <sup>2</sup>Applied Bioinformatics group, Tuebingen, Germany; <sup>3</sup>University Medical Center, Goettingen, Goettingen, Germany
- ThP 460 **Structural Mass Spectrometric Analysis of FOXO Transcription Factor/DNA Response Element Interaction;** Hynek Mrazek<sup>1</sup>; John Mangrum<sup>2</sup>; Matteo Scalabrin<sup>2</sup>; Petr Man<sup>1,3</sup>; Daniele Fabris<sup>2</sup>; Petr Novak<sup>1,3</sup>; <sup>1</sup>Institute of Microbiology, ASCR, Prague, Czech Republic; <sup>2</sup>The RNA Institute, University at Albany, Albany, NY; <sup>3</sup>Faculty of Sciences, Charles University, Prague, Czech Republic
- ThP 461 **An Electrochemistry-Assisted Cross-Linking Method for Probing Protein Conformational Structures by Mass Spectrometry;** Qiuling Zheng<sup>1</sup>; Hao Zhang<sup>2</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Ohio University, Athens, OH; <sup>2</sup>Washington University in St. Louis, St. Louis, MO
- ThP 462 **Defining Structural Dynamics of Protein Complexes Using Quantitative Cross-linking Mass Spectrometry;** Clinton Yu<sup>1</sup>; Haibin Mao<sup>2</sup>; Eric Novitsky<sup>1</sup>; Shenheng Guan<sup>3</sup>; Scott Rychnovsky<sup>1</sup>; Ning Zheng<sup>2</sup>; Lan Huang<sup>1</sup>; <sup>1</sup>University of California, Irvine, Irvine, CA; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>University of California, San Francisco, San Francisco, CA
- ThP 463 **Improved Identification of Cross-Linked Peptides via an Optimized 2D High-/Low-pH RPLC-MSn Workflow;** Alex Huszagh; Wang Xiaorong; Yingying Yang; Clinton Yu; Eric James Novitsky; Scott Rychnovsky; Lan Huang; *University of California, Irvine, Ca*
- ThP 464 **Protein Interactions and Topologies in Antibiotic Resistant *Acinetobacter baumannii* Cells;** Xia Wu; Juan D. Chavez; Chunxiang Zheng; Arti Navare; Devin Schweppe; Jimmy K. Eng; Pradeep K. Singh; Colin Manoil; James E. Bruce; *University of Washington, Seattle, WA*
- ThP 465 **Protein Interaction Topologies in Cells: A View from the Inside;** James Bruce; Juan Chavez; Arti Navare; Devin Schweppe; Chunxiang Zheng; Xia Wu; *University of Washington, Seattle, WA*
- ThP 466 **Quantifying Protein-Protein Interactions with Protein Interaction Reporter Technology;** Juan Chavez; Chunxiang Zheng; Jimmy K. Eng; James Bruce; *University of Washington, Seattle, WA*
- ThP 467 **Probing Conformation of G Protein-Coupled Receptor 110 by Chemical Crosslinking and Mass Spectrometry;** Bill Huang; Ji-Won Lee; Hee-Yong Kim; *NIAAA/NIH, Rockville, MD*
- ThP 468 **Diazo Crosslinkers as Structural Probes for MS-based Elucidation of Nucleic Acids and Protein-Nucleic Acid Complexes;** Matteo Scalabrin; Sugyan Dixit; Daniele Fabris; *University at Albany, The RNA Institute, Albany, NY*
- Ion Mobility: Fundamentals, 469 - 482**
- ThP 469 **UVPD and IMS-MS: Photodissociation of Ions Selected by Drift-Time Separation and/or m/z Ratio;** Jeff Brown<sup>1</sup>; Bruno Bellina<sup>3</sup>; Kevin Giles<sup>1</sup>; Mike Morris<sup>1</sup>; Isabelle Compagnon<sup>2</sup>; Perdita Barran<sup>3</sup>; <sup>1</sup>Waters Corporation, Wilmslow, UK; <sup>2</sup>Université Lyon 1, Lyon, France; <sup>3</sup>The University of Manchester, Manchester, UK
- ThP 470 **Additional Models of a Mammalian Cryptochrome – E3 Ubiquitin Ligase Complex Restrained by Results from Ion Mobility Mass Spectrometry;** Samuel Marionni; Weiman Xing; Ning Zheng; Matthew Bush; *University of Washington, Seattle, WA*
- ThP 471 **Exploring the Relationship between Incremental and Conformational Contributions to the Collision Cross Section of Nucleic Acid-Ligand Complexes;** Jennifer Lippens<sup>1</sup>; Bill Redick<sup>1</sup>; Katharyn Wendt<sup>1</sup>; Srivathsan Ranganathan<sup>1</sup>; Jacob Miner<sup>2</sup>; Angel Garcia<sup>2</sup>; D Fabris<sup>1</sup>; <sup>1</sup>The RNA Institute, University at Albany, Albany, NY; <sup>2</sup>Rensselaer Polytechnic Institute (RPI), Troy, NY
- ThP 472 **Novel Real-Time Dual Filtering Technique for Multiplexed IM-QTOF All-Ions Analysis of Complex Protein Digests;** Bruce Wang; William Frazer; Christian Klein; Ruwan Kurulugama; Edward Darland; George Stafford; Gregor Overney; *Agilent Technologies, Santa Clara, CA*
- ThP 473 **Using Differential Mobility Spectrometry to Measure the Interactions of Hormone Peptides with Divalent Metal Ions and Solvent Molecules;** Chang Liu<sup>1</sup>; J. Larry Campbell<sup>1</sup>; J.C. Yves Leblanc<sup>1</sup>; Jefry Shields<sup>2</sup>; John S. Janiszewski<sup>2</sup>; <sup>1</sup>AB SCIEX, Concord, ON, Canada; <sup>2</sup>Pfizer Inc., Groton, CT
- ThP 474 **Limits to the Mobility-Selected Current Transmitted and to the Chemical Background in a Differential Mobility Analyzer (DMA);** Mario Amo-Gonzalez<sup>2</sup>; Juan Fernandez De La Mora<sup>1</sup>; <sup>1</sup>Yale University - Mechanical Engineering Department, New Haven, CT; <sup>2</sup>SEADM, Boecillo, Valladolid, Spain
- ThP 475 **Electrical Mobilities of Near-Spherical, Positively- and Negatively-Charged Ionic Liquid Nanodrops in Monatomic and Polyatomic gases: Influence of Ion-Induced Dipole Interactions;** Juan Fernández-García; Juan Fernández de la Mora; *Yale University, New Haven, CT*
- ThP 476 **Tandem Transversal Modulation IMS and Linear Trap Quadrupole MS: Towards a Functional Ion Mobility System for Ion Trap MS;** Miriam Macia<sup>1</sup>; Cesar Barrios<sup>1,2</sup>; Guillermo Vidal de Miguel<sup>1</sup>; <sup>1</sup>SEADM S.L., Boecillo, SPAIN; <sup>2</sup>University of Valladolid, Valladolid, Spain
- ThP 477 **Enhanced Separation Capacity via Vapor Doping in Tandem Transversal Modulation IMS-IMS-MS;** Vivek Rawat<sup>2</sup>; Chris Hogan<sup>2</sup>; Guillermo Vidal de Miguel<sup>1</sup>; <sup>1</sup>SEADM S.L., Boecillo, Spain; <sup>2</sup>University of Minnesota, Minneapolis, Minnesota
- ThP 478 **Development of the Periodic Focusing Differential Mobility Analyzer (PFDMA)- a portable, high resolution ion mobility spectrometer;** Kent Gillig; Chung-Hsuan Chen; *Academia Sinica, Taipei, Taiwan*
- ThP 479 **A Molecular Modeling Study on the Collision Cross Section for Ion Mobility Spectrometry;** Glenn E. Spangler; *Technispan LLC, Lutherville, MD*
- ThP 480 **Validation of an Improved Momentum-Transfer Theory for Ion Mobility Using Accurate Hard-Sphere Kinetic Computations;** William F. Siems<sup>1</sup>; Larry Viehland<sup>2</sup>; Herbert H. Hill, Jr<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Chatham University, Pittsburgh, PA
- ThP 481 **AT-Hook Peptide and Protein Isomerization Dynamics: Solution vs Gas-Phase;** Emily Schenk<sup>1</sup>; Genevieve Gozo<sup>1</sup>; Mark Ridgeway<sup>2</sup>; Melvin A. Park<sup>2</sup>; Fenfei Leng<sup>1</sup>; Francisco Fernandez Lima<sup>1</sup>; <sup>1</sup>Florida International University, Miami, FL; <sup>2</sup>Bruker Daltonic, Inc., Billerica, MA
- ThP 482 **Understanding Global Ion Mobility Separation Differences of Biomolecules in Alternative Drift Gases;** Jody C. May<sup>1</sup>; Katrina L. Leaprot<sup>1</sup>; Nichole M. Lareau<sup>1</sup>; Ruwan T. Kurulugama<sup>2</sup>; George C. Stafford<sup>2</sup>; Alex Mordehai<sup>2</sup>; John C. Fjeldsted<sup>2</sup>; John A. Mclean<sup>1</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>Agilent Technologies, Santa Clara, CA



## Ion Mobility: Applications, 483 - 512

- ThP 483 **Data-Independent Analysis of Proteomic Samples Utilizing in-Frame Collision Energy Ramping by Drift Tube based Ion Mobility Mass Spectrometry;** Christian Klein<sup>1</sup>; Ed Darland<sup>1</sup>; Bill Frazer<sup>1</sup>; Kevin Crowell<sup>2</sup>; Bill Barry<sup>1</sup>; Ruwan Kurulugama<sup>1</sup>; Bruce Wang<sup>1</sup>; Alex Mordehai<sup>1</sup>; Gregor Overney<sup>1</sup>; George Stafford<sup>1</sup>; John Fjeldsted<sup>1</sup>; <sup>1</sup>Agilent Technologies, Inc, Santa Clara, CA; <sup>2</sup>Pacific Northwest National Lab, Richland, WA
- ThP 484 **Evaluation of a High Performance Ion Mobility-MS Platform for Structural Measurements in Different Drift Gases Combined with Computational Strategies;** Ruwan T. Kurulugama<sup>1</sup>; Alex Mordehai<sup>1</sup>; Nathan Sanders<sup>1</sup>; Sarah M. Stow<sup>2</sup>; Jody C. May<sup>2</sup>; John A. McLean<sup>2</sup>; George C. Stafford<sup>1</sup>; John C. Fjeldsted<sup>1</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Vanderbilt University, Nashville, TN
- ThP 485 **Structural Mass Spectrometry of Protein Modification by Unique Oxidation Processes;** Libin Xu<sup>1,2</sup>; Jay G. Forsythe<sup>1,2</sup>; Jody C. May<sup>1,2</sup>; Keri A. Tallman<sup>1,2</sup>; Ned A. Porter<sup>1,2</sup>; John A. McLean<sup>1,2</sup>; <sup>1</sup>Department of Chemistry, Vanderbilt University, Nashville, TN; <sup>2</sup>VICB, Vanderbilt University, Nashville, TN
- ThP 486 **Combined Electron Transfer Dissociation-Ion Mobility-Collision Induced Dissociation-Mass Spectrometry Techniques for the Characterization of Proteins, Glycans, and Glycoproteins;** Nichole M. Lareau; Jody C. May; John A. McLean; Vanderbilt University, Nashville, TN
- ThP 487 **Structural Analysis of Protein Complexes using Integrated Crosslinking and Ion Mobility-Mass Spectrometry;** Billy Samulak; Philip Andrews; Brandon Ruotolo; University of Michigan, Ann Arbor, MI
- ThP 488 **Site-Directed Mutagenesis of Amyloid  $\beta$  to Elucidate Binding Location of Leucine-Enkephaline Using Ion Mobility - Mass Spectrometry;** Molly Soper; Brandon Ruotolo; University Of Michigan, Ann Arbor, MI
- ThP 489 **Ion Mobility Mass Spectrometry and Chemical Crosslinking Reveal the 3D Architecture of the Urease Pre-Activation Complex;** Joseph Eschweiler<sup>1</sup>; Mark Farrugia<sup>2</sup>; Robert Hausinger<sup>2</sup>; Brandon Ruotolo<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>Michigan State University, East Lansing, MI
- ThP 490 **Kinase Inhibitor Discovery through Ion Mobility-Mass Spectrometry: New Targets and Larger Libraries;** Jessica Rabuck-Gibbons<sup>1</sup>; Matthew Soellner<sup>2</sup>; Brandon Ruotolo<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Michigan, Ann Arbor, MI; <sup>2</sup>College of Pharmacy, University of Michigan, Ann Arbor, MI
- ThP 491 **Characterization of  $\beta$ -Cyclodextrin-Cholesterol-Ca<sup>2+</sup> Complexes by Drift Tube Ion Mobility (IMS-MS);** Alfred L. Yergey<sup>1</sup>; Christian Klein<sup>2</sup>; Stephanie Cologna<sup>1</sup>; Paul S. Blank<sup>1</sup>; Ruwan Kurulugama<sup>2</sup>; Alex Mordehai<sup>2</sup>; William Barry<sup>2</sup>; Ed Darland<sup>2</sup>; Peter S. Backlund<sup>1</sup>; <sup>1</sup>NIH, Bethesda, MD; <sup>2</sup>Agilent Technologies, Santa Clara, CA
- ThP 492 **Discrimination of Epimeric Glycans and Glycopeptides using Travelling Wave Ion-Mobility Mass Spectrometry: towards a Comprehensive Carbohydrate Sequencing Strategy;** Christopher Gray<sup>1</sup>; Peter Both<sup>1</sup>; Anthony Green<sup>1</sup>; Robert Šardžik<sup>1</sup>; Josef Voglmeir<sup>2</sup>; Dominique Richardson<sup>1</sup>; Goran Widmalm<sup>4</sup>; Sabine Flitsch<sup>1</sup>; Rob Field<sup>3</sup>; Claire Eyers<sup>5</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>Nanjing Agricultural University, Nanjing, China; <sup>3</sup>John Innes Centre, Norwich, UK; <sup>4</sup>Stockholm University, Stockholm, Sweden; <sup>5</sup>University of Liverpool, Liverpool, UK
- ThP 493 **Large-Scale Structural Analysis of Proteolytic Peptides with C-terminal and N-terminal Lysine Residues;** Christopher Lietz; Qing Yu; Xueqin Pang; Lingjun Li; University of Wisconsin, Madison, WI
- ThP 494 **IMS-MS Analysis of the Protein Complex GroEl Reveals Dimers, Trimers, Heptamers, and 11-mers with Widely Different Compactness;** Juan Fernandez De La Mora<sup>1</sup>; Chris Hogan<sup>2</sup>; <sup>1</sup>Yale University - Mechanical Engineering Department, New Haven, CT; <sup>2</sup>University of Minnesota, Minneapolis, Minnesota
- ThP 495 **Ion Mobility-Mass Spectrometry for Molecular Nanomaterials;** Kellen M. Harkness<sup>1</sup>; Andrzej Balinski<sup>2</sup>; Jay G. Forsythe<sup>2</sup>; David E. Cliffel<sup>2</sup>; John A. McLean<sup>2</sup>; Francesco Stellacci<sup>1</sup>; <sup>1</sup>Ecole Polytechnique Federale de Lausanne, Lausanne, CH; <sup>2</sup>Vanderbilt University, Nashville, TN
- ThP 496 **Simultaneous Quantification of Acridinium and its Metabolites in Human Plasma using LC-MS/MS Coupled with SelexION™ Technology;** Qingguo Tian<sup>1</sup>; Haodan Yuan<sup>1</sup>; Jordi Aubets<sup>2</sup>; Josep Jansat<sup>2</sup>; Daksha Desai-Krieger<sup>1</sup>; Andreas Grill<sup>1</sup>; <sup>1</sup>Forest Laboratories, Inc., Farmingdale, NY; <sup>2</sup>Almirall S.A., Sant Feliu de Llobregat, Spain
- ThP 497 **Solving Selectivity Challenges in Qualitative and Quantitative Analysis of Drugs and Metabolites;** Kaoru Karasawa<sup>1</sup>; Suma Ramagiri<sup>2</sup>; Carmai Seto<sup>2</sup>; Natalia Penner<sup>3</sup>; <sup>1</sup>AB SCIEX, Tokyo, Japan; <sup>2</sup>AB SCIEX, Concord, ON; <sup>3</sup>Biogen Idec, Cambridge, MA
- ThP 498 **Comprehensive Two-Dimensional Separation of Alcohol Ethoxylates Coupling Ion Mobility-Mass Spectrometry and Hydrophilic Interaction Chromatography Using a Customized Sub-2  $\mu$ m Column;** Qiang Ma<sup>1,2</sup>; Xi Chen<sup>3</sup>; Hua Bai<sup>1</sup>; Chao Wang<sup>1</sup>; <sup>1</sup>Chinese Academy of Inspection and Quarantine, Beijing, China; <sup>2</sup>Purdue University, West Lafayette, IN; <sup>3</sup>Waters Corporation, Shanghai, China
- ThP 499 **Separation of Aromatic Amino Acids Enantiomers by traveling Wave Ion Mobility – Mass Spectrometry;** Virginie Domalain<sup>1</sup>; Marie Hubert-Roux<sup>1</sup>; Catherine Lange<sup>1</sup>; Jacques Rouden<sup>2</sup>; Carlos Afonso<sup>1</sup>; <sup>1</sup>Normandie Univ UMR 6014, FR 3038; Univ Rouen; CNRS, Mont Saint Aignan, France; <sup>2</sup>Normandie Univ UMR 6507, FR 3038; ENSICAEN; CNRS, Caen, France
- ThP 500 **An Investigation of 3-methylxanthine Supramolecular Complexes using Field Asymmetric Waveform and Drift Tube Ion Mobility Spectrometry Combined with Mass Spectrometry;** Kayleigh Arthur; James Reynolds; Colin Creaser; Loughborough University, Loughborough, UK
- ThP 501 **ATP-induced Reduction in Conformational Flexibility of a Membrane-embedded Rotary ATPase: Evidence from Ion Mobility Mass Spectrometry;** Min Zhou<sup>1,2</sup>; Argyris Politis<sup>1,3</sup>; Roberta.B Davies<sup>4,5</sup>; Ildir Liko<sup>1</sup>; Kuan-Jung Wu<sup>1</sup>; Alastair G. Stewart<sup>4,5</sup>; Daniela Stock<sup>4,5</sup>; Carol V. Robinson<sup>1</sup>; <sup>1</sup>University of Oxford, Oxford, UK; <sup>2</sup>Nanjing University of Science and Technology, Nanjing, China; <sup>3</sup>University of Ulster, Ulster, UK; <sup>4</sup>The Victor Chang Cardiac Research Institute, Darlinghurst, Australia; <sup>5</sup>The University of New South Wales, Sydney, Australia
- ThP 502 **Formation of Intramolecular H-bonds Retains Discrete Conformations of Cyclic peptides;** Suk-Joon Hyung; Xidong Feng; Ye Che; Justin Stroh; Michael Shapiro; Pfizer, Groton, CT
- ThP 503 **Contribution of Ion Mobility for Structural Analysis and Analytical Chemistry: the Use of Selective IMS Shift Reagents;** Christopher Kune; Johann Far; Cédric Delvaux; Gauthier Eppe; Edwin De Pauw; Mass spectrometry laboratory, University of Liège, Liège, Belgique
- ThP 504 **Characterization of the Retinal Protonated Schiff Base in the Gas Phase by Photoisomerization Action Spectroscopy;** Neville Coughlan; Katherine Catani; Brian Adamson; Evan Bieske; University of Melbourne, Melbourne, Australia

- ThP 505 **Differential Mobility Spectrometry as a Measure of ion Solvation: The Roles of Solvents and Ionic Structures for Separating Quinoline-Based Drugs;** J. Larry Campbell<sup>1</sup>; J.C. Yves Leblanc<sup>1</sup>; Chang Liu<sup>1</sup>; John Janiszewski<sup>2</sup>; W. Scott Hopkins<sup>3</sup>; Gene F. Ye<sup>3</sup>; <sup>1</sup>AB SCIEX, Concord, ON, ON; <sup>2</sup>Pfizer Inc., Groton, CT; <sup>3</sup>University of Waterloo, Waterloo, ON
- ThP 506 **Differential Mobility Spectrometry for Gas-Phase Fractionation Increases Proteome Coverage and Improves Ion Library Creation for SWATH™ Acquisition;** Mark Cafazzo<sup>1</sup>; Christie L Hunter<sup>2</sup>; Samuel L Bader<sup>3</sup>; Robert L Moritz<sup>3</sup>; <sup>1</sup>AB SCIEX, Framingham, MA; <sup>2</sup>AB SCIEX, Foster City, CA; <sup>3</sup>ISB, Seattle, WA
- ThP 507 **Enhanced Separation and Ion Prefiltering using a High Performance Ion Mobility Device Coupled with the LTQ series of Mass Spectrometers;** Adam M Graichen<sup>1</sup>; Robert Jackson<sup>1</sup>; Ching Wu<sup>1</sup>; Mark Osgood<sup>1</sup>; Dirk Nolting<sup>2</sup>; Alexander Makarov<sup>2</sup>; <sup>1</sup>Excellims Corporation, Acton, MA; <sup>2</sup>Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 508 **Electrospray Ionization Mechanisms for Large Polyethylene Glycol Chains studied through IMS-IMS separation;** Carlos Larriba Andaluz<sup>1</sup>; Juan Fernandez De La Mora<sup>2</sup>; David Clemmer<sup>3</sup>; <sup>1</sup>University of Minnesota, Minneapolis, MN; <sup>2</sup>Yale University - Mechanical Engineering Department, New Haven, CT; <sup>3</sup>Indiana University, Bloomington, IN
- ThP 509 **Analysis of Positional Poly(Pyridylalkyl Methacrylate) Isomers by Ion Mobility and Electrospray Ionization Mass Spectrometry;** Michelle Kushnir; Chrys Wesdemiotis; University of Akron, Akron, OH
- ThP 510 **Characterization of Giant Calixarenes by MALDI MS and Ion Mobility Spectrometry;** Esra Altuntas<sup>1</sup>; Marion Rollet<sup>1</sup>; Didier Gignes<sup>1</sup>; Vincent Huc<sup>2</sup>; Laurence Charles<sup>1</sup>; <sup>1</sup>Aix-Marseille University, Marseille, France; <sup>2</sup>University Paris-Sud, Paris, France
- ThP 511 **Absolute Quantitation of an Amyloidogenic HIV infection-enhancing Human Semen Peptide using MALDI TOF IM-MS;** Haichuan Liu<sup>1</sup>; Nadia Roan<sup>2,3</sup>; Jason Neidleman<sup>3</sup>; Susan Fisher<sup>1</sup>; Warner Greene<sup>3</sup>; H. Ewa Witkowska<sup>1</sup>; <sup>1</sup>UCSF Sandler-Moore Mass Spectrometry Core Facility, San Francisco, CA; <sup>2</sup>Department of Urology, University of California, San Francisco, CA; <sup>3</sup>Gladstone Institute of Virology and Immunology, San Francisco, CA
- ThP 512 **Data-independent MS<sup>F</sup> with Ion Mobility Identifies GPX4 as a New Target for Anti-Cancer Drugs;** Lewis M. Brown<sup>1</sup>; Rohitha SriRamaratnam<sup>1</sup>; Wan Seok Yang<sup>1</sup>; Matthew E. Welsch<sup>1</sup>; Kenichi Shimada<sup>1</sup>; Rachid Skouta<sup>1</sup>; Vasanthi S. Viswanathan<sup>2</sup>; Jaime H. Cheah<sup>2</sup>; Paul A. Clemons<sup>2</sup>; Alykhan F. Shamji<sup>2</sup>; Clary B. Clish<sup>2</sup>; Albert W. Girotti<sup>3</sup>; Virginia W. Cornish<sup>1</sup>; Stuart L. Schreiber<sup>2</sup>; Brent R. Stockwell<sup>1,4</sup>; <sup>1</sup>Columbia University, New York, NY; <sup>2</sup>Broad Institute of Harvard and MIT, Cambridge, MA; <sup>3</sup>Medical College of Wisconsin, Milwaukee, WI; <sup>4</sup>Howard Hughes Medical Institute, New York, NY
- Nucleic Acids, 513 - 526**
- ThP 513 **Energetics Comparison of the Venturi Easy Ambient Sonic-spray Ionization and Development of an Original Dual Sprayer Device;** Bessem Brahim<sup>1</sup>; Denis Lesage<sup>1</sup>; Sandra Alves<sup>1</sup>; Marcos Eberlin<sup>2</sup>; Richard Cole<sup>1</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>UPMC (Paris 6), Paris, France; <sup>2</sup>UNICAMP, Campinas, Brazil
- ThP 514 **Sequence-scrambling in Collision-induced Dissociation of Oligonucleotides;** Brett Harper; Elizabeth Neumann; Touradj Solouki; Baylor University, Waco, TX
- ThP 515 **Charge and Signal Enhancement in Negative Mode Electrospray Mass Spectrometry of DNA Oligomers: Effects of Additives and Solvent Compositions;** You-Jun Fu; Paritosh Pande; Ashis Basu; Department of Chemistry, University of Connecticut, Storrs, CT
- ThP 516 **A Method for RNA Epigenetics: Enhancing the Comparative Analysis of RNA Digests for Modification Mapping via Isotope Enrichment;** Collin Wetzel; Patrick Limbach; University of Cincinnati, Cincinnati, OH
- ThP 517 **An Exclusion List Strategy to Improve Detection of Modified Oligonucleotides from RNA;** Xiaoyu Cao; Patrick Limbach; University of Cincinnati, Cincinnati, OH
- ThP 518 **Alternative Ammonium Acetate Mobile Phases for LC-MS/MS Analysis of Oligonucleotides;** Kirk Gaston; Patrick Limbach; University of Cincinnati, Cincinnati, OH
- ThP 519 **Unbiased identification of Protein-RNA Contact Sites in vivo at Amino Acid and Nucleotide Resolution after UV Cross-Linking;** Katharina Kramer<sup>1</sup>; Timo Sachsenberg<sup>2</sup>; Benedikt Beckmann<sup>3</sup>; Saadia Qamar<sup>1</sup>; Matthias W. Hentze<sup>3</sup>; Oliver Kohlbacher<sup>2</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; <sup>2</sup>University of Tübingen, Tübingen, Germany; <sup>3</sup>European Molecular Biology Laboratory EMBL, Heidelberg, Germany
- ThP 520 **Direct Identification and Characterization of Human Cellular microRNAs by Liquid Chromatography – Tandem Mass Spectrometry and Database Searching;** Hiroshi Nakayama<sup>1,2</sup>; Yoshio Yamauchi<sup>3</sup>; Masato Taoka<sup>3</sup>; Toshiaki Isobe<sup>2,3</sup>; <sup>1</sup>RIKEN, Wako, Japan; <sup>2</sup>CREST, JST, Tokyo, Japan; <sup>3</sup>Tokyo Metropolitan University, Tokyo, Japan
- ThP 521 **Accurate Identification of small RNAs Loaded into the RNA-Induced Silencing Complex by Immunocapture LC-MS;** Kristin L. Geddes; Charles D. Thompson; Mark T. Cancilla; Merck, West Point, PA
- ThP 522 **Quantification of DNA Adducts of 1, 3-Butadiene in vivo Using NanoLC/ESI<sup>+</sup> High Resolution MS<sup>3</sup> Mass Spectrometry (nanoLC/ESI<sup>+</sup>-HRMS<sup>3</sup>);** Dewakar Sangaraju; Peter Villalta; Natalia Tretyakova; University of Minnesota, Minneapolis, MN
- ThP 523 **Determination of N7-methyl-Guanine DNA Adducts by Liquid Chromatography – Tandem Mass Spectrometry;** Benjamin Moeller<sup>1</sup>; Leonard Collins<sup>2</sup>; Marcie Grimes<sup>1</sup>; Philip Kuehl<sup>1</sup>; Steven Belinsky<sup>1</sup>; James Swenberg<sup>1</sup>; Jacob McDonald<sup>1</sup>; <sup>1</sup>Lovelace Respiratory Research Institute, Albuquerque, NM; <sup>2</sup>University of North Carolina, Chapel Hill, NC
- ThP 524 **High Resolution LC/MS/MS Study of the Interactions of Inorganic Mercury (II) with Nucleic Acids Rich in Thymine;** Janna Anichina; Andre Schreiber; Takeo Sakuma; AB SCIEX, Concord, Canada
- ThP 525 **LC ESI MS Analysis of RNA using Metabolic and Chemical Labeling Methods;** Alison Nwokeoji; An-Wen Kung; Sakharam Waghmare; Mark Dickman; University of Sheffield, Sheffield, UK
- ThP 526 **GMP-Compliant Analysis of Large RNA/DNA Hybrids in Preparation of a Clinical Trial;** Roger E. Moore; Denise A. Keen; Piotr Swiderski; Bogdan-Gabriel Gugiu; Christopher Lincoln; Markus Kalkum; City of Hope, Duarte, CA
- Traditional Chinese Medicine, 527 - 530**
- ThP 527 **Rapid Screening and Quantitative Analysis of 87 Pesticide Residues in Traditional Chinese Medicinal Herbs by Liquid Chromatography-Tandem Mass Spectrometry;** Zhi Cheng<sup>2</sup>; Meiling Lu<sup>3</sup>; Rong Zhang<sup>1</sup>; Ying Liu<sup>1</sup>; Minglin Wang<sup>2</sup>; Jinhua Wang<sup>1</sup>; <sup>1</sup>Beijing Entry-Exit Inspection&Quarantine Bureau, Beijing, China; <sup>2</sup>Shandong Agriculture University, Taian, China; <sup>3</sup>Agilent Technologies Beijing, Beijing, China

- ThP 528 **Determination of Synthetic Adulterants in Dietary Supplements and Traditional Chinese Medicines (TCM) using liquid Chromatography-Tandem Mass Spectrometry with Triggered MRM;** [Yue Song](#)<sup>1</sup>; Shao-Zhen Wang<sup>1</sup>; Man-Yu Zhang<sup>1</sup>; Wen-Yen Lee<sup>1</sup>; Shan-An Chan<sup>2</sup>; <sup>1</sup>Agilent, Shanghai, China; <sup>2</sup>Agilent Taipei, Taiwan
- ThP 529 **Identify Chemical and Herbal Components of an Unknown TCM Product Using LC/MS Coupled with a Novel Informatics Platform;** Lirui Qiao<sup>1</sup>; JIng Huang<sup>1</sup>; Diane Diehl<sup>2</sup>; [Kate Yu](#)<sup>2</sup>; <sup>1</sup>Waters China, Shanghai, China; <sup>2</sup>Waters Corporation, Milford, MA
- ThP 530 **Rapid Identification of Complex Constituents in Cordyceps Cicadae using High Resolution Mass Spectrometry with Targeted and Non-Targeted Processing Workflows;** Bo Tan<sup>1</sup>; Yizhun Zhu<sup>1</sup>; [Ting Liu](#)<sup>2</sup>; Kerong Zhang<sup>2</sup>; Cheng Yang<sup>2</sup>; <sup>1</sup>School of Pharmacy Fudan University, Shanghai, CHINA; <sup>2</sup>AB Sciex Company, Shanghai, China
- High Mass Accuracy / High Performance MS: Applications, 531 - 547**
- ThP 531 **A Miniature Capillary Electrophoresis Mass Spectrometry System;** [Yinna Zhang](#)<sup>1</sup>; Zejian Huang<sup>2</sup>; Wei Xu<sup>1</sup>; <sup>1</sup>Beijing Institute Of Technology, Beijing, China; <sup>2</sup>Chinese Scientific Metrology Institute, Beijing, China
- ThP 532 **The Characterization of Polysorbates and the Identification of Their Breakdown Products by Tandem High Speed Mass Spectrometry;** [Stephen Rumbelow](#)<sup>1</sup>; James Ferguson<sup>2</sup>; Johnnie Brown<sup>2</sup>; Keith Goodman<sup>2</sup>; <sup>1</sup>Croda Inc, New Castle, DE; <sup>2</sup>AB SCIEX, Framingham, MA
- ThP 533 **Ultra High Performance Liquid Chromatography Tandem Quadrupole-Time of Flight Mass Spectrometry for the Identification of Major Impurities in Synthesized Pharmaceuticals;** [Tao Bo](#); Zheng-Xiang Zhang; We Du; Agilent Technologies (China), Beijing, China
- ThP 534 **Systematic Analysis of Urinary Proteome using Curated Spectral Library;** [Nina Khristenko](#); Adèle Bourmaud; Suruchi Gutgutia; Sebastien Gallien; Bruno Domon; Luxembourg Clinical Proteomics Center, Strassen, Luxembourg
- ThP 535 **Bioanalytical Method Development for the Quantitative Analysis of a Polymer CAPA for Stability Study in Phosphate Buffered Saline;** [Xiaohui Chen](#); Stephanie Dodd; Upendra Argikar; Jakal Amin; Panos Hatsis; Novartis, Cambridge, MA
- ThP 536 **Rapid Differentiation of isobaric Drugs using a Novel Direct Sample Analysis Source, CID, and Accurate Mass TOF Mass Spectrometry;** [Robert J. Seward](#); Bonnie Marmor; Andrew Tyler; PerkinElmer, Waltham, MA
- ThP 537 **Identification and Quantification of Contaminants in Compressor Oil by High Resolution LCMS;** [Zhibin Zhang](#)<sup>1</sup>; Kate Comstock<sup>2</sup>; <sup>1</sup>Emerson Climate Technology, Sidney, OH; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 538 **Determination of Ribavirin Triphosphate in Rat Blood and Liver by Liquid Chromatography/High-Resolution Accurate Mass Spectrometry;** Yi Tao; [Hui Hong](#); Lirong Fan; Xin Zhang; WuXi AppTec Co., Shanghai, CHINA
- ThP 539 **Q Exactive Quantitation of Deuterium Enriched Isotopomers;** [Greg Waitt](#); Jon D. Williams; Todd Shearer; GlaxoSmithKline, Research Triangle Park, NC
- ThP 540 **FTMS-based Isotopic Simulator Improves Accuracy of Mass and Intensity Measurements;** Hans Pfaff; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 541 **ESI-Q-TOF Structural Characterization of Prominent MS/MS Product Ions of Veterinary Drugs for Improved Regulatory Monitoring;** [Alberto Nuñez](#)<sup>1</sup>; Steve Lehotay<sup>1</sup>; Lucia Geis-Asteggianti<sup>2</sup>; <sup>1</sup>USDA-ARS-ERRC, Wyndmoor, PA; <sup>2</sup>University of Maryland, College Park, MD
- ThP 542 **Proof of Principle Study: Non-Targeted Differential Analysis of Drug-Spiked Dog Urine vs. Control Urine;** [Hemakanthi De Alwis](#); Upul Nishshanka; U.S. Food and Drug Administration, Laurel, MD
- ThP 543 **Quantification of Triamcinolone Acetonide in Rabbit Plasma by Supported Liquid Extraction Followed by UHPLC-QTOF High Resolution Mass Spectrometry;** [Damon Papac](#); Alan Mueller; Navigen, Salt Lake City, UT
- ThP 544 **Detection of Persistent Organic Pollutants using Atmospheric Pressure Gas Chromatography and a Novel Acquisition Mode for Quadrupole Time-of-Flight MS;** Lauren Mullin<sup>1</sup>; Adam Ladak<sup>2</sup>; Kendon Graham<sup>1</sup>; Ingrid Ericson Jogsten<sup>3</sup>; [Gareth Cleland](#)<sup>1</sup>; Bert van Bavel<sup>3</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>Waters Corporation, Beverly, MA; <sup>3</sup>MTM Research Centre, Örebro University, Örebro, Sweden
- ThP 545 **Increasing Protein Sequence Coverage Exploring Alternative Enzymes in Combination with Decision-Tree Based Tandem Mass Spectrometry on the Orbitrap Fusion<br>abp="982">"; [Onno Bleijerveld](#)<sup>1</sup>; Liesbeth Hoekman<sup>1</sup>; A.F. Maarten Altelaar<sup>1,2</sup>; <sup>1</sup>The Netherlands Cancer Institute, Amsterdam, The Netherlands; <sup>2</sup>Utrecht University, Utrecht, Netherlands**
- ThP 546 **Rapid Automated Direct Infusion Ultrahigh Resolution Mass Spectrometry of siRNA and Their Metabolites from Various in vitro Biomatrices;** [Kristen Kwasnjuk](#); Christopher Kochansky; BaoJen Shyong; Charles Thompson; Mark Cancilla; Merck & Co., Inc., West Point, PA
- ThP 547 **New Algorithms and Workflow for Significantly Improved Untargeted 2-Sample-Comparison using High-Resolution Data from TOF/Q-TOF Mass Spectrometers;** [Frank Kuhlmann](#); Xiangdong Li; Agilent Technologies, Santa Clara, CA
- Environmental Analysis: General, 549 - 574**
- ThP 549 **Investigation of NOx Effect on Secondary Organic Aerosol Composition with Ultra-High Resolution 15 T FT-ICR Mass Spectrometry;** [Sun Jong Baek](#)<sup>1</sup>; Jun Hyun Park<sup>1</sup>; Ho-Jin Lim<sup>2</sup>; Hyun Sik Kim<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Chungbuk, South Korea; <sup>2</sup>Kyungpook National University, Daegu, South Korea
- ThP 550 **Chemical Mechanisms of Atmospheric Aging of Secondary Organic Aerosol;** [Peijun Tu](#); Murray Johnston; University of Delaware, Newark, DE
- ThP 551 **Rapid Separation of Hexabromocyclododecane Diastereomers and Enantiomers using a Novel Method Combining Supercritical Fluid Chromatography and MS/MS Detection;** [Lauren Mullin](#)<sup>1</sup>; Ingrid Ericson Jogsten<sup>2</sup>; Jennifer Burgess<sup>1</sup>; Andy Aubin<sup>1</sup>; Dawei Geng<sup>2</sup>; Kendon Graham<sup>1</sup>; Bert van Bavel<sup>2</sup>; <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>MTM Research Centre, Örebro University, Örebro, Sweden
- ThP 552 **Analytical Methods Assessment and Developments of Alternative Flame Retardants;** [Tan Guo](#); Yunzhui Wang; Myrto Petreas; JuneSoo Park; Department of Toxic Substance Control, Berkeley, CA
- ThP 553 **Secondary Organic Aerosol from Gas Phase Methylsiloxane Oxidation: Products and Reaction Mechanisms;** [Yue Wu](#); Murray Johnston; University of Delaware, Newark,
- ThP 554 **Identification of Intermediates from Ozone Oxidation of Oseltamivir Phosphate using an Ion Trap - Time of Flight Mass Spectrometry;** [Hong Youngmin](#)<sup>1,2</sup>; Jaewoo Song<sup>1</sup>; Ingyu Lee<sup>2</sup>; Hyunook Kim<sup>2</sup>; <sup>1</sup>Dong-il Shimadzu, Seoul, Republic of Korea; <sup>2</sup>The University of Seoul, Seoul, Republic of Korea

- ThP 555 **Comparing X!Tandem and Sequest Algorithms for Soil Metaproteomes;** Krystalle S. Diaz<sup>1</sup>; Eun-Hae Kim<sup>1</sup>; Robert M. Jones<sup>1</sup>; Ben J. Woodcroft<sup>2</sup>; Manesh B. Shah<sup>3</sup>; Gene W. Tyson<sup>2</sup>; Nathan C. Verberkmoes<sup>4</sup>; Virginia I. Rich<sup>1</sup>; <sup>1</sup>University of Arizona, Tucson, AZ; <sup>2</sup>University of Queensland, Queensland, Australia; <sup>3</sup>Oak Ridge National Laboratories, Oak Ridge, TN; <sup>4</sup>New England Biolabs Inc, Ipswich, MA
- ThP 556 **Non-Target and Post-Target Analysis of Organic Environmental Contaminants in River Sediments;** Jonathan Byer<sup>1</sup>; Brad Hill<sup>2</sup>; Joe Binkley<sup>1</sup>; <sup>1</sup>Leco Corporation, St Joseph, MI; <sup>2</sup>Environment Canada, Burlington, ON
- ThP 557 **Environmental Forensics Analysis in Proximity to Unconventional Drilling Activity: Air and Soil Contamination Study Initiated through Amateur Documentation and Collection;** Doug Carlton<sup>1</sup>; Sabra Ramirez<sup>1</sup>; Zacariah Hildenbrand<sup>1,2</sup>; Brian Fontenot<sup>1</sup>; Jayme Walton<sup>1,3</sup>; Kevin Schug<sup>1</sup>; <sup>1</sup>The University of Texas at Arlington, Arlington, TX; <sup>2</sup>Inform Environmental, LLC, Dallas, TX; <sup>3</sup>SWCA Environmental Consultants, Arlington, TX
- ThP 558 **Determination of inositol Phosphates in Lake Sediments with Ion-Exchange Chromatography Coupled with Mass Spectrometry;** Julia V Paraskova; Emil Rydin; Per J R Sjöberg; *Department of Chemistry - BMC, Uppsala University, Uppsala, Sweden*
- ThP 559 **Analysis of Naphthenic Acids in Oil Sands Process Water (OSPW) using LC/TOF;** Avinash Dalmia; Thomas White; *Perkinelmer, Shelton, CT*
- ThP 560 **A Streamlined Workflow for the Rapid Detection and Identification of Unknown Contaminants in Environmental Samples using Semi Permeable Membrane Devices;** David Hardy<sup>1</sup>; Praveen Kuty<sup>2</sup>; Anthony Gravel<sup>2</sup>; <sup>1</sup>ACD/Labs, Bracknell, UK; <sup>2</sup>Natural Resources Wales, Llanelli, Wales
- ThP 561 **Determination of Aroclor 1254 and 1260 in Soil Samples by Headspace Solid Phase Microextraction – GC/MS using Partial Least-Squares Regression;** Mengliang Zhang; Peter de B. Harrington; *Ohio University, Athens, OH*
- ThP 562 **One Step Extraction, Clean Up and Direct-to-vial Concentration For PCBs in Soil and Sediment;** Justin Blau; Lawrence Kramer; *Fluid Management Systems, Watertown, MA*
- ThP 563 **Automated Solid Phase Extraction of Semi-Volatile Organic Compounds (AB8270SIM) in Water;** Rudolf Addink; Lawrence Kramer; *Fluid Management Systems, Watertown, MA*
- ThP 564 **EPA 1664A: Oil and Grease by Solid Phase Extraction (SPE);** Alex Sharopov; Rudolf Addink; *Fluid Management Systems, Watertown, MA*
- ThP 565 **Qualitative and Quantitative Analysis of Contaminants of Emerging Concern in Biosolids Using Dilute-and-Shoot UHPLC-Orbitrap MS Method;** Ahmed Mostafa<sup>1</sup>; Paul Yang<sup>2</sup>; Jonathan Beck<sup>3</sup>; Maciej Bromirski<sup>4</sup>; Dipankar Ghosh<sup>3</sup>; Charles Yang<sup>3</sup>; Lynda McCarthy<sup>1</sup>; <sup>1</sup>Ryerson University, Toronto, Canada; <sup>2</sup>Ontario Ministry of the Environment, Etobicoke, Canada; <sup>3</sup>Thermo Fisher Scientific, San Jose, CA; <sup>4</sup>Thermo Fisher Scientific GmbH, Bremen, N/A
- ThP 566 **Environmental Analysis of Poly- and Perfluoroalkyl Compounds using a Q-Exactive Orbitrap: Optimization for a Laser Diode Thermal Desorption Method;** Gabriel Munoz<sup>2,3</sup>; Sung Vo Duy<sup>1</sup>; H el ene Budzinski<sup>3</sup>; Pierre Labadie<sup>3</sup>; Jinxia Liu<sup>4</sup>; S ebastien Sauv e<sup>1</sup>; <sup>1</sup>Universit e de Montreal, Montreal, Canada; <sup>2</sup>Universit e de Bordeaux, Talence, France; <sup>3</sup>CNRS, Talence, France; <sup>4</sup>McGill University, Montreal, Canada
- ThP 567 **Use of Automated Sample Preparation in ISO 17025 Accreditation;** Donald Tang; Tom Hall; *Fluid Management Systems, Watertown, MA*
- ThP 568 **Comprehensive Analysis of Brominated Flame Retardants using HESI, APCI and APPI on a TSQ Quantiva;** Mark Dreyer; Maria Prieto Conaway; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*
- ThP 569 **Petroleum Analysis by Orbitrap Elite Mass Spectrometry with Multiple Ionization Methods;** Pengxiang Yang<sup>1</sup>; Keith Waddell<sup>1</sup>; Brian Ruddy<sup>2</sup>; Matt Ashby<sup>2</sup>; Leonard Nyadong<sup>3</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>Taxon Biosciences, Tiburon, CA; <sup>3</sup>Phillips 66, Houston, TX
- ThP 570 **Application of Ultra-High Resolution Tandem Mass Spectrometry in Non-Targeted Analysis of Emerging Environmental Contaminants;** Lee Ferguson<sup>1</sup>; Gordon Getzinger<sup>1</sup>; Heather Stapleton<sup>1</sup>; Jonathan Beck<sup>2</sup>; <sup>1</sup>Duke University, Durham, NC; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 571 **Using GC Triple Quadrupole MS in Full scan, SIM and SRM to provide the highest coverage for regulated methods;** Paul Silcock<sup>1</sup>; Dwain Cardona<sup>2</sup>; Cristian Cojocariu<sup>1</sup>; Alexander Semyonov<sup>2</sup>; David Steiniger<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, Runcorn, UK; <sup>2</sup>Thermo Fisher Scientific, Austin, TX
- ThP 572 **Nationwide Survey of Nitrosamines by SPE Optimization with fully automated GC-EI-MS/MS;** Jaewon Choi<sup>1</sup>; YD Kim<sup>1</sup>; JM Jung<sup>2</sup>; HJ Huebschmann<sup>3</sup>; <sup>1</sup>Kwater, Daejeon, South Korea; <sup>2</sup>Thermo Fisher Scientific, Seoul, Korea; <sup>3</sup>Thermo Fisher Scientific, Singapore, Singapore
- ThP 573 **Analysis of Environmental Samples with a Novel Atmospheric Pressure GC Source Coupled to High-Resolution TOF-MS;** Thomas Arthen-Engeland<sup>1</sup>; Andreas Stelter<sup>1</sup>; Armin Holle<sup>1</sup>; Joe Anacleto<sup>2</sup>; Carsten Baessmann<sup>1</sup>; <sup>1</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup>Bruker Daltonics, Milton, ON, Canada
- ThP 574 **Portable Digital Linear Ion Trap Mass Spectrometer Used for VOCs On-line Detections;** Zhengxu Huang<sup>1</sup>; Wei Gao<sup>1</sup>; Li Ding<sup>3</sup>; Wenjian Sun<sup>3</sup>; Lulu Sun<sup>2</sup>; Bing Xue<sup>2</sup>; Gongyu Jiang<sup>3</sup>; Hui Mu<sup>3</sup>; Zhen Zhou<sup>1,2</sup>; <sup>1</sup>Jinan University, Guangzhou, Guangdong, China; <sup>2</sup>Hexin Analytical Instrument Co., Ltd, Guangzhou, Guangdong, China; <sup>3</sup>Shimadzu Research Laboratory (Shanghai) Co., Ltd., Shanghai, China

## Forensics, 575 - 604

- ThP 575 **Approaching the Ideal Forensic GC-MS;** Tal Alon<sup>1,3</sup>; Alexander Fialkov<sup>1</sup>; Aviv Amirav<sup>1,2</sup>; <sup>1</sup>Tel-Aviv University, Tel-Aviv, Israel; <sup>2</sup>Aviv Analytical, Tel Aviv, Israel; <sup>3</sup>Afeka Academic College of Engineering, Tel Aviv, Israel
- ThP 576 **Low Level Determination Of Synthetic Cannabinoids (SPICE) And Metabolites From Oral Fluid Using A Novel C18-Based Stationary Phase By UHPLC-MS/MS;** Alan McKeown<sup>1</sup>; Carl Zimmerman<sup>2</sup>; <sup>1</sup>Advanced Chromatography Technologies Ltd, Aberdeen, UK; <sup>2</sup>MAC-MOD Analytical Inc., Chadds Ford, PA
- ThP 577 **Analysis of Organic Gunshot Residue from Clothing by Solid Phase Microextraction with Gas Chromatography-Mass Spectrometry;** Brent Casper<sup>1</sup>; Bert C. Lynn<sup>2</sup>; <sup>1</sup>Univ of Kentucky, Lexington, KY; <sup>2</sup>University of Kentucky, Lexington, KY
- ThP 578 **Determining the Efficacy of Antimicrobial Solutions at Preserving Accelerant Residues in Soil Using Headspace Sorptive Extraction and GC-EI-MS;** Nicholas Vercruysse; *George Mason University, Fairfax, VA*

- ThP 579 **Exploring the Integration of PSI-FAIMS-MS for Forensic Applications;** Chia-Wei Tsai<sup>1,2</sup>; Christopher A. Tipple<sup>3</sup>; Richard A. Yost<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>2</sup>CFSRU, Visiting Scientist Program, FBI Laboratory, Quantico, VA; <sup>3</sup>CFSRU, FBI Laboratory Division, Quantico, VA
- ThP 580 **Analysis of Plastic Explosives by Comprehensive Multidimensional GC-MS (GC×GC-ToF);** Chia-Wei Tsai<sup>1,2</sup>; Sarah M. Kile<sup>3</sup>; Christopher A. Tipple<sup>4</sup>; <sup>1</sup>CFSRU, Visiting Scientist Program, FBI Laboratory, Quantico, VA; <sup>2</sup>Department of Chemistry, University of Florida, Gainesville, FL; <sup>3</sup>Explosives Unit, FBI Laboratory Division, Quantico, VA; <sup>4</sup>CFSRU, FBI Laboratory Division, Quantico, VA
- ThP 581 **Quantitation of Dyes in Forensic Fibers using UHPLC-TOF and Building a Dye Database using Accurate Mass;** Sharanya Reddy; Sergey Rakov; PerkinElmer, Shelton, CT
- ThP 582 **Screening and Quantification of Opiates in Urine and Serum by UHPLC-TOF;** Sharanya Reddy; Nonie Danna; PerkinElmer, Shelton, CT
- ThP 583 **Screening and Quantification of Benzodiazepams in Urine and Serum by LC-TOF;** Sharanya Reddy; Leslie Sullivan; George Perkins; PerkinElmer, Shelton, CT
- ThP 584 **Screening and Quantification of the SAMHSA (NIDA) Panel in Urine and Serum using LC-Time of Flight Mass Spectrometry;** Avinash Dalmia; Noelle Elliott; Joanne Mather; Bonnie Marmor; George Perkins; PerkinElmer, Shelton, CT
- ThP 585 **Comparison of Forensic Tandem Mass Spectral Data Obtained on Portable Instrumentation to an Established Reference Library;** Adam O'Leary; Seth Hall<sup>1</sup>; Herbert Oberacher<sup>2</sup>; Christopher Mulligan<sup>1</sup>; <sup>1</sup>Illinois State University, Normal, IL; <sup>2</sup>Innsbruck Medical University, Innsbruck, Austria
- ThP 586 **Establishing a Surface Swabbing Protocol Compatible with Ambient Sampling Mass Spectrometers for On-site Forensic Evidence Screening;** Alex Swiontek; Seth Hall; Adam O'Leary; Christopher Mulligan; Illinois State University, Normal, IL
- ThP 587 **Simultaneous Screening and Quantitation of Ten Amphetamines in Urine by On-line SPE-LC/MS Method;** Helmy Rabaha<sup>1</sup>; Sweet Chin Lim<sup>1</sup>; Zhe Sun<sup>2</sup>; Jie Xing<sup>2</sup>; Zhaoqi Zhan<sup>2</sup>; <sup>1</sup>Department of Scientific Service, Ministry of Health, Brunei Darussalam; <sup>2</sup>Customer Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive, #02-01/08, Singapore 118264
- ThP 588 **The Analysis of Cannabinoids and Their Metabolites in Human Urine by LC-MS/MS;** Frances Carroll; Restek, Bellefonte, PA
- ThP 589 **Evaluation of Drugs of Abuse Extraction from Oral Fluid using Supported Liquid Extraction prior to GC/MS and LC/MS Analysis;** Lee Williams<sup>1</sup>; Rhys Jones<sup>1</sup>; Helen Lodder<sup>1</sup>; Adam Senior<sup>1</sup>; Alan Edgington<sup>1</sup>; Geoff Davies<sup>1</sup>; Steve Jordan<sup>1</sup>; Claire Desbrow<sup>1</sup>; Victor Vandell<sup>2</sup>; Frank Kero<sup>2</sup>; <sup>1</sup>Biotage GB Limited, Cardiff, UK; <sup>2</sup>Biotage LLC, Charlotte, NC
- ThP 590 **Screening of Forensic and Clinical Samples by SWATH Acquisition and Processing by High Resolution / High Accuracy Reference Spectra;** Stefan König; Susanne Nussbaumer; Thomas Wüthrich; Werner Bernhard; Wolfgang Weinmann; Institut für Rechtsmedizin, Universität Bern, Bern, Switzerland
- ThP 591 **Rapid and Simple Determination of Benzodiazepines, Zolpidem and Their Metabolites using Direct Injection Liquid Chromatography-Tandem Mass Spectrometry;** Yu-Dong Jeong<sup>1</sup>; Sunglll Suh<sup>2</sup>; Moon Kyo In<sup>2</sup>; Junghan Song<sup>3</sup>; Jin Young Kim<sup>2</sup>; Ki-Jung Paeng<sup>1</sup>; <sup>1</sup>Yonsei University, Wonju, South Korea; <sup>2</sup>Supreme Prosecutors' office, Seoul, South Korea; <sup>3</sup>Seoul National University Bundang Hospital, Bundang, South Korea
- ThP 592 **Simultaneous Analysis for Forensic Drugs in Human Blood and Urine using Ultra-High Speed LC-MS/MS;** Toshikazu Minohata<sup>1</sup>; Keiko Kudo<sup>2</sup>; Kiyotaka Usui<sup>3</sup>; Noriaki Shima<sup>4</sup>; Munehiro Katagi<sup>4</sup>; Noriaki Ikeda<sup>2</sup>; Hitoshi Tsuchihashi<sup>5</sup>; Koichi Suzuki<sup>5</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Kyushu University, Fukuoka, Japan; <sup>3</sup>Tohoku University Graduate School of Medicine, Sendai, Japan; <sup>4</sup>Osaka Prefectural Police, Osaka, Japan; <sup>5</sup>Osaka Medical Collage, Takatsuki, Japan
- ThP 593 **LC-MS Identification of Etanercept in Equine Plasma for Doping Control;** Fuyu Guan<sup>1</sup>; Cornelius Uboh<sup>2</sup>; Lawrence Soma<sup>3</sup>; <sup>1</sup>University of Pennsylvania, West Chester, PA; <sup>2</sup>Pennsylvania Equine Toxicology and Research Center, West Chester, PA; <sup>3</sup>University of Pennsylvania, Kennett Square, PA
- ThP 594 **Elucidation of the Biotransformation Pathways of New Designer Drugs by Chromatography-Mass Spectrometry following in vitro Metabolism Studies;** Xavier De La Torre; Caterina Covelli; Monica Mazzarino; Mario Nardone; Alessandra Stampella; Francesco Botrè; Laboratorio Antidoping FMSI, Rome, Italy
- ThP 595 **LC-MS/MS Analytical Procedure to Detect Small Peptides in Biological Samples: Evaluation of Different SPE Extraction Sorbents and Protocols;** Monica Mazzarino; Valeria Calvaresi; Xavier de la Torre; Chiara Sebastianelli; Francesco Botrè; Laboratorio Antidoping FMSI, Rome, Italy
- ThP 596 **Characterization of E-Cigarettes Liquid Contents and Transformation Products by LC-MS, GC-MS and ICP-MS Techniques;** Claudio Medana<sup>1</sup>; Cecilia Sala<sup>1</sup>; Raffaele Pellegrino<sup>2</sup>; Riccardo Aigotti<sup>1</sup>; Federica Dal Bello<sup>1</sup>; Giancarlo Bianchi<sup>2</sup>; Enrico Davoli<sup>2</sup>; <sup>1</sup>University of Turin, Torino, ITALY; <sup>2</sup>Mario Negri Institute, Milano, N/A
- ThP 597 **Rapid Characterization of Methylone Analogues by Direct Analysis in Real Time Quadrupole Time-of-Flight;** Seongshin Gwak; Jose Almirall; Florida International University, Miami, FL
- ThP 598 **Analysis of Cathinones in Plasma Using LC-MS/MS;** Jonathan Ho<sup>1</sup>; Shu-Yuan Cheng<sup>2</sup>; Theron Ng-A-Quei<sup>2</sup>; Bruce Eng<sup>1</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Inc., Somerset, NJ; <sup>2</sup>John Jay College of Criminal Justice, CUNY, New York, NY
- ThP 599 **Determination of Opiates, Amphetamines and Cocaine in Whole Blood, Plasma and Urine by UHPLC-MS/MS using a QuEChERS Sample Preparation;** Sylvain Dulaurent<sup>1</sup>; Mikael Levi<sup>1</sup>; Jean-Michel Gaulier<sup>2</sup>; Stephane Moreau<sup>3</sup>; Pierre Marquet<sup>2,4</sup>; <sup>1</sup>Shimadzu France, Noisiel, France; <sup>2</sup>CHU Limoges, Department of Pharmacology and Toxicology, Limoges, France; <sup>3</sup>Shimadzu Europe, Albert-Hahn Strasse 6-10, Duisburg, Germany; <sup>4</sup>Univ Limoges, Limoges, France
- ThP 600 **Determination of Δ9-tetrahydrocannabinol and Two of its Metabolites in Whole Blood, Plasma and Urine by UHPLC-MS/MS using QuEChERS Sample Preparation;** Sylvain Dulaurent<sup>1</sup>; Mikael Levi<sup>2</sup>; Jean-Michel Gaulier<sup>1</sup>; Stephane Moreau<sup>3</sup>; Pierre Marquet<sup>1,4</sup>; <sup>1</sup>Chu Limoges, Department of Pharmacology and Toxicology, Limoges, France; <sup>2</sup>ShimadzuFrance, Noisiel, France; <sup>3</sup>Shimadzu Europe, Albert-Hahn Strasse 6-10, Duisburg, Germany; <sup>4</sup>Univ Limoges, Limoges, France
- ThP 601 **Methods for Characterizing the Performance of Ambient Pressure Ionization Sources;** Tim Brewer<sup>1</sup>; Thomas Forbes<sup>2</sup>; Leonard Demoranville<sup>3</sup>; Shin Muramoto<sup>2</sup>; Edward Sisco<sup>4</sup>; Greg Gillen<sup>2</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, MD; <sup>3</sup>Centre College, Danville, KY; <sup>4</sup>University of Maryland, College Park, MD

- ThP 602 **Using an Ambient Sampling, Portable Mass Spectrometer for the Direct Analysis of Species Related to Desomorphine (“Krokodil”) Synthesis**; Seth Hall; Adam O’Leary; Angelica Traub; Christopher Mulligan; *Illinois State University, Normal, IL*
- ThP 603 **A Sensitive and Comprehensive Method for the Screening and Confirmation of Drugs of Abuse in oral fluid by LC-QTOF**; Sheher Bano Mohsin; Andre Szczesniowski; *Agilent Technologies, Schaumburg, IL*
- ThP 604 **An Analysis of Philadelphia Currency Contaminated with Cocaine**; Brooks F. Mirabella; Karen S. Wendling; *Chestnut Hill College, Philadelphia, PA*
- Food “omics”: MS Characterization of Food and Nutritional Supplements, 605 - 633**
- ThP 605 **Molecular Gastronomy of Coffee: Using Gas Chromatography Mass Spectrometry to Investigate Roles of Origin, Roasting & Storage on Flavor Components**; Steven B. Foster; Stephanie I. Allred; Emily P. Erdman; Jane Hsi; Dallas P. Milligan; Anna Marie Rowell; Josie M. Smith; Ronald L. Halterman; *University of Oklahoma, Department of Chemistry &, Norman, OK*
- ThP 606 **Characterization of Marine Dietary Supplements using Travelling Wave Ion Mobility Mass Spectrometry Coupled to UPLC**; Fereshteh Zandkarimi<sup>1</sup>; Mirela Galusca<sup>2</sup>; Jeffrey Morr <sup>1</sup>; Claudia S. Maier<sup>1</sup>; <sup>1</sup>*Oregon State University, Corvallis, OR*; <sup>2</sup>*University of Arad, Arad, Romania*
- ThP 607 **The Complimentary Use of MALDI-TOF MS Protein Fingerprinting and SSTR Genetic Profiling for the Identification and Characterization of Brewer’s Yeast**; Sarah Marie Lyons<sup>1</sup>; Hend Ibrahim<sup>1</sup>; Dana Sedin<sup>2</sup>; Kelly Tretter<sup>2</sup>; Drew Bombard<sup>2</sup>; Jessica Prenni<sup>1</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*New Belgium, Fort Collins, CO*
- ThP 608 **Brewing a Better Beer: Application of UPLC-MS Metabolomics to Develop Non-Volatile Markers of Beer Stability during Storage**; Adam Heuberger<sup>1</sup>; Kaylyn Kirkpatrick<sup>1</sup>; Lindsay Guerdrum<sup>2</sup>; Dana Sedin<sup>2</sup>; Jessica Prenni<sup>1</sup>; <sup>1</sup>*Colorado State University, Fort Collins, CO*; <sup>2</sup>*New Belgium Brewing Company, Fort Collins, CO*
- ThP 609 **Merits of fast, High Resolution Time-of-Flight Mass Spectrometry for the Aroma Profiling of Cheese Samples at Different Maturity Levels**; Thomas M. Groeger<sup>1</sup>; Ralf Zimmermann<sup>1,2</sup>; Muammer Kaplan<sup>3</sup>; Elmas Oktem<sup>3</sup>; Wibke Peters<sup>4</sup>; Juergen Wendt<sup>4</sup>; <sup>1</sup>*JMSC, CMA Helmholtz Zentrum Muenchen, Neuherberg, Germany*; <sup>2</sup>*JMSC, Analytical Chemistry, University of Rostock, Rostock, Germany*; <sup>3</sup>*TUBITAK Marmara Research Centre Food Institute, Gebze, Turkey*; <sup>4</sup>*LECO European LSCA Centre, Moenchengladbach, Germany*
- ThP 610 **MALDI-TOF-MS Screening of Skim Milk Powder for Economically Motivated Adulteration with Foreign Proteins: An Inter-laboratory Feasibility of Concept Demonstration**; Peter Scholl<sup>1</sup>; Samantha Farris<sup>1</sup>; Roman Romero<sup>2</sup>; Peter Harrington<sup>3</sup>; Jeffrey Moore<sup>4</sup>; Petra Lutter<sup>5</sup>; <sup>1</sup>*US FDA, Baltimore, MD*; <sup>2</sup>*Nestl  Research Centre, Lausanne, Switzerland*; <sup>3</sup>*Ohio University, Athens, OH*; <sup>4</sup>*US Pharmacopeial Convention, Rockville, MD*; <sup>5</sup>*Nestl  Quality Assurance Center, Weiding, Germany*
- ThP 611 **Proteomics Deciphers Dairy and Bakery Recipes Used in Ancient China**; Anna Shevchenko<sup>1</sup>; Yimin Yang<sup>2</sup>; Changsui Wang<sup>2</sup>; Andrej Shevchenko<sup>1</sup>; <sup>1</sup>*MPI of Molecular Cell Biology and Genetics, Dresden, Germany*; <sup>2</sup>*University of Chinese Academy of Sciences, Beijing, China*
- ThP 612 **Differentiation of Whiskies with Data Fusion of Organic and Inorganic Features**; Catherine Stacey<sup>1</sup>; Mark Upton<sup>2</sup>; Robert Hoults<sup>2</sup>; <sup>1</sup>*PerkinElmer, Waltham, MA*; <sup>2</sup>*PerkinElmer, Seer Green, UK*
- ThP 613 **Top-Down, High-Throughput Proteomics using a New LC-MS Platform Provides New Ammunition against Pervasive Fish Fraud in less than 1 hour**; Daniel Lopez Ferrer<sup>1</sup>; Michael Blank<sup>1</sup>; Monica Carrera<sup>2</sup>; Jose M. Gallardo<sup>2</sup>; Michael Andersen<sup>3</sup>; Nicolais Bache<sup>1</sup>; Andreas Huhmer<sup>1</sup>; <sup>1</sup>*Thermo Fisher Scientific, San Jose, CA*; <sup>2</sup>*CSIC, Vigo, SPAIN*; <sup>3</sup>*Thermo Fisher Scientific, Odense, Denmark*
- ThP 614 **Profiling 100+ Years of Port-style Wines Using UHPLC/QTOF-MS**; Anthony L. Robinson<sup>1</sup>; Jerry Zweigenbaum<sup>2</sup>; Robert Trengrove<sup>3</sup>; Susan E. Ebeler<sup>4</sup>; Thomas S. Collins<sup>4</sup>; <sup>1</sup>*Treasury Wine Estates, Nuriootpa, SA, Australia*; <sup>2</sup>*Agilent Technologies, Wilmington, DE*; <sup>3</sup>*Murdoch University, Murdoch, WA, Australia*; <sup>4</sup>*UC Davis, Department of Viticulture & Enology, Davis, CA*
- ThP 615 **Characterization of Flavors and Origin of Tequila and Agave Distillates Using Accurate Mass GC/QTOF and Mass Profiler Professional**; Rafael Acosta<sup>1</sup>; Dale Walker<sup>2</sup>; Ron Honnold<sup>2</sup>; <sup>1</sup>*Agilent Technologies, Mexico City, Mexico*; <sup>2</sup>*Agilent Technologies, Santa Clara, CA*
- ThP 616 **Vitamin D and 25-Hydroxy Vitamin D in Human Milk by LC-MSMS**; Guy L. Dufresne; *Health Canada food lab, Longueuil, Canada*
- ThP 617 **Characterization of Food Products by GC×GC-TOFMS and GC-high resolution TOFMS: A Food “omics” Approach**; Elizabeth Humston-Fulmer; Jeffrey Patrick; Joe Binkley; David Alonso; *Leco Corporation, St. Joseph, MI*
- ThP 618 **Evaluation of Volatiles in Edible Oils by SPME-DART-QTOF**; Susan Seegers; Tiffanie West; *Bunge North America, Bradley, IL*
- ThP 619 **Quality Control of Cooking Oils by GC-MS Profiling and Spectral Fingerprinting**; Pui Hei Chan<sup>1</sup>; Yue Zhu<sup>2</sup>; Karl, W. K. Tsim<sup>1</sup>; Henry Lam<sup>1</sup>; <sup>1</sup>*The Hong Kong University of Science and Technology, Kowloon, Hong Kong*; <sup>2</sup>*Nanjing University of Chinese Medicine, Nanjing, China*
- ThP 620 **A Novel Technique to Increase Sensitivity for the Analysis of Volatile Compounds with DART-MS**; Yuki Kudou<sup>1</sup>; Takehito Sagawa<sup>2</sup>; Takao Nishiguchi<sup>1</sup>; Kazumasa Kinoshita<sup>1</sup>; <sup>1</sup>*BioChromato, Fujisawa, Japan*; <sup>2</sup>*S&B Foods, Tokyo, Japan*
- ThP 621 **Health Sustaining Components Analysis by LC-MS in Heavy Fermented “Miso”**; Atsuko Takahashi<sup>1</sup>; Hiromitsu Watanabe<sup>2</sup>; Yuichiro Miyasaka<sup>3</sup>; Tsuyoshi Esaki<sup>1</sup>; Hajime Mizuno<sup>1</sup>; Tsutomu Masujima<sup>1</sup>; <sup>1</sup>*Quantitative Biology Center (QBiC), RIKEN, Suita, Japan*; <sup>2</sup>*Prof. Emeritus Hiroshima Univ., Hiroshima, Japan*; <sup>3</sup>*Miyasaka Brewery CO., Ltd., Tokyo, Japan*
- ThP 622 **Metabolite Profiling of Edible Bird’s Nest using GC/MS and LC/MS**; Sam Li<sup>1</sup>; Yong Guan Chua<sup>1</sup>; Lai Peng Leong<sup>1</sup>; Bosco Bloodworth<sup>2</sup>; <sup>1</sup>*National University of Singapore, Singapore, SINGAPORE*; <sup>2</sup>*Health Sciences Authority, Singapore, Singapore*
- ThP 623 **Mass Spectrometry Approach for Identification of Porcine and Bovine Gelatin Biomarkers in Food Commodities**; Wan Noor Faradalila Wan Jamaluddin<sup>1</sup>; Venkatesha Gaddemane<sup>2</sup>; Fanny Widjaja<sup>2</sup>; Chee Sian Gan<sup>2</sup>; Dzulkifly Mat Hashim<sup>1</sup>; <sup>1</sup>*Universiti Putra Malaysia, Serdang, Malaysia*; <sup>2</sup>*Agilent Technologies, Singapore, Singapore*
- ThP 624 **Characterization of Proanthocyanidin Content in Dietary Supplement Standard Reference Materials by Two-Dimensional Liquid Chromatography with High-Resolution Mass Spectrometry**; Benjamin Place; Catherine Rimmer; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 625 **Detection and Quantitation of PDE-5 Inhibitor Adulterants in Herbal Supplements**; Kevin Krock; *Shimadzu Scientific Instruments, Pleasanton, CA*

- ThP 626 **Identification of Undeclared Designer Anabolic Steroids in a Vitamin-B Dietary Supplement: Mass Spectral Clues for Forensic Investigation;** Jonathan J. Litzau; Travis M. Falconer; Mary B. Jones; Sarah E. Voelker; *U.S. Food & Drug Administration, Cincinnati, OH*
- ThP 627 **Nitration of Some Flavonoids Found in Beer;** Larry Sallans; Stephen Macha; *University of Cincinnati, Cincinnati, OH*
- ThP 628 **Characterization of Phosvitin Digests Using MALDI-TOF Mass Spectrometry;** Himali Samaraweera<sup>1</sup>; Sun Hee Moon<sup>1</sup>; Eun Joo Lee<sup>2</sup>; Jennifer E. Grant<sup>3</sup>; Jordan Fouks<sup>4</sup>; Joo Won Suh<sup>5</sup>; Dong Ahn<sup>1,6</sup>; <sup>1</sup>Dept. of Animal Science, Iowa State University, Ames, IA; <sup>2</sup>Dept. of Food and Nutrition, Univ. Wisconsin-Stout, Menomonie, WI; <sup>3</sup>Dept. of Biology, Univ. Wisconsin-Stout, Menomonie, WI; <sup>4</sup>Applied Science Program, Univ. Wisconsin-Stout, Menomonie, WI; <sup>5</sup>Center for Nutraceutical/Pharmaceutical Materials, Yongin, South Korea; <sup>6</sup>Dept. of Animal Science and Tech., Suncheon National, Suncheon, South Korea
- ThP 629 **Quantitative Analysis of Hops Bittering Acids by Direct Analysis Electrospray Ionization Mass Spectrometry;** Gregg Hasman Jr; Andre Venter; *Western Michigan University, Kalamazoo, MI*
- ThP 630 **Simultaneous Screening of Multiple Plant-Based Allergens and Gluten using Liquid Chromatography-Mass Spectrometry;** Jennifer Sealey Voyksner<sup>1</sup>; Robert Voyksner<sup>1</sup>; Jerry Zweigenbaum<sup>2</sup>; <sup>1</sup>LCMS Limited, Durham, NC; <sup>2</sup>Agilent Technologies, Willmington, DE
- ThP 631 **Novel Endogenous Iron-Binding Compounds in Wines Discovered through Exploitation of Iron's Characteristic Isotopic Signature;** Oliver Baars; David H. Perlman; *Princeton University, Princeton, NJ*
- ThP 632 **A LCMS Method for the Detection of Cocoa Butter Substitutes, Replacers, and Equivalents in Commercial Chocolate-like Products;** Jared Russell; Kevin Krock; Liling Fang; Will Bankert; *Shimadzu Scientific Instruments, Inc., Pleasanton, CA*
- ThP 633 **High Throughput Characterization of Katsuoibushi using DART-MS with High-Speed Polarity Switching;** Shun Wada<sup>1</sup>; Keiko Matsumoto<sup>2</sup>; Jun Watanabe<sup>2</sup>; Teruhisa Shiota<sup>3</sup>; <sup>1</sup>Inst. of oil & fats, other foods Inspection, Tokyo, Japan; <sup>2</sup>Shimadzu Corporation, Kyoto, Japan; <sup>3</sup>AMR, Tokyo, Japan
- Metabolomics: General, 634 - 653**
- ThP 634 **Mass Spectrometry-based Metabolomics Analysis Reveals Age-related Pathway Changes in *Drosophila melanogaster*;** Yuping Cai; Yuan Guo; Zhengqiang Zhu; *IRCB, Chinese Academy of Sciences, Shanghai, China*
- ThP 635 **Development of a Targeted Metabolic LC-MS/MS Assay to Assess Nanotoxicity In *C. Elegans*;** Jeanita Pritchett; Ashley Beasley-Green; Bryant Nelson; *National Institute of Standards and Technology, Gaithersburg, MD*
- ThP 636 **Large-scale Metabolic Profiling of Saponins in *M. truncatula* Ecotypes;** Zhentian Lei; Bonnie Watson; David Huhman; Shelagh Henson; Lloyd Sumner; *The Samuel Roberts Noble Foundation, Ardmore, OK*
- ThP 637 **Metabolic Pathway Directed Targeted Metabolomics by Mining High Resolution Full Scan MS Data Sets – a Food Metabolomics Case Study;** Heiko Neuweger; Klaus Meyer; Verena Tellström; Aiko Barsch; *Bruker Daltonik, Bremen, Germany*
- ThP 638 **Targeted Metabolomic Analysis to Interrogate the Role of cellular Retinol-Binding Protein, Type 1 in retinoic Acid Biosynthesis;** Jianshi Yu; Jace Jones; Keely Pierzchalski; Maureen Kane; *University of Maryland at Baltimore, Baltimore, MD*
- ThP 639 **Study of How Variation in Fragmentation Energy Affects Our Ability to Apply MS/MS Information to small Molecule Formula Assignment;** Jane Razumovskaya; Ralf Tautenhahn; Tim Stratton; Sachin Deshpande; *Thermo Fisher Scientific, San Jose, CA*
- ThP 640 **Development of a Software Toolbox for Systematic Annotation of Plant Metabolomes;** Feng Qiu; Dennis D. Fine; Daniel J. Wieritt; Zhentian Lei; Lloyd W. Sumner; *The Samuel Roberts Noble Foundation, Ardmore, OK*
- ThP 641 **High Sensitivity Analysis of Metabolites in Serum Using Simultaneous SIM and MRM Modes in a Triple Quadrupole GC/MS/MS;** Shuichi Kawana<sup>1</sup>; Yukihiko Kudo<sup>2</sup>; Kenichi Obayashi<sup>2</sup>; Laura Chambers<sup>3</sup>; Richard Whitney<sup>3</sup>; Haruhiko Miyagawa<sup>2</sup>; <sup>1</sup>Shimadzu, Osaka, Japan; <sup>2</sup>Shimadzu, Kyoto, Japan; <sup>3</sup>Shimadzu Scientific Instruments, Columbia, MD
- ThP 642 **Metabolite Profiling of Active Metabolites of Vitamin A in Lung Epithelial Cells;** Wenjing Li<sup>1</sup>; Jace W. Jones<sup>1</sup>; Jianshi Yu<sup>1</sup>; Keely Pierzchalski<sup>1</sup>; Pu-Ting Xu<sup>2</sup>; Isabel L. Jackson<sup>2</sup>; Zeljko Vujaskovic<sup>2</sup>; Gregory Tudor<sup>3</sup>; Catherine Booth<sup>3</sup>; Thomas J. MacVittie<sup>2</sup>; Maureen A. Kane<sup>1</sup>; <sup>1</sup>University of Maryland, School of Pharmacy, Baltimore, MD; <sup>2</sup>University of Maryland, School of Medicine, Baltimore, MD; <sup>3</sup>Epistem Ltd, Manchester, UK
- ThP 643 **Examination of Multi-Vitamin and -Mineral Supplementation Effects on Saliva Metabolomics;** LeeCole Legette; Elizabeth Hardard; Jaewoo Choi; Jan F. Stevens; *Oregon State University, Corvallis, OR*
- ThP 644 **Identification of Natural Substrates of Spermidine/ spermine acetyltransferase 2 (SAT2) by metabolomic approaches;** Han-Jia Lin<sup>1</sup>; Yu-Ling Peng<sup>1</sup>; Hsien-Hong Chang<sup>2</sup>; <sup>1</sup>Taiwan Ocean University, Keelung, Taiwan; <sup>2</sup>National Taiwan Ocean University, Keelung, Taiwan
- ThP 645 **Improvements of Salicylic Acid Detection in Engineered *Escherichia coli* Cells Using HPLC and GC-MS Techniques;** Trong Khoa Pham<sup>1</sup>; Martynas Serys-Kubertavicius<sup>1</sup>; Joy Mukherjee<sup>1</sup>; Catherine A. Biggs<sup>1</sup>; Felix Dafnis-Calas<sup>2</sup>; Stephan Heeb<sup>2</sup>; Miguel Camara<sup>2</sup>; Natalio Krasnogor<sup>3</sup>; Phillip C. Wright<sup>1</sup>; <sup>1</sup>CHELSI Institute, The University of Sheffield, Sheffield, UK; <sup>2</sup>School of Life Sciences, University of Nottingham, Nottingham, UK; <sup>3</sup>School of Computing Science, Newcastle University, Newcastle, UK
- ThP 646 **Tracking Nocardiozine Biosynthesis with Liquid Chromatographic Accurate Tandem Mass Spectrometry: Tryptophan Diketopiperazine Fragmentation in Positive and Negative Ion Modes;** Angela M. Hansen<sup>1</sup>; Norah Alqahtani<sup>2</sup>; Suheel Porwal<sup>2</sup>; Rajesh Viswanathan<sup>2</sup>; Jonathan A. Karty<sup>1</sup>; <sup>1</sup>Indiana University, Bloomington, IN; <sup>2</sup>Case Western Reserve University, Cleveland, OH
- ThP 647 **Development of a Multi-Omics Approach using a Single Extraction;** John Bowden<sup>1</sup>; Tracey Schock<sup>1</sup>; Miki Watanabe<sup>1</sup>; Satomi Kohno<sup>2</sup>; <sup>1</sup>NIST, Charleston, SC; <sup>2</sup>Medical University of South Carolina, Charleston, SC
- ThP 648 **Isotopic Tracer Analysis Provides Insight to the Mechanism of Action Aminoxyacetate and Inhibition of tumor Cell Proliferation;** Fang Wang; Eugene Melamud; Kim Arndt; Jeremy Myers; *Oncology Research, Pfizer WRD, Pearl River, NY*
- ThP 649 **Automated Data Acquisition and Analysis Workflows for Metabolomics Analysis of Plant-Microbe Interactions and <sup>13</sup>C Incorporation by GC/MS;** Stefan Jenkins<sup>1</sup>; Shengjing Shi<sup>2,3</sup>; Beibei Huang<sup>2</sup>; Marcus Schicklberger<sup>1</sup>; Mary Firestone<sup>1,2</sup>; Romy Chakraborty<sup>1</sup>; David Wemmer<sup>1,2</sup>; Trent Northen<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>University of Oklahoma, Oklahoma City, OK

- ThP 650 **Metabolomics: The Study of Serum Metabolites and Traumatic Injury**; Janine Johnson; *University of Connecticut, Storrs, CT*
- ThP 651 **Serum Metabolomics from a Brazilian Population using GC-MS**; Kallyandra Padilha<sup>1</sup>; Gabriela Venturini<sup>1</sup>; Celso Blatt<sup>2</sup>; Alexandre Pereira<sup>1</sup>; <sup>1</sup>Heart Institute, Sao Paulo, Brazil; <sup>2</sup>Agilent Technologies, Barueri, Brazil
- ThP 652 **PMR: Plant & Microbial Metabolomics Resource**; Manhoi Hur; Joon-Yong Lee; Ling Li; Eve Syrkin Wurtele; *Iowa State University, Ames, IA*
- ThP 653 **The Wheat Defenseome under Challenge by Fungal Pathogens - A Metabolite MRM Atlas Approach**; Joel Gummer<sup>1</sup>; Catherine Rawlinson<sup>2</sup>; Kar-Chun Tan<sup>3</sup>; Richard McCulloch<sup>2</sup>; Aiko Barsch<sup>4</sup>; Joe Anacleto<sup>5</sup>; Richard Oliver<sup>3</sup>; Robert Trengove<sup>1,2</sup>; <sup>1</sup>Metabolomics Australia, Murdoch University, Perth, Australia; <sup>2</sup>Separation Science and Metabolomics Laboratory, Perth, Australia; <sup>3</sup>Dept. Environment & Agriculture, Curtin University, Perth, Australia; <sup>4</sup>Bruker Daltonics, Bremen, Germany; <sup>5</sup>Bruker Daltonics, Milton, Canada
- Metabolomics: Clinical Applications, 654 - 664**
- ThP 654 **Investigation of Serum Metabolome Changes in Postmenopausal Women after Administration of Phytoestrogenic Dietary Supplements**; Caleb Nienow<sup>1</sup>; Jeff Dahl<sup>2</sup>; Richard B. Van Breemen<sup>3</sup>; <sup>1</sup>University of Illinois at Chicago, Chicago, IL; <sup>2</sup>Shimadzu, Columbia, MD; <sup>3</sup>University of Illinois, Chicago, IL
- ThP 655 **Detection of Recurrent Breast Cancer by Metabolite Profiling: Initial Validation Results**; Haiwei Gu<sup>1,2</sup>; Danijel Djukovic<sup>1,2</sup>; Robert Ballas<sup>3</sup>; Narasimhamurthy Shanaiah<sup>2</sup>; G.A. Nagana Gowda<sup>1</sup>; Frederic Waldman<sup>4</sup>; Beverly Handy<sup>5</sup>; Daniel Raftery<sup>1,2</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Matrix-Bio, Inc., Fort Wayne, IN; <sup>3</sup>Biomarker Associates, Inc., Newark, DE; <sup>4</sup>Quest Diagnostics, San Juan Capistrano, CA; <sup>5</sup>The University of Texas M.D. Anderson Cancer Center, Houston, TX
- ThP 656 **Metabolomics Analysis Reveals Dietary Components in Nipple Aspirate Fluid**; Jessica A. Miller<sup>1</sup>; Patricia A. Thompson<sup>1</sup>; Andrew Baker<sup>2</sup>; H-H Sherry Chow<sup>1</sup>; <sup>1</sup>University of Arizona Cancer Center, Tucson, AZ; <sup>2</sup>Waters Corporation, Milford, CT
- ThP 657 **Pathway-Centric Integrative Analysis Identifies RRM2 as a Prognostic Marker in Breast Cancer Associated with Poor Survival and Tamoxifen Resistance**; Nagireddy Putluri; *Baylor College of Medicine, Houston, TX*
- ThP 658 **Pathway-Based Integrative Analysis Reveals a Key Role for the Hexosamine Biosynthetic Pathway in Prostate Cancer Progression**; Arun Sreekumar; *Baylor College of Medicine, Houston, TX*
- ThP 659 **Targeted LC-MS/MS Metabolic Profiling for Monitoring Colon Cancer Progression**; Jiangjiang Zhu<sup>1</sup>; Danijel Djukovic<sup>1</sup>; Lingli Deng<sup>2</sup>; Haiwei Gu<sup>1</sup>; Daniel Raftery<sup>1,3</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Xiamen University, Xiamen, P.R. China; <sup>3</sup>Fred Hutchinson Cancer Research Center, Seattle, Washington
- ThP 660 **Comprehensive Profiling of Bioactive Lipids in Human Plasma: Understanding Biochemical Effects of Pulmonary Rehabilitation on COPD Patients**; Chen Zhang; Sherman Gorbis; John Wang; A. Daniel Jones; *Michigan State University, East Lansing, MI*
- ThP 661 **Lipidomics of Alzheimer's Disease using an Integrated Microfluidic-Ion Mobility-MS Device**; Steven Lai; Angela Doneanu; James Murphy; James Langridge; Giuseppe Astarita; *Waters Corporation, Milford, MA*
- ThP 662 **In vivo LC/MS-based Metabolic Flux Analysis to Delineate Nucleotide Metabolism in Diabetes**; Anna Mathew; Jaeman Byun; Pradeep Kayampilly; Farsad Afshinnia; Subramaniam Pennathur; *University of Michigan, Ann Arbor, MI*
- ThP 663 **Preliminary Screening of Dried Blood Serum Spots (DBS) for Organic Components by On-Line Supercritical Fluid Extraction- Gas Chromatography/ Mass Spectrometry**; Bruce A. Benner; Jessica Reiner; *NIST, Gaithersburg, MD*
- ThP 664 **In-situ, Real-Time Analysis of Upper Gastrointestinal Mucosa by the Direct Combination of Rapid Evaporative Ionization Mass Spectrometry (REIMS) and Endoscopy**; Juzheng Huang; Cristina Guallar-Hoyas; Sacheen Kumar; Nima Abbassi-Ghadi; Emrys Jones; Jonathan Hoare; George Hanna; Zoltan Takats; *Faculty of Medicine, Imperial College London, London, UK*
- Drug Metabolism: Quantitative Analysis, 665 - 684**
- ThP 665 **Quantitative Analysis of Tricyclic Antidepressants in Urine by Rapidfire Coupled with Triple Quadrupole Mass Spectrometry**; Flaubert Mbeunkui; Sarah Sullivan; R. Brent Dixon; *Physician's Choice Laboratory Services, Rock Hill, SC*
- ThP 666 **Determination of Serum Protein Binding of Lipophilic Compounds by Ultracentrifugation and LC-MS/MS Analysis**; Jun Zhang; Dieter Drexler; Brian McAuliffe; Chris Cianci; Wilson Shou; *Bristol-Myers Squibb Company, Wallingford, CT*
- ThP 667 **Quantification of Active Pharmaceutical Ingredient by Triple Quadrupole ICP-MS**; Naoki Sugiyama<sup>1</sup>; Yasumitsu Ogra<sup>2</sup>; Yasumi Anan<sup>2</sup>; <sup>1</sup>Agilent Technologies Japan, Hachioji-shi, Japan; <sup>2</sup>Showa Pharmaceutical University, Machida-shi, Japan
- ThP 668 **Simultaneous Determination of Zolmitriptan and its metabolite in Human Plasma Using LC-MS/MS Techniques**; Moo-Young Kim; Marsha Luna; Rochelle Burke; Julie Showalter; Yansheng Liu; *KCAS, Shawnee, KS*
- ThP 669 **A Sensitive HPLC-MS/MS Method for the Quantitative Determination of Bromocriptine in Human Prolactinoma Tissues**; Qingce Zang<sup>1</sup>; Yang Liu<sup>2</sup>; Jiuming He<sup>1</sup>; Xiaofei Yue<sup>1</sup>; Ruiping Zhang<sup>1</sup>; Renzhi Wang<sup>2</sup>; Zeper ABLIZ<sup>1</sup>; <sup>1</sup>Institute of Materia Medica, CAMS&PUMC, Beijing, China; <sup>2</sup>Peking Union Medical College Hospital, CAMS&PUMC, Beijing, China
- ThP 670 **Robust Quantitative Droplet-Based Liquid Microjunction Surface Sampling HPLC-MS/MS System**; Vilmos Kertesz; Gary J. Van Berkel; *Oak Ridge National Laboratory, Oak Ridge, TN*
- ThP 671 **Quantitation of Anacetrapib, Stable-Isotope Labeled-Anacetrapib (Microdose), and Four Metabolites in Human Plasma Using Liquid Chromatography Tandem Mass Spectrometry**; Cynthia M. Chavez-Eng; Ryan Lutz; Dina Goykhman; Kevin Bateman; *Merck & Co., West Point, PA*
- ThP 672 **Rapid Development of Analytical Method for Antiepileptic Drugs in Plasma using UHPLC Method Scouting System Coupled to LC/MS/MS**; Miho Kawashima<sup>1</sup>; Satoshi Masuda<sup>2</sup>; Ikuko Yano<sup>2</sup>; Kazuo Matsubara<sup>2</sup>; Kiyomi Arakawa<sup>3</sup>; Qiang Li<sup>3</sup>; Yoshihiro Hayakawa<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Tokyo, JAPAN; <sup>2</sup>Kyoto University Hospital, Kyoto, Japan; <sup>3</sup>Shimadzu Corporation, Kyoto, Japan



- ThP 673 **Stereospecific Metabolite Profiling of Racemic Warfarin using 2D LC/MS Q-TOF Analysis;** Siji Joseph<sup>1</sup>; Smriti Khera<sup>2</sup>; Murali Subramanian<sup>3</sup>; <sup>1</sup>Agilent technologies, Bangalore, INDIA; <sup>2</sup>Agilent Technologies, Santa Clara, CA, US; <sup>3</sup>Biocon BMS, Syngene Internationl, Bangalore, India
- ThP 674 **An SFC-MS/MS Detection Method for the *in vivo* Quantitation of the Ganglionic Blocker Hexamethonium;** Sarah M Osgood; Amanda J King-Ahmad; Christopher L Holliman; *Pfizer, Groton, CT*
- ThP 675 **Indirect and Direct LC/MS Methods for Quantification of Ribavirin and Its Phosphate Metabolites in Biological Samples;** Chao Li; Feng Wang; Greg Waitt; Jon Williams; Chris Barringer; Vishal Shah; David Wagner; Glenn Smith; John Dunn; *GlaxoSmithKline, Research Triangle Park, NC*
- ThP 676 **Measurement of Serum Concentrations of Olaparib by LC-MS/MS-MRM;** Huseyin Kayadibi; Christopher Ryan; Farbod Fazlollahi; Julian Whitelegge; Kym Faulk; *Pasarow Mass Spectrometry Laboratory, UCLA, Los Angeles, CA*
- ThP 677 **Bioanalysis of an Oligonucleotide Class Macromolecule from Urine and Skin Tissue Using Liquid Chromatography - Tandem Mass Spectrometry;** Hang Zeng<sup>1</sup>; Eugene Kadar<sup>1</sup>; Elisabeth Lonie<sup>2</sup>; John Nowak<sup>2</sup>; Rick Steenwyk<sup>1</sup>; <sup>1</sup>Pfizer, Inc., Groton, CT; <sup>2</sup>Pfizer, Inc., Andover, MA
- ThP 678 **Ketamine CYP3A Mediated Metabolism Study using Mammalian Liver S9 Fractions, cDNA Expressed Enzymes and Liquid Chromatography Tandem Mass Spectrometry;** Raphaël Santamaria; Floriane Pailleux; Francis Beaudry; *Université de Montréal, St-Hyacinthe, CANADA*
- ThP 679 **Comparative Cellular Pharmacology of a  $\beta$ -D-2'-C-methyl-2,6-diaminopurine ribonucleoside phosphoramidate RS-1389 with INX189 and IDX184 in Rat, Dog, Monkey and Human Hepatocytes;** Sijia Tao<sup>1</sup>; Longhu Zhou<sup>1</sup>; Shaoman Zhou<sup>1</sup>; Jong-Hyun Cho<sup>1</sup>; Steven J. Coats<sup>2</sup>; Raymond F. Schinazi<sup>1</sup>; <sup>1</sup>Emory University School of Medicine, Atlanta, GA; <sup>2</sup>RFS Pharma LLC, Tucker, GA
- ThP 680 **Determination of the Bioavailability Characteristics of a Novel TMZ Based Therapeutic via CEMS for the Treatment of Brain Cancer;** Neloni R Wijeratne<sup>1</sup>; Ruth M. Alvarez<sup>1</sup>; Ahyoung Joo<sup>1</sup>; Thomas Chen<sup>2</sup>; Hee-Yeon Cho<sup>2</sup>; Axel H. Schonthal<sup>2</sup>; Florence M Hofman<sup>2</sup>; Chitra Ratnayake<sup>3</sup>; Jonathan E Katz<sup>1</sup>; <sup>1</sup>CAMM/USC, Los Angeles, CA; <sup>2</sup>USC, Los Angeles, CA; <sup>3</sup>AB Sciex, Brea, CA
- ThP 681 **Occidofungin Kinetics in Blood Plasma following Different Routes of Administration in a Murine Model;** Akshaya Ravichandran<sup>1</sup>; Jamie Humphries<sup>2</sup>; Lawrence Dangott<sup>1</sup>; Jerome Escano<sup>1</sup>; Wanjin Tang<sup>1</sup>; James Smith<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>ThermoScientific, Austin, TX
- ThP 682 **Development of a Quantitative LCMS Method for the Peptide RF9 in Equine Plasma;** Curtis Korthanke<sup>1</sup>; Lawrence Dangott<sup>1</sup>; Jamie Humphries<sup>2</sup>; Marcel Amstalden<sup>1</sup>; Gary Williams<sup>1</sup>; <sup>1</sup>Texas A&M University, College Station, TX; <sup>2</sup>ThermoScientific, Austin, TX
- ThP 683 **Profiling the Anti-Tumor Ability of Vitamin D Metabolites by UPLC-MS;** Liu Chia-Hsiun; Chiang Kun-Chun; Hsu Pang-Hung; *Keelung, R.O.C.*
- ThP 684 **The Effects of Obesity on Anesthetic Drug Distribution – Absolute Quantitation of Propofol in Human Plasma by GC-MS/MS;** Karolina M. Krasinska<sup>1</sup>; Jerry Ingrande<sup>2</sup>; Allis S. Chien<sup>1</sup>; <sup>1</sup>SUMS, Stanford University, Stanford, CA; <sup>2</sup>Department of Anesthesiology, Stanford University, Stanford, CA
- Ion Activation / Dissociation, 685 - 702**
- ThP 685 **Activated-Ion Electron Transfer Dissociation for the Improved Fragmentation of Intact Protein Cations;** Nicholas Riley; Christopher Rose; Timothy Rhoads; Michael Westphall; Joshua Coon; *University of Wisconsin, Madison, Wisconsin*
- ThP 686 **Improved ETD Duty Cycle and Spectral Signal to Noise Ratio in a Dual Cell Linear Ion Trap;** Christopher Mullen<sup>1</sup>; Lee Earley<sup>1</sup>; Jean-Jacques Dunyach<sup>1</sup>; John E. P. Syka<sup>1</sup>; Jeffrey Shabanowitz<sup>2</sup>; A. Michelle English<sup>2</sup>; Donald F. Hunt<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, San Jose, CA; <sup>2</sup>University of Virginia, Charlottesville, VA
- ThP 687 **Structure of Arene-Linked Dinuclear Ruthenium(II) Organometallics–Peptide Complexes;** Laure Menin; Benjamin S. Murray; Luc Patiny; Yury O. Tsybin; Paul J. Dyson; *Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*
- ThP 688 **Electron Capture Dissociation of Sodiated Peptides on modified SCIEX Q-Star quadrupole-TOF mass spectrometer;** Valery G. Voinov; Samuel Bennett; Peter Hoffman; Joseph Beckman; Douglas Barofsky; *Oregon State University, Corvallis, OR*
- ThP 689 **ECD, ECD/CID and HPLC ECD MRM of Phosphorylated Peptides in a Triple Quadrupole Mass Spectrometer;** Kenneth Newton<sup>1</sup>; Valery Voinov<sup>2</sup>; Samuel Bennett<sup>2</sup>; Peter Hoffman<sup>2</sup>; Douglas Barofsky<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Oregon State University, Corvallis, OR
- ThP 690 **Characterization of Surface Induced Dissociation in a Multi-Reflecting TOF - TOF Mass Spectrometer;** Aleksey Vorobyev; Andrey Trufanov; Sergey Kirillov; Anatoly Verenchikov; *MSC-CG, Bar, Montenegro*
- ThP 691 **Investigation of Fragmentation of Tryptophan Nitrogen Radical Cation;** Andrii Piatkivskiy<sup>1</sup>; Marshall Happ<sup>1</sup>; Justin Kai-Chi Lau<sup>2</sup>; Alan C. Hopkinson<sup>2</sup>; Victor Ryzhov<sup>1</sup>; <sup>1</sup>Northern Illinois University, Dekalb, IL; <sup>2</sup>York University, Toronto, Ontario, Canada
- ThP 692 **Evaluation of Dissociation Techniques for Non-Targeted Analyte Identification;** Travis Falconer; Enrique Yanes Santos; *US Food & Drug Administration, Cincinnati, OH*
- ThP 693 **Novel Application of Electron Induced Dissociation (EID) for Steroid Fragmentation;** Christopher J. Thompson<sup>1</sup>; Guilong (Charles) Cheng<sup>2</sup>; <sup>1</sup>Bruker Daltonics Inc., Billerica, MA; <sup>2</sup>Alexion Pharmaceutical Inc., Cheshire, CT
- ThP 694 **Fragmentation of Isotope Labeled and Unlabeled Azo Compounds;** Martin Clemen; Tassilo Muskat; Jürgen Grotemeyer; *Inst. f. Phys. Chem der CAU zu Kiel, Kiel, Germany*
- ThP 695 **Ion–Molecule Reactions and Separation of <sup>238</sup>U/<sup>238</sup>Pu Isobars in the Collision/reaction Cell of Tandem Inductively Coupled Plasma Mass Spectrometer;** Mohamed A. Amr; Saeed H. Al-Meer; *Qatar University, Doha, Qatar*
- ThP 696 **Development of a Tune Method, Based on theoretical Studies, for the Comparison of CID Spectra from Various Instrumental Platforms;** Farid Ichou<sup>1</sup>; Adrian Schwarzenberg<sup>1</sup>; Denis Lesage<sup>1</sup>; Sandra Alves<sup>1</sup>; Richard B. Cole<sup>1</sup>; Xavier Machuron-Mandard<sup>2</sup>; Christophe Junot<sup>3</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>University Paris VI (UPMC) case 45 UMR 7201 CNRS, Paris Cedex 05, France; <sup>2</sup>Atomic Energy Commission, Arpajon Cedex, France; <sup>3</sup>CEA, LEMM, DSV/ibitec-S/SPI, 91191 Gif-sur-Yvette, France
- ThP 697 **Soft Supercharging of Biomolecular Ions in Electrospray Ionization Mass Spectrometry;** Xu Ning; Konstantin Chingjin; Eric Handberg; Huanwen Chen; *East China Institute of Technology, Nanchang, China*

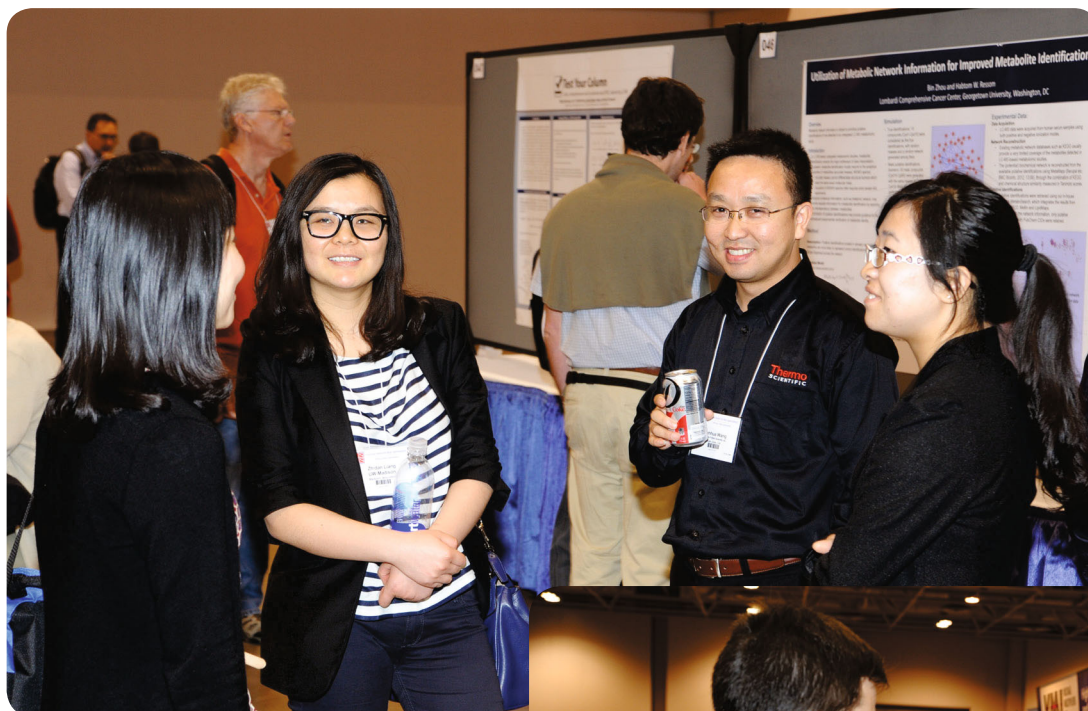
- ThP 698 **Differentiation of Isomeric Branched Side-Chain Amino Acids by Electron Activated Dissociation;** Wendy Zhong<sup>1</sup>; Xiang Yu<sup>2</sup>; <sup>1</sup>Merck, Summit, NJ; <sup>2</sup>Northwestern University, Evanston, IL
- ThP 699 **Are Acylium Ions Proton Donors or Hydride Acceptors in the Fragmentation of Protonated Amides?;** Yunfeng Chai; Yuanjiang Pan; Zhejiang University, Hangzhou, China
- ThP 700 **Modeling the Dissociation of Cyclodextrin Dimer Ions and their Inclusion Complexes;** Justin Renaud; Kevin Berland; Paul Michael Mayer; University of Ottawa, Ottawa, Canada
- ThP 701 **Characterisation of Point Mutations in Hemoglobin Chains using Top Down Mass Spectrometry;** Krisztina Rádi<sup>1</sup>; Julia Smith<sup>2</sup>; James Scrivens<sup>1</sup>; <sup>1</sup>University of Warwick - Life Sciences, Coventry, UK; <sup>2</sup>Bruker, Coventry, UK
- ThP 702 **Heterolytic or Homolytic Bond Cleavage: Possible Pathways for Generating Ions 170 and 171 from Dansylated Compounds under Electrospray Ionization;** Jianshuang Wang; Brian Dean; Xiao Ding; Genentech, South San Francisco, CA
- Carbohydrates, 709 - 734**
- ThP 709 **MALDI in-Source Decay Fragmentation of Glycans with Iron Oxide Nanoparticle Matrices;** Qiaoli Liang; Yaolin Xu; Thomas Macher; Yuping Bao; Carolyn Cassady; University of Alabama, Tuscaloosa, AL
- ThP 710 **Linkage and Stereo-Structure Determination of Oligosaccharides by Microwave Assisted Partial Acid Hydrolysis and MS<sup>n</sup> (n>2);** Jia Ren; Purdue University, West Lafayette, IN
- ThP 711 **Mechanistic Investigation on the Negative Electron Transfer Dissociation of Heparan Sulfate Disaccharide ΔHexA2S-GlcNs;** Yiqun Huang; Yu Huang; Joseph Zaia; Catherine E. Costello; Cheng Lin; Boston University School of Medicine, Boston, MA
- ThP 712 **Use of Ion Mobility and Negative Ion Fragmentation for Isomer Separation and Structural Determination of N-Linked Glycans from HIV-Derived gp120;** David J. Harvey<sup>1,2</sup>; Max Crispin<sup>1</sup>; Kevin Pagel<sup>3</sup>; Matthew Edgeworth<sup>2</sup>; Weston Struwe<sup>4</sup>; James Scrivens<sup>2</sup>; <sup>1</sup>University of Oxford, Department of Biochemistry, Oxford, UK; <sup>2</sup>University of Warwick, Coventry, UK; <sup>3</sup>Fritz Haber Institute of the Max Planck Society, Berlin, Germany; <sup>4</sup>University of Oxford, Department of Chemistry, Oxford, UK
- ThP 713 **An Integrated Mass Spectrometry Pipeline for Site-specific N-Glycopeptide Identification;** Chen-Chun Chen<sup>1,2</sup>; Wan-Chih Su<sup>3</sup>; Mira Anne Dela Rosa<sup>3</sup>; Yu-Ju Chen<sup>1,3</sup>; <sup>1</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>2</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan; <sup>3</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- ThP 714 **Improved Glycopeptide Analysis by Optimized Digestion and Enrichment Protocol;** Wan-Chih Su<sup>1</sup>; Chen-Chun Chen<sup>2,3</sup>; Rofe-Amor Obena<sup>1</sup>; Yu-Ju Chen<sup>1,2</sup>; <sup>1</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan; <sup>2</sup>Department of Chemistry, National Taiwan University, Taipei, Taiwan; <sup>3</sup>Genomics Research Center, Academia Sinica, Taipei, Taiwan
- ThP 715 **MALDI and ESI MS-based Analysis of Oligosaccharides using 4-(diphenylphosphine)-benzeneamine as Non-Reductive Amination Derivatizing Agent;** Yan Liu; Jie peng Gan; Hang Yuan; Yu fen Zhao; School of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China
- ThP 716 **Progress towards Elucidating the Octasaccharide Glycan Structures on the S-layer Glycoproteins of the Archaea Methanosarcina mazei by Mass Spectrometry;** Deborah R. Leon<sup>1</sup>; Cheng Lin<sup>2</sup>; Rebecca Glaskin<sup>1</sup>; Nancy Leymarie<sup>3</sup>; Rachel R. Ogorzalek Loo<sup>4</sup>; Joseph A. Loo<sup>4</sup>; Robert P. Gunsalus<sup>4</sup>; Catherine E. Costello<sup>3</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Boston University, Boston, MA; <sup>3</sup>Boston University School of Medicine, Boston, MA; <sup>4</sup>UCLA, Los Angeles, CA
- ThP 717 **Discrimination of Isomeric Hexoses by Variable-Wavelength Infrared Photodissociation Fingerprints;** Yanglan Tan; Nicolas Polfer; Department of Chemistry, University of Florida, Gainesville, FL
- ThP 718 **Development of a Rapid and Sensitive Method Based on LC-MS/MS Detection and Quantification of Glycosaminoglycans in Cells;** Guoyun Li<sup>1,2</sup>; Lingyun Li<sup>2</sup>; Bo Yang<sup>2</sup>; Changhu Xue<sup>1</sup>; Robert Linhart<sup>2</sup>; <sup>1</sup>Ocean University of China, Qingdao, China; <sup>2</sup>Rensselaer Polytechnic Institute, Troy, New York
- ThP 719 **Identifying Gangliosides by ESI-CID-MS: The Need for High and Low Collision Energy for Glycolipid Characterization on Release from Protein-Glycolipid complexes;** Aneika Loney; Nobar Jalili; John Klassen; University of Alberta, Edmonton, Canada
- ThP 720 **Quantitative Measurement of Sialic Acid in Culture Medium and Cell Surface;** Dan Wang<sup>1</sup>; Huan Nie<sup>2</sup>; Evgeny Ozhegov<sup>1</sup>; Aiming Zhou<sup>1</sup>; Xue-Long Sun<sup>1</sup>; <sup>1</sup>Cleveland state university, Cleveland, Ohio; <sup>2</sup>Harbin Institute of Technology, Harbin, China
- ThP 721 **Comparison of Fragmentation Pattern of Constitutive Disaccharides Isomers between GC-EI/CI/FI-MS;** Takeshi Furuhashi<sup>1</sup>; Keisuke Ishii<sup>2</sup>; Kazuo Tanaka<sup>2</sup>; Wolfram Weckwerth<sup>3</sup>; Takemichi Nakamura<sup>4</sup>; <sup>1</sup>RIKEN, Yokohama City, JAPAN; <sup>2</sup>JEOL, Tachikawa, Japan; <sup>3</sup>Wien Universität, Vienna, Austria; <sup>4</sup>RIKEN Wako, Wako city, Japan
- ThP 722 **Automating Mass Spectrometry-Based Quantitative Glycomics using Tandem Mass Tag (TMT) Reagents with SimGlycan;** Ningombam Sanjib Meitei<sup>1</sup>; Arun Apte<sup>2</sup>; Sergei Snovida<sup>3</sup>; Julian Saba<sup>4</sup>; John Rogers<sup>3</sup>; <sup>1</sup>PREMIER Biosoft, Indore, India; <sup>2</sup>PREMIER Biosoft, Palo Alto, CA; <sup>3</sup>Thermo Fisher Scientific, Rockford, IL; <sup>4</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 723 **Preliminary Development of a Shotgun Heparin/Heparan Sulfate Array using Multi-Dimensional Fractionation;** David Fischler; Tong Zhang; Joshua S. Sharp; Complex Carbohydrate Research Center, UGA, Athens, GA
- ThP 724 **Analysis of Heparan Sulfate in Human Serum: Significant Differences in Healthy Vs Rheumatoid Arthritis Patients;** Jenny K. Sabol; Wei Wei; Youjin Seo; Armann Andaya; Julie A. Leary; University of California Davis, Davis, CA
- ThP 725 **Investigating Changes in the Gas-Phase Conformation of Antithrombin III Upon Binding of Arixtra Using Traveling Wave Ion Mobility Spectrometry (TWIMS);** Yuejie Zhao<sup>1</sup>; Lingyun Li<sup>2</sup>; Robert J. Linhardt<sup>2</sup>; Jon Amster<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Rensselaer Polytechnic Institute, Troy, NY
- ThP 726 **GAG-ID: Heparan Sulfate and Heparin Glycosaminoglycan High-Throughput Identification Software;** Yulun Chiu; Rongrong Huang; Ron Orlando; Joshua S. Sharp; CCRC, University of Georgia, Athens, GA
- ThP 727 **Structural Analysis of Isomeric Chondroitin Sulfate Oligosaccharides Using Regioselective 6-O-desulfation Method and Tandem Mass Spectrometry;** Shu Ting Chen; Guor-Rong Her; National Taiwan University, Taipei, Taiwan

- ThP 728 **Investigation of Matrix Effects on INLIGHT™ Tagging and Optimization of Reversed-Phase nanoLC-MS for Improved Detection of N-linked Glycans;** Elizabeth S. Hecht; Amber C. Cook; David C. Muddiman; *North Carolina State University, Raleigh, NC*
- ThP 729 **Stability Analysis of Oligosaccharides;** Lauren D. Wu; Angela Zivkovic; Sarah Totten; L. Renee Ruhaak; Carlito B. Lebrilla; *University of California, Davis, CA*
- ThP 730 **Characterizing the Mode of Action of Dermatatan Sulfate Epimerase 1 using a Hydrogen/Deuterium Exchange Method;** Yang Mao<sup>1</sup>; Emil Tykesson<sup>2</sup>; Xiaofeng Shi<sup>3</sup>; Anders Malmström<sup>2</sup>; Joseph Zaia<sup>1</sup>; <sup>1</sup>*Boston University School of Medicine, Boston, MA*; <sup>2</sup>*Lund University, Lund, Sweden*; <sup>3</sup>*New England Biolabs, Ipswich, MA*
- ThP 731 **CZE-ESI-MS Analysis of INLIGHT™ Tagged N-Glycans for Improved Separation and Limit of Detection using Neutral and Charged Hydrophobic Hydrazide Reagents;** James Mccord<sup>1</sup>; Amber Cook<sup>1</sup>; Liangliang Sun<sup>2</sup>; Morteza Khaleedi<sup>1</sup>; Norman Dovichi<sup>2</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*University of Notre Dame, South Bend, IN*
- ThP 732 **Analysis of Carbohydrates and Derivatized Carbohydrates Using Matrix Assisted Ionization Vacuum-Ion Mobility Spectrometry-Mass Spectrometry;** Bryan Harless; Tarick El-Baba; Sarah Trimpin; *Wayne State University, Detroit, MI*
- ThP 733 **Biomarker Discovery Efforts for Ovarian Cancer: Using Association Analysis for Elucidating Unique N-Glycome Profiles Generated from Matched Human Plasma;** Amber Cook<sup>1</sup>; Hunter Walker<sup>1</sup>; Amber Taylor<sup>1</sup>; Chad Brown<sup>1</sup>; Alison Motsinger<sup>1</sup>; William Cliby<sup>2</sup>; James Petite<sup>1</sup>; David C. Muddiman<sup>1</sup>; <sup>1</sup>*North Carolina State University, Raleigh, NC*; <sup>2</sup>*Mayo Clinic College of Medicine, Rochester, MN*
- ThP 734 **Identification of Sulfation Patterns for Heparan Sulfate Mixtures using High Resolution Tandem Mass Spectrometry;** Han Hu<sup>1</sup>; Yu Huang<sup>2</sup>; Yu Xia<sup>3</sup>; Joseph Zaia<sup>2</sup>; <sup>1</sup>*Boston University, Boston, MA*; <sup>2</sup>*Boston University School of Medicine, Boston, MA*; <sup>3</sup>*McGill University, Montreal, Canada*
- Agriculture, 735 - 737**
- ThP 735 **Quantitative Label-Free Shotgun Proteomic Analysis of Cabernet sauvignon Cells Exposed to Hot and Cold Temperature Stresses;** Iniga S. George<sup>1</sup>; Dana Pascovici<sup>2</sup>; Paul A. Haynes<sup>1</sup>; <sup>1</sup>*Macquarie University, Sydney, Australia*; <sup>2</sup>*Australian Proteome Analysis Facility, Macquarie University, Sydney, Australia*
- ThP 736 **The Analysis of Foliates in Pulse Crops by LC-MS/MS;** Randy W. Purves<sup>1,2</sup>; Ashokkumar Kaliyaperumal<sup>2</sup>; Stephen J. Ambrose<sup>1</sup>; Thomas D. Warkentin<sup>2</sup>; Albert Vandenberg<sup>2</sup>; <sup>1</sup>*National Research Council, Saskatoon, Canada*; <sup>2</sup>*University of Saskatchewan, Saskatoon, Canada*
- ThP 737 **High Mass Accuracy FT-ICR for Characterization of the Soybean Metabolome;** Troy Wood<sup>1</sup>; Jerod Hurst<sup>1</sup>; William Friesen<sup>2</sup>; <sup>1</sup>*University at Buffalo, Buffalo, NY*; <sup>2</sup>*SUNY at Buffalo, Buffalo, NY*
- Instrumentation: General, 738 - 764**
- ThP 738 **High Sensitivity Selective-Reagent-Ionization Time-of-Flight Mass Spectrometry (SRI-TOF-MS);** Alfons Jordan<sup>1</sup>; Kostiantyn Breiev<sup>1</sup>; Christian Lindinger<sup>1</sup>; Gernot Hanel<sup>1</sup>; Eugen Hartungen<sup>1</sup>; Jens Herbig<sup>1</sup>; Simone Jürschik<sup>1</sup>; Matteo Lanza<sup>1</sup>; Philipp Sulzer<sup>1</sup>; Tilmann D. Märk<sup>1,2</sup>; <sup>1</sup>*IONICON Analytik GmbH., Innsbruck, Austria*; <sup>2</sup>*University of Innsbruck, Innsbruck, Austria*
- ThP 739 **A Portable Fast Gas Chromatograph - Mass Spectrometer and Its Field Applications;** Lian Duan; Qiao Ma; JiaHui Deng; Rong Zhu; YingZhi Liu; LiPeng Liu; Yi Zheng; ShuangLai Han; *Focused Photonics(Hangzhou),Inc., HangZhou, China*
- ThP 740 **Extension of an In-house CE-ESI System to an Ion Trap Mass Spectrometer;** Rosemary Onjiko; Peter Nemes; *George Washington University, Washington, DC*
- ThP 741 **Detecting and Removing Data Artifacts in Hadamard Transform Ion Mobility-Mass Spectrometry Measurements;** Spencer A. Prost<sup>1</sup>; Kevin L. Crowell<sup>1</sup>; Erin S. Baker<sup>1</sup>; Yehia M. Ibrahim<sup>1</sup>; Brian H. Clowers<sup>2</sup>; Matthew E. Monroe<sup>1</sup>; Gordon A. Anderson<sup>1</sup>; Richard D. Smith<sup>1</sup>; Samuel H. Payne<sup>1</sup>; <sup>1</sup>*Pacific Northwest National Laboratory, Richland, WA*; <sup>2</sup>*Washington State University, Pullman, WA*
- ThP 742 **Investigation of the Influence of Laser Spot Size and Ion Trajectory to Mass Resolving Power of Dual-Polarity Time-of-Flight Mass Spectrometer;** Yi-Hong Cai; Yin-Hung Lai; Hsun Lee; Yi-Sheng Wang; *Genomics Research Center, Academia Sinica, Taipei, Taiwan*
- ThP 743 **Top Down Protein Analysis by Ultraviolet Photodissociation (UVPD) in an Orbitrap Tribrid Mass Spectrometer;** Dustin Holden<sup>1</sup>; Jesse Canterbury<sup>2</sup>; Eugene Zhuk<sup>2</sup>; Nick Izgarian<sup>2</sup>; Jae Schwartz<sup>2</sup>; Jennifer Brodbelt<sup>1</sup>; <sup>1</sup>*The University of Texas, Austin, TX*; <sup>2</sup>*Thermo Fisher Scientific, San Jose, CA*
- ThP 744 **Design & Development of a New, High Performance 20kV HED Detector with Improved Efficiency and Low Noise Characteristics;** Michael Flanagan; Michael Ugarov; Layne Howard; Anabel Fandino; *Agilent Technologies, Santa Clara, CA*
- ThP 745 **A High-Performance Parallel Computational Platform for Ion Optics And Ion Motion Dynamics Simulations using Graphics Processing Units of Desktop Computers;** Konstantin Novoselov<sup>1</sup>; Nina N. Popova<sup>2</sup>; Alexander M. Popov<sup>2</sup>; Vladimir M. Doroshenko<sup>1</sup>; Alexander Misharin<sup>1</sup>; <sup>1</sup>*MassTech, Columbia, MD*; <sup>2</sup>*Moscow State University, Moscow, Russia*
- ThP 746 **Identification and Affinity- Quantification of  $\beta$ -amyloid and  $\alpha$ -synuclein Polypeptides using Online SAW-Biosensor- Mass Spectrometry;** Stefan Slamnoiu<sup>1</sup>; Camelia Vlad<sup>1,2</sup>; Mihaela Stumbaum<sup>1,2</sup>; Adrian Moise<sup>1</sup>; Nicole Engel<sup>1,3</sup>; Kathrin Lindner<sup>1</sup>; Mar Vilanova<sup>5</sup>; Mireia Diaz<sup>5</sup>; Christiaan Karreman<sup>1</sup>; Marcel Leist<sup>1</sup>; Thomas Ciossek<sup>4</sup>; Bastian Hengerer<sup>4</sup>; Marta Vilaseca<sup>5</sup>; Michael Przybylski<sup>1</sup>; <sup>1</sup>*University of Konstanz, Konstanz, Germany*; <sup>2</sup>*SAW- Instruments, Bonn, Germany*; <sup>3</sup>*Technical University of Vienna, Vienna, Austria*; <sup>4</sup>*Boehringer Ingelheim Pharma, Biberach, Germany*; <sup>5</sup>*Institute for Research in Biomedicine Barcelona, Barcelona, Spain*
- ThP 747 **3D Simulation of Quadrupole Mass Filters with Offset and Tilted Rods;** David Langridge; *Waters, Wilmslow, UK*
- ThP 748 **Extending the Linear Dynamic Range of Quadrupole Detectors;** Richard Moulds; Daniel J Kenny; Kenneth Worthington; Steven Pringle; *Waters Corporation, Manchester, UK*
- ThP 749 **Design and Performance of a Highly Compact Single Quadrupole Mass Spectrometer;** Daniel J Kenny; Dave Gordon; Richard Moulds; Kate Whyatt; Marcus Dawber; Ian Trivett; Howard Read; *Waters Corporation, Manchester, UK*
- ThP 750 **Triple Stage Quadrupole Mass Spectrometer with Enhanced Sensitivity to Product Ions;** Oleg Silivra; Harald Oser; Terry Olney; *Thermo Fisher Scientific, San Jose, CA*

- ThP 751 **Space Charge Effects in a Coaxial Two-Mirror Electrostatic Multi-Reflection Mass Analyzer**; Dmitry Grinfeld<sup>1</sup>; Anastassios Giannakopoulos<sup>1</sup>; Igor Kopaev<sup>2</sup>; Mikhail Monastyrskiy<sup>2</sup>; Michael Skoblin<sup>3</sup>; Alexander Makarov<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>General Physics Institute of Rus. Acad. Sci., Moscow, Russia; <sup>3</sup>Institute for energy problems of chemical physics, Moscow, Russia
- ThP 752 **Combined Experimental and Theoretical Study of the Spatial and Velocity Distributions of Ions Stored in a RF Ion Trap**; Christian Hock; Dmitry Grinfeld; Anastassios Giannakopoulos; Richard Heming; Alexander Makarov; Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany
- ThP 753 **Fourier Transform Based Apex Triggered Quantitation Enhanced Data-Dependent (QED) Scanning**; Qingyu Song; Michael W. Senko; Eric Hemenway; Mary Blackburn; Thermo Fisher Scientific, San Jose, CA
- ThP 754 **Putting Scattering to the Right Use – Discrimination of Ion Species of Different Sizes by the Decay Rate in FTMS**; Konstantin Aizikov; Dmitry Grinfeld; Eugen Damoc; Alexander Makarov; Thermo Fisher Scientific, Bremen, Germany
- ThP 755 **Evaluation of a Collision Cell with Axial Field for Achieving High Speed SRM in a Triple Stage Quadrupole Mass Spectrometer**; Oleg Silivra; Harald Oser; Joshua Maze; Terry Olney; Thermo Fisher Scientific, San Jose, CA
- ThP 756 **Improved Control of Ion Populations for Orbitrap Mass Analysis**; Philip M Remes; Jesse D. Canterbury; Michael W. Senko; Thermo Fisher Scientific, San Jose, CA
- ThP 757 **Ion Collision Cross Section Measurements in Quadrupole Ion Traps Using a Time-frequency Analysis Method**; Muyi He; Yu Chen; Wei Xu; Beijing Institute of Technology, Beijing, China
- ThP 758 **Multi-Ported Pulsed Valve Interface for a Linear Quadrupole Ion Trap for Rapid Screening of Multiple Functional Group Selective Ion-Molecule Reactions**; Tiffany Jarrell; James Riedeman; Mark Carlsen; Randall Replogle; Timothy Selby; Hilikka Kenttämä; Purdue University, West Lafayette, IN
- ThP 759 **Optimizing Ion Optical Rail for Coupling a Drift Tube to a Mass Spectrometer**; Alex Mordehai; Nathan Sanders; Ruwan Kurulugama; Mark Werlich; Agilent Technologies, Santa Clara, CA
- ThP 760 **Simulation of Ion Trajectories through An Entire Mass Spectrometer - Incorporation of a Full Gas Dynamic Field with Electric Field**; Xiaoyu Zhou; Zheng Ouyang; Purdue University, West Lafayette, Indiana
- ThP 761 **Improvement of Pulse Height Distribution in Superconducting Strip Ion Detectors for TOF MS**; Nobuyuki Zen; Shigetomo Shiki; Masahiro Ukibe; Masaki Koike; Masataka Ohkubo; AIST, Tsukuba, Japan
- ThP 762 **A Quadrupole Orbitrap Benchtop Instrument with a High Field Analyzer Applied to In-Depth, Single Shot Proteomics**; Richard Alexander Scheltema<sup>1</sup>; Jan-Peter Hauschild<sup>2</sup>; Oliver Lange<sup>2</sup>; Eduard Denisov<sup>2</sup>; Nicolaie Eugen Damoc<sup>2</sup>; Andreas Kuehn<sup>2</sup>; Mann Matthias<sup>1</sup>; <sup>1</sup>Max Planck Institute, Martinsried, Germany; <sup>2</sup>Thermo Fisher Scientific, Bremen, Germany
- ThP 763 **Data Independent Acquisition on a Q Exactive Plus Prototype with a High-Field Orbitrap**; Jarrett Egerton<sup>1</sup>; Richard S. Johnson<sup>1</sup>; Ying Sonia Ting<sup>1</sup>; Dario Amodei<sup>2</sup>; Brendan MacLean<sup>1</sup>; Donald Marsh<sup>1</sup>; Parag Mallick<sup>2</sup>; Michael J. MacCoss<sup>1</sup>; <sup>1</sup>University of Washington, Seattle, WA; <sup>2</sup>Stanford University, Palo Alto, California
- ThP 764 **Plasma Generation for High Sensitivity ICP-MS**; Louiri Kalinitchenko<sup>1</sup>; Steven Hosemans<sup>2</sup>; Peter Zdaril<sup>2</sup>; Jeffrey Sim<sup>2</sup>; <sup>1</sup>Bruker, Fremont, CA; <sup>2</sup>Bruker, Preston, Australia
- LCMS Sample Preparation, 765 - 784**
- ThP 765 **Simplified Strategy for Rapid Reproducible Quantitation of Monoclonal Antibodies in Plasma**; John O'Grady<sup>1</sup>; Hongxia (Jessica) Wang<sup>2</sup>; Kevin Meyer<sup>1</sup>; Zhiqi Hao<sup>2</sup>; <sup>1</sup>Perfinity Biosciences, Inc, West Lafayette, IN; <sup>2</sup>Thermo Fisher Scientific, San Jose, CA
- ThP 766 **A Rapid and Reproducible Immuno-MS Platform from Sample Collection to Quantitation of IgG**; Rachel Lieberman<sup>1</sup>; David Colquhoun<sup>1</sup>; Jeremy Post<sup>1</sup>; Brian Feild<sup>1</sup>; Scott Kuzdzal<sup>1</sup>; Fred Regnier<sup>2</sup>; <sup>1</sup>Shimadzu Scientific Instruments, Columbia, MD; <sup>2</sup>Novilytic L.L.C., W. North Webster, IN
- ThP 767 **Detection of Neutralizing Antibodies in Human Serum by a Ligand Binding-LC/MS/MS Hybrid Approach**; Xiao Liu; Ben Badillo; Huiyu Zhou; BioMarin Pharmaceutical Inc, Novato, CA
- ThP 768 **A Novel Approach to Increase Sensitivity and Selectivity in LC-MS/MS Quantitation of Proteins by Selectively Removing Albumin from Plasma/Serum Samples**; Guowen Liu; Jim Shen; Yue Zhao; Aida Angeles; Mark Arnold; Bristol-Myers Squibb, Princeton, NJ
- ThP 769 **Comparison of LC Methodology and Sample Preparation for Label-Free Quantitative Analysis of the Serum Proteome**; Jeffrey F. Kuhn<sup>1</sup>; Leesa Deterding<sup>2</sup>; <sup>1</sup>NIEHS, Research Triangle Park, NC; <sup>2</sup>NIEHS/NIH/DHHS, Research Triangle Park, NC
- ThP 770 **Analysis of Fibrinogen Methionine Oxidation in Plasma from Trauma Patients by nanoLC-ESI-MS/MS**; Yi Wang<sup>1</sup>; Nathan White<sup>2</sup>; Dominic Chung<sup>1,2</sup>; Xiaoyun Fu<sup>1,2</sup>; <sup>1</sup>Puget Sound Blood Center, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- ThP 771 **Histology-Guided Microdissection-Based Proteomic and Glycomic Profiling of Tissue Sections**; Le Meng; Lilla Turiak; Chun Shao; Qi Wang; Joseph Zaia; Boston University School of Medicine, Boston, MA
- ThP 772 **Optimizing an Extraction Method for Reducing Humic Acid Interferences in MS-based Proteome Measurements of Environmental Soil Samples**; Chen Qian; Karuna Chourey; Robert Hettich; Oak Ridge National Laboratory, Oak Ridge, TN
- ThP 773 **Cumulomics - Optimization of Sample Preparation for Low Amount Cumulus Samples**; Claudia Fortes<sup>1</sup>; Bernd Roschitzki<sup>1</sup>; Jasmin Walter<sup>2</sup>; Ralph Schlapbach<sup>1</sup>; <sup>1</sup>Functional Genomics Center Zurich, Zurich, Switzerland; <sup>2</sup>Vetsuisse Faculty, Zurich, Switzerland
- ThP 774 **How to reproducibly Collect, Ship and Share Extremely Diluted Proteome Samples**; Florian Bonn; Jürgen Bartel; Knut Büttner; Michael Hecker; Dörte Becher; Andreas Otto; University Greifswald, Greifswald, Germany
- ThP 775 **Investigation of Difference between LC-UV and LC-MS Peptide Maps Caused by Residual Alkylation Reagent Iodoacetamide**; Hongwei Xie; Song klapoetke; KBI Biopharma, Durham, NC
- ThP 776 **The Removal of LC-MS Contaminants in Shotgun Proteomics**; Ellen Scheerlinck; Kathleen Van Steendam; Paulien Meert; Maarten Dhaenens; Dieter Deforce; Laboratory of Pharmaceutical Biotechnology, University Ghent, Belgium
- ThP 777 **Evaluation of Stain-Free Chemistry for GeLC-MS Applications**; Sricharan Bandhakavi<sup>1</sup>; Kate Smith<sup>1</sup>; Todd Markowski<sup>2</sup>; <sup>1</sup>Bio-Rad Laboratories, Hercules, CA; <sup>2</sup>University of Minnesota, Minneapolis, MN



- ThP 778 **Yeast and Human Protein Extracts for Mass Spectrometry Performance Monitoring and Method Development;** Sergei Saveliev; Ethan Strauss; Mike Rosenblatt; Marjeta Urh; *Promega Corporation, Madison, WI*
- ThP 779 **Selecting the Right Tool for In-Gel and In-Solution Protein Digestion;** Marjeta Urh; *Promega, Madison, WI*
- ThP 780 **Investigation of Different Denaturants in Mouse Brain Tissue Sample Preparation for LC/MS Based Discovery Proteomics;** Qiaozhen (Cheryl) Lu; Kojo Abdul-Hadi; Peter Juhasz; Ru Wei; *Biogen Idec, Cambridge, MA*
- ThP 781 **A Small-Scale, Flexible, yet Automated Protein Digestion and Peptide Desalting Process;** Kojo Abdul-Hadi<sup>1</sup>; Martin Technau<sup>2</sup>; Qiaozhen (Cheryl) Lu<sup>1</sup>; Bekim Bajrami<sup>1</sup>; Nathan Swentko<sup>3</sup>; Peter Juhasz<sup>1</sup>; Ru Wei<sup>1</sup>; <sup>1</sup>*Biogen Idec, Cambridge, MA*; <sup>2</sup>*Intavis AG, Cologne, Germany*; <sup>3</sup>*Intavis AG, Chicago, IL*
- ThP 782 **Automated SDS Removal and Protein Digestion in a Disposable Two-Stage Spin Cartridge for Bottom-up MS Analysis;** Alan A. Doucette; Andrew Crowell; Samantha Rudolph; *Dalhousie University, Halifax, Canada*
- ThP 783 **Porous Polymer Monolith Micro-Sample Preparation Devices for Filtration, Digestion and Direct At-Line Solid Phase Extraction-Mass Spectrometry;** Esme Candish<sup>1, 2</sup>; Wei Boon Hon<sup>1, 3</sup>; Hans-Jürgen Wirth<sup>3</sup>; Andrew Gooley<sup>1, 3</sup>; Robert A. Shellie<sup>1</sup>; Emily F. Hilder<sup>1</sup>; <sup>1</sup>*ACROSS, Hobart, Australia*; <sup>2</sup>*SGE Analytical Science, Ringwood, Australia*; <sup>3</sup>*Trajan Scientific & Medical, Ringwood, Australia*
- ThP 784 **LC/MS Protein Quantification and Characterization Enabled by a Sample Preparation Platform that Automates Purification, Digestion, and Cleanup;** Steve Murphy; Jason Russell; Michael Bovee; *Agilent Technologies, Inc., Madison, WI*



## INDEX OF AUTHORS

Ababat, Mary	MP 713	Aebersold, Ruedi	ThP 257	Albers, Christian	MP 289
Abate, Daniel	MP 625	Aebersold, Ruedi	TOD pm 4:10	Alberta, John A.	TP 007
Abate, Daniel	TP 654	Aebersold, Ruedi	TP 181	Alberti, James	WP 769
Abate-Pella, Daniel	TP 667	Aebersold, Ruedi	WP 155	Albone, Earl	TP 238
Abbas, Esraa Y.	TP 563	Aebi, Markus	MP 152	Albrecht, Benjamin	WP 486
Abbassi-Ghadi, Nima	ThP 664	Aerts, Johannes M.F.G.	MP 265	Albrecht, Lauren	TOG am 08:50
Abbassi-Ghadi, Nima	TP 375	Aerts, Jordan T.	TP 640	Albrecht, Sascha	TP 736
Abbatiello, Susan E.	ThOC am 10:10	Afchine, Armin	TP 736	Albrecht, Simone	ThOH am 09:30
Abbatiello, Susan E.	ThP 217	Afiuni, Somi	TP 428	Aldrich, Joshua	WOE pm 4:10
Abbott, Richard	WP 644	Afjehi-Sadat, Leila	ThOF pm 2:30	Aleksic, Maja	ThP 249
Abdelhameed, Ali S.	MP 725	Afonso, Carlos	ThP 499	Aleyunas, Yun	TP 629
Abdelmoula, Walid M.	MP 027	Afonso, Carlos	TP 369	Alessi, Dario	WP 200
Abdelmoula, Walid M.	TP 015	Afonso, Carlos	TP 406	Alexandrov, Theodore	MOH pm 4:10
Abdi, Fadi	MP 238	Afonso, Carlos	TP 775	Alexandrov, Theodore	MP 020
Abdulkaker, Abdullah A.	TP 563	Afonso, Carlos	WOC pm 2:50	Alexandrov, Theodore	MP 021
Abdul-Hadi, Kojo	ThP 780	Afonso, Carlos	WP 679	Alexandrov, Theodore	ThOA pm 2:50
Abdul-Hadi, Kojo	ThP 781	Afsar Minhas, Fayyaz-ul-Amir	ThOG am 08:50	Alexandrov, Theodore	ThOG am 09:30
Abdullah, Laila	MP 116	Afshinnia, Farsad	ThP 662	Alexandrov, Theodore	TP 008
Abdullah, Laila	MP 246	Aga, Diana	TP 553	Alexandrov, Theodore	TP 047
Abdullah, Laila	MP 266	Agar, Jeffrey	TP 546	Alexandrova, Ludmila	TP 507
Abdullah, Laila	WOF am 09:50	Agar, Jeffrey N.	MP 147	Alexandrova, Sonya	ThP 062
Abelin, Jennifer	WOG pm 2:30	Agar, Jeffrey N.	ThP 130	Alexandrova, Sonya	ThP 064
Abelin, Jennifer G.	WOD am 08:50	Agar, Nathalie Y. R.	TP 007	Aleyunas, Yun	WP 637
Abello, Nicolas	WP 055	Agar, Nathalie Y.R.	TP 055	Alfano, Massimo	ThP 293
Abenmoha, Elie	WP 047	Agius, Gareth	ThP 089	Alfaro, Clint M.	MP 312
Abliiz, Zeper	ThP 669	Agnew, Brian	TP 146	Alghafly, Hashim	MP 780
Ablonczy, Zsolt	MP 022	Agrawal, Rakesh	MP 574	Al-Gizawiy, Mona	MP 428
Ablonczy, Zsolt	TP 070	Aguilar, Julieta	TP 019	Al-Gizawiy, Mona	ThP 280
Aboufazel, Forouzan	MP 142	Aguirre, J. Dafhne	WP 112	Ali, Ahmed M.	MP 202
Aboulaich, Nabila	TP 243	Agyekum, Isaac	TP 329	Ali, Liaqat	WP 072
Abou-Samra, Abdul	TP 488	Agyekum, Isaac	WOD pm 3:10	Ali, Zahid	MP 713
Abraham, Paul	TP 675	Ahlers, Stephen T.	ThP 306	Aliman, Michel	MP 690
Abraham, Sheela	WP 114	Ahlf, Dorothy	TP 006	Al-Janabi, Wissam	TP 143
Abrahamson, Dale	MOH pm 2:30	Ahmad, Shadab	ThP 450	Al-Janabi, Wissam	TP 488
Abramov, Tigran	TOG pm 3:30	Ahmad, Shadab	WP 515	Al-Janabi, Wissam	WP 241
Abramowski, Pierre	TP 054	Ahmad, Yasmeen	ThP 089	Aljarod, Omar Y.	TP 563
Abshiru, Nebiyu	TP 113	Ahmad Rusmili, Muhamad Rusdi	TP 303	Alkanaimsh, Salem	TP 258
Abubacker, Thaminum Ansari	TP 529	Ahmed, Arif	MP 300	Alkhatib, Ghalib	TP 107
Abzalimov, Rinat R.	ThP 090	Ahmed, Musahid	TP 381	Alla, Ravi Chandran Reddy	TP 292
Ackerman, Luke	WP 403	Ahmed, Saima	MP 680	Allard, Rene	TP 445
Ackermann, Gail	MOH pm 4:10	Ahmed, Saima	MP 747	Allard, Rene	WP 138
Acosta, Rafael	ThP 615	Ahmed, Saima	ThOE pm 4:10	Allard, Rene	WP 137
Acosta, Rafael	TP 308	Ahmed, Sartaj	MP 255	Alleaume, Anne-Marie	TP 202
Acosta, Rafael	TP 557	Ahn, Dong	ThP 628	Allen, Lloyd	WP 753
Acosta-Martin, Adelina E	WP 156	Ahn, Natalie	ThP 193	Allen, Mike	WP 040
Adachi, Tomoko	TP 711	Ahn, Tae-Hyuk	TP 125	Allen, Mike	WP 480
Adam, Gregory	MP 536	Ahrens, Maike	MP 431	Allen, Samuel J.	MOC pm 3:30
Adam, Melody	TP 506	Ahrens, Maike	TP 481	Allen, Samuel J.	WP 669
Adamec, Jiri	TOB pm 2:30	Aich, Udayanath	TP 337	Allentoff, Alban	TOE am 09:30
Adamo, Martin L.	ThP 385	Aichel, Fabian	MP 052	Allis, C. David	WOG am 09:50
Adams, Chris	ThP 308	Aichler, Michaela	MP 021	Allison, John	MP 011
Adams, Chris	TOA pm 3:30	Aigotti, Riccardo	ThP 596	Allison, Timothy	WOH pm 3:50
Adams, Craig	TP 575	Aikawa, Masanori	WP 018	Allmaier, Guenter	TP 053
Adams, Craig	WP 569	Aikawa, Masanori	WP 070	Allred, Brent Mckay	WP 574
Adams, Kendra	TP 209	Ainley, Steve	MOF pm 2:50	Allred, Stephanie I.	ThP 605
Adams, Paul D.	TP 175	Ainley, Steven	WP 627	Almaguer, Ashley	WP 774
Adams, Rachel	MP 264	Ait-Aissa, Selim	TP 309	Al-Majdoub, Mahmoud	ThP 107
Adams, Rachel	ThP 332	Aiyetan, Paul	ThP 156	Almeer, Saeed	WP 341
Adams, Brian	ThP 504	Aizikov, Konstantin	ThP 754	Al-Meer, Saeed H.	MP 334
Addink, Rudolf	MP 552	AK, Vinayak	TP 512	Al-Meer, Saeed H.	ThP 695
Addink, Rudolf	ThP 564	Akarish, Abel	MP 067	Almeida, Lucas Ferreira	ThP 307
Addink, Rudolf	ThP 563	Akinsanya, Billy	TOE am 09:30	Almirall, Jose	ThP 597
Addink, Rudolf	WP 578	Akinsanya, Karen	ThOE am 09:10	Al-Naqshabandi, Mohammed	ThP 362
Adelfinskaya, Yelena	MOA am 09:30	Akinsanya, Karen	TP 061	Alon, Tal	ThP 575
Adelfinskaya, Yelena A.	MP 054	Akiyama, Hisako	ThP 397	Alon, Tal	TP 608
Ademowo, Stella	ThP 433	Aksamija, Zlatan Aksamija	ThOB pm 2:50	Alon, Tal	WOA am 10:10
Adhikari, Jagat	ThP 085	Aksenov, Alexander	TP 133	Alonso, Ana Paula	MP 415
Adkins, Josh N.	TP 324	Akyildiz, Erdal	WP 410	Alonso, David	MP 607
Adkins, Joshua	MOG pm 3:30	Akyüz, Mehmet	TP 302	Alonso, David	MP 655
Adler, Michael	WP 107	Akyüz, Mehmet	TP 307	Alonso, David	ThP 617
Adler, Ryan S.	TP 519	Al Outa, Amani	ThP 297	Alonso, David	TP 603
Adney, Emily M.	WP 253	Alalwiat, Ahlam	MOA pm 2:30	Alonso, David	WP 307
Advani, Jayshree	MP 255	Alalwiat, Ahlam	TP 253	Alonso, David	WP 588
Advani, Jayshree	MP 270	Alaoui Sosse, Saad	WP 549	Alpert, Andrew J.	WP 039
Aebersold, Ruedi	MOG pm 3:50	Alary, Jean-François	MP 656	Alpert, Andrew J.	WP 091
Aebersold, Ruedi	MP 260	Albenne, Cecile	WP 076	Alpert, Andrew J.	WP 162
Aebersold, Ruedi	MP 432	Alberici, Rosana M.	MP 362	Alqahtani, Norah	ThP 646
Aebersold, Ruedi	ThOE pm 3:50	Alberici, Rosana M.	TP 729	Al-Qahtani, Muneera T.	MP 334
Aebersold, Ruedi	ThP 035			Al-Saad, Khalid A.	TP 563

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Al-Saad, Khalid A.....	WP 341	Anderson, Gordon.....	TOC am 08:30	Ao, Minghui.....	WOF pm 4:10
Alt, Carsten.....	WP 465	Anderson, Gordon A.....	MP 654	Aoki, Jun.....	ThP 012
Altaf, Awais.....	MP 414	Anderson, Gordon A.....	MP 677	Aoki-Kinoshita, Kiyoko F.....	ThP 165
Altehaar, A.F. Maarten.....	MP 263	Anderson, Gordon A.....	ThP 741	Aoyama, Chiaki.....	MP 766
Altehaar, A.F. Maarten.....	ThP 212	Anderson, Gordon A.....	TOB am 09:50	Apetri, Adrian.....	ThP 119
Altehaar, A.F. Maarten.....	ThP 545	Anderson, Gordon A.....	TP 324	Apffel, Alex.....	MOC pm 3:10
Altehaar, A.F. Maarten.....	TP 052	Anderson, Gordon A.....	TP 716	Apffel, Alex.....	MP 637
Alterman, Michail.....	ThP 313	Anderson, Gordon A.....	TP 714	Aponte, Julia.....	WP 368
Altmaier, Stephan.....	MP 741	Anderson, Gordon A.....	TP 717	Appelblad, Patrik.....	WP 597
Alton, Dominick J.....	MP 712	Anderson, Kit.....	ThP 370	Apps, Peter.....	WP 455
Altuntas, Esra.....	ThP 510	Anderson, Kristin A.....	TP 112	Apte, Arun.....	MP 238
Altuntas, Esra.....	TP 780	Anderson, Kyle.....	MP 234	Apte, Arun.....	ThP 722
Aluwihare, Lihini.....	TP 549	Anderson, Leigh.....	TP 462	Aquino, Veronica.....	TP 146
Alvarez, Narciso.....	TP 632	Anderson, Leigh.....	WP 517	Arabyan, Narine.....	TP 333
Alvarez, Ruth.....	TP 195	Anderson, Lissa.....	TP 188	Arakawa, Kiyomi.....	MP 739
Alvarez, Ruth M.....	ThP 680	Anderson, Malcolm.....	MP 181	Arakawa, Kiyomi.....	MP 755
Alves, Gelio.....	MP 042	Anderson, Melanie.....	WP 108	Arakawa, Kiyomi.....	ThP 672
Alves, Sandra.....	MP 587	Anderson, Michelle A.....	MP 446	Arakawa, Kiyomi.....	TP 560
Alves, Sandra.....	MP 628	Anderson, N. Leigh.....	WP 518	Arakawa, Kiyomi.....	WP 628
Alves, Sandra.....	ThP 513	Anderson, Stacey E.....	ThP 309	Arakawa, Ryuichi.....	MP 067
Alves, Sandra.....	ThP 696	Anderson, Timothy.....	TP 671	Arampatzidou, Maria.....	ThP 146
Alves, Sandra.....	TP 414	Andersson, Malin.....	MP 003	Araujo, John.....	ThP 423
Alwis, K. Udeni.....	TP 476	Ando, Yosuke.....	MP 267	Arcaro, Kathleen F.....	MP 423
Amann, Joseph.....	ThP 296	Andolfo, Annapaola.....	ThP 293	Archakov, Alexander I.....	TP 081
Amann, Kerstin.....	TP 056	Andren, Per.....	TOH am 08:30	Archer, Jieutonne.....	WOB pm 3:30
Amano, Junko.....	ThP 162	Andren, Per E.....	MP 026	Ard, Shaun.....	MOD am 08:30
Amao, Michiko.....	WP 102	Andren, Per E.....	TP 012	Ardnt, Kim.....	ThP 294
Amato, Nicholas J.....	WP 366	Andren, Per E.....	TP 013	Arens, Nadja.....	MP 416
Ambrose, Stephen J.....	ThP 736	Andren, Per E.....	TP 046	Arevalo, Ricardo.....	ThP 369
Amin, Jakal.....	ThP 535	Andren, Per E.....	TP 016	Arevalo, Ricardo.....	TP 711
Amirav, Aviv.....	ThP 575	Andren, Per E.....	TP 047	Arevalo, Ricardo.....	TP 710
Amirav, Aviv.....	TP 608	Andren, Per E.....	WP 012	Arevalo Jr., Ricardo.....	TOA pm 2:30
Amirav, Aviv.....	WOA am 10:10	Andreotti, Amy H.....	WP 221	Argikar, Upendra.....	ThP 535
Ammazzini, Sara.....	TP 770	Andrews, Andrew.....	MP 227	Argmann, Carmen.....	MP 260
Amodei, Dario.....	ThP 035	Andrews, Christine L.....	TOF pm 3:30	Arif, Ahmed.....	WOA pm 2:30
Amodei, Dario.....	ThP 763	Andrews, Matthew.....	MP 049	Arike, Liisa.....	MP 210
Amo-Gonzalez, Mario.....	ThP 474	Andrews, Philip.....	ThP 454	Arike, Liisa.....	MP 211
Amr, Mohamed A.....	MP 334	Andrews, Philip.....	ThP 487	Aristotelus, Antonopolous.....	ThP 161
Amr, Mohamed A.....	ThP 695	Andrews, Philip.....	WP 258	Arita, Masanori.....	WP 604
Amr, Mohamed A.....	WP 341	Andreyeva, Alina.....	WP 689	Arlt, Heike.....	ThP 405
Amstalden, Marcel.....	ThP 682	Andriamaharavo, N. Rabe.....	MP 048	Armengaud, Jean.....	TP 225
Amster, Jon.....	MP 703	Andriamaharavo, Nirina R.....	MP 604	Armentrout, Peter.....	MOD am 08:30
Amster, Jon.....	ThOH pm 3:50	Andrien, Bruce.....	TP 148	Armentrout, Peter.....	ThP 188
Amster, Jon.....	ThP 725	Andrzejewski, Denis.....	TP 217	Armistead, Paul.....	ThOC am 09:30
Amster, Jon.....	TP 329	Ane, Jean-Michel.....	ThOG pm 3:10	Arndt, James.....	ThP 105
Amster, Jon.....	WOD pm 3:10	Ané, Jean-Michel.....	MP 405	Arndt, James.....	TP 540
An, Bo.....	TP 245	Ané, Jean-Michel.....	TP 669	Arndt, Kim.....	MOE am 10:10
An, Bo.....	WP 193	Angel, Peggì.....	WP 002	Arndt, Kim.....	ThP 648
An, Eunkyung.....	MP 269	Angeles, Aida.....	ThP 768	Arnold, Eddy.....	TOF am 09:50
An, Eunkyung.....	WP 141	Angeles, Aida.....	WP 188	Arnold, Mark.....	MOF pm 3:30
An, Hyun Joo.....	ThOA am 09:50	Angeletti, Ruth.....	MP 421	Arnold, Mark.....	MP 074
An, Hyun Joo.....	ThOH pm 3:10	Angeletti, Ruth Hogue.....	WP 165	Arnold, Mark.....	MP 366
An, Hyun Joo.....	ThP 168	Angerer, Tina.....	ThP 011	Arnold, Mark.....	ThP 768
An, Hyun Joo.....	TP 257	Angerer, Tina B.....	TP 010	Arnold, Mark.....	TOE am 09:30
An, Hyun Joo.....	TP 328	Angermann, Bastian.....	MP 269	Arnold, Mark.....	TP 501
An, Hyun Joo.....	WP 066	Anglin, Bobbi.....	WP 099	Arnold, Mark.....	WP 188
An, Ran.....	ThP 259	Anichina, Janna.....	ThP 524	Arnold, Mark.....	WP 543
An, Rong.....	MP 730	Anish, Chakkumkal.....	TP 160	Arnold, Mark.....	WP 534
An, Yanming.....	ThP 164	Anjo, Sandra.....	ThP 101	Arnold, Mark E.....	WP 636
Anacleto, Joe.....	ThP 573	Anjo, Sandra.....	ThP 315	Arnold, Randy J.....	WP 185
Anacleto, Joe.....	ThP 653	Ankley, Gary.....	TP 311	Arnotskaya, Natalia.....	WP 207
Anaev, EC.....	TP 449	Annangudi, Suresh.....	MOA am 09:30	Arnott, David.....	ThOF pm 2:30
Anagnostopoulos, Dimitrios.....	ThP 087	Annangudi, Suresh.....	ThP 318	Arnott, David.....	WP 048
Anan, Yasumi.....	ThP 667	Annangudi Palani, Suresh Babu.....	WP 024	Arnould, Mark.....	TP 788
Anand, Swati.....	MP 239	Ansong, Charles.....	MOG pm 3:30	Aronova, Sofia.....	MP 600
Ananieva, Irina.....	WP 423	Ansong, Charles.....	WOE pm 4:10	Aronova, Sofia.....	ThOA pm 3:50
Ananieva, Irina.....	WP 713	Anstadt, Emily.....	MP 251	Aronova, Sofia.....	WP 360
Ancheva, Lina.....	ThP 442	Anstadt, Emily.....	WP 502	Aronova, Sofia.....	WP 566
Andaya, Armann.....	MP 101	Anta, Cristina.....	MP 733	Aros-Calt, Sandrine.....	TP 224
Andaya, Armann.....	ThP 724	Anteer, Wissam.....	TP 139	Arra, M.....	TP 434
Andersen, Amity.....	ThOD pm 4:10	Antoine, Rodolphe.....	MOD am 09:10	Array, Tabiwang N.....	ThP 321
Andersen, Michael.....	ThP 613	Antoine, Rodolphe.....	MP 731	Arrey, Tabiwang.....	WOF am 10:10
Andersen, Simon I.....	WOA pm 3:50	Antoine, Rodolphe I.....	WP 177	Arrey, Tabiwang N.....	MP 186
Anderson, Brian.....	TOA am 08:50	Antonaccio, Carla.....	TP 769	Arrey, Tabiwang N.....	ThP 317
Anderson, Brooke.....	MP 415	Antonucci, Vincent.....	MP 511	Arriaga, Edgar.....	MP 218
Anderson, David M.....	MP 022	Antony, Marie Lue.....	TP 615	Arshavsky, Vadim.....	TP 147
Anderson, David M.....	TP 070	Antwi, Kwasi.....	WP 192	Arslanoglu, Julie.....	MP 011
Anderson, Gordon.....	MOC pm 3:10	Antzutkin, Oleg.....	MOB am 09:10	Arslanoglu, Julie.....	MP 068
Anderson, Gordon.....	ThOB am 10:10	Anupriya, Anupriya.....	TP 357	Artaev, Slava.....	WP 709

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

## INDEX OF AUTHORS

Artaev, Viatcheslav .....	MP 660	Aubry, Anne-Françoise .....	WP 636	Baek, Sun Jong .....	ThP 549
Artaev, Viatcheslav .....	ThOB pm 3:10	Auclair, Jared R. ....	MP 147	Baes, Myriam.....	TP 015
Artaev, Viatcheslav .....	WOA pm 3:10	Auclair, Jared R. ....	ThP 130	Baessmann, Carsten .....	MOE pm 3:30
Artaev, Viatcheslav .....	WP 753	Auer, Manfred .....	TP 381	Baessmann, Carsten .....	MP 289
Artavanis-Tsakonas, Spyros .....	TP 145	Auger, Serge .....	MP 284	Baessmann, Carsten .....	MP 723
Artemenko, Konstantin .....	MP 135	Auger, Serge .....	MP 533	Baessmann, Carsten .....	ThP 253
Arthen-Engeland, Thomas .....	ThP 573	Auger, Serge .....	ThP 411	Baessmann, Carsten .....	ThP 573
Arthen-Engeland, Thomas .....	TP 750	Auger, Serge .....	TP 556	Baessmann, Carsten .....	TP 655
Arthur, Kayleigh .....	ThP 500	Auger, Serge .....	TP 607	Baessmann, Carsten .....	WP 727
Arthur, Kayleigh .....	TP 402	Auger, Serge .....	WP 361	Baeumlisberger, Dominic .....	ThP 141
Arvidsson, Torbjörn .....	TP 566	Auger, Serge .....	WP 626	Baeumlisberger, Marion .....	ThP 141
Aryal, Uma .....	WP 088	Auger, Serge .....	WP 634	Baeza, Josue .....	MP 121
Arzola, Lucas .....	TP 258	Aurand, Craig .....	MP 732	Bag, Soumabha .....	TP 350
Asano, Natsuyo .....	WP 628	Aurand, Craig .....	MP 773	Bag, Soumabha .....	TP 741
Asante, Fred .....	MP 190	Aurand, Craig .....	WP 642	Bagatela, Bianca .....	TP 025
Asara, John .....	WP 047	Auray-Blais, Christiane .....	WP 441	Bagdany, Miklos .....	WP 230
Asara, John M .....	WOD am 09:50	Aust, Daniela .....	TP 057	Baggerman, Geert.....	MOG pm 3:10
Asara, John M .....	WP 583	Austad, John .....	ThOA pm 3:30	Baggerman, Geert .....	TP 482
Asara, John M .....	WP 608	Austin, Daniel .....	MP 696	Baggerman, Geert .....	WP 469
Asare Okai, Papa Nii .....	MOC am 08:30	Austin, Daniel .....	MP 707	Baghla, Rahul .....	WP 103
Ascencio-Ibanez, Jose Trinidad .....	WOE pm 3:50	Austin, Daniel E .....	ThP 370	Bagrov, VA .....	TP 449
Aseev, Oleg .....	ThOD pm 3:10	Austin, Daniel E .....	TP 713	Bahman, Sanjivan .....	TP 274
Ashby, Matt .....	ThP 569	Austin, Daniel E .....	MP 687	Bai, Bing .....	WP 139
Ashcroft, Alison E. ....	Special	Austin, Daniel E .....	MP 706	Bai, Dina .....	MOE am 08:30
Ashcroft, Alison E. ....	ThP 106	Austin, Samantha .....	WOA am 09:50	Bai, Dina .....	MOH am 10:10
Ashcroft, Alison E. ....	WOH pm 3:10	Austliid Taskén, Kristin .....	ThP 433	Bai, Dina .....	TP 188
Ashcroft, Alison E. ....	WP 201	Auwaerter, Volker .....	MP 289	Bai, Hao .....	WP 706
Ashline, David .....	ThOH pm 3:30	Auwerx, Johan .....	MP 260	Bai, Hua .....	ThP 498
Ashline, David .....	ThP 139	Avtonomov, Dmitry .....	MP 035	Bailey, Aaron O. ....	ThP 328
Ashline, David .....	TP 332	Avtonomov, Dmitry .....	WP 045	Bailey, Derek J. ....	ThP 068
Ashline, David .....	TP 335	Awaiye, Kayode .....	WP 549	Bailey, Derek J. ....	ThP 178
Ashton, Simon .....	TP 282	Awan, Almas Taj .....	WP 711	Bailey, Jonathan .....	TP 554
Askenazi, Manor .....	ThOG am 10:10	Awasthi, Shivangi .....	TP 377	Bailey, Robert .....	TP 152
Askenazi, Manor .....	TP 082	Awasthi, Shivangi .....	TP 386	Bailey, Robert .....	WP 197
Aslanian, Aaron .....	ThP 021	Awazu, Kunio .....	ThP 012	Bailey, Robert .....	WP 196
Aslanian, Aaron .....	TP 483	Axelsen, Paul .....	MP 169	Bailloux, Isabelle .....	TP 293
Aslebagh, Roshanak .....	MP 423	Ayabe, Miho .....	WP 183	Bain, Ryan .....	ThOA am 08:30
Aspinall-O'Dea, Mark .....	WP 114	Ayaz Guner, Serife .....	WP 057	Bain, Ryan .....	TP 387
Assimon, Victoria A. ....	WP 228	Aycirieux, Sophie .....	MP 241	Baird, Zane .....	MP 394
Assunção, Nilson .....	MP 464	Aydin, Egemen .....	TP 666	Baird, Zane .....	TP 398
Astarita, Giuseppe .....	ThP 417	Aylward, Frank .....	MP 569	Bais, Preeti .....	MP 466
Astarita, Giuseppe .....	ThP 661	Ayoub, Daniel .....	MOB am 09:30	Baiwir, Dominique .....	MP 441
Astarita, Giuseppe .....	TOH am 09:50	Ayoub, Daniel .....	MOE am 08:50	Baiwir, Dominique .....	ThP 256
Astarita, Giuseppe .....	TP 643	Ayoub, Daniel .....	WP 172	Baiwir, Dominique .....	TP 176
Astarita, Giuseppe .....	WP 022	Ayzikov, Konstantin .....	TOB am 10:10	Bajardi-Taccioli, Adriana .....	WP 081
Astarita, Giuseppe .....	WP 586	Azad, Sassan .....	ThP 267	Bajrami, Bekim .....	ThP 781
Astigarraga, Egoitz .....	MP 006	Azargun, Mohammad .....	MOD am 10:10	Baker, Andrew .....	ThP 656
Ata, Şevket .....	TP 302	Azhakaprakalam, Vinayak .....	MP 481	Baker, Andrew .....	TP 629
Ata, Şevket .....	TP 307	Azzara, Anthony .....	ThOE am 08:30	Baker, Andy .....	ThP 392
Atakay, Mehmet .....	TP 785	Baade, Brian .....	MP 068	Baker, Bonnie .....	MP 268
Athanas, Michael .....	MP 058	Baars, Oliver .....	ThP 631	Baker, Bonnie .....	ThP 176
Athanas, Michael .....	TP 652	Baba, Hideo .....	MP 431	Baker, Christopher .....	TP 767
Athanassopoulos, Constantinos M. ....	TP 511	Baba, Takashi .....	WOD pm 2:50	Baker, David .....	TP 285
Atkins, Patricia .....	TP 691	Babeluk, Rita .....	WP 140	Baker, David .....	TP 282
Atlasevich, Natalya .....	MP 068	Babu, Sudheer .....	WP 717	Baker, David .....	WP 351
Attie, Alan D. ....	WOD am 10:10	Babu, Suresh .....	WP 204	Baker, Erin .....	MOC pm 3:10
Attwa, Mohamed W. ....	MP 725	Babu CV, Suresh .....	TP 262	Baker, Erin .....	ThOB am 10:10
Attwa, Mohamed W. ....	MP 726	Babu CV, Suresh .....	MP 097	Baker, Erin .....	TOC am 08:30
Attygalle, Athula .....	WP 320	Bache, Nicolais .....	ThP 613	Baker, Erin .....	WP 698
Attygalle, Athula .....	WP 409	Bachmann, Brian .....	ThOG pm 2:50	Baker, Erin S. ....	MP 677
Attygalle, Athula B. ....	MP 050	Bachmeier, Corbin .....	MP 116	Baker, Erin S. ....	ThP 741
Attygalle, Athula B. ....	MP 331	Bachmeier, Corbin .....	MP 246	Baker, Lane .....	WOB am 08:30
Attygalle, Athula B. ....	MP 478	Bachschmid, Markus .....	WP 195	Baker, Mark S. ....	WP 079
Attygalle, Athula B. ....	TP 346	Bachschmid, Markus M. ....	MOH am 08:50	Baker, Paul .....	WP 777
Attygalle, Athula B. ....	WP 383	Bachschmid, Markus M. ....	MP 120	Baker, Peter R .....	ThP 027
Attygalle, Athula B. ....	WP 552	Bachschmid, Markus M. ....	MP 465	Baker, Peter R .....	ThP 048
Atwood, James A. ....	WP 237	Backfish, Gisela .....	MP 639	Baker, Scott .....	WP 088
Aubele, Michaela .....	MP 004	Backlund, Peter S. ....	MP 437	Balakrishnan, Indran .....	TP 222
Aubele, Michaela .....	TP 052	Backlund, Peter S. ....	ThP 491	Balakrishnan, Lavanya .....	MP 255
Aubets, Jordi .....	ThP 496	Backos, Don .....	MP 117	Balan, Venkatesh .....	MP 564
Aubin, Andy .....	ThP 551	Bader, Gary D. ....	MP 255	Balasubramaniam, Deepa .....	ThP 118
Aubriet, Frédéric .....	MP 576	Bader, Noor M. ....	TP 563	Balbuena, Tiago S. ....	ThP 453
Aubry, Anne .....	MP 366	Bader, Samuel .....	TP 181	Balcer, Jesse .....	MOA am 09:30
Aubry, Anne .....	WP 487	Bader, Samuel L .....	ThP 506	Balcer, Jesse L. ....	MP 054
Aubry, Anne .....	WP 534	Badgett, Majors .....	ThP 331	Baldauf, Nicholas .....	TP 276
Aubry, Anne-Francoise .....	MP 074	Badiei, Hamid .....	ThOB am 08:50	Baldwin, Ian T. ....	MP 615
Aubry, Anne-Francoise .....	TOE am 09:30	Badiei, Hamid .....	WP 749	Balimane, Praveen .....	WP 639
Aubry, Anne-Francoise .....	WP 543	Badillo, Ben .....	ThP 767	Balinski, Andrzej .....	ThP 495
Aubry, Anne-Françoise .....	MOF pm 3:30	Badran, Ismail .....	TP 721	Ball, Lauren .....	ThP 166

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



Ball, Lauren .....	TP 128	Barnaby, Omar .....	MP 457	Bataglion, Giovana .....	MP 332
Ball, Lauren .....	WP 071	Barnaby, Omar .....	MP 747	Bataglion, Giovana .....	WP 685
Balland, Alain .....	TP 152	Barnes, Alan J .....	MP 762	Bateman, Kevin .....	MP 639
Balland, Alain .....	WP 196	Barnes, Alan J .....	WP 641	Bateman, Kevin .....	ThP 671
Balland, Alain .....	WP 197	Barnes, Brian .....	WP 720	Bateman, Kevin .....	TP 492
Ballard, Billy .....	MP 595	Barnes, Ian .....	TP 737	Bateman, Kevin .....	TP 626
Ballas, Robert .....	ThP 655	Barnes, Jeremy .....	MP 076	Bateman, Kevin .....	WP 108
Balloon, Allison .....	ThOG pm 3:10	Barnes, Stephen .....	MP 586	Bateman, Kevin .....	WP 184
Balloon, Allison .....	ThP 327	Barnes, Stephen .....	TP 680	Bateman, Kevin .....	WP 547
Balluff, Benjamin .....	MP 004	Barney, Brandon L .....	ThP 370	Bateman, Randall .....	TP 448
Balluff, Benjamin .....	MP 027	Barney, Brandon L .....	TP 713	Batezelli, Alessandro .....	TP 584
Balluff, Benjamin .....	TP 049	Barnidge, David .....	ThP 349	Bathon, Joan M .....	WP 497
Balluff, Benjamin .....	TP 052	Barnidge, David .....	ThP 345	Batoon, Patrickhenry .....	MP 320
Balog, Aaron .....	MP 180	Barofsky, Douglas .....	ThP 688	Batov, Ilya .....	MP 340
Balog, Julia .....	TP 215	Barofsky, Douglas .....	ThP 689	Batruch, Ihor .....	TP 244
Balog, Julia .....	WP 424	Barr, John R .....	MP 529	Batta, Rachit .....	MP 463
Baltes, Mathias .....	WP 746	Barr, John R .....	ThP 382	Battaglioli, Eric .....	MP 517
Bamba, Takeshi .....	MP 613	Barr, John R .....	TP 155	Bath, Tanveer .....	TP 175
Bamba, Takeshi .....	ThP 375	Barran, Perdita .....	ThP 469	Bath, Tanveer .....	WP 093
Bamba, Takeshi .....	ThP 378	Barran, Perdita .....	TOD am 09:30	Baudys, Jakub .....	MP 529
Bamba, Takeshi .....	WP 283	Barreda-Gómez, Gabriel .....	MP 006	Bauer, Michael .....	ThP 054
Bandeira, Nuno .....	MOG am 09:30	Barentine, Emily .....	TP 712	Bauer, Oliver Bolle .....	TP 031
Bandeira, Nuno .....	MOH pm 4:10	Barrera, Joe .....	TP 490	Baughman, Joshua M .....	WOD am 10:10
Bandeira, Nuno .....	MP 043	Barre, Caroline .....	TP 406	Baum, Heidi .....	MP 597
Bandeira, Nuno .....	MP 056	Barrett, Jeffrey .....	WP 646	Baumann, Bernd .....	MP 451
Bandeira, Nuno .....	MP 207	Barrett, Ryan A .....	WP 705	Baumann, Christian .....	WP 496
Bandeira, Nuno .....	TP 087	Barrey, Emily .....	MP 732	Baumann, Stephan .....	ThOA pm 3:50
Bandeira, Nuno .....	TP 088	Barrey, Emily .....	MP 773	Baumgartner, Roland .....	WP 140
Bandeira, Nuno .....	TP 182	Barrey, Emily .....	MP 774	Bavari, Sina .....	WP 010
Bandeira, Nuno .....	TP 229	Barrey, Emily .....	WP 642	Baycin Hizal, Deniz .....	TP 431
Bandhakavi, Sricharan .....	MP 164	Barringer, Chris .....	ThP 675	Baykut, Goekhan .....	MOB am 08:50
Bandhakavi, Sricharan .....	ThP 044	Barrios, Cesar .....	ThP 476	Baykut, Gökhan .....	TP 609
Bandhakavi, Sricharan .....	ThP 777	Barros, Lorena .....	MP 355	Baynes, John W .....	MP 506
Bando, Kiyoko .....	MOF pm 3:10	Barrow, Kory .....	TP 067	Bazenet, Chantal .....	ThP 163
Bando, Yasuhiko .....	TP 383	Barrow, Mark .....	MOB am 09:10	Beach, Daniel .....	MP 353
Banerjee, Kaushik .....	TP 762	Barrow, Mark .....	MOD pm 3:10	Beach, Daniel .....	WP 773
Banerjee, Sarbajit .....	TP 066	Barrow, Mark .....	WP 329	Beals, John .....	MP 213
Banfield, Jill .....	ThP 332	Barrow, Mark .....	WP 729	Beals, John .....	TOG am 10:10
Banfield, Jill .....	TP 660	Barry, Bill .....	ThP 483	Bean, Mark .....	TOF pm 4:10
Banfield, Jillian .....	TP 125	Barry, Cornelius S .....	TP 646	Bearss, David .....	WP 464
Bang, Eunjung .....	ThP 271	Barry, Jeremy .....	ThP 007	Beasley, Rebecca .....	TP 596
Bankert, Will .....	ThP 632	Barry, Jeremy .....	TOH am 08:50	Beasley, Rebecca L .....	MP 550
Banks, Charles .....	MP 154	Barry, Jeremy .....	TP 011	Beasley-Green, Ashley .....	ThP 268
Banks, Douglas .....	TOF am 10:10	Barry, William .....	WP 011	Beasley-Green, Ashley .....	ThP 635
Banks, J. Fred .....	MP 286	Barry, III, Clifton E .....	ThP 491	Beaty, Thomas C .....	MP 350
Banks, Peter A .....	ThOE pm 4:10	Barsch, Aiko .....	TP 030	Beaudry, Francis .....	ThP 678
Bantscheff, Marcus .....	MP 041	Barsch, Aiko .....	MP 614	Beaudry, Francis .....	TP 174
Bantscheff, Marcus .....	ThP 046	Barsch, Aiko .....	MP 615	Beaumont, Maribel .....	WP 184
Bantscheff, Marcus .....	ThOB pm 3:50	Barsch, Aiko .....	ThP 637	Beausoleil, Sean A .....	TOD pm 3:50
Bao, Jiangyin .....	MP 619	Barsch, Aiko .....	ThP 653	Beauvois, Romain .....	WP 522
Bao, Ya-Fei .....	WP 422	Barsch, Aiko .....	TP 655	Beauvois, Romain .....	WP 535
Bao, Yuping .....	ThP 709	Barsch, Aiko .....	TP 750	Beauvois, Romain .....	WP 545
Baranyáné Ganzler, Katalin .....	TP 263	Barsnes, Harald .....	MP 033	Beccari, Melinda .....	MP 459
Barbas, Coral .....	MP 582	Barsnes, Harald .....	WP 029	Bechara, Etelvino J. H .....	MP 115
Barbas, Coral .....	MP 584	Bartel, Jürgen .....	ThP 774	Becher, Dörte .....	ThP 071
Barbier, Pasale .....	ThP 351	Bartels, Michael .....	WP 490	Becher, Dörte .....	ThP 774
Barbosa Domont, Gilberto .....	MP 159	Barthel, Jochen .....	TP 736	Becher, Francois .....	MP 527
Barbu, Ioana .....	WP 055	Barthélemy, Nicolas .....	TP 472	Becher, Francois .....	MP 528
Barbuto, Alexandre .....	WP 460	Bartlett, Michael .....	WP 486	Becher, François .....	TP 472
Barcelo, Damia .....	WP 562	Bartlett, Michael G .....	MP 170	Becher, Isabelle .....	ThOB pm 3:50
Barceló, Damià .....	TP 551	Bartlett, Michael G .....	TP 304	Bechill, Michael .....	TP 292
Barcenas, Mariana .....	WP 443	Bartlett, Michael G .....	TP 568	Becht, Steve .....	TP 261
Bardoni, Barbara .....	ThP 081	Bartmess, John .....	WP 377	Becht, Steven .....	TP 260
Barefoot, Nathan .....	TP 345	Bartmess, John E .....	TP 743	Beck, Alain .....	MOE am 08:50
Baretton, Gustavo .....	TP 057	Barton, Chris .....	WP 194	Beck, Alain .....	MOE am 09:50
Baretton, Gustavo .....	TP 051	Barton, Geran .....	MOB pm 3:50	Beck, Alain .....	TP 149
Barile, Daniela .....	WOE am 08:50	Barut, Miloš .....	TP 447	Beck, Alain .....	TP 247
Barinaga, Charles J .....	ThOB pm 4:10	Barut, Miloš .....	WP 135	Beck, Alain .....	WP 265
Barington, Torben .....	ThP 347	Barylyuk, Konstantin .....	WOF am 09:10	Beck, Alain .....	WP 269
Barker, Gary .....	MOG am 09:10	Basak, Trayambak .....	TP 436	Beck, Birgit .....	TP 667
Barket, Dennis .....	MOA am 10:10	Basile, Franco .....	TP 606	Beck, Erling .....	TP 500
Barket, Dennis .....	MOB pm 2:30	Basile, Franco .....	WP 003	Beck, Florian .....	TP 105
Barket, Dennis .....	MP 530	Bassignani, Phil .....	WP 573	Beck, Jonathan .....	ThP 565
Barkley, Robert M .....	WP 280	Bastos, Wagner .....	TP 584	Beck, Jonathan .....	ThP 570
Barksdale, Stephanie .....	TP 188	Bastos, Wagner L .....	TP 586	Beck, Jonathan .....	TP 284
Barlaz, Morton .....	WP 574	Basu, Ashis .....	ThP 515	Beck, Jonathan .....	TP 579
Barletta, Frank .....	WP 272	Basu, Sankha S .....	TP 310	Beck, Jonathan .....	TP 578
Barlow, James .....	TP 564	Basu, Sankha S .....	WOH am 08:50	Beck, Kirsten .....	WOH pm 2:50
Barmin, VV .....	TP 449	Basu, Uttiya .....	MP 150	Beck, Michael W .....	TOF pm 3:50

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Beck, Scarlet	MP 723	Benicky, Julius	WP 089	Bernier, Morgan	TOD am 09:10
Becker, Alicia	TP 259	Benjamin, Elfrida	WOH am 10:10	Bernstein, Kenneth	ThP 386
Becker, Chris	MOE am 09:10	Benner, Bruce A.	ThP 663	Bernstein, Laurence E.	MOG am 09:30
Becker, Chris	MOG pm 2:50	Bennett, Alexander	TP 688	Berry, Rodney	TP 143
Becker, Chris	MP 149	Bennett, Keiryn L.	MP 228	Berry, Rodney	TP 139
Becker, Chris	TP 074	Bennett, Keiryn L.	WOF pm 2:50	Berry, Rodney	TP 488
Becker, Chris	TP 091	Bennett, Mark	TP 265	Berry, Rodney	WP 241
Becker, Chris	WP 041	Bennett, Michael	WP 430	Bertin, John	MP 512
Becker, Gerald	TOF am 10:10	Bennett, Rachel V.	WOB pm 2:30	Bertin, Jonathan	TP 495
Becker, Gerald W.	TP 185	Bennett, Samuel	ThP 688	Bérubé, Eugénie-Raphaëlle	WP 544
Becker, Katja	MP 468	Bennett, Samuel	ThP 689	Besenfelder, Urban	MP 135
Becker, Katja	TP 071	Benson, Samantha L.	WP 329	Besra, Gurdyal	ThP 394
Becker, Matthew	TP 253	Bentayeb, Karim	WP 403	Bessadóttir, Margrét	ThP 401
Becker, Michael	MP 021	Benter, Thorsten	MOD pm 4:10	Bessant, Conrad	MOG am 09:10
Becker, Michael	ThOG am 09:30	Benter, Thorsten	MP 299	Bessant, Conrad	ThP 034
Becker, Michael	TP 008	Benter, Thorsten	MP 315	Bethard, Jennifer	TP 128
Becker, Stefan	ThP 401	Benter, Thorsten	MP 524	Bethel, Wes	MP 024
Beckman, Joseph	ThP 688	Benter, Thorsten	MP 684	Betowski, Don	WP 579
Beckmann, Benedikt	ThP 519	Benter, Thorsten	MP 690	Beu, Steve	MOB am 10:10
Beckmann, Janine	TP 008	Benter, Thorsten	TP 734	Beu, Steve C.	MP 648
Bedman, Timothy	MP 038	Benter, Thorsten	TP 737	Beu, Steven C.	MP 699
Bedner, Mary	WP 451	Benter, Thorsten	TP 735	Beuning, Penny J.	WP 223
Beech, Iwona	ThP 010	Benter, Thorsten	TP 733	Beurskens, Frank J.	TP 237
Beecher, Chris	TP 653	Benter, Thorsten	TP 732	Beutel, Bruce	TOF pm 3:30
Beekman, Christopher	WP 680	Benter, Thorsten	TP 731	Beynon, Robert J.	MP 265
Beger, Richard	MP 267	Benter, Thorsten	TP 736	Beynon, Robert J.	MP 272
Begley, Ben	WP 480	Bentivegna, Valerie	WP 478	Bezard, Erwan	TP 016
Begley, Timothy	MP 359	Bentley, Adam	TP 502	Bezstarosti, Karel	ThP 239
Begley, Timothy	WP 403	Bentzley, Catherine	TP 570	Bhagwat, Nikhil	MP 101
Beglinger, Katherine	TP 429	Benvenuti, Mark	MP 338	Bhandari, Deepak	ThP 004
Beglinger, Katherine	WP 457	Benvenuti, Mark	WP 347	Bhandari, Deepak	TP 476
Behar, Françoise	TP 605	Beniz, Frederick W.	TP 305	Bhandari, Dhaka	TP 020
Behrens, Beate	TP 287	Benzing, Thomas	ThP 314	Bhandari, Dhaka Ram	TOH pm 2:30
Behring, Jessica	WP 195	Berchem, Guy	ThP 254	Bhandarkar, Deepti	TP 496
Behring, Jessica B.	MP 120	Berchem, Guy	TP 485	Bhandarkar, Deepti	TP 497
Behring, Jessica B.	MP 465	Berden, Giel	MP 322	Bhandarkar, Deepti	TP 498
Beik, Samantha	ThP 033	Berden, Giel	ThOD pm 3:30	Bhandarkar, Deepti	WP 350
Beilman, Greg	TP 656	Berden, Giel	ThOD pm 3:50	Bhanu, Natarajan V.	ThP 070
Bekker-Jensen, Dorte B.	MP 109	Berden, Giel	TP 364	Bhardwaj, Shilpa R.	TOA pm 3:30
Belanger, Philippe	MP 490	Berden, Giel	TP 365	Bhat, Ajay	TP 436
Belbin, Thomas	MP 421	Berejnaia, Olga	ThOE am 09:10	Bhat, Gowri	MP 075
Belford, Michael	TP 294	Bereman, Michael	ThP 288	Bhat, Gowri	ThOE am 09:10
Belford, Michael	WP 762	Berezovski, Maxim	MOC am 10:10	Bhat, Vadi	WP 133
Belford, Michael	WP 763	Berg, Amanda	MP 710	Bhat, Vadiraja	ThP 303
Belford, Michael W.	WP 761	Berg, Amanda	WP 159	Bhat, Vadiraja	TP 427
Belgacem, Omar	ThP 351	Berg, Amanda	WP 754	Bhat, Vadiraja B.	ThP 280
Belgacem, Omar	TP 222	Berg, Thorsten	WOF am 09:10	Bhatia, Vivek N.	TP 095
Belger Krody, Sumru	WP 305	Bergdahl, Andreas	MP 588	Bhattacharya, Anannya	WOF pm 2:50
Belinsky, Steven	ThP 523	Berger, Judith	MP 021	Bhattacharya, Arup	WP 373
Belisle, Pascal	MP 533	Berger, Scott	MP 512	Bhattacharya, Sharmila	TOA pm 3:30
Belkina, Natalia	ThP 204	Berger, Sebastian	TP 187	Bhattacharya, Subhra	MP 737
Bell, Bruce	MP 325	Berger, Shelley L.	ThOF pm 2:30	Bhattacharya, Subhra	MP 779
Bell, Dave	MP 732	Bergeron, Michel	ThP 287	Bhattacharya, Nabanita	MP 550
Bell, Dave	MP 773	Berg-Lyon, Donna	MOH pm 4:10	Bhawal, Ruchika	ThP 244
Bell, David	WP 532	Bergo, Vladislav	MP 199	Bhawal, Ruchika	ThP 245
Bell, David	WP 642	Bergquist, Jonas	MP 135	Bhone, Ankush	TP 761
Bell, David S.	WP 623	Bergquist, Jonas	TP 455	Bhone, Ankush	TP 762
Bellanger, Laurent	TP 225	Bergquist, Jonas	WP 489	Bhone, Ankush	TP 763
Bellin, Melena	ThOE pm 4:10	Bergsdorf, Christian	ThP 094	Bhosale, Santosh	WP 028
Bellina, Bruno	ThP 469	Bergthaler, Andreas	WOF pm 2:50	Bhosale, Santosh	WP 504
Belmont, Mark	TP 755	Beris, Photis	MP 148	Bhuin, Radha Gobinda	TP 350
Belmonte Valles, Noelia	WP 360	Berkaw, Mary	TP 128	Bhujwalla, Zaver	MOH pm 3:50
Belov, Arseniy M.	TOC pm 2:30	Berland, Kevin	ThP 700	Bi, Sheng	MP 652
Belov, Mike	WOF am 09:30	Berleman, James	TP 381	Bi, Xiaobao	ThP 126
Belov, Mikhail	TOD am 08:30	Bern, Marshall	MOE am 09:10	Biacchi, Michael	WP 269
Belsky, Jennifer L.	MP 469	Bern, Marshall	ThP 222	Bian, Cunjuan	MP 649
Belsky, Jennifer L.	TP 730	Bern, Marshall	WP 041	Bian, Fang	TP 439
Belton, Amy	TP 432	Bern, Marshall W.	MP 149	Bian, Liangqiao	TP 490
Beltrao, Pedro	ThP 314	Bern, Marshall W.	TP 074	Bianchi, Giancarlo	ThP 596
Beltzung, Etienne	TP 096	Bern, Marshall W.	TP 091	Biarç, Jordane	WP 177
Beltzung, Etienne	TP 098	Bern, Marshall W.	WP 065	Biasioli, Franco	MP 663
Bemis, Kyle	MP 019	Bern, Marshall W.	WP 088	Bícego, Mária	MP 332
Ben Hamidane, Hisham	ThP 175	Bernal, Corina	TP 679	Bienstock, Rachelle	MP 072
Benchaar, Sabrina	WP 197	Bernet, Pascal	ThP 094	Bier, Mark E.	TOC pm 3:30
Benchaar, Sabrina	WP 196	Bernhard, Werner	ThP 590	Bier, Mark E.	TP 133
Benes, Cyril	MP 257	Bernhardt, Oliver M.	ThOE pm 2:30	Bierbaum, Veronica M.	MP 321
Benet, Zachary	MP 261	Bernhardt, Oliver M.	TP 086	Bierbaum, Veronica M.	TOA pm 3:50
Ben-Hur, Asa	ThOG am 08:50	Bernhardt, Oliver M.	WP 722	Bierbaum, Veronica M.	TP 356
Benicky, Julius	ThP 139	Bernier, Matthew	ThOA pm 3:10	Bierkandt, Thomas	WP 410

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Bieske, Evan.....	ThP 504	Blakney, Greg T.....	MOB am 10:10	Bokhart, Mark.....	WP 452
Biffinger, Justin C.....	MP 278	Blakney, Greg T.....	MP 084	Bokhart, Mark T.....	ThP 006
Biggs, Catherine A.....	ThP 645	Blakney, Greg T.....	WP 734	Bokiniec, Phill.....	WP 234
Bilgraer, Raphaël.....	MP 235	Blakney, Gregory T.....	MP 699	Boldyrev, Alexey.....	TOA pm 4:10
Billign, Tsion.....	MP 469	Blanc, Adi.....	ThP 133	Bollig, Klaus.....	TP 583
Bilker, Warren.....	ThP 282	Blanco, Cristian.....	TP 416	Bollinger, James G.....	TOG pm 3:50
Bilodeau, Jason.....	MP 493	Blanco-Tirado, Cristian.....	TP 588	Bombard, Drew.....	ThP 607
Bilodeau, Jason.....	MP 494	Blanco-Tirado, Cristian.....	TP 587	Bomgarden, Ryan.....	MP 206
Bilodeau, Jason.....	MP 496	Blank, Michael.....	ThP 613	Bomgarden, Ryan.....	MP 652
Bilodeau, Jason.....	MP 485	Blank, Michael.....	WP 510	Bomgarden, Ryan.....	ThOF am 09:50
Bindila, Laura.....	TP 424	Blank, Michael A.....	ThP 222	Bomgarden, Ryan.....	ThP 170
Binek, Aleksandra.....	ThP 336	Blank, Michael A.....	WP 150	Bomgarden, Ryan.....	ThP 211
Binette, Marie-Josée.....	MP 531	Blank, Paul S.....	ThP 491	Bomgarden, Ryan.....	WP 481
Bingham, Patrick.....	MP 540	Blankenship, Robert E.....	ThOF am 10:10	Bonacina, Luigi.....	MOD am 09:10
Binkley, Joe.....	MOA pm 4:10	Blanksby, Stephen J.....	MP 248	Bond, Nathan.....	MP 566
Binkley, Joe.....	MP 607	Blanksby, Stephen J.....	ThOD am 10:10	Bondarenko, Alexandra.....	TP 389
Binkley, Joe.....	MP 655	Blanksby, Stephen J.....	TP 371	Bondarenko, Andrey.....	WOG pm 4:10
Binkley, Joe.....	ThP 556	Blankson, Joel.....	WOF pm 4:10	Bondarenko, Andrey.....	WP 017
Binkley, Joe.....	ThP 617	Blasberg, Jim.....	MP 751	Bondarenko, Andrey.....	WP 037
Binkley, Joe.....	TP 603	Blaske, Franziska.....	TP 032	Bondarenko, Pavel.....	MOE pm 2:50
Binkley, Joe.....	TP 753	Blatnik, Matthew.....	MOF pm 4:10	Bondarenko, Pavel.....	TP 240
Binkley, Joe.....	TP 792	Blatnik, Renata.....	ThP 343	Bondarenko, Pavel.....	TP 642
Binkley, Joe.....	WP 307	Blatt, Celso.....	ThP 651	Bondarenko, Pavel.....	WP 254
Binkley, Joe.....	WP 588	Blau, Justin.....	ThP 562	Bondarenko, Pavel V.....	WP 606
Binneboese, Laura.....	TP 506	Bleecker, Jennifer.....	MP 515	Bondesson, Ulf.....	MP 352
Binz, Pierre-Alain.....	WP 029	Bleiholder, Christian.....	MOC pm 4:10	Bondesson, Ulf.....	TP 628
Biosvert, Jessica.....	MP 257	Bleijerveld, Onno.....	ThP 545	Bonds, Kari.....	MP 597
Birdsall, Robert.....	TP 158	Blenkinsopp, Paul.....	ThP 011	Bonduriansky, Russell.....	MP 438
Birdsall, Robert.....	TP 236	Blethrow, Justin.....	WP 185	Bone, Kathleen.....	TP 648
Birdsall, Robert.....	WP 274	Blethrow, Justin.....	WP 270	Bones, Jonathan.....	ThOH am 09:30
Birka, Marvin.....	WP 442	Blick, Robert.....	ThOB pm 2:50	Bones, Jonathan.....	WP 189
Birsan, Alex.....	MP 284	Bloem, Esther.....	ThP 112	Boniface, J. Jay.....	ThP 285
Birsan, Alex.....	WP 361	Blomgren, Anders.....	WP 440	Bonifay, Vincent.....	TP 666
Birsan, Alex.....	WP 626	Blonder, Josip.....	MP 132	Bonifay, Vincent.....	TP 665
Birsan, Alex.....	WP 634	Bloodworth, Bosco.....	ThP 622	Bonilla, Leo.....	MP 124
Bischof, Julia.....	ThP 250	Bloomfield, Nic.....	MP 721	Bonilla, Leo.....	WP 235
Bischofberger, Allen.....	WP 640	Bloomfield, Nic.....	ThP 316	Bonn, Florian.....	ThP 774
Bischoff, Rainer.....	TOA am 10:10	Bloomfield, Nic.....	ThP 330	Bonneil, Eric.....	ThOC am 08:30
Bischoff, Rainer.....	TOE am 09:10	Blount, Benjamin.....	TP 476	Bonneil, Eric.....	TP 108
Bischoff, Rainer.....	WP 147	Blum, Lorenz.....	ThP 257	Bonnel, David.....	MP 025
Bishop, Barney.....	TP 188	Bo, Tao.....	MP 337	Bonnel, David.....	TOH am 09:10
Bishop, Steven.....	WP 215	Bo, Tao.....	MP 730	Bonnel, David.....	TP 009
Bitterman, Peter.....	MP 429	Bo, Tao.....	ThP 533	Bonnel, David.....	TP 034
Bittremieux, Wout.....	MP 032	Bo, Tao.....	TP 533	Bonnel, David.....	TP 050
Bjorling, Dale.....	MP 448	Bo Li Lu, Jessica.....	TP 621	Bonnel, David.....	TP 249
Bjorling, Dale.....	TP 454	Boanca, Gina.....	MP 154	Bonner, Ron.....	MP 057
Blachon, Gregory.....	ThP 411	Bobba, Sudheer.....	MP 645	Bonner, Ron.....	MP 629
Blachon, Gregory.....	TP 607	Bober, Magdalena.....	TP 086	Bonner, Ron.....	TP 673
Blachon, Gregory.....	WP 361	Bobst, Cedric.....	TOE am 10:10	Bonzón-Kulichenko, Elena.....	ThP 336
Blackburn, Kevin.....	MP 410	Bobst, Cedric E.....	ThP 116	Boone, Eric.....	MP 554
Blackburn, Kevin.....	WOE pm 3:50	Bochnowski, Alisa.....	MP 261	Boons, Geert-Jan.....	ThOH pm 4:10
Blackburn, Kevin.....	WP 098	Böcker, Sebastian.....	MP 030	Boons, Geert-Jan.....	TP 320
Blackburn, Mary.....	MP 742	Böcker, Sebastian.....	ThOG am 08:30	Boon-Spijker, Mariëtte.....	ThP 112
Blackburn, Mary.....	ThP 568	Bodnar, Edward.....	ThP 145	Booth, Catherine.....	ThP 642
Blackburn, Mary.....	ThP 753	Boege, Fritz.....	WP 248	Booth, Catherine.....	TP 299
Blackburn, Mary.....	TP 284	Boehm, Gitte.....	ThP 215	Booth, Catherine.....	TP 437
Blackler, Adele.....	WP 141	Boehm, Guenter.....	MP 632	Booth, Catherine.....	TP 688
Blackmer, James.....	ThOH pm 2:50	Boehm, Guenter.....	TP 746	Booth, Catherine.....	WP 601
Blackwell, Anne.....	TP 468	Boehm, Guenter.....	WP 174	Bootharaju, M. S.....	TP 398
Blackwell, Anne.....	WP 602	Boeke, Jef D.....	WP 253	Bora, Adriana.....	TP 468
Blackwell, Anne E.....	MP 589	Boekelheide, Kim.....	WP 581	Boram, Sharon.....	MP 781
Blackwell, Anne E.....	WP 290	Boenzi, Sara.....	WP 431	Borbridge, Lisa.....	TP 480
Blackwell, Benny.....	ThP 450	Boersema, Paul.....	ThP 329	Borchers, Christoph.....	MP 037
Blades, Michael.....	MP 674	Boeuf, Amandine.....	MOE am 09:50	Borchers, Christoph.....	ThP 026
Blades, Michael W.....	MP 675	Boeuf, Amandine.....	MP 450	Borchers, Christoph.....	ThP 049
Blagoev, Blagoy.....	TP 126	Boggess, Andrew.....	MP 557	Borchers, Christoph.....	ThP 056
Blagojevic, Voislav.....	WP 778	Bohme, Diethard K.....	WP 778	Borchers, Christoph.....	ThP 050
Blair, Ian A.....	MP 509	Bohn, Paul.....	TP 006	Borchers, Christoph.....	ThP 252
Blair, Ian A.....	TP 103	Boinay, Ryan.....	TOF pm 3:30	Borchers, Christoph.....	ThP 262
Blair, Ian A.....	TP 310	Boissinot, Maurice.....	ThP 287	Borchers, Christoph.....	ThP 361
Blair, Ian A.....	WOH am 08:50	Boiteau, Rene.....	MP 609	Borchers, Christoph.....	ThP 360
Blair, Ian A.....	WP 499	Bojko, Barbara.....	MP 603	Borchers, Christoph.....	ThP 455
Blair, Ian A.....	WP 479	Bojko, Barbara.....	MP 770	Borchers, Christoph.....	TOG pm 3:10
Blake, Thomas.....	MP 194	Bojko, Barbara.....	ThOB am 09:50	Borchers, Christoph.....	TP 014
Blake, Thomas.....	ThP 429	Bojko, Barbara.....	ThP 408	Borchers, Christoph.....	TP 255
Blakeman, Kenion.....	MOB pm 3:10	Bojko, Barbara.....	TP 521	Borchers, Christoph.....	TP 484
Blakeman, Kenion.....	MP 691	Bojko, Barbara.....	WP 750	Borchers, Christoph.....	TP 544
Blakeman, Kenion.....	TP 738	Bokhart, Mark.....	TOH am 08:50	Borchers, Christoph.....	WOG pm 3:10
Blakeslee, Wes.....	MP 117	Bokhart, Mark.....	TP 011	Borchers, Christoph.....	WP 471

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Borchers, Christoph.....	WP 611	Bovee, Michael.....	ThP 784	Brem, Gottfried.....	MP 135
Borchers, Christoph.....	WP 610	Bové, Judith V.M.G.....	TP 049	Brenna, Tom.....	MP 335
Borchers, Christoph.....	WP 654	Bowden, John.....	ThP 377	Bresnick, Emery.....	MP 460
Borén, Mats.....	MP 426	Bowden, John.....	ThP 647	Bretnall, Alison.....	WP 527
Borén, Mats.....	WP 012	Bowden, Michaela.....	WP 475	Breuker, Kathrin.....	ThP 088
Borges, Rodrigo.....	ThOA am 09:30	Bowen, Ben.....	MP 024	Brewer, Heather.....	WOE pm 4:10
Borgmann-Winter, Karin.....	ThP 282	Bowen, Ben.....	MP 627	Brewer, Sarah.....	TP 676
Borgmann-Winter, Karin E.....	WP 148	Bowen, Benjamin.....	TP 660	Brewer, Tim.....	ThP 601
Borisov, Oleg.....	MOE pm 4:10	Bowen, Chester.....	TP 465	Brewer, Tim.....	WP 291
Borisov, Oleg.....	MOG pm 2:50	Bowen, Chester L.....	MP 781	Brewer, William.....	MP 772
Borisov, Oleg.....	WP 190	Bowen, Chester L.....	TOE am 09:50	Brewster, Dave.....	TP 190
Borkowski, Andrew.....	MOH pm 4:10	Bowen, Chester L.....	TP 464	Brian, Haab.....	TP 068
Bormotov, Denis.....	TP 409	Bowen, Michael.....	TP 431	Bridgewater, Brandi.....	TP 662
Bornemann, Stephen.....	WP 684	Bowers, Michael T.....	MOC pm 4:10	Bridoux, Maxime.....	WP 396
Bornschein, Russell.....	WP 675	Bowles, Dawn E.....	TOA pm 2:50	Brière, Jean-François.....	WP 679
Boronina, Tatiana N.....	MP 187	Boxer, Adam.....	MP 457	Brignol, Nastry.....	WOH am 10:10
Borotto, Nicholas.....	ThP 115	Boyaci, Ezel.....	MP 770	Brill, Laurence.....	WP 092
Borotto, Nicholas.....	ThP 114	Boyce, Greg.....	TOH am 09:50	Brinc, Davor.....	TP 244
Borthwick, Andy.....	WP 022	Boyce, Gregory.....	MP 002	Brinch-Pedersen, Henrik.....	MP 409
Bortoli, Stella.....	WP 554	Boyce, Gregory.....	TP 218	Brinckerhoff, William.....	MP 697
Borton, Christopher.....	WP 777	Boyce, Gregory.....	WP 002	Brinckerhoff, William.....	ThP 369
Borton, David.....	MOA am 09:50	Boychenko, Alexander.....	WP 147	Brinckerhoff, William.....	ThP 365
Bossée, Anne.....	WOC pm 2:50	Boyd, Alison.....	MP 415	Brinckerhoff, William.....	ThP 364
Boston, Penelope J.....	ThP 366	Boyd, David.....	TP 216	Brinckerhoff, William.....	TOA pm 2:30
Boswell, Paul.....	MP 625	Boyd, Jessica.....	WOC pm 4:10	Brinckerhoff, William.....	TP 712
Boswell, Paul.....	TP 654	Boyd, Robert.....	WOH am 10:10	Brinckerhoff, William.....	TP 711
Boswell, Paul.....	TP 667	Boyes, Barry.....	ThP 142	Brinckerhoff, William.....	TP 710
Boswell, Paul.....	WP 720	Boyes, Barry.....	TP 110	Brinckerhoff, William B.....	ThP 366
Boswell, Paul G.....	WP 721	Boyes, Barry.....	TP 331	Brindley, Amanda.....	ThP 172
Boswell, Sarah W.....	MP 680	Boyes, Barry.....	WP 080	Brink, Andreas.....	MP 639
Both, Peter.....	ThP 492	Boylan, Kristin.....	TP 428	Brinkkötter, Paul.....	ThP 314
Bothner, Brian.....	MP 276	Boyles, Matthew.....	WP 153	Brinkman-Van der Linden, Els.....	ThP 119
Bothner, Brian.....	TP 656	Boyne, Michael.....	MOE pm 3:50	Brinson, Robert G.....	TP 256
Bothner, Brian.....	WP 311	Boyne, Michael.....	ThP 143	Brinza-Nichita, Norica.....	MP 162
Botrè, Francesco.....	ThP 594	Brabeck, Gregory.....	MP 669	Brion, François.....	TP 309
Botrè, Francesco.....	ThP 595	Brabeck, Gregory.....	MP 670	Britain, Scott.....	ThP 405
Bottalico, Lisa.....	MP 509	Bracha, Shay.....	ThP 286	Brito, Rui.....	ThP 101
Bottalico, Lisa.....	WP 479	Bracha, Shay.....	WOD am 08:30	Britton, David.....	ThOE am 08:50
Botting, Gregory.....	WP 481	Bracht, Thilo.....	MP 431	Britton, David.....	ThP 215
Bou-Assaf, George.....	ThP 134	Bracht, Thilo.....	TP 481	Britton, Laura-Mae.....	MP 236
Bouchard, Luc.....	MP 498	Brachthaeuser, Yessica.....	TP 732	Britton, Laura-Mae.....	MP 237
Bouchard, Luc.....	MP 497	Brachthaeuser, Yessica.....	TP 734	Brivanlou, Ali.....	MP 592
Boucher, Christina.....	TP 088	Bracken, Jack D.....	MP 131	Brkić, Boris.....	MP 521
Boucheron, Nicole.....	MP 228	Bradford, Chad L.....	ThP 285	Brnakova, Zuzana.....	WP 075
Boudah, Samia.....	MP 581	Bradley, Joel C.....	ThP 178	Broadbelt, Kevin.....	MP 747
Boudah, Samia.....	ThP 391	Brady, Donita.....	MP 082	Broadbelt, Kevin.....	ThP 279
Boudah, Samia.....	TP 224	Brahim, Bessem.....	ThP 513	Broadwell, David.....	WP 105
Boudah, Samia.....	WP 281	Bramanti, Emilia.....	TP 770	Brockhaus, Albrecht.....	MP 690
Boudreau, Nadine.....	MP 491	Brambl, Robert.....	MP 605	Brockhaus, Albrecht.....	TP 733
Boudreau, Nadine.....	MP 490	Branchfield, Kelsey.....	TP 168	Brockman, Adrienne.....	WP 570
Boudreau, Nadine.....	MP 494	Brand, Martin.....	TP 127	Brockman, Stephen.....	MP 605
Boudreau, Nadine.....	MP 498	Brand, Martin D.....	WP 118	Brockman, Stephen A.....	MP 413
Boudreau, Nadine.....	MP 493	Brandenburg, Armd.....	WP 050	Brockmann, Klaus.....	MP 690
Boudreau, Nadine.....	MP 497	Brandt, Cameron.....	ThP 103	Brockmann, Klaus J.....	TP 734
Boudreau, Nadine.....	MP 496	Branson, Owen E.....	MP 229	Broadbelt, Jennifer.....	ThP 110
Boudreau, Nadine.....	MP 485	Branson, Owen E.....	ThP 292	Broadbelt, Jennifer.....	ThP 108
Boudreau, Nadine.....	MP 486	Brant, David M.....	MP 678	Broadbelt, Jennifer.....	ThP 743
Boudreau, Nadine.....	MP 488	Brantley, Matthew.....	MP 047	Broadbelt, Jennifer.....	TOB am 08:30
Boudreau, Nadine.....	MP 489	Brantley, Matthew.....	WP 657	Broadbelt, Jennifer.....	TOD am 09:50
Boudreau, Nadine.....	MP 492	Brantley, Matthew.....	WP 658	Broadbelt, Jennifer.....	TP 162
Boudreau, Nadine.....	MP 495	Brantley, Stephen.....	TP 463	Broadbelt, Jennifer.....	TP 289
Boudreau, Nadine.....	TP 517	Brar, Satinder Kaur.....	TP 556	Broadbelt, Jennifer.....	WP 175
Boudreau, Paul.....	MP 056	Braswell, Elise.....	WOE pm 3:50	Broadbelt, Jennifer.....	WP 176
Bouhifd, Mounir.....	WP 581	Brauer, Jonathan.....	ThP 010	Broadbelt, Jennifer.....	WP 368
Boulanger, Madeleine.....	WOE am 09:50	Braulke, Thomas.....	WP 656	Broadbelt, Jennifer S.....	ThP 350
Boulanger, Nathalie.....	MP 450	Braun, Arkady.....	WP 423	Broadbelt, Jennifer S.....	TOE pm 2:30
Boulcault, Jean.....	TP 414	Bray, Fabrice.....	MP 083	Broadbelt, Jennifer S.....	WP 261
Boulton, David.....	TP 501	Bray, Fabrice.....	TP 719	Brodie, Nicholas.....	ThP 360
Bourassa, Sylvie.....	ThP 287	Brechlin, Peter.....	MP 157	Brodie, Nicholas.....	ThP 361
Bourderieux, Matthieu.....	WP 145	Breckels, Lisa M.....	WP 738	Broeckling, Corey.....	ThOG am 08:50
Bourmaud, Adèle.....	ThP 534	Breen, Christopher.....	WP 645	Broeckling, Corey.....	WP 550
Bouslimani, Amina.....	MOH pm 4:10	Breen, Edmond.....	WP 019	Broeckling, Corey.....	WP 720
Bouslimani, Amina.....	MP 020	Breidinger, Sheila.....	WP 108	Broeckling, Cory.....	MP 418
Bouslimani, Amina.....	MP 056	Breidinger, Sheila.....	WP 652	Broeker, Jenny.....	MP 225
Boutaghou, Mohamed Nazim.....	WP 161	Breiev, Kostiantyn.....	ThP 738	Bromirski, Maciej.....	MP 186
Boutaghou, Mohamed Nazim.....	WP 211	Breinholt, Jens.....	ThP 135	Bromirski, Maciej.....	MOD pm 4:10
Boutal, Hervé.....	MP 528	Breitkopf, Susanne.....	WOD am 09:50	Bromirski, Maciej.....	ThP 565
Boutte', Angela M.....	ThP 306	Breitkopf, Susanne.....	WP 608	Bromirski, Maciej.....	TOG pm 2:50
Bova, Geroge Steven.....	MP 432	Breitwieser, Florian.....	MP 228	Bromirski, Maciej.....	TP 280

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Bromirski, Maciej.....	TP 578	Bu, Jiexun.....	TP 341	Bushman, G. Guy.....	TP 223
Bromirski, Maciej.....	WP 265	Bu, yahao.....	WP 015	Bushman, Wade.....	MP 448
Bronsema, Kees.....	TOE am 09:10	Buch, Arnaud.....	ThP 369	Bushman, Wade.....	TP 454
Bronsert, Peter.....	TP 172	Buchan, Alison.....	MP 775	Busman, Mark.....	TP 268
Brookes, Catherine.....	WP 527	Buchbinder, Susan.....	WOF pm 4:10	Busnel, Jean-Marc.....	TP 247
Brooks, Bernard.....	ThP 314	Buchholz, Lisa.....	TP 531	Büter, Lars.....	MP 477
Brooks Jackson, Jay.....	WOF pm 4:10	Buchou, Thierry.....	WOG am 09:50	Büter, Lars.....	TP 612
Bros, Pauline.....	WP 447	Buck, Lynette.....	TP 239	Büter, Lars.....	TP 611
Brouard, Mark.....	ThP 002	Buckanovich, Ronald.....	WP 501	Büttner, Knut.....	ThP 774
Broudin, Simon.....	MP 581	Buckenmaier, Stephan.....	TP 192	Button, Julie.....	ThOA pm 2:50
Broudin, Simon.....	ThP 391	Budgeon, Alan.....	TP 676	Butzmann, Lars.....	MP 041
Broudin, Simon.....	TP 577	Budzinski, Hélène.....	ThP 566	Butzmann, Lars.....	ThP 046
Broudin, Simon.....	WP 281	Buhse, Lucinda.....	ThP 143	Buzalaf, Marília Afonso Rabelo.....	ThP 307
Broughton, Howard.....	TP 543	Bui, Huy.....	MP 716	Buzalaf, Marília Afonso Rabelo.....	MP 461
Brouns, Stan J. J.....	ThP 458	Bui, Huy.....	WP 681	Byer, Jonathan.....	ThP 556
Brouwer, Hendrik-Jan.....	MP 093	Buil, Alfonso.....	ThP 257	Byer, Jonathan.....	TP 753
Brouwer, Hendrik-Jan.....	TP 622	Buisson, Corinne.....	TP 293	Byram, Gregory.....	ThP 450
Brown, Chad.....	ThP 733	Bukowski, Michael.....	MP 089	Byrd, Gary.....	WP 339
Brown, Eric W.....	MP 333	Bulayeva, Nataliya.....	MP 290	Byrdwell, William C.....	ThP 412
Brown, Gary.....	TP 711	Bulgarelli, Adriana.....	MP 464	Byrne, Keren.....	WOE pm 2:30
Brown, Hilary.....	WP 309	Bullock, Brandon.....	TP 146	Byrnes, Andrew.....	ThOA am 09:10
Brown, Jeff.....	MP 181	Bunch, Josephine.....	MP 001	Bythell, Benjamin.....	TP 778
Brown, Jeff.....	MP 674	Bunch, Josephine.....	MP 028	Bythell, Benjamin J.....	TP 599
Brown, Jeff.....	MP 675	Bunch, Josephine.....	MP 253	Bythell, Benjamin J.....	WP 706
Brown, Jeff.....	ThP 469	Bunch, Josephine.....	TP 041	Byun, Jaeman.....	MP 597
Brown, Jeff.....	TOC pm 3:50	Bunch, Josephine.....	TP 232	Byun, Jaeman.....	ThP 395
Brown, Jeff.....	WP 280	Bunch, Josephine.....	WP 013	Byun, Jaeman.....	ThP 662
Brown, Jeff.....	WP 748	Bunch, Josephine.....	WP 386	Bzdek, Bryan.....	MOA am 09:10
Brown, Johnie.....	ThP 532	Bunch, Josephine.....	WP 384	Bzdek, Bryan.....	ThP 368
Brown, Kristy J.....	ThOE am 09:50	Bundy, Jonathan.....	TP 155	Cabral, Elaine Cristina.....	TP 025
Brown, Kristy J.....	MP 163	Bunk, David.....	ThP 268	Cabral, Elaine Cristina.....	WP 379
Brown, Kristy J.....	MP 424	Bunkenborg, Jakob.....	WP 043	Cabrera, Karin.....	MP 741
Brown, Kristy J.....	TP 467	Bunn, Jonathan.....	TP 604	Cabreres, Oscar.....	MP 776
Brown, Lauren.....	WP 760	Bunnik, Evelien.....	ThOF pm 3:30	Cabreres, Oscar.....	MP 772
Brown, Lewis M.....	MP 150	Burant, Charles.....	MP 597	Cafazzo, Mark.....	ThP 506
Brown, Lewis M.....	ThP 512	Burant, Charles.....	MP 636	Cai, Cheng Yuan.....	WP 357
Brown, Lindsay.....	WP 600	Buratti, Martin.....	ThOG am 09:50	Cai, Chengyuan.....	WP 731
Brown, Nicole.....	TOF am 09:50	Burch, Tanya.....	ThP 392	Cai, Jian.....	TP 305
Brown, Robert.....	ThP 105	Burdette, Carolyn.....	WP 509	Cai, Min.....	TP 486
Brown, Robert.....	ThP 193	Bure, Corinne.....	MP 241	Cai, Qian.....	MP 113
Brown, Simon.....	ThP 376	Burg, Dominic.....	WP 468	Cai, Tanxi.....	MP 222
Brown, Stephen.....	MP 597	Burg, Maurice.....	ThP 052	Cai, Wenxuan.....	ThP 078
Brown, Steven.....	MOB am 09:10	Burg, Maurice B.....	WP 255	Cai, Xiaohan.....	WP 533
Brownridge, Philip.....	MP 272	Burgess, Jefferey.....	WP 454	Cai, Yang.....	ThP 353
Brownstein, Naomi.....	MP 230	Burgess, Jennifer.....	MP 338	Cai, Yi.....	MP 396
Bruce, James.....	ThOC pm 3:50	Burgess, Jennifer.....	ThP 551	Cai, Yi-Hong.....	ThP 742
Bruce, James.....	ThP 223	Burgess, Jennifer.....	WP 347	Cai, Yi-Hong.....	WP 691
Bruce, James.....	ThP 465	Burgess, Jennifer.....	WP 349	Cai, Yuping.....	ThP 634
Bruce, James.....	ThP 466	Burgess, Michael.....	TP 426	Cain, Joel.....	TP 131
Bruce, James.....	WOF pm 3:30	Burgett, Anthony.....	WOB pm 3:10	Cajka, Tomas.....	ThP 406
Bruce, James E.....	ThP 464	Burggraf, Larry.....	MP 302	Cajka, Tomas.....	WP 286
Bruce, James E.....	WOH pm 2:50	Burk, Piia.....	MP 313	Calabrese, Antonio N.....	WOH pm 3:10
Bruchmann, Andreas.....	WP 174	Burke, Kathleen.....	ThP 105	Calafat, Antonia.....	WP 461
Bruckner, James.....	TP 304	Burke, Meghan.....	MP 136	Calderon, Angela.....	MP 468
Bruckner, James V.....	TP 568	Burke, Nicole.....	TP 362	Calderón, Angela I.....	WP 324
Bruckner, Raphael.....	TP 145	Burke, Rob.....	TOE am 08:50	Calderón, Angela I.....	WP 319
Bruderer, Roland M.....	ThOE pm 2:30	Burke, Rochelle.....	ThP 668	Caldwell, Anna.....	MP 561
Bruderer, Roland M.....	TP 086	Burke, Jr., Terrence R.....	MP 189	Callahan, John.....	TP 217
Bruderer, Roland M.....	WP 722	Burkhardt, Julia Maria.....	MP 087	Callahan, John H.....	WP 333
Bruening, Merlin.....	MP 204	Burlingame, Alma.....	ThP 037	Callery, Patrick S.....	TP 038
Bruhn, Laurakay.....	MP 637	Burns, Kyle.....	TP 538	Calligaris, David.....	TP 007
Bruinen, Anne.....	TOH pm 3:10	Burnum-Johnson, Kristin.....	MOC pm 3:10	Callister, Stephen.....	TP 203
Bruins, Andries P.....	MP 298	Burrows, Jon.....	WP 141	Callister, Stephen.....	TP 229
Bruinsma, Marieke.....	WP 478	Burssens, Guy.....	MP 771	Calvaresi, Valeria.....	ThP 595
Brumbach, Michael.....	TP 789	Burstein, David.....	TP 660	Camafeita, Emilio.....	ThP 336
Brun, Virginie.....	MP 527	Burton, Lyle.....	MP 057	Camara, Johanna.....	WP 453
Brun, Virginie.....	MP 528	Burton, Lyle.....	MP 629	Camara, Johanna.....	WP 509
Brunel, Jean-Michel.....	ThP 351	Burzykowski, Tomasz.....	WP 031	Camara, Miguel.....	ThP 645
Brunner, Katherine.....	TP 146	Buse, Joshua.....	ThOF am 09:50	Camenzind, Alex.....	TOG pm 3:10
Bruning, John.....	ThP 137	Bush, David.....	TP 149	Cameron, R. Andrew.....	ThP 310
Brunisholz, Rene.....	MP 200	Bush, David R.....	WP 065	Camicioli, Richard.....	MP 594
Brunner, Reto.....	ThP 094	Bush, David R.....	MP 147	Cammack, Lidia.....	TP 215
Bruss, Jon.....	ThP 435	Bush, David R.....	TOC pm 2:30	Cammarata, Michael.....	ThP 110
Bruun Schjødt, Christine.....	ThP 135	Bush, Matthew.....	ThOC pm 4:10	Cammarata, Michael.....	ThP 108
Bryan, Caroline.....	WOE pm 3:50	Bush, Matthew.....	ThP 093	Camp, David.....	WOE am 08:30
Brylev, Vladimir.....	WP 027	Bush, Matthew.....	ThP 470	Camp, David G.....	WP 513
Brzak, Kathy.....	WP 490	Bush, Matthew F.....	MOC pm 3:30	Camp II, David G.....	TP 324
Bu, Jiexun.....	TP 339	Bush, Matthew F.....	MOD am 09:30	Camp, II, David.....	WOG pm 2:50
Bu, Jiexun.....	TP 340	Bush, Matthew F.....	WP 669	Campbell, Colin.....	TOE pm 3:50

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Campbell, Elizabeth.....	MP 167	Cardenas, Michelle.....	TP 712	Casadonte, Rita.....	TP 057
Campbell, J. Larry.....	ThOC am 08:50	Cardenas, Silvia.....	TP 679	Casadonte, Rita.....	TP 051
Campbell, J. Larry.....	ThP 473	Cardenas-Valencia, Andres.....	MP 553	Casadonte, Rita.....	TP 056
Campbell, J. Larry.....	ThP 505	Cardinal, Kristen.....	MP 645	Casillas, Linda.....	MP 512
Campbell, J. Larry.....	WOD pm 2:50	Cardona, Dwain.....	ThP 571	Casina, Veronica C.....	ThP 128
Campbell, Larry.....	WP 779	Cardona, Dwain.....	WP 359	Caspary, Guy.....	WP 198
Campbell, Sharon L.....	MP 179	Cardoso, Felipe.....	TP 585	Casper, Brent.....	ThP 577
Campopiano, Dominic.....	MP 182	Cardoso, Josiane de O.....	TP 614	Cassady, Carolyn.....	ThP 181
Campos, Alex.....	WP 092	Cardozo, Karina Helena Morais.....	TP 435	Cassady, Carolyn.....	ThP 709
Campuzano, Iain D G.....	MP 184	Cardozo, Karina Helena Morais.....	WP 434	Cassady, Carolyn J.....	ThP 182
Campuzano, Iain D G.....	TOE pm 3:10	Carlage, Tyler.....	WP 081	Cassady, Carolyn J.....	MP 319
Canagaratna, Manjula.....	TOA pm 3:10	Carlsen, Mark.....	ThP 758	Cassady, Carolyn J.....	ThP 180
Cañas, Benito.....	MP 355	Carlson, Erin E.....	MP 618	Cassou, Catherine A.....	WOB am 09:10
Cancilla, Mark.....	ThOE am 09:30	Carlson, Timothy S.....	TP 324	Castaneda, Carlos.....	ThP 235
Cancilla, Mark.....	ThP 546	Carlsson, Henrik.....	WP 456	Castanheira, Pedro.....	ThP 101
Cancilla, Mark.....	TOE am 08:50	Carlton, Doug.....	ThP 557	Castellanos, Laura.....	TP 416
Cancilla, Mark T.....	ThP 521	Carney, Peter.....	TP 723	Castellanos-García, Laura J.....	TP 588
Candish, Esme.....	ThP 783	Caron, Danielle.....	TP 130	Castelli, Florence.....	MP 581
Canevarolo, Rafael.....	WP 460	Caron, Danielle.....	TP 108	Castello, Alfredo.....	TP 202
Canki, M.....	TP 434	Caron, Kevin.....	WOC pm 3:50	Castillo, Mary Joan.....	ThP 194
Cannon, Joe.....	TOB am 08:30	Caron, Nicolas.....	MP 288	Castillo, Mary Joan.....	TP 486
Cannon, Joe.....	WP 176	Caron, Pierre-Yves.....	MP 495	Castoro, John.....	WP 527
Cannon, Joe R.....	TOE pm 2:30	Caron, Pierre-Yves.....	MP 494	Castro, Begoña.....	TP 064
Cannon, Presley.....	ThP 156	Caron, Pierre-Yves.....	MP 486	Castro, Brian.....	TP 416
Cansell, Maud.....	MP 241	Caron-Lizotte, Olivier.....	TP 108	Castro, Brian.....	TP 588
Cantarel, Brandi.....	MP 264	Caron-Lizotte, Olivier.....	TP 113	Castro, Sergio.....	ThP 088
Canterbury, Jesse.....	ThP 743	Carpen, Olli.....	ThP 276	Castro-Perez, Jose.....	ThOE am 09:10
Canterbury, Jesse D.....	MP 717	Carpenter, Anna.....	WP 640	Castro-Perez, Jose.....	TP 061
Canterbury, Jesse D.....	ThP 756	Carpy, Alejandro.....	ThP 043	Castro-Perez, Jose.....	TP 459
Cantone, Joseph L.....	ThP 421	Carr, Peter.....	WP 720	Catalano, Carlos.....	ThP 093
Cantor, Jerome.....	ThP 448	Carr, Steven.....	TP 082	Catani, Katherine.....	ThP 504
Cantor, Jerome.....	TP 450	Carr, Steven A.....	MOG am 08:30	Catherman, Adam.....	WOH pm 3:30
Cantrell, Pamela.....	TOH am 09:50	Carr, Steven A.....	MP 126	Caudill, Marie.....	ThP 426
Cantrell, Pamela.....	WP 405	Carr, Steven A.....	ThOC am 10:10	Caudle, Michael.....	ThP 304
Cantu, Theresa.....	ThP 377	Carr, Steven A.....	ThOE am 10:10	Caudy, Amy.....	TP 638
Cao, Fan.....	WP 004	Carr, Steven A.....	ThP 039	Causon, Jason.....	MP 578
Cao, Lejje.....	TP 100	Carr, Steven A.....	ThP 205	Cavanaugh, Craig.....	MP 691
Cao, Li.....	TP 439	Carr, Steven A.....	ThP 217	Cavanaugh, Craig.....	TP 738
Cao, Li.....	WP 088	Carr, Steven A.....	TOG am 08:30	Cavdar, Huseyin Avni.....	MP 763
Cao, Rui.....	ThP 270	Carr, Steven A.....	TP 177	Cazares, Lisa H.....	WP 010
Cao, Song.....	TP 082	Carr, Steven A.....	TP 426	Cecchini, Tiphaine.....	TP 219
Cao, Song.....	TP 433	Carr, Steven A.....	TP 433	Cece, Esra Nurten.....	MP 639
Cao, Song.....	TP 438	Carr, Steven A.....	TP 438	Cech, Nadja.....	WP 476
Cao, Xiaoyan.....	WP 643	Carr, Steven A.....	WOD am 08:50	Cech, Nadja B.....	MP 312
Cao, Xiaoyu.....	ThP 517	Carr, Steven A.....	WOG am 08:50	Cechner, Karen.....	WP 530
Cao, Xing-Jun.....	TP 114	Carr, Steven A.....	WOG pm 2:30	Celik, Murat.....	MP 763
Cao, Zhijun.....	WP 249	Carré, Vincent.....	MP 576	Çelikbıçak, Ömür.....	MP 066
Cao, Zhijun.....	WP 470	Carreira, Ricardo J.....	MP 027	Çelikbıçak, Ömür.....	MP 475
Cao, Zhiyun.....	ThP 320	Carreira, Ricardo J.....	TP 005	Cellar, Nicholas.....	TP 276
Cao, Zhiyun.....	ThP 344	Carrera, Monica.....	MP 355	Cellar, Nick.....	TP 277
Capangpangan, Rey Y.....	WP 492	Carrera, Monica.....	ThP 613	Celum, Connie.....	WOF pm 4:10
Capodanno, Eric.....	WP 351	Carrick, Emma.....	WP 114	Cerciello, Ferdinando.....	ThP 296
Capono, Clifford.....	MP 056	Carrillo-Carrasco, Nuria.....	MP 514	Cerna, Vera.....	ThP 354
Cappadona, Salvatore.....	ThP 220	Carroll, Frances.....	MP 281	Černigoj, Urh.....	WP 135
Cappiello, Achille.....	MP 722	Carroll, Frances.....	ThP 588	Ceroni, Alessio.....	WP 050
Cappiello, Achille.....	TP 764	Carroll, James.....	WP 273	Cervantes, Serena.....	ThOF pm 3:30
Caprioli, Richard.....	MOB am 09:50	Carruthers, Anthony.....	MP 134	Cesnik, Anthony J.....	MOG am 08:50
Caprioli, Richard.....	MOH pm 2:30	Carter, Christy.....	MP 240	Cessna, Allan.....	TP 554
Caprioli, Richard.....	MP 017	Carter, Claire L.....	ThP 390	Ceven, Jim.....	TP 271
Caprioli, Richard.....	ThP 008	Carter, Claire L.....	TP 067	Cha, Sangwon.....	WP 289
Caprioli, Richard.....	ThP 009	Carter, Claire L.....	TP 299	Chacón-Patiño, Martha L.....	TP 588
Caprioli, Richard.....	TP 070	Carter, Dominique.....	WP 245	Chacón-Patiño, Martha L.....	TP 587
Caprioli, Richard.....	TP 058	Carter, Melissa.....	MP 194	Chaerkady, Raghothama.....	MP 255
Caprioli, Richard.....	TP 091	Carter, Melissa.....	ThP 429	Chaerkady, Raghothama.....	MP 440
Caprioli, Richard.....	WP 001	Carter, Spencer J.....	TP 519	Chaerkady, Raghothama.....	ThP 082
Caprioli, Richard M.....	MP 014	Cartron, Michael.....	ThP 172	Chaerkady, Raghothama.....	ThP 204
Caprioli, Richard M.....	MP 015	Caruso, Michael.....	TP 139	Chaerkady, Raghothama.....	ThP 219
Caprioli, Richard M.....	MP 022	Caruso, Michael.....	TP 143	Chaerkady, Raghothama.....	TP 431
Caprioli, Richard M.....	MP 023	Caruso, Michael.....	TP 488	Chaerkady, Raghothama.....	TP 427
Caprioli, Richard M.....	MP 029	Caruso, Michael.....	WP 241	Chaerkady, Raghothama.....	WP 511
Caprioli, Richard M.....	TP 042	Carvalho, José.....	ThP 101	Chafin, Dana.....	TP 759
Caprioli, Richard M.....	TP 039	Carvalho, Paulo Costa.....	TP 686	Chagovets, Vitaliy.....	MP 245
Caprioli, Richard M.....	TP 030	Carvalho, Valdemir Melechco.....	TP 435	Chagovets, Vitaliy.....	MP 303
Caprioli, Richard M.....	TP 073	Carver, Chris.....	WP 668	Chagovets, Vitaliy.....	ThP 396
Capriotti, Carol.....	MP 512	Carver, Chris.....	WP 666	Chahine, Ramez.....	WP 498
Capriotti, Fabiana.....	TP 764	Carver, Jeremy.....	MP 043	Chai, J.....	MP 264
Carbone, David.....	ThP 296	Carver, Jeremy.....	MP 056	Chai, Yunfeng.....	ThP 699
Cardasis, Helene.....	ThP 234	Carver, Mark.....	MP 167	Chai, Yunfeng.....	TP 352
Cardasis, Helene.....	WP 069	Casado, Marta.....	TP 639	Chaibva, Maxmore.....	ThP 105

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

## INDEX OF AUTHORS



Chait, Brian.....	MOE am 09:30	Chapman, Richard.....	WP 280	Chen, Hauh-Jyun Candy.....	MP 112
Chait, Brian.....	TOC pm 4:10	Chapple, Iain.....	MP 098	Chen, Hauh-Jyun Candy.....	ThP 444
Chait, Brian T.....	MP 165	Charles, Laurence.....	ThP 510	Chen, Hong.....	WP 360
Chait, Brian T.....	MP 160	Charles, Laurence.....	TP 781	Chen, Hsin-Chang.....	TP 312
Chait, Brian T.....	TP 132	Charles, Laurence.....	TP 780	Chen, Huan.....	MOA am 08:30
Chait, Brian T.....	WP 253	Charles, Laurence.....	WP 682	Chen, Huan.....	MP 550
Chait, Brian T.....	WP 743	Charles, Philip.....	ThP 342	Chen, Huan.....	MP 555
Chakrabarty, Shubhashis.....	MP 301	Charrier, Jean Philippe.....	ThP 023	Chen, Huanwen.....	MP 357
Chakraborty, Romy.....	ThP 649	Charrier, Jean-Philippe.....	TP 219	Chen, Huanwen.....	ThP 697
Chalkley, Robert.....	ThP 027	Charrietier, Yannick.....	TP 219	Chen, Huanwen.....	TP 391
Chalkley, Robert.....	ThP 048	Charusanti, Pep.....	MP 056	Chen, Huanwen.....	TP 388
Chalkley, Robert.....	WP 029	Chassy, Alexander.....	ThP 406	Chen, Hui-Yuan.....	MP 306
Chalmers, Michael.....	TP 543	Chatterjee, Aditi.....	MP 255	Chen, Ivy.....	WP 057
Chalmers, Michael.....	WOH pm 2:30	Chattopadhyay, Sandip.....	MP 520	Chen, Jenny.....	WP 144
Chalupová, Jana.....	TP 490	Chatzi, K.....	WP 229	Chen, Jenny.....	WP 263
Chamberlin, Chad.....	TOF pm 3:30	Chaudhary, Ashish.....	TP 712	Chen, Jie.....	WP 430
Chambers, Andrew.....	ThP 262	Chauhan, Sitara.....	MP 125	Chen, Jin.....	WOF pm 3:50
Chambers, Andrew.....	TOG pm 3:10	Chauhan, Vinita.....	MP 012	Chen, Jing.....	MP 785
Chambers, Andrew.....	TP 484	Chaurand, Pierre.....	MP 012	Chen, Jing.....	ThOH am 10:10
Chambers, Andrew.....	WOG pm 3:10	Chaurand, Pierre.....	MP 013	Chen, Jing.....	TP 478
Chambers, Andrew.....	WP 654	Chaurand, Pierre.....	TOH pm 3:50	Chen, Kai-Yun.....	WP 246
Chambers, Erin.....	WP 123	Chavali, Aparna.....	MP 728	Chen, Kuo-Chiang.....	ThP 275
Chambers, Erin E.....	WP 125	Chavali, Aparna.....	MP 729	Chen, Lee Chuin.....	TP 725
Chambers, Laura.....	ThP 641	Chavan, Sandip.....	MP 255	Chen, Lee Chuin.....	TP 727
Chambers, Matt.....	WP 029	Chavez, Juan.....	ThOC pm 3:50	Chen, Li.....	ThP 040
Chamot-Rooke, Julia.....	ThOF am 09:10	Chavez, Juan.....	ThP 466	Chen, Lijun.....	MP 432
Chamot-Rooke, Julia.....	WP 059	Chavez, Juan.....	ThP 465	Chen, Lijun.....	ThOH am 10:10
Champion, Matthew.....	MP 080	Chavez, Juan.....	WOF pm 3:30	Chen, Lijun.....	ThP 451
Champion, Matthew M.....	TP 228	Chavez, Juan D.....	ThP 464	Chen, Lijun.....	TP 477
Chan, Daniel.....	ThP 040	Chavez-Eng, Cynthia M.....	ThP 671	Chen, Lin.....	WP 630
Chan, Daniel.....	ThP 295	Chavez-Eng, Cynthia M.....	TP 492	Chen, Lin-Zhi.....	WP 519
Chan, Daniel W.....	ThP 451	Chavez-Eng, Cynthia M.....	WP 567	Chen, Liuxi.....	WP 662
Chan, George H.M.....	WP 582	Che, Ye.....	ThP 502	Chen, Pei.....	WP 338
Chan, Holly.....	MOD pm 3:10	Cheah, Jaime H.....	ThP 512	Chen, Pei.....	WP 337
Chan, Kelvin.....	WP 480	Cheema, Amrita.....	MP 061	Chen, Qing.....	TP 632
Chan, Leanne Jade.....	TP 175	Cheema, Amrita.....	WP 583	Chen, Qiuying.....	MP 592
Chan, Pik Kay.....	WP 606	Cheema, Jasparl.....	WP 171	Chen, Qiuying.....	MP 579
Chan, Pui Hei.....	ThP 619	Cheetham, Janet.....	WP 718	Chen, Shanshan.....	TP 758
Chan, Shan-An.....	MP 346	Chelbi-alix, Mounira.....	TP 108	Chen, Shanyan.....	ThP 302
Chan, Shan-An.....	ThP 528	Chelsky, Daniel.....	TP 445	Chen, Shao-Kuan.....	ThP 275
Chan, Shan-An.....	TP 279	Chelsky, Daniel.....	WP 137	Chen, Shao-Nong.....	WP 325
Chan, Shan-An.....	WP 356	Chelsky, Daniel.....	WP 138	Chen, Shu Ting.....	ThP 727
Chan, Stephen.....	MP 203	Chemnitzner, Rene.....	MP 665	Chen, Shu-Hua.....	WP 662
Chan, Tak Wah Dominic.....	ThP 151	Chemnitzner, René.....	MP 333	Chen, Shu-Hui.....	ThP 152
Chan, T-W. Dominic.....	MP 658	Chen, Chein-Hung.....	MP 425	Chen, Shu-Ting.....	ThP 434
Chan, T-W. Dominic.....	MP 657	Chen, Alan.....	MOC am 08:30	Chen, Sixue.....	WP 062
Chance, Mark.....	ThP 356	Chen, Amanda.....	MP 602	Chen, Sophia.....	WP 213
Chance, Mark.....	ThP 355	Chen, Bicui.....	WP 629	Chen, Suming.....	MP 400
Chance, Mark.....	TP 233	Chen, Bingming.....	MP 010	Chen, Susan.....	TP 515
Chance, Mark R.....	TP 118	Chen, Bingming.....	WP 006	Chen, Tao.....	MP 357
Chance, Mark R.....	MP 169	Chen, Chein-Hung.....	TP 330	Chen, Thomas.....	ThP 680
Chance, Mark R.....	WP 603	Chen, Chein-Hung.....	TP 687	Chen, Tien-Hao.....	ThOF am 09:30
Chandler, Kevin B.....	WP 075	Chen, Chen-Chun.....	ThP 714	Chen, Tong.....	MOB am 10:10
Chandramohan, Govindarajan.....	TP 528	Chen, Chen-Chun.....	ThP 713	Chen, Tong.....	MP 699
Chandramohan, Govindarajan.....	TP 529	Chen, Chia-Yang.....	WP 521	Chen, Tsung-Chi.....	MP 677
Chandramohan, Govindarajan.....	WP 539	Chen, Chien-Lun.....	ThP 291	Chen, Tsung-Chi.....	ThOB am 10:10
Chandranayak, Sidaiah.....	TP 647	Chen, Chien-Lun.....	WP 493	Chen, Tsung-Chi.....	TOB am 09:50
Chaney, Sarah B.....	MP 229	Chen, Chung-Hsuan.....	MP 304	Chen, Tsung-Chi.....	TOC am 08:30
Chang, Ching-Yun.....	MOG pm 3:50	Chen, Chung-Hsuan.....	MP 393	Chen, Tsung-Chi.....	TP 714
Chang, Hsien-Hong.....	ThP 644	Chen, Chung-Hsuan.....	MP 425	Chen, Wei.....	MP 118
Chang, Hui.....	WOH am 10:10	Chen, Chung-Hsuan.....	MP 662	Chen, Wei.....	ThP 324
Chang, Linda.....	TP 468	Chen, Chung-Hsuan.....	ThP 478	Chen, Weibin.....	MP 745
Chang, Michelle.....	MP 637	Chen, Chung-Hsuan.....	TP 330	Chen, Weibin.....	TP 156
Chang, Ming-Chu.....	MP 425	Chen, Chung-Hsuan.....	TP 687	Chen, Weibin.....	TP 157
Chang, Wei-Hung.....	MP 624	Chen, Chung-Hsuan.....	WP 246	Chen, Weibin.....	TP 158
Chang, Ya-Hui.....	WP 422	Chen, Cindy.....	TP 502	Chen, Weibin.....	TP 235
Chang, Yan Zin.....	MP 343	Chen, Daijie.....	WP 252	Chen, Weibin.....	TP 236
Chang, Yung-Yu.....	WP 462	Chen, David.....	MP 150	Chen, Weibin.....	TP 265
Chang, Yu-Sun.....	ThP 291	Chen, Dazhou.....	WP 404	Chen, Weibin.....	TP 541
Chang, Yu-Ting.....	MP 425	Chen, Dunlu.....	ThOE am 09:10	Chen, Weibin.....	WP 023
Chang, Yuwei.....	TP 120	Chen, Fangfang.....	ThP 436	Chen, Weibin.....	WP 274
Chang, Zhen.....	WP 239	Chen, Guodong.....	MOE pm 3:10	Chen, Weichao.....	ThOC am 09:10
Chanover, Nancy J.....	ThP 366	Chen, Guodong.....	MP 172	Chen, Weichao.....	WP 620
Chapman, Jessica R.....	WP 111	Chen, Guodong.....	MP 180	Chen, Weiqiang.....	WP 136
Chapman, John.....	ThP 325	Chen, Guodong.....	ThP 441	Chen, Wei-Qiang.....	TP 447
Chapman, John D.....	TP 400	Chen, Guodong.....	TP 541	Chen, Wei-Qiang.....	WP 135
Chapman, Kent.....	ThP 393	Chen, Hao.....	MP 329	Chen, Weiwei.....	TP 322
Chapman, Kent.....	TOH pm 4:10	Chen, Hao.....	ThP 461	Chen, Weiwu.....	ThP 016
Chapman, Kent.....	TP 037	Chen, Hao.....	TP 397	Chen, Weixuan.....	ThP 230

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Chen, Weixuan.....	TP 191	Chernobrovkin, Alexey.....	ThP 248	Choi, Jong-Soon.....	ThOA am 09:50
Chen, Wen-Jen.....	MP 435	Chernobrovkin, Alexey.....	TOF pm 3:10	Choi, Jong-Soon.....	ThOH pm 3:10
Chen, Xi.....	ThP 498	Chernobrovkin, Alexey L.....	TP 081	Choi, Jong-Soon.....	ThP 312
Chen, Xi.....	TP 258	Chernookiy, Dmitriy.....	MP 694	Choi, Minjung.....	ThP 133
Chen, Xian.....	MP 179	Chernookiy, Dmitriy.....	MP 693	Choi, Sung W.....	WP 118
Chen, Xian.....	ThP 206	Chernyavsky, Ilya.....	ThOG am 09:30	Cholet, Sophie.....	ThP 140
Chen, Xian.....	ThP 290	Cherrier, Martin.....	MP 761	Cholia, Shreyas.....	MP 024
Chen, Xian.....	TP 433	Chervet, Jean-Pierre.....	MP 093	Chong, Patrick.....	TP 216
Chen, Xiaofeng.....	WP 633	Chervet, Jean-Pierre.....	TP 622	Choo, Edna F.....	WP 005
Chen, Xiaohong.....	MP 735	Chesnik, Marla.....	MP 428	Chopra, Shilpi.....	WP 720
Chen, Xiaohong.....	WP 432	Chesnik, Marla A.....	ThP 280	Chornoguz, Olesya.....	ThP 339
Chen, Xiaohui.....	ThP 535	Chesnov, Serge.....	MP 200	Chou, Chi-Chi.....	TP 207
Chen, Xin.....	WP 736	Chevolleau, Sylvie.....	TP 649	Chou, Jo-Han.....	MP 382
Chen, Xuan.....	WP 210	Chew, Yin Ling.....	MP 342	Chou, Jo-Han.....	WP 415
Chen, Y. Ann.....	TP 463	Chew, Yin Ling.....	MP 351	Chou, Robert.....	TP 240
Chen, Yet-Ran.....	MP 624	Chhoy, Peter.....	TP 112	Chou, Wayne.....	ThP 228
Chen, Yi-Chen (Ivy).....	ThP 065	Chhuon, Cerina.....	WP 145	Choudhary, Chunaram.....	WP 257
Chen, Yi-Lun.....	TP 399	Chi, Hao.....	WP 054	Choudhary, Jyoti.....	WP 160
Chen, Yi-Lun.....	WP 346	Chi, Hao.....	WP 053	Chouinard, Christopher D.....	MP 376
Chen, Ying.....	ThOE am 09:10	Chi, Jingduan.....	WP 541	Chourey, Karuna.....	MP 277
Chen, Yi-Ting.....	ThP 291	Chia-Hsiun, Liu.....	ThP 683	Chourey, Karuna.....	ThP 772
Chen, Yi-Ting.....	WP 493	Chiang, Su-Yin.....	TP 312	Chourey, Prem.....	WP 062
Chen, Yi-Yun.....	TP 121	Chiang, Vincent.....	MP 209	Chow, H-H Sherry.....	ThP 656
Chen, Yu.....	MP 648	Chiarelli, M. Paul.....	MP 324	Chowdhry, Babur.....	WP 695
Chen, Yu.....	ThOF pm 3:10	Chiarelli, M. Paul.....	WP 559	Chowdhury, Goutam.....	MP 645
Chen, Yu.....	ThP 757	Chiarelli, M. Paul.....	WP 563	Chowdhury, Saiful.....	ThP 245
Chen, Yu.....	TP 720	Chicher, Johana.....	TP 247	Chowdhury, Saiful.....	ThP 244
Chen, Yu.....	TP 720	Chicher, Johana.....	WP 498	Chowdhury, Saiful.....	ThP 223
Chen, Yuan-Shek.....	TP 504	Chick, Joel.....	WOG am 09:10	Chrisler, William.....	WOG pm 2:50
Chen, Yuan-Shek.....	TP 508	Chick, Joel M.....	MOG pm 2:30	Christiansen, Jesper.....	MP 409
Chen, Yuan-Shek.....	TP 684	Chien, Allis.....	ThP 308	Christianson, Chad.....	MP 711
Chen, Yuan-Shek.....	WP 533	Chien, Allis.....	TP 507	Christison, Terri.....	MP 596
Chen, Yue.....	MOG pm 4:10	Chien, Allis S.....	ThP 684	Christison, Terri.....	MP 634
Chen, Yue.....	MP 033	Chien, Allis S.....	TOA pm 3:30	Christoforou, Andy.....	WP 738
Chen, Yue.....	MP 104	Chien, Du-Shieng.....	WP 488	Chu, Caroline S.....	TP 246
Chen, Yue.....	WOG am 09:50	Chien, Ko-Yi.....	TP 458	Chu, Feixia.....	WP 482
Chen, Yue.....	WP 259	Chien, Peter.....	MP 185	Chu, Kuan Yu.....	MP 305
Chen, Yufei.....	TP 535	Chilewski, Shannon.....	TOE am 09:30	Chu, Kung-Hui.....	MP 563
Chen, Yu-Ju.....	ThP 713	Chilton, John.....	MP 033	Chu, Rosalie.....	WOE am 08:30
Chen, Yu-Ju.....	ThP 714	Chingin, Konstantin.....	ThP 697	Chu, Rosey.....	TP 676
Chen, Yu-Ju.....	WP 492	Chingin, Konstantin.....	TP 388	Chu, Xiaogang.....	WP 407
Chen, Yu-Luan.....	WP 537	Chiorean, Gabriela.....	MP 443	Chua, Yong Guan.....	ThP 622
Chen, Yung-Hsiang.....	MP 499	Chiou, Thomas S.-H.....	MP 435	Chuang, Yung-Kun.....	MP 304
Chendo, Christophe.....	TP 780	Chiplunkar, Sanket.....	TP 763	Chubatyi, Nicholas.....	WP 387
Chendo, Christophe.....	WP 682	Chiplunkar, Sanket.....	TP 761	Chughtai, Kamila.....	MOH pm 3:50
Cheney, Carolyn M.....	MP 229	Chiplunkar, Sanket.....	TP 762	Chui, David H. K.....	WP 445
Cheng, Chu-Nian.....	MP 384	Chiron, Lionel.....	TP 719	Chumbley, Chad W.....	TP 030
Cheng, Cliff C.....	MP 131	Chiron, Lionel.....	WP 729	Chumsae, Chris.....	TP 102
Cheng, Dong.....	ThOE am 08:30	Chitranshi, Priyanka.....	TP 489	Chun, Chanlan.....	WOE pm 4:10
Cheng, Guilong.....	TP 730	Chitranshi, Priyanka.....	WP 548	Chung, Dominic.....	ThP 770
Cheng, Guilong (Charles).....	ThP 693	Chiu, Norman.....	WP 694	Chung, Duk-Won.....	ThOF pm 3:30
Cheng, Guilong (Charles).....	TP 148	Chiu, Yulun.....	ThP 726	Chung, Haena.....	WP 240
Cheng, Hong.....	ThP 405	Chiu, Yulun.....	TP 320	Chung, Hyo (Helen).....	TP 239
Cheng, Jianlin.....	ThP 302	Chiuu, Daisie.....	WP 636	Chung, Lisa M.....	MP 219
Cheng, Jie.....	ThP 356	Chiva, Cristina.....	ThP 220	Chung, Myung.....	TP 188
Cheng, Kai.....	WP 068	Chlopicki, Stefan.....	ThP 445	Chung, Nickesha.....	ThOA am 09:10
Cheng, Keding.....	TP 213	Chmelka, Franziska.....	MP 776	Chung, Ray.....	ThP 163
Cheng, Lin-Yang.....	MOG pm 3:50	Cho, David S.....	TP 743	Chung, Ting.....	ThP 291
Cheng, Lin-Yang.....	ThP 257	Cho, Hee-Yeon.....	ThP 680	Chung, Ting.....	WP 493
Cheng, Menglin.....	TP 062	Cho, Hyun-Deok.....	TP 509	Chung, Wai Keen.....	TP 243
Cheng, Michael.....	TP 591	Cho, Jin-Young.....	ThP 024	Churchill, Gary A.....	MOG pm 2:30
Cheng, Michael T.....	WOA am 09:10	Cho, Jong-Hyun.....	ThP 679	Churchwell, Mona I.....	TP 499
Cheng, Shu-Yuan.....	ThP 598	Cho, Kevin.....	MP 602	Churchwell, Mona I.....	TP 624
Cheng, Sy Chyi.....	TP 382	Cho, Kun-Ching.....	MP 563	Churlaud, Florence.....	TP 775
Cheng, Sy-Chyi.....	MP 389	Cho, Sool Yeon.....	WP 116	Chuzel, Olivier.....	WP 682
Cheng, Ting-Jen.....	WP 246	Cho, Wonryeon.....	WP 084	Ci, Bo.....	MP 118
Cheng, Xin.....	TP 238	Cho, Yi-Tzu.....	WP 422	Cianci, Chris.....	ThP 666
Cheng, Yaofeng.....	MP 197	Cho, Yunju.....	WOA pm 2:30	Cianferani, Sarah.....	MOE am 09:50
Cheng, Yupeng.....	TP 396	Choi, Bernard.....	TP 460	Cianferani, Sarah.....	MP 157
Cheng, Zhi.....	ThP 527	Choi, Bernard.....	WP 184	Cianferani, Sarah.....	ThP 095
Cheng, Zhongyi.....	MP 232	Choi, Caitlin.....	ThP 040	Cianferani, Sarah.....	WP 265
Cheng, Zhongyi.....	TP 100	Choi, Cheol Ho.....	MP 300	Ciccimaro, Eugene.....	MP 622
Cheng, Zhongyi.....	TP 123	Choi, Cheol Ho.....	WOA pm 2:30	Ciccimaro, Eugene F.....	TP 693
Cheng, Zhongyi.....	TP 122	Choi, Eun-kyeong.....	TP 214	Ciccimaro, Eugene F.....	WP 725
Cheng, Zhongyi.....	TP 674	Choi, Hyungwon.....	MP 258	Ciccimaro, Eugene F.....	WP 732
Cheng, Zhongyi.....	WP 259	Choi, Jaewon.....	ThP 572	Cichewicz, Robert.....	TP 220
Cheong, Nam-Yong.....	WP 580	Choi, Jaewon.....	TP 580	Cichewicz, Robert.....	WP 330
Cheow, Esther.....	WP 061	Choi, Jaewoo.....	MP 598	Cicotte, Steven.....	MOG pm 2:30
Chernobrovkin, Alexey.....	MOG am 10:10	Choi, Jaewoo.....	ThP 643	Cifková, Eva.....	ThP 396

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



Ciossek, Thomas.....	ThP 746	Cohen, Jerry D.....	MP 611	Comstock, Kate.....	ThP 537
Cipollo, John.....	MP 681	Cohen, Jerry D.....	TP 641	Comstock, Kate.....	TP 530
Cipollo, John.....	ThP 164	Cohen, Lucinda.....	TP 460	Comstock, Kate.....	TP 791
Cisowska, Tamara.....	WP 325	Cohen, Richard.....	WP 195	Conforti, Franco.....	ThP 439
Ciszek, Jacob W.....	MP 324	Cohen, Richard A.....	MP 120	Conjelko, Timothy.....	WP 421
Claesen, Jürgen.....	WP 031	Cohen, Richard A.....	MP 465	Conley, Sandra K.....	MP 437
Clancy, Trevor.....	ThP 433	Cohen, Ryan.....	MP 484	Connelly, Jennifer.....	MP 428
Clark, Daniel.....	WP 260	Cohen, Ryan.....	MP 511	Connolly, Joanne B.....	MP 409
Clark, Hillary.....	WP 112	Cohen, Ryan.....	MP 685	Connolly, Joanne B.....	ThP 036
Clark, Robert.....	MP 251	Cohen-kaminsky, Sylvia.....	MP 025	Connolly, Joseph.....	MP 161
Clark, Robert B.....	WP 502	Cojocariu, Cristian.....	ThP 571	Connolly, Michael.....	ThP 184
Clark, Sean.....	WOH am 10:10	Cojocariu, Cristian.....	WP 359	Connolly, Paul.....	MP 281
Clarke, David.....	TOE pm 3:50	Colangelo, Christopher M.....	MP 219	Conrad, Charles A.....	MP 427
Clarke, David J.....	MP 182	Colby, Greg.....	TP 145	Conrad, Stephen M.....	MP 354
Claude, Christian.....	WP 047	Cole, Daniel.....	MP 565	Conrads, Kelly A.....	ThP 202
Claude, Emmanuelle.....	ThP 001	Cole, Daniel.....	MP 566	Conrads, Thomas P.....	ThP 202
Claude, Emmanuelle.....	TP 004	Cole, Jason.....	ThOG pm 3:10	Contamin, Bénédicte.....	TP 423
Clausen, Rasmus.....	TOF pm 2:30	Cole, Jason.....	WP 359	Conti, Elena.....	WOG am 09:30
Clauser, Karl.....	ThP 039	Cole, Laura E.....	WP 111	Conteras, Stephanie.....	WOE am 08:50
Clauser, Karl.....	TP 082	Cole, Richard.....	ThP 513	Conwell, Darwin.....	ThP 279
Clauser, Karl.....	TP 426	Cole, Richard.....	WP 173	Conwell, Darwin L.....	ThOE pm 4:10
Clauser, Karl R.....	MOG am 08:30	Cole, Richard B.....	MP 587	Cook, Amber.....	ThP 731
Clauser, Karl R.....	ThOE am 10:10	Cole, Richard B.....	ThP 696	Cook, Amber.....	ThP 733
Clauser, Karl R.....	ThP 205	Cole, Richard B.....	TP 293	Cook, Amber.....	WP 030
Clauser, Karl R.....	TOG am 08:30	Cole, Richard B.....	TP 414	Cook, Amber C.....	ThP 728
Clauser, Karl R.....	TP 438	Cole, Richard B.....	TP 524	Cook, Jamie Elsilia.....	ThP 365
Cleary, Michele.....	TP 061	Cole, Robert.....	ThP 082	Cook, Kelsey D.....	TP 743
Cleeve, Matthew.....	MP 767	Cole, Robert.....	ThP 219	Cook, Kevin.....	MP 338
Cleeve, Matthew.....	MP 768	Cole, Robert.....	TP 431	Cook, Kevin.....	WP 637
Cleland, Gareth.....	ThP 544	Cole, Robert N.....	TP 427	Cooke, Ira.....	MP 033
Cleland, Gareth.....	WP 349	Cole, Robert N.....	WP 511	Cooke, Ira.....	ThP 045
Cleland, Timothy P.....	ThP 247	Cole, Robert N.....	MP 187	Cooks, Graham.....	ThOA am 08:30
Clemen, Martin.....	ThP 694	Coleman, Gary D.....	TP 668	Cooks, R. Graham.....	MP 394
Clements, James.....	WP 015	Coletta, Ricardo.....	WP 460	Cooks, R. Graham.....	TP 387
Clemmer, David.....	ThP 233	Colgrave, Michelle.....	WOE pm 2:30	Cooks, R. Graham.....	TP 398
Clemmer, David.....	ThP 508	Colinge, Jacques.....	MP 228	Cooks, R. Graham.....	TP 741
Clemmer, David E.....	MOC pm 2:50	Colinge, Jacques.....	WOF pm 2:50	Cooks, R. Graham.....	WP 021
Clemons, Paul A.....	ThP 512	Collins, Andrew.....	ThP 034	Cooks, R. Graham.....	WP 412
Clendinen, Chaevien.....	TP 044	Collins, Ben.....	MP 432	Cool, Lydia.....	TP 776
Clerici, Lorella.....	MP 148	Collins, Ben.....	ThOE pm 3:50	Cool, Lydia.....	TP 784
Clerici, Lorella.....	WP 156	Collins, Ben.....	ThP 257	Cooley, Michael.....	TP 230
Cliby, William.....	ThP 733	Collins, Leonard.....	ThP 523	Coon, Joshua.....	ThOG pm 3:10
Cliffel, David E.....	ThP 495	Collins, Thomas S.....	ThP 614	Coon, Joshua.....	ThP 685
Clifton-Bligh, Roderick.....	MP 449	Cologna, Stephanie.....	ThP 491	Coon, Joshua J.....	ThP 068
Clinckemaillie, Tom.....	TP 024	Cologna, Stephanie M.....	MP 437	Coon, Joshua J.....	ThP 177
Clingenpeel, Amy C.....	TP 598	Coloma, Luis.....	WP 339	Coon, Joshua J.....	ThP 178
Clinton, Steven K.....	ThP 292	Colquhoun, David.....	MP 262	Coon, Joshua J.....	ThP 179
Clish, Clary B.....	ThP 512	Colquhoun, David.....	ThOE pm 3:30	Coon, Joshua J.....	ThP 327
Clouse, Steven D.....	MP 410	Colquhoun, David.....	ThP 229	Coon, Joshua J.....	ThP 348
Clowers, Brian H.....	ThP 741	Colquhoun, David.....	ThP 766	Coon, Joshua J.....	TP 669
Clowers, Brian H.....	WP 692	Colquhoun, David.....	TP 146	Coon, Joshua J.....	WOA am 09:50
Coadou, Gael.....	WOC pm 2:50	Colquhoun, David.....	WP 161	Coon, Joshua J.....	WOD am 10:10
Coats, Steven J.....	ThP 679	Colquhoun, David.....	WP 602	Cooper, Allen.....	MP 069
Cobbaert, Christa M.....	WP 518	Colsch, Benoit.....	MP 587	Cooper, Bret.....	TP 668
Cobbold, Mark.....	MOH am 10:10	Colsch, Benoit.....	MP 581	Cooper, Bret.....	WOE pm 3:30
Cobbold, Simon A.....	MP 271	Colsch, Benoit.....	ThP 391	Cooper, Helen.....	TP 041
Cobbold, Simon A.....	TP 101	Colsch, Benoit.....	WP 281	Cooper, Helen J.....	WP 765
Coburn, Steven.....	MOD pm 2:50	Colucci, Wilson.....	WP 195	Cooper, Helen J.....	MP 253
Cochran, Chip.....	MP 069	Colucci, Wilson S.....	MP 120	Cooper, Helen J.....	TOD pm 3:30
Cochran, Elizabeth.....	MP 428	Colucci, Wilson S.....	MP 465	Cooper, Helen J.....	TP 232
Cochran, Jack.....	WOC pm 2:30	Combariza, Marianny.....	TP 416	Cooper, Helen J.....	WP 082
Cochran, Jack.....	WP 557	Combariza, Marianny Y.....	TP 587	Cooper, Helen J.....	WP 764
Cochran, Jack.....	WP 570	Combariza, Marianny Y.....	TP 588	Coopersmith, Brad.....	TP 693
Cockwell, Paul.....	MP 098	Combe, Peter.....	ThP 066	Copie, Valerie.....	MP 276
Cocuron, Jean-Christophe.....	MP 415	Comi, Troy.....	WP 399	Corbett, John.....	TP 104
Cody, Robert.....	WP 292	Comi, Troy J.....	MP 387	Corbett, John.....	WP 058
Cody, Robert B.....	MP 385	Cominetti, Ornella.....	ThP 255	Corcoran, Henry.....	WP 720
Cody, Robert B.....	ThP 415	Comisar, Wendy.....	WP 652	Cordwell, Stuart.....	TP 131
Cody, Robert B.....	WP 336	Commodore, Juliette J.....	ThP 182	Corea, Oliver.....	TP 676
Cody, Robert B.....	WP 576	Compagnon, Isabelle.....	ThP 469	Corilo, Yuri.....	WOA pm 2:50
Coelho, Fernando.....	WP 685	Compton, Laine.....	WP 740	Corilo, Yuri E.....	MOA am 08:30
Coelho Graça, Didia.....	MP 148	Compton, Philip.....	MP 676	Corilo, Yuri E.....	TP 595
Coelho Graça, Didia.....	WP 156	Compton, Philip.....	TOD am 08:30	Corilo, Yuri E.....	TP 601
Coffey, Chelsea.....	MP 091	Compton, Philip.....	TOE pm 3:30	Corilo, Yuri E.....	TP 602
Cohen, Daniel.....	TP 541	Compton, Philip.....	TP 234	Corilo, Yuri E.....	TP 597
Cohen, Herbert.....	WP 743	Compton, Philip.....	WOH pm 3:30	Corilo, Yuri E.....	WOA am 09:30
Cohen, Jerry.....	MP 412	Compton, Philip D.....	ThP 060	Corman, Bruno.....	TP 577
Cohen, Jerry D.....	MP 413	Compton, Philip D.....	TP 196	Cornett, Shannon.....	MP 008
Cohen, Jerry D.....	MP 605	Comstock, Kate.....	MP 641	Cornish, Timothy.....	MP 697

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Cornish, Timothy.....	ThP 365	Cradic, Kendall .....	WP 726	Cudre Correia De Almeida, Sandrine .....	MP 632
Cornish, Virginia W.....	ThP 512	Cramer, Rainer .....	MP 407	Cuevas Polo, Nerea .....	ThP 279
Corona, Alejandro.....	MP 453	Cramer, Rainer .....	TP 420	Cuevas Polo, Nerea .....	TP 187
Corr, Jay .....	TP 518	Cramer, Rainer .....	WP 748	Cui, Dan.....	WP 659
Corradini, Eleonora.....	ThP 301	Crappé, Jeroen.....	TP 078	Cui, He.....	MP 378
Correa, Deleon .....	ThOA am 09:30	Craven, Kirsten.....	TP 777	Cui, Jiankun.....	ThP 302
Correia, Carlos R. D. ....	MP 367	Crawford, Elizabeth .....	ThP 413	Cui, Jianyong.....	MP 330
Corso, Jasmin.....	MP 198	Crawford, Fiona .....	MP 116	Cui, Weidong .....	MP 111
Corso, Jasmin.....	ThP 203	Crawford, Fiona .....	MP 246	Cui, Yaya .....	WOE pm 4:10
Cortes, Diego.....	WP 127	Crawford, Fiona .....	MP 266	Cullins, Charles .....	MP 553
Cortes, Laetitia .....	TP 423	Crawford, Fiona .....	WOE am 09:50	Culotta, Valeria .....	WP 112
Corthesy, John.....	WP 510	Crawford, James .....	ThP 357	Culp, Amanda .....	TP 635
Corthésy, John.....	ThP 255	Crawford, Matthew .....	MP 287	Cummings, Brian .....	TP 304
Corvaia, Nathalie .....	MOE am 09:50	Crawford, Matthew .....	MP 532	Cummings, Brian S.....	TP 568
Cossins, Ben .....	WP 056	Crawford, Matthew .....	TOG pm 4:10	Cummings, Steven .....	TP 341
Cossoul, Emilie.....	TP 775	Crawford, Matthew .....	WP 429	Cummins, David .....	TP 543
Costa-Leonardo, Ana Maria.....	MP 562	Creaser, Colin.....	ThOC am 09:10	Cunha, Isabela .....	MP 464
Costanzo, Michael T. ....	WP 397	Creaser, Colin.....	ThP 500	Cunha de Miranda, Barbara K.....	TP 269
Costello, Catherine E.....	MOH am 08:50	Creaser, Colin.....	TP 402	Cunningham, Debbie L.....	ThP 316
Costello, Catherine E.....	MP 120	Creaser, Colin.....	TP 390	Cunningham, Debbie L.....	WP 764
Costello, Catherine E.....	MP 465	Creaser, Colin S.....	MP 522	Cunningham, Robert .....	MP 206
Costello, Catherine E.....	ThOH pm 2:30	Creasy, David .....	WP 029	Cupo, Al.....	TOF am 08:50
Costello, Catherine E.....	ThP 057	Creech, Amanda.....	WOG pm 2:30	Curk, Tomaz .....	TP 202
Costello, Catherine E.....	ThP 159	Creese, Andrew .....	MP 098	Curran, Patrick.....	TOF pm 3:30
Costello, Catherine E.....	ThP 711	Creese, Andrew .....	WP 765	Currie, Cameron .....	MP 569
Costello, Catherine E.....	ThP 716	Creese, Andrew J.....	TP 216	Curtis, Matthew.....	TP 308
Costello, Catherine E.....	TP 095	Creese, Andrew J.....	TOD pm 3:30	Curtis, Matthew.....	TP 557
Costello, Catherine E.....	TP 223	Creese, Andrew J.....	WP 082	Curtis, Maurice A.....	TP 060
Costello, Catherine E.....	TP 242	Creese, Andrew J.....	WP 764	Cusanovich, Darren.....	MP 212
Costello, Catherine E.....	TP 323	Creran, Brian .....	WP 701	Cutak, Benjamin .....	MP 751
Costello, Catherine E.....	WOE pm 2:30	Crich, David .....	TP 322	Cuthbertson, Daniel.....	MP 589
Costello, Catherine E.....	WP 059	Crispin, Max.....	ThP 171	Cutler, Paul.....	TP 172
Costello, Catherine E.....	WP 195	Cristea, Ileana M. ....	MP 158	Cutts, John .....	MP 586
Costello, Catherine E.....	WP 445	Cristea, Ileana M. ....	ThP 171	Cvacka, Josef .....	TP 401
Costello, Catherine E.....	WP 674	Cristea, Ileana M. ....	ThP 340	Cvačka, Josef.....	MP 030
Cotham, Victoria C.....	WP 261	Cristea, Ileana M. ....	TP 451	Czar, Martin F.....	ThOD pm 2:30
Cotham, William E.....	MP 506	Cristea, Ileana M. ....	WOE pm 3:50	Czentnar, Zoltan .....	MP 292
Cotern, Margaret .....	MP 167	Cristea, Ileana M. ....	WP 244	Czernekova, Lydie .....	ThP 149
Cottine Hitchcock, Jennifer.....	MP 471	Crittenden, Christopher M.....	ThP 350	D'Arienzo, Celia .....	ThP 441
Cotton, Jerome .....	TP 577	Crocker, Madison.....	MP 246	D'Ulivo, Alessandro .....	TP 770
Coughlan, Christina .....	ThP 304	Crocker, Madison.....	MP 266	Da Costa, Caitlyn.....	TP 390
Coughlan, Neville .....	ThP 504	Croft, Marie.....	MP 645	da Fonseca, Micaella P.....	MP 159
Counter, Christopher .....	MP 082	Croley, Timothy.....	MP 364	da Silva, Bianca F.....	TP 614
Coupier, Bruno.....	MP 693	Croley, Timothy R.....	WP 333	Da Silva, Gabriel.....	TP 355
Coupier, Bruno.....	MP 694	Crone, Catharina .....	ThP 317	Dabrowski, Wojtek .....	ThP 055
Cousins, Lisa .....	MP 339	Crone, Catharina .....	WP 301	Dacostasousa, Leonardo.....	MP 564
Cousins, Lisa .....	TP 521	Crosby, Meredith .....	TP 300	Dafnis-Calas, Felix .....	ThP 645
Cousins, Lisa M.....	MP 656	Crosland, Susan .....	Special	Dagher, Zeina .....	WP 498
Cousins, Matthew .....	WOE pm 4:10	Crossley, Janna .....	ThP 393	Dahl, Jeff .....	ThP 654
Coutouly, Marie-Aude .....	TP 719	Crossley, Janna .....	ThP 417	Dahl Andersen, Mette .....	ThP 135
Coutouly, Marie-Aude .....	WP 729	Crossley, Janna .....	TP 643	Dai, Hongping .....	MP 053
Couvillon, Anthony .....	MP 122	Crossman, Alan .....	TP 016	Dai, Hongping .....	TP 662
Couzens, Amber L.....	MP 258	Crouch, Rosalie .....	MP 022	Dai, Jenny.....	MP 517
Covelli, Caterina .....	ThP 594	Crouch, Rosalie.....	TP 070	Dai, Jianliang .....	WP 060
Cover, Timothy L.....	MP 123	Crow, Brian .....	MP 194	Dai, Jianliang .....	WP 458
Covey, Thomas.....	TP 518	Crow, Brian .....	ThP 429	Dai, Jie.....	WP 044
Covey, Thomas.....	WP 696	Crow, Marni.....	ThP 340	Dai, Lixin.....	WP 253
Covey, Thomas.....	WP 771	Crowe, Matthew.....	TOA am 09:30	Dai, Lunzhi.....	TP 112
Covey, Thomas R.....	WP 772	Crowell, Andrew.....	ThP 261	Dai, Lunzhi.....	WOG am 09:50
Cowan, David .....	ThP 163	Crowell, Andrew.....	ThP 782	Dai, Mingji.....	TP 353
Cowart, Emily .....	WP 222	Crowell, Kevin.....	MOC pm 3:10	Dai, Susie .....	ThP 123
Cox, Brian M.....	TP 063	Crowell, Kevin.....	MOG pm 3:30	Dai, Susie .....	TP 678
Cox, David .....	WP 295	Crowell, Kevin.....	ThP 483	Dai, Yuqin .....	WP 591
Cox, David .....	WP 357	Crowell, Kevin L.....	MP 677	Dal Bello, Federica .....	ThP 596
Cox, Holly .....	ThP 437	Crowell, Kevin L.....	ThP 741	Dalby, Kevin.....	ThP 350
Cox, Jonathan .....	ThOB am 10:10	Crowell, Kevin L.....	TP 324	Dale, Bruce E .....	MP 564
Cox, Jonathan T.....	MP 677	Crowley, Jan .....	TP 651	Dale, Stephanie .....	TP 035
Cox, Jonathan T.....	TP 324	Crozier, Thomas .....	MP 151	Dalko, Anita .....	WP 540
Cox, Jonathan T.....	TP 715	Crozier, Thomas .....	ThP 089	Dalko, Anita .....	WP 546
Cox, Jonathan T.....	WP 745	Cruikshank-Quinn, Charmion .....	TP 446	Dallas, Dave .....	WOE am 08:50
Cox, Juergen .....	MP 198	Cruz, Karen .....	WP 460	Dalmia, Avinash .....	ThP 416
Cox, Juergen .....	MP 723	Crynen, Gogce .....	MP 116	Dalmia, Avinash .....	ThP 559
Cox, Richard .....	MOD am 08:30	Crynen, Gogce .....	MP 246	Dalmia, Avinash .....	ThP 584
Coy, Stephen .....	WP 776	Crynen, Gogce .....	MP 266	Dalmia, Avinash .....	TP 267
Coy, Stephen L.....	TP 659	Crynen, Gogce .....	WOE am 09:50	Dalmia, Avinash .....	WP 408
Coy, Stephen L.....	WP 775	Cseke, Leland.....	TP 680	Daly, Charlotte E.....	TP 487
Coyaud, Étienne.....	MP 258	Cubberley, Richard .....	ThP 249	Damacharla, Divyasri .....	TP 139
Cozma, Claudia.....	WP 656	Cubison, Mike .....	TOA pm 3:10	Damacharla, Divyasri .....	TP 143
Crabtree, Nathaniel .....	ThP 054	Cubrilovic, Dragana.....	WOE am 09:10	Damacharla, Divyasri .....	WP 241

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

## INDEX OF AUTHORS



Damale, Shailesh .....	TP 496	Datar, Ajit .....	TP 761	De Pauw, Edwin .....	WOE am 09:50
Damale, Shailesh .....	TP 497	Datar, Ajit .....	WP 350	de S. Galaverna, Renan .....	TP 586
Damale, Shailesh .....	TP 498	Date, Sachiko .....	MOF pm 3:10	De Saeger, Sarah .....	ThOA pm 2:30
Damale, Shailesh .....	WP 350	Date, Sachiko .....	MP 417	de Souza, Emanuel .....	WOE pm 4:10
Damgaard Poulsen, Hanne .....	MP 409	Date, Sachiko .....	WP 594	Dean, Brian .....	MP 499
Dammer, Eric .....	MP 216	Datta, Keshava K. ....	MP 255	Dean, Brian .....	ThP 428
Dammer, Eric .....	WP 178	Daub, Henrik .....	ThP 019	Dean, Brian .....	ThP 702
Dammer, Eric .....	WP 237	Dauly, Claire .....	WP 281	Dean, Ralph A. ....	MP 119
Damoc, Eugen .....	MP 186	Dautry, Sébastien .....	ThOF am 09:10	Deane, Fiona .....	TP 205
Damoc, Eugen .....	MP 653	Dave, Jitendra R. ....	ThP 306	Dear, Gordon .....	MP 647
Damoc, Eugen .....	ThP 190	David, Frank .....	ThOA pm 3:50	Dearden, David V. ....	TOB am 08:50
Damoc, Eugen .....	ThP 754	Davidovic, Laetitia .....	ThP 081	Dearden, David V. ....	TP 357
Damoc, Eugen .....	TOB am 10:10	Davidson, Kimberly .....	ThOC pm 4:10	DeArmond, Patrick .....	WP 579
Damoc, Eugen .....	TOD am 08:30	Davies, Donna .....	ThP 439	Debaene, Francois .....	ThP 095
Damoc, Eugen .....	TP 136	Davies, Geoff .....	MP 341	Debaene, Francois .....	WP 265
Damoc, Eugen .....	WOA pm 3:30	Davies, Geoff .....	MP 756	Debaene, François .....	MOE am 09:50
Damoc, Eugen .....	WOF am 09:30	Davies, Geoff .....	MP 757	Debaene, Francoise .....	MP 157
Damoc, Nicolaie Eugen .....	ThP 762	Davies, Geoff .....	MP 758	DeBenedetto, Christopher .....	TP 040
Dan, Vi .....	TP 504	Davies, Geoff .....	MP 760	Debernardi, Alexandra .....	WOG am 09:50
Dancel, Maria Cristina A. ....	TP 786	Davies, Geoff .....	MP 761	Deblois, Christian .....	WP 564
Dandekar, Abhaya .....	TP 258	Davies, Geoff .....	MP 783	Deboer, Gerrit .....	MOA am 09:30
Dandekar, Satya .....	ThP 153	Davies, Geoff .....	ThP 589	DeBoer, Gerrit J. ....	MP 054
Dandliker, Peter .....	TOF pm 3:30	Davies, Roberta.B .....	ThP 501	Debois, Delphine .....	TP 418
D'Andrea, Annalisa .....	WP 465	Davies, Sherri .....	TOG am 08:30	DeBord, John .....	TP 209
Dane, A. John .....	ThP 415	Davies, Sherri .....	TP 082	Debrauwer, Laurent .....	TP 309
Dane, A. John .....	WP 336	Davies, Sherri R. ....	MOG am 08:30	Debrauwer, Laurent .....	TP 649
Dane, A. John .....	WP 576	Davies, Sherri R. ....	ThP 039	deCastro, B. Rey .....	TP 476
Dane, John .....	MP 385	Davies, Sherri R. ....	ThP 170	Dechaume, Dominique .....	TP 219
Dane, John .....	WP 292	Davies, Sherri R. ....	ThP 205	DeChenne, Sharon .....	MP 711
Danell, Allison S. ....	ThP 096	Davies, Sherri R. ....	TP 169	Decker, Petra .....	MP 289
Danell, Ryan M. ....	ThP 369	Davies, Sherri R. ....	TP 173	Dee, Stacy .....	MP 287
Danell, Ryan M. ....	TOA pm 2:30	Davies, Sherri R. ....	TP 433	Dee, Stacy .....	MP 532
Danell, Ryan M. ....	TP 710	Davies, Sherri R. ....	TP 438	Dee, Stacy .....	TOG pm 4:10
Daneshfar, Rambod .....	ThP 099	Davies, Sherri R. ....	WOG pm 3:50	Dee, Stacy .....	WP 429
Dang, Katherine .....	TP 765	Davin, Laurence .....	TP 676	Deeb, Ruba .....	MP 579
Dang, Xibei .....	ThOF pm 3:10	Davis, Alan E. ....	ThP 170	Deeds, Jonathan R. ....	MP 354
Dang, Xibei .....	TOE pm 4:10	Davis, Darryl .....	MOE pm 4:10	Deelder, Andre .....	ThP 026
Dangott, Lawrence .....	ThP 682	Davis, Eric .....	MP 735	Deelder, André .....	MP 004
Dangott, Lawrence .....	ThP 681	Davis, Jasmine C. C. ....	ThOH am 08:50	Deelder, André .....	TP 052
Danielewicz, Megan .....	TP 381	Davis, Jennifer .....	MP 038	Deelder, André M. ....	TP 161
Daniels, Casey M. ....	TP 111	Davis, Katherine .....	TOA am 09:30	Deepak, Saligrama Adavigowda .....	TP 647
Danielson, Steve .....	MP 125	Davis, R. Duane .....	ThP 267	Deery, Mike .....	WOD am 09:30
Danielson, Steven .....	MP 104	Davoli, Enrico .....	ThP 596	Deese, Alan .....	TP 503
Danielson, Steven .....	WP 510	Davoli, Enrico .....	TP 029	DeFelice, Brian .....	MP 591
Danielson, Steven R. ....	WP 118	Dawaher, Maria .....	TP 550	DeFelice, Brian .....	WP 286
Danis, Paul .....	MP 386	Dawber, Marcus .....	ThP 749	Deforce, Dieter .....	ThP 776
Danna, Nonie .....	ThP 582	Dayon, Loïc .....	ThP 255	Deforce, Dieter .....	WP 294
Dansky, Hayes .....	ThOE am 09:10	Dayon, Loïc .....	WP 510	Defoy, Daniel .....	ThP 287
Dantonio, Sue .....	WP 327	De Alwis, Hemakanthi .....	ThP 542	Degenhardt, Dani .....	TP 554
Darebna, Petra .....	ThP 139	de Andrade, Lidiane Maria .....	TP 413	Degenstein, John .....	MP 575
Darie, Costel .....	MP 106	de Azambuja, Francisco .....	MP 367	Degenstein, John .....	MP 574
Darie, Costel .....	MP 162	de Faria, Bernadete .....	MP 115	Degenstein, John .....	MP 577
Darie, Costel .....	TP 429	De Filippos, Amanda .....	WP 778	Degenstein, John .....	WOA am 08:50
Darie, Costel .....	WP 457	de Graaf, Erik L. ....	MP 263	Degnan, Andrew .....	MP 643
Darie, Costel C. ....	MP 423	de Graaf, Erik L. ....	ThP 212	Degout-Charrette, Elodie .....	TP 219
D'Arienzo, Celia .....	TP 693	de Graaf, Marieke A. ....	TP 049	DeGraan-Weber, Nick .....	ThP 189
D'Arienzo, Celia .....	WP 725	De Grave, Kurt .....	ThP 022	DeGraw, Tyler .....	MP 510
Dari, Ekaterina .....	MP 617	de Jong, Ad P.J.M. ....	WOE am 10:10	DeGruttola, Heather .....	WP 208
Dariolli, Rafael .....	TP 435	de Jong, Felice .....	TP 653	Deguchi, Jiro .....	MOF pm 3:10
Daris, Kristi .....	TP 239	de Jong, Rob N. ....	TP 237	Degueldre, Michel .....	WOE am 09:50
Darland, Ed .....	MOC pm 3:10	De Keulenaer, Sarah .....	TP 078	DeHaan, John .....	ThOA am 09:10
Darland, Ed .....	MP 585	de La Cal, Miguel A. ....	MP 584	DeHaven, Corey .....	MP 053
Darland, Ed .....	ThP 483	de la Torre, Xavier .....	ThP 595	DeHaven, Corey .....	TP 662
Darland, Ed .....	ThP 491	De La Torre, Xavier .....	ThP 594	Deiningger, Soeren .....	TP 051
Darland, Edward .....	ThP 472	de Lima, Maria do Carmo A. ....	TP 614	Deiningger, Sören-Oliver .....	TP 056
Dartois, Veronique .....	TP 023	De Marchi, Umberto .....	WP 510	Deiningger, Sören-Oliver .....	TP 057
Dartois, Veronique .....	TP 026	De Meester, Ellen .....	TP 078	deJong, Ebbing .....	MP 164
Dartois, Veronique .....	WP 553	De Moor, Bart .....	MP 029	Dekker, Lennard .....	ThP 064
Darula, Zsuzsa .....	ThP 231	De Moor, Bart .....	MP 022	Dekker, Lennard .....	ThP 062
Darville, Lancia .....	TP 140	de Morais, Erica T. ....	TP 586	Dekker, Lennard .....	ThP 209
Darzi, Ara .....	TOG pm 3:30	de Munter, Stephanie .....	TP 015	Dekker, Lennard .....	WP 151
Dasari, Surendra .....	ThP 272	de Oliveira, Luciana Gonzaga .....	ThP 453	Dekker, Nicholas .....	MP 265
Dasari, Surendra .....	ThP 345	de Oliveira Cardoso, Josiane .....	TP 621	Dekker, Tim .....	MP 004
Daskalopoulou, Stella .....	TOH pm 3:50	De Pauw, Edwin .....	MOC pm 2:30	Dekkers, Dick .....	ThP 239
Datar, Ajit .....	TP 496	De Pauw, Edwin .....	MP 441	DeKroon, Robert M. ....	WP 250
Datar, Ajit .....	TP 497	De Pauw, Edwin .....	ThP 256	Dela Rosa, Mira Anne .....	ThP 713
Datar, Ajit .....	TP 498	De Pauw, Edwin .....	ThP 503	Dela Rosa, Mira Anne C. ....	WP 492
Datar, Ajit .....	TP 763	De Pauw, Edwin .....	TP 176	Delaby, Constance .....	WP 447
Datar, Ajit .....	TP 762	De Pauw, Edwin .....	TP 418	Delanghe, Bernard .....	ThP 222

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Delaria, Kathy.....	WP 278	Destefano, Joseph.....	TP 110	Ding, Li.....	ThP 574
DeLeon, Venetra.....	WP 524	Deterding, Leesa.....	MP 072	Ding, Li.....	TOG am 08:30
DeLeon-Pennell, Kristine.....	ThP 156	Deterding, Leesa.....	ThP 404	Ding, Li.....	TP 082
Delgass, W. Nicholas.....	MP 574	Deterding, Leesa.....	ThP 769	Ding, Li.....	TP 433
Delinsky, David.....	WP 480	Dettmer-Wilde, Katja.....	TP 750	Ding, Li.....	TP 438
Dell, Anne.....	ThP 161	Deupree, Susan.....	WP 040	Ding, Ming.....	TP 115
Delporte, Cedric.....	ThOH am 09:30	Deutsch, Eric W.....	ThP 031	Ding, Xiao.....	MP 499
Delporte, Cedric.....	WP 189	Devine, Lauren.....	WP 511	Ding, Xiao.....	ThP 428
Delsuc, Marc-André.....	TP 719	Devine, Megan.....	TP 188	Ding, Xiao.....	ThP 702
Delsuc, Marc-André.....	WP 729	Devine, Paul W A.....	WP 201	Ding, Xuan (Jo-Ann).....	TP 208
Delvaux, Cédric.....	ThP 503	Dewald, Carolin.....	ThP 071	Ding, Yan.....	TP 759
Delvenne, Philippe.....	MP 441	Dewald, Hans.....	TP 149	Ding, Ying.....	ThP 042
Demers, Roger.....	WP 480	Dewald, Hans.....	WP 065	Dinglasan, Rhoel.....	TP 146
Demers, Sarah.....	ThP 411	Dewhurst, Mark W.....	ThP 084	Dinglasan, Rhoel R.....	WP 446
Demina, Olga.....	TOA pm 4:10	Dexter, Alexander.....	MP 253	Dinh, Phuoc.....	WP 597
Demmers, Jeroen.....	ThP 239	Dey, Anwasha.....	WOD am 10:10	Dion, Annick.....	MP 284
Demoranville, Leonard.....	ThP 601	Dey, Gourav.....	MP 255	Dionisio, Giuseppe.....	MP 409
DeMuth, J. Corinne.....	MP 081	Dey, Gourav.....	MP 270	Dioumaeva, Irina.....	MP 784
Demyanyuk, Vitalii.....	ThP 062	Dey, Subhakar.....	MP 517	DiPasquale, Robert.....	MP 005
Deng, Cecilia.....	ThP 045	Dey, Subhakar N.....	ThOC am 08:50	Discenza, Lorell.....	TP 693
Deng, Fei.....	WP 046	Dhabaria, Avantika.....	MP 137	Distler, Ute.....	TP 084
Deng, Helen.....	WP 540	Dhaenens, Maarten.....	ThP 776	DiTillio, Giacomo.....	MP 275
Deng, Helen Deng.....	WP 122	Dhaenens, Maarten.....	WP 294	DiTondo, Beth.....	TP 035
Deng, JiaHui.....	ThP 739	Dhandapani, Ramkumar.....	WP 720	Dittmann, Monika.....	TP 192
Deng, Lingli.....	MP 443	Dharmarajan, Venkat.....	ThP 136	Dittmar, Gunnar.....	WP 174
Deng, Lingli.....	ThP 659	Dharmasiri, Udara.....	ThOC am 09:30	Dittwald, Piotr.....	WP 035
Deng, Liulin.....	MP 658	Dharsee, Moyez.....	ThP 433	Dixit, Sugyan.....	ThP 468
Deng, Liulin.....	MP 657	Dhople, Vishnu.....	ThP 250	Dixon, David A.....	MP 319
Deng, Lu.....	ThP 269	Dhummakupt, Elizabeth.....	WP 647	Dixon, Jack E.....	WP 226
Deng, Shuang.....	WP 088	Di Bussolo, Joseph.....	MP 753	Dixon, Peter.....	MP 583
Deng, Zhiyou.....	WOG am 09:50	Di Donna, Leonardo.....	TP 511	Dixon, R. Brent.....	ThP 665
Denicola, Chris.....	MP 290	Di Poto, Cristina.....	MP 580	Dixon, Roger.....	MP 594
Denisov, Eduard.....	MP 653	Di Poto, Cristina.....	TP 756	Dizdaroglu, Miral.....	WP 707
Denisov, Eduard.....	ThP 762	Diamandis, Eleftherios P.....	TP 244	Djukanović, Ratko.....	WP 468
Denisov, Eduard.....	TOB am 10:10	Diamond, Michael.....	TP 488	Djukovic, Danijel.....	MP 443
Denisov, Eduard.....	TOD am 08:30	Diamond, Scott L.....	TP 103	Djukovic, Danijel.....	ThP 655
Denisov, Eduard.....	TP 136	Diana Di Mavungu, José.....	ThOA pm 2:30	Djukovic, Danijel.....	ThP 659
Denisov, Eduard.....	WOA pm 3:30	Dias Lima Jedlicka, Leticia.....	MP 115	do Amaral, Fernanda.....	WOE pm 4:10
Denisov, Eduard.....	WOF am 09:30	Diaz, Krystalle S.....	ThP 555	do Nascimento, Claudio Augusto Oller.....	TP 413
Denniff, Philip.....	WP 640	Diaz, Mireia.....	ThP 746	Dobi, Albert.....	WP 513
Dennis, Elise A.....	ThOB pm 4:10	DiBussolo, Joseph.....	MP 671	Dobos, Karen.....	ThP 234
Dennis, Jon.....	WP 069	Dick, Bernhard.....	WP 671	Dobson, Gareth.....	ThOA am 09:10
Dennis, Jonathan H.....	ThOF pm 3:10	Dick, Lawrence.....	MP 144	Dodd, Stephanie.....	ThP 535
Dennis, Jonathan H.....	TOE pm 4:10	Dickhut, Clarissa.....	ThP 225	Dodder, Nathan.....	TP 549
Dennison, Andrew.....	WP 751	Dickinson, Danielle N.....	MP 375	Dodds, Eric.....	TP 452
Denslow, Nancy.....	ThP 449	Dickinson, Danielle N.....	WP 394	Dodds, Eric D.....	MP 142
Denu, John.....	MP 121	Dickman, Mark.....	ThP 172	Dodds, Eric D.....	WP 078
Deperaita, Galahad.....	TP 159	Dickman, Mark.....	ThP 525	Dodds, Eric D.....	WP 370
Dephoure, Noah E.....	ThP 319	Diedrich, Jolene.....	MP 065	Dodds, Eric D.....	WP 593
Derbyshire, Emily R.....	ThP 359	Diedrich, Jolene K.....	WP 730	Dodds, Eric D.....	WP 676
Deredge, Daniel.....	ThP 121	Diefenbach, Otto.....	ThP 119	Dodds, Eric D.....	WP 677
Dermenjian, Renee.....	MP 484	Diehl, Diane.....	ThP 529	Dodds, Eric D.....	WP 678
Dernovics, Mihaly.....	WP 362	Dieters-Castator, Dylan.....	MP 458	Dodge, Jeffrey.....	TP 543
Derogis, Priscilla BMC.....	ThP 407	Dietz, Lisa.....	MP 452	Doellinger, Joerg.....	ThP 055
Derpmann, Valerie.....	MP 524	Díez-García, Javier.....	TP 064	Doerge, Daniel R.....	TP 499
Derpmann, Valerie.....	TP 732	Digiuseppe-Champion, Patricia.....	TP 228	Doerge, Daniel R.....	TP 624
Derrick, Jeffrey S.....	TOF pm 3:50	Dijke, Peter ten.....	WP 257	Doherty, John.....	WP 528
Derst, Christian.....	TP 167	Dijkstra, Jouke.....	MP 027	Doherty, John.....	WP 645
Desai, Abhishek.....	ThP 384	Dijkstra, Jouke.....	TP 015	Doherty, Margaret.....	ThOH am 09:30
Desai, Manik.....	MP 487	Diken, Eric.....	ThOA am 09:10	Dohnalkova, Alice.....	WOE pm 4:10
Desai, Varsha G.....	WP 470	Dikler, Sergei.....	MP 008	Dojahn, Joerg.....	MP 198
Desai-Krieger, Daksha.....	ThP 496	Dikler, Sergei.....	TP 055	Dojahn, Jörg.....	WP 496
Desai-Krieger, Daksha.....	WP 100	Dill, Brian.....	ThP 338	Döll, Stefanie.....	MP 416
Desai-Krieger, Daksha.....	WP 526	Dillin, Andrew.....	MP 218	Dollinger, Gavin.....	ThP 102
Desaire, Heather.....	ThOH am 08:30	Dinallo, Roger.....	WP 507	Domalain, Virginie.....	ThP 499
Desaire, Heather.....	WP 260	Diner, Benjamin.....	ThP 340	Domanski, Dominik.....	MP 037
Desbrow, Claire.....	MP 341	Diner, Benjamin.....	WOF pm 3:50	Domanski, Dominik.....	ThP 026
Desbrow, Claire.....	MP 758	Diner, Ian.....	WP 178	Domingues, Roménia.....	WP 460
Desbrow, Claire.....	MP 783	Dines, Trevor.....	WP 695	Dominguez, Celia.....	WP 480
Desbrow, Claire.....	MP 757	Ding, Caroline.....	MP 472	Domon, Bruno.....	ThP 254
Desbrow, Claire.....	MP 756	Ding, Caroline.....	MP 641	Domon, Bruno.....	ThP 322
Desbrow, Claire.....	ThP 589	Ding, Caroline.....	WP 650	Domon, Bruno.....	ThP 442
Deshiere, Alexandre.....	MP 262	Ding, Chuanfan.....	WOD pm 2:30	Domon, Bruno.....	ThP 534
Deshpande, Sachin.....	ThP 639	Ding, Chuan-fan.....	TP 718	Domon, Bruno.....	TP 485
Deshpande, Samir.....	ThP 077	Ding, Haiyan.....	TP 674	Domont, Gilberto.....	TP 686
Deshpande, Samir.....	ThP 333	Ding, Hua.....	ThP 018	Donald, W. Alex.....	TP 355
DeSilva, Binodh.....	TOE am 09:30	Ding, Jie.....	MP 645	Donaldson, Paul J.....	TP 039
Destá, Zeruesenay.....	TP 621	Ding, Li.....	MOG am 08:30	Donaldson, Robert P.....	TP 135

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Doneanu, Angela.....	MP 750	Drake, Richard R.....	TP 068	Dumenil, Guillaume.....	WP 059
Doneanu, Angela.....	ThP 661	Drake, Robert.....	MP 474	Dumond, Jenna.....	ThP 052
Doneanu, Catalin.....	MP 745	Drebot, Mike.....	TP 213	Dumond, Jenna F.....	WP 255
Doneanu, Catalin.....	TP 235	Dreher, Wolfgang.....	MP 021	Dumont, Quentin.....	TP 293
Doneanu, Catalin.....	TP 693	Dremina, Elena.....	WP 503	Dunbar, Brett D.....	TP 522
Donegan, Michael P.....	TP 522	Drews, Oliver.....	WP 517	Dunbar, Robert C.....	MP 322
Dong, Chen.....	MP 330	Drews, Oliver.....	WP 518	Duncan, Bradley.....	WP 701
Dong, Huifang.....	TP 431	Drexler, Dieter.....	ThP 666	Duncan, Katherine.....	MP 020
Dong, Jia.....	ThP 114	Drexler, Dieter M.....	MP 376	Duncan, Kyle D.....	MP 556
Dong, Meng-Qiu.....	ThP 051	Drexler, Dieter M.....	ThP 421	Duncan, Kyle D.....	WP 746
Dong, Michael.....	TP 512	Dreyer, Mark.....	MP 742	Dungan, Leo.....	WOH am 10:10
Dong, Mingming.....	WP 068	Dreyer, Mark.....	ThP 568	Dunham, Wade H.....	MP 258
Dong, Qian.....	WP 051	Driver, Joshua.....	MP 703	Dunk, Paul W.....	WP 705
Dong, Xiaofeng.....	MP 357	Drogui, Patrick.....	TP 556	Dunn, John.....	ThP 675
Dong, Xueming.....	ThP 126	Droit, Arnaud.....	ThP 287	Dunwell, Jim.....	MP 407
Dong, Yiyang.....	WP 407	Drouin, Elise E.....	WOF pm 2:30	Dunyach, Jean-Jacques.....	ThP 686
Donnarumma, Fabrizio.....	MP 724	Drouin, Nicolas.....	ThP 446	Dunyach, Jean-Jacques.....	TP 740
Donnarumma, Fabrizio.....	WP 032	Drury, Tony.....	MP 289	Dunyach, Jean-Jacques.....	WP 763
Donnell, Deborah.....	WOF pm 4:10	Drury, Tony.....	WP 353	Dunyach, Jean-Jacques.....	WP 761
Donoghue, Helen.....	ThP 394	D'Silva, Kyle.....	MOD pm 4:10	Dunyach, Jean-Jacques.....	WP 762
Donohoe, Greg.....	TP 540	D'souza, Rochelle CJ.....	WP 257	Duong, Duc.....	MP 216
Donohoe, Gregory.....	MP 590	Du, Alicia Y.....	TP 469	Duong, Duc.....	WP 178
Donohoe, Gregory.....	WP 672	Du, Dan.....	ThOD pm 4:10	Duong, Duc.....	WP 237
Doonan, Robert James.....	TOH pm 3:50	Du, Lin.....	TP 220	Dupre, Mathieu.....	MP 528
Doran, Michael.....	TP 673	Du, Lin.....	WP 330	Dupre, Mathieu.....	MP 527
Dorfer, Viktoria.....	TP 075	Du, Peicheng.....	MP 421	Dupree, Emmalyn.....	WP 457
Dörig, Pablo.....	TP 742	Du, We.....	ThP 533	Dupree, Ray.....	MOB am 09:10
Dorman, Dr. Frank.....	WP 570	Du, Y. Melodie.....	WP 021	Durand, Kirt L.....	ThOD am 08:50
Dorman, Frank.....	ThOA am 10:10	Dua, Ajit.....	TP 274	Durant, Joe.....	MOE pm 2:30
Dorman, Frank.....	TP 392	Duan, Jiana.....	ThOH pm 3:50	Durazo, Armando.....	WP 340
Dorman, Frank.....	WOC pm 2:30	Duan, Lian.....	ThP 739	Durban, Jordi.....	WOE am 09:50
Dorman, Frank.....	WP 557	Duan, Xiaokun.....	MP 378	Durbin, Kenneth.....	TOE pm 3:30
Doroshenko, Vladimir M.....	ThP 745	Duan, Xiaokun.....	WP 416	Durette, Chantal.....	TP 108
Dorrell, Lucy.....	ThP 342	Duan, Xiaokun.....	WP 404	Durighello, Emie.....	TP 225
Dorrestein, Kathleen.....	MOH pm 4:10	Duan, Xiaokun.....	WP 407	Dürnberger, Gerhard.....	TP 098
Dorrestein, Kathleen.....	MP 020	Duan, Xiaokun.....	WP 414	Dürnberger, Gerhard.....	TP 096
Dorrestein, Pieter.....	MOH pm 4:10	Dubay, George.....	MP 738	Duschl, Albert.....	WP 153
Dorrestein, Pieter.....	MP 020	Dubay, George.....	TP 768	Dusenbury, Katharine H.....	WP 170
Dorrestein, Pieter.....	MP 056	Dubay, George.....	TP 769	Dutta, Bamaprasad.....	ThOF pm 3:50
Dorrestein, Pieter.....	ThOA pm 2:50	Dube, Danielle.....	ThP 150	Dutta, Bhaskar.....	MP 261
Dorrestein, Pieter.....	TP 019	Dubey, Jitender P.....	TP 223	Dutton, Rachel.....	ThOA pm 2:50
Dorschel, Craig.....	WP 637	Dubey, Naveen.....	WP 531	Duursma, Marc C.....	WOB am 08:50
Dortch, Kristin.....	WOC pm 3:50	Dubey, Ritvik.....	WP 466	Dvorkin, Mikhail.....	ThP 064
Dorywalska, Magdalena Dorywalska.....	WP 278	Dubikovskaya, Elena.....	WP 172	Dvorkin, Mikhail.....	ThP 062
Dossmann, Héloïse.....	TP 369	Dubois, Laura.....	ThP 267	Dwivedi, Prabha.....	TP 729
Dossmann, Héloïse.....	TP 524	Dubois, Laura G.....	TOA pm 2:50	Dwivedi, Prabha.....	TP 730
Doster, Douglas.....	TP 746	Ducancel, Frederic.....	WOE am 09:50	Dwivedi, Prabha.....	TP 728
Douce, David.....	WP 665	Duchoslav, Eva.....	MP 057	Dwivedi, Prabha.....	WP 378
Douce, David.....	WP 667	Duchoslav, Eva.....	MP 629	Dwivedi, Sutopa.....	MP 270
Douce, David.....	WP 668	Duchoslav, Eva.....	TP 627	Dworski, Shaalee.....	TP 065
Douce, David S.....	TP 618	Duchoslav, Eva.....	WP 618	Dyachenko, Andrey.....	WOF am 09:30
Douce, David S.....	TP 751	Ducret, Axel.....	TP 171	Dyakov, Yuri.....	MP 306
Doucette, Alan.....	ThP 261	Ducruix, Celine.....	TP 577	Dyakov, Yuri A.....	MP 305
Doucette, Alan A.....	ThP 782	Ducruix, Céline.....	TP 224	Dybkov, Olexandr.....	ThP 456
Douglass, Jacqueline.....	TOG am 09:10	Duczak, Jr, Nicholas.....	MP 678	Dymm, Braydon L.....	MP 712
Douglass, Kevin.....	MP 316	Duda, Robert.....	TOC pm 3:30	Dyson, Barry.....	TP 157
Dovich, Norman.....	MP 080	Dudek, Nadine.....	ThP 342	Dyson, Paul J.....	ThP 687
Dovich, Norman.....	ThP 198	Dueker, Stephen.....	WP 636	Dzerk, A.....	MP 507
Dovich, Norman.....	ThP 731	Dueñas, Maria.....	TP 037	E Horb, Marko.....	TP 180
Dovich, Norman.....	TP 194	Duewel, Henry.....	ThP 260	Earley, Lee.....	MP 084
Dovich, Norman J.....	TOB pm 3:50	Duff, Robert.....	TP 241	Earley, Lee.....	MP 146
Dow, Alex.....	MP 575	Duffy, Kaitlyn.....	WP 775	Earley, Lee.....	ThP 686
Dowell, James.....	MP 121	Dufield, Dawn.....	TP 251	Early, Bryan.....	ThP 059
Dowlatshahipour, Masoumeh.....	TP 018	Dufield, Dawn.....	TP 479	Early, Bryan.....	ThP 058
Dowsey, Andrew.....	ThP 034	Dufield, Dawn.....	WP 271	Early, Bryan.....	WOH pm 3:30
Doyle, Michael.....	TP 541	Dufour, Anthony.....	MP 576	Early, Bryan.....	WP 157
Doyle, Michael L.....	MOE pm 3:10	Dufresne, Craig.....	MP 219	Early, Bryan P.....	ThP 060
Drabner, Georg.....	MP 077	Dufresne, Guy L.....	ThP 616	Early, Michael.....	MP 164
Drabner, Georg.....	WP 049	Dufresne, Martin.....	MP 012	Easter, John.....	WP 487
Draghici, Sorin.....	TP 139	Dufresne, Martin.....	TOH pm 3:50	Easter, John.....	WP 636
Draghici, Sorin.....	TP 143	Duggan, Brendan.....	MP 056	Easterling, Mike.....	TP 610
Draghici, Sorin.....	TP 488	Duggan, Jeffrey.....	MP 515	Easton, Mckay.....	MP 574
Draghici, Sorin.....	WP 241	Dugourd, Philippe.....	MOD am 09:10	Easton, Mckay.....	WOA am 08:50
Draher, Jonathan.....	TP 277	Dugourd, Philippe.....	MP 731	Eather, Samuel.....	ThP 376
Draher, Jonathan.....	TP 276	Dugourd, Philippe.....	WP 177	Eatough, David.....	WP 666
Drake, Charles G.....	MP 255	Dührkop, Kai.....	ThOG am 08:30	Eberink, Eduard.....	ThP 112
Drake, Richard.....	ThP 166	Dulaurent, Sylvain.....	ThP 600	Ebel, Wolfgang.....	TP 238
Drake, Richard.....	TP 065	Dulaurent, Sylvain.....	ThP 599	Ebeler, Susan.....	MP 347
Drake, Richard R.....	TP 069	Dumas, Sébastien J.....	MP 025	Ebeler, Susan.....	ThOA pm 3:50

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Ebeler, Susan E.....	ThP 614	EK, Bo.....	TP 455	Engen, John R.....	MOE pm 3:10
Eberlin, Livia.....	MP 019	EK, Patrik.....	MP 451	Engen, John R.....	MOF am 09:30
Eberlin, Marcos.....	MP 332	Ek Dahl, Anja.....	MP 205	Engen, John R.....	ThP 130
Eberlin, Marcos.....	MP 390	Ekelöf, Måns.....	MP 078	Engen, John R.....	ThP 132
Eberlin, Marcos.....	ThOA am 09:30	Ekpo, Francesca.....	WP 524	Engen, John R.....	TOF am 09:10
Eberlin, Marcos.....	ThP 513	Ekroos, Kim H.....	TP 443	Engen, John R.....	WP 223
Eberlin, Marcos.....	TP 231	El Aalamat, Yousef.....	MP 029	Engen, John R.....	WP 221
Eberlin, Marcos.....	TP 584	El Aalamat, Yousef.....	MP 022	Englander, S. Walter.....	ThP 128
Eberlin, Marcos.....	WP 685	El Khatib, Soraya.....	MP 362	Englander, Walter.....	MOF am 08:30
Eberlin, Marcos.....	WP 709	El-Baba, Tarick.....	MP 538	English, A. Michelle.....	MP 084
Eberlin, Marcos N.....	WP 406	El-Baba, Tarick.....	ThP 732	English, A. Michelle.....	MP 146
Eberlin, Marcos N.....	MP 362	El-Baba, Tarick.....	TP 288	English, A. Michelle.....	ThP 686
Eberlin, Marcos N.....	TP 586	El-Baba, Tarick.....	TP 790	English, Michelle.....	MOE am 08:30
Eberlin, Marcos N.....	WOA pm 3:30	El-Baba, Tarick.....	WOB am 09:50	English, Robert D.....	MP 290
Eberlin, Marcos N.....	WP 711	El-Baba, Tarick.....	WP 702	Engtrakul, Juntyma.....	WP 620
Ebert, Benjamin.....	WOG am 08:50	Elbert, Thomas.....	WP 471	Eninger, Timo.....	ThP 081
Ebhardt, H. Alexander.....	TOD pm 4:10	Elci, S. Gokhan.....	WP 701	Enke, Chris.....	WOB am 08:30
Ecelberger, Scott.....	MP 697	Elci, Sukru Gokhan.....	WP 703	Enke, Christie G.....	Special
Ecelberger, Scott.....	ThP 365	El-Elimat, Tamam.....	WP 321	Enke, Christie G.....	ThOB pm 4:10
Echterbille, Julien.....	WOE am 09:50	El-Hawiet, Amr.....	ThP 097	Enke, Christie G.....	WOC am 10:10
Eckey, Maren.....	MP 193	Eliane, Jean-Pierre.....	MP 126	Enyedi, Attila.....	WP 424
Eckler, Larry.....	MP 193	Elias, Joshua E.....	TP 170	Eo, Su-Jin.....	WP 580
Economou, A.....	WP 229	Elias, Joshua E.....	ThP 334	Eom, Han Young.....	TP 509
Economou, Anastassios.....	WP 219	Eliuk, Shannon.....	MP 717	Eppe, Gauthier.....	ThP 503
Economou, Christos.....	ThP 394	Elizabeth, Roshan.....	TP 113	Eppe, Gauthier.....	TP 418
Eddie, Brian.....	MP 279	El-Khatib, Ahmed H.....	MP 178	Epstein, Marsha.....	TP 501
Edelman, Aleksander.....	WP 145	Ellerby, Lisa M.....	WP 118	Epure, Emily.....	TP 494
Edelmann, Mariola.....	TP 208	Elliott, Marie.....	MP 618	Erdman, Emily P.....	ThP 605
Edgar, John S.....	TP 403	Elliott, Noelle.....	ThOA am 10:10	Erdmann, Raf.....	TP 141
Edgar, Scott.....	ThP 325	Elliott, Noelle.....	ThP 584	Erdmann-Gilmore, Petra.....	ThP 170
Edgeworth, Matthew.....	ThP 120	Ellis, Matthew.....	TOG am 08:30	Erdmann-Gilmore, Petra.....	TP 173
Edgeworth, Matthew.....	ThP 712	Ellis, Matthew.....	TP 082	Erdmann-Gilmore, Petra.....	WOG pm 3:50
Edgington, Alan.....	MP 341	Ellis, Matthew.....	TP 169	Erguido, Izaskun.....	MP 006
Edgington, Alan.....	MP 760	Ellis, Matthew J.....	MOG am 08:30	Erickson, Alison.....	MP 264
Edgington, Alan.....	MP 757	Ellis, Matthew J.....	ThP 039	Erickson, Brian K.....	ThP 214
Edgington, Alan.....	MP 758	Ellis, Matthew J.....	ThP 170	Ericson Jogsten, Ingrid.....	ThP 544
Edgington, Alan.....	MP 759	Ellis, Matthew J.....	ThP 205	Ericson Jogsten, Ingrid.....	ThP 551
Edgington, Alan.....	MP 761	Ellis, Matthew J.....	TP 173	Erlemann, Karl-Rudolf.....	WP 179
Edgington, Alan.....	MP 783	Ellis, Matthew J.....	TP 438	Ernest, McGahee.....	WOC pm 3:50
Edgington, Alan.....	ThP 589	Ellis, Matthew J.....	TP 433	Ernst, Robert.....	ThP 337
Edison, Arthur S.....	TP 044	Ellis, Matthew J.....	WOG pm 3:50	Ernst, Robert.....	TP 291
Edvardsson, Vidar O.....	WP 448	Ellis, Megan.....	WP 210	Ernst, Robert K.....	TP 286
Edwards, Alistair.....	MP 719	Ellis, Shane.....	TOH pm 3:10	Ernst, Robert K.....	WP 288
Edwards, Alistair.....	MP 718	Ellis, Shane.....	WOC am 09:50	Esaki, Tsuyoshi.....	MOF pm 3:10
Edwards, Alistair V.G.....	TP 124	Ellis, Shane R.....	MP 397	Esaki, Tsuyoshi.....	MP 417
Edwards, Laura.....	WOC pm 3:50	Ellis, Shane R.....	ThOB pm 2:30	Esaki, Tsuyoshi.....	ThP 621
Edwards, Laura E.....	WP 098	Ellis, Shane R.....	WOB am 08:50	Esaki, Tsuyoshi.....	WP 594
Edwards, Nathan.....	MP 061	Ellis, Wade.....	WOB am 10:10	Escano, Jerome.....	ThP 681
Edwards, Nathan.....	MP 125	Ellis, Wade C.....	MP 391	Eschrich, Steven.....	TP 463
Edwards, Nathan.....	WOH pm 4:10	Ellmeier, Wilfried.....	MP 228	Eschweiler, Joseph.....	ThP 489
Edwards, Nathan.....	WP 075	ElMasri, Marwan.....	ThP 178	Escobar, Hernando.....	WP 439
Edwards, Nathan J.....	MP 137	ElNaggar, Mariam S.....	TP 023	Escudier, Bernard.....	WP 145
Edwards, Nathan J.....	ThP 235	Elnaggar, Mariam S.....	TP 026	Escudier, Estelle.....	WP 145
Efstathiou, Eleni.....	ThP 423	Elsasser, Suzanne.....	TOF am 09:10	Esfandiary, Reza.....	WP 215
Egea, Pascal.....	ThP 092	Elseberg, Tim.....	MP 667	Esko, Jeffrey.....	WP 226
Egekwa, Chioma.....	TP 668	Emdal, Kristina B.....	MP 109	Espada, Alfonso.....	MP 733
Egertson, Jarrett.....	MOG am 09:50	Emdal, Kristina B.....	TP 126	Espada, Alfonso.....	TP 543
Egertson, Jarrett.....	ThP 326	Emert-Sedlak, Lori A.....	ThP 132	Espinosa, Juan.....	TP 543
Egertson, Jarrett.....	ThP 763	Emery, Maurice.....	WP 495	Esplin, Sean.....	MP 239
Egertson, Jarrett.....	WP 737	Emery, Samantha.....	TP 211	Esposito, Christopher L.....	WP 435
Eggleston-Rangel, Roxana.....	ThP 147	Emmer, Asa.....	MP 078	Espourteille, Francois.....	MP 671
Ehler, Sven.....	MOD pm 2:50	Emmer, Asa.....	TP 411	Espourteille, Francois A.....	WP 435
Ehling, Stefan.....	TP 277	Emmerich, Tanja.....	MP 246	Esquenazi, Eduardo.....	MP 056
Ehret-Sabatier, Laurence.....	MP 450	Emmerich, Tanja.....	MP 266	Esteban-Fernández, Diego.....	MP 178
Ehrmann, Brandie M.....	MP 312	Emory, Joshua.....	WP 107	Etienne, Chris.....	ThOF am 09:50
Ehrmann, Frederick.....	ThP 095	Enche, Julien.....	WOC pm 2:50	Etienne, Chris.....	WP 121
El Khoury, Maroun.....	TP 530	Enders, Jeffrey.....	MP 771	Eto, Yuzuru.....	WP 102
Eichholz, Todd.....	TP 575	Enders, Jeffrey.....	WP 536	Ettefagh, Keivan.....	WP 476
Eichner, Daniel.....	ThP 437	Eng, Bruce.....	ThP 598	Ettrich, Rudiger.....	MP 183
Eijkel, Gert.....	MOH pm 3:50	Eng, Jimmy.....	ThP 031	Ettrichova, Olga.....	MP 183
Eijkel, Gert.....	TP 015	Eng, Jimmy K.....	ThP 464	Euzen, Ronan.....	TOG pm 2:50
Eijkel, Gert.....	WOC am 09:50	Eng, Jimmy K.....	ThP 466	Evain-Brion, Danièle.....	MP 235
Eikel, Daniel.....	MOB pm 4:10	Engel, Marc E.....	MP 336	Evans, Adam.....	MP 208
Eiriksson, Finnur F.....	WP 448	Engel, Nicole.....	ThP 746	Evans, Adam.....	ThP 305
Eiriksson, Finnur F.....	ThP 401	Engel, Victoria A.....	ThP 302	Evans, Adam R.....	ThP 320
Eisenacher, Martin.....	MP 431	Engelen, Jeannine.....	TP 287	Evans, Anne.....	MP 053
Eisenacher, Martin.....	TP 481	Engen, John.....	ThP 131	Evans, Anne.....	TP 662
Eiserberg, Gene.....	MP 641	Engen, John.....	TP 539	Evans, Charles.....	MP 636
Ejsing, Christer.....	WOH am 08:30	Engen, John.....	WP 220	Evans, Christopher.....	MP 714

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

## INDEX OF AUTHORS



Evans, Christopher A.....	TP 464	Fandino, Anabel.....	ThP 744	Fell, Lorne.....	MP 608
Evans, James.....	MP 116	Fandino, Anabel.....	TP 179	Fell, Lorne.....	WP 588
Evans, James.....	MP 246	Fandino, Anabel.....	WP 355	Feller, Stephan.....	TP 683
Evans, James.....	MP 266	Fandino, Anabel.....	WP 560	Fellers, Ryan.....	ThP 058
Evans, Kendra R.....	MP 712	Fang, Bin.....	TP 463	Fellers, Ryan.....	ThP 059
Evans, Kenneth.....	ThP 433	Fang, Chunli.....	WP 473	Fellers, Ryan.....	TOE pm 3:30
Evans, Peter.....	TP 217	Fang, Jing.....	TP 240	Fellers, Ryan.....	WP 157
Evans, Vanessa.....	MOG am 09:10	Fang, Jing.....	TP 541	Fellers, Ryan T.....	ThP 060
Evans-Nguyen.....	WP 309	Fang, Liling.....	ThP 632	Fenaille, Francois.....	MP 528
Evans-Nguyen, Theresa.....	WP 345	Fang, Meng.....	MP 514	Fenaille, Francois.....	MP 527
Evans-Nguyen, Theresa.....	WP 769	Fang, Meng.....	WP 106	Fenaille, Francois.....	MP 587
Evard, Hanno.....	MP 722	Fang, Pengfei.....	ThP 129	Fenaille, Francois.....	ThP 140
Everest-Dass, Arun.....	TP 327	Fang, Xiang.....	MP 650	Fenaille, François.....	TP 224
Everett, Allen.....	ThP 300	Fang, Xiping.....	WP 488	Fenaille, François.....	TP 472
Everley, Robert.....	MP 133	Fang, Xiping.....	WP 529	Feng, Bo.....	MP 126
Everley, Robert A.....	ThP 214	Fang, Xiping.....	WP 630	Feng, Changgeng.....	ThP 181
Everley, Robert A.....	TOD pm 3:50	Fang, Yigang.....	TP 381	Feng, Duan.....	WP 166
Everley, Robert A.....	TOG am 09:50	Faou, Pierre.....	ThP 045	Feng, Jing.....	TP 250
Evers, Waltraud.....	WP 517	Far, Johann.....	ThP 503	Feng, Jinhua.....	MP 094
Ewan, Richard.....	WP 200	Farber, Robert M.....	ThP 032	Feng, Ju.....	WP 088
Ewing, Andrew.....	ThP 011	Farenc, Mathilde.....	TP 406	Feng, Shun.....	WP 473
Ewing, Andrew.....	TP 033	Farese, Ann.....	TP 688	Feng, Xidong.....	ThP 502
Ewing, Andrew.....	TP 018	Farese, Ann M.....	TP 067	Feng, Yuehan.....	ThP 329
Ewing, Andrew G.....	TP 059	Farhat, Zein.....	ThP 297	Feng, Ziding.....	WP 060
Eyers, Claire.....	ThP 492	Faria, Bernadete.....	MP 464	Feng, Ziding.....	WP 458
Eyers, Claire.....	WP 056	Faria, Morse.....	WP 127	Fenner, Madeline.....	WP 376
Eyers, Claire E.....	MP 272	Faria, Tiago.....	ThP 101	Fenselau, Catherine.....	MP 125
Eyers, Claire E.....	TP 164	Farias, Santiago.....	WP 278	Fenselau, Catherine.....	MP 136
Eysberg, Martin.....	TP 622	Farnood, Ramin.....	TP 578	Fenselau, Catherine.....	MP 137
Ezan, Eric.....	TP 225	Farnsworth, Charles L.....	ThP 073	Fenselau, Catherine.....	ThP 235
Faber, Johann.....	ThP 135	Farnsworth, Charles L.....	TP 117	Fenselau, Catherine.....	WOH pm 4:10
Faber, Scott.....	ThP 447	Farnsworth, Paul.....	MP 379	Fenton, Anne.....	ThP 153
Fabrik, Ivo.....	ThP 201	Farnsworth, Paul.....	WOB am 10:10	Fenyo, David.....	MOE am 09:30
Fabris, D.....	ThP 471	Farnsworth, Paul B.....	MP 391	Fenyo, David.....	MOG am 08:30
Fabris, D.....	TP 434	Farres, Mireia.....	TP 637	Fenyo, David.....	MP 040
Fabris, D.....	WP 374	Farris, Samantha.....	ThP 610	Fenyo, David.....	MP 149
Fabris, Daniele.....	MOC am 08:30	Farrokhi, Vahid.....	MP 251	Fenyo, David.....	ThP 039
Fabris, Daniele.....	ThP 460	Farrokhi, Vahid.....	WP 502	Fenyo, David.....	ThP 170
Fabris, Daniele.....	ThP 468	Farrugia, Mark.....	ThP 489	Fenyo, David.....	TOB pm 3:10
Facchine, Kevin.....	TP 394	Farutin, Victor.....	WP 173	Fenyo, David.....	TOG am 08:30
Fack, Fred.....	TP 050	Fasciotti, Maira.....	MP 570	Fenyo, David.....	TP 082
Fadel, Elie.....	MP 025	Fasciotti, Maira.....	TP 586	Fenyo, David.....	TP 089
Faerber, Franz.....	MP 041	Faserl, Klaus.....	ThP 226	Fenyo, David.....	TP 433
Faerber, Franz.....	ThP 046	Faserl, Klaus.....	ThP 242	Fenyo, David.....	TP 438
Fagbami, Lola.....	ThP 217	Fattinger, Christof.....	TP 742	Fenyő, David.....	TP 173
Fagbami, Lola.....	TP 177	Faull, Kym.....	MP 250	Fenyő, David.....	WOG pm 3:50
Fagbami, Lola.....	WOD am 08:50	Faull, Kym.....	MP 626	Feraudet-Tarisse, Cécile.....	MP 527
Fagbami, Lola.....	WOG pm 2:30	Faull, Kym Francis.....	ThP 676	Ferguson, James.....	ThP 532
Fagerquist, Clifton K.....	TP 210	Faull, Richard L.M.....	ThP 422	Ferguson, Lee.....	ThP 570
Fahey, Albert J.....	WP 299	Favara, Sarah.....	TP 060	Ferguson, Michael.....	MP 151
Fahrenholz, Timothy.....	ThP 447	Favara, Sarah.....	WP 645	Fermann, Martin.....	WOB pm 3:30
Fahrmann, Johannes.....	MP 430	Favero, Fabricio F.....	WP 711	Fernandes, Mileni Silva.....	ThP 307
Fair-Wandland, Sarah.....	MP 280	Favre, Amélie.....	TOG pm 2:50	Fernandes, Nancy.....	WP 482
Fair-Wandland, Sarah.....	TP 514	Fawzi, Elham.....	WP 341	Fernandes da Silva, Viviane.....	MP 570
Falaux, Emeline.....	TP 034	Fayad, Paul.....	WP 296	Fernandez, Facundo.....	MP 379
Falconer, Travis.....	ThP 692	Fayad, Paul.....	WP 565	Fernandez, Facundo M.....	TP 728
Falconer, Travis M.....	ThP 626	Fazlollahi, Farbod.....	MP 250	Fernandez, Facundo M.....	TP 729
Falconet, Denis.....	TP 408	Fazlollahi, Farbod.....	MP 626	Fernandez, Facundo M.....	TP 730
Falconet, Denis.....	WOB pm 2:50	Fazlollahi, Farbod.....	ThP 422	Fernandez, Facundo M.....	WOB pm 2:30
Falk, Bryce.....	TP 258	Fazlollahi, Farbod.....	ThP 676	Fernandez, Jose A.....	TP 064
Falsarella Carazzolle, Macelo.....	MP 562	Fee, Erin.....	WP 587	Fernandez, Roberto.....	TP 064
Famigliini, Giorgio.....	MP 722	Feeney, Caitlin.....	ThP 205	Fernández, Facundo.....	MP 599
Famigliini, Giorgio.....	TP 764	Feeney, Caitlin.....	WOG pm 2:30	Fernández, Facundo M.....	MP 274
Fan, Zengwei.....	MP 330	Feeney, Maria.....	WP 503	Fernández, Facundo M.....	TP 664
Fan, Chao.....	WP 166	Feenstra, Adam.....	TOH am 09:30	Fernández, Facundo M.....	WP 378
Fan, Chih-Huang.....	MP 112	Feger, Bryan J.....	TOA pm 2:50	Fernández, José A.....	MP 006
Fan, Hui.....	MP 076	Fehse, Boris.....	TP 054	Fernández, Roberto.....	MP 006
Fan, Hui.....	TP 490	Feig, Martin.....	ThP 250	Fernandez De La Mora, Juan.....	ThP 474
Fan, Hui.....	TP 505	Feil, Robert.....	ThP 301	Fernandez De La Mora, Juan.....	ThP 494
Fan, Jun.....	MOG am 09:10	Feil, Susanne.....	ThP 301	Fernandez De La Mora, Juan.....	ThP 508
Fan, Jun.....	ThP 034	Feild, Brian.....	ThP 766	Fernández de la Mora, Juan.....	ThP 475
Fan, Jun.....	TP 757	Feild, Brian.....	WP 161	Fernandez Lima, Francisco.....	ThP 481
Fan, Lirong.....	ThP 538	Feild, Brian J.....	WP 211	Fernandez Lima, Francisco.....	TP 209
Fan, Sheng-Bo.....	ThP 051	Feilden, Andrew.....	TP 791	Fernández-Alba, Amadeo.....	WP 360
Fan, Sheng-Bo.....	WP 053	Feldman, Daniel R.....	TP 007	Fernández-García, Juan.....	ThP 475
Fan, Xing.....	WP 389	Feldman, Daniel R.....	TP 055	Fernandez-Lima, Francisco.....	MP 249
Fan, Xuxin.....	TOC pm 2:50	Feldman, Jonathan.....	TOC pm 3:30	Fernandez-Martinez, Javier.....	MP 165
Fandino, Anabel.....	MP 518	Feldmann, Jorg.....	WP 342	Fernandez-Martinez, Javier.....	TP 132
Fandino, Anabel.....	MP 702	Feldmesser, Marta.....	TP 227	Fernandez-Metzler, Carmen.....	MP 268

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Fernandez-Metzler, Carmen.....	ThP 176	Fitzgerald, Michael C.....	ThP 359	Fournaise, Erik.....	MP 013
Ferrando - Climent, Laura.....	TP 551	Fitzgibbons, Timothy P.....	ThP 402	Fournier, Frederic.....	ThP 287
Ferrarini, Alessia.....	MP 582	Fitzhenry, Matthew.....	TP 327	Fowler, Carol.....	WP 716
Ferraris, Joan.....	ThP 052	Fjeldsted, John.....	ThP 483	Fowler, Carol B.....	WP 236
Ferraris, Joan D.....	WP 255	Fjeldsted, John C.....	ThP 482	Fox, Gerad.....	MP 069
Ferreira, Christina.....	MP 019	Fjeldsted, John C.....	ThP 484	Fox, Jay.....	WP 460
Ferreira, Tanare.....	TP 576	Flanagan, John.....	WOH am 10:10	Frahm, Jennifer L.....	WP 192
Ferrieri, Richard.....	WOE pm 4:10	Flanagan, Michael.....	MP 702	Francavilla, Chiara.....	MP 109
Ferzoco, Alessandra.....	TP 709	Flanagan, Michael.....	ThP 744	Francavilla, Chiara.....	TP 126
Ferzoco, Alessandra.....	WP 759	Flanigan, Paul.....	TP 407	Francavilla, Chiara.....	WP 093
Feschenko, Marina.....	WP 081	Flanigan, Paul.....	WOB pm 3:30	France, Greg.....	MP 349
Fessler, Michael.....	ThP 404	Flarakos, Jimmy.....	MP 038	Franceschi, Christine.....	TP 219
Feyerherm, Fred.....	TP 308	Flarakos, Jimmy.....	TP 040	Francisco, Joseph S.....	MP 323
Fhaner, Cassie.....	ThOG pm 2:30	Flarakos, Jimmy.....	TP 502	Francisco, Joseph S.....	ThP 192
Fhaner, Cassie J.....	ThP 409	Flarakos, Jimmy.....	WP 528	Franco, Catarina.....	ThP 310
Fialkov, Alexander.....	ThP 575	Flarakos, Jimmy.....	WP 645	Franco, Marcos.....	MP 390
Fialkov, Alexander.....	TP 608	Flatley, Brian.....	ThP 433	Franco, Marcos.....	ThOA am 09:30
Fialkov, Alexander.....	WOA am 10:10	Fleischer, Tracey C.....	ThP 285	Franco, Rodrigo.....	TP 452
Fidelis, Carlos.....	WP 406	Fletcher, John.....	ThP 011	Franco, Rodrigo.....	WP 593
Fiebig, Lukas.....	TP 338	Fletcher, John.....	TP 033	Franco Cairo, João Paulo.....	MP 562
Fiedler, Katherine L.....	ThOA pm 4:10	Fletcher, John S.....	TP 010	Francois, Yannis.....	TP 247
Fiehn, Oliver.....	MP 430	Flett, Fiona.....	ThP 104	Francois, Yannis.....	WP 269
Fiehn, Oliver.....	MP 591	Fleury, Normand.....	MP 288	Franco-Ruiz, Mariana.....	WOE pm 3:50
Fiehn, Oliver.....	MP 608	Flick, Jeff S.....	ThP 285	Frank, Hans.....	WP 478
Fiehn, Oliver.....	MP 616	Flitsch, Sabine.....	ThP 492	Frankevich, Vladimir.....	MP 303
Fiehn, Oliver.....	MP 630	Florens, Laurence.....	MP 044	Franzke, Joachim.....	TP 272
Fiehn, Oliver.....	MP 606	Florens, Laurence.....	ThOF pm 3:30	Fraser, Bruce.....	MP 419
Fiehn, Oliver.....	ThOG am 09:10	Flowers, Sarah.....	WP 072	Fraser, Bruce.....	WP 625
Fiehn, Oliver.....	ThP 406	Floyd, Melissa.....	ThP 365	Fraser, Iain.....	MP 261
Fiehn, Oliver.....	WP 286	Floyd, Mellisa.....	ThP 366	Fraser, Iain.....	TOG am 09:30
Fiehn, Oliver.....	WP 589	Flug, Tom.....	TP 746	Fraser-Liggett, Claire.....	MP 264
Field, Jennifer.....	WP 574	Foehr, Sophia.....	TP 202	Frazer, Bill.....	ThP 483
Field, Rob.....	ThP 492	Foglio, Mary Ann.....	WP 711	Frazer, William.....	MP 716
Fields, Scott.....	WP 465	Fokar, Mohamed.....	WP 615	Frazer, William.....	ThP 472
Fierke, Carol.....	TOC pm 3:10	Foley, Casey.....	TP 790	Frazer, William.....	WP 681
Figard, Ben.....	MP 290	Foley, Casey.....	WOB am 09:50	Fredenhagen, Andreas.....	MOD pm 2:30
Figard, Benjamin.....	ThP 430	Folk, William R.....	ThP 302	Frederick, Brian.....	MP 568
Figg, C. Adrian.....	TP 786	Fonslow, Bryan.....	MP 220	Fredrickson, Jim.....	MP 569
Filgueiras, Paulo.....	WP 460	Fontenot, Brian.....	ThP 557	Fredriksson, Elisabeth.....	MP 352
Fillgrove, Kerry.....	MP 639	Forbes, Matthew W.....	MP 202	Freeman, Dilys.....	ThP 376
Fillgrove, Kerry.....	TP 626	Forbes, Thomas.....	ThP 601	Freeman, Rob.....	MP 290
Fillmore, Thomas.....	TOA am 08:50	Forbes, Thomas.....	WP 302	Freeman Jr, Robert M.....	TP 180
Fillmore, Thomas.....	WOE am 08:30	Forbes, Thomas.....	WP 291	Frei, Balz.....	WP 436
Fillmore, Thomas.....	WOG pm 2:50	Forbes, Thomas.....	WP 380	Freiberg, Alexander.....	TP 072
Fillmore, Thomas L.....	TP 169	Ford, Amina.....	ThP 270	Freihoff, Sandy-Dominic.....	TP 581
Fillmore, Thomas L.....	WP 513	Ford, Michael.....	MP 212	Freire d'Eça Nogueira Santos, Karina.....	WOE pm 4:10
Finan, Michael.....	TP 425	Foreman, Daniel P.....	ThOB am 09:10	Freissinet, Caroline.....	ThP 369
Findsen, Eric.....	MOD pm 3:30	Formanovsky, Andrey.....	WP 027	Freitas, Michael A.....	MP 229
Fine, Dennis.....	MP 607	Formolo, Trina.....	MOE am 09:10	Freitas, Michael A.....	MP 442
Fine, Dennis D.....	MP 614	Formolo, Trina.....	MOE pm 4:10	Freitas, Michael A.....	ThP 292
Fine, Dennis D.....	ThP 640	Formolo, Trina.....	TP 252	Frejno, Martin.....	TP 683
Fingerhut, Stefanie.....	TP 031	Formolo, Trina.....	WP 214	Frese, Christian.....	TP 052
Fink, John.....	WP 620	Fornace, Albert.....	WP 776	Frese, Christian K.....	TP 202
Finke, Juliane C.....	WP 715	Fornace, Albert J. Jr.....	TP 659	Frese, Christian K.....	WOE am 10:10
Finley, Daniel.....	TOF am 09:10	Fornelli, Luca.....	MOE am 08:50	Freund, Dana.....	TP 667
Finn, Steve.....	WP 475	Fornelli, Luca.....	WP 172	Freund, Dana M.....	MP 413
Fioramonte, Mariana.....	ThP 452	Forngren, Benita.....	TP 046	Freund, Dana M.....	MP 605
Firestone, Mary.....	ThP 649	Forni, Amanda.....	TP 397	Freund, Dana M.....	TP 641
Firth, Laurence.....	TP 215	Forsythe, Jay G.....	ThP 485	Frewen, Barbara.....	ThP 450
Fischer, Bernd.....	TP 202	Forsythe, Jay G.....	ThP 495	Frewen, Barbara.....	WP 515
Fischer, Lukas.....	MP 663	Forsythe, Jay G.....	TOC am 09:50	Frey, Brian.....	WP 239
Fischer, Roman.....	ThP 342	Fort, Kyle.....	WP 670	Frey, Brian L.....	MOG am 08:50
Fischer, Steven M.....	ThP 061	Fort, Kyle L.....	MOC pm 2:50	Frey, Brian L.....	ThP 221
Fischer, Steven M.....	WP 591	Fort, Kyle L.....	WP 661	Frey, Robert.....	TP 767
Fischler, David.....	ThP 723	Fortes, Claudia.....	ThP 773	Fridén, Mikael.....	WP 326
Fish, Jan.....	WP 171	Fortin, Tanguy.....	TP 219	Fridgen, Travis.....	MOD am 10:10
Fisher, Christine M.....	TP 339	Fortunato de Carvalho Rocha, Werickson.....	MP 570	Fridy, Peter.....	MOE am 09:30
Fisher, Christine M.....	TP 340	Foster, Fred.....	MP 772	Fridy, Peter.....	TP 132
Fisher, Christine M.....	TP 395	Foster, Leonard.....	TP 137	Frieden, Carl.....	WP 217
Fisher, Keith.....	ThP 358	Foster, Leonard.....	WP 069	Friedman, Alicia.....	WOB am 08:30
Fisher, Susan.....	MP 436	Foster, Matthew W.....	TOA pm 2:50	Friedman, Evan.....	WP 652
Fisher, Susan.....	ThP 511	Foster, Matthew W.....	TP 450	Friedrich, Jochen.....	MOB am 08:50
Fitzek, Stefanie.....	TP 153	Foster, Matthew W.....	WOG pm 3:30	Friedrich, Katrin.....	TP 051
FitzGerald, Garret A.....	TP 103	Foster, Steven B.....	ThP 605	Friedrich, Nils.....	WP 342
Fitzgerald, Lisa A.....	MP 278	Fouks, Jordan.....	ThP 628	Friedt, Wolfgang.....	TP 020
Fitzgerald, Maria.....	WP 638	Fountain, Kenneth.....	MP 745	Friend, Jordan.....	WP 740
Fitzgerald, Michael C.....	ThP 084	Fountain, Kenneth.....	WP 123	Fries, David.....	MOB pm 3:50
Fitzgerald, Michael C.....	ThP 085	Fountain, Kenneth.....	WP 125	Fries, Susanne.....	TP 103

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



Friese, Olga.....	WP 273	Gaffrey, Matthew J.....	MP 100	Garcia, Antonia.....	MP 584
Friesen, William.....	ThP 737	Gagen, Karen.....	TP 061	Garcia-Garcia, Aracely.....	TP 452
Friesen, William.....	TP 066	Gahoual, Rabah.....	TP 247	Garcia-Garcia, Aracely.....	WP 593
Friso, Giulia.....	ThP 075	Gairloch, Elena.....	MP 760	Garcia-Reiriz, Alejandro.....	TP 639
Fritsche, Kevin L.....	ThP 302	Gairloch, Elena.....	MP 761	Garcia-Reyes, Juan F.....	TP 272
Fritschen, Uwe.....	WP 715	Gairloch, Elena.....	MP 759	Garcia-Reyes, Juan F.....	WP 362
Fritz, Kristofer.....	MP 117	Gairloch, Elena.....	MP 756	Gardner, Ben.....	MP 069
Fritz, Kristofer.....	ThP 304	Galassie, Allison.....	WP 243	Gardner, Michael.....	ThP 382
Frizzell, Norma.....	MP 506	Galaverna, Renan.....	WP 685	Garg, Neha.....	MP 020
Froehlich, John.....	WP 142	Galaverna, Renan S.....	MP 362	Garg, Neha.....	MP 056
Froehlich, Sophie.....	TP 053	Galayda, Katherine-Jo.....	TP 671	Garimella, Sandilya.....	MP 677
Frost, Dustin.....	ThP 169	Galeva, Nadya.....	WP 503	Garimella, Sandilya.....	ThOB am 10:10
Frye, Stephen.....	TP 201	Galindo Casas, Meritxell.....	WP 278	Garimella, Sandilya.....	TOC am 08:30
Fryer, Doug.....	MP 778	Gallagher, Elyssia S.....	TP 256	Garimella, Sandilya.....	WP 698
Fu, Dax.....	ThP 356	Gallagher, Richard T.....	TP 618	Garimella, Sandilya V. B.....	TP 714
Fu, Qin.....	WP 497	Gallardo, Jose M.....	ThP 613	Garimella, Sandilya V.B.....	TOB am 09:50
Fu, Xiaoyun.....	ThP 770	Gallardo, Jose Manuel.....	MP 355	Garimella, Sandilya V.B.....	TP 716
Fu, Yan.....	TP 523	Gallien, Sebastien.....	ThP 254	Garimella, Sandilya V.B.....	TP 717
Fu, You-Jun.....	ThP 515	Gallien, Sebastien.....	ThP 322	Garofolo, Fabio.....	WP 132
Fu, Zhengwei.....	TP 674	Gallien, Sebastien.....	ThP 442	Garofolo, Fabio.....	WP 179
Fu, Zongming.....	ThP 300	Gallien, Sebastien.....	ThP 534	Garofolo, Fabio.....	WP 180
Fuchs, Beate.....	MP 252	Gallien, Sebastien.....	TP 485	Garofolo, Fabio.....	WP 181
Fuchser, Jens.....	MP 549	Gallo, Richard.....	MOH pm 4:10	Garofolo, Fabio.....	WP 267
Fuerst, Peter.....	WP 360	Galusca, Mirela.....	ThP 606	Garofolo, Fabio.....	WP 268
Fuesler, John.....	ThP 340	Galvez-Peralta, Marina.....	TP 038	Garofolo, Fabio.....	WP 523
Fujii, Makiko.....	MP 005	Gamage, Chaminda M.....	MP 395	Garofolo, Fabio.....	WP 545
Fujii, Takashi.....	MP 417	Gambardella, Janice.....	TOE am 09:30	Garofolo, Fabio.....	WP 544
Fujimoto, Grant.....	MOG pm 3:30	Gambin, Anna.....	ThP 191	Garofolo, Fabio.....	WP 538
Fujimoto, Grant M.....	TP 169	Gambin, Anna.....	WP 035	Garofolo, Fabio.....	WP 535
Fujimura, Yoshinori.....	MP 062	Gamble, Donald S.....	TP 558	Garofolo, Fabio.....	WP 525
Fujimura, Yoshinori.....	WP 282	Gamble, Heather A.....	TP 558	Garofolo, Fabio.....	WP 522
Fujita, Ai.....	MOF pm 3:10	Gamboa da Costa, Goncalo.....	MP 769	Garofolo, Fabio.....	WP 532
Fujita, Ai.....	MP 196	Gamboa Da Costa, Goncalo.....	TP 489	Garoutte, Aaron Joseph.....	MP 564
Fujita, Ai.....	WP 594	Gamboa da Costa, Goncalo.....	WP 548	Garrard, Kenneth.....	WP 030
Fujita, Setsuko.....	MOF pm 3:10	Gamez, Roberto.....	TP 410	Garraway, Levi.....	WOG am 08:50
Fujito, Yuka.....	TP 560	Gan, Chee Sian.....	MP 358	Garrett, Timothy.....	MP 240
Fukakusa, Shunsuke.....	MP 067	Gan, Chee Sian.....	ThP 623	Garrett, Timothy.....	MP 631
Fukuda, Yasunori.....	MOF pm 3:10	Gan, Jie peng.....	ThP 715	Garrett, Timothy.....	MP 785
Fukusaki, Eiichiro.....	MP 613	Gan, Jinping.....	WOF am 08:30	Garrett, Wesley M.....	TP 668
Fukusaki, Eiichiro.....	ThP 378	Gan, Jinrui.....	TP 012	Garside, John.....	TP 723
Fukusaki, Eiichiro.....	ThP 375	Ganapathy, Ramesh.....	WP 121	Gasch, Audrey P.....	ThP 378
Fukusaki, Eiichiro.....	WP 283	Gandhi, Abhishek.....	WP 103	Gasch, Audrey P.....	ThP 327
Fukuyama, Yuko.....	MP 130	Gandhi, Adarsh.....	TP 045	Gaston, Kirk.....	ThP 518
Fung, Eliza.....	MP 366	Gandhi, Tejas.....	ThOE pm 2:30	Gatèk, Jiří.....	ThP 396
Fung, Shane.....	ThP 222	Gandhi, Tejas.....	TP 086	Gates, Ashley.....	WP 557
Fung, Shan-Yu.....	WP 150	Gandhi, Tejas.....	WP 722	Gatti, Daniel M.....	MOG pm 2:30
Funk, Carrie.....	MP 639	Gang, David.....	TP 432	Gatto, Laurent.....	MP 682
Funk, Carrie.....	TP 625	Gangam, Rekha.....	WP 383	Gatto, Laurent.....	WOD am 09:30
Funk, Carrie.....	WP 616	Gano, Lindsey B.....	TP 446	Gatto, Laurent.....	WP 738
Funk, Carrie.....	WP 618	Gao, Chan.....	MP 618	Gaulier, Jean-Michel.....	ThP 599
Furlong, Michael.....	MP 074	Gao, Chao.....	TP 396	Gaulier, Jean-Michel.....	ThP 600
Furlong, Michael.....	WP 636	Gao, Hongying.....	ThP 443	Gault, Joseph.....	WP 059
Furr, Jonathan.....	WP 461	Gao, Hongying.....	WP 631	Gauss, Robert.....	MP 152
Furtado, Milton.....	WP 545	Gao, Jing.....	MP 357	Gauthier, Lauren.....	MP 126
Furtado, Milton.....	WP 544	Gao, Peng.....	ThP 166	Gauthier, Nicholas.....	MP 215
Furtado, Milton.....	WP 538	Gao, Qi.....	ThP 352	Gautier, Violette.....	WOG am 09:30
Furtado, Milton.....	WP 535	Gao, Wei.....	ThP 574	Gavin, Anne-Claude.....	ThP 072
Furtado, Milton.....	WP 532	Gao, Xiaoli.....	ThP 385	Gavrilov, Dimitar.....	WP 655
Furtado, Milton.....	WP 525	Gao, Yang.....	MP 143	Gawron, Daria.....	TP 078
Furtado, Milton.....	WP 522	Gao, Yuan.....	WP 249	Gazis, Paul.....	MP 679
Furtado, Milton.....	WP 523	Gao, Yuan.....	WP 470	Gbormittah, Francisca.....	WP 077
Furtos, Alexandra.....	TP 530	Gao, Yuqian.....	WOG pm 2:50	Ge, Ying.....	MP 110
Furuhashi, Takeshi.....	ThP 721	Gaquerel, Emmanuel.....	MP 615	Ge, Ying.....	ThP 065
Fusco, James C.....	WP 470	Garabedian, Alyssa.....	MP 249	Ge, Ying.....	ThP 078
Fushman, David.....	ThP 235	Garate, Jone.....	MP 006	Ge, Ying.....	WP 057
Fux, Elie.....	MP 638	Garcia, Angel.....	ThP 471	Ge, Ying.....	WP 162
Gabashvili, Alexandra.....	ThP 197	Garcia, Benjamin.....	MP 237	Gebhardt, Christoph.....	TP 750
Gabelica, Valérie.....	MOC am 09:30	Garcia, Benjamin.....	WP 097	Gebhardt, Christoph.....	WP 727
Gabelica, Valérie.....	TOC am 08:50	Garcia, Benjamin A.....	ThP 070	Gebreab, Fana.....	TP 145
Gabelle, Audrey.....	TP 472	Garcia, Benjamin A.....	ThP 237	Geddes, Donna.....	WP 587
Gabelle, Audrey.....	WP 447	Garcia, Benjamin A.....	WP 067	Geddes, Kristin.....	ThOE am 09:30
Gabriel, Stefan J.....	TP 417	Garcia, Benjamin A.....	MP 099	Geddes, Kristin L.....	ThP 521
Gabriel, Stefan Johannes.....	MOA pm 3:50	Garcia, Benjamin A.....	MP 095	Geer, M. Ariel.....	ThP 084
Gabryelski, Wojciech.....	WP 773	Garcia, Benjamin A.....	MP 236	Geib, Timon.....	WP 452
Gaddemane, Venkatesha.....	MP 358	Garcia, Benjamin A.....	ThOF pm 2:30	Geiger, Tamar.....	MP 433
Gaddemane, Venkatesha.....	ThP 623	Garcia, Benjamin A.....	TP 099	Geis-Asteggiante, Lucia.....	MP 137
Gaddis, LaQuasha.....	TP 759	Garcia, Benjamin A.....	TP 114	Geis-Asteggiante, Lucia.....	ThP 541
Gadi, Sneha.....	TP 561	Garcia, Benjamin A.....	TP 184	Gelb, Abby S.....	WP 676
Gaffrey, Matthew.....	WOG pm 2:50	Garcia, Gustavo A.....	TP 369	Gelb, Abby S.....	WP 678

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Gelb, Michael.....	WP 443	Giannone, Richard J.....	MP 129	Gingras, Anne-Claude.....	TP 087
Gemmill, Robert.....	ThP 166	Giannone, Richard J.....	MP 746	Gingras, Anne-Claude.....	TP 138
Gemperline, Erin.....	MP 405	Giannoukos, Stamatios.....	MP 521	Gingras, Anne-Claude.....	TP 182
Geng, Dawei.....	ThP 551	Giansanti, Piero.....	ThP 212	Gingras, Anne-Claude.....	TP 181
Gengeliczki, Zsolt.....	TP 263	Gibbs, Allison.....	TP 067	Ginsberg, Henry.....	MP 075
Genin, Eric.....	MP 623	Giblin, Daryl.....	MP 173	Gioino, Paula.....	MP 463
Gennity, Ingrid.....	MP 591	Giblin, Daryl.....	MP 324	Giordano, Braden C.....	WP 401
Genovese, Luca.....	ThP 293	Giblin, Daryl.....	TP 348	Giordano, Laurent.....	TP 781
Genovese, Raymond F.....	ThP 306	Gibson, Bradford.....	TP 127	Giordano, Silvia.....	TP 029
Gentry, Gary.....	MOB pm 2:30	Gibson, Bradford W.....	WP 118	Giovannelli, Jean François.....	ThP 023
George, Bijesh.....	MP 255	Gibson, Bradford W.....	WP 113	Giovannucci, Dr. David.....	WP 459
George, Cameron.....	MP 518	Gibson, John K.....	ThOD pm 3:50	Girault, Hubert.....	TP 389
George, Christian.....	WP 146	Gibson, John K.....	TP 364	Giremus, Audrey.....	ThP 023
George, Ed.....	MP 689	Gidden, Jennifer.....	ThP 127	Girod, Marion.....	WP 177
George, Iniga S.....	ThP 735	Giddings, Katherine.....	WP 311	Girotti, Albert W.....	ThP 512
Gerber, Bernd.....	WP 146	Gierliński, Marek.....	ThP 338	Girshenko, Savva.....	WP 709
Gerencser, Akos A.....	WP 118	Gies, Anthony P.....	MOA pm 3:30	Giuffrè, Robert.....	TP 427
Gerfault, Laurent.....	ThP 023	Gieschen, Andy.....	TP 246	Giusti, Pierre.....	TP 406
Gerling, John.....	WP 309	Gigmes, Didier.....	ThP 510	Giza, Jennifer.....	WP 374
Germain, Ronald.....	MP 269	Gigmes, Didier.....	TP 780	Gizzi, Michael.....	WP 310
German, Bruce.....	WOE am 08:50	Giguere, Sophie.....	MP 158	Glaskin, Rebecca.....	ThP 716
Germansderfer, Philip.....	WP 572	Gikas, Evangelos.....	WP 600	Glaskin, Rebecca S.....	ThOH pm 2:30
Gernert, Claus.....	MP 326	Gil, Geun-Cheol.....	TP 445	Glaskin, Rebecca S.....	WP 674
Geromanos, Scott.....	TP 157	Gil, Geun-Cheol.....	WP 138	Glass, Keely.....	MP 738
Geromanos, Scott J.....	ThP 274	Gil, Geun-Cheol.....	WP 137	Glass, Keely.....	TP 768
Gerritsen, Karin G. F.....	MP 477	Gil, Sophie.....	MP 235	Glass, Keely.....	TP 769
Gerritsma, Jort.....	WP 055	Gilad, Yoav.....	MP 212	Glatt, Sebastian.....	ThP 072
Gershenson, Anne.....	ThP 122	Gilbert, Jeffrey.....	MOA am 09:30	Glauner, Thomas.....	MP 356
Gershon, Paul.....	ThP 228	Gilbert, Jeffrey.....	ThP 318	Glauner, Thomas.....	MP 702
Gershon, Paul.....	WP 039	Gilbert, Jeffrey.....	WP 024	Glauner, Thomas.....	WP 355
Gershon, Paul.....	WP 094	Gilbert, Jeffrey R.....	MP 054	Glaven, Sarah.....	MP 279
Gerstmair, Anja.....	MP 041	Gilbert, Joshua.....	TP 341	Glaven, Sarah M.....	MP 278
Gerstmair, Anja.....	ThP 046	Gilbert, Joshua D.....	TP 339	Glavin, Danny.....	TP 712
Gerszten, Robert.....	TP 426	Gilbert, Joshua D.....	TP 340	Gleason, Carol.....	TOE am 09:30
Gervasi, Gaspard.....	TP 224	Gilbert, Tony.....	TP 724	Gledhill, Antonietta.....	WP 347
Gervasi, Gaspard.....	TP 219	Gilbert-López, Bienvenida.....	TP 272	Glick, James.....	TP 040
Gerwick, William.....	MP 056	Giles, David.....	ThP 350	Glick, James.....	WP 373
Gesell Salazar, Manuela.....	ThP 250	Giles, Kevin.....	MP 181	Glick, James.....	WP 775
Gessel, Megan M.....	MOH pm 2:30	Giles, Kevin.....	ThP 469	Glish, Gary.....	ThOC am 09:30
Gessulat, Siegfried.....	MP 041	Giles, Kevin.....	TP 722	Glish, Gary.....	WP 768
Gessulat, Siegfried.....	ThP 046	Giles, Kevin.....	TP 723	Glish, Gary L.....	MP 327
Gestwicki, Jason E.....	WP 228	Giles, Kevin.....	WOA pm 2:30	Glish, Gary L.....	TP 349
Gethings, Lee A.....	MP 265	Giles, Roger.....	WP 689	Glish, Gary L.....	TP 372
Gethings, Lee A.....	ThP 036	Gill, Christopher G.....	MP 556	Glish, Gary L.....	TP 561
Gethings, Lee A.....	WP 126	Gill, Christopher G.....	WP 746	Glish, Gary L.....	WP 770
Getie-Kebtie, Melkamu.....	ThP 313	Gill, Jason.....	MP 563	Glocker, Michael O.....	ThP 107
Getnet, Derese.....	MP 255	Gillen, Greg.....	ThP 601	Glocker, Michael O.....	ThP 277
Getnet, Derese.....	ThP 219	Gillen, Greg.....	WP 291	Glocker, Michael O.....	WP 146
Getnet, Derese.....	TOG am 09:10	Gillen, Greg.....	WP 302	Glocker, Michael O.....	WP 715
Getty, Stephanie.....	MP 697	Gillen, Greg.....	WP 380	Glueckmann, Matthias.....	MP 238
Getty, Stephanie.....	ThP 364	Gilles, Christopher.....	WP 649	Glukhov, Evgenia.....	MP 056
Getty, Stephanie.....	ThP 365	Gilles, Nicolas.....	WOE am 09:50	Glunde, Kristine.....	MOH pm 3:50
Getty, Stephanie.....	ThP 366	Gillespie, Alison.....	TP 152	Glunde, Kristine.....	TP 062
Getty, Stephanie.....	ThP 369	Gillespie, Bradley.....	MP 514	Go, Christopher.....	MP 258
Getty, Stephanie.....	TOA pm 2:30	Gillet, Ludovic.....	ThOE pm 3:50	Go, Christopher.....	TP 638
Getty, Stephanie.....	TP 710	Gillet, Ludovic CJ.....	MP 432	Go, Eden.....	ThOH am 08:30
Getzinger, Gordon.....	ThP 570	Gillet, Ludovic CJ.....	ThP 257	Go, Eden.....	WP 260
Geum Sook, Hwang.....	MP 482	Gillet, Sylvie.....	MP 235	Godat, Becky.....	TP 234
Gevaert, Kris.....	WP 129	Gillette, Michael.....	TOG am 08:30	Godbey, Jeffrie.....	MP 054
Geyer, Roland.....	MP 771	Gillette, Michael A.....	MOG am 08:30	Gode, David.....	WP 697
Geyer, Roland.....	WP 293	Gillette, Michael A.....	ThOE am 10:10	Godoi, Marla.....	WP 685
Ghaemmaghami, Sina.....	WP 232	Gillette, Michael A.....	ThP 205	Gödörházy, Lajos.....	MP 404
Gharahdaghi, Farzin.....	MP 073	Gillette, Michael A.....	TP 426	Godoy, Patricio.....	MP 452
Ghashghaei, Troy.....	WP 011	Gillette, Michael A.....	TP 438	Goepfert, Tyler.....	MP 275
Ghassabi Kondalaji, Samaneh.....	WP 699	Gillig, Kent.....	MP 662	Goesmann, Fred.....	ThP 369
Ghassemian, Majid.....	MP 207	Gillig, Kent.....	ThP 478	Goesmann, Fred.....	TOA pm 2:30
Ghazi, Arjumand.....	WP 117	Gilliland, Jr., William M.....	TP 739	Goessens, Wil.....	WP 151
Ghislain, Thierry.....	MP 576	Gilmore, Ian.....	WP 384	Goethals, Bart.....	MP 032
Ghorai, Suman.....	TOH pm 3:30	Gilmore, Ian S.....	MP 001	Goethals, Bart.....	WP 042
Ghorai, Suman.....	TP 748	Gilmore, Ian S.....	WP 013	Goguen, Robert.....	MP 365
Ghosh, Banibrata.....	WP 612	Gilmore, Ian S.....	WP 386	Goguen, Robert.....	ThP 413
Ghosh, Dipankar.....	ThP 565	Gimelshein, Natalia.....	MP 381	Goguen, Robert.....	TP 269
Ghosh, Dipankar.....	TP 284	Gimelshein, Natalia.....	MP 383	Goh, Evelyn.....	MP 350
Ghosh, Dipankar.....	TP 578	Gimelshein, Natalia.....	WP 385	Gokulrangan, Giridharan.....	ThP 355
Ghosh, Dipankar.....	TP 580	Gimelshein, Sergey.....	MP 383	Gold, David.....	TP 431
Giannakopoulos, Anastassios.....	ThP 751	Gimelshein, Sergey.....	MP 381	Goldin, Robert.....	TOG pm 3:30
Giannakopoulos, Anastassios.....	ThP 752	Gimelshein, Sergey.....	WP 385	Goldin, Robert D.....	TP 375
Giannone, Richard.....	MP 276	Gingras, Anne-Claude.....	MP 258	Goldin, Robert D.....	WP 020

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Goldman, Radoslav.....	ThP 139	Gordiyenko, Yuliya.....	ThOC pm 2:30	Grant, Kyle G.....	WP 098
Goldman, Radoslav.....	WP 075	Gordon, Dave.....	ThP 749	Grant, Melissa.....	MP 098
Goldman, Radoslav.....	WP 089	Gornbein, Jeffrey.....	MP 626	Grant, Paaqua A.....	ThOB am 09:10
Goldstein, Matthew.....	WP 303	Gorre, Elsa.....	MP 018	Grant, Russell.....	MP 287
Golf, Ottmar.....	MOH pm 3:10	Gorrochategui, Eva.....	WP 719	Grant, Russell.....	TOG pm 4:10
Golf, Ottmar.....	MP 404	Gorsh, Amy.....	WP 726	Grant, Russell.....	WP 134
Golf, Ottmar.....	ThP 379	Gorshkov, Alexander V.....	WP 164	Grant, Russell.....	WP 429
Golf, Ottmar.....	TP 375	Gorshkov, Mikhail.....	WP 135	Grant, Russell.....	WP 428
Golf, Ottmar.....	WP 020	Gorshkov, Mikhail V.....	TP 081	Grant, Russell P.....	MP 532
Gollapalli, Kishore.....	WP 235	Gorshkov, Mikhail V.....	WP 136	Grãos, Mário.....	ThP 101
Gomer, Richard.....	TP 209	Gorshkov, Mikhail V.....	WP 164	Grapov, Dmitry.....	MP 071
Gomes, Alexander.....	TP 486	Gorskho, Mikhail V.....	WP 172	Grapov, Dmitry.....	MP 430
Gomes, Alexandre.....	TP 585	Gorynski, Krzysztof.....	MP 770	Grapov, Dmitry.....	ThOG am 09:10
Gomes, Alexandre F.....	MP 367	Göschl, Lisa.....	MP 228	Grasso, Luigi.....	TP 238
Gomes, Helineia O.....	TP 594	Gosciny, Severine.....	WP 666	Graumann, Johannes.....	ThP 175
Gomez, Joe.....	TP 446	Gosciny, Séverine.....	WP 667	Gravell, Anthony.....	ThP 560
Gómez-Escudero, Andrea.....	TP 587	Goshawk, Jeff.....	WP 666	Gravell, Anthony.....	WP 566
Gómez-Ríos, German Augusto.....	ThOB am 09:50	Goshe, Michael.....	MP 411	Gravenstein, Nikolaus.....	WP 397
Gómez-Ríos, German Augusto.....	TP 749	Goshe, Michael B.....	MP 410	Graves, Lee M.....	TP 173
Gómez-Ríos, Germán Augusto.....	TP 521	Goshe, Michael B.....	WOE pm 3:50	Graves, Steven.....	MP 239
Gómez-Ríos, Germán Augusto.....	WP 750	Goshe, Michael B.....	WP 098	Graves, Steven.....	WOE am 09:30
Gomi, Masahiro.....	WP 143	Goswami, Devrishi.....	TOF am 09:50	Gray, Alexander.....	MP 599
Gonçalves Santos, Vanessa.....	TP 586	Goswami, Devrishi.....	TP 543	Gray, Andrea.....	ThP 167
Gong, Chao.....	TOE am 09:30	Goswami, Hareshwar.....	WOE pm 2:30	Gray, Christopher.....	ThP 492
Gong, Haiqing.....	WP 390	Goswami, Neha.....	ThP 175	Gray, Donald.....	MP 510
Gong, Jiachang.....	MP 366	Goto, Takaaki.....	MP 105	Gray, Jesse.....	MP 513
Gong, Xiaoyun.....	TP 379	Goto, Takaaki.....	MP 107	Gray, L Earl.....	WP 461
Gonnsen, Zachary.....	TP 711	Goto, Takaaki.....	MP 108	Gray, Murray.....	TP 589
Gonthier, Renaud.....	TP 495	Goto, Takaaki.....	MP 096	Gray, Murray R.....	TP 588
Gonzales Arandilla, Alba.....	ThP 338	Goto, Takaaki.....	WP 131	Gray, Nicola.....	WP 596
Gonzales-Cope, Michelle.....	ThOF pm 2:30	Goto Silva, Livia.....	MP 159	Grayson, Michael A.....	Special
Gonzalez, Antonio.....	MOH pm 4:10	Gotoh, Naohiro.....	WP 283	Grayson, Scott.....	TP 790
Gonzalez, Ariel.....	MP 246	Gottschalk, Bart.....	MOG pm 4:10	Greaves, Rod.....	MP 302
Gonzalez, Ariel.....	MP 266	Gottschalk, Bart.....	MP 033	Grebe, Stefan.....	WP 726
Gonzalez, Faviel.....	ThP 034	Gottwald, Sven.....	TP 020	Greco, Todd M.....	ThP 171
Gonzalez, Frank J.....	TP 659	Gough, Peter.....	MP 512	Greco, Todd M.....	WP 244
Gonzalez, Pau.....	TP 064	Gouin, Charlotte.....	WOE am 09:50	Greco, Todd M.....	WP 244
Goo, Young Ah.....	MP 039	Gouveia, Felipe C.....	TP 594	Greeley, Laura.....	MP 411
Goo, Young Ah.....	ThP 325	Govan, Annie Bea.....	WP 117	Green, Anthony.....	ThP 492
Goo, Young Ah.....	TP 386	Govindan, Subramanian.....	TP 160	Green, Felicia M.....	WP 386
Goo, Young Ah.....	TP 400	Govorukhina, Natalia.....	WP 147	Green, Kari.....	ThP 263
Goo, Young Ah.....	TP 437	Gowda, G.A. Nagana.....	ThP 655	Green, Karin.....	ThP 403
Goo, Youngah.....	ThP 276	Gowda, Harsha.....	MP 270	Green, Karin.....	ThP 402
Goodchild, Ann.....	WP 234	Gowda, Harsha.....	MP 256	Green, Kathleen.....	TOG am 08:50
Goodlet, David.....	WP 751	Gowda, Harsha.....	MP 255	Green, Martin.....	MP 287
Goodlett, David.....	ThP 093	Goyallon, Arnaud.....	ThP 140	Green, Martin.....	TOG pm 4:10
Goodlett, David.....	ThP 276	Goykman, Dina.....	ThP 671	Green, Martin.....	TP 724
Goodlett, David.....	ThP 325	Goykman, Dina.....	TP 492	Green, Martin.....	WP 134
Goodlett, David.....	TP 377	Goykman, Dina.....	WP 547	Green, Martin.....	WP 429
Goodlett, David.....	TP 403	Gozo, Genevieve.....	ThP 481	Green, Martin.....	WP 428
Goodlett, David.....	TP 400	Gozzo, Fabio.....	TP 585	Green, Martin K.....	MP 532
Goodlett, David.....	TP 386	Gozzo, Fabio C.....	ThP 138	Green Tringe, Susannah.....	WOE pm 4:10
Goodlett, David.....	WOB pm 4:10	Gozzo, Fabio C.....	ThP 452	Greene, Warner.....	ThP 511
Goodlett, David.....	WP 028	Gozzo, Fabio C.....	MP 367	Greenhaw, James.....	MP 267
Goodlett, David.....	WP 504	Gozzo, Fabio C.....	ThP 453	Greenhouse, Robert.....	TP 507
Goodlett, David R.....	MP 039	Gräber, Martin.....	WOF am 09:10	Greenlief, C. Michael.....	ThP 302
Goodlett, David R.....	TP 286	Grabowska, Agnieszka K.....	ThP 343	Greenwood, Tiffany.....	MOH pm 3:50
Goodlett, David R.....	TP 437	Grafelman, D.....	MP 507	Greer, Joseph.....	ThP 059
Goodlett, David R.....	WOB am 08:50	Graham, David.....	ThOE pm 3:30	Greer, Joseph B.....	ThP 060
Goodlett, David R.....	WOC am 08:50	Graham, David.....	ThP 229	Greer, Sylvester.....	WP 175
Goodlett, David R.....	WP 288	Graham, David.....	ThP 273	Greer, Tyler.....	MP 448
Goodman, Haddon.....	TP 220	Graham, David.....	WP 602	Greer, Tyler.....	ThP 169
Goodman, Haddon.....	WP 330	Graham, David R.....	MP 262	Greer, Tyler.....	TP 454
Goodman, Keith.....	ThP 532	Graham, David R.....	TP 146	Gregorich, Zachery.....	MP 110
Goodwin, Cody.....	MP 585	Graham, David R.....	TP 468	Gregorich, Zachery.....	ThP 065
Goodwin, Cody.....	ThOG pm 2:50	Graham, Jill.....	MP 185	Gregorich, Zachery R.....	ThP 078
Goodwin, Cody R.....	TOB pm 2:50	Graham, Kendon.....	ThP 544	Gregory, Simon.....	MP 601
Goodwin, Douglas.....	WP 324	Graham, Kendon.....	ThP 551	Greicius, Michael.....	ThP 308
Goodwin, Richard.....	TOH am 08:30	Graham, Kendon.....	WP 347	Greiner, Annette.....	MP 024
Goodwin, Richard.....	TP 046	Graichen, Adam.....	WP 758	Greiner, Martin.....	ThP 446
Goodwin, Richard.....	WP 012	Graichen, Adam M.....	ThP 507	Greis, Ken.....	ThP 210
Goodwin, Richard J. A.....	TP 016	Granato, Daniela.....	WP 460	Gren, Eric.....	MP 069
Gooley, Andrew.....	ThP 783	Grand, Noël.....	ThP 369	Grensemann, Hans.....	MP 052
Gopalan, Venkat.....	ThOF am 09:30	Grandy, Jonathan.....	TP 749	Grensemann, Hans.....	MP 472
Gopen, Quinton.....	MP 250	Grangeat, Pierre.....	ThP 023	Grensemann, Hans.....	WP 650
Gor, Baptiste.....	WP 447	Grant, Christopher M.....	MP 272	Greulich, Heidi.....	ThP 217
Goracci, Laura.....	MP 639	Grant, David.....	WP 466	Grey, Angus C.....	TP 039
Gorbis, Sherman.....	ThP 660	Grant, David.....	WP 586	Grey, Angus C.....	TP 060
Gordish-Dressman1, Heather.....	ThOE am 09:50	Grant, Jennifer E.....	ThP 628	Griep-Raming, Jens.....	ThOG pm 3:10

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Grieshaber, Sarah E.....	MOA pm 2:30	Grunewald, Kay.....	ThP 171	Gumin, Joy.....	WP 238
Grieves, Nigel.....	WP 625	Grüning, Anja.....	TP 583	Gummer, Joel.....	ThP 653
Griffin, Jeddidah.....	MP 166	Grunseich, Christopher.....	ThP 313	Gummer, Joel.....	WP 587
Griffin, Julian L.....	WP 285	Grzetic, Josipa.....	ThOD pm 3:30	Guna, Mircea.....	WOC am 09:10
Griffin, Pat.....	WOH pm 2:30	Grzetic, Josipa.....	TP 365	Gunaratne, Don.....	ThOD pm 4:10
Griffin, Patrick.....	ThP 136	Gu, Christine (Chunang).....	MP 363	Gunawardena, Harsha.....	TP 433
Griffin, Patrick.....	ThP 137	Gu, Chunang (Christine).....	TP 503	Gunawardena, Harsha P.....	MP 179
Griffin, Patrick.....	TOF am 09:50	Gu, Chunang (Christine).....	TP 512	Gunawardena, Harsha P.....	ThP 290
Griffin, Patrick.....	TP 543	Gu, Haiwei.....	MP 443	Gunawardena, Harsha P.....	WP 250
Griffin, Patrick R.....	ThP 335	Gu, Haiwei.....	ThP 655	Gunawardena, Harsha P.....	WP 463
Griffin, Patrick R.....	TP 094	Gu, Haiwei.....	ThP 659	Gundberg, Caren M.....	ThP 247
Griffin, Tim.....	MOG pm 4:10	Gu, Hongbo.....	MP 122	Gundermann, Nick.....	MP 356
Griffin, Tim.....	MP 033	Gu, Hongbo.....	ThP 073	Gundlach-Graham, Alexander W.....	ThOB pm 4:10
Griffin, Tim.....	MP 104	Gu, Hongbo.....	TP 117	Gundry, Rebekah L.....	WP 212
Griffin, Tim.....	MP 429	Gu, Hongbo.....	TP 457	Guner, Huseyin.....	ThP 065
Griffin, Tim.....	ThP 044	Gu, Huidong.....	WP 534	Gunner, Serife A.....	ThP 078
Griffin, Tim.....	TP 077	Gu, Liqing.....	MP 208	Gunnness, Patrina.....	WP 154
Griffin, Timothy.....	MP 049	Gu, Ming.....	MP 666	Gunning, Patrick.....	ThP 125
Griffin, Timothy.....	TP 428	Gu, Ming.....	TP 248	Gunnlaugsdóttir, Helga.....	WP 342
Griffith, Emily.....	ThP 288	Gu, Ming.....	TP 547	Gunsalus, Robert.....	MP 016
Griffiths, William James.....	MP 244	Gu, Ming.....	TP 572	Gunsalus, Robert.....	WOG am 10:10
Grill, Andreas.....	ThP 496	Gu, Ming.....	TP 755	Gunsalus, Robert P.....	ThP 716
Grill, Andreas.....	WP 100	Gu, Ming.....	WP 352	Guo, Ailan.....	MP 122
Grill, Andreas.....	WP 526	Gu, Rong-Fang.....	MP 153	Guo, Baochuan.....	MP 508
Grimes, Marcie.....	ThP 523	Gu, Sheng.....	ThP 109	Guo, Dan.....	TP 351
Grimm, Rudolf.....	ThP 168	Gu, Zezong.....	ThP 302	Guo, Dongfa.....	MP 330
Grimm, Rudolf.....	TP 257	Guallar-Hoyas, Cristina.....	MP 404	Guo, Hua.....	MOD am 08:30
Grimm, Rudolf.....	WP 066	Guallar-Hoyas, Cristina.....	ThP 664	Guo, Jia.....	MP 100
Grinfeld, Dmitry.....	ThP 754	Guan, Fuyu.....	ThP 593	Guo, Jia.....	WOG pm 2:50
Grinfeld, Dmitry.....	ThP 751	Guan, Shenheng.....	ThP 037	Guo, Jingshu.....	WP 485
Grinfeld, Dmitry.....	ThP 752	Guan, Shenheng.....	ThP 462	Guo, Jingzhong (Tim).....	WP 190
Grinfeld, Dmitry.....	TP 136	Guan, Shenheng.....	WP 228	Guo, Lei.....	TP 685
Grinstein, Veronika.....	MP 150	Guan, Ting.....	MP 635	Guo, Lei.....	WP 251
Gritsenko, Marina.....	WOG pm 2:50	Guan, Wei.....	ThOE am 08:50	Guo, Lizhi.....	ThP 436
Grober, Jay.....	MP 536	Guan, Wei.....	TP 463	Guo, Manman.....	ThP 328
Groeber, Elizabeth A.....	TP 522	Guan, Xiaoyan.....	MP 084	Guo, Min.....	ThP 139
Groeger, Thomas M.....	ThP 609	Guan, Xiaoyan.....	WP 735	Guo, Mingquan.....	MP 610
Groen, Aaron C.....	MP 259	Guarani-Pereira, Virginia.....	TP 145	Guo, Mingquan.....	TP 645
Groenewold, Gary.....	MP 392	Guazzotti, Sergio.....	TP 755	Guo, Tan.....	ThP 552
Groessl, Michael.....	WP 671	Guazzotti, Sergio.....	TP 754	Guo, Tiannan.....	WP 155
Groetsch, Helga.....	ThP 072	Gucek, Marjan.....	ThP 052	Guo, Tianyang.....	WP 407
Gronert, Scott.....	MP 091	Gucek, Marjan.....	WP 255	Guo, Wei.....	MP 110
Gronert, Scott.....	TP 354	Gucinski, Ashley.....	MOE pm 3:50	Guo, Xiaofeng.....	MP 254
Gronert, Scott.....	TP 359	Gucinski, Ashley.....	ThP 143	Guo, Xuejiang.....	ThP 238
Groopman, John D.....	WP 511	Gudihal, Ravindra.....	MP 085	Guo, Xuejiang.....	WP 149
Gros, Meritxell.....	TP 551	Gudihal, Ravindra.....	MP 097	Guo, Yibo.....	WP 640
Gross, Juergen.....	TP 384	Gudihal, Ravindra.....	TP 262	Guo, Yike.....	WP 468
Gross, Michael.....	MP 172	Gudihal, Ravindra.....	WP 204	Guo, Yuan.....	ThP 634
Gross, Michael.....	MP 173	Gueiros-Filho, Federico.....	MP 159	Guo, Yueshui.....	ThP 238
Gross, Michael.....	ThP 107	Gueneva-Boucheva, Kristina.....	WP 507	Guo, Zhongwu.....	TP 319
Gross, Michael.....	TP 159	Guenther, Sabine.....	WP 020	Gupta, Anshul.....	TOH am 08:30
Gross, Michael.....	WP 217	Guéraud, Françoise.....	TP 649	Gupta, Manoj Kumar.....	MP 270
Gross, Michael.....	WP 231	Guerdrum, Lindsay.....	ThP 608	Gupta, Sayan.....	ThP 356
Gross, Michael L.....	MP 111	Guerrera, Ida Chiara.....	WP 145	Gurdak, Elzbieta.....	WP 386
Gross, Michael L.....	MP 324	Guerrero, Alonna.....	TP 505	Gushue, Jennifer.....	MP 600
Gross, Michael L.....	ThOF am 10:10	Guerrero, Andres.....	TP 221	Gushue, Jennifer.....	WP 360
Gross, Michael L.....	ThP 362	Guerrero, Andres.....	TP 258	Gushue, Jennifer.....	WP 566
Gross, Michael L.....	ThP 363	Guerrero, Andres.....	WOG am 08:50	Guterres, Sheila.....	MP 115
Gross, Michael L.....	TP 348	Guerrero, Andres.....	WP 086	Guterres, Sheila.....	WP 140
Gross, Steven.....	MP 579	Guerrero, Candace.....	WP 367	Gutgutia, Suruchi.....	ThP 254
Gross, Steven.....	MP 592	Guerrero, Candace R.....	WP 366	Gutgutia, Suruchi.....	ThP 534
Grosse-Coosmann, Florian.....	ThP 317	Guettler, Thomas.....	MP 259	Guthals, Adrian.....	MP 043
Grosser, Tilo.....	TP 103	Gugiu, Bogdan-Gabriel.....	ThP 386	Guthals, Adrian.....	MP 207
Grossgarten, Mandy.....	TP 032	Gugiu, Bogdan-Gabriel.....	ThP 526	Guthals, Adrian.....	TP 088
Grossmann, Jonas.....	WP 154	Gugiu, Gabriel B.....	WP 472	Guther, Lucia.....	MP 151
Grote, Eric.....	ThP 300	Guha, Udayan.....	ThP 204	Gutierrez, Marcelino.....	MP 056
Grottemeyer, Jurgen.....	MP 326	Guilbaud, Rudolf.....	TP 423	Guttikar, Swati.....	WP 103
Grottemeyer, Jurgen.....	TP 361	Guillette, Jr., Louis J.....	ThP 377	Guttman, Miklos.....	TOF am 08:50
Grottemeyer, Jürgen.....	ThP 694	Guimarães, Gustavo.....	MP 464	Gwak, Seongshin.....	ThP 597
Grotz, Diane.....	TP 626	Guimarães Neto, Manoel J.R.....	TP 594	Gygi, Melanie.....	TP 145
Grotz, Diane E.....	MP 639	Guimarães Pereira, Gonçalo.....	MP 562	Gygi, Steven.....	MP 133
Grover, Himanshu.....	MP 040	Guingab-Cagmat, Joy.....	ThP 306	Gygi, Steven.....	ThP 174
Grover, Himanshu.....	ThP 039	Guise, Amanda.....	MP 158	Gygi, Steven.....	ThP 319
Grover, Himanshu.....	TP 089	Gul, Nizamettin.....	WP 107	Gygi, Steven.....	TP 145
Grozovsky, Renata.....	TP 332	Güler, Ülkü.....	MP 066	Gygi, Steven.....	TP 180
Grubb, Mary.....	WP 622	Gullick, Darren.....	TP 304	Gygi, Steven.....	TP 430
Gruenhagen, Jason.....	TP 503	Gullick, Darren R.....	TP 568	Gygi, Steven P.....	ThP 214
Gruia, Flaviu.....	MP 094	Gulvik, Christopher.....	MP 775	Gygi, Steven P.....	MOG pm 2:30

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Gygi, Steven P.....	MP 259	Hamm, Gregory.....	TOH am 09:10	Hanson, Jeff.....	MP 637
Gygi, Steven P.....	TOD pm 3:50	Hamm, Gregory.....	TP 009	Hansson, Annelie.....	MP 352
Gygi, Steven P.....	TOG am 09:50	Hamm, Gregory.....	TP 034	Hansson, Annelie.....	TP 628
Gygi, Steven P.....	WOG am 09:10	Hamm, Gregory.....	TP 249	Hansson, Gunnar C.....	MP 211
Ha, Emmeline.....	TP 135	Hammann, Philippe.....	TP 247	Hansson, Gunnar C.....	MP 210
Haab, Brian.....	TP 069	Hammann, Philippe.....	WP 498	Hao, Changtong.....	MP 339
Haack, Alexander.....	TP 731	Hammer, Elke.....	ThP 250	Hao, Changtong.....	TP 630
Haas, Bernd.....	ThOG am 09:50	Hammer, Emily.....	MP 167	Hao, Changtong.....	WP 558
Haas, Wilhelm.....	MP 257	Hammer, Neal D.....	TP 073	Hao, Chi.....	ThP 051
Haberer, Kirsten.....	MOD pm 4:10	Hammock, Bruce.....	MP 430	Hao, Ling.....	MP 448
Haberer, Kirsten.....	MP 684	Hammond, Dean E.....	MP 272	Hao, Ling.....	TP 454
Haberl, Peter.....	WP 050	Hampton, Andrew.....	MP 692	Hao, Piliang.....	ThP 157
Hacker, Timothy.....	MP 110	Hamuro, Lora.....	WP 188	Hao, Piliang.....	TP 097
Hacker, Timothy.....	ThP 065	Han, Chanyoung.....	ThOA am 09:50	Hao, Rui.....	WP 259
Hadiwikarta, Wahyu.....	MOG pm 3:10	Han, Dohyun.....	MP 128	Hao, Zhiqi.....	ThP 765
Hadjisavvas, Andreas.....	WP 491	Han, Dohyun.....	WP 014	Hao, Zhiqi.....	TP 154
Haftchenary, Sina.....	ThP 125	Han, Guanghui.....	ThOE pm 3:30	Hao, Zhiqi.....	TP 264
Hager, Jim. W.....	WOD pm 2:50	Han, Jiyou.....	TP 441	Hao, Zhiqi.....	WP 202
Hägglund, Per.....	WP 043	Han, Jun.....	TP 014	Hao, Zhiqi.....	WP 264
Hagler, Clay D.....	TP 324	Han, Jun.....	WP 471	Hao, Zhiqi.....	WP 262
Hahlbrock, Jennifer.....	TP 084	Han, Jun.....	WP 610	Hao, Zhiqi.....	WP 263
Hahm, Cynthia.....	MP 518	Han, Jun.....	WP 611	Haper, Jamie.....	TP 067
Hahm, Eun-Ryeong.....	TP 615	Han, Ling.....	ThP 098	Happ, Marshall.....	ThP 691
Hahn, Chang-Gyu.....	ThP 282	Han, Linjie.....	TOC am 09:30	Haq, Daniel.....	WP 208
Hahn, Chang-Gyu.....	WP 148	Han, Sang Beom.....	TP 509	Hara, Manami.....	MP 430
Hahn, Si Houn.....	TP 473	Han, Sang Woo.....	TP 199	Hardardt, Elizabeth.....	ThP 643
Hahne, Hannes.....	MP 041	Han, Sean.....	WP 272	Harden, Charles.....	TOC am 09:10
Hahne, Hannes.....	MP 193	Han, Seongah.....	ThOE am 09:10	Harden, Charles.....	WP 693
Hahne, Hannes.....	MP 191	Han, ShuangLai.....	ThP 739	Harden, Leslie.....	TP 230
Hahne, Hannes.....	ThOB am 09:30	Han, Wei.....	MP 594	Hardie, Darryl.....	TP 484
Hahne, Hannes.....	ThOB pm 3:50	Han, Wei.....	TP 655	Hardy, David.....	ThP 560
Hahne, Hannes.....	ThP 046	Han, Xianlin.....	ThP 399	Hardy, David.....	WP 025
Hains, Peter.....	TP 205	Han, Xianlin.....	WOH am 09:30	Harel, Michal.....	MP 433
Hajkova Leary, Dagmar.....	MP 279	Han, Xuemei.....	ThP 021	Hargiss, Leonard O.....	WP 710
Hakala, Kevin.....	ThP 076	Han, Xuemei.....	TP 091	Hariparsad, Nirosh.....	WP 620
Hakansson, Kristina.....	MP 090	Han, Xuemei.....	TP 483	Harkness, Kellen M.....	ThP 495
Hakansson, Kristina.....	TP 344	Han, Yong-Hae.....	WP 639	Harless, Bryan.....	ThP 732
Hakansson, Kristina.....	WOD pm 4:10	Han, Yumiao.....	WP 097	Harless, Bryan.....	WOB am 09:50
Hakansson, Kristina.....	WP 335	Hanchard, Julia.....	TP 638	Harman, Victoria M.....	MP 272
Hakansson, Kristina.....	WP 369	hancock, william.....	WP 077	Harmon, Patricia.....	TP 787
Hakenberg, Oliver.....	ThP 277	Hancock, William S.....	WP 079	Harnly, James.....	WP 338
Hakimi, Amirmansoor.....	TP 487	Handberg, Eric.....	MP 357	Harper, Brett.....	MP 047
Halabalaki, Maria.....	WP 600	Handberg, Eric.....	ThP 697	Harper, Brett.....	ThP 514
Halada, Petr.....	WP 167	Handberg, Eric.....	TP 388	Harper, Brett.....	WP 657
Halade, Ganesh.....	ThP 156	Handberg, Eric.....	TP 391	Harper, Brett.....	WP 658
Hale, Robert.....	MP 331	Handique, Dheeraj.....	TP 763	Harper, J. Wade.....	TP 145
Hale, Wendi.....	WP 335	Handique, Dheeraj.....	TP 762	Harper, Ross.....	MP 530
Halford, Edward.....	ThP 002	Handique, Dheeraj.....	TP 761	Harrelson, Jane.....	WP 184
Halket, John M.....	MP 048	Handy, Beverly.....	ThP 655	Harrer, Marques.....	ThOB am 10:10
Halket, John M.....	MP 561	Hanel, Gernot.....	MP 663	Harriman, Brian.....	TP 665
Hall, Adam.....	MP 523	Hanel, Gernot.....	ThP 738	Harrington, Peter.....	ThP 610
Hall, Adam B.....	WP 775	Haney, Paul.....	WP 121	Harrington, Peter.....	WP 026
Hall, Chassidy.....	TP 249	Haney, Paul.....	WP 514	Harrington, Peter B.....	WP 343
Hall, Maura.....	TP 550	Hang, Jiliang.....	WP 576	Harrington, Peter de B.....	ThP 561
Hall, Nathan.....	ThP 045	Hangauer, David.....	WP 015	Harris, Myanna Y.....	TP 324
Hall, Roger.....	ThP 054	Hanke, Sabrina.....	MOF pm 3:50	Harris, Rachel.....	WP 770
Hall, Ronald.....	TP 500	Hanke, Sabrina.....	MP 445	Harris, Thomas.....	MP 421
Hall, Seth.....	ThP 585	Hanke, Tomas.....	ThP 342	Harris, Timothy.....	TP 145
Hall, Seth.....	ThP 586	Hankin, Joseph A.....	WP 280	Harris, William A.....	MP 375
Hall, Seth.....	ThP 602	Hanley, John.....	TP 480	Harris, William A.....	WP 394
Hall, Seth.....	WP 310	Hanley, Patrick.....	MP 325	Harrison, Alex G.....	ThP 185
Hall, Stacy.....	ThP 149	Hanley-Bowdoin, Linda.....	MP 411	Harrison, Michelle.....	TP 505
Hall, Tom.....	ThP 567	Hanna, George.....	ThP 664	Harrison, Rane.....	TP 539
Hall, Tom.....	TP 271	Hanneken, Anne.....	TP 070	Harron, Andrew.....	MP 534
Hall, Tom.....	WP 571	Hanneman, Andrew.....	ThOH pm 3:30	Harshman, Sean W.....	MP 229
Hall, Tom.....	WP 578	Hanneman, Andrew.....	TP 332	Harst, Andreas.....	WP 242
Halligan, Brian.....	MP 428	Hanot, Vincent.....	WP 666	Hart, Ariel.....	MP 266
Halterman, Ronald L.....	ThP 605	Hanot, Vincent.....	WP 667	Hart, Ariel.....	WOF am 09:50
Halusa, Goran.....	ThP 025	Hanozin, Emeline.....	MOC pm 2:30	Hart, Bradley.....	MP 285
Halushka, Marc K.....	MP 255	Hanrieder, Jorg.....	TP 059	Hart, Gerald.....	ThOE pm 3:30
Hamada, Jun-ichiro.....	MP 447	Hanrieder, Jörg.....	MP 786	Hart, Philippa.....	TP 222
Hamann, Mark T.....	WP 324	Hanrieder, Jörg.....	TP 033	Hart, Sarah R.....	WP 171
Hamerly, Timothy.....	MP 276	Hansen, Angela M.....	ThP 646	Hartlein, Tom.....	TP 564
Hamester, Meike.....	MP 333	Hansen, Brett J.....	MP 706	Hartman, Blaine.....	WOA pm 4:10
Hamester, Meike.....	MP 665	Hansen, Christopher.....	TP 355	Hartmann, Peter.....	WP 587
Hamilton, Chad A.....	ThP 202	Hansen, Christopher S.....	TP 371	Hartmer, Ralf.....	MOE pm 3:30
Hamilton, Jason.....	WOH am 09:50	Hansen, Doug A.....	WP 335	Hartmer, Ralf.....	MP 148
Hamler, Rick.....	WOH am 10:10	Hansen, Rebecca.....	TP 022	Hartmer, Ralf.....	MP 157
Hamm, Gregory.....	MP 025	Hansen, Rebecca.....	TP 043	Hartmer, Ralf.....	WP 156

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Hartsock, Wendy	MP 756	Haynes, Paul	WP 234	Hegeman, Adrian D.	MP 605
Hartung, Thomas	WP 581	Haynes, Paul A.	ThP 735	Hegeman, Adrian D.	MP 611
Hartungen, Eugen	MP 663	Hayward, Penny	WP 738	Hegeman, Adrian D.	TP 641
Hartungen, Eugen	ThP 738	Hazama, Hisanao	ThP 012	Heidbrink Thompson, Jenny	TP 243
Harvey, Alex	WP 080	Hazen, Stanley	WP 286	Heien, Michael	WP 099
Harvey, David J.	ThP 712	He, Huan	TP 456	Heijs, Bram	TP 005
Harvey, Stephen B.	MP 454	He, Huan	TP 774	Heiling, Sven	MP 615
Hase, Prashant	TP 762	He, Jiangtao	ThP 448	Heilman, Heather	MP 753
Hase, Prashant	TP 763	He, Jiangtao	TP 450	Heinen, Kaitlin	MP 567
Hase, Prashant	TP 761	He, Jintang	WOG pm 2:50	Heipel, Mark	ThP 103
Hasegawa, Hideki	MP 661	He, Jintang	WP 513	Heischmann, Svenja	TP 446
Hasegawa, Hideki	TP 744	HE, Jiuming	ThP 669	Held, Jason	TP 127
Haserick, John	ThP 159	He, Kun	WP 054	Held, Jason M.	ThP 170
Hashi, Yuki	TP 281	He, Muiyi	ThP 757	Heldmann, Stefan	MP 021
Hashi, Yuki	TP 396	He, Muiyi	TP 351	Helenius, Katja	WOD am 09:50
Hashi, Yuki	TP 757	He, Qingyu	WP 016	Helperich, William G.	TP 499
Hashi, Yuki	WP 393	He, Si-Min	ThP 051	Helfrich, Forrest	ThP 440
Hashi, Yuki	WP 739	He, Si-Min	WP 053	Helin, Kristian	WOG am 08:30
Hashimoto, Bryce	TP 258	He, Si-Min	WP 054	Heller, Rexford T.	MP 672
Hashimoto, Hiroaki	MP 526	He, Tieming	TP 100	Helm, Dominic	ThOB am 09:30
Hashimoto, Yuichiro	MP 661	He, Timothy	ThP 405	Helm, Dominic	ThOB pm 3:50
Hashimoto, Yuichiro	TP 744	He, Xiang	MP 293	Helm, Paul A.	WP 575
Haslam, Stuart	ThP 161	He, Zeying	TP 758	Helmy, Roy	MP 392
Hasman, David	WP 322	Headley, John	TP 554	Hembrough, Todd	WP 141
Hasman Jr., Gregg	ThP 629	Heaney, Liam	TP 402	Hemenway, Eric	ThP 753
Hassan, Lyla	WP 391	Heath, Ester	TP 551	Heming, Richard	ThP 752
Hassan, Noman	MP 463	Heath, John K.	ThP 216	Henderson, Clark M.	TOG pm 3:50
Hassell, Kerry	MP 280	Heath, John K.	WP 764	Henderson, Colin	MP 214
Hassell, Kerry	TP 514	Heath, William	MOA pm 3:30	Henderson, Douglas B.	MP 375
Hassing, Robbert-Jan	WP 151	Hebeler, Romano	MP 614	Henderson, Douglas B.	WP 394
Hassiss, Maria	MP 436	Hebert, Alex	ThP 177	Henderson, Holly	MP 199
Hastings, Mike	MOA am 09:30	Hebert, Alex	ThP 327	Henderson, Holly	MP 380
Hastings, Mike	TP 531	Hebert, Alexander S.	ThP 068	Henderson, Hope	MP 218
Hatcher, Nathan	TP 061	Hebert, Alexander S.	ThP 179	Henderson, Jeffrey	TP 651
Hatcher, Nathan	WP 184	Hebert, Alexander S.	ThP 178	Henderson, Jeffrey P.	TP 348
Hatcher, Patrick	MP 573	Hebert, Alexander S.	WOD am 10:10	Henderson, Michelle	MP 218
Hatcher, Patrick	WOA pm 4:10	Hecht, Elizabeth S.	ThP 728	Henderson, Peter J. F.	WOH pm 3:10
Hatcher, Patrick G.	TP 605	Heck, Albert	TP 052	Hendricks, Nathan	ThOD pm 2:50
Hathout, Yetrib	MP 163	Heck, Albert	WOF am 09:30	Hendrickson, Chris L.	WP 734
Hathout, Yetrib	MP 424	Heck, Albert J. R.	ThP 301	Hendrickson, Christopher L.	MOB am 10:10
Hathout, Yetrib	ThOE am 09:50	Heck, Albert J. R.	TP 237	Hendrickson, Christopher L.	MP 084
Hathout, Yetrib	TP 467	Heck, Albert J.R.	MP 263	Hendrickson, Christopher L.	MP 648
Hatsis, Panos	ThP 535	Heck, Albert J.R.	ThP 212	Hendrickson, Christopher L.	MP 699
Hattem, Gaye	MP 156	Heck, Albert J.R.	TP 136	Hendrickson, Ronald	MP 036
Hauberg-Lotte, Lena	MP 021	Heck, Albert J.R.	WOE am 10:10	Hendrikse, Jan	MP 531
Hauck, Brian	TOC am 09:10	Heck, Albert J.R.	WOG am 09:30	Hendrix, Roger	TOC pm 3:30
Hauck, Brian	WP 693	Heckendorf, Christian	MP 120	Hengerer, Bastian	ThP 746
Haugh, Jason M.	WP 098	Heckendorf, Christian	MP 465	Hengstler, Jan	MP 452
Haughey, Norm	TP 468	Heckendorf, Christian	ThP 057	Henion, Jack	MP 395
Haura, Eric	TP 463	Heckendorf, Christian	WP 445	Henion, Jack	TP 277
Hauschild, Jan-Peter	MP 653	Heckendorf, Christian F.	TP 095	Henion, Jack	WP 644
Hauschild, Jan-Peter	ThP 762	Hecker, Michael	ThP 071	Henrich, Marco L.	ThP 072
Hauschild, Jan-Peter	TOB am 10:10	Hecker, Michael	ThP 774	Henrich, Christoph	MP 472
Hauser, Nicolas J.	TP 534	Hedberg, Christian	ThP 225	Henricson, Erik	ThOE am 09:50
Hausinger, Robert	ThP 489	Hedeland, Mikael	TP 566	Henry, Ryan	MP 227
Hauskins, Collin	ThP 103	Hedeland, Mikael	TP 628	Henschker, Christian	ThP 071
Havard, Guy	MP 488	Hedgepeth, William	WP 182	Hensley, Dr. Kenneth	WP 459
Havard, Guy	MP 489	Hedlund, Gustaf	MP 205	Hensley, Kenneth	WP 392
Havard, Guy	MP 491	Hedrick, Victoria	WP 169	Henson, Shelagh	ThP 636
Havard, Guy	MP 496	Heeb, Stephan	ThP 645	Hentze, Matthias W.	ThP 519
Havugimana, Pierre C.	ThP 060	Heegaard, Niels HH.	WP 467	Hentze, Matthias W.	TP 202
Hawke, David	MP 219	Heemskerk, Anthonius A.M.	WP 065	Hepler, John	TOF am 09:50
Hawke, David	WP 165	Heemskerk, Antonius	TP 149	Her, Guor-Rong	ThP 727
Hawkins, Aaron R.	MP 706	Heemskerk, Johan	TP 105	Heratch, Kithsiri	MP 075
Hawkridge, Adam	MP 064	Heeren, Ron	MOH pm 3:50	Herath, Kithsiri	ThOE am 09:10
Hawkridge, Adam	ThP 251	Heeren, Ron	WOC am 09:50	Herath, Kithsiri	WP 320
Haxo, Ted	WP 191	Heeren, Ron M.A.	MP 397	Herbele, Henry	WP 460
Hay, Ronald T.	ThP 241	Heeren, Ron M.A.	MP 704	Herbig, Jens	MP 663
Hayakawa, Yoshihiro	MP 739	Heeren, Ron M.A.	MP 703	Herbig, Jens	ThP 738
Hayakawa, Yoshihiro	MP 755	Heeren, Ron M.A.	ThOB pm 2:30	Hercules, David M.	TOC am 09:50
Hayakawa, Yoshihiro	ThP 672	Heeren, Ron M.A.	TOH pm 3:10	Herdering, Christina	MP 667
Hayakawa, Yoshihiro	TP 560	Heeren, Ron M.A.	TP 015	Herman, Joseph L.	MP 280
Hayden, Kevin	ThP 009	Heeren, Ron M.A.	TP 062	Herman, Joseph L.	TP 514
Hayen, Heiko	TP 272	Heeren, Ron M.A.	TP 597	Hermelin, Sylvain	MOD am 09:10
Hayen, Heiko	TP 287	Heeren, Ron M.A.	WOB am 08:50	Hermes, Jeffrey	MP 536
Hayes, Michael J.	MP 038	Heesom, Kate	MOG am 09:10	Hermjakob, Henning	MP 031
Hayes, William	MP 069	Hegeman, Adrian	TP 667	Hermjakob, Henning	ThP 034
Haynes, Paul	MP 273	Hegeman, Adrian D.	MP 412	Hernandez, Belinda	WP 475
Haynes, Paul	TP 211	Hegeman, Adrian D.	MP 413	Hernandez, Diana	MP 249

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Hernandez, Oscar	TOD pm 2:30	Hilger, Maximiliane	TOF am 09:30	Hoffman, Eric P	ThOE am 09:50
Hernandez, Oscar	TP 368	Hilger, Maximiliane	WP 049	Hoffman, Nathan	MP 669
Hernandez, Oscar	TP 372	Hilger, Ryan T.	TOB am 09:10	Hoffman, Nathan	MP 670
Herodes, Koit	MP 313	Hill, Alex R.	MP 522	Hoffman, Peter	ThP 689
Herold, David	MP 207	Hill, Brad	ThP 556	Hoffman, Peter	ThP 688
Herold, Michael	MP 638	Hill, Dennis	WP 466	Hoffman, Ron M.	TP 743
Herold, Michael	WP 592	Hill, Herbert	TP 432	Hoffman, Ronald	WP 116
Heron, Scott	MP 039	Hill, Herbert	WP 673	Hoffman, Tim L.	ThOC am 08:50
Heron, Scott	ThP 093	Hill, Herbert H.	WP 774	Hoffmann, Andreas	MP 431
Heron, Scott	TP 377	Hill, John	ThP 143	Hoffmann, Jonathan	TP 423
Heron, Scott	TP 400	Hill, Matthew	ThP 400	Hoffmann, Roland	ThP 389
Heron, Scott	TP 403	Hill, Ryan	WP 110	Hoffmann, William D.	MOB pm 3:30
Heron, Scott	WOB pm 4:10	Hill, Ryan	WP 120	Hoffmeister, Karin	TP 332
Heron, Scott	WP 751	Hill, Jr, Herbert H.	ThP 480	Hofman, Florence M.	ThP 680
Heron, Scott R.	WOB am 08:50	Hill, Jr., Herbert	TOC am 09:10	Hofmann, Daniela	WOF am 09:10
Heroux, Maxime	MP 428	Hill, Jr., Herbert	WP 693	Hogan, Chris	ThP 477
Heroux, Maxime S.	ThP 280	Hilliard, Mark	TP 156	Hogan, Chris	ThP 494
Herren, Luke	TP 227	Hilliard, Mark	WP 023	Hogan, Christopher	ThOC pm 4:10
Hershfeld, Kaylee	WP 303	Hilmer, Jonathan	WP 311	Hogberg, Helena	WP 581
Hersi, Siham S.	TP 563	Hilton, Donald	WP 461	Hoh, Eunha	TP 549
Hersman, Elisabeth	WP 331	Hilton, Gina	ThP 288	Højlund, Kurt	TP 488
Hersman, Elisabeth	WP 332	Himly, Martin	WP 153	Hoke, Robert	TP 311
Hertz-Schuenemann, Romy	MOD pm 2:50	Himmaty, Farhan	MP 443	Holcapek, Michal	MP 245
Hervey IV, William Judson	MP 278	Hines, Jolaine	WP 726	Holcapek, Michal	ThP 410
Hervey IV, William Judson	MP 279	Hines, Kelly	MP 595	Holčapek, Michal	ThP 396
Hesketh, Geoffrey	MP 258	Hinks, David	WP 306	Holcomb, Jennifer	WP 118
Hess, Nancy J.	TOA am 08:50	Hinrichs, Kai-Uwe	MP 549	Holden, Dustin	ThP 743
Hess, Philipp	WOC pm 2:50	Hirabayashi, Yoshio	ThP 397	Holden, Dustin	TOB am 08:30
Hess, Sonja	MP 225	Hirano, Ichiro	WP 130	Holden, Kyle	WP 117
Hess, Sonja	MP 226	Hirano, Takashi	TP 321	Holland, Patricia	MP 287
Hess, Sonja	ThOF pm 2:50	Hirao, Yoshiko	MP 739	Holland, Patricia	TOG pm 4:10
Hess, Sonja	ThP 147	Hiraoka, Kenzo	TP 727	Holland, Patricia	WP 429
Hess, Sonja	ThP 240	Hiraoka, Kenzo	TP 725	Holland, Patricia	WP 428
Hess, Sonja	ThP 310	Hiraoka, Kenzo	TP 726	Holland, Patricia L.	MP 532
Hettich, Robert	MP 129	Hiraoka, Kenzo	WP 381	Holle, Armin	ThP 573
Hettich, Robert	MP 277	Hird, Simon	TP 285	Holliman, Christopher	ThP 443
Hettich, Robert	MP 264	Hird, Simon	TP 282	Holliman, Christopher L.	ThP 674
Hettich, Robert	MP 276	Hird, Simon	TP 564	Holman, Hoi-Ying	TP 745
Hettich, Robert	MP 746	Hirschey, Matthew D.	TP 112	Holman, Stephen W.	MP 272
Hettich, Robert	ThP 332	Hirtz, Christophe	TP 472	Holmberg, Sydney	TP 759
Hettich, Robert	ThP 772	Hirtz, Christophe	WP 447	Holmes, Daniel	TOG pm 3:10
Hettich, Robert	TP 125	Hitchcock, Charles	MP 442	Holmes, Elaine	TOG pm 3:30
Hettich, Robert	TP 675	Hittle, Lauren	TP 291	Holmes, Paula	TP 728
Hettick, Justin M.	ThP 309	Hixson, Kim K.	TP 676	Holtkamp, Michael	WP 442
Hetzler, Martin	ThOC pm 3:10	Hnatyshyn, Serhiy	MP 622	Holyoake, Tessa	WP 114
Heuberger, Adam	ThP 608	Hnatyshyn, Serhiy	WP 732	Hommersom, Bob	MP 397
Heuberger, Adam	WP 720	Ho, Chun Loong	ThP 126	Hommersom, Bob	WOB am 08:50
Hewetson, John	MP 419	Ho, Emmie N.M.	WP 582	Hon, Wei Boon	ThP 783
Hewetson, John	WP 625	Ho, Hsiu-O	TP 382	Hong, Huang	MP 643
Hewitt, Josh	MP 625	Ho, Jenny T.C.	WP 510	Hong, Hui	ThP 538
Hewitt, Josh	TP 654	Ho, Johnny K.	MP 375	Hong, Jiyong	ThP 084
Hezel, Lori	ThP 431	Ho, Johnny K.	WP 394	Hong, Kwan Soo	TP 048
Hibbs, John A.	WP 552	Ho, Jonathan	ThP 598	Hong, Paula	MP 728
Hickok, Durlin	ThP 285	Ho, Stacy	WP 638	Hong, Qiuting	ThP 155
Hicks, Leslie	MP 114	Hoang, Khoa	MP 534	Hong, Qiuting	ThP 153
Hicks, Leslie	MP 414	Hoang, Khoa	TP 380	Hong, Qiuting	TP 119
Hicks, Leslie M.	MP 103	Hoang, Van	MP 144	Hong, Qiuting	WP 087
Hicks, Leslie M.	MP 102	Hoare, Jonathan	ThP 664	Hong, Teresa	ThP 386
Hidalgo, Manuel	ThP 294	Hobbs, Deborah	WP 436	Hong, Teresa B.	WP 472
Hidy, Bruce	MP 505	Hobbs, G. Aaron	MP 179	Honnold, Ron	ThP 615
Hidy, Bruce	MP 764	Hochart, Guillaume	TP 009	Honnold, Ron	TP 557
Hidy, Bruce	WP 127	Hochart, Guillaume	TP 050	Hood, Brian L.	ThP 202
Hieftje, Gary	WOB am 08:30	Hochstrasser, Denis	MP 148	Hooda, Ruchi	WP 615
Hieftje, Gary M.	ThOB pm 4:10	Hochstrasser, Denis	WP 156	Hoofnagle, Andrew	ThP 025
Higazi, Daniel	ThP 120	Hock, Christian	ThP 752	Hoofnagle, Andrew N.	TOG pm 3:50
Higazi, Daniel	WP 201	Hodek, Petr	ThP 354	Hoog, Jeremy	TP 173
Higbee, Alan J.	WOA am 09:50	Hodgkins, Chris	WP 425	Hoog, Jeremy	WOG pm 3:50
Higgins, Leeann	MP 033	Hodgson, Wayne C.	TP 303	Hoopes, J. Todd	TP 256
Higgins, LeeAnn	MP 049	Hoefkens, Jens	WP 050	Hoopmann, Michael R.	ThP 031
Higgins, LeeAnn	MP 104	Hoefler, Heinz	TP 052	Hoopmann, Michael R.	WP 766
Higgins, Leeann	MP 429	Hoehne, Steven	TP 506	Hoover, Michael E.	MP 229
Higgins, Leeann	TP 076	Hoek, Kristen	WP 243	Hooyberghs, Jef	MOG pm 3:10
Higgs, Jessica M.	MP 687	Hoekman, Liesbeth	ThP 545	Hop, Cornelis	ThP 357
Hike, Hiroshi	TP 383	Hoepfner, Morgan	ThP 117	Hop, Cornelis	WP 712
Hildebrand, Diana	ThOB pm 2:50	Hoermann, Katrin	WOF pm 2:50	Hop, Marcel	MP 499
Hildenbrand, Zacariah	ThP 557	Hoerth, Patric	MP 715	Hopcroft, Lisa	WP 114
Hilder, Emily F.	ThP 783	Hofele, Romina	ThP 456	Hopfer, Helene	MP 347
Hilderbrand, Amy	WP 049	Hoffman, Eric	TP 467	Hopfgartner, Gerard	MP 629
Hilgart, Ian	ThP 286	Hoffman, Eric P.	MP 424	Hopfgartner, Gerard	MP 632

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Hopfgartner, Gerard.....	TOA am 10:10	Hsu, Chuan-Chih.....	ThP 079	Huang, Min Zong.....	WP 346
Hopfgartner, Gerard.....	WP 614	Hsu, Chuan-Chih.....	TP 670	Huang, Min Zong.....	WP 415
Hopfgartner, Gérard.....	MP 057	Hsu, Hsu Chen.....	MP 305	Huang, Paul.....	MOF pm 4:10
Hopkins, W. Scott.....	ThP 505	Hsu, Kuo-Tung.....	MP 306	Huang, Qianyang.....	WP 530
Hopkinson, Alan C.....	ThP 691	Hsu, Kuo-Tung.....	MP 307	Huang, Richard.....	MOE pm 3:10
Hoppe, Carolyn.....	WP 445	Hsu, Pang-Hung.....	ThP 053	Huang, Richard.....	MP 172
Hoppe, Stephanie.....	ThP 343	Hu, Alex.....	TP 083	Huang, Rongrong.....	ThP 726
Hoppel, Charles L.....	ThP 431	Hu, Amanda.....	MP 236	Huang, Rongrong.....	TP 320
Hoppel, Charles L.....	WP 595	Hu, Bin.....	WP 375	Huang, Roy (TY).....	TP 531
Hopper, Erin.....	MP 072	Hu, Chang-Deng.....	WP 163	Huang, Tai-Chung.....	MP 255
Horáková, Jana.....	MP 135	Hu, Changqin.....	WP 414	Huang, Tai-Chung.....	ThP 219
Horan, Andrew.....	MOA am 09:10	Hu, Han.....	ThP 734	Huang, Taohong.....	TP 281
Horan, Andrew.....	MP 297	Hu, Hanfeng.....	ThP 187	Huang, Taohong.....	TP 757
Horie, Kanta.....	TOB pm 3:30	Hu, Jian-Zhi.....	WP 088	Huang, Taohong.....	WP 393
Horn, David.....	TP 264	Hu, Jiehui.....	WP 731	Huang, Taohong.....	WP 629
Horn, David.....	WP 202	Hu, Liping.....	TP 206	Huang, Taohong.....	WP 739
Horn, David.....	WP 262	Hu, Peibin.....	MP 337	Huang, Xian.....	TP 151
Horn, David.....	WP 263	Hu, Qingyuan.....	TP 475	Huang, Xiaodong.....	TP 779
Horn, David.....	TOC pm 2:30	Hu, Qingyuan.....	TP 474	Huang, Xiaohua.....	MP 643
Horn, David M.....	WP 065	Hu, Roger.....	WOG pm 2:30	Huang, Yeou-Lih.....	TP 399
Horn, David M.....	ThP 328	Hu, Shen.....	MP 596	Huang, Yeou-Lih.....	WP 346
Horn, Heiko.....	ThP 243	Hu, Shen.....	MP 634	Huang, Yingying.....	MP 596
Horn, Patrick.....	ThP 393	Hu, Valerie.....	MP 439	Huang, Yingying.....	MP 623
Horner, Julie.....	TP 294	Hu, Weimin.....	ThP 436	Huang, Yingying.....	MP 634
Hornshaw, Martin.....	WP 510	Hu, Wenbing.....	MOF am 08:30	Huang, Yingying.....	WP 287
Horowitz, Jeffrey.....	TP 139	Hu, Wenbing.....	ThP 128	Huang, Yining.....	ThP 142
Horowitz, Jeffrey.....	TP 488	Hu, Ye.....	WP 021	Huang, Yining.....	TP 331
Horsley, Andrew.....	MP 523	Hu, Yingwei.....	ThP 232	Huang, Yining.....	WP 080
Horswill, Alexander.....	WP 476	Hu, Yingwei.....	TP 092	Huang, Yiqun.....	ThP 711
Horuath, Thomas.....	TP 493	Hu, Yingwei.....	WP 252	Huang, Yiqun.....	TP 323
Hosamani, Ravikumar.....	TOA pm 3:30	Hu, Yunli.....	ThOH am 09:50	Huang, Yu.....	ThOH pm 4:10
Hosemans, Steven.....	ThP 764	Hu, Yunli.....	ThOH pm 2:50	Huang, Yu.....	ThP 711
Hosfield, Chris.....	TP 234	Hu, Yunli.....	ThP 154	Huang, Yu.....	ThP 734
Hoshi, Tomoomi.....	WP 393	Hu, Zeping.....	WP 607	Huang, Yu.....	WOF pm 2:30
Hosseingholizadeh, Ahmad.....	TP 085	Hu, Zhou.....	WP 159	Huang, Yu-Chen.....	MP 624
Hosseinzadehshahri, Leila.....	TP 036	Hua, Honghui.....	WP 416	Huang, Yue.....	TP 377
Hoteling, Andrew J.....	TP 787	Hua, Serenus.....	ThOH pm 3:10	Huang, Yue.....	TP 386
Hou, Aixin.....	MP 550	Hua, Serenus.....	ThP 168	Huang, Yue.....	TP 400
Hou, Guixue.....	ThP 323	Hua, Serenus.....	TP 257	Huang, Yue.....	TP 403
Hou, Guixue.....	WP 016	Hua, Serenus.....	TP 328	Huang, Yue.....	WOB am 08:50
Hou, Guixue.....	WP 152	Hua, Serenus.....	WP 066	Huang, Yue.....	WOB pm 4:10
Hou, Hongwei.....	TP 475	Hua, Zhendong.....	WP 298	Huang, Yu-Min.....	MP 384
Hou, Hongwei.....	TP 474	Huan, Tao.....	TP 655	Huang, Yuting.....	TP 452
Hou, Jingguo.....	TP 493	Huan, Tao.....	WP 605	Huang, Yuting.....	WP 593
Hou, Jingguo.....	TP 506	Huang, Amy.....	MP 738	Huang, Yuting.....	WP 677
Hou, Ming-Feng.....	WP 422	Huang, Amy.....	TP 768	Huang, Yuting.....	WP 678
Hou, Shuyu.....	MP 572	Huang, Amy.....	TP 769	Huang, Yuting.....	WP 676
Hou, Shuyu.....	TP 508	Huang, Beibei.....	ThP 649	Huang, Zejian.....	ThP 531
Hou, Sijian.....	WP 121	Huang, Bill.....	ThP 467	Huang, Zhengxu.....	ThP 574
Hou, Singyuk.....	WP 723	Huang, Chengsi.....	MP 229	Huang, Zhi-Qiang.....	ThP 149
Houde, Damian.....	TP 539	Huang, Chengsi.....	ThP 259	Hubbard, Simon.....	ThP 034
Houde, Damian.....	WP 081	Huang, Chengsi.....	TP 227	Hubbard, Simon J.....	MP 272
Houel, Stephane.....	TP 157	Huang, Chi-Jung.....	ThP 275	Huber, Christian.....	WP 153
Houel, Stephane.....	TP 265	Huang, Chun-Hao.....	MP 435	Huber, Jason D.....	TP 038
Houel, Stephane.....	TP 541	Huang, Dai-Yong.....	MP 346	Huber, Nicole.....	ThOG am 09:50
Houk, R.S.....	TP 671	Huang, Eric.....	MP 569	Hubert-Roux, Marie.....	ThP 499
Hoult, Robert.....	ThP 612	Huang, Eric.....	TP 677	Hubert-Roux, Marie.....	TP 406
Houser, Whitney.....	WP 364	Huang, Fan.....	MP 560	Hubert-Roux, Marie.....	TP 775
Housman, Kathleen.....	WP 107	Huang, Fan.....	TP 590	Hubert-Roux, Marie.....	WP 679
Houson, Hailey.....	MP 056	Huang, Gang.....	WP 196	Huc, Ivan.....	TOC am 08:50
Houten, Sander.....	MP 260	Huang, Guang.....	WP 473	Huc, Vincent.....	ThP 510
Hovmand, Lars.....	TOA pm 2:30	Huang, Guangming.....	MP 399	Hudak, Edward.....	MP 536
Howard, Audrey M.....	MP 506	Huang, He.....	WOG am 09:50	Hudgens, Jeffrey W.....	TP 256
Howard, Cecil.....	TOD am 09:10	Huang, Hehe.....	MP 348	Hudson, Aaron.....	ThP 316
Howard, Erinn C.....	MP 278	Huang, Huilian.....	WP 338	Hudson, Billy.....	MOH pm 2:30
Howard, Layne.....	ThP 744	Huang, Jeffrey.....	MP 214	Hudson, John.....	WP 308
Howe, Kevin.....	ThP 173	Huang, Jincui.....	WP 087	Hudson, Yvette R.....	MP 375
Howitt, Crispin.....	WOE pm 2:30	Huang, Jincui.....	WP 086	Hudson, Yvette R.....	WP 394
Howland, Matthew.....	MP 012	Huang, Jing.....	ThP 529	Huebner, Kay.....	MP 229
Hoyes, Emmy.....	WP 280	Huang, Junfeng.....	WP 473	Huebschmann, HJ.....	ThP 572
Hoyes, John B.....	MP 695	Huang, Juzheng.....	ThP 664	Huestis, Marilyn.....	TP 045
Hribar, James.....	WP 494	Huang, Ke.....	MP 644	Hughes, Chris.....	WP 126
Hruban, Ralph H.....	MP 255	Huang, Lan.....	ThP 463	Hughes, Christopher.....	TP 189
Hrudey, Steve.....	WOC pm 4:10	Huang, Lan.....	ThP 462	Hughes, Christopher J.....	ThOB pm 3:50
Hrudey, Steve.....	WP 567	Huang, Lin.....	WOC pm 3:10	Hughes, Cole.....	ThP 437
Hsi, Jane.....	ThP 605	Huang, Lingyi.....	MP 644	Hughes, Nicola.....	WP 122
Hsiao, He-Hsuan.....	MP 744	Huang, Min Zong.....	MP 382	Hughes, Nicola.....	WP 540
Hsieh, Ming-Yueh.....	MP 744	Huang, Min Zong.....	MP 402	Hughes, Nicola.....	WP 546
Hsieh, Ping-Kun.....	TP 121	Huang, Min Zong.....	TP 399	Hughes, Sarah.....	TP 505

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Huhman, David.....	MP 607	Iacob, Roxana E.....	ThP 130	Ishii, Haruhiko.....	WOG am 09:50
Huhman, David.....	ThP 636	Iacobuzio-Donahue, Christine A.....	MP 255	Ishii, Keisuke.....	ThP 721
Huhmer, Andreas.....	MP 652	Ianowski, Juan.....	MP 463	Ishii, Masaru.....	MP 269
Huhmer, Andreas.....	ThP 222	Iavarone, Anthony.....	MP 444	Ishikawa, Daisuke.....	WP 372
Huhmer, Andreas.....	ThP 613	Ibáñez, Borja.....	ThP 336	Ishikawa, Hideaki.....	WP 372
Huhmer, Andreas.....	TP 337	Ibrahim, Adel.....	ThP 241	Islam, Nazrul.....	TP 668
Hühmer, Andreas.....	WP 737	Ibrahim, Hend.....	MP 418	Ismailoglu, Ismail.....	MP 592
Huhtinen, Kaisa.....	ThP 276	Ibrahim, Hend.....	ThP 607	Isobe, Toshiaki.....	ThP 520
Hui, John O.....	ThP 246	Ibrahim, Hend.....	WP 550	Isobe, Toshiaki.....	WP 372
Humbert, Marc.....	MP 025	Ibrahim, Marianne.....	WP 498	Isoherranen, Nina.....	TP 400
Hummon, Amanda B.....	ThP 207	Ibrahim, Yehia.....	MOC pm 3:10	Isserlin, Ruth.....	MP 255
Hummon, Amanda B.....	ThP 200	Ibrahim, Yehia.....	ThOB am 10:10	Iurascu, Marius.....	WP 656
Hummon, Amanda B.....	TOH am 10:10	Ibrahim, Yehia.....	ThOG pm 4:10	Ivanov, Alexander.....	TP 149
Hummon, Amanda B.....	TP 006	Ibrahim, Yehia.....	TOC am 08:30	Ivanov, Alexander R.....	MP 147
Hummon, Amanda B.....	WP 632	Ibrahim, Yehia.....	WP 698	Ivanov, Alexander R.....	MP 219
Humphreys, W. Griff.....	WP 639	Ibrahim, Yehia.....	WP 767	Ivanov, Alexander R.....	TOB pm 3:10
Humphreys, W. Griffith.....	WOF am 08:30	Ibrahim, Yehia M.....	MP 677	Ivanov, Alexander R.....	TOC pm 2:30
Humphreys, William.....	WP 622	Ibrahim, Yehia M.....	ThP 741	Ivanov, Alexander R.....	TP 089
Humphries, Jamie.....	ThP 681	Ibrahim, Yehia M.....	TOB am 09:50	Ivanov, Alexander R.....	WP 065
Humphries, Jamie.....	ThP 682	Ibrahim, Yehia M.....	TP 717	Ivanov, Mark V.....	TP 081
Humphries, Jamie K.....	WP 621	Ibrahim, Yehia M.....	TP 716	Ivanov, Mark V.....	WP 164
Humston-Fulmer, Elizabeth.....	ThP 617	Ibrahim, Yehia M.....	TP 714	Iverson, Line V.....	WP 467
Huncik, Kevin.....	TP 567	Ichetovkin, Iliia.....	ThP 285	Iverson, Suzanne.....	TP 046
Hung, Chia.....	TP 651	Ichihara, Suguru.....	TOB pm 3:30	Ivey, Richard.....	ThP 218
Hung, Ruei-Hung.....	MP 389	Ichise, Ryutarō.....	ThP 165	Ivleva, Vera.....	TP 158
Hung, Sheng-Wei.....	MP 306	Ichou, Farid.....	ThP 696	Ivosev, Gordana.....	TP 085
Hung, Sunny.....	TOF pm 4:10	Ide, Jennifer L.....	TP 055	Ivosev, Gordana.....	TP 181
Hunt, Donald.....	MOH am 10:10	Ifa, Demian.....	TP 025	Iwabuchi, Haruo.....	MOF pm 3:10
Hunt, Donald.....	TOG am 08:50	Ifa, Demian.....	WP 379	Iwamoto, Shinichi.....	TP 166
Hunt, Donald.....	TP 188	Ihling, Christian.....	ThOF am 08:30	Iwata, Hiroshi.....	WP 018
Hunt, Donald F.....	MOE am 08:30	Ihssane, Bouchaib.....	WP 549	Iyer, Ramsunder.....	MP 746
Hunt, Donald F.....	MP 084	Ikeda, Erika.....	MP 476	Iyer, Rashi.....	MP 585
Hunt, Donald F.....	MP 146	Ikeda, Noriaki.....	ThP 592	Iyer, Srinivas.....	MP 585
Hunt, Donald F.....	ThP 686	Ikeda, Toru.....	MP 525	Izgarian, Nick.....	ThP 743
Hunter, Christie.....	MP 748	Ikram, A.....	TP 444	Izumi, Shunsuke.....	MP 130
Hunter, Christie.....	ThP 316	Ilagan, Robielyn.....	MP 727	Izumi, Takashi.....	MOF pm 3:10
Hunter, Christie.....	ThP 406	Ilchenko, Sergei.....	MP 169	Izumi, Yoshihiro.....	ThP 375
Hunter, Christie.....	ThP 407	Ileka, Kevin.....	WP 369	Jabbour, Rabih.....	ThP 077
Hunter, Christie.....	ThP 425	Iliopoulos, Othon.....	WP 077	Jabbour, Rabih.....	ThP 333
Hunter, Christie.....	TP 085	Iliuk, Anton.....	ThP 079	Jabs, Wolfgang.....	MOE pm 3:30
Hunter, Christie.....	WP 068	Ilonen, Jorma.....	WP 028	Jabs, Wolfgang.....	MP 148
Hunter, Christie.....	WP 497	Imamura, Amanda.....	TP 576	Jabs, Wolfgang.....	MP 157
Hunter, Christie.....	WP 635	Imhoff, Werner.....	MP 157	Jabs, Wolfgang.....	WP 156
Hunter, Christie L.....	ThOE pm 3:50	Imperial, Julita.....	MP 149	Jachtenberg, Jan-Willem.....	ThP 209
Hunter, Christie L.....	ThP 506	Imperial, Lorelie.....	WOB am 09:50	Jacksén, Johan.....	MP 078
Hunter, Christie L.....	TP 184	Impey, Gary.....	WP 268	Jacksén, Johan.....	MP 451
Hunter, Neil.....	MP 101	In, Moon Kyo.....	ThP 591	Jacksén, Johan.....	TP 411
Hunter, Neil.....	ThP 172	In, Yongha.....	MP 537	Jackson, Angela.....	ThP 026
Huo, Yin.....	TP 281	Indeykina, Maria.....	ThP 086	Jackson, Ayanna U.....	MP 054
Huppertz, Laura.....	MP 289	Indeykina, Maria I.....	TP 409	Jackson, Bruce.....	MP 239
Hur, Manhoi.....	ThP 652	Ingalls, Stephen T.....	ThP 431	Jackson, Bruce.....	WOE am 09:30
Hurme, Reini.....	TP 443	Ingalls, Stephen T.....	WP 595	Jackson, Glen P.....	MOB pm 3:30
Hurst, Harrell E.....	TP 305	Ingelsson, Martin.....	WP 489	Jackson, Isabel.....	TP 067
Hurst, Jerod.....	ThP 737	Ingendoh, Arnd.....	MP 615	Jackson, Isabel.....	TP 688
Hurt, Matthew.....	MOA am 09:50	Ingrande, Jerry.....	ThP 684	Jackson, Isabel L.....	ThP 390
Hurt, Matthew.....	MP 577	Inoue, Takahiro.....	TP 166	Jackson, Isabel L.....	ThP 642
Hurt, Matthew.....	MP 574	Interthal, Heidrun.....	ThP 104	Jackson, Isabel L.....	TP 299
Hurt, Matthew.....	TP 591	Inutan, Ellen.....	MP 538	Jackson, Lauren S.....	ThOA pm 4:10
Hurt, Matthew.....	WOA am 09:10	Inutan, Ellen.....	TP 163	Jackson, Lidia.....	MP 181
Huszagh, Alex.....	ThP 463	Inutan, Ellen.....	WOB am 09:50	Jackson, Philip.....	ThP 172
Hutchinson, Carolyn.....	MP 567	Ippoliti, Paul.....	TP 177	Jackson, Robert.....	MP 386
Hutchinson, Carolyn.....	MP 566	Ipsaro, Jonathan J.....	WP 170	Jackson, Robert.....	WP 507
Hutchinson, Carolyn.....	MP 565	Ipsen, Andreas.....	ThOB pm 3:30	Jackson, Robert.....	WP 758
Huttlin, Edward L.....	TOD pm 3:50	Iraneta, Pamela.....	MP 782	Jackson, Shelley N.....	MOH pm 2:50
Huttlin, Edward L.....	TP 145	Isaac, Giorgis.....	ThP 392	Jackson, Shelley N.....	ThP 387
Hutton, Erica.....	WP 524	Isaac, Giorgis.....	ThP 393	Jackson, Shelley N.....	TP 002
Huynh, Minh V.....	MP 179	Isaac, Giorgis.....	ThP 417	Jackson, Shelley N.....	TP 063
Hwang, Geum-Sook.....	TP 048	Isaac, Giorgis.....	WP 022	Jacob, Harrys K. C.....	ThP 204
Hwang, Kyubaek.....	TP 080	Isaacs, Jennifer S.....	TOE pm 4:10	Jacob, Sara.....	TP 238
Hwang, Kyu-Baek.....	ThP 020	Isailovic, Dr. Dragan.....	WP 459	Jacobs, Jon M.....	MP 100
Hwang, Leekyoung.....	ThP 078	Isailovic, Dragan.....	MOD pm 3:30	Jacobs, Ryan.....	WP 481
Hwang, Minsook.....	TP 258	Isailovic, Dragan.....	TP 292	Jacobs, William R.....	WP 111
Hwang, Sunil.....	WP 240	Isailovic, Dragan.....	WP 392	Jacobsen, Søren.....	WP 467
Hyche, Justin.....	WP 191	Iseberg, Samantha.....	ThOC am 09:30	Jacobson, Kenneth A.....	TP 773
Hyde, Shellie.....	TP 170	Iseberg, Samantha.....	TP 372	Jacobson, Rachelle.....	MP 439
Hye, Abdul.....	ThP 163	Iseberg, Samantha.....	WP 770	Jacoby, Rachelle.....	ThP 422
Hyöty, Heikki.....	WP 028	Ishida, Mayu.....	TP 193	Jadoul, Laure.....	TP 418
Hyung, Suk-Joon.....	ThP 502	Ishigai, Masaki.....	WP 183	Jaffe, Jacob.....	ThP 205
Iacob, Roxana E.....	MOE pm 3:10	Ishihama, Yasushi.....	TOB pm 3:30	Jaffe, Jacob D.....	ThP 217

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Jaffe, Jacob D.....	TP 177	Jenkins, Stefan.....	ThP 649	Jin, Song.....	ThP 078
Jaffe, Jacob D.....	WOD am 08:50	Jenkins, Stefan.....	TP 660	Jin, Song.....	WP 162
Jaffe, Jacob D.....	WOG pm 2:30	Jennings, Keith R.....	Special	Jing, Chen.....	MP 432
Jaffray, Ellis G.....	ThP 241	Jennische, Eva.....	TP 018	Jobst, Karl.....	TP 392
Jagmin, Jeff.....	ThP 416	Jensen, Kristian.....	MP 075	Jobst, Karl.....	WOC pm 2:30
Jagtap, Pratik.....	MOG pm 4:10	Jensen, Ole.....	MP 034	Jobst, Karl J.....	WP 575
Jagtap, Pratik.....	MP 033	Jensen, Ole.....	ThP 258	Jobst, Karl J.....	WP 576
Jagtap, Pratik.....	MP 049	Jensen, Ole Nørregaard.....	MP 719	Jockusch, Rebecca A.....	MOC am 09:50
Jagtap, Pratik.....	MP 104	Jensen, Ole Nørregaard.....	MP 718	Jockusch, Rebecca A.....	ThOD pm 2:30
Jagtap, Pratik.....	MP 429	Jensen, Ole Nørregaard.....	WOG am 08:30	Jockusch, Rebecca A.....	TP 343
Jagtap, Pratik.....	ThP 044	Jensen, Pernille Foged.....	TOF am 09:30	Jockusch, Rebecca A.....	TP 370
Jagtap, Pratik.....	TP 077	Jeong, Clara.....	WP 562	Jodari, Farman.....	MP 347
Jagtap, Pratik.....	TP 076	Jeong, Mark.....	MP 117	Joh, Yoonsung.....	TP 080
Jahn, Sandra.....	MP 632	Jeong, Seul-Ki.....	ThP 024	Johansen, Eric.....	MOC pm 2:30
Jahouh, Farid.....	MP 516	Jeong, Seunghyup.....	TP 328	Johansen, Eric.....	ThP 067
Jain, Shobhit.....	MP 255	Jeong, Yu-Dong.....	ThP 591	Johansen, Eric.....	TP 184
Jaiswal, Mihir.....	ThP 054	Jeremic, Aleksander.....	TP 135	Johansen, Eric.....	WP 185
Jalah, Rashmi.....	WP 211	Jernerén, Fredrik.....	MP 786	Johansen, Eric.....	WP 270
Jalili, Nobar.....	ThP 719	Jerome, Morganne.....	TP 213	Johansson, Mats W.....	ThP 348
James, Lindsey.....	TP 201	Jersie-Christensen, Rosa R.....	ThP 321	John, Jaya John.....	ThP 002
Jamil, Amer.....	MP 414	Jertz, Roland.....	MOB am 08:50	John, Manohar.....	MP 466
Jander, Georg.....	WP 589	Jhang, Siou-Sian.....	MP 389	Johns, Doug.....	TP 459
Jang, Yu Jin.....	TP 441	Jhang, Siou-Sian.....	MP 402	Johns, Douglas.....	ThOE am 09:10
Janicki, Susan.....	MP 095	Jhilal, Faycal.....	WP 549	Johns, Douglas G.....	TP 061
Janis, Gregory.....	WP 720	Ji, Chengjie.....	TP 545	Johnson, Adam.....	ThP 357
Janiszewski, John.....	MOF pm 2:50	Ji, Injung.....	ThOH pm 3:10	Johnson, Andrew R.....	MP 618
Janiszewski, John.....	MP 639	Ji, Qin.....	MOF pm 3:30	Johnson, Benjamin.....	MP 643
Janiszewski, John.....	ThP 424	Ji, Qin.....	TP 501	Johnson, Casey.....	MP 711
Janiszewski, John.....	ThP 505	Ji, Qingin.....	ThP 033	Johnson, Christine.....	MP 206
Janiszewski, John.....	TP 625	Ji, Weihua.....	WP 497	Johnson, Christopher.....	TP 711
Janiszewski, John.....	WP 627	Ji, Yuhuan.....	MOH am 08:50	Johnson, Darryl.....	MP 194
Janiszewski, John.....	WP 617	Jia, Chenxi.....	MOH am 09:10	Johnson, Darryl.....	ThP 429
Janiszewski, John.....	WP 618	Jia, Echo W.....	MP 378	Johnson, David W.....	WP 431
Janiszewski, John S.....	ThP 473	Jia, Shiling.....	TP 469	Johnson, Dennis A.....	WP 774
Jankowska, Ewa.....	MP 681	Jia, Wei.....	WP 298	Johnson, Eric.....	MP 536
Jansat, Josep.....	ThP 496	Jia, Weitao.....	WP 276	Johnson, Gary L.....	TP 173
Janzen, Stefanie.....	TP 153	Jia, Xiaoying.....	ThP 073	Johnson, Grant.....	ThOD pm 4:10
Japertas, Pranas.....	WP 025	Jia, Xiaoying.....	TP 117	Johnson, James.....	MOG pm 4:10
Jara, Jose.....	TP 584	Jia, Xinqiao.....	MOA pm 2:30	Johnson, James.....	MP 033
Jariwala, Freneil.....	WP 383	Jian, Wenying.....	WP 390	Johnson, James.....	MP 049
Jariwala, Freneil B.....	WP 552	Jiang, Carol.....	MP 738	Johnson, James.....	ThP 044
Jarratt, Rebecca E.....	WP 678	Jiang, Carol.....	TP 769	Johnson, James.....	TP 077
Jarratt, Rebecca E.....	WP 676	Jiang, Carol.....	TP 768	Johnson, Jamie L.....	WP 511
Jarrell, Tiffany.....	MP 575	Jiang, Chang.....	MP 337	Johnson, Janine.....	ThP 650
Jarrell, Tiffany.....	ThP 758	Jiang, Fan.....	TP 107	Johnson, Jay S.....	WP 742
Jarrell, Tiffany.....	TP 589	Jiang, Gongyu.....	ThP 574	Johnson, Joshua L.....	TP 623
Jarrett, Harry.....	TP 412	Jiang, Hao.....	MP 074	Johnson, Katina.....	MP 072
Jarrett, Nikki.....	WP 121	Jiang, Hao.....	TOE am 09:30	Johnson, Keith.....	WP 208
Jarrold, Martin.....	MP 698	Jiang, Hongxia.....	MP 734	Johnson, Kevin J.....	WP 382
Jaruga, Pawel.....	WP 707	Jiang, Hua.....	WP 253	Johnson, Michael.....	ThP 131
Jarvis, Jacqueline M.....	TP 599	Jiang, Hua.....	WP 569	Johnson, Michael.....	WP 483
Jarvis, Jacqueline M.....	TP 598	Jiang, Huafang.....	TP 520	Johnson, Pete.....	MOA am 09:30
Jarvis, Jacqueline M.....	WOA pm 3:50	Jiang, Hui.....	WP 520	Johnson, Pete L.....	MP 054
Jarvis, Jacqueline M.....	WP 706	Jiang, Jie.....	MP 357	Johnson, Richard S.....	ThP 763
Jarvis, Michael J. Y.....	WP 308	Jiang, Lu.....	MOH pm 3:50	Johnson, Robert.....	TP 040
Jarvis, Michael J. Y.....	WP 295	Jiang, Lu.....	TP 062	Johnson, Rudolph.....	MP 194
Jaulhac, Benoît.....	MP 450	Jiang, Shan.....	MP 009	Johnson, Rudolph.....	ThP 429
Jaumot, Joaquim.....	TP 639	Jiang, Taijiao.....	MP 222	Johnson, Ryan.....	MOD am 08:30
Javahery, Reza.....	MP 656	Jiang, Tao.....	TP 344	Johnson, Ted W.....	TP 028
Javahery, Reza.....	TP 374	Jiang, Wen.....	WP 597	Johnson, Will.....	MP 688
Jayachandran, Vignesh.....	ThP 045	Jiang, Wentao.....	WP 706	Johnston, Murray.....	MOA am 09:10
Jayaram, Savita.....	MP 255	Jiang, Xi.....	ThP 098	Johnston, Murray.....	MP 297
Jayaraman, Dhileepkumar.....	TP 669	Jiang, Xiaoming.....	TP 645	Johnston, Murray.....	ThP 368
Jayasekara, M. P. Suresh.....	TP 773	Jiang, Xiaoyue.....	MP 652	Johnston, Murray.....	ThP 367
Jayasundera, Keerthi.....	ThP 357	Jiang, Xuntian.....	WP 520	Johnston, Murray.....	ThP 550
Jayne, John T.....	TOA pm 3:10	Jiang, Yanjie.....	WP 173	Johnston, Murray.....	ThP 553
Jean, Nicolas.....	MP 493	Jiang, Ying.....	WP 723	Jois, Bhavna.....	ThP 122
Jean, Nicolas.....	MP 491	Jiang, You.....	MP 650	Jolliffe, Charles.....	TP 374
Jean Beltran, Pierre.....	WP 244	Jiang, Yutao.....	TP 681	Jonakin, Kelli.....	WP 124
Jecmen, Tomas.....	ThP 354	Jiang, Yuxuan.....	WP 088	Jonakin, Kelli.....	WP 270
Jedrychowski, Mark.....	MP 133	Jiang, Zheng.....	ThP 324	Jones, A. Daniel.....	MP 564
Jedrychowski, Mark P.....	ThP 214	Jiang, Ziwen.....	WP 723	Jones, A. Daniel.....	MP 619
Jedrychowski, Mark P.....	TOG am 09:50	Jiao, Lili.....	MP 610	Jones, A. Daniel.....	ThP 660
Jehmlich, Nico.....	ThP 250	Ji-Jeong, Ryu.....	MP 482	Jones, A. Daniel.....	TOA am 08:30
Jelbmann, Astrid.....	TP 031	Jimenez, Jose L.....	TOA pm 3:10	Jones, A. Daniel.....	TP 646
Jelinek, Christine.....	ThOE pm 3:30	Jin, Chunfen.....	TP 589	Jones, A. Daniel.....	WP 612
Jenkins, Rand.....	MP 505	Jin, Feng.....	MOB pm 3:30	Jones, Andrew.....	MP 031
Jenkins, Rand.....	MP 764	Jin, Fulai.....	WOG am 09:50	Jones, Andrew.....	ThP 034
Jenkins, Rand.....	WP 127	Jin, Jian.....	TP 173	Jones, Andrew R.....	ThP 036

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Jones, Andrew W.....	TOD pm 3:30	Julia, Smith.....	WP 444	Kaltashov, Igor.....	WP 216
Jones, Chad.....	TOB am 08:50	Julian, Ryan R.....	MP 145	Kaltashov, Igor A.....	ThP 090
Jones, Christina.....	MP 599	Julian, Ryan R.....	ThOD am 09:30	Kaltashov, Igor A.....	ThP 116
Jones, Christina M.....	MP 274	Julian, Ryan R.....	ThOD pm 2:50	Kaltashov, Igor A.....	TOE am 10:10
Jones, Dan.....	ThP 045	Julian, Ryan R.....	TOD pm 3:10	Kalu appulage, Danajaya.....	ThP 430
Jones, Donald J.L.....	TP 487	Julian, Ryan R.....	TP 129	Kamakura, Takeo.....	TOB pm 3:30
Jones, E. Ellen.....	TP 065	Julien, Jean-Philippe.....	TOF am 08:50	Kamali Sarvestani, Afrand.....	MP 564
Jones, Emrys.....	MP 004	Jun, Zhang.....	TP 185	Kamani, Mustafa.....	TP 065
Jones, Emrys.....	ThP 664	Jung, Hanyoung.....	TP 214	Kamel, Amin.....	TP 623
Jones, Emrys.....	TOG pm 3:30	Jung, Hyun-Jin.....	TP 441	Kamendi, Harriet.....	TP 300
Jones, Emrys A.....	MOH pm 3:10	Jung, Jette.....	TP 212	Kamga, Albert.....	TP 605
Jones, Emrys A.....	ThP 379	Jung, Jin Woo.....	TP 048	Kamita, Masahiro.....	WP 143
Jones, Emrys A.....	TP 375	Jung, JM.....	ThP 572	Kamlage, Beate.....	WP 592
Jones, Gareth Rhys.....	TP 751	Jung, Kook.....	WP 240	Kamphuis, Lars.....	MP 419
Jones, Jace.....	ThP 638	Jung, Stephan.....	ThP 215	Kan, Zhong-yuan.....	MOF am 08:30
Jones, Jace.....	WP 601	Jung, Sunhee.....	TP 473	Kan, Zhong-yuan.....	ThP 128
Jones, Jace W.....	MP 039	Jung, Young-Rim.....	MP 360	Kanamori-Kataoka, Mieko.....	MP 525
Jones, Jace W.....	ThP 390	Jung, Yura.....	TP 509	Kanamori-Kataoka, Mieko.....	MP 526
Jones, Jace W.....	ThP 642	Jungju, Seo.....	MP 482	Kanazawa, Mitsuhiro.....	WP 604
Jones, Jace W.....	TP 067	Jungmichel, Stephanie.....	ThP 243	Kandukuri, Surya.....	WP 546
Jones, Jace W.....	TP 299	Jungmichel, Stephanie.....	WP 109	Kandukuri, Surya.....	WP 540
Jones, Jace W.....	TP 688	Junninen, Heikki.....	TOA pm 3:10	Kane, Maureen.....	ThP 638
Jones, Jamey.....	MP 395	Junnotula, Venkatraman.....	MP 501	Kane, Maureen.....	TP 688
Jones, Lisa.....	MP 175	Junot, Christophe.....	MP 527	Kane, Maureen.....	WP 601
Jones, Lisa M.....	MP 174	Junot, Christophe.....	MP 528	Kane, Maureen A.....	MP 039
Jones, Mary B.....	ThP 626	Junot, Christophe.....	MP 581	Kane, Maureen A.....	ThP 390
Jones, Matt.....	MP 513	Junot, Christophe.....	MP 587	Kane, Maureen A.....	ThP 642
Jones, Michael.....	ThP 393	Junot, Christophe.....	ThP 140	Kane, Maureen A.....	TP 067
Jones, Rhys.....	MP 341	Junot, Christophe.....	ThP 391	Kane, Maureen A.....	TP 299
Jones, Rhys.....	MP 783	Junot, Christophe.....	ThP 696	Kane, Maureen A.....	TP 437
Jones, Rhys.....	MP 761	Junot, Christophe.....	TP 224	Kang, Hee-Gyoo.....	TP 441
Jones, Rhys.....	MP 760	Junot, Christophe.....	TP 472	Kang, Huan.....	WP 464
Jones, Rhys.....	MP 759	Junot, Christophe.....	TP 577	Kang, Sohye.....	WP 254
Jones, Rhys.....	MP 758	Junot, Christophe.....	WP 281	Kang, Yang.....	TP 186
Jones, Rhys.....	MP 757	Junqueira, Magno.....	MP 159	Kang, Yang.....	WP 772
Jones, Rhys.....	MP 756	Junqueira, Magno.....	TP 686	Kang, Young-Moon.....	ThP 312
Jones, Rhys.....	ThP 589	Jürschik, Simone.....	ThP 738	Kani, Kian.....	TP 195
Jones, Robert M.....	ThP 555	Justice, Nicholas.....	TP 125	Kannan, Gunasekaran.....	ThP 246
Jones, Jr, Elliot.....	MP 197	Kabe, Yasuaki.....	ThP 111	Kanyo, Jean.....	TP 572
Jones-Lepp, Tammy.....	WP 579	Kaboord, Barb.....	WP 514	Kao, Yi-Ying.....	TP 382
Jonsson, Tobias.....	WP 597	Kadar, Eugene.....	ThP 677	Kapinos, Brendon.....	MOF pm 2:50
Joo, Ahyoung.....	ThP 680	Kadek, Alan.....	MP 183	Kapinos, Brendon.....	ThP 424
Joo, Ahyoung.....	TP 195	Kadi, Adnan A.....	MP 726	Kapinos, Brendon.....	WP 627
Joore, Jos.....	ThP 209	Kadi, Adnan A.....	MP 725	Kaplan, Desmond.....	MP 689
Jorabchi, Kaveh.....	ThOB am 08:50	Kadiyala, Pathanjali.....	TP 501	Kaplan, Desmond.....	ThP 266
Jorabchi, Kaveh.....	TP 273	Kadiyala, Vivek.....	ThOE pm 4:10	Kaplan, Desmond.....	TP 178
Jorabchi, Kaveh.....	WOB am 09:30	Kafle, Amol.....	WP 775	Kaplan, Desmond.....	WP 670
Jorabchi, Kaveh.....	WP 749	Kafle, Amol.....	WP 776	Kaplan, Muammer.....	ThP 609
Jordan, Alfons.....	MP 663	Kafonek, C.....	MP 507	Kaplon, Joanna.....	MP 263
Jordan, Alfons.....	ThP 738	Kaftan, Filip.....	MP 030	Kapono, Cliff.....	MP 020
Jordan, Steve.....	MP 341	Kagan, Jacob.....	WP 513	Kapp, Eugene.....	WP 029
Jordan, Steve.....	MP 758	Kahen, Kaveh.....	ThOB am 08:50	Karamanou, S.....	WP 229
Jordan, Steve.....	MP 783	Kahen, Kaveh.....	WP 749	Karamanou, Spyridoula.....	WP 219
Jordan, Steve.....	MP 757	Kahler, Ty.....	MP 281	Karancsi, Tamás.....	MP 404
Jordan, Steve.....	ThP 589	Kai-Chi Lau, Justin.....	ThP 691	Karas, Michael.....	ThP 141
Jorge, Lucie.....	ThP 389	Kailas, Ajay.....	TP 002	Karasawa, Kaoru.....	ThP 497
Jorge Cerrudo, Inmaculada.....	ThP 336	Kailemia, Muchena J.....	TP 329	Karateev, Grigory.....	WP 172
Jorgensen, Thomas J.D.....	WP 219	Kailemia, Muchena J.....	WOD pm 3:10	Karch, Kelly.....	ThP 237
Jørgensen, T.J.D.....	WP 229	Kailich, Tobias.....	WP 049	Karch, Kelly R.....	MP 099
José Daroda, Romeu.....	MP 570	Kaiser, Nathan.....	MOB am 10:10	Karch, Kelly R.....	TP 184
Joseph, Jincy.....	MP 568	Kaiser, Nathan.....	WP 734	Karger, Barry.....	TP 149
Joseph, Prasanth.....	TP 274	Kaiser, Nathan K.....	MP 084	Karger, Barry L.....	MP 147
Joseph, Raji E.....	WP 221	Kaiser, Nathan K.....	MP 648	Karger, Barry L.....	TOB pm 3:10
Joseph, Siji.....	MP 481	Kaiser, Nathan K.....	MP 699	Karger, Barry L.....	TOC pm 2:30
Joseph, Siji.....	ThP 673	Kaiser, Nathan K.....	TP 720	Karger, Barry L.....	TP 089
Joseph, Siji.....	TP 513	Kaiser, Nathan K.....	WP 705	Karger, Barry L.....	WP 065
Josephs, Jonathan L.....	WP 622	Kajihara, Shigeki.....	TP 166	Karikari, Nana Kofi.....	TP 061
Joshi, Preeti.....	MP 158	Kajita, Ryo.....	MP 096	Kariv, Ilona.....	TOF pm 3:30
Joshi, Vivek.....	TP 190	Kalb, Suzanne R.....	MP 529	Karki, Santosh.....	TP 407
Jouanin, Isabelle.....	TP 649	Kalinitchenko, Iouri.....	ThP 764	Karlsson, Niclas.....	WP 072
Joy, Rosa.....	WOF am 09:50	Kaliyaperumal, Ashokkumar.....	ThP 736	Karlsson, Oskar.....	MP 003
Jozefowicz, Anna Maria.....	MP 416	Kalkum, Markus.....	ThP 386	Karlsson, Oskar.....	MP 786
Ju, Yue.....	MP 138	Kalkum, Markus.....	ThP 526	Karlsson, Oskar.....	TP 013
Juba, Melanie.....	TP 188	Kalkum, Markus.....	WP 472	Karpov, Dmitry S.....	TP 081
Juehne, Tom.....	ThP 260	Käll, Lukas.....	WP 034	Karpova, Maria A.....	TP 081
Juelich, Terry.....	TP 072	Kallback, Patrik.....	MP 026	Karreman, Christiaan.....	ThP 746
Juhasz, Peter.....	ThP 780	Kallback, Patrik.....	TP 012	Karst, Uwe.....	MP 007
Juhasz, Peter.....	ThP 781	Kalli, Anastasia.....	ThOF pm 2:50	Karst, Uwe.....	MP 477
Juhl Jensen, Lars.....	ThP 243	Kalmeyer, Vadim.....	WP 354	Karst, Uwe.....	MP 667

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Karst, Uwe.....	MP 709	Kehler, Jonathan.....	TP 466	Kerner, Alexander.....	MP 445
Karst, Uwe.....	TP 031	Kehler, Jonathan.....	TP 465	Kerns, Ed.....	MP 514
Karst, Uwe.....	TP 032	Keifer, David.....	ThOC pm 3:30	Kero, Frank.....	MP 341
Karst, Uwe.....	TP 555	Keil, Adam.....	MOB pm 2:30	Kero, Frank.....	MP 756
Karst, Uwe.....	TP 611	Keil, Adam.....	MP 530	Kero, Frank.....	MP 783
Karst, Uwe.....	TP 612	Keilich, Lauren C.....	ThP 274	Kero, Frank.....	MP 769
Karst, Uwe.....	WP 442	Keirse, Jeremy.....	ThP 263	Kero, Frank.....	MP 761
Karty, Jonathan A.....	ThP 646	Kelchtermans, Pieter.....	MP 032	Kero, Frank.....	MP 760
Kashuba, Angela.....	TOH am 08:50	Kelchtermans, Pieter.....	MP 682	Kero, Frank.....	MP 759
Kashuba, Angela.....	TP 011	Kelkar, Dhanashree.....	MP 270	Kero, Frank.....	MP 757
Kashuba, Angela.....	WP 011	Kelkar, Dhanashree S.....	MP 255	Kero, Frank.....	MP 758
Kashuba, Angela D. M.....	ThP 006	Kelkar, Jitendra.....	TP 497	Kero, Frank.....	ThP 589
Kashyap, Manoj.....	ThP 204	Kelkar, Jitendra.....	TP 496	Kerr, Candace L.....	TP 427
Kasi, Mohan.....	TP 529	Kelkar, Jitendra.....	TP 498	Kerr, Candace L.....	MP 255
Kasi, Mohan.....	TP 528	Kelkar, Jitendra.....	TP 763	Kerr, Richard.....	TOF pm 3:50
Kasi, Mohan.....	WP 328	Kelkar, Jitendra.....	TP 761	Kersten, Hendrik.....	MOD pm 4:10
Kasi, Mohan.....	WP 539	Kelkar, Jitendra.....	TP 762	Kersten, Hendrik.....	MP 299
Kaspar, Stephanie.....	MP 416	Kelkar, Jitendra.....	WP 350	Kersten, Hendrik.....	MP 315
Kaspar, Stephanie.....	MP 723	Kelleher, Neil L.....	MP 676	Kersten, Hendrik.....	MP 684
Kaspar, Stephanie.....	ThP 253	Kelleher, Neil L.....	ThP 058	Kersten, Hendrik.....	TP 737
Kaspar, Stephanie.....	WP 727	Kelleher, Neil L.....	ThP 060	Kersten, Hendrik.....	TP 732
Kasper, Tina.....	WP 410	Kelleher, Neil L.....	ThP 059	Kersten, Hendrik.....	TP 734
Kass, David A.....	TP 477	Kelleher, Neil L.....	ThP 144	Kertesz, Vilmos.....	ThP 670
Kasten, Tom.....	TP 448	Kelleher, Neil L.....	TOD am 08:30	Kery, Vladimir.....	TP 206
Katagi, Munehiro.....	ThP 592	Kelleher, Neil L.....	TOE pm 3:30	Keshavjee, Shaf.....	ThP 267
Kato, Dawn.....	MP 559	Kelleher, Neil L.....	TP 196	Keshet, Uri.....	TP 608
Katselis, George.....	MP 463	Kelleher, Neil L.....	TP 234	Keshishian, Hasmik.....	TP 426
Katsumura, Koichi.....	MP 460	Kelleher, Neil L.....	WOH pm 3:30	Kesimer, Mehmet.....	ThP 270
Katz, Jonathan.....	TP 195	Kelleher, Neil L.....	WP 157	Kessler, Benedikt.....	ThP 342
Katz, Jonathan E.....	ThP 680	Keller, Mark P.....	WOD am 10:10	Keunen, Olivier.....	TP 050
Katzman, Shana.....	WP 118	Kelley, David.....	MP 075	Kevala, Karl R.....	ThP 384
Katzmann, Jerry.....	ThP 345	Kelley, James A.....	MP 189	Keyes, Philip.....	WP 710
Kaufman, Eric.....	ThP 010	Kelley, Richard.....	WP 438	Khairallah, George N.....	MOD am 08:50
Kaufman, Eric.....	TP 665	Kellie, John.....	TOE am 08:30	Khairallah, George N.....	TP 355
Kaupmees, Karl.....	MP 313	Kellmann, Markus.....	MP 186	Khakinejad, Mahdiar.....	TP 540
Kauppila, Tiina J.....	MP 299	Kellmann, Markus.....	MP 653	Khakinejad, Mahdiar.....	WP 699
Kauppila, Tiina J.....	MP 315	Kellmann, Markus.....	ThP 317	Khaledi, Morteza.....	ThP 731
Kauppila, Tiina J.....	TP 401	Kellmann, Markus.....	ThP 321	Khalfallah, Faiza.....	WP 248
Kauppila, Tiina J.....	WP 378	Kellmann, Markus.....	TOB am 10:10	Khan, Aafaque A.....	MP 255
Kaur, Parminder.....	ThP 355	Kellmann, Markus.....	TP 280	Khan, Arshad.....	WP 516
Kaur, Parminder.....	TP 233	Kellmann, Markus.....	TP 298	Khan, Nasrin.....	MOC am 10:10
Kaur, Surinder.....	WP 277	Kellmann, Markus.....	WOF am 10:10	Khan, Zareen.....	TP 762
Kawachi, Nicole.....	MP 421	Kellmann, Markus.....	WP 301	Khan, Zia.....	MP 121
Kawahara, Kazuki.....	MP 067	Kelln, Wayne.....	MP 069	Khan, Zia.....	MP 212
Kawahara, Rebeca.....	WP 460	Kelly, Brian.....	MP 414	Khanna, Richie.....	WOH am 10:10
Kawai, Takayuki.....	TOA am 09:10	Kelly, Isabelle.....	ThP 287	Kharchenko, Andriy.....	MP 704
Kawai, Yosuke.....	MP 247	Kelly, Paul F.....	MP 522	Kharchenko, Andriy.....	MP 703
Kawamukai, Takatomo.....	TP 383	Kelly, Ryan.....	MOC pm 3:10	Kharybin, Oleg.....	MOB am 08:50
Kawamura, Hidehisa.....	TP 604	Kelly, Ryan.....	TP 715	Khatri, Kshitij.....	WP 008
Kawana, Shuichi.....	ThP 641	Kelly, Ryan T.....	TOB pm 4:10	Khatri, Kshitij.....	WP 085
Kawano, Shin-ichi.....	TP 281	Kelm, Jens.....	WP 154	Khatri, Kshitij.....	WP 674
Kawano, Shin-ichi.....	TP 757	Kelstrup, Christian D.....	ThP 321	Khera, Smriti.....	ThP 673
Kawano, Shin-ichi.....	WP 393	Kempf, Juergen.....	MP 289	Khiron Rokhas, Maria.....	MP 078
Kawano, Shin-ichi.....	WP 739	Kempf, Valerie.....	WP 480	Khmelniskii, Artem.....	TP 015
Kawasaki, Hideya.....	MP 067	Kenar, Erhan.....	MP 052	Khochbin, Saadi.....	WOG am 09:50
Kawasaki, Kumiko.....	WP 143	Kennedy, George.....	TP 228	Khodonov, Andrey.....	TOA pm 4:10
Kawashima, Miho.....	ThP 672	Kennedy, Jacob.....	ThP 025	Khojasteh, Cyrus.....	ThP 357
Kawashima, Miho.....	WP 449	Kennedy, Jacob.....	ThP 218	Khojasteh, Cyrus.....	WP 712
Kayadibi, Huseyin.....	ThP 676	Kennedy, Joseph H.....	WP 400	Khoo, Kay-Hooi.....	ThP 160
Kayampilly, Pradeep.....	ThP 662	Kennedy-Gabb, Sonya.....	TP 394	Khoo, Kay-Hooi.....	TP 121
Kaylor, Adam.....	MP 379	Kenney, Jim.....	MP 781	Khoo, Kay-Hooi.....	TP 207
Kaylor, Adam.....	TP 728	Kenny, Daniel J.....	ThP 748	Khot, Lav R.....	WP 774
Kaylor, Adam.....	TP 730	Kenny, Daniel J.....	ThP 749	Khristenko, Nina.....	ThP 534
Kaylor, Adam.....	WOB am 10:10	Kenny, Tara.....	WP 010	Khunjar, Wendell.....	TP 553
Ke, Yan.....	WP 633	Kent, Michael S.....	MOF am 09:30	Khurana, Siddhartha.....	WP 531
Ke, Yuyong.....	TP 495	Kenttamaa, Hiikka.....	MP 575	Kibbey, Richard.....	ThP 424
Ke, Zhenlian.....	WP 184	Kenttamaa, Hiikka.....	ThOD am 09:50	Kiehne, Andrea.....	MOE pm 3:30
Keasling, Jay D.....	TP 175	Kenttamaa, Hiikka I.....	WOA am 08:50	Kiehne, Andrea.....	MP 292
Kedia, Komal.....	WOE am 09:30	Kenttamaa, Hiikka.....	MOA am 09:50	Kiehne, Andrea.....	WP 063
Keefer, Christopher.....	TP 625	Kenttamaa, Hiikka.....	MP 577	Kiernan, Urban.....	WP 192
Keegan, Sarah.....	MOE am 09:30	Kenttamaa, Hiikka.....	MP 775	Kiernan, Urban.....	WP 266
Keegan, Sarah.....	TP 089	Kenttamaa, Hiikka.....	ThP 758	Kieser, William E.....	MP 656
Keelor, Joel.....	MP 379	Kenttamaa, Hiikka.....	TP 360	Kil, Yong.....	MOE am 09:10
Keelor, Joel.....	WOB am 10:10	Kenttamaa, Hiikka.....	TP 358	Kil, Yong.....	MOG pm 2:50
Keelor, Joel D.....	TP 729	Kenttamaa, Hiikka.....	TP 589	Kil, Yong.....	WP 041
Keen, Denise A.....	ThP 526	Keppel, Theodore.....	MOF am 08:50	Kil, Yong J.....	TP 091
Kehasse, Amanuel.....	TP 095	Kerjaschki, Donscho.....	TP 053	Kil, Yong Joo.....	TP 074
Kehler, Jonathan.....	TOE am 08:30	Kerner, Alexander.....	MOF pm 3:50	Kilby, Greg.....	MP 199
Kehler, Jonathan.....	TOE am 09:50	Kerner, Alexander.....	MP 310	Kilby, Greg.....	TOH am 09:50

Program code: M,T,W, Th = Day    O = Oral, P = Poster    Time or poster number

# INDEX OF AUTHORS



Kilby, Greg.....	WP 405	Kim, Sunghwan.....	MP 300	Kjeldsen, Frank.....	MP 718
Kilby, Greg W.....	MP 002	Kim, Sunghwan.....	WOA pm 2:30	Kjellström, Anna.....	ThP 394
Kilby, Greg W.....	TP 218	Kim, Taehee.....	MP 086	Klaeger, Susan.....	ThOB am 09:30
Kilby, Greg W.....	WP 002	Kim, Unyong.....	TP 509	Klaeger, Susan.....	TP 683
Kilby, Karen.....	MP 470	Kim, Woong-Ki.....	WP 240	Klaene, Joshua.....	WP 373
Kile, Sarah M.....	ThP 580	Kim, Yangsun.....	MP 537	Klammer, Martin.....	ThP 019
Kilgour, David.....	WOB pm 4:10	Kim, Yangsun.....	TP 214	Klapoetke, Song.....	ThP 775
Kilgour, David P. A.....	WP 329	Kim, YD.....	ThP 572	Klapoetke, Song.....	WP 074
Kilgour, David P.A.....	TP 386	Kim, Yeoun Jin.....	ThP 254	Klapoetke, Song.....	WP 209
Kilgour, David P.A.....	WOC am 08:50	Kim, Yeoun-Jin.....	TP 485	Klassen, John.....	ThP 097
Killeen, Kevin.....	TP 334	Kim, Younghwan.....	MP 300	Klassen, John.....	ThP 098
Killeen, Kevin.....	WP 205	Kim, Young-Mo.....	MOC pm 3:10	Klassen, John.....	ThP 099
Kilpatrick, Eric.....	TP 266	Kim, Young-Mo.....	MP 569	Klassen, John.....	ThP 719
Kilpatrick, Eric L.....	TP 252	Kim, Youngsoo.....	MP 128	Klassen, John.....	TOC pm 2:50
Kilpatrick, Lisa.....	MOE am 09:10	Kim, Youngsoo.....	WP 014	Klebe, Gerhard.....	ThP 095
Kilpatrick, Lisa.....	MOE pm 4:10	Kim Hor Hee, Daryl.....	WP 449	Kleber, Markus.....	TP 443
Kilpatrick, Lisa.....	WP 214	Kimmel, Joel.....	TOA pm 3:10	Klee, Sonja.....	TP 733
Kilpatrick, Lisa E.....	TP 252	Kindzey, Michael.....	WP 191	Kleensang, Andre.....	WP 581
Kim, Albert.....	WP 006	Kind, Tobias.....	MP 616	Klein, Adam.....	TP 022
Kim, Andrew.....	TP 328	Kind, Tobias.....	TP 667	Klein, Christian.....	ThP 472
Kim, Bong-Joon.....	TP 509	King, Christina.....	WP 117	Klein, Christian.....	ThP 483
Kim, Bum Jin.....	ThOA am 09:50	King, Fred.....	WP 227	Klein, Christian.....	ThP 491
Kim, Byung Chul.....	TOC pm 3:10	King, Jeremy.....	ThOF am 10:10	Klein, Christian.....	TOC am 08:50
Kim, Chang Soo.....	WP 703	King, Richard.....	MP 268	Klein, Christian.....	WP 680
Kim, Chul Wook.....	ThP 312	King, Richard.....	ThP 176	Klein, Christian.....	WP 681
Kim, Do Yong.....	WP 670	King, Simon.....	ThP 002	Klein, Dustin.....	TP 289
Kim, Doyong.....	TOD pm 3:30	King, Victoria.....	MP 268	Klein, Ian.....	MP 577
Kim, Eun-Hae.....	ThP 555	King-Ahmad, Amanda J.....	ThP 674	Klein, Jon.....	WP 494
Kim, Evelyn.....	MP 456	Kingston, H. M. Skip.....	ThP 447	Klein, Patrick J.....	TP 491
Kim, Hee-Yong.....	ThP 384	Kingston, H.M. "Skip".....	WP 508	Klein, Theo.....	ThP 222
Kim, Hee-Yong.....	ThP 467	Kingston, H.M. Skip.....	MP 557	Klein, Theo.....	WP 150
Kim, Helen.....	MP 586	Kini, R. Manjunatha.....	WP 101	Klich, Amna.....	ThP 023
Kim, Helen.....	TP 680	Kinose, Fumi.....	TP 463	Klinger, Alexandra.....	MP 169
Kim, Hokeun.....	ThP 020	Kinoshita, Kazumasa.....	MOA pm 3:10	Klitze, Clécio.....	TP 603
Kim, Hugh I.....	WOA pm 2:30	Kinoshita, Kazumasa.....	ThP 620	Klopotowski, Sebastian.....	TP 732
Kim, Hye-Jung.....	ThP 281	Kinross, James.....	TOG pm 3:30	Klopotowski, Sebastian.....	TP 737
Kim, Hyesoo.....	TP 427	Kinross, James.....	TP 375	Klopotowski, Sebastian.....	TP 731
Kim, Hyong-Ha.....	WP 206	Kinross, James.....	WP 020	Kloske, John.....	MP 553
Kim, Hyun Sik.....	ThP 549	Kinsel, Gary R.....	MP 308	Knaan, Tal.....	MP 056
Kim, Hyunook.....	ThP 554	Kirillov, Sergey.....	ThOB pm 3:10	Knaden, Markus.....	MP 030
Kim, Hyunseok Kim.....	ThOB pm 2:50	Kirillov, Sergey.....	ThP 690	Knapp, Richard.....	WP 638
Kim, Hyunwoo.....	TP 080	Kirk, Benjamin.....	ThOD am 10:10	Knebel, Axel.....	WP 200
Kim, Jaehan.....	TP 328	Kirk, Jonathan.....	TP 477	Knebelmann, Bertrand.....	WP 145
Kim, Jeesu.....	MP 537	Kirk, Kiaran.....	MP 271	Knecht, Dana.....	MP 714
Kim, Jeongkwon.....	MP 086	Kirkpatrick, Christine.....	MP 414	Knegt, Lena.....	WP 651
Kim, Jeongkwon.....	TP 421	Kirkpatrick, Donald.....	WP 048	Knemeyer, Ian.....	TP 626
Kim, Jin Young.....	ThP 591	Kirkpatrick, Donald S.....	WOD am 10:10	Knierman, Michael.....	MP 080
Kim, JinHee.....	TOB pm 2:30	Kirkpatrick, Kaylyn.....	ThP 608	Knight, James DR.....	MP 258
Kim, Jo-Il.....	TP 527	Kirkwood, Jay.....	MP 418	Knight, Rob.....	MOH pm 4:10
Kim, Jong-Hoon.....	TP 441	Kirkwood, Kathryn.....	ThP 089	Knip, Mikael.....	WP 028
Kim, Jung Hoe.....	ThP 168	Kirmess, Kristopher.....	MP 308	Knochenmuss, Richard.....	TOA pm 3:10
Kim, Junghyun.....	TP 509	Kirsch, Dieter.....	WP 300	Knochenmuss, Richard.....	WP 671
Kim, Ki Hun.....	MP 676	Kirschbaum, Clemens.....	WP 471	Knolhoff, Ann M.....	WP 333
Kim, Kwang-Youl.....	ThP 024	Kirschner, Marc W.....	MP 259	Knoppova, Barbora.....	ThP 149
Kim, Kyoungmi.....	ThP 155	Kirschner, Marc W.....	TOG am 09:50	Knox, J. David.....	TP 213
Kim, Kyoung-Kon.....	WP 157	Kirschner, Marc W.....	TP 180	Knust, Matthias.....	ThP 346
Kim, Michael.....	MOG pm 2:50	Kiselar, Janna.....	MP 169	Knyazkov, Denis A.....	WP 410
Kim, Michael.....	WP 041	Kiselar, Janna.....	ThP 355	Knych, Heather.....	TP 628
Kim, Michael.....	WP 049	Kiselar, Janna.....	TP 233	Ko, Yeon Jae.....	TP 709
Kim, Min Sik.....	TOG am 09:10	Kiss, Tamás.....	TP 263	Ko, Yeon Jae.....	WP 759
Kim, Min-Sik.....	MP 256	Kissel, Ed.....	ThOA am 09:10	Koal, Therese.....	ThOG am 09:50
Kim, Min-Sik.....	MP 255	Kissick, David.....	TP 001	Kobarg, Jan Hendrik.....	MP 021
Kim, Min-Sik.....	MP 440	Kita, Adriana.....	TP 148	Kobayashi, Hiroshi.....	TP 193
Kim, Min-Sik.....	ThP 219	Kita, Yoshihiro.....	ThP 398	Kobayashi, Norifumi.....	WP 474
Kim, Mi-Young.....	MP 360	Kitagawa, Norton.....	ThP 061	Kobayashi, Tamaki.....	WP 446
Kim, Moo-Young.....	ThP 668	Kitagawa, Norton.....	WP 591	Kobeissy, Firas.....	ThP 297
Kim, Sanggoo.....	TP 747	Kitahara, Yoshiro.....	WP 102	Koch, Alexander.....	TP 078
Kim, Sangtae.....	MOG am 09:50	Kitano, Riki.....	MP 419	Koch, Boris P.....	MP 549
Kim, Sangtae.....	MOG pm 3:30	Kitchens, Robert.....	TP 082	Koch, Heiner.....	ThOB am 09:30
Kim, Sangtae.....	MP 033	Kitchens, Robert.....	TP 173	Koch, Heiner.....	WP 095
Kim, Sangtae.....	TP 083	Kitchens, Robert.....	WOG pm 3:50	Koch, Marianne.....	TP 447
Kim, Sang-Yoon.....	ThP 254	Kitova, Elena.....	ThP 099	Koch, Marianne.....	WP 140
Kim, Sang-Yoon.....	ThP 322	Kitova, Elena.....	ThP 098	Kochansky, Christopher.....	ThOE am 09:30
Kim, Seung Joong.....	TP 132	Kitova, Elena.....	ThP 097	Kochansky, Christopher.....	ThP 546
Kim, Somang.....	MP 639	Kitova, Elena.....	TOC pm 2:50	Köcher, Thomas.....	TP 098
Kim, Somang.....	TP 626	Kiyonami, Reiko.....	ThP 324	Kochert, Brent.....	ThP 131
Kim, Sung Tae.....	WP 703	Kiyonami, Reiko.....	WP 144	Kochhar, Rashi.....	TP 497
Kim, Sung Tae.....	WP 723	Kiyonami, Reiko.....	WP 737	Kochhar, Rashi.....	TP 496
Kim, Sung woo.....	ThP 303	Kjeldsen, Frank.....	MP 719	Kochhar, Rashi.....	TP 498

Program code: M,T,W, Th = Day    O = Oral, P = Poster    Time or poster number

# INDEX OF AUTHORS

Kochhar, Rashid.....	WP 350	Kostrzewa, Markus.....	TP 212	Kristl, Theresa.....	WP 153
Koebel, Knut.....	ThOF am 08:30	Kostyukevich, Yury.....	TP 325	Krivacic, Cody.....	MP 540
Koh, Young Ho.....	ThP 271	Kostyukevich, Yury.....	WP 724	Krivos, Kady.....	WP 334
Kohira, Takahiro.....	ThP 398	Kotch, Frank.....	TP 236	Krock, Kevin.....	ThP 632
Kohl, Michael.....	MP 431	Kotch, Frank.....	WP 274	Krock, Kevin.....	ThP 625
Kohlbacher, Oliver.....	MP 052	Kotchey, Gregg P.....	WP 706	Kroep, Judith.....	MP 004
Kohlbacher, Oliver.....	ThP 457	Kothapalli, Naga Rama.....	WOB pm 3:10	Kröger, Sabrina.....	TP 031
Kohlbacher, Oliver.....	ThP 458	Kou, Qiang.....	TP 090	Krogh, Erik T.....	MP 556
Kohlbacher, Oliver.....	ThP 459	Koudsi, Georges.....	WP 522	Krogh, Erik T.....	WP 746
Kohlbacher, Oliver.....	ThP 519	Koudstaal, P.J.....	TP 444	Krokhin, Oleg.....	TP 183
Kohno, Satomi.....	ThP 647	Koulakiotis, Nikolaos Stavros.....	ThP 087	Krolkowski, Piotr.....	WP 559
Koike, Masaki.....	ThP 761	Koulman, Albert.....	WP 285	Kroll, Kai.....	MOD pm 4:10
Kolarich, Daniel.....	TP 160	Kounadis, Diamantis.....	MP 668	Kroll, Kai.....	MP 684
Kölbl, Heinz.....	TP 447	Koury, Olivia.....	MP 588	Kroll, Kai.....	TP 737
Kolippakkam, Deepak.....	TP 145	Kousar, Sumaira.....	MP 414	Kronewitter, Scott R.....	WP 745
Koll, Hans.....	WP 049	Koutalos, Yannis.....	TP 070	Kronewitter, Scott R.....	TP 324
Koller, Antonius.....	MP 219	Koutalos, Yiannis.....	MP 022	Krönke, Jan.....	WOG am 08:50
Kolli, Venkata.....	WP 078	Kovalev, Sergei.....	WP 207	Kros, J.M.....	TP 444
Kollipara, Laxmikanth.....	MP 452	Kovtoun, Viatcheslav V.....	MP 673	Kroto, Harold W.....	WP 705
Komarov, Alexandre.....	MP 340	Kowalski, Matt.....	TOF pm 4:10	Krovvidi, Ravi K.....	MP 124
Komatsuzaki, Ryo.....	MP 678	Kowalski, Michael P.....	WP 497	Krovvidi, Ravi Kumar.....	WP 235
Komatsuzaki, Ryo.....	WP 196	Kowalski, Paul.....	TP 413	Krstic, Marko.....	TOG pm 2:50
Komives, Elizabeth.....	MP 207	Kowalski, Timothy.....	TP 460	Krug, Karsten.....	ThP 043
Komives, Elizabeth.....	ThP 118	Koy, Cornelia.....	ThP 107	Krug, Karsten.....	ThP 080
Koncar, Gerald.....	WP 144	Koy, Cornelia.....	ThP 277	Krug, Karsten.....	WP 242
Kondo, Tomohide.....	MP 525	Koy, Cornelia.....	WP 715	Krug, Oliver.....	TP 628
Konermann, Lars.....	MOF am 10:10	Koza, Stephan.....	MP 745	Kruger, Jordan.....	MP 061
Konermann, Lars.....	ThP 124	Kozak, Marta.....	MP 285	Krüger, Marcus.....	ThP 314
Konermann, Lars.....	TOF am 08:30	Kozak, Marta.....	MP 282	Krüger, Sascha.....	TP 361
Kong, Andy.....	MP 258	Kozak, Marta.....	MP 283	Krumwiede, Dirk.....	MOD pm 4:10
Kong, Andy.....	WOD am 09:10	Kozhinov, Anton N.....	MOB am 09:30	Krupp, Eva.....	WP 342
Kong, Jeffrey.....	MP 158	Kozhinov, Anton N.....	MP 701	Kruppa, Gary.....	TP 212
Kong, Xianglei.....	TP 366	Kozhinov, Anton N.....	MP 700	Krutchinsky, Andrew N.....	WP 743
Kongmanas, Kessiri.....	MP 250	Kozicki, Antje.....	MOE pm 3:30	Kruve, Anneli.....	MP 313
König, Iwo.....	ThOD pm 2:30	Kozin, Sergey.....	ThP 086	Krystek, Stanley R.....	MOE pm 3:10
König, Stefan.....	ThP 590	Kozlov, Boris.....	MP 651	Ku, Kuo-Lung.....	WP 599
König, Stefan.....	WP 293	Kozlov, Boris.....	ThOB pm 3:10	Ku, Wei-Chi.....	ThP 275
König, Tim.....	ThP 314	Kozlov, Boris.....	WOA pm 3:10	Kubanek, Julia.....	MP 274
Konijnenberg, A.....	WP 229	Kozlov, Dmitry N.....	ThOG am 09:30	Kubo, Akiko.....	TP 017
Konijnenberg, Albert.....	TOC pm 3:50	Kraemer, Thomas.....	ThOE pm 3:10	Kudo, Keiko.....	ThP 592
Kononikhin, Alexey.....	ThP 086	Kraj, Agnieszka.....	MP 093	Kudo, Yukihiro.....	ThP 641
Kononikhin, Alexey.....	TOA pm 4:10	Kraj, Agnieszka.....	TP 622	Kudo, Yuta.....	MP 108
Kononikhin, Alexey.....	TP 325	Krajewski, Logan C.....	TP 595	Kudou, Yuki.....	MOA pm 3:10
Kononikhin, Alexey.....	TP 409	Kramer, Gertjan.....	MP 265	Kudou, Yuki.....	ThP 620
Kononikhin, Alexey.....	WP 724	Kramer, Katharina.....	ThP 457	Kudou, Yuki.....	TP 782
Kononikhin, AS.....	TP 449	Kramer, Katharina.....	ThP 458	Kudryavtsev, Igor.....	WP 207
Kool, Jeroen.....	WOF am 10:10	Kramer, Katharina.....	ThP 459	Kudtarkar, Parul.....	ThP 310
Koolen, Hector.....	TP 585	Kramer, Katharina.....	ThP 519	Kudva, Indira.....	MP 466
Koomen, John.....	ThOE am 08:50	Kramer, Lawrence.....	ThP 563	Kuehl, Philip.....	ThP 523
Koomen, John.....	TP 463	Kramer, Lawrence.....	ThP 562	Kuehn, Andreas.....	ThP 317
Kooren, Joel.....	ThP 044	Kramer, Lawrence.....	TP 270	Kuehn, Andreas.....	ThP 321
Kopaev, Igor.....	ThP 751	Kramer, Lawrence.....	WP 572	Kuehn, Andreas.....	ThP 762
Kopec, Rachel.....	ThOA pm 3:10	Krasinska, Karolina M.....	ThP 684	Kuepper, Marius.....	ThP 343
Koppenaar, David W.....	MP 100	Krasnogor, Natalio.....	ThP 645	Kuharev, Joerg.....	ThP 015
Koppenaar, David W.....	MP 654	Krasnomowitz, Justin.....	ThP 368	Kuharev, Jörg.....	TP 084
Koppenaar, David W.....	ThOB pm 4:10	Krastins, Bryan.....	ThP 450	Kuhlmann, Frank.....	ThP 547
Koppenaar, David W.....	TOE pm 2:50	Krastins, Bryan.....	TP 244	Kuhlmann, Katja.....	MP 431
Koppenol-Raab, Marijke.....	MP 261	Krastins, Bryan.....	WP 192	Kuhlmann, Katja.....	TP 141
Koppenol-Raab, Marijke.....	MP 269	Kraus, Olga.....	TP 054	Kuhlmann, Katja.....	TP 481
Koppenol-Raab, Marijke.....	WP 256	Krechmer, Jordan.....	TOA pm 3:10	Kuhn, Eric.....	ThP 217
Kopylov, Arthur.....	ThP 248	Kremser, Leopold.....	ThP 226	Kuhn, Eric.....	TP 177
Korade, Zeljka.....	ThOG pm 2:50	Krieger, José Eduardo.....	TP 435	Kuhn, Jeffrey F.....	MP 072
Korbakis, Dimitrios.....	TP 244	Kriegsmann, Jörg.....	TP 056	Kuhn, Jeffrey F.....	ThP 769
Korfmacher, Walter.....	WP 638	Kriegsmann, Jörg.....	TP 057	Kuhn, Karsten.....	ThP 215
Korhonen, Anna.....	WP 257	Kriegsmann, Jörg.....	TP 051	Kuhn, Lauriane.....	TP 247
Korsgren, Pernilla.....	MP 205	Kriegsmann, Mark.....	TP 051	Kuhn, Lauriane.....	WP 498
Korshun, Vladimir.....	WP 027	Kriegsmann, Mark.....	TP 056	Kühnöl, Jürgen.....	MOD pm 2:30
Korte, Andrew.....	MP 473	Kriegsmann, Mark.....	TP 057	Kuijper, Joseph.....	ThP 103
Korte, Andrew.....	ThP 003	Krijgsveld, Jeroen.....	MP 223	Kukacka, Zdenek.....	MP 183
Korte, Andrew.....	TP 037	Krijgsveld, Jeroen.....	TP 202	Kukacka, Zdenek.....	ThOF am 08:50
Korte, Andy.....	TOH am 09:30	Krijgsveld, Jeroen.....	TP 189	Kukaev, EN.....	TP 449
Korte, Birgit.....	MP 431	Krishnan, Anita.....	MP 155	Kukaev, Evgeny.....	TP 409
Korte, Birgit.....	TP 481	Krishnan, Anita.....	WP 717	Kukleniyik, Zsuzsanna.....	ThP 382
Korthanck, Curtis.....	ThP 682	Krishnan, Chenni.....	MP 735	Kukleniyik, Zsuzsanna.....	TP 155
Kosjek, Tina.....	TP 551	Krisp, Christoph.....	MP 221	Kükre, Başak.....	ThP 119
Kostakis, Ioannis.....	ThP 087	Krisp, Christoph.....	ThOE pm 2:50	Kukula, Maciej.....	TP 490
Kostel, Stephen.....	TP 190	Kristensen, Anders.....	TP 137	Kulej, Katarzyna.....	TP 144
Koster, Emile.....	WP 651	Kristensen, Jesper.....	TOF pm 2:30	Kulikova, Inna.....	WOE pm 3:50
Kostiainen, Risto.....	TP 401	Kristin Burnum-Johnson, Kristin.....	MP 569	Kuljanin, Miljan.....	MP 455

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

## INDEX OF AUTHORS



Kulkarni, Purva	MP 030	Kwiatkowski, Christopher	TOF pm 4:10	Lai, Yi-Chieh	WP 521
Kullolli, Majinda	ThP 146	Kwiatkowski, Marcel	WP 744	Lai, Yin-Hung	MP 309
Kulman, John	ThP 134	Kwiecien, Nicholas	ThP 177	Lai, Yin-Hung	ThP 742
Kultima, Kim	WP 489	Kwiecien, Nicholas W.	ThP 348	Lai, Zijuan	MP 630
Kumano, Shun	TP 744	Kwiecien, Nicholas W.	TOC am 09:50	Lai, Zon	TP 172
Kumar, Anoop	TP 532	Kwon, Do Yeon	ThP 084	Laiakis, Evagelia	WP 776
Kumar, Anoop	WP 103	Kwon, Ja-Young	MP 127	Laibinis, Paul	MP 017
Kumar, Anoop	WP 531	Kwon, Keehwan	ThP 283	Lajeunesse, André	WP 296
Kumar, Anuj	WP 258	Kwon, Yong-il	TP 328	Lajoie, Gilles	MP 458
Kumar, Ashwani	MP 270	Kynast, Philipp	MP 030	Lakatta, Edward	ThP 300
Kumar, Manish	MP 255	Kyriacou, Kyriacos	WP 491	Lakbub, Jude	WP 260
Kumar, Manish	MP 270	Kyung, Hyunsook	MP 107	Lakshmanan, Rajeswari	TP 150
Kumar, Praveen	MP 255	Laaksonen, Reijo	TP 443	Lakshmi, N.S	MP 085
Kumar, Ruby	TP 163	Lababidi, Sami	WOA am 08:30	Lakshminarasimhan, Mahadevan	MP 156
Kumar, Ruby	TP 198	Labadie, Pierre	ThP 566	Lalli, Priscila	WOA pm 2:50
Kumar, Ruby	WOB am 09:50	Labrie, Fernand	TP 495	Lalli, Priscila M.	TP 601
Kumar, Sacheen	ThP 664	Labuz, Krzysztof	MP 620	Lalli, Priscila M.	TP 602
Kumar Raghuraman, Bharath	MP 434	LaCava, John	WP 253	LaLone, Carlie	TP 311
Kumar Raghuraman, Bharath	WP 478	Lacey, Ernest	TP 211	Lalor, Patricia F.	TP 041
Kump, Matthew	TP 652	Lachance, Sylvain	MP 492	Lam, Henry	MP 255
Kuna, Sunnie	ThP 150	Lachance, Sylvain	MP 485	Lam, Henry	ThP 031
Kun-Chun, Chiang	ThP 683	Lachance, Sylvain	MP 488	Lam, Henry	ThP 232
Kune, Christopher	ThP 503	Lachance, Sylvain	MP 493	Lam, Henry	ThP 619
Kung, An-Wen	ThP 525	Lachance, Sylvain	MP 494	Lam, Henry	TP 092
Künne, Tim	ThP 458	Lachance, Sylvain	MP 496	Lam, Henry	TP 226
Kunz, Ryan	TOG am 09:50	Lachance, Sylvain	MP 498	Lam, Henry	WP 252
Kuo, Chao-Jen	MP 435	Lachance, Sylvain	MP 486	Lam, Justine	TP 028
Kuo, Mei-Yi	TP 654	Lachance, Sylvain	TP 517	Lam, Tukiet T.	TP 572
Kuo, Ya-Po	MP 425	Łącki, Mateusz	ThP 191	Lam, Zamas	TP 633
Kuo, Yin-Ming	MP 227	Lacorte, Sílvia	WP 719	Lam, Zamas	TP 634
Kurian, Ritika	WP 484	LaCourse, Margaret	TP 373	Lam, Zamas	TP 616
Kurimata, Naoko	MP 525	LaCourse, Margret	TP 405	LaMarch, Brian L.	TOB am 09:50
Kurnin, Igor	MP 651	LaCourse, William	ThP 167	Lamarche, Brian	ThOB am 10:10
Kuroda, Marcelo	WP 240	LaCourse, William	TP 405	Lamarche, Brian L.	MP 677
Kuroguchi, Masaki	ThP 162	LaCourse, William	TP 404	LaMarche, Brian L.	TP 324
Kurono, Sadamu	WP 474	LaCourse, William R.	MP 403	Lamarr, William A.	WP 437
Kurtin, Paul J.	ThP 272	LaCourse, William R.	TP 373	Lambert, Jean Philippe	TP 087
Kurulugama, Ruwan	MOC pm 3:10	Lacoursiere, Jean	MP 284	Lambert, Jean-Philippe	MP 258
Kurulugama, Ruwan	ThP 472	Lacoursiere, Jean	WP 626	Lambert, Jean-Philippe	TP 181
Kurulugama, Ruwan	ThP 483	Lacoursiere, Jean	WP 634	Lamblin, Anne-Francoise	MP 033
Kurulugama, Ruwan	ThP 491	Lacoux, Xavier	TP 219	Lamborg, Carl	MP 275
Kurulugama, Ruwan	ThP 759	Lacroix, Bruno	ThP 023	Lame, Mary	WP 123
Kurulugama, Ruwan	WP 674	Ladak, Adam	ThP 544	Lame, Mary	WP 125
Kurulugama, Ruwan	WP 680	Ladak, Adam	TP 392	Lammert, Steve	MP 696
Kurulugama, Ruwan	WP 681	Ladak, Adam	TP 629	Lamoliatte, Frederic	ThOC am 08:30
Kurulugama, Ruwan T.	ThP 482	Ladak, Adam	WOC pm 2:30	Lamoliatte, Frederic	TP 108
Kurulugama, Ruwan T.	ThP 484	Ladakhin, Alexey	WP 022	Lamoliatte, Frederic	TP 130
Kusai, Akihiko	TP 604	Ladwig, Paula	WP 231	Lamond, Angus	MP 151
Kusano, Hideaki	TP 782	Laeyendecker, Oliver	ThP 349	Lamond, Angus	ThP 089
Kusch, Sebastian	MP 052	LaFayette, Amber	WOF pm 4:10	Lamontagne, Julie	WP 137
Kushnir, Mark M.	WP 439	Lafitte, Daniel	WP 537	Lamourette, Patricia	MP 527
Kushnir, Michelle	ThP 509	Lafontaine, Catherine	ThP 531	Lamourette, Patricia	MP 528
Kushnir, Stuart	WP 640	Lafontaine, Nadine	MP 671	Lampinen Salomonsson, Matilda	MP 352
Kusinski, Matthew	TP 542	Lafrance, Claude-Paul	MP 494	Lampron, Nancy	MP 495
Kussmann, Martin	ThP 255	Laganowsky, Arthur	WP 714	Lamsa, Anne	MP 056
Kussmann, Martin	WP 510	Lage, Sergio	WOH pm 3:50	Laņas, Fernando	TP 576
Kuster, Bernhard	MP 041	Lagojda, Andreas	MP 006	Lance, Raymond	TP 069
Kuster, Bernhard	MP 191	Lah, James	WP 301	Landgraf, Richardt G.	MP 115
Kuster, Bernhard	MP 193	Lahaie, Mathieu	WP 178	Landt Larsen, Ane	ThP 347
Kuster, Bernhard	ThOB am 09:30	Lahaie, Mathieu	WP 535	Landuyt, Bart	WP 469
Kuster, Bernhard	ThOB pm 3:50	Lahaie, Mathieu	WP 522	Lane, Catherine	WP 072
Kuster, Bernhard	ThP 046	Lähdesmäki, Harri	WP 028	Lane, Douglas	WP 010
Kuster, Bernhard	TP 052	Lahesmaa, Riita	ThP 276	Lane, Lydie	WP 029
Kuster, Bernhard	TP 683	Lahesmaa, Riitta	WP 028	Lane, Monica	WP 506
Kuster, Bernhard	WP 095	Lahesmaa, Riitta	WP 504	Lanekoff, Ingela	MOH pm 3:30
Kutilek, Victoria	TOF pm 3:30	Lai, Ching	WP 587	Lanekoff, Ingela	TOH pm 2:50
Kutty, Praveen	ThP 560	Lai, Christopher C.	MP 189	Lang, Frederick	WP 238
Kutty, Praveen	WP 566	Lai, Ming-Tain	MP 536	Lang, Johnsie	WP 574
Kuzdzal, Scott	ThP 766	Lai, Raymond	TP 648	Lang, Lisa	WP 297
Kuzdzal, Scott	WP 161	Lai, Steven	ThP 417	Lang Jr, Frederick F.	MP 427
Kuzdzal, Scott	WP 649	Lai, Steven	ThP 661	Lange, Catherine	ThP 499
Kuzdzal, Scott A.	WP 211	Lai, Steven	TP 629	Lange, Christoph	TP 212
Kuznetsova, Ksenia	ThP 248	Lai, Steven	TP 643	Lange, Oliver	MP 653
Kvam, Allison	MP 566	Lai, Steven	WP 022	Lange, Oliver	ThP 762
Kwak, June M.	ThOB am 09:10	Lai, Steven	WP 466	Lange, Oliver	TOB am 10:10
Kwasnjuk, Kristen	ThOE am 09:30	Lai, Steven	WP 586	Lange, Stefan	TP 018
Kwasnjuk, Kristen	ThP 546	Lai, Szu-Hsueh	MP 304	Langejuergen, Jens	MP 388
Kweon, Hye Kyong	ThP 454	Lai, Wen-Ter	MP 435	Langenkamp, Anja	TP 171
Kweon, Hye Kyong	WP 258	Lai, Xianyin	ThP 264	Langer, Julia	MP 583

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Langner, Markus.....	TP 732	Laube, Audra H.....	ThP 149	Lee, Caroline.....	TP 634
Langridge, David.....	ThP 747	Lauber, Matthew.....	MP 745	Lee, Caroline.....	TP 616
Langridge, David.....	TP 723	Laude, Nicholas.....	WP 099	Lee, Cheng S.....	TOB pm 4:10
Langridge, James.....	ThP 001	Laue, Alexander.....	MP 690	Lee, Chung-Fan.....	WOG am 08:30
Langridge, James.....	ThP 036	Laughlin, Brian C.....	WP 400	Lee, Chung-Tien.....	ThP 456
Langridge, James.....	ThP 392	Laukens, Kris.....	MP 032	Lee, Chuping.....	MP 306
Langridge, James.....	ThP 393	Laukens, Kris.....	MP 682	Lee, Dave Chi Hoo.....	TP 164
Langridge, James.....	ThP 417	Laukens, Kris.....	WP 042	Lee, Dong-Gi.....	ThP 312
Langridge, James.....	ThP 661	Laurini, Erik.....	WP 682	Lee, Dongkun.....	WP 289
Langridge, James.....	TOH am 09:50	Lauzon, Nidia.....	MP 012	Lee, Ed.....	MP 696
Langridge, James.....	TP 643	Lavallée, Richard.....	WP 532	Lee, Eun Joo.....	ThP 628
Langridge, James.....	WP 022	Lavallée, Richard.....	WP 525	Lee, Eunice.....	MP 598
Langridge, James.....	WP 126	Lavallée, Richard.....	WP 538	Lee, Hangyeore.....	ThP 020
Langridge, James.....	WP 586	LaViolette, Peter.....	MP 428	Lee, Han-Ho.....	MP 127
Langridge, James I.....	MP 265	Lavoie, Pamela.....	WP 441	Lee, HooKeun.....	TP 441
Langridge, James I.....	ThOB pm 3:50	Law, Alex.....	ThP 157	Lee, Howard.....	WP 400
Langridge-Smith, Patrick.....	TP 403	Lawless, Craig.....	MP 272	Lee, Hsun.....	MP 309
Langridge-Smith, Pat.....	TOE pm 3:50	Lawson, John A.....	TP 103	Lee, Hsun.....	ThP 742
Langridge-Smith, Patrick.....	WP 751	Lay, Jackson, Jr.....	ThP 346	Lee, Hyoung-Joo.....	MP 127
Lankin, David C.....	WP 325	Lay Jr., Jackson O.....	ThP 127	Lee, Hyoung-Joo.....	ThP 024
Lannfelt, Lars.....	WP 489	Lazar, Alexandru.....	WP 210	Lee, Ingyu.....	ThP 554
Lansing, Jonathan.....	WP 173	Lazar, Juliana.....	TP 079	Lee, Jae Jin.....	WP 224
Lanthalier, Karin.....	MP 272	Le, Dung.....	WP 681	Lee, Jae Won.....	WP 283
Lantin, Patrice.....	TP 517	Le, Nhat.....	TP 359	Lee, Jeong.....	WP 194
Lanucara, Francesco.....	TP 164	Le Blanc, Yves.....	WOD pm 2:50	Lee, Jihyeon.....	MP 086
Lanucara, Francesco.....	WP 056	Le Brech, Yann.....	MP 576	Lee, Jin-Gyun.....	WP 240
Lanza, Matteo.....	ThP 738	Le Fol, Vincent.....	TP 309	Lee, Ji-Won.....	ThP 467
Lao, Julie.....	TP 460	Le Marchand, Loic.....	WP 485	Lee, Ji-Young.....	MP 360
Lapek, John.....	MP 257	Le Roch, Karine.....	ThOF pm 3:30	Lee, John C.....	ThP 385
Lapointe, Joseph.....	MP 365	Leach, Steven D.....	MP 255	Lee, Jong Wha.....	WOA pm 2:30
Lapointe, Joseph.....	ThP 415	Leach III, Franklin E.....	MP 654	Lee, Joon-Yong.....	ThP 652
Lapointe, Joseph.....	TP 269	Leach III, Franklin E.....	TOE pm 2:50	Lee, Kelly.....	TOF am 08:50
Laprévotte, Olivier.....	MP 235	Leamon, Christopher P.....	TP 491	Lee, Kelvin H.....	MP 572
Laphorn, Cris.....	WP 695	Leaprot, Katrina L.....	ThP 482	Lee, Kimberly.....	ThP 073
Larance, Mark.....	MP 151	Leaprot, Katrina L.....	WP 688	Lee, Kimberly.....	TP 109
Larance, Mark.....	ThP 089	Leary, Dagmar Hajkova.....	MP 278	Lee, Kimberly A.....	MP 122
Lareau, Nichole M.....	ThOD pm 2:50	Leary, Julie A.....	MOC pm 3:50	Lee, Kimberly A.....	TP 117
Lareau, Nichole M.....	ThP 482	Leary, Julie A.....	MP 101	Lee, Kong-Joo.....	WP 224
Lareau, Nichole M.....	ThP 486	Leary, Julie A.....	ThP 724	Lee, Linda S.....	ThOE pm 4:10
Larkin, Selena.....	TP 462	Lebedev, Albert T.....	ThP 190	Lee, Ling Y.....	WP 079
Larkins, Katherine P.B.....	ThP 216	Lebedev, Albert T.....	WP 709	Lee, Melissa.....	TP 332
Larney, Francis.....	TP 554	Lebel, Philippe.....	TP 530	Lee, Mike.....	WP 158
Larraillet, Vincent.....	TOF am 09:30	Leber, Amanda.....	WP 192	Lee, Min Jung.....	MP 127
Larraillet, Vincent.....	WP 049	Lebev Pereira, Claney.....	TP 160	Lee, Min-Yi.....	MP 435
Larriba Andaluz, Carlos.....	ThP 508	Leblanc, André.....	TP 204	Lee, Oona.....	ThP 394
Larsen, Barbara S.....	TP 311	Leblanc, André.....	WOF am 08:50	Lee, Richard.....	TP 190
Larsen, Brett.....	TP 087	Leblanc, J.C. Yves.....	MP 721	Lee, Richard.....	WP 142
Larsen, Brett.....	TP 182	Leblanc, J.C. Yves.....	ThOC am 08:50	Lee, Sangkyu.....	WP 259
Larsen, Martin R.....	ThP 202	Leblanc, J.C. Yves.....	ThP 330	Lee, Sang-Won.....	ThP 020
Larsen, Martin R.....	ThP 213	Leblanc, J.C. Yves.....	ThP 473	Lee, Seon Hwa.....	MP 096
Larsen, Martin R.....	TP 124	Leblanc, J.C. Yves.....	ThP 505	Lee, Seon Hwa.....	MP 105
Larsen, Martin R.....	TP 144	Leblanc, J.C. Yves.....	TP 516	Lee, Seon Hwa.....	MP 107
Larsen, Martin Røssel.....	MP 718	LeBlanc, Yves.....	WP 779	Lee, Seon Hwa.....	MP 108
Larsen, Martin Røssel.....	MP 719	Lebrilla, Carlito.....	MOA pm 2:50	Lee, Seon Hwa.....	WP 131
Larsen, Sara Charlotte.....	WP 109	Lebrilla, Carlito.....	ThP 155	Lee, Sung-Hyeon.....	ThP 168
Larsson, Ola.....	MP 429	Lebrilla, Carlito.....	ThP 153	Lee, Tae.....	TP 199
Lashin, Vitaly.....	WP 025	Lebrilla, Carlito.....	TP 119	Lee, Victoria.....	MP 265
Laskay, Unige.....	MOE am 08:50	Lebrilla, Carlito.....	TP 221	Lee, Wen-Hwa.....	TP 121
Laskay, Unige A.....	WP 172	Lebrilla, Carlito.....	TP 258	Lee, Wen-Yen.....	ThP 528
Laskin, Alexander.....	MP 554	Lebrilla, Carlito.....	TP 259	Lee, Wen-Yen.....	TP 279
Laskin, Julia.....	MOH pm 3:30	Lebrilla, Carlito.....	TP 333	Lee, Wen-Yen.....	WP 356
Laskin, Julia.....	MP 554	Lebrilla, Carlito.....	WOE am 08:50	Lee, Yin-Yu.....	MP 307
Laskin, Julia.....	ThOD pm 4:10	Lebrilla, Carlito.....	WP 086	Lee, Yin-Yu.....	MP 306
Laskin, Julia.....	TOH pm 2:50	Lebrilla, Carlito.....	WP 087	Lee, Yong-Yook.....	WP 240
Lasne, Françoise.....	TP 293	Lebrilla, Carlito B.....	ThOH am 08:50	Lee, Yoon-Suk.....	WP 580
Laszlo, Kenneth J.....	MOD am 09:30	Lebrilla, Carlito B.....	ThP 729	Lee, Young Jin.....	MP 473
Lateed, Syed Salman.....	MP 481	Lecchi, Paolo.....	TP 273	Lee, Young Jin.....	MP 565
Lateef, Syed.....	TP 512	Lechaplais, Christophe.....	MP 617	Lee, Young Jin.....	MP 566
Lateef, Syed Salman.....	MP 124	Ledford, Edward.....	MP 600	Lee, Young Jin.....	MP 567
Lateef, Syed Salman.....	TP 513	Ledford, William.....	MP 600	Lee, Young Jin.....	ThP 003
Lateef, Syed Salman.....	TP 647	Leduc, Richard.....	ThP 059	Lee, Young Jin.....	TP 022
Laterza, Rosa.....	TP 447	Leduc, Richard.....	ThP 058	Lee, Young Jin.....	TP 037
Latour, Sylvain.....	WP 544	Leduc, Richard.....	WP 157	Lee, Young Jin.....	TP 043
Lattanzio, Veronica.....	MP 338	Ledvina, Aaron.....	WP 551	Lee, Young-Jin.....	TOH am 09:30
Lau, Adam.....	TP 186	Lee, Albert.....	ThP 082	Lee, Yuan Tseh.....	MP 306
Lau, Joseph.....	TP 332	Lee, Amanda.....	ThP 235	Lee, Yuan-Tseh.....	MP 305
Lau, Stanley.....	TP 226	Lee, Anita.....	TP 460	Lee, Yuan-Tseh.....	MP 307
Lau, Thomas.....	MP 126	Lee, Bruce.....	WP 580	Lee, Zachary.....	MP 154
Lau, Wilma.....	WP 049	Lee, Caroline.....	TP 633	Leenstra, Sieger.....	ThP 209

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



Lees-Miller, Susan.....	ThP 117	Leurs, Ulrike.....	TOF pm 2:30	Li, Hao.....	WP 389
Lefebvre, Matthew.....	TP 451	Levacher, Vincent.....	WP 679	Li, Honglan.....	ThP 020
Lefebvre, Michel.....	MP 288	Levesque, Ann.....	MP 488	Li, Hongli.....	MP 361
Leff, Richard.....	TP 500	Levesque, Ann.....	MP 497	Li, Huilin.....	MP 145
Lefkowitz, Robert.....	ThP 133	Levesque, Ann.....	MP 498	Li, Huilin.....	MP 184
Lefsrud, Mark.....	TP 677	Levesque, Ann.....	MP 486	Li, Huilin.....	TOD am 08:50
Legette, LeeCole.....	ThP 643	Levesque, Ann.....	MP 489	Li, Huilin.....	TOE pm 3:10
Legleiter, Justin.....	ThP 105	Levesque, Ann.....	MP 490	Li, Jiannong.....	TP 463
Legouffe, Raphael.....	MP 025	Levesque, Ann.....	MP 491	Li, Jianzhong.....	MP 730
Legouffe, Raphael.....	TP 009	Levesque, Ann.....	MP 492	Li, Jilong.....	ThP 302
Lehmann, Sylvain.....	TP 472	Levesque, Ann.....	MP 493	Li, Jin.....	WP 275
Lehmann, Sylvain.....	WP 447	Levesque, Ann.....	MP 494	Li, Jing.....	WP 231
Lehotay, Steve.....	ThP 541	Levesque, Ann.....	MP 495	Li, Jingning.....	WP 190
Lehotay, Steven.....	ThOC am 09:50	Levesque, Ann.....	MP 496	Li, Jinqing.....	WP 463
Lei, Qing Paula.....	WP 199	Levesque, Ann.....	MP 485	Li, Jinxi.....	WP 062
Lei, Shulei.....	TP 452	Levesque, Ann.....	TP 517	Li, Jinying.....	MP 330
Lei, Shulei.....	WP 593	Levesque, Carine.....	MP 497	Li, Jiwen.....	TP 760
Lei, Zhentian.....	ThP 636	Levesque, Jean-Francois.....	WP 620	Li, Jun.....	MP 224
Lei, Zhentian.....	ThP 640	Levey, Allan.....	WP 178	Li, Jun.....	ThP 013
Leiserowitz, Gary.....	ThP 155	Levi, Mikael.....	MP 345	Li, Jun.....	ThP 014
Leist, Marcel.....	ThP 746	Levi, Mikael.....	ThP 600	Li, Jun.....	WP 015
Leite, Aline Lima.....	MP 461	Levi, Mikael.....	ThP 599	Li, Jun.....	WP 232
Leite, Aline Lima.....	ThP 307	Levi, Mikael.....	WP 351	Li, Junyu.....	WP 633
Leito, Ivo.....	MP 313	Levin, David.....	TP 183	Li, Ke Sherry.....	ThP 363
Leize-Wagner, Emmanuelle.....	TP 247	Levin, Yishai.....	ThP 015	Li, Laisheng.....	TP 391
Leize-Wagner, Emmanuelle.....	WP 269	Levin, Yishai.....	ThP 197	Li, Lan.....	TP 684
Leize-Wagner, Emmanuelle.....	WP 498	Levine, Douglas.....	ThP 295	Li, Lan.....	WP 533
Lekkas, Alexander.....	MP 668	Levine, Douglas A.....	TP 169	Li, Liang.....	MP 594
Lelieveldt, Boudewijn F.P.....	MP 027	Levis, Robert.....	TP 407	Li, Liang.....	MP 597
Lemeer, Simone.....	WP 095	Levis, Robert.....	WOB pm 3:30	Li, Liang.....	TP 648
Lemière, Filip.....	WP 042	Levit, Matthew.....	WP 107	Li, Liang.....	TP 650
Lemieux, George.....	MP 436	Levitsky, Lev I.....	WP 172	Li, Liang.....	TP 655
Lemoff, Andrew.....	MP 254	Levitsky, Lev I.....	WP 164	Li, Liang.....	WP 605
Lemoine, Jerome.....	TP 219	Levitt, Nick.....	MOF pm 2:50	Li, Linfan.....	TOB am 09:30
Lemoine, Jérôme.....	WP 177	Levitt, Nick.....	WP 627	Li, Ling.....	ThP 652
Lemonakis, Nikolaos.....	WP 600	Levram-Ellisman, Varda.....	ThOC pm 3:10	Li, Linge.....	MP 764
Leney, Aneika.....	ThP 719	Lewis, David A.....	ThP 042	Li, Lingjun.....	MOH am 09:10
Leney, Aneika.....	TOC pm 2:50	Lewis, Monique.....	TP 143	Li, Lingjun.....	MP 010
Leng, Fenfei.....	ThP 481	Lewis, Monique.....	TP 139	Li, Lingjun.....	MP 009
Lenkey, Krisztián.....	TP 263	Lewis, Monique.....	TP 488	Li, Lingjun.....	MP 405
Lentz, David.....	WP 597	Lewis, Monique.....	WP 241	Li, Lingjun.....	MP 448
Lenz, Christof.....	MP 198	Lewis, Norman.....	TP 676	Li, Lingjun.....	MP 460
Lenz, Christof.....	ThP 203	Lewis, Robert.....	WP 665	Li, Lingjun.....	ThOH am 09:10
Lenz, Christof.....	ThP 456	Lewis, Zachery.....	TP 221	Li, Lingjun.....	ThP 169
Lenz, Christof.....	ThP 459	Leymarie, Nancy.....	ThP 716	Li, Lingjun.....	ThP 493
Leon, Carlos.....	WP 286	Leymarie, Nancy.....	WP 007	Li, Lingjun.....	TP 168
Leon, Deborah R.....	ThP 716	Leymarie, Nancy.....	WP 008	Li, Lingjun.....	TP 422
Leonard, Buckbinder.....	MOF pm 4:10	Leymarie, Nancy.....	WP 085	Li, Lingjun.....	TP 454
Leonardis, Aleš.....	MP 028	L'HOSTIS, Guillaume.....	TP 224	Li, Lingjun.....	WOE am 09:10
Leong, Lai Peng.....	ThP 622	Li, Ailin.....	MP 706	Li, Lingjun.....	WP 006
Leprince, Françoise.....	WP 396	Li, Anyin.....	TP 398	Li, Lingyun.....	ThP 718
Lerari, Thilo.....	TP 141	Li, Changku.....	TP 281	Li, Lingyun.....	ThP 725
Lermyte, Frederik.....	ThP 191	Li, Changkun.....	TP 757	Li, Lingyun.....	TP 254
Lermyte, Frederik.....	TOC pm 3:50	Li, Changkun.....	WP 393	Li, Lingyun.....	TP 329
Lerner, Raissa.....	TP 424	Li, Changkun.....	WP 629	Li, Lingyun.....	WOD pm 3:10
Leroux, Fanny.....	TP 577	Li, Changkun.....	WP 739	Li, Lixin.....	WP 736
Lesage, Denis.....	ThP 513	Li, Chao.....	ThP 675	Li, Mei.....	WP 122
Lesage, Denis.....	ThP 696	Li, Chen.....	TP 154	Li, Mei.....	WP 540
Lesage, Denis.....	TP 369	Li, Chen.....	WP 044	Li, Mei.....	WP 546
Lesch, Andreas.....	TP 389	Li, Dan.....	ThP 438	Li, Min.....	TP 535
Lescuyer, Pierre.....	MP 148	Li, Ding.....	TP 396	Li, Min.....	WP 306
Lescuyer, Pierre.....	TP 093	Li, Donghui.....	ThP 253	Li, Ming.....	ThP 281
Lescuyer, Pierre.....	WP 156	Li, Fei.....	MP 203	Li, Pan.....	MOC am 08:30
Lesiak, Ashton.....	WP 292	Li, Fei.....	ThP 390	Li, Pei.....	MP 170
Lesiak, Ashton.....	WP 336	Li, Fei.....	WP 601	Li, Pei.....	WP 486
Lesslie, Michael.....	TP 342	Li, Fengyao.....	MP 329	Li, Peter.....	TP 154
Lesur, Antoine.....	ThP 442	Li, Fred.....	WP 776	Li, Qiang.....	ThP 672
Leszyk, John.....	MP 134	Li, Frederick.....	MP 523	Li, Qiang.....	TP 396
Leszyk, John D.....	WOF pm 3:10	Li, Frederick.....	WP 775	Li, Qianqian.....	WOE pm 3:10
Letarte, Sylvain.....	MP 533	Li, Fumin.....	WP 541	Li, Qing K.....	MP 432
Letarte, Sylvain.....	WP 361	Li, Gang.....	MP 664	Li, Qingrun.....	WP 044
Letarte, Sylvain.....	WP 626	Li, Gangqiang.....	MP 664	Li, Qing-Run.....	WP 090
Letarte, Sylvain.....	WP 634	Li, Gongyu.....	MP 399	Li, Qiyao.....	WP 239
Letourneau, Dane R.....	MP 556	Li, Guoyun.....	ThP 718	Li, Quanzi.....	MP 209
Leung, Anthony K.L.....	TP 111	Li, Hang.....	MP 398	Li, Rongxia.....	WP 044
Leung, Kelvin SY.....	MP 593	Li, Hang.....	TP 135	Li, Ruizhi.....	TP 103
Leung, Lisa.....	TP 286	Li, Hao.....	TP 520	Li, Run.....	WP 633
Leung, Lisa M.....	WP 288	Li, Hao.....	TP 523	Li, Sam.....	ThP 622

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Li, Shelly	TP 730	Liao, Chih-Yu	MP 306	Lin, David	ThP 262
Li, Sheng	ThP 133	Liao, Chih-Yu	MP 307	Lin, Han-Jia	MP 624
Li, Sheng	WP 226	Liao, Debra	TP 515	Lin, Han-Jia	ThP 644
Li, Shuaicheng	WP 064	Liao, Guanhua	TP 366	Lin, Hao	ThP 016
Li, Shunqiang	ThP 170	Liao, Guochao	TP 319	Lin, Hao	ThP 017
Li, Shunqiang	TP 169	Liao, Guojian	TP 122	Lin, Hening	MP 118
Li, Shunqiang	TP 173	Liao, James C.	WP 589	Lin, Hening	TP 203
Li, Shunqiang	WOG pm 3:50	Liao, Wei-Li	WP 141	Lin, Hou-Yu	MP 307
Li, Shuwei	ThP 302	Liao, Zhongping	MP 213	Lin, Hou-Yu	MP 306
Li, Siyang	TOB pm 3:10	Liao, Zhongping	TOG am 10:10	Lin, Hua	WP 213
Li, Siyang	TP 089	Liao, Jie	WP 413	Lin, Hung-Yu	MP 063
Li, Su-Chen	TP 456	Liba, Amir	TP 692	Lin, Jason Ching-Yao	TP 207
Li, Sujun	WP 038	LiCata, Vince	ThP 121	Lin, Jia-Der	WP 691
Li, Tuo	ThP 340	Licea Perez, Hermes	MP 501	Lin, Jung-Lee	MP 304
Li, Tuo	WOF pm 3:50	Licea Perez, Hermes	MP 714	Lin, Jung-Lee	MP 393
Li, Wei	MP 209	Lichtenberger, Emily	TP 535	Lin, Jung-Lee	TP 330
Li, Wenjing	ThP 642	Lichti, Cheryl	ThP 041	Lin, Jung-Lee	TP 687
Li, Wenjing	TP 437	Lichti, Cheryl	WP 032	Lin, Karen	WP 611
Li, Wenkui	WP 528	Lichti, Cheryl	WP 238	Lin, Liang	ThP 323
Li, Wenkui	WP 645	Lichtman, Joshua S.	ThP 334	Lin, Liang	WP 016
Li, Wenyu	TP 460	Lieberenz, Marcus	MP 041	Lin, Liang	WP 152
Li, Wenzhou	TP 241	Lieberenz, Marcus	ThP 046	Lin, Longze	WP 337
Li, Wenzhou	WP 196	Lieberman, Rachel	ThP 766	Lin, Min	MP 647
Li, Xiang	ThP 364	Lieberman, Rachel	WP 161	Lin, Ninghang	ThOB am 08:50
Li, Xiang	ThP 365	Liebler, Daniel C.	ThP 281	Lin, Ninghang	WP 749
Li, Xiang	ThP 366	Liederer, Bianca	MP 499	Lin, Pei-Yi	WP 492
Li, Xiang	TOA pm 2:30	Liem, Michael	ThP 045	Lin, Qishan	MP 752
Li, Xiang	TP 710	Lietz, Christopher	MOH am 09:10	Lin, Roman	MP 738
Li, Xiangdong	ThP 547	Lietz, Christopher	MP 010	Lin, Roman	TP 769
Li, Xianyu	TP 442	Lietz, Christopher	ThP 493	Lin, Shanhua	WP 262
Li, Xiaohua	WP 553	Lietz, Christopher	TP 168	Lin, Shirley	TP 261
Li, Xiaojin	TP 779	Lightfield, Alan	ThOC am 09:50	Lin, Shiwen	MP 161
Li, Xiaoyan	MP 177	Lih, Fred Bjorn	ThP 404	Lin, Shu	ThOF pm 2:30
Li, Xingde	TP 003	Ligand, Jaanus	MP 313	Lin, Shu	ThP 267
Li, Xing-Fang	WOC pm 4:10	Liko, Idlir	ThP 501	Lin, Shu	TP 099
Li, Xing-Fang	WP 561	Liko, Idlir	WOH pm 3:50	Lin, Tzu-Yung	MP 654
Li, Xing-Fang	WP 567	Lill, Jennie	ThOF pm 2:30	Lin, Tzu-Yung	TOE pm 2:50
Li, Xiuqin	WP 404	Lilley, Kathryn S.	WOD am 09:30	Lin, Yan-Ping	TP 765
Li, Xuanwen	TP 103	Lilley, Kathryn S.	WP 738	Lin, Ya-Ping	TP 330
Li, Xuesong	TOC am 08:50	Lilly, Taylor	MP 381	Lin, Ya-Ping	TP 687
Li, Yafeng	MP 400	Lilly, Taylor	MP 383	Lin, Yong Y	ThP 448
Li, Yalan	MOA am 08:50	Lilly, Taylor	WP 385	Lin, Yong Y	TP 450
Li, Yanhong	TP 258	Lim, Hee-Joung	TP 441	Lin, Yuehe	ThOD pm 4:10
Li, Yifan	WP 751	Lim, Ho-Jin	ThP 549	Lin, Zheng	MOE pm 3:10
Li, Yihan	TP 196	Lim, Jihyeon	MP 421	Lin, Zheng	TP 541
Li, Yiming	MP 094	Lim, Jong-Sun	MP 127	Lin, Zhenxin	WP 060
Li, Yinghe	MP 514	Lim, Mi Hee	TOF pm 3:50	Lin, Zhenxin	WP 458
Li, Yinghe	WP 106	Lim, Sungmin	TP 747	Lin, Zhenxin	WP 500
Li, Yinyin	MOE am 09:30	Lim, Swee Chin	MP 535	Lin, Zhewang	MP 118
Li, Yongmin	ThOC am 09:10	Lim, Swee Chin	ThP 587	Lin, Ziqing	TP 353
Li, Yongmin	MP 620	Lima, Diogo B.	TP 686	Lincoln, Christopher	ThP 526
Li, Yong-Xi	ThP 435	Limbach, Patrick	MP 392	Lindberg, Johan	TP 046
Li, Yong-Xi	TP 494	Limbach, Patrick	ThP 517	Lindemann, Claudia	TP 141
Li, Yong-Xi	WP 104	Limbach, Patrick	ThP 518	Lindemann, Stephen	MP 569
Li, Yong-Xi	WP 633	Limbach, Patrick	ThP 516	Lindinger, Christian	MP 663
Li, Yuanli	ThP 270	Limbach, Patrick	WP 363	Lindinger, Christian	ThP 738
Li, Yue	WP 402	Limbach, Patrick	WP 364	Lindner, Herbert H.	ThP 226
Li, Yueqi	WP 739	Limper, Andy	MP 429	Lindner, Herbert H.	ThP 242
Li, Yu-Teh	TP 456	Lin, Aaron	ThP 171	Lindner, Ingo	WP 049
Li, Zhendong	TP 655	Lin, Andrew	TP 205	Lindner, Kathrin	ThP 746
Li, Zhenyu	MP 161	Lin, Baiwei	TP 681	Lindner, Martin	ThP 055
Li, Zhi	TP 203	Lin, Baochuan	MP 279	Lindsay, John	WP 047
Li, Zhou	TP 125	Lin, Baochuan	MP 278	Lindsey, Merry	ThP 156
Li, Zixuan	MP 176	Lin, Changqing	TP 523	Lindsey Rose, Kristie	TP 073
Liang, Hui-Chung	ThP 163	Lin, Cheng	MOH am 08:50	Lineberger, W. Carl	MP 321
Liang, Qiaoli	ThP 709	Lin, Cheng	ThOH pm 2:30	Ling, Changying	WP 239
Liang, Renxing	TP 666	Lin, Cheng	ThOH pm 4:10	Ling, Victor	TP 159
Liang, Shun-Hsin	WP 450	Lin, Cheng	ThP 711	Ling, Victor	WP 610
Liang, Suh-Yuen	TP 121	Lin, Cheng	ThP 716	Ling, Yee-Soon	TP 312
Liang, Tao	TP 286	Lin, Cheng	TP 323	Linhardt, Robert J.	ThP 725
Liang, Wenzhong	TP 523	Lin, Cheng	WP 007	Linhardt, Robert J.	TP 254
Liang, Wenzhong	TP 520	Lin, Chen-Lung Steve	MP 435	Linhardt, Robert J.	TP 329
Liang, Yuexue	WP 051	Lin, Chenwei	ThOE am 10:10	Linhardt, Robert J.	WOD pm 3:10
Liang, Yuxue	MP 051	Lin, Chenwei	ThP 218	Linhardt, Robert	ThP 718
Liang, Yuxue	WP 119	Lin, Chenwei	TOG am 08:30	Link, Andrew	WP 243
Liang, Zhenmin	TP 480	Lin, Chih-Ming	ThP 275	Link, Marek	ThP 201
Liang, Zhidan	WOE am 09:10	Lin, Chih-Yuan	MP 305	Linscheid, Michael	MP 178
Liao, Che-I	WP 599	Lin, Ching Ying	TP 768	Linton, Kenneth J.	WP 082
Liao, Chen-Chung	TP 120	Lin, Chun-Hung	TP 207	Liotta, Lance	TP 440

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Lippa, Katrice.....	WP 451	Liu, Siqi.....	WP 016	Lodder, Helen.....	MP 758
Lippens, Jennifer.....	ThP 471	Liu, Siqi.....	WP 152	Lodder, Helen.....	MP 783
Lipshutz, David.....	MP 512	Liu, Tao.....	TP 169	Lodder, Helen.....	ThP 589
Lipton, Mary.....	MP 569	Liu, Tao.....	WOE am 08:30	Lodén, Henrik.....	TP 013
Lipton, Mary.....	TP 676	Liu, Tao.....	WOG pm 2:50	Loessl, Philip.....	ThOF am 08:30
Lipton, Mary.....	WP 088	Liu, Tao.....	WP 513	Löffler, Frank.....	MP 277
Liras, Jennifer.....	MP 126	Liu, Ting.....	ThP 530	Loftus, Neil.....	TP 285
Lis, Rosina.....	WP 475	Liu, Ting.....	TP 296	Loftus, Neil.....	TP 282
Lisa, Miroslav.....	MP 245	Liu, Ting.....	TP 619	Loftus, Neil.....	WP 614
Lisa, Miroslav.....	ThP 396	Liu, Ting.....	WP 731	Loftus, Neil J.....	MP 762
Lisa, Miroslav.....	ThP 410	Liu, Weiguo.....	WP 710	Loftus, Neil J.....	WP 641
Lisitsa, Andrey.....	ThP 248	Liu, Wei-ting.....	MP 056	Logan, Timothy.....	WP 585
Lisitsa, Andrey V.....	TP 081	Liu, Xia.....	MP 232	Loginov, Denis.....	TP 007
Littau, Sally.....	WP 454	Liu, Xia.....	TP 123	Logothetis, Christopher.....	ThP 423
Littlewood, Peter.....	WP 620	Liu, Xiao.....	ThP 767	Logsdon, Aric F.....	TP 038
Litzau, Jonathan J.....	ThP 626	Liu, Xiaodong.....	TP 337	Lohnes, Karen.....	MP 016
Liu, Aihua.....	MP 502	Liu, Xiaodong.....	WP 262	Lohr, Kelly.....	ThP 304
Liu, Aihua.....	ThP 438	Liu, Xiaofen.....	WP 252	Lohse, Brian.....	TOF pm 2:30
Liu, Baohong.....	TP 389	Liu, Xiaojing.....	WP 584	Loike, John.....	MP 068
Liu, Chang.....	ThOC am 08:50	Liu, Xiaoqian.....	ThP 300	Lok, David.....	MP 513
Liu, Chang.....	ThP 473	Liu, Xiaoqian.....	WP 497	Lombard, Camille.....	TP 197
Liu, Chang.....	ThP 505	LIU, Xiaowei.....	TP 758	Londry, Frank.....	WP 696
LIU, Chang.....	TP 758	Liu, Xiaowen.....	ThP 064	Long, Carrie M.....	ThP 309
Liu, Chao.....	WP 054	Liu, Xiaowen.....	ThP 062	Long, Ernest.....	MP 727
Liu, Chao.....	WP 053	Liu, Xiaowen.....	ThP 065	Long, Tran.....	MP 599
Liu, Charles C.....	MP 378	Liu, Xiaowen.....	TP 090	Long, William.....	MP 500
Liu, Charles C.....	WP 407	Liu, Xiaowen.....	WP 046	Longuespée, Rémi.....	MP 441
Liu, Charles C.....	WP 416	Liu, Xiaowen.....	WP 064	Longuespée, Rémi.....	TP 418
Liu, Charles C.....	WP 413	Liu, Xiaoxiao.....	TP 646	Lonie, Elisabeth.....	ThP 677
Liu, Charles C.....	WP 414	Liu, Xiaoxin.....	MP 277	Lonie, Elisabeth.....	TP 479
Liu, Cheng Bin.....	ThP 388	Liu, Xiaoxuan.....	TP 781	Loo, Joseph.....	WOG am 10:10
Liu, Chih-Wei.....	TP 163	Liu, Xin.....	WP 632	Loo, Joseph A.....	MOD am 09:50
Liu, Chih-Wei.....	TP 198	Liu, Xueting.....	MP 056	Loo, Joseph A.....	MP 016
Liu, Chih-Wei.....	WOB am 09:50	Liu, Yan.....	ThOH am 09:10	Loo, Joseph A.....	MP 145
Liu, Chin-Chi.....	ThP 121	Liu, Yan.....	ThP 715	Loo, Joseph A.....	MP 184
Liu, Chongming.....	TP 346	LIU, Yang.....	ThP 669	Loo, Joseph A.....	MP 314
Liu, Chuan.....	MOD pm 2:50	Liu, Yang.....	WP 610	Loo, Joseph A.....	MP 467
Liu, Chuanfa.....	ThP 126	Liu, Yansheng.....	MOG pm 3:50	Loo, Joseph A.....	ThP 092
Liu, Cui.....	ThP 206	Liu, Yansheng.....	MP 432	Loo, Joseph A.....	ThP 716
Liu, Cynthia.....	MOA am 10:10	Liu, Yansheng.....	ThP 257	Loo, Joseph A.....	TOD am 08:50
Liu, Danting.....	WP 530	Liu, Yansheng.....	ThP 668	Loo, Joseph A.....	TOE pm 3:10
Liu, Guifang.....	MP 330	Liu, Yijun.....	WP 585	Loo, Joseph A.....	TP 150
Liu, Guowen.....	ThP 768	Liu, Ying.....	ThP 527	Loo, Joseph A.....	TP 471
Liu, Guowen.....	TP 501	Liu, Yinggao.....	MP 734	Loo, Rachel O.....	MP 016
Liu, Guowen.....	WP 188	Liu, Yingzhi.....	ThP 739	Loo, Rachel O.....	MP 145
Liu, Guowen.....	WP 543	Liu, Yong.....	TP 474	Loo, Rachel O.....	TP 150
Liu, Guowen.....	WP 534	Liu, Yong.....	TP 475	Loo, Rachel R. Ogorzalek.....	TOE pm 3:10
Liu, Haichuan.....	ThP 511	Liu, Yonggang.....	TP 306	Looser, Ralf.....	MP 638
Liu, Haijun.....	MP 111	Liu, Zhaogui.....	MP 400	Lootsma, Wayne.....	MOF pm 2:50
Liu, Haijun.....	ThOF am 10:10	Liu, Zhaoyang.....	TP 783	Lootsma, Wayne.....	WP 627
Liu, Hanlan.....	TP 024	Liu, Zhen.....	TP 562	Lopes, Andrey.....	TP 025
Liu, Hongcheng.....	TP 148	Liu, Zhi-Yu.....	ThP 275	Lopez, Linda.....	MP 596
Liu, Hongji.....	WP 199	Liu, Charles C.....	WP 404	Lopez, Linda.....	MP 634
Liu, Hongzhi.....	WP 546	Liuni, Peter.....	MP 531	Lopez, Mary.....	WP 515
Liu, Hongzhi.....	WP 540	Livchak, Stephania.....	MP 153	Lopez, Mary F.....	WP 192
Liu, Huafen.....	TP 619	Livingston, Brittny.....	WP 196	Lopez, Mary F.....	ThP 450
Liu, Huiling.....	MP 427	Liyanage, Rohana.....	ThP 127	Lopez, Mary F.....	TP 244
Liu, Jane.....	TP 501	Llewellyn, Gareth.....	ThP 394	López, Juan Antonio.....	ThP 336
Liu, Jia.....	WP 083	Llinás, Manuel.....	MP 271	Lopez de Alda, Miren.....	TP 551
Liu, Jiangjiang.....	WP 747	Llinás, Manuel.....	TP 101	Lopez Ferrer, Daniel.....	MP 652
Liu, JianHua.....	WP 618	Lloyd, John R.....	TP 773	Lopez Ferrer, Daniel.....	ThP 613
Liu, Jinny L.....	MP 278	Lloyd, Kenneth.....	MP 134	Lopez Gonzalez, Cesar.....	TP 784
Liu, Jinqi.....	ThOE am 09:10	Lo, Andy.....	MP 446	Lopez-Avila, Viorica.....	TP 752
Liu, Jinxia.....	ThP 566	Loadman, Paul.....	WP 491	Lopez-Casas, Pedro P.....	ThP 294
Liu, Junyang.....	TP 760	Lobas, Anna.....	WP 136	Lorcheim, Paul.....	TP 636
Liu, LiPeng.....	ThP 739	Lobas, Anna A.....	WP 164	Lorent, Urszula.....	TP 494
Liu, Min.....	WP 718	Lobas, Anna A.....	WP 172	Lorente, José A.....	MP 582
Liu, Minjing.....	MOH am 08:50	Lobodin, Vladislav.....	TP 596	Lorente, José A.....	MP 584
Liu, Pengyuan.....	TP 397	Lobodin, Vladislav V.....	MOA am 08:30	Lorenz, Matthias.....	ThOB am 08:30
Liu, Ping.....	TP 106	Locasale, Jason.....	WP 584	Loroch, Stefan.....	TP 105
Liu, Qian.....	ThP 130	Lochridge, Jackie.....	TP 347	Lorphelin, Alain.....	TP 225
Liu, Qian.....	TP 546	Lock, Stephen.....	MP 344	Lössl, Philip.....	WOG am 09:30
Liu, Qiang.....	TP 662	Lockhart, Sybil.....	WP 191	Lou, Sha.....	TP 049
Liu, Renmeng.....	WP 009	Lockman, Paul R.....	TP 038	Lou, Xiaomin.....	WP 016
Liu, Serah.....	TP 154	Lockwood, Sarah Y.....	WP 632	Lou, Xiaomin.....	WP 152
Liu, Sherry.....	MP 503	Loda, Massimo.....	WP 475	Louie, Katherine.....	MP 024
Liu, Sherry.....	TP 519	Lodder, Helen.....	MP 341	Louis, Edouard.....	ThP 256
Liu, Shuo.....	MOC am 09:10	Lodder, Helen.....	MP 757	Loukotkova, Lucie.....	TP 489
Liu, Siqi.....	ThP 323	Lodder, Helen.....	MP 756	Loukotkova, Lucie.....	WP 548

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Loureiro, Liliana.....	ThP 101	Luo, Qingjie .....	TP 398	Maccoss, Michael J. ....	MOG am 09:50
Loutelier-Bourhis, Corinne.....	WOC pm 2:50	Luo, Quanzhou .....	TP 239	Maccoss, Michael J. ....	ThP 035
Loutelier-Bourhis, Corinne.....	WP 679	Luo, Quanzhou .....	WP 196	Maccoss, Michael J. ....	ThP 326
Love, Chasity.....	ThOD am 08:50	Luo, Yongyi .....	WP 638	MacCoss, Michael J. ....	ThP 763
Love, Chasity B. ....	MP 323	Luo, Yue .....	MP 580	MacCoss, Michael J. ....	TOG pm 3:50
Love, Christopher J. ....	TP 007	Luo, Yue .....	TP 756	Maccoss, Michael J. ....	TP 083
Love, Katie.....	ThP 114	Luongo, Carl .....	TP 341	Maccoss, Michael J. ....	WOG pm 4:10
Lovestone, Simon.....	ThP 163	Lupo, Sharon.....	MP 281	Maccoss, Michael J. ....	WP 017
Lovrics, Anna.....	ThP 379	Lupo, Sharon.....	WP 450	Maccoss, Michael J. ....	WP 037
Low-De'carie, Etienne .....	TP 677	Luptak, Andrej.....	WP 094	Maccoss, Michael J. ....	WP 115
Lowe, David.....	ThP 120	Luszczek, Elizabeth.....	TP 656	Maccoss, Michael J. ....	WP 737
Lowe, David.....	WP 201	Lusk, Todd .....	MP 504	Macrehan, William .....	TP 690
Lowenthal, Mark .....	MOE pm 4:10	Lutisan, Juraj .....	MP 623	MacDonald, Matthew L.....	ThP 042
Lowenthal, Mark .....	TP 266	Lutisan, Juraj .....	TP 526	MacDonald, Matthew L.....	WP 148
Loziuk, Philip .....	MP 209	Lutowski, Corinne.....	TP 163	Macek, Boris.....	MP 215
Lu, Bingwen.....	MOE am 10:10	Lutowski, Corinne.....	TP 288	Macek, Boris.....	ThP 043
Lu, Bingwen.....	ThP 294	Lutowski, Corinne.....	WOB am 09:50	Macek, Boris.....	ThP 080
Lu, Congcong .....	ThP 091	Lutter, Petra .....	ThP 610	Macek, Boris.....	ThP 081
Lu, Dezhao .....	TP 619	Luttrell, Louis .....	TP 128	Macek, Boris.....	WP 242
Lu, Guotao .....	MP 487	Lutz, Beat .....	TP 424	MacGilvray, Matthew E.....	ThP 178
Lu, Guotao .....	MP 635	Lutz, Eric .....	WP 454	Macha, Stephen .....	ThP 627
Lu, Guotao .....	TP 283	Lutz, Ryan .....	ThP 671	Machado, Andrea .....	MP 390
Lu, Guotao .....	WP 624	Lutz, Ryan .....	TP 492	Machado, Jandyson .....	ThOA am 09:30
Lu, Guotao .....	WP 643	Lutz, Ryan .....	WP 547	Machado Santos, Jandyson .....	TP 586
Lu, I-Chung .....	MP 305	Lux, François .....	MP 731	Machaidze, Revaz .....	TP 007
Lu, I-Chung .....	MP 306	Luzzatto Knaan, Tal.....	MP 020	Macher, Bruce .....	MP 453
Lu, I-Chung .....	MP 307	Lv, Tingting .....	WP 752	Macher, Thomas.....	ThP 709
Lu, Jacquie .....	MP 233	Ly, Justin Q. ....	WP 005	Macherla, Venkat .....	MP 056
Lu, Jie .....	MOA am 08:30	Ly, Melissa .....	WP 208	Macherone, Anthony.....	TP 453
Lu, Jonathan .....	ThP 037	Ly, Van .....	WP 636	Macherone, Anthony.....	WP 421
Lu, Mei .....	MP 329	Lyashkov, Alexey .....	MP 262	Machtejevas, Egidijus.....	MP 741
Lu, Meiling .....	MP 348	Lyashkov, Alexey .....	ThOE pm 3:30	Machtejevas, Egidijus.....	WP 284
Lu, Meiling .....	ThP 527	Lyashkov, Alexey .....	TP 468	Machuron-Mandard, Xavier.....	ThP 696
Lu, Qiaozhen (Cheryl) .....	ThP 781	Lyczko, Jadwiga .....	WP 773	Machuron-Mandard, Xavier.....	TP 524
Lu, Qiaozhen (Cheryl) .....	ThP 780	Lyianage, Rohana .....	ThP 346	Machuron-Mandard, Xavier.....	WP 396
Lu, Shan .....	ThP 051	Lyle, Charles .....	TP 753	Macia, Miriam .....	ThP 476
Lu, Tian-Sheng .....	ThP 435	Lyman, Michael .....	ThOE am 09:30	Mack, Anne.....	MP 500
Lu, Xiaodong .....	WOD am 08:50	Lynch, Eric J. ....	WP 774	Mackay, C Logan .....	ThP 104
Lu, Xiaodong .....	WOG pm 2:30	Lynch, Tom .....	TP 390	Mackay, C. Logan .....	MP 182
Lu, Xiaojun.....	WP 194	Lynn, Bert C. ....	MP 559	Mackay, C. Logan .....	TOE pm 3:50
Lu, Xiaoning.....	MP 774	Lynn, Bert C. ....	MP 560	Mackay, C. Logan .....	TOH am 08:30
Lu, Xiaoning.....	WP 623	Lynn, Bert C. ....	ThP 577	Mackay, C. Logan .....	WP 751
Lu, Yali .....	TP 243	Lyons, Greg .....	WP 400	Mackie, Ken .....	TP 198
Lu, Yali .....	WP 190	Lyons, Kathryn.....	WP 480	Mackie, Ken .....	TP 288
Lu, Yanyan .....	TP 242	Lyons, Sarah Marie .....	ThP 607	Mackintosh, Susan A.....	TP 549
Lu, Yinfei .....	WP 744	Lyssiotis, Costas .....	WOD am 09:50	Maclea, Brendan .....	MOG am 09:50
Lu, Zhike.....	WOG am 09:50	Lyssiotis, Costas.....	WP 608	Maclea, Brendan .....	MP 219
Lubahn, Dennis B. ....	ThP 302	Lyubarskaya, Yelena .....	WP 081	Maclea, Brendan .....	ThP 025
Lubeck, Markus .....	MP 723	Ma, Bin .....	ThP 016	Maclea, Brendan .....	ThP 035
Lubeck, Markus .....	WP 727	Ma, Danjun .....	TP 139	Maclea, Brendan .....	ThP 763
Lubman, David .....	WP 458	Ma, Danjun .....	TP 143	Maclea, Brendan .....	WOG pm 4:10
Lubman, David M. ....	MP 446	Ma, Danjun .....	TP 488	MacLeod, Kenneth .....	MP 214
Lubman, David M. ....	ThP 289	Ma, Danjun .....	WP 241	Macmahon, Shaun .....	MP 359
Lubman, David M. ....	TP 421	Ma, Jiamin .....	MP 378	Macovei, Alina .....	MP 162
Lubman, David M. ....	WP 060	Ma, Jun .....	WOE pm 3:10	MacVittie, Thomas .....	TP 688
Lubman, David M. ....	WP 501	Ma, Li .....	MP 197	MacVittie, Thomas .....	WP 601
Lubman, David M. ....	WP 500	Ma, Li.....	TOA am 09:50	MacVittie, Thomas J.....	ThP 642
Lucey, Brendan.....	TP 448	Ma, Lifu.....	ThOD am 10:10	MacVittie, Thomas J.....	TP 067
Luchini, Alessandra .....	TP 440	Ma, Mingming .....	TP 531	Macvittie, Thomas J.....	TP 299
Luebberstedt, Marc .....	MP 585	Ma, Qiang .....	ThP 498	MacVittie, Thomas J.....	TP 437
Luhn, Steven .....	WP 300	Ma, Qiao .....	ThP 739	Maddalo, Gianluca.....	MP 263
Lui, James .....	WP 587	Ma, Shuguang .....	ThP 357	Madden, Stephen .....	ThP 061
Luiders, T.M. ....	TP 444	Ma, Shuguang .....	WP 712	Maddock, Janine .....	ThP 454
Luiders, Theo.....	ThP 064	Ma, Shuren .....	ThP 448	Madhaven, Subha .....	MP 061
Luiders, Theo.....	ThP 209	Ma, Shuren .....	TP 450	Madsen, James .....	WP 173
Luiders, Theo.....	WP 151	Ma, Xiaoxiao .....	ThOD am 08:50	Madugundu, Anil.....	MP 270
Luiders, Theo M. ....	ThP 062	Ma, Xiaoxiao .....	ThOG pm 3:50	Madugundu, Anil.....	MP 255
Luizete, Milena .....	TP 415	Ma, Xiaoxiao .....	TP 290	Madupu, Ramana .....	ThP 284
Luk, Emily .....	WP 622	Ma, Xiaoxiao .....	WP 388	Maeda, Junko .....	MP 405
Lukacs, Gergely.....	WP 230	Ma, Xin .....	ThOF am 09:30	Maeda, Junko .....	TP 669
Luna, Leah.....	MP 054	Ma, Xin .....	TOD am 09:10	Maeder, Muriel.....	TP 423
Luna, Leah.....	WP 490	Ma, Yan .....	MP 616	Maegley, Karen.....	MP 540
Luna, Marsha.....	ThP 668	Ma, Yan .....	TP 667	Maekawa, Masamitsu.....	WP 131
Lund, Riika .....	ThP 276	Ma, Yinfa.....	TP 575	Maes, Evelyne .....	MOG pm 3:10
Lunyak, Victoria V.....	ThP 450	Ma, Yinfa.....	WP 569	Maes, Evelyne .....	TP 482
Luo, Dahai .....	ThP 126	Ma, Yonggang.....	ThP 156	Maes, Evelyne .....	WP 042
Luo, Gang.....	WP 619	Maass, Peter .....	MP 021	Maes, Evelyne .....	WP 469
Luo, Hein .....	MP 515	MacAleese, Luke.....	MOD am 09:10	Magagnotti, Cinzia.....	ThP 293
Luo, Jiejian .....	MP 222	Macatangay, Ariel .....	TP 729	Maganga, Clisy.....	WP 679

Program code: M,T,W, Th = Day    O = Oral, P = Poster    Time or poster number

# INDEX OF AUTHORS

Magera, Mark J.....	WP 655	Maljers, Louis.....	MP 720	Marcoux, Julien.....	MP 183
Magliery, Thomas.....	ThP 113	Maljers, Louis.....	TP 278	Marcoux, Marie-Josée.....	MP 490
Magni, Ruben.....	TP 440	Malkin, Mark.....	MP 428	Marcum, Christopher.....	MP 575
Magnuson, Matthew.....	MP 520	Mallard, Wm. Gary.....	MP 048	Marcum, Christopher.....	MP 775
Mahaffy, Paul.....	ThP 369	Mallet, Claude.....	TP 573	Maréchal, Éric.....	TP 408
Mahaffy, Paul.....	TOA pm 2:30	Mallick, Parag.....	MP 019	Maréchal, Éric.....	WOB pm 2:50
Mahaffy, Paul.....	TP 710	Mallick, Parag.....	ThP 035	Marek, Ales.....	WOD pm 3:30
Mahaffy, Paul.....	TP 711	Mallick, Parag.....	ThP 763	Marginean, Ioan.....	TP 324
Mahaffy, Paul.....	TP 712	Mallisho, Abdullah.....	TP 139	Marginean, Ioan.....	TP 715
Mahajan, Mukesh.....	MP 512	Mallisho, Abdullah.....	TP 143	Mari, Yelenis.....	ThP 335
Mahan, Amber R.....	MP 054	Mallisho, Abdullah.....	WP 241	Mari, Yelenis.....	TP 094
Mahan, Elizabeth.....	TOE am 08:50	Malmberg, Per.....	TP 018	Marimuthu, Arivusudar.....	MP 255
Mahat, Rajendra.....	TP 606	Malmstrom, David.....	TOG pm 3:10	Marimuthu, Arivusudar.....	ThP 204
Mahe, Pierre.....	ThP 023	Malmström, Anders.....	ThP 730	Marin Vicente, Consuelo.....	TOF pm 3:10
Maher, Christopher.....	MOG am 08:30	Malosse, Christian.....	WP 059	Marino, John P.....	TP 256
Maher, Christopher.....	TP 082	Malys, Brian.....	MP 018	Marionni, Samuel.....	ThP 470
Maher, Christopher A.....	TP 438	Malysheva, Olga.....	ThP 426	Märk, Lukas.....	MP 663
Maher, Christopher A.....	TP 433	Man, Petr.....	MP 183	Märk, Tilmann D.....	MP 663
Maheux, Maxim.....	WP 714	Man, Petr.....	ThOF am 08:50	Märk, Tilmann D.....	ThP 738
Mahieu, Nathaniel G.....	MP 602	Man, Petr.....	ThP 460	Marker, Paul.....	MP 448
Mahmud Khalil, Saleh.....	TP 071	Man, Petr.....	WP 167	Marker, Paul.....	TP 454
Mahon, John-Emmett.....	WP 370	Manadas, Bruno.....	ThP 101	Markham, Dan.....	WP 490
Mahrouche, Louiza.....	TP 108	Manadas, Bruno.....	ThP 315	Marko-Varga, György.....	WP 032
Mahrouche, Louiza.....	WP 138	Mance, Austen.....	TP 292	Markowski, Todd.....	MP 033
Mahsut, Ablatt.....	MP 075	Mancuso, Francesco Mattia.....	ThP 220	Markowski, Todd.....	MP 049
Mahsut, Ablatt.....	ThOE am 09:10	Manda, Srikanth S.....	MP 255	Markowski, Todd.....	MP 104
Mai, Anna.....	MOF pm 3:30	Manda, Srikanth S.....	MP 256	Markowski, Todd.....	MP 429
Maier, Claudia.....	ThP 286	Mandal, Mridul Kanti.....	WP 381	Markowski, Todd.....	ThP 777
Maier, Claudia.....	WOC pm 3:10	Mandal, Rupasri.....	ThP 269	Markowski, Todd.....	TP 076
Maier, Claudia.....	WOD am 08:30	Mandi, Nagnath.....	WP 717	Marks, Christopher R.....	TP 665
Maier, Claudia S.....	ThP 277	Manes, Nathan.....	MP 261	Marmor, Bonnie.....	ThP 536
Maier, Claudia S.....	ThP 380	Manes, Nathan.....	MP 269	Marmor, Bonnie.....	ThP 584
Maier, Claudia S.....	ThP 606	Manes, Nathan.....	ThP 074	Maroui, Mohamed Ali.....	TP 108
Maier, Stefan.....	TP 052	Mangrum, John.....	MP 064	Marquet, Pierre.....	ThP 599
Maile, Tobias.....	ThOF pm 2:30	Mangrum, John.....	ThP 251	Marquet, Pierre.....	ThP 600
Maile, Tobias.....	WP 048	Mangrum, John.....	ThP 460	Marquis, Robert.....	MP 512
Maitra, Anirban.....	MP 255	Mani, D. R.....	MOG am 08:30	Marrero, Jorge.....	WP 060
Maitra, Sushmit.....	WP 505	Mani, D. R.....	ThOE am 10:10	Marrero, Jorge.....	WP 458
Maitre, Philippe.....	TOD pm 2:30	Mani, D. R.....	ThP 205	Marriner, Gwendolyn A.....	TP 030
Maitre, Philippe.....	TP 368	Mani, D. R.....	TOG am 08:30	Marroquin-Guzman, Margarita.....	MP 600
Maitre, Philippe.....	TP 372	Mani, D. R.....	TP 438	Marsden, Philip.....	MP 233
Maity, Sankar.....	ThP 423	Mani, D. R.....	TP 426	Marsh, Don.....	ThP 035
Maity, Tapan.....	ThP 204	Mani, D. R.....	ThP 025	Marsh, Donald.....	ThP 763
Majdi, Ellie.....	ThP 427	Mani, Jan.....	TP 134	Marshall, Alan.....	TP 596
Majdi, Ellie.....	TP 558	Manicke, Nicholas.....	ThOA am 08:50	Marshall, Alan G.....	MOA am 08:30
Majdi, Ellie.....	WP 648	Manicke, Nicholas E.....	WP 400	Marshall, Alan G.....	MOB am 10:10
Majmudar, Jaimeen.....	MOH am 09:50	Manicke, Nicholas E.....	MP 285	Marshall, Alan G.....	MP 084
Majumdar, Ranajoy.....	WP 215	Mann, Jessica.....	MP 261	Marshall, Alan G.....	MP 550
Majumdar, Tapan.....	TP 502	Mann, Matthias.....	MP 723	Marshall, Alan G.....	MP 555
Mak, Chun Kong.....	MP 709	Mann, Matthias.....	WP 257	Marshall, Alan G.....	MP 648
Makarov, Alexander.....	MOD pm 4:10	Manning, Janet.....	ThP 210	Marshall, Alan G.....	MP 699
Makarov, Alexander.....	MP 653	Manohar, Venkat.....	TP 528	Marshall, Alan G.....	ThOF pm 3:10
Makarov, Alexander.....	ThP 190	Manohar, Venkat.....	TP 529	Marshall, Alan G.....	ThP 129
Makarov, Alexander.....	ThP 507	Manohar, Venkat.....	WP 328	Marshall, Alan G.....	TOE pm 4:10
Makarov, Alexander.....	ThP 751	Manohar, Venkat.....	WP 539	Marshall, Alan G.....	TP 456
Makarov, Alexander.....	ThP 752	Manoil, Colin.....	ThP 464	Marshall, Alan G.....	TP 600
Makarov, Alexander.....	ThP 754	Manoj, Ghaste.....	TP 643	Marshall, Alan G.....	TP 595
Makarov, Alexander.....	TOB am 10:10	Manolakos, Spiros.....	WP 769	Marshall, Alan G.....	TP 597
Makarov, Alexander.....	TOD am 08:30	Mansour, Tarek.....	TP 408	Marshall, Alan G.....	TP 599
Makarov, Alexander.....	TP 136	Manura, John.....	TP 767	Marshall, Alan G.....	TP 601
Makarov, Alexander.....	WOA pm 3:30	Manzini, M. Chiara.....	TP 197	Marshall, Alan G.....	TP 602
Makarov, Alexander.....	WOF am 09:30	Mao, Chuanbin.....	WP 741	Marshall, Alan G.....	TP 598
Makarov, Alexander.....	WP 760	Mao, Haibin.....	ThP 462	Marshall, Alan G.....	TP 720
Makarov, Vasily.....	MP 651	Mao, Lu.....	TP 720	Marshall, Alan G.....	WOA am 09:30
Makboul, Makboul A.....	WP 319	Mao, Pan.....	TP 740	Marshall, Alan G.....	WOA pm 3:50
Makepeace, Karl.....	ThP 049	Mao, Yang.....	ThOH pm 4:10	Marshall, Alan G.....	WP 705
Makriyannis, Alexandros.....	ThP 131	Mao, Yang.....	ThP 730	Marshall, Alan G.....	WP 706
Malakar, Dipankar.....	MP 155	Maor, Maya.....	ThP 197	Marshall, Alan G.....	WP 735
Malakar, Dipankar.....	TP 436	Mapolelo, Mmili M.....	WOA pm 3:50	Marshall, Alan G.....	WP 734
Malaker, Stacy.....	MOH am 10:10	Maranda, Bruno.....	WP 441	Marshall, Connie.....	ThP 199
Malanoski, Anthony.....	MP 279	Marathi, Ramya.....	TP 467	Marshall, Dana.....	MP 595
Malanoski, Anthony P.....	MP 278	Marathi, Ramya L.....	ThOE am 09:50	Marshall, Darrell.....	TP 452
Malech, Harry.....	ThP 313	Marcano, Francia.....	TP 585	Marshall, Darrell.....	WP 593
Maleki, Hossein.....	MP 590	March, Raymond.....	TP 673	Marshall, David.....	ThOD am 10:10
Maleki, Hossein.....	TP 540	Marchand, Adrien.....	MOC am 09:30	Marshall, Harvey E.....	WOG pm 3:30
Maleknia, Simin D.....	MP 438	Marchetti-Deschmann, Martina.....	TP 053	Marshall, Peter.....	WP 013
Maleknia, Simin D.....	ThP 358	Marchionni, Mark A.....	TP 055	Marsico, Alyssa.....	WP 701
Malih, Paymaneh.....	TP 195	Marciano, David.....	ThP 137	Marsili, Ray.....	MOA pm 4:10
Malinao, Maria Christina.....	TP 206	Marcobal, Angela.....	ThP 334	Marszalkowskil, Frank.....	MP 782

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Martello, Rita	WP 109	Matsuda, Fumio	WP 130	Mccomb, Mark E	ThP 057
Martens, Jonathan	ThOD pm 3:30	Matsuda, Shuichi	MOF pm 3:10	McComb, Mark E	TP 095
Martens, Jonathan	TP 365	Matsuda, Takahisa	WP 143	Mccomb, Mark E	WP 195
Martens, Lennart	MP 033	Matsumoto, Keiko	ThP 633	Mccomb, Mark E	WP 445
Martens, Lennart	MP 032	Matsumoto, Keiko	TP 510	McConville, Patricia	MP 728
Martens, Lennart	MP 682	Matsumoto, Takafumi	WP 477	McConville, Patricia	MP 729
Martens, Lennart	TP 105	Matsunobu, Takehiko	WOH am 09:10	Mccord, James	ThP 731
Martin, Amanda C	TP 641	Matsuo, Jiro	MP 005	McCorrister, Stuart	TP 213
Martin, Brent	MOH am 09:50	Matsuura, Nariaki	WP 474	Mccorrister, Stuart	TP 216
Martin, Christopher E	TP 160	Matsuura, Shuji	WP 474	McCoy, Joe-Ann	WP 338
Martin, Jesse	MP 161	Matthew, David	ThOA am 09:10	McCubbin, Patrick	ThP 333
Martin, Jonathan	WOC pm 3:30	Mathews, Clayton	MP 785	McCullagh, Michael	WP 668
Martinez, Jairo Rene	TP 679	Mathews, David	MOG am 09:10	McCullagh, Michael	WP 667
Martinez, Marissa	ThP 082	Mathias, Mann	ThP 762	McCullagh, Michael	WP 666
Martinez, MPaz	MP 582	Mattivi, Fulvio	TP 643	McCullagh, Michael	WP 695
Martinez Arias, Alfonso	WP 738	Matyas, Gary R	WP 211	McCullagh, Mike	TP 618
Martinez Ferrando, Isabel	MP 262	Mauldin-Jeronimo, Eric	ThP 306	McCullers, Jonathan	ThP 164
Martinez-Aguilar, Juan	MP 449	Maurer, Verena	ThP 242	McCulloch, Richard	ThP 653
Martinez-Arias, Alfonso	WOD am 09:30	Maurizot, Victor	TOC am 08:50	McDaniel, Michael	ThP 199
Martinez-Caro, Leticia	MP 584	Mauviel, Guillion	MP 576	McDonald, Craig	ThOE am 09:50
Martinez-Fonts, Kirby	TOE pm 2:30	Mawuenyega, Kwasi	TP 448	McDonald, Jacob	ThP 583
Martinez-Lozano Sinues, Pablo	WOB pm 3:50	Maxwell, Brad	MP 366	Mcdonald, Jeff	ThP 521
Martini, Tatiana	MP 461	Maxwell, G. Larry	ThP 202	McDonald, John	MP 599
Martino, Paul	MP 166	Maxwell, Robert	ThP 266	McDonald, Karen	TP 258
Martino, Paul	MP 167	Maxwell, Robert	TP 178	McDonald, Stephen	WP 637
Martins, Júlia	TP 576	May, Jody C	ThP 482	Mcdonald, W. Hayes	MP 123
Martosella, James	WP 083	May, Jody C	ThP 484	Mcdonnell, Liam	MP 004
Marupaka, Ramesh	MP 604	May, Jody C	ThP 485	Mcdonnell, Liam	MP 027
Marvin, Rachel	WP 392	May, Jody C	ThP 486	McDonnell, Liam	TP 005
Marvin, Rachel	WP 459	May, Jody C	TOC am 09:50	Mcdonnell, Liam	TP 052
Marwaha, S.S	TP 274	May, Jody C	WP 688	McDonnell, Liam A	TP 049
Marx, Harald	MP 041	May, Jody C	WP 687	McEwen, Charles	WP 376
Marx, Harald	ThP 046	Mayer, Paul Michael	ThP 700	McEwen, Charles	WP 387
Marx, Kristina	MOE pm 3:30	Mayne, Leland	MOF am 08:30	Mcewen, Charles N	MP 301
Marx, Kristina	WP 063	Mayne, Leland	ThP 128	Mcewen, Charles N	MP 534
Marx, Kristina	WP 076	Mayrand-Provencher, Laurence	WP 523	McEwen, Charles N	TP 380
Mary, Sandrine	WP 447	Mayrand-Provencher, Laurence	WP 532	McFarland, Melinda	TP 217
März, Winfried	TP 443	Mayrhofer, Corina	MP 135	Mcfarland, Melinda A	WP 333
Marzilli, Lisa	WP 208	Mays, Jared	MP 474	Mcgee, William	TP 345
Mascini, Nadine E	TP 062	Maze, Joshua	ThP 755	Mcgee, William	WP 169
Mashl, R. Jay	TP 433	Maziarz, Margaret	MP 045	McGonigal, Maura	ThOA am 10:10
Mason, Jeffrey	WP 716	Maziarz, Margaret	MP 046	McGown, Steven R	MP 290
Mason, Jeffrey T	WP 236	Mazzarino, Monica	ThP 594	Mcgrath, Sara C	MP 354
Masselot, Alexandre	WP 048	Mazzarino, Monica	ThP 595	McGrath, Sara C	ThOA pm 4:10
Massi, Jennifer	TP 284	Mazzotti, Fabio	TP 511	Mcguigan, Megan	TP 759
Massoli, Paola	TOA pm 3:10	Mazzucchelli, Gabriel	MP 441	Mcguire, Jeffrey	TP 301
Masson, Eric	MP 329	Mazzucchelli, Gabriel	ThP 256	McHale, Kevin J	MP 242
Massonnet, Philippe	MOC pm 2:30	Mazzucchelli, Gabriel	TP 176	Mchale, Kevin J	MP 243
Mastovska, Katerina	ThOA pm 3:30	Mbeunkui, Flaubert	ThP 665	McHugh, Timothy	TP 222
Masuda, Satohiro	ThP 672	MCAdam, Kevin	MOD pm 2:50	McHugh, Vince	WP 693
Masujima, Tsutomu	MOF pm 3:10	Mcalister, Graeme	MP 717	McHugh, Vincent	TOC am 09:10
Masujima, Tsutomu	MP 196	McAlister, Graeme C	ThP 214	Mcllvin, Matthew	MP 275
Masujima, Tsutomu	MP 247	McAlister, Graeme C	MP 259	Mcllvin, Matthew	WP 112
Masujima, Tsutomu	MP 417	McAllister, Erin	ThP 066	McInerney, Michael	WOG am 10:10
Masujima, Tsutomu	ThP 621	McAllister, Fiona E	TP 170	McIntire, Gregory	MP 471
Masujima, Tsutomu	WP 594	McAllister, Tim	TP 554	Mcintire, Gregory	WP 536
Mat Hashim, Dzulkify	MP 358	McArthur, Justin C	TP 468	McIntire, Ph.D., Gregory	MP 479
Mat Hashim, Dzulkify	ThP 623	McAuliffe, Brian	ThP 666	Mcintire, Ph.D., Gregory	MP 480
Matassa, Luca	TP 684	McCall, Eimear	MP 338	McIntosh, Daniel G	MP 699
Matassa, Luca	WP 533	McCann, Kevin	MP 291	Mcintosh, Ian	WP 659
Matassa, Luca C	TP 504	McCarthy, Jason W	TP 227	McIntyre, W	TP 434
Matchett, Michael	MP 736	McCarthy, Lynda	ThP 565	Mckay, Matthew	ThOE pm 2:50
Matern, Dietrich	WP 655	Mccarthy, Sean	MP 046	Mckenna, Amy	MP 550
Matheis, Katerina	WP 284	Mccarthy, Sean	MP 045	McKenna, Amy M	MOA am 08:30
Mather, Joanne	ThP 584	McCarthy, Sean	MP 728	Mckenna, Amy M	MP 555
Mathess, Scott	MP 380	McCarty, Nael A	TP 664	Mckenna, Amy M	TP 597
Mathew, Anna	MP 597	McCaskill, David	MOA am 09:30	McKenna, Amy M	TP 600
Mathew, Anna	ThP 662	McCaskill, David	ThP 318	Mckenna, Amy M	WOA pm 3:50
Mathias, Rommel	TP 451	Mccaskill, David	WP 024	McKenna, Chris	ThP 018
Mathias, Rommel	WP 244	McClatchy, Daniel B	ThP 021	McKenzie, Christine	TP 355
Mathivanan, Suresh	ThP 045	McClory, Andrew	TP 503	McKenzie, James	TOG pm 3:30
Mathur, Premendu P	MP 256	Mcclory, Phillip	MP 090	McKeown, Alan	ThP 576
Matic, Ivan	ThP 241	Mcclure, Evelyn	MP 462	McKinney, Kimberly	WP 240
Matic, Katarina	ThP 043	Mcclure, Evelyn	WP 295	McKinsey, Timothy	MP 117
Matic, Katarina	ThP 081	Mcclure, Thomas	MP 058	Mclafferty, Fred W	ThP 088
Matouschek, Andreas	TOE pm 2:30	Mcclure, Thomas	TP 652	McLaren, David	ThOE am 09:10
Matros, Andrea	MP 416	McCluskey, Adam	TP 205	McLaren, David	TP 061
Matson, Jacob	ThP 228	Mccomb, Mark E	MP 120	McLean, John	MP 595
Matsubara, Kazuo	ThP 672	Mccomb, Mark E	MP 465	Mclean, John A	MP 585

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

McLean, John A. ....	ThOD pm 2:50	Mehta, Anand .....	TP 068	Merrill, Anna E. ....	WOD am 10:10
McLean, John A. ....	ThOG pm 2:50	Mehta, Anand .....	TP 069	Mertens, Inge.....	MOG pm 3:10
McLean, John A. ....	ThP 482	Mehta, Kurren.....	WOG pm 3:30	Mertens, Inge.....	TP 482
McLean, John A. ....	ThP 485	Mehus, Aaron.....	WP 454	Mertens, Inge.....	WP 469
McLean, John A. ....	ThP 486	Meier, Florian.....	WP 452	Mertens, Koen .....	ThP 112
McLean, John A. ....	ThP 495	Meier, Jacob.....	WP 664	Mertins, Philipp.....	MOG am 08:30
McLean, John A. ....	ThP 484	Meier, Jacob.....	WP 663	Mertins, Philipp.....	ThOE am 10:10
McLean, John A. ....	TOB pm 2:50	Meier, Scott.....	WP 514	Mertins, Philipp.....	ThP 039
McLean, John A. ....	TOC am 09:50	Meier-Schellersheim, Martin.....	MP 269	Mertins, Philipp.....	ThP 205
McLean, John A. ....	WP 687	Meija, Juris .....	TP 770	Mertins, Philipp.....	TOG am 08:30
McLean, John A. ....	WP 688	Meijer, Alexander.....	ThP 112	Mertins, Philipp.....	TP 082
McLeish, Kenneth.....	WP 494	Meikle, A. Wayne.....	WP 439	Mertins, Philipp.....	TP 438
McLellan, Michael.....	TOG am 08:30	Meinema, Anne.....	TOA am 10:10	Mertins, Philipp.....	TP 433
McLellan, Michael.....	TP 082	Meirrelles, Gabriela.....	WP 460	Mertins, Philipp.....	TP 426
McLellan, Michael.....	TP 433	Meiring, Hugo D.....	WOE am 10:10	Mesaros, Clementina.....	MP 509
McLellan, Michael.....	TP 438	Meissen, John.....	MP 608	Mesaros, Clementina.....	WP 499
McLoughlin, Niaobh.....	ThOH am 09:30	Meissen, John.....	MP 606	Mesaros, Clementina.....	WP 479
McLoughlin, Niaobh.....	TP 156	Meitei, Ningombam Sanjib.....	ThP 722	Mesker, Wilma.....	MP 004
McLoughlin, Niaobh.....	WP 023	Mekhssian, Kevork.....	WP 267	Mesri, Mehdi.....	ThP 025
McLoughlin, Niaobh.....	WP 189	Mekhssian, Kevork.....	WP 522	Mess, Jean-Nicholas.....	WP 132
McLucky, Morgan.....	TOG pm 2:30	Melamud, Eugene.....	ThP 648	Mess, Jean-Nicholas.....	WP 181
McLucky, Morgan.....	WP 747	Melani, Rafael D.....	TP 686	Mess, Jean-Nicholas.....	WP 179
McLucky, Scott.....	MP 143	Melechco Carvalho, Valdemir.....	MP 459	Mess, Jean-Nicholas.....	WP 267
McLucky, Scott.....	MP 248	Melechco Carvalho, Valdemir.....	WP 434	Mess, Jean-Nicholas.....	WP 268
McLucky, Scott.....	TP 341	Melichar, Bohuslav.....	ThP 396	Messaoudi, Melina.....	TP 423
McLucky, Scott.....	TP 345	Melki, Ronald.....	ThOF am 09:10	Mester, Zoltán.....	TP 770
McLucky, Scott.....	TP 362	Melko, Joshua.....	MOD am 08:30	Metalnikov, Pavel.....	MP 340
McLucky, Scott.....	WP 169	Mellacheruvu, Dattatreya.....	TP 138	Methe, Esther.....	WP 305
McLucky, Scott A.....	MP 081	Melles, Gerrit.....	WP 478	Metz, Thomas.....	MOC pm 3:10
McLucky, Scott A.....	TOB am 09:10	Mellors, J. Scott.....	TP 739	Metz, Thomas.....	MP 569
McLucky, Scott A.....	TP 340	Melnik, Alexey.....	MP 020	Meurer, Eduardo.....	MP 332
McLucky, Scott A.....	TP 339	Melnik, Alexey.....	MP 056	Meuwis, Marie Alice.....	MP 441
McLucky, Scott A.....	TP 395	Melo, Matilde.....	ThP 101	Meuwis, Marie-Alice.....	ThP 256
McMahon, Adam.....	MP 762	Melo-Braga, Marcella.....	ThP 213	Meyer, Barbara.....	ThP 376
McMahon, Adam.....	WP 641	Mencken, Thomas.....	TOE am 09:50	Meyer, Helmut.....	MP 431
McMahon, Kelly.....	ThP 036	Mencken, Thomas.....	TP 465	Meyer, Helmut E.....	TP 141
McManus, Francis.....	TP 130	Mendes, Maria Anita.....	TP 413	Meyer, Helmut E.....	TP 481
McManus, Kevin.....	TP 506	Mendes, Vera.....	ThP 101	Meyer, Jesse.....	MP 207
McMartin, Dena.....	TP 554	Mendis, Lakshini.....	TP 060	Meyer, Kevin.....	ThP 765
McMillan, Nancy.....	ThP 366	Mendoza, Luis.....	ThP 031	Meyer, Kevin.....	WP 202
McMillen, Chelsea L.....	ThP 180	Mendoza, Vanessa.....	ThP 115	Meyer, Kevin W.....	WP 161
McNally, Mary Ellen.....	TP 743	Mendoza, Vivienne.....	ThOE am 09:10	Meyer, Klaus.....	ThP 637
McNamara, John.....	WP 124	Mendoza, Vivienne.....	TP 061	Meyer, Markus.....	MP 292
McNamara, Michael.....	ThP 286	Mendrick, Donna.....	MP 267	Meyer, Markus.....	WP 063
McNerney, MaryEllen.....	MP 366	Menendez, Camino.....	ThP 294	Meyer, Markus.....	WP 156
McQueen, Peter D.....	TP 183	Meng, Da.....	WP 088	Meyer, Matthew.....	ThP 025
McShane, Adam.....	ThP 194	Meng, Jia-Ming.....	ThP 051	Meyer, Matthew R.....	TP 173
Mcshane, Adam.....	TP 486	Meng, Jia-Ming.....	WP 053	Meyer, Matthew R.....	WOG pm 3:50
McVey, Patrick.....	TP 671	Meng, Juncui.....	MP 536	Meyer, Melissa.....	WP 541
McWilliams, Lisa.....	ThP 382	Meng, Kai.....	TP 582	Meyer, Morten.....	ThP 213
Meads, Mark.....	ThOE am 08:50	Meng, Kai.....	WP 360	Meyer, Sören.....	TP 031
Meakin, Julie.....	TP 213	Meng, Le.....	ThP 771	Meyer, Stephen.....	TP 711
Mechin, Nathalie.....	TP 293	Meng, Le.....	WP 007	Mezcua Peral, Milagros.....	WP 360
Mechref, Yehia.....	ThOH am 09:50	Meng, Le.....	WP 008	Mezencev, Roman.....	MP 599
Mechref, Yehia.....	ThOH pm 2:50	Meng, Min.....	MP 503	Mezyl, Jakub.....	TP 526
Mechref, Yehia.....	ThP 154	Meng, Min.....	MP 502	Michael, Nicholas.....	ThP 048
Mechref, Yehia.....	ThP 148	Meng, Min.....	ThP 438	Michalski, Annette.....	MP 723
Mechref, Yehia.....	ThP 297	Meng, Min.....	TP 519	Michalski, Annette.....	WP 727
Mechref, Yehia.....	TP 107	Meng, Tzu-Ching.....	TP 121	Michelmann, Karsten.....	WP 690
Mechtler, Karl.....	TP 075	Meng, Ying.....	MP 730	Michelmann, Karsten.....	WP 686
Mechtler, Karl.....	TP 098	Menger, Robert.....	TP 044	Michelsen, Klaus.....	WP 225
Mechtler, Karl.....	TP 096	Menikarachchi, Lochana.....	WP 586	Michon, José.....	WP 525
Mechtler, Karl.....	WP 091	Menin, Laure.....	ThP 687	Middaugh, C.....	WP 215
Medana, Claudio.....	ThP 596	Menin, Laure.....	WP 418	Midey, Anthony.....	MP 386
Medard, Guillaume.....	WP 095	Menon, Sreelakshmy.....	MP 481	Mielczarek, Przemyslaw.....	MP 620
Médard, Guillaume.....	TP 683	Menschaert, Gerben.....	TP 078	Migliorini Figueira, Ana Carolina.....	ThP 138
Medin, Jeffrey.....	TP 065	Mercadante, Julie.....	TP 570	Miingi, Nyokabi.....	TP 500
Mediniha, Leonardo.....	TP 576	Merchant, Michael.....	WP 494	Mijakovic, Ivan.....	ThP 080
Medlock, Jan.....	ThP 286	Merchant, Michael L.....	TP 305	Mikaia, Anzor I.....	MP 295
Medzihradzsky, Katalin F.....	ThP 231	Mercier, Catherine.....	ThP 023	Mikaia, Anzor I.....	TP 569
Meehan, Michael.....	MOH pm 4:10	Meredith, Jere E.....	ThP 421	Mikami, Toshiyuki.....	WP 477
Meehan, Michael.....	MP 056	Merkel, Dietrich.....	WP 496	Mike, McCullagh.....	WP 665
Meek, Claudia.....	TP 500	Merrihew, Gennifer.....	ThP 326	Mikes, Romana.....	WP 153
Meert, Paulien.....	ThP 776	Merrihew, Gennifer.....	WP 115	Mikkonen, Saara.....	TP 411
Megger, Dominik.....	MP 431	Merrill, Anna.....	ThP 177	Miladi, Mahsan.....	TP 347
Megger, Dominik Andre.....	TP 481	Merrill, Anna.....	ThP 327	Miladinović, Saša M.....	ThOE pm 2:30
Mehl, John.....	ThP 441	Merrill, Anna E.....	ThP 068	Miladinović, Saša M.....	WP 722
Mehl, John T.....	TP 693	Merrill, Anna E.....	ThP 178	Milagre, Humberto.....	TP 231

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Milagre, Humberto	TP 415	Misuno, Kaori	MP 596	Mollah, Sahana	ThP 407
Milavancev, Milan	ThP 286	Misuno, Kaori	MP 634	Mollah, Sahana	TP 184
Mildenberg, Benjamin	MP 199	Mita, Paolo	WP 253	Mollah, Sahana	WP 124
Milnichik, Andrew	TP 238	Mitchell, Chris	MP 270	Mollah, Sahana	WP 633
Millan Martin, Silvia	ThOH am 09:30	Mitchell, Christopher J	MP 255	Molloy, Kelly R	WP 253
Millan Martin, Silvia	WP 189	Mitchell, Matthew	TP 662	Molloy, Mark	MP 449
Millar, Alan	TP 061	Mitchell, Todd W	ThP 376	Molloy, Mark	TP 327
Miller, Amanda	WP 196	Mitchison, Timothy J	MP 259	Molloy, Mark P	MP 221
Miller, Christine	ThP 061	Mitne-Neto, Miguel	MP 459	Molloy, Mark P	ThOE pm 2:50
Miller, Christine	ThP 433	Mitra, Kaushik	TP 632	Molnárné Guricza, Lilla	TP 592
Miller, Christine	TP 179	Mitra, Vikram	ThP 215	Mommen, Geert P.M	WOE am 10:10
Miller, Emily	ThP 443	Mitran, Sorin	MP 693	Monastyrskiy, Mikhail	ThP 751
Miller, Emily	TP 028	Mitrano, Amy	MP 212	Moncur, John	WP 455
Miller, Frederick	MP 072	Mitri, Zahi	ThP 423	Mondegue, Florence	WOC pm 2:50
Miller, Jeff	MP 197	Mitroshkov, Alexandre	MP 377	Money, Ryan	ThP 029
Miller, Jessica A.	ThP 656	Mittler, Gerhard	MP 092	Monge, Maria Eugenia	MP 599
Miller, Logan	ThP 447	Mittler, Ron	ThP 417	Monge, Maria Eugenia	TP 664
Miller, Logan	WP 508	Mittler, Ron	TP 643	Moniz, Heather	MP 176
Miller, Luke	TP 662	Mitulovic, Goran	TP 447	Monkkonen, Lucas	ThP 093
Miller, Martin	MP 215	Mitulovic, Goran	WP 140	Monks, Stephen	MP 161
Miller, P	MP 507	Mitulovic, Goran	WP 136	Monroe, Matthew	MOC pm 3:10
Miller, Paul	ThOE am 09:10	Mitulović, Goran	WP 135	Monroe, Matthew	TP 676
Miller, Paul	TP 459	Miura, Daisuke	MP 062	Monroe, Matthew	WOE am 08:30
Miller, R.J. Dwayne	WP 744	Miura, Daisuke	WP 282	Monroe, Matthew E	ThP 741
Miller, Rebecca L	MP 272	Miyagawa, Haruhiko	ThP 641	Monroe, Matthew E	TP 169
Miller, Ryan	MP 059	Miyagi, Masaru	ThP 298	Monroe, Matthew E	TP 324
Miller, Ryan	MP 060	Miyamoto, Satoshi	TOH am 09:10	Montague, Hannah	MP 246
Miller, Vaughn	WP 437	Miyamoto, Sayuri	ThP 407	Montague, Hannah	MP 266
Miller-Stein, Cindy	WP 652	Miyamoto, Suzanne	ThP 155	Montellier, Emilie	WOG am 09:50
Millie, David	MOB pm 3:50	Miyasaka, Yuichiro	ThP 621	Montenegro Burke, Rafael	ThOG pm 2:50
Milligan, Dallas P	ThP 605	Miyazaki, Yu	TP 166	Montminy, Valérie	MP 492
Mills, Andrew	WOB pm 3:30	Mizuno, Hajime	MOF pm 3:10	Moody, Sally A	ThOB am 09:10
Mills, David	TP 221	Mizuno, Hajime	MP 196	Mookala, Naidu	WP 717
Mills, Mark	ThP 002	Mizuno, Hajime	MP 247	Mookherjee, Abhigya	ThP 188
Milovancev, Milan	WOD am 08:30	Mizuno, Hajime	MP 417	Moon, Jeong Hee	TP 199
Minnaugh, Megan	MP 515	Mizuno, Hajime	ThP 621	Moon, Sun Hee	ThP 628
Min, Lie	MP 572	Mizuno, Hajime	WP 594	Moon, Sungyoon	MP 128
Minambres, Rebeca	WOE am 09:50	Mo, Jingjie	MP 172	Moore, Bradley	MP 056
Minamisawa, Toshikazu	TP 321	Mo, Jingjie	TP 541	Moore, Cedric	WP 716
Minardi, Carina	TP 273	Mo, Shunyan	ThP 402	Moore, Chad	MP 503
Minardi, Carina	WOB am 09:30	Mo, WenJun (David)	MP 063	Moore, Chad	ThP 438
Miner, Jacob	ThP 471	Mo, Wenjun (David)	TP 243	Moore, Ian	WP 186
Ming Hui, Chen	WP 466	Mochida, Isao	TP 604	Moore, Jeffrey	ThP 610
Mingham, Rosane	WP 460	Mock, Hans-Peter	MP 416	Moore, Jessica L	TP 073
Minkler, Paul E	ThP 431	Mody, Rustom	WP 717	Moore, John	TOF am 08:50
Minkler, Paul E	WP 595	Moehlig, Aaron	MP 328	Moore, Kassandra	TP 387
Minkoff, Benjamin	MP 406	Moehring, Thomas	MP 186	Moore, Kenneth	MP 063
Minnich, Anne	WP 487	Moeller, Benjamin	ThP 523	Moore, Richard	WOF pm 4:10
Minnikin, David	ThP 394	Moeller Christensen, Gitte Julie	MOH pm 4:10	Moore, Roger E	ThP 526
Minogue, Catherine	TP 669	Moench, Paul	TP 040	Moore, Ronald	ThOG pm 4:10
Minogue, Catherine E	ThP 327	Moghaddas Gholami, Amin	MP 041	Moore, Ronald	WOE am 08:30
Minohata, Toshikazu	ThP 592	Moghaddas Gholami, Amin	ThP 046	Moore, Ronald	WOG pm 2:50
Mirabal, Alex	TP 789	Moghieb, Ahmed	ThP 449	Moore, Ronald J	MP 100
Mirabella, Brooks F	ThP 604	Möginger, Uwe	TP 160	Moore, Ronald J	TP 169
Miranda, Cristobal L	MP 598	Mohamed, Ahmed A	WP 513	Moore, Ronald J	TP 324
Mirnaghi, Fatemeh	ThOB am 09:50	Mohammadi, Amir	TP 033	Moore, Ronald J	WP 745
Mirnezami, Reza	TOG pm 3:30	Mohammed, Yassene	MP 037	Moore, William	WP 681
Mirnezami, Reza	TP 375	Mohammed, Yassene	ThP 026	Moorthy, Ganesh	WP 646
Mirokhin, Yuri	MP 048	Mohan, Shekher	WP 397	Mora, Johanna	TOE am 09:30
Mirokhin, Yuri	ThOG am 10:10	Mohanty, Ajeet Kumar	MP 270	Moradian, Annie	MP 225
Mirokhin, Yuri	WP 051	Mohanty, Sujit	MOA am 08:50	Moradian, Annie	MP 226
Mironov, Gleb	MOC am 10:10	Moharrum, Ahmad M	WP 319	Moradian, Annie	ThOF pm 2:50
Mironov, Konstantin	TP 409	Mohien, Ceereena	MP 262	Morais, Erica	TP 584
Mirsalis, Jon	WP 465	Mohsin, Sheher Bano	MP 754	Moran, Dawn	MP 275
Mirza, Shama	MP 428	Mohsin, Sheher Bano	ThP 603	Mordehai, Alex	MOC pm 3:10
Mirza, Shama P	ThP 280	Moini, Mehdi	WP 305	Mordehai, Alex	ThP 482
Mirzaei, Hamid	MP 254	Moini, Mehdi	WP 304	Mordehai, Alex	ThP 484
Mirzaei, Mehdi	WP 234	Moise, Adrian	ThP 746	Mordehai, Alex	ThP 491
Mirzakhanyan, Yeva	WP 094	Molden, Rosalynn	MP 095	Mordehai, Alex	ThP 483
Mischerikow, Nikolai	WP 091	Molden, Rosalynn	ThP 070	Mordehai, Alex	ThP 759
Misek, David	MP 456	Molden, Rosalynn	WP 097	Mordehai, Alex	WP 674
Misek, Jiri	WP 094	Moldoveanu, Serban	MP 470	Mordehai, Alex	WP 681
Misharin, Alexander	ThP 745	Moldoveanu, Zina	ThP 149	Moreau, Stephane	MP 345
Mishra, Ashok	WP 717	Molhoj, Michael	WP 049	Moreau, Stephane	ThP 599
Mishra, Satish	ThP 278	Molina, Henrik	WP 043	Moreau, Stephane	ThP 600
Misselwitz, Michelle	WP 570	Molina, Patricia	TP 159	Moremen, Kelley	MP 176
Mistrik, Robert	MP 623	Molina-Díaz, Antonio	TP 272	Moresco, James	MP 065
Mistrik, Robert	TP 526	Molina-Díaz, Antonio	WP 362	Morgan, Caroline	MP 302
Mistrik, Robert	TP 525	Molina-Martin, Manuel	TP 543	Morgan, Ling	ThP 432

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Morgan, Marsha	TP 476	Moyano, Daniel F.	WP 703	Munoz, Nathalie	WP 585
Morgenstern, David	MP 149	Moyer, Mary	TP 201	Munske, Gerhard	ThP 223
Morgner, Nina	ThOC pm 2:30	Mrazek, Hynek	ThP 460	Muntean, Felician	MP 689
Morihiro, Motohiko	MOF pm 3:10	Mrazek, Hynek	WP 167	Muntel, Jan	MP 680
Morimoto, Kentaro	TP 166	Mriziq, Khaled	MP 743	Muntel, Jan	MP 747
Morin, Eric	MP 485	Mriziq, Khaled	ThP 067	Muntel, Jan	ThOE pm 4:10
Morin, Louis-Philippe	WP 180	Mriziq, Khaled	ThP 425	Muntel, Jan	TP 187
Morin, Paul	TP 541	Mrzljak, Ladislav	WP 480	Muntha, KesavaReddy	MP 364
Morin, Paul E.	MOE pm 3:10	Msallaty, Zaher	TP 143	Muralidharan, Sridevi	MP 273
Morin Jaskiewicz, Nicole	WP 482	Msallaty, Zaher	TP 139	Muramoto, Shin	ThP 601
Moritz, Albrecht	ThP 219	Msallaty, Zaher	TP 488	Muramoto, Shin	WP 302
Moritz, Robert	TP 181	Msallaty, Zaher	WP 241	Muramoto, Shin	WP 380
Moritz, Robert L.	ThP 031	Mu, Hui	ThP 574	Murao, Naoaki	WP 183
Moritz, Robert L.	ThP 506	Mu, Ruipu	TP 575	Murase, Masaki	TP 166
Moritz, Robert L.	WP 766	Mucci, Lorelei	ThP 433	Murata, Kazuyuki	MP 108
Morlais, Isabelle	WP 446	Muddiman, Dave	MP 209	Murphy, Angus	TP 668
Moroco, Jamie A.	ThP 132	Muddiman, David	TP 011	Murphy, Anne	ThOE pm 3:30
Morosi, Lavinia	TP 029	Muddiman, David	WP 452	Murphy, Beth Ann	ThOE am 09:10
Morowitz, Michael	ThP 332	Muddiman, David C.	MP 119	Murphy, Denise	MP 131
Morr, Mary	TOG pm 4:10	Muddiman, David C.	ThP 006	Murphy, James	MP 750
Morré, Jeffrey	ThP 606	Muddiman, David C.	ThP 007	Murphy, James	ThP 661
Morreau, Johannes	TP 052	Muddiman, David C.	ThP 728	Murphy, James	WP 742
Morrice, Nicholas	WP 200	Muddiman, David C.	ThP 731	Murphy, Jim	TP 693
Morris, Arvia	WP 198	Muddiman, David C.	ThP 733	Murphy, Keeley	MP 671
Morris, Ayodele	MP 471	Muddiman, David C.	TOH am 08:50	Murphy, Keeley	MP 678
Morris, Ayodele	WP 536	Muddiman, David C.	WP 011	Murphy, Keeley	MP 620
Morris, Caleb B.	WP 687	Muddiman, David C.	WP 030	Murphy, Robert	WP 280
Morris, Michael	WP 748	Mueller, Alan	ThP 543	Murphy, Steve	ThP 784
Morris, Mike	MP 404	Mueller, André C.	WOF pm 2:50	Murphy, Steve	TP 177
Morris, Mike	MP 674	Mueller, Anja	TP 776	Murphy, Steve	WP 096
Morris, Mike	MP 675	Mueller, Benjamin	TP 153	Murphy, Steven	TP 109
Morris, Mike	ThP 469	Mueller, Christoph W.	ThP 072	Murr, Annette	ThP 250
Morris, Mike	TP 215	Mueller, David	MP 524	Murray, Benjamin S.	ThP 687
Morris, Mike	WP 280	Mueller, David	TP 734	Murray, David	ThP 345
Morrison, Kendall	TP 206	Mueller, David	TP 732	Murray, David	ThP 349
Morrison, Lindsay	ThP 113	Mueller, Mathias	MP 653	Murray, Jacolin	WP 577
Morrison, Sean	WOH am 10:10	Mueller, Mathias	ThP 317	Murray, Kermit K.	MP 724
Morsa, Denis	MOC pm 2:30	Mueller, Mathias	TOB am 10:10	Murray, Kermit K.	MP 780
Morton, Joseph	TP 218	Mueller, Susanne	MP 152	Murray, Kermit K.	TOH pm 3:30
Morton, Thomas	MP 328	Mueller, Wade	MP 428	Murray, Kermit K.	TP 590
Moruz, Luminita	WP 034	Muhammad, Rizwan	WP 546	Murray, Kermit K.	TP 748
Moruz, Luminita	WP 129	Muirhead, Laura	TP 375	Murray, Kermit K.	WP 004
Morzan, Ezequiel M.	WOB pm 2:30	Mukherjee, Gargee	ThP 277	Murria, Priya	MP 574
Moseley, Arthur	ThP 267	Mukherjee, Joy	ThP 645	Murria, Priya	MP 577
Moseley, Arthur	WP 586	Mulhern, Daniel	MP 122	Murria, Priya	WOA am 08:50
Moseley, M. Arthur	TOA pm 2:50	Mulier, Kristine	TP 656	Murthy, Krishna R.	MP 255
Moseley, M. Arthur	TP 457	Mullan, Michael	MP 246	Murthy, Shashi	TP 089
Moseley, M. Arthur	TP 470	Mullan, Michael	MP 266	Murthy, Shashi K.	TOB pm 3:10
Moseley, M. Arthur	WOG pm 3:30	Mullan, Mike	MP 116	Musah, Rabi	ThP 415
Mosher, Deane	ThP 348	Mullen, Christopher	MP 084	Musah, Rabi	WP 292
Moshin, Jenny	MP 293	Mullen, Christopher	MP 146	Musah, Rabi	WP 336
Moshkovskii, Sergei	ThP 248	Mullen, Christopher	ThP 686	Muscalu, Alina	WP 575
Moshkovskii, Sergei A.	TP 081	Müllen, Klaus	WP 683	Musil, Stanislav	WP 342
Moskovets, Eugene	MP 383	Muller, Bruno	TP 224	Muskat, Tassilo	ThP 694
Moskovets, Eugene	MP 381	Muller, Ludovic	MOH pm 2:50	Musselman, Brian	MP 386
Moskovets, Eugene	WP 385	Muller, Ludovic	ThP 387	Musselman, Brian	MP 523
Moss, William John	WP 446	Muller, Ludovic	TP 002	Musselman, Brian	ThP 413
Mostafa, Ahmed	ThP 565	Muller, Ludovic	TP 063	Musselman, Brian	TP 269
Mostovenko, Ekaterina	ThP 041	Muller, Markus	TP 093	Musselman, Brian D.	MP 365
Mostovenko, Ekaterina	WP 032	Mullett, Steven	WP 158	Musselman, Brian D.	ThP 415
Mostovenko, Ekaterina	WP 238	Mulligan, Christopher	ThP 585	Mustacich, Debbie J.	WP 436
Motari, Edwin M.	TP 223	Mulligan, Christopher	ThP 586	Musuku, Adrien	WP 549
Motorykin, Ievgen	WOD am 08:30	Mulligan, Christopher	ThP 602	Musunuri, Sravani	WP 489
Motsinger, Alison	ThP 733	Mulligan, Christopher	WP 310	Muthanna, Mohamed S.	TP 563
Mou, Si	ThP 198	Mulligan, Christopher	WP 411	Muthu, Kesavan	WP 328
Mou, Si	TOB pm 3:50	Mullin, Lauren	ThP 544	Muthusamy, Babylakshmi	MP 255
Mougios, Vassilios	WP 600	Mullin, Lauren	ThP 551	Muthusamy, Nagendran	WP 011
Moulder, Robert	ThP 276	Mullin, Lauren	WP 349	Mwangi, Joseph	WP 694
Moulder, Robert	WP 028	Mullin, Robert J.	TP 249	Myers, Andrew	TP 463
Moulder, Robert	WP 504	Mulvey, Claire	WOD am 09:30	Myers, Anne	TP 392
Moulds, Richard	ThP 748	Mulvey, Claire	WP 738	Myers, Anne	WOC pm 2:30
Moulds, Richard	ThP 749	Mulvey, Michael	TP 216	Myers, Anne L.	WP 575
Mount, Andrew	WP 751	Mun, Dong-Gi	ThP 020	Myers, Jeremy	MOE am 10:10
Moura, Lyzette	TP 585	Mundt, Max	WP 095	Myers, Jeremy	ThP 294
Mousavi, Fatemeh	MP 603	Muneeeruddin, Khaja	WP 216	Myers, Jeremy	ThP 648
Mousavi, Fatemeh	WOE pm 2:50	Muneshwar, Praveen	WP 717	Myers, Nichole R.	TP 522
Movahed, Navid	TP 656	Munger, Steven C.	MOG pm 2:30	Myhill, Sophie	WP 013
Mowry, Curtis	TP 789	Munoz, Gabriel	ThP 566	Mylott, William R.	WP 127
Moxley, Richard IV	TP 468	Munoz, Ignacio	WP 480	Myung, Seoung-Woon	WP 580

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Na, Chan-Hyun.....	ThP 311	Nayak, Ajay P.....	ThP 309	Nguyen, Bich.....	TP 445
Na, Keun.....	MP 127	Naz, Shama.....	MP 584	Nguyen, Bich.....	WP 138
Na, Seungjin.....	MP 043	Nazari, Milad.....	ThP 006	Nguyen, Bich.....	WP 137
Na, Seungjin.....	TP 229	Nazarov, Erkinjon.....	WP 771	Nguyen, Don.....	MP 056
Naboulsi, Wael.....	MP 431	Ndah, Elvis.....	TP 078	Nguyen, Elizabeth.....	ThP 276
Nachtigall, Jonny.....	MP 638	Nebuloni, Manuela.....	ThP 293	Nguyen, Hong Hanh.....	WOG am 10:10
Nadler, Wiebke.....	MOF pm 3:50	Nechyporenko, Anatoliy.....	MP 448	Nguyen, Huong (Ivy).....	ThP 183
Nadler, Wiebke.....	MP 310	Needham, Shane.....	MP 711	Nguyen, Son N.....	TOE am 10:10
Nadon, Celine.....	TP 213	Neely, Benjamin.....	TP 069	Nguyen, Tran Xuan Phong.....	ThP 095
Naegele, Edgar.....	TP 571	Neely, Benjamin A.....	ThP 166	Nguyen, Tung-Vi.....	TP 578
Naes, Benjamin E.....	WP 299	Neeson, Kieran.....	WP 666	Nguyen, Vien.....	WP 233
Nagai, Toshiharu.....	WP 283	Neeson, Kieran J.....	WP 668	Nguyen-khoa, Thao.....	WP 145
Nagao, Tatsuhiko.....	MP 062	Nefzger, Hartmut.....	TOC am 09:50	Ni, Chi-Kung.....	MP 307
Nagaraj, Nagarjuna.....	WP 257	Negreira, Noelia.....	TP 551	Ni, Chi-Kung.....	MP 306
Nagaraju, Kanneboyina.....	MP 424	Nehme, Benjamin.....	ThP 287	Ni, Chi-Kung.....	MP 305
Nagaraju, Kanneboyina.....	ThOE am 09:50	Neidleman, Jason.....	ThP 511	Ni, Zhong-Hai.....	WP 389
Nagaraju, Kanneboyina.....	TP 467	Nelsen, David.....	MP 069	Niakan, Kathy.....	WOD am 09:30
Nagashima, Hisayuki.....	MP 526	Nelson, Bryant.....	ThP 635	Nichols, Charles.....	MP 321
Nagashima, Hisayuki.....	MP 525	Nelson, Bryant C.....	WP 707	Nichols, Charles.....	TP 356
Nagel, Alexis.....	WP 071	Nelson, Jenny.....	WP 342	Nichols, Frank.....	MP 251
Nagilla, Rakesh.....	MP 512	Nelson, Karen.....	ThP 283	Nichols, Frank C.....	WP 502
Nagore, Linda.....	TP 412	Nelson, Karen.....	ThP 284	Nichols, William.....	TP 787
Nagornov, Konstantin O.....	MOB am 09:30	Nelson, Ornella.....	TP 203	Nicholson, Jeremy.....	TOG pm 3:30
Nagornov, Konstantin O.....	MP 700	Nelson, William.....	MP 569	Nicholson, Jeremy.....	WP 596
Nagornov, Konstantin O.....	MP 701	Nemati, Reza.....	MP 251	Nickbarg, Elliott.....	MP 131
Nagoya, Tomoki.....	MP 525	Nemati, Reza.....	WP 502	Nickbarg, Elliott.....	TOF pm 3:30
Nagoya, Tomoki.....	MP 526	Nemes, Peter.....	MP 361	Nickel, Christoph.....	WP 196
Nagy, Lauren.....	ThP 153	Nemes, Peter.....	ThP 740	Nicklaus, Michele.....	TP 642
Nagyhazi, Orsolya.....	WP 424	Nemes, Peter.....	TP 197	Nicklay, Joshua.....	MP 195
Najdekr, Lukas.....	TP 526	Nemes, Peter.....	TP 640	Nicklay, Joshua.....	WP 266
Najjar, Rami.....	MP 122	Nerland, Donald E.....	TP 305	Niclou, Simone P.....	TP 050
Nakabayashi, Ryo.....	MP 621	Nesmith, Barry.....	MP 689	Nicol, Gordon.....	MP 751
Nakagawa, Tetsuya.....	TP 027	Nesvizhskii, Alexey.....	MP 035	Nicol, Gordon.....	ThP 260
Nakajima, Chihiro.....	MP 130	Nesvizhskii, Alexey.....	MP 258	Nicolardi, Simone.....	TP 161
Nakajima, Kazuki.....	ThP 397	Nesvizhskii, Alexey.....	ThP 028	Nicolle, Sarah.....	WP 444
Nakajima, Takeshi.....	WP 143	Nesvizhskii, Alexey.....	TP 138	Nicora, Carrie.....	WOG pm 2:50
Nakajima, Tomoyuki.....	WP 474	Nesvizhskii, Alexey.....	WOD am 09:10	Nie, Huan.....	ThP 720
Nakajima, Yoji.....	MP 005	Nesvizhskii, Alexey.....	WP 045	Nie, Shuai.....	ThP 409
Nakamura, Junya.....	WP 282	Nesvizhskii, Alexey.....	WP 119	Nie, Song.....	MP 446
Nakamura, Takemichi.....	ThP 721	Neta, Pedatsur.....	MP 051	Nie, Song.....	TP 421
Nakanishi, Tsuyoshi.....	TP 017	Nethero, William C.....	TP 522	Nie, Song.....	WP 458
Nakanishi, Tsuyoshi.....	WP 613	Nette, Geoffrey.....	TP 295	Nie, Song.....	WP 500
Nakata, Mitsutoshi.....	MP 447	Neu, Volker.....	TP 742	Nie, Yongxin.....	MP 734
Nakayama, Hiroshi.....	ThP 520	Neubauer, Rebecca.....	TP 373	Nie, Yongxin.....	ThP 142
Nakayama, Hiroshi.....	WP 372	Neubauer, Rebecca.....	TP 404	Nie, Zongxiu.....	MP 400
Nakayama, Kenji.....	TP 166	Neubauer, Rebecca.....	TP 405	Niederkofler, Eric.....	WP 192
Nakazawa, Takashi.....	MP 067	Neubert, Hendrik.....	MP 126	Niederkofler, Eric.....	WP 266
Nam, Younwoo.....	TOF pm 3:50	Neubert, Hendrik.....	TOF pm 2:50	Nieh, Christina.....	TP 792
Nambi, Subhalaxmi.....	WOF pm 3:10	Neubert, Thomas.....	WP 583	Niehaus, Rebecca.....	MP 007
Nandakumar, Renu.....	TP 452	Neumann, Drexel.....	WP 237	Niehoff, Ann-Christin.....	TP 031
Nandi, Somen.....	TP 258	Neumann, Elizabeth.....	ThP 514	Nielsen, Michael Lund.....	ThP 243
Nanjappa, Vishalakshi.....	MP 255	Neumann, Steffen.....	ThOG am 08:50	Nielsen, Michael Lund.....	WP 109
Nanni, Paolo.....	ThP 329	Neupert, Susanne.....	TP 167	Niemi, Lydia.....	TP 550
Nantel, Julien.....	WP 523	Neuweger, Heiko.....	ThP 637	Nien, Pei-Yung.....	WP 422
Napoli, Anna.....	TP 511	Nevin, Austin.....	MP 083	Nienow, Caleb.....	ThP 654
Narayan, Alison R.....	WP 335	Nevin, Philip.....	WP 223	Nieves, Edward.....	MP 421
Narayanan, Rahul.....	WP 412	Newbold, Jane.....	WP 444	Niggeloh, Verena.....	MP 077
Narayanasamy, Suresh.....	MP 091	Newitt, John.....	MP 180	Nightlinger, Nancy.....	TP 152
Nardone, Mario.....	ThP 594	Newman, Jason.....	ThP 042	Nightlinger, Nancy.....	WP 196
Narendran, Parth.....	MP 098	Newsome, G. Asher.....	WP 382	Nightlinger, Nancy.....	WP 197
Nargund, Sandhya.....	WP 449	Newsome, G. Asher.....	WP 401	Niimi, Hironobu.....	MP 005
Nargund, Shilpa.....	WP 198	Newton, Kenneth.....	ThP 689	Nijholt, Diana A.T.....	TP 444
Nascimento, Heliara.....	TP 584	Nezami Ranjbar, Mohammad R.....	MP 580	Nika, Heinz.....	WP 165
Nascimento, Heliara D. L.....	TP 586	Nezami Ranjbar, Mohammad R.....	TP 756	Nikolaev, EN.....	TP 449
Nash, John.....	MP 574	Ng, Andrew.....	WP 232	Nikolaev, Eugene.....	MOB am 08:50
Nash, John.....	TP 360	Ng, Carl.....	WP 277	Nikolaev, Eugene.....	MP 704
Nash, John J.....	WOA am 08:50	Ng, Katharine.....	ThP 334	Nikolaev, Eugene.....	ThP 086
Nash, Tara E.....	MP 410	Ng, Leong L.....	TP 487	Nikolaev, Eugene.....	TOA pm 4:10
Nath, Avindra.....	TP 468	Ng, Ryan.....	WP 118	Nikolaev, Eugene.....	TP 325
Nath, Nidhi.....	TP 234	Ng, Shok-Li.....	WP 246	Nikolaev, Eugene.....	TP 409
Navare, Arti.....	ThOC pm 3:50	Ng, Wailap.....	TP 120	Nikolaev, Eugene.....	WP 724
Navare, Arti.....	ThP 465	Ng, Jing Cheng.....	MP 342	Nikolau, Basil.....	WP 589
Navare, Arti.....	ThP 464	Ng, Jing Cheng.....	TP 275	Nikolic, Dejan.....	WP 325
Navare, Arti.....	WOH pm 2:50	Ng-A-Qui, Theron.....	ThP 598	Nikolic, Dejan.....	WP 331
Navarro, Meritxell.....	TP 639	Ngo, Tuan.....	ThP 228	Nikolic, Dejan.....	WP 332
Navarro, Pedro.....	TP 084	Ngounou, Armand.....	MP 106	Nikolos, Ioannis.....	MP 668
Navas, Natalia.....	ThOH am 09:30	Ngounou, Armand.....	TP 429	Nilson A., Assuncao.....	MP 115
Navas, Natalia.....	WP 189	Ngounou Wetie, Armand G.....	MP 423	Nilsson, Anna.....	MP 026
Nawaz, Sadat.....	TP 564	Nguyen, Amelia Y.....	MP 100	Nilsson, Anna.....	TOH am 08:30

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Nilsson, Anna.....	TP 012	Nouri, Eslam.....	WP 232	Oefner, Peter J.....	TP 750
Nilsson, Anna.....	TP 013	Nouri, Eslam.....	WP 598	Oeh, Jason.....	MP 499
Nilsson, Anna.....	TP 046	Nouri-Nigjeh, Eslam.....	TP 245	Oehler, Rudolf.....	WP 140
Nilsson, Anna.....	TP 016	Nouta, Jan.....	WP 518	Oei, Maria.....	MP 136
Nilsson, Anna.....	TP 047	Novak, Jan.....	ThP 149	Oeljeklaus, Silke.....	TP 134
Nilsson, Anna.....	WP 012	Novak, Jan.....	WP 073	Oelke, Claudine.....	MP 645
Nilsson, Bjorn.....	TP 072	Novak, Petr.....	MP 183	Oellerich, Thomas.....	MP 198
Nilsson, Carol.....	ThP 041	Novak, Petr.....	ThOF am 08:50	Oellerich, Thomas.....	ThP 203
Nilsson, Carol.....	TP 072	Novak, Petr.....	ThP 139	Oetjen, Janina.....	MP 021
Nilsson, Carol.....	WP 032	Novak, Petr.....	ThP 354	Oetjen, Janina.....	ThOG am 09:30
Nilsson, Carol.....	WP 238	Novak, Petr.....	ThP 460	Oetjen, Janina.....	TP 008
Nilsson, Carol L.....	MP 427	Novick, Scott.....	ThP 137	Ogawa, Osamu.....	TP 166
Nilsson, Erik.....	WOB pm 4:10	Novick, Scott.....	TP 543	Ogiwara, Atsushi.....	WP 604
Nilsson, Ulrika.....	WP 456	Novitsky, Eric.....	ThP 462	Oglesbee, Devin.....	WP 655
Nimkar, Subodh.....	MP 743	Novitsky, Eric James.....	ThP 463	Ögmundsdóttir, Helga.....	ThP 401
Nimkar, Subodh.....	ThP 067	Novoselov, Konstantin.....	ThP 745	Ögmundsdóttir, Margrét H.....	ThP 401
Nimkar, Subodh.....	ThP 425	Nowak, John.....	ThP 677	Ogorzalek Loo, Rachel.....	MP 467
Nin, Nicolas.....	MP 584	Nowak, Timothy.....	MP 511	Ogorzalek Loo, Rachel.....	WOG am 10:10
Nin, Nicolás.....	MP 582	Nowling, Tamara.....	TP 065	Ogorzalek Loo, Rachel R.....	MOD am 09:50
Ning, Xu.....	ThP 697	Nshanian, Michael.....	MP 314	Ogorzalek Loo, Rachel R.....	MP 314
Ninomiya, Satoshi.....	TP 726	Ntai, Ioanna.....	WP 157	Ogorzalek Loo, Rachel R.....	ThP 716
Ninonuevo, Milady.....	ThP 266	Nti-Addae, Yaw.....	WP 024	Ogorzalek Loo, Rachel R.....	TOD am 08:50
Ninonuevo, Milady.....	TP 178	Nuccio, Art.....	ThP 074	Ogra, Yasumitsu.....	ThP 667
Nirujogi, Raja Sekhar.....	MP 255	Nuccio, Arthur.....	MP 261	O'Grady, John.....	ThP 765
Nirujogi, Raja Sekhar.....	MP 270	Nudelman, Ilona.....	MOE am 09:30	O'Grady, John.....	WP 202
Nirujogi, Raja Sekhar.....	MP 256	Nunez, Antonio.....	WP 510	Ogura, Tairo.....	MP 613
Nirujogi, Raja Sekhar.....	ThP 208	Núñez, Alberto.....	ThP 541	Ogura, Tairo.....	WP 130
Nirujogi, Raja Sekhar.....	ThP 278	Núñez Galindo, Antonio.....	ThP 255	Ogura, Tairo.....	WP 628
Nishida, Yuya.....	WP 113	Nunn, Brook L.....	MP 274	Ogurtsov, Aleksey.....	MP 042
Nishiguchi, Takao.....	ThP 620	Nuño Ayala, Mario.....	ThP 336	Oh, Han Bin.....	MP 201
Nishiumi, Shin.....	ThP 375	Nury, Catherine.....	ThOF am 09:10	Oh, Ken.....	MP 164
Nishshanka, Upul.....	MP 050	Nusinow, David.....	MP 133	Oh, Myung Jin.....	ThP 168
Nishshanka, Upul.....	ThP 542	Nusinow, David.....	ThP 174	Oh, Myung Jin.....	TP 257
Nissen, Silke.....	MP 277	Nusinow, David.....	WOG am 09:10	Oh, Myung Jin.....	WP 066
Nita-Lazar, Aleksandra.....	MP 269	Nusinow, David P.....	TOG am 09:50	Oh, Yeonyee.....	MP 119
Nita-Lazar, Aleksandra.....	MP 261	Nussbaumer, Susanne.....	ThP 590	O'Hair, Richard A. J.....	MOD am 08:50
Nita-Lazar, Aleksandra.....	ThP 074	Nussbaumer, Susanne.....	WP 293	O'Hair, Richard A. J.....	TP 355
Nita-Lazar, Aleksandra.....	TOG am 09:30	Nwokeoji, Alison.....	ThP 525	O'Hair, Richard A. J.....	ThOD am 09:10
Nita-Lazar, Aleksandra.....	WP 256	Nwosu, Charles.....	TP 260	Ohashi, Yoko.....	TP 321
Nitsche, Andreas.....	ThP 055	Nyadong, Leonard.....	ThP 569	Ohira, Masayoshi.....	MP 766
Niu, Beifang.....	TP 433	Nyalwidhe, Julius.....	ThP 392	Ohkubo, Masataka.....	ThP 761
Niu, Ben.....	MP 173	Nyberg, Joel.....	ThP 252	Ohlemacher, Shannon.....	TP 348
Niu, Ben.....	ThP 362	Nye, Leanne.....	MP 583	Ohlund, Leanne.....	TP 631
Niu, Shuai.....	TOC pm 3:10	Nye-Wood, Mitchell G.....	TP 039	Ohmori, Takeshi.....	MP 525
Niu, Shuai.....	WP 675	O'Connor, Peter B.....	MP 654	Ohmori, Takeshi.....	MP 526
Niu, Xin.....	WP 149	O'Leary, Adam.....	ThP 602	Ohmura, Mitsuyo.....	TP 017
Niu, Xinnan.....	WP 243	O'Rourke, Joseph R.....	MOH pm 2:50	Ohsawa, Isaac.....	MP 525
Nixon, Peter.....	TP 723	O'Rourke, Joseph R.....	ThP 387	Ohsawa, Isaac.....	MP 526
Nixson, Christopher.....	MP 364	O'bach, R. Scott.....	WP 631	Ohtsuki, Sumio.....	MP 447
Nobe, Yuko.....	WP 372	Obar, Robert.....	TP 145	Oishi, Haruki.....	WP 474
Noble, William Stafford.....	MOG am 09:50	Obayashi, Kenichi.....	ThP 641	Ojanperä, Ilkka.....	MP 289
Noble, William Stafford.....	TP 083	Obena, Rofe-Amor.....	ThP 714	Okahashi, Nobuyuki.....	WP 130
Noestheden, Matthew.....	WP 358	Obena, Rofeamor P.....	WP 492	Okhonin, Victor.....	MOC am 10:10
Nofsinger, Brian.....	WP 040	Oberacher, Herbert.....	ThP 585	Okonkwo, Ozioma.....	TP 422
Nofsinger, Brian.....	WP 480	Oberlies, Nicholas.....	WP 321	Oktem, Berk.....	MP 383
Noguchi, Tsuyoshi.....	WP 477	Obermayr, Philipp.....	WP 135	Oktem, Elmas.....	ThP 609
Nogueira, Fabio CS.....	TP 686	Oberreit, Derek.....	ThOC pm 4:10	Okuda, Koji.....	TP 604
Nogueira Eberlin, Marcos.....	MP 570	Obolensky, Oleg.....	ThP 195	Okumu, Anna.....	ThP 308
Noguera, Daniel R.....	WOA am 09:50	O'Brien, Jeremy T.....	TP 745	Okumu, Anna.....	TOA pm 3:30
Nolan, Krystal D.....	TOE pm 4:10	O'Brien, John.....	TOD am 09:50	Okumura, Akihiko.....	MP 526
Nolen, Greg T.....	WP 249	O'Brien, John P.....	ThP 350	Okuno, Toshiaki.....	WOH am 09:10
Nolting, Dirk.....	ThP 507	O'Brien, Jonathon.....	ThP 290	Olah, Timothy.....	ThP 441
Nolting, Dirk.....	WP 760	O'Brien Johnson, Reid.....	MP 467	Olah, Timothy.....	TP 693
Nomerotski, Andrei.....	ThP 002	Obuchi, Wataru.....	MP 447	Olah, Timothy.....	WP 725
Noon, Kathleen.....	WP 245	Ochiai, Shoko.....	WP 537	Olah, Timothy.....	WP 732
Noon, Kathleen R.....	WP 212	O'Connell, Lauren.....	WP 339	Olaitan, Abayomi.....	TP 347
Norheim, Randolph V.....	MP 654	O'Connor, Peter.....	WP 729	Olaitan, Abayomi D.....	MP 296
Norheim, Randolph V.....	TOB am 09:50	O'Connor, Peter B.....	MOB am 09:10	Olajos, Marcell.....	TP 263
Norheim, Randolph V.....	TP 714	O'Connor, Peter B.....	WP 329	Old, William.....	ThP 193
Norheim, Randy.....	ThOB am 10:10	O'Connor, Wayne.....	MP 273	O'Leary, Adam.....	ThP 585
Noritake, Yuka.....	MOA pm 3:10	Odijk, Mathieu.....	TP 611	O'Leary, Adam.....	ThP 586
Norris, James.....	TP 065	Odwin-DaCosta, Shelly.....	WP 581	O'Leary, Adam.....	WP 310
Norris, Jeremy L.....	MP 014	Oe, Tomoyuki.....	MP 107	O'Leary, Timothy.....	WP 716
Northen, Trent.....	MP 024	Oe, Tomoyuki.....	MP 108	O'Leary, Timothy J.....	WP 236
Northen, Trent.....	ThP 649	Oe, Tomoyuki.....	MP 105	Olinares, Paul Dominic B.....	MP 160
Northen, Trent.....	TP 381	Oe, Tomoyuki.....	MP 096	Oliphant, Joe.....	MP 696
Northen, Trent.....	TP 660	Oe, Tomoyuki.....	WP 131	Oliveira, Beatriz.....	ThP 171
Norton, Isaiah.....	TP 007	Öeckl, Patrick.....	MP 451	Oliveira, Lydie.....	MP 581

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Oliveira, Regina V.....	TP 614	Osaka, Kosuke.....	MP 766	Padovan, Julio C.....	WP 743
Oliveira dos Santos, Luana.....	ThP 138	Osburn, Sandra.....	ThOD am 09:10	Paek, Eunok.....	ThP 020
Oliveira Vidal, Ramon.....	MP 562	Osei, Michael.....	WP 285	Paek, Eunok.....	TP 080
Oliver, Richard.....	ThP 653	Oser, Harald.....	ThP 750	Paeng, Ki-Jung.....	ThP 591
Olivera, Baldomera.....	MP 149	Oser, Harald.....	ThP 755	Paes Leme, Adriana.....	WP 460
Olivieri, Silvana.....	WP 545	Osgood, Mark.....	ThP 507	Paes Leme, Adriana Franco.....	MP 562
Olivos, Hernando.....	TP 629	Osgood, Mark.....	WP 758	Pagel, Kevin.....	ThP 712
Olivos, Hernando.....	WP 586	Osgood, Sarah M.....	ThP 674	Pagel, Kevin.....	TOC am 10:10
Olivova, Petra.....	WP 506	O'Shea, Thomas.....	TP 024	Pagels, Shirin.....	WP 519
Olkowicz, Mariola.....	ThP 445	O'Shea, Tom.....	WP 638	Pager, C.....	TP 434
Olney, Terry.....	ThP 750	Oss, Merit.....	MP 313	Paglia, Giuseppe.....	WP 586
Olney, Terry.....	ThP 755	Østergaard, Ole.....	WP 467	Pagliano, Enea.....	TP 770
Olsen, Jesper V.....	WP 093	Ostrand-Rosenberg, Susan.....	MP 125	Pagliarini, David J.....	ThP 327
Olsen, Jesper V.....	MP 109	Ostrand-Rosenberg, Suzanne.....	MP 137	Pagnotti, Vincent.....	MP 301
Olsen, Jesper V.....	ThP 321	Ostrand-Rosenberg, Suzanne.....	MP 136	Pai, Pei-Jing.....	ThP 232
Olsen, Jesper V.....	TP 126	Ostrand-Rosenberg, Suzanne.....	WOH pm 4:10	Pai, Pei-Jing.....	TP 092
Olsen, Khris.....	MP 377	Ota, Shigenori.....	MP 766	Pai, Pei-Jing.....	WP 252
Olsen, Nora.....	WP 774	Otake, Yosuke.....	WP 143	Paik, Bradford A.....	MOA pm 2:30
Olson, Peter.....	ThP 294	Othman, Iekhsan.....	TP 303	Paik, Young-Ki.....	MP 127
Olsthoorn, Maurien.....	WP 055	Otsuka, Yuya.....	TP 321	Paik, Young-Ki.....	ThP 024
Olthuis, Wouter.....	TP 611	Otte, Gabriel L.....	ThOF pm 2:30	Pailleux, Floriane.....	ThP 678
Oman, Trent.....	WP 110	Ottesen, Jennifer.....	TOD am 09:10	Pailleux, Floriane.....	TP 174
Oman, Trent.....	WP 120	Ottl, Johannes.....	ThP 094	Paiva, Anthony.....	MP 639
Ómarsdóttir, Sesselja S.....	ThP 401	Otto, Andreas.....	ThP 071	Paiva, Felipe.....	WP 460
O'meally, Robert.....	MP 187	Otto, Andreas.....	ThP 774	Paizs, Bela.....	TOD pm 2:30
O'Meally, Robert.....	ThP 082	Otto, Joseph J.....	ThP 265	Pajand Birjandi, Afsoon.....	ThP 408
O'meally, Robert.....	ThP 219	Otto, Markus.....	MP 451	Pak, Huisong.....	TP 093
O'Meally, Robert.....	ThP 339	Otto, Mike.....	TP 056	Pakrasi, Himadri B.....	MP 111
O'Meally, Robert.....	WP 511	Otto, Mike.....	TP 051	Pakrasi, Himadri B.....	MP 100
Onami, Ichio.....	WP 183	Ottwell, Anne.....	TP 057	Palandra, Joe.....	TOF pm 2:50
O'Neil Slawewcki, Stacy.....	TOF pm 4:10	Ouellet, Michel.....	TP 203	Palaniswamy, M Sundaram.....	MP 085
O'Neill, Emily.....	MP 011	Oulamine, Youssef.....	MP 025	Palaniswamy, M Sundaram.....	WP 204
O'Neill, Terry.....	MP 520	Oulyadi, Hassan.....	TP 775	Palanjian, Sevag.....	TP 270
Ong, Shao-En.....	TP 111	Ouyang, Chuanzi.....	WP 006	Palazoglu, Mine.....	MP 606
Ong, Ta-Hsuan.....	TP 001	Ouyang, Zheng.....	MOB pm 2:50	Pallante, Giovanni.....	WP 603
Onifer, Tiffany M.....	TOC am 09:50	Ouyang, Zheng.....	ThOG pm 3:50	Palma, Pierangela.....	MP 722
Onjiko, Rosemary.....	ThP 740	Ouyang, Zheng.....	ThP 760	Palma, Pierangela.....	TP 764
Onjiko, Rosemary M.....	TP 197	Ouyang, Zheng.....	TOB am 09:30	Palmbiad, Magnus.....	MP 037
Onjiko, Rosemary M.....	TP 640	Ouyang, Zheng.....	TOG pm 2:30	Palmbiad, Magnus.....	MP 368
Ono, Masaya.....	WP 143	Ouyang, Zheng.....	TP 353	Palmbiad, Magnus.....	ThP 026
Onodera, Jun.....	TP 604	Ouyang, Zheng.....	TP 385	Palmbiad, Magnus.....	TP 161
Onor, Massimo.....	TP 770	Ouyang, Zheng.....	WP 021	Palmer, Andrew D.....	ThOG am 09:30
Onorato, Joelle.....	ThOE am 08:30	Ouyang, Zheng.....	WP 388	Palmer, Martin.....	TP 724
Onorato, Joelle.....	WP 487	Ouyang, Zheng.....	WP 747	Palmisano, Giuseppe.....	TP 124
Onsongo, Getiria.....	ThP 044	Ovchinnikova, Olga.....	ThP 004	Palsson, Bernhard O.....	WP 586
Onsongo, Getiria.....	TP 077	Ovchinnikova, Olga S.....	ThOB am 08:30	Palsson, Runolfur.....	WP 448
Oomens, Jos.....	MP 322	Ovchinnikova, Olga S.....	ThP 005	Palvannanathan, Raman.....	TP 529
Oomens, Jos.....	ThOD pm 3:30	Overall, Christopher M.....	ThP 222	Palvannanathan, Raman.....	TP 528
Oomens, Jos.....	ThOD pm 3:50	Overall, Christopher M.....	WP 150	Palvannanathan, Raman.....	WP 539
Oomens, Jos.....	TP 364	Overmyer, Katherine.....	MP 636	Pamelard, Fabien.....	MP 025
Oomens, Jos.....	TP 365	Overney, Gregor.....	MP 716	Pamelard, Fabien.....	TP 009
Oppenshaw, Anna P.....	MP 391	Overney, Gregor.....	ThP 472	Pamukcu, Matt.....	WP 508
Oppenshaw, Matthew.....	ThP 351	Overney, Gregor.....	ThP 483	Pamuku, Matt.....	ThP 447
Oppenheimer, Stacey R.....	TP 028	Overney, Gregor.....	WP 681	Pan, Chongle.....	MP 264
Opperman, Kay.....	WP 121	Ovitt, Tina.....	MP 767	Pan, Chongle.....	MP 627
Opperman, Kay.....	WP 514	Ovod, Vitaliy.....	TP 448	Pan, Chongle.....	TP 125
Oppermann, Felix.....	ThP 019	Owen, Benjamin.....	TP 589	Pan, Fengyun.....	WP 298
Oppermann, Madalina.....	TP 298	Owens, Kevin.....	WP 590	Pan, Jingxi.....	TP 014
Oppermann, Madalina.....	WP 510	Oyler, Jonathan.....	MP 018	Pan, Jingxi.....	TP 255
Opuni, Kwabena F.M.....	ThP 107	Ozcan, Sureyya.....	WP 107	Pan, Jingxi.....	TP 544
O'Reilly, Katherine.....	ThP 439	Ozdemir, Abdil.....	TP 259	Pan, Jiongwei.....	WP 371
Orfanopoulos, Ioannis.....	MP 668	Ozdemir, Abdil.....	MP 393	Pan, Kuan-Ting.....	ThP 203
Organtini, Kari.....	TP 392	Ozdemir, Abdil.....	TP 133	Pan, Li.....	MOH am 08:30
Organtini, Kari.....	WOC pm 2:30	Ozer, Sinan.....	WP 239	Pan, Li.....	ThP 079
Orlando, Ron.....	MP 734	Ozhegov, Evgeny.....	ThP 720	Pan, Ning.....	WOB pm 3:10
Orlando, Ron.....	ThP 142	Paape, Rainer.....	MOE pm 3:30	Pan, Ning.....	WP 009
Orlando, Ron.....	ThP 331	Paape, Rainer.....	TP 056	Pan, Ning.....	WP 395
Orlando, Ron.....	ThP 726	Paape, Rainer.....	WP 518	Pan, Ning.....	WP 741
Orlando, Ron.....	TP 110	Paape, Rainer.....	WP 517	Pan, Shenmin.....	MP 727
Orlando, Ron.....	TP 331	Pachl, Fiona.....	MP 191	Pan, Xiang.....	MP 400
Orlando, Ron.....	WP 080	Pachl, Fiona.....	ThOB am 09:30	Pan, Yanbo.....	TP 694
Orlando, Thomas M.....	TP 729	Pacholarz, Kamila.....	TOD am 09:30	Pan, Yi.....	MP 075
Orlowicz, Sean.....	WP 433	Packer, Nicolle.....	TP 327	Pan, Yuanjiang.....	ThP 699
Orr, Bonnie.....	TOE am 09:50	Packer, Nicolle H.....	WP 079	Pan, Yuanjiang.....	TP 352
Orr, Bonnie.....	TP 464	Padden, Juliet.....	TP 481	Panchal, Rekha.....	WP 010
Orr, Bonnie.....	WP 655	Padilha, Kallyandra.....	ThP 651	Pande, Paritosh.....	ThP 515
Orsini, Joseph.....	TP 639	Padmanaban, Arunkumar.....	MP 124	Pandey, Akhilesh.....	MP 256
Ortiz, Elena.....	TP 639	Padovan, Julio C.....	MP 160	Pandey, Akhilesh.....	MP 270
Orton, Daniel.....	MOC pm 3:10			Pandey, Akhilesh.....	MP 255
Ory, Daniel S.....	WP 520				

Program code: M,T,W, Th = Day    O = Oral, P = Poster    Time or poster number

# INDEX OF AUTHORS

Pandey, Akhilesh	MP 440	Parker, Karen	TP 170	Patterson, Rainey	MP 631
Pandey, Akhilesh	ThP 082	Parker, Kenneth	TP 419	Patti, Gary J.	MP 602
Pandey, Akhilesh	ThP 077	Parker, Kevin	WP 398	Pattison, Christine	TP 618
Pandey, Akhilesh	ThP 208	Parker, Kevin E.	TP 376	Pau, Stanley	TP 738
Pandey, Akhilesh	ThP 204	Parker, Lindsay	WP 234	Paul, John	MOB pm 3:50
Pandey, Akhilesh	ThP 219	Parker, Robert	ThOE pm 2:50	Paul, Lake	WP 169
Pandey, Akhilesh	ThP 278	Parker, Ryan	ThP 108	Pauli, Guido F.	WP 325
Pandey, Akhilesh	TOG am 09:10	Parker, William	ThP 267	Paulo, Joao	TP 145
Pandey, Niranjan	MP 187	Parker, William R.	ThP 350	Paulo, Joao	TP 430
Pandhal, Jags	MP 571	Parkinson, Erika	ThP 249	Paulovich, Amanda	ThOE am 10:10
Pang, Shaokun	TP 045	Parks, Derek	WP 105	Paulovich, Amanda	ThP 025
Pang, Xueqin	ThP 493	Parmar, Rubina	TOE am 08:50	Paulovich, Amanda	ThP 218
Pang, Yongle	MP 204	Parnell, Jonathan	ThP 118	Paulovich, Amanda	TOG am 08:30
Pang-Hung, Hsu	ThP 683	Paron, Igor	MP 723	Pavlopoulos, Antonis	WP 240
Paniagua, Eric	ThP 032	Parr, Vic	ThP 002	Pavlov, Julius	WP 409
Panic-Jankovic, Tanja	WP 136	Parrain, Jean-Luc	WP 682	Pavlov, Julius	WP 383
Panic-Janković, Tanja	WP 135	Parren, Paul W.H.I.	TP 237	Pawlak, Sebastian	WP 179
Panin, Alexandre	MP 340	Parrish, Whitney A.	ThP 096	Pawliszyn, Janusz	MP 603
Pankiewicz, Vania	WOE pm 4:10	Parsons, Lisa	MP 681	Pawliszyn, Janusz	MP 770
Pankratz, Todd	MP 645	Pasa-Tolic, Ljiljana	MOG pm 3:30	Pawliszyn, Janusz	ThOB am 09:50
Panne, Ulrich	MOA pm 3:50	Pasa-Tolic, Ljiljana	ThP 062	Pawliszyn, Janusz	ThP 408
Panne, Ulrich	TP 417	Pasa-Tolic, Ljiljana	ThP 064	Pawliszyn, Janusz	TP 521
Pannell, Lewis	TP 425	Pasa-Tolic, Ljiljana	TP 676	Pawliszyn, Janusz	TP 749
Pannell, Lewis	WP 144	Pasa-Tolic, Ljiljana	WOE pm 4:10	Pawliszyn, Janusz	WOE pm 2:50
Pannell, Lewis K.	MP 683	Paša-Tolić, Ljiljana	MP 654	Pawliszyn, Janusz	WP 750
Pannell, Lewis K.	ThP 265	Paša-Tolić, Ljiljana	TOA am 08:50	Pawłowski, Jake	WP 081
Panse, Christian	WP 154	Paša-Tolić, Ljiljana	TOE pm 2:50	Payne, Sam	MOG pm 3:30
Pantazides, Brooke	MP 194	Paša-Tolić, Ljiljana	WP 088	Payne, Samuel	TP 229
Panutdaporn, Nantika	ThP 126	Pasay, Jered	TP 003	Payne, Samuel	WOE am 08:30
Pap, Ildiko	ThP 394	Pascal, Bruce	ThP 137	Payne, Samuel H.	MOG am 09:50
Papac, Damon	ThP 543	Pascal, Bruce	TOF am 09:50	Payne, Samuel H.	ThP 741
Papanastasiou, Dimitris	MP 668	Pascal, Bruce	TP 543	Payne, Samuel H.	TP 083
Papanastasiou, M.	WP 229	Pascal, Bruce	WOH pm 2:30	Payne, Samuel H.	TP 169
Papanastasiou, Malvina	WP 219	Pascal, Bruce D.	ThP 335	Payne, Samuel H.	TP 324
Papetti, Moreno	TP 126	Pascal, Bruce D.	TP 094	Pe Benito, Melanie	TP 501
Papoulias, Panagiotis	MP 302	Pascale, Benlian	WP 447	Peacock, Patricia M.	WP 323
Papoutsakis, E. Terry	MP 572	Pascovici, Dana	ThOE pm 2:50	Peacock, Samantha N.	WP 170
Pappin, Darryl J.C.	ThP 032	Pascovici, Dana	ThP 735	Peake, David	WP 287
Pappin, Darryl J.C.	WP 170	Passarelli, Melissa K.	WP 013	Peake, David A.	MP 242
Parameswarappa, Sharavathi	TP 160	Pastore, Glaucia	WP 406	Peake, David A.	MP 243
Paramithiotis, Eustache	TP 423	Pastorelli, Roberta	TP 029	Peake, David A.	TP 294
Paranhos-Baccalà, Glaucia	TP 423	Patapoff, Thomas	WP 218	Pearson, Roger	TP 746
Parapatics, Katja	WOF pm 2:50	Patel, Anil	TP 677	Pearson, Terry	TP 462
Paraskova, Julia V.	ThP 558	Patel, Bhavin	WP 121	Pearson, Terry W.	WP 518
Pardo, Sammy	ThP 076	Patel, Bhavin	WP 514	Pease, Joe	TP 681
Pardo, Sammy	ThP 385	Patel, Bhavin	WP 737	Peat, Brian	TP 746
Paris, Alain	MP 587	Patel, Bhavish	MP 561	Peay, Marling G.	MP 505
Paris, Alain	MP 628	Patel, Dharmesh	WP 103	Peccinini, Rosângela G.	TP 614
Paris, Daniel	WOF am 09:50	Patel, Himakshi	WP 208	Pechan, Tibor	ThP 186
Park, Ben	TOG am 09:10	Patel, Jinal	WOD am 08:50	Pechanova, Olga	TP 644
Park, Dayoung	TP 333	Patel, Jinal	WOG pm 2:30	Peddada, Shyamal	MP 072
Park, Heejin	TP 080	Patel, Manisha	TP 446	Peddicord, Michael	TP 248
Park, Hwa Chun	ThP 312	Patel, Mitesh	ThP 427	Pedevilla, Hannes	ThOG am 09:50
Park, Jeong-Jin	TP 432	Patel, Mitesh	WP 648	Pedrosa, Fabio	WOE pm 4:10
Park, Ji-Won	TP 199	Patel, Rakesh	MP 530	Peeper, Daniel S.	MP 263
Park, Jonghoo	ThOB pm 2:50	Patel, Rutika	MP 190	Peer, Markus	MP 294
Park, Jong-Min	TP 527	Patel, Shirishkumar	WP 717	Peers, Graham	MP 558
Park, Jong-Moon	TP 441	Pates, George	TP 360	Pehrson, Bret	MOE pm 2:30
Park, Joo-il	TP 604	Patil, Pratap	MP 410	Peikert, Christian	TP 134
Park, Jun Hyun	ThP 549	Patil, Arun	MP 270	Pekar-Second, Tonya	MP 226
Park, JuneSoo	ThP 552	Patil, Arun H.	MP 255	Pelander, Anna	MP 289
Park, Kyu Hwan	MP 537	Patil, Ujwal	ThP 353	Pellarin, Riccardo	TP 132
Park, Kyu Hwan	TP 214	Patiny, Luc	ThP 687	Pellati, Federica	MP 582
Park, Melvin	WP 664	Patole, Chhaya	MP 407	Pellegrino, Raffaele	ThP 596
Park, Melvin	WP 690	Paton, Martin	TP 515	Pelletier, Laurence	MP 258
Park, Melvin A.	ThP 481	Patrick, Amanda	ThP 227	Pelletier, Nathalie	MP 485
Park, Melvin A.	TP 329	Patrick, Jeff	TP 661	Pelletier, Nathalie	MP 492
Park, Melvin A.	WP 663	Patrick, Jeffrey	MP 607	Pelletier, Nathalie	MP 497
Park, Melvin A.	WP 670	Patrick, Jeffrey	MP 608	Pelletier, Nathalie	MP 498
Park, Melvin A.	WP 686	Patrick, Jeffrey	ThP 617	Pelot, Robert	MP 116
Park, Robin	ThP 021	Patrick, Jeffrey	TP 603	Pelot, Robert	MP 246
Park, Sang-Je	ThP 312	Patrick, Jeffrey	TP 753	Pelot, Robert	MP 266
Park, Young	TP 238	Patrick, John	WP 660	Pena-Abaurrea, Miren	WP 575
Parker, Carol	ThP 050	Patrie, Steven	ThP 069	Pence, Lisa	MP 267
Parker, Evan	MOA pm 2:50	Patrie, Steven	TP 104	Peng, Baijie	MP 625
Parker, Evan	TP 119	Patrie, Steven	WP 058	Peng, Baijie	TP 654
Parker, Evan	WP 086	Patterson, Heath	TOH pm 3:50	Peng, Chao	TP 112
Parker, Glendon	WP 311	Patterson, Khiry	TP 364	Peng, Chao	WOG am 09:50
Parker, Jennifer L.	MP 119	Patterson, Rainey	MP 408	Peng, Junmin	MP 217

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Peng, Junmin.....	WP 139	Peru, Kerry M.....	TP 554	Piatkowska, Elzbieta.....	WP 171
Peng, Kuan-Chieh.....	ThP 053	Pesce, Michael.....	WP 426	Picard, Pierre.....	MP 284
Peng, Liming.....	MP 735	Peshkin, Leonid.....	MP 259	Picard, Pierre.....	MP 533
Peng, Liming.....	WP 432	Peshkin, Leonid.....	TOG am 09:50	Picard, Pierre.....	ThP 411
Peng, Ling.....	TP 781	Peshkin, Leonid.....	TP 180	Picard, Pierre.....	TP 607
Peng, Tan.....	TP 306	Peter, Gary F.....	MP 408	Picard, Pierre.....	WP 361
Peng, Xiaojun.....	MP 232	Peterman, Scott.....	MP 195	Picard, Pierre.....	WP 507
Peng, Xiaojun.....	TP 100	Peterman, Scott.....	ThP 211	Picard, Pierre.....	WP 626
Peng, Xiaojun.....	TP 123	Peterman, Scott.....	ThP 450	Picard, Pierre.....	WP 634
Peng, Xiaojun.....	TP 122	Peterman, Scott.....	WP 192	Picard De Muller, Gaël.....	MP 025
Peng, Yao.....	MP 056	Peterman, Scott.....	WP 266	Picca, Anna.....	WP 118
Peng, Ying.....	ThP 065	Peterman, Scott.....	WP 515	Piceni, Renzo.....	MP 632
Peng, Ying.....	WP 057	Peters, Calvin.....	MP 412	Pichler, Peter.....	TP 075
Peng, Yu-Ling.....	ThP 644	Peters, Kevin.....	WP 398	Pick, Horst.....	TP 389
Peng, Zhenlei.....	TP 760	Peters, Kevin C.....	TP 376	Picklo, Matthew.....	MP 089
Peng, Zhou.....	TP 345	Peters, Wibke.....	ThP 609	Pickup, Kathryn.....	TP 618
Penk, Steffen.....	WP 519	Petersen, Amelia.....	ThOG pm 3:10	Picot, Valentina.....	TP 423
Pennathur, Subramaniam.....	MP 597	Petersen, Elijah J.....	WP 707	Picotti, Paola.....	ThP 329
Pennathur, Subramaniam.....	ThP 395	Peterson, Amelia.....	MP 653	Pieczkolan, Jerzy.....	WP 179
Pennathur, Subramaniam.....	ThP 662	Peterson, Amelia.....	TOB am 10:10	Piehowski, Paul.....	MP 569
Penner, Natalia.....	MP 483	Peterson, Amelia C.....	MOD pm 4:10	Piehowski, Paul.....	WP 516
Penner, Natalia.....	MP 642	Peterson, Emily R.....	MP 278	Pieper, Rembert.....	ThP 283
Penner, Natalia.....	ThP 497	Peterson, Teresa E.....	TP 682	Pieper, Rembert.....	ThP 284
Penner, Natasha.....	MP 639	Petite, James.....	ThP 733	Pierce, Andrew.....	WP 114
Pennington, Ross.....	MOA am 09:10	Petrareanu, Catalina.....	MP 162	Pierrard, Marie-Aline.....	ThP 254
Pennington, Stephen.....	TP 433	Petrea, Myrto.....	ThP 552	Pierre, Fabrice.....	TP 649
Pennington, Stephen.....	WP 475	Petricoin, Emanuel.....	TP 440	Piersimoni, Lolita.....	ThP 454
Penny, Sarah.....	MOH am 10:10	Petrochenko, Evgeniy.....	ThP 050	Pierson, Nicholas A.....	MOC pm 2:50
Penrose, Jane.....	MP 579	Petrochenko, Evgeniy.....	ThP 056	Pierzchalski, Keely.....	ThP 390
Pensabene, Virginia.....	TOB pm 2:50	Petrochenko, Evgeniy.....	ThP 049	Pierzchalski, Keely.....	ThP 638
Penzlin, Anke.....	ThP 055	Petrochenko, Evgeniy.....	ThP 360	Pierzchalski, Keely.....	ThP 642
Pepin, Robert.....	ThOD am 08:30	Petrochenko, Evgeniy.....	ThP 361	Pierzchalski, Keely.....	TP 688
Pepin, Robert.....	WOD pm 3:30	Petrochenko, Evgeniy.....	ThP 455	Pieterse, Mervin.....	WP 478
Perazzo, Fábio.....	TP 025	Petsko, Gregory A.....	ThP 130	Pietrasiewicz, Alicia.....	TP 519
Percy, Andrew.....	ThP 252	Pettersson, Curt.....	TP 566	Pietrowski, Detlef.....	WP 136
Percy, Andrew.....	TP 484	Pettit, Michael.....	MP 047	Pikalov, Ioannis.....	MP 192
Percy, Andrew.....	WOG pm 3:10	Pettit, Michael.....	WP 658	Pike, Ian.....	MP 244
Percy, Andrew.....	WP 654	Pettit, Michael E.....	WP 657	Pike, Ian.....	ThOE am 08:50
Pereckas, Michael.....	WP 212	Pétursdóttir, Ásta.....	WP 342	Pike, Ian.....	ThP 163
Pereira, Alberto.....	WOC pm 3:30	Petyuk, Vladislav.....	WP 516	Pikin, OV.....	TP 449
Pereira, Alexandre.....	ThP 651	Petyuk, Vladislav A.....	TP 169	Pillai, Manoj.....	TP 274
Pereira, Alexandre da Costa.....	TP 435	Petzold, Chris.....	TP 175	Pillai, Manoj.....	TP 436
Pereira, C. A. M.....	WP 668	Peukert, Manuela.....	MP 416	Pillai, Manoj.....	TP 532
Pereira, Heloisa Aparecida Barbosa da Silva.....	MP 461	Pevzner, Pavel.....	ThP 064	Pillai, Manoj.....	WP 103
Pereira, Luisa.....	MP 742	Pevzner, Pavel A.....	ThP 062	Pillai, Manoj.....	WP 531
Pereira, Rosana.....	TP 584	Pfaff, Hans.....	MP 472	Pilo, Alice.....	MP 143
Pereira, Rosana C. L.....	TP 586	Pfaff, Hans.....	ThP 540	Pilon, Pierre.....	MP 531
Pereira, Rosana C. L.....	TP 594	Pfannkoch, Edward.....	MP 776	Pimenova, Tatiana.....	TP 171
Perera, Ann.....	MP 466	Pfannkoch, Edward.....	MP 772	Pimentel, Adam.....	TP 789
Perez, Johnny.....	TP 407	Pfeiffer, Conrad.....	TP 407	Piña, Benjamín.....	TP 637
Perez, Jonas.....	MP 194	Pham, Huong T (Nicole).....	ThOD am 09:30	Piña, Benjamín.....	TP 639
Perez, Jose.....	ThOA am 09:30	Pham, Melinda.....	WP 557	Pinkse, Martijn.....	MP 434
Perez, Marta.....	ThOD pm 3:10	Pham, Trong Khoa.....	ThP 083	Pinkse, Martijn.....	WOF am 10:10
Pérez, José J.....	TP 664	Pham, Trong Khoa.....	ThP 645	Pinkse, Martijn.....	WP 478
Pérez, Lisa M.....	WP 700	Pham, Victoria.....	WP 048	Pinnick, Veronica.....	ThP 364
Pérez, Sandra.....	TP 551	Phan, Nhu.....	TP 033	Pinnick, Veronica.....	ThP 369
Perez-Oliva, Ana.....	WP 200	Phan, Trang.....	TP 780	Pinnick, Veronica.....	TOA pm 2:30
Pérez-Ortega, Patricia.....	WP 362	Phelan, Vanessa.....	MP 056	Pinnick, Veronica.....	TP 710
Perkins, George.....	ThP 583	Phelan, Vanessa.....	TP 019	Pino, Lindsay.....	ThOC am 10:10
Perkins, George.....	ThP 584	Phelps, Mandy.....	WOH am 09:50	Pino, Lindsay.....	ThP 217
Perkins, George.....	WP 408	Philip, John.....	MP 036	Pinsolle, Alexandre.....	MP 241
Perkins, George.....	WP 695	Phillips, Jennifer.....	WP 111	Pinto, Antonio.....	MP 065
Perkins, Mathew.....	WP 574	Phillips, Julian.....	MP 294	Pinto, Antonio F. M.....	WP 730
Perkins, Simon.....	MP 031	Phillips, Andrew J.....	ThP 274	Pinto, Shirley.....	ThOE am 09:10
Perlman, David H.....	MP 271	Phillips, Jonathan.....	ThP 120	Pinto, Sneha.....	MP 270
Perlman, David H.....	ThP 631	Phinney, Brett.....	MP 219	Pinto, Sneha M.....	MP 255
Perlman, David H.....	TP 101	Phinney, Brett.....	WP 512	Pinto, Sneha M.....	ThP 208
Permentier, Hjalmar.....	TOA am 10:10	Phinney, Brett S.....	MP 071	Piotrowski, Mary.....	MOF pm 2:50
Pernas, Lucia Espona.....	ThP 035	Phinney, Karen.....	MOE pm 4:10	Piotrowski, Mary.....	WP 617
Pérot-Taillandier, Marie.....	TP 369	Phinney, Karen.....	ThP 268	Piper, Kristin.....	WP 587
Perou, Charles.....	TP 082	Phinney, Karen.....	TP 252	Pirani, Parisa.....	ThP 353
Perreault, Héléne.....	ThP 145	Phinney, Karen.....	TP 266	Pirhalla, Jill.....	MP 647
Perret, Alain.....	MP 617	Phinney, Karen.....	WP 214	Pirhalla, Jill L.....	TP 620
Perry, Cydne.....	ThP 426	Phinney, Karen.....	WP 453	Pirkle, James.....	ThP 382
Perry, Richard.....	WP 398	Phu, Lilian.....	WP 048	Pirman, David.....	WP 617
Perry, Richard.....	WP 399	Phu, My.....	TP 258	Pirmoradian, Mohammad.....	MOG am 10:10
Perry, Richard H.....	MP 387	Phung, Wilson.....	ThP 357	Pirmoradian, Mohammad.....	TOF pm 3:10
Perry, Richard H.....	TP 376	Pi, Na.....	WP 355	Pirrone, Gregory F.....	MOF am 09:30
Person, Jonathan.....	WP 411	Piatkivskyi, Andrii.....	ThP 691	Pirrotte, Patrick.....	TP 440

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Pisitkun, Trairak.....	ThP 314	Portner, Christoph.....	TP 581	Pretzel, Jette.....	TP 071
Pitta, Ivan R.....	TP 614	Portner, Christoph.....	WP 568	Previs, Stephen.....	MP 075
Pitteri, Sharon.....	ThP 146	Porto Da Silva, Carla.....	MOH pm 4:10	Previs, Stephen.....	ThOE am 09:10
Pitzalis, Emanuela.....	TP 770	Porto Da Silva, Carla.....	MP 020	Previs, Stephen.....	TP 061
Place, Benjamin.....	ThP 624	Porto Da Silva, Carla.....	MP 056	Previs, Stephen.....	TP 459
Place, Benjamin.....	WP 509	Porwal, Suheel.....	ThP 646	Previs, Stephen.....	WP 320
Place, Benjamin.....	WP 577	Poshkus, Jennifer.....	MP 753	Prévost, Michèle.....	WP 565
Plant, Steve.....	MP 783	Posocco, Paola.....	WP 682	Pricl, Sabrina.....	WP 682
Plath, Logan.....	TP 133	Possolo, Antonio.....	WP 453	Pridatchenko, Marina L.....	WP 164
Pleik, Stefanie.....	WP 300	Post, Jeremy.....	ThP 766	Prideaux, Brendan.....	TP 026
Plesofsky, Nora.....	MP 605	Post, Jeremy.....	WP 649	Prideaux, Brendan.....	TP 023
Plewa, Michael.....	WP 562	Postigo, Cristina.....	WP 562	Prideaux, Brendan.....	WP 553
Plowey, Edward.....	ThP 308	Postovit, Lynne-Marie.....	MP 458	Prien, Justin.....	MOE pm 4:10
Ploy, Marie-Cécile.....	WP 059	Pott, Leona Louise.....	TP 481	Prieto, DaRue A.....	MP 132
Plumb, Robert.....	WP 596	Potter, Oscar.....	TP 334	Prieto Conaway, Maria.....	ThP 568
Plummer, Chelsea E.....	MP 319	Potter, Oscar.....	WP 083	Prieto Conaway, Maria C.....	MP 285
Plummer, Kim.....	ThP 045	Potts, Gregory K.....	ThP 179	Prieto Conaway, Maria C.....	WP 650
Plymire, Daniel.....	TP 104	Poudyal, Hemant.....	WP 600	Prince, John.....	MP 059
Plymire, Daniel.....	WP 058	Poulson-Ellestad, Kelsey L.....	MP 274	Prince, John.....	MP 060
Pocai, Alessandro.....	TP 460	Pour, Masoumeh.....	TP 033	Prince, John.....	ThP 030
Podar, Mircea.....	MP 129	Pourkaveh, Shiva.....	WP 191	Prince, John.....	ThP 029
Podar, Mircea.....	MP 276	Powell, Andrew T.....	MP 706	Prince, John.....	WP 036
Podgorski, David C.....	MOA am 08:30	Powell, Jonathan.....	ThP 339	Prince, John.....	WP 464
Podgorski, David C.....	MP 555	Powell, Kendall.....	WP 480	Pringle, Steven.....	MP 404
Poetzsch, Michael.....	ThOE pm 3:10	Powell, Matthew.....	MP 199	Pringle, Steven.....	ThP 748
Pogliano, Kit.....	TP 019	Powell, Matthew.....	MP 380	Pringle, Steven.....	TP 215
Pohl, Chris.....	TP 337	Powell, Matthew.....	WP 740	Pringle, Steven.....	TP 722
Poirier, Michael.....	TOD am 09:10	Powell, Robyn.....	MP 469	Pringle, Steven.....	TP 723
Polaczek, Christine.....	TP 732	Power, Mary.....	TP 660	Pripuzova, Natalia.....	ThP 313
Polcelli, Wagner.....	WP 379	Powers, Marcel.....	MP 011	Pritchard, Jonathan.....	MP 212
Polfer, Nicolas.....	ThP 227	Powers, Robert.....	TP 452	Pritchett, Jeanita.....	ThP 635
Polfer, Nicolas.....	ThP 717	Powers, Robert.....	WP 593	Progent, Frédéric.....	WP 396
Polfer, Nicolas.....	TP 363	Powers, Thomas.....	TP 069	Prokai, Laszlo.....	WP 233
Polfer, Nicolas.....	TP 367	Poyer, Salomé.....	WOC pm 2:50	Prokai-Tatrai, Katalin.....	WP 233
Politi, Katerina.....	ThP 274	Pradeep, T.....	TP 350	Prosser, Simon J.....	MOB pm 4:10
Politis, Argyris.....	ThP 501	Pradeep, T.....	TP 398	Prosser, Simon J.....	MP 395
Polozova, Alla.....	MP 094	Pradeep, T.....	WP 412	Prosser, Simon J.....	MP 666
Polpitiya, Ashoka D.....	ThP 285	Pradhan, Sujana.....	MP 612	Prost, Spencer.....	ThOB am 10:10
Polson, Craig.....	ThP 421	Prado, Ana Carolina.....	WP 460	Prost, Spencer A.....	MP 677
Polt, Robin.....	WP 099	Prado, Mindy.....	ThOF am 10:10	Prost, Spencer A.....	ThP 741
Polyakova, Olga.....	WP 709	Prakash, Amol.....	ThP 450	Prost, Spencer A.....	TOB am 09:50
Polyukh, Christina A.....	TP 324	Prakash, Amol.....	WP 192	Protzel, Chris.....	ThP 277
Pompach, Petr.....	ThOF am 08:50	Prakash, Amol.....	WP 515	Provencher, Gilles.....	MP 288
Pompach, Petr.....	ThP 139	Prakash, Chandra.....	MP 483	Prudhomme, Jacques.....	ThOF pm 3:30
Ponniah, Gomathinayagam.....	TP 148	Prakash, Chandra.....	MP 642	Prystowsky, Michael.....	MP 421
Ponnusamy, Babu.....	ThP 161	Prasad, Namrata.....	MP 436	Przybyciel, Matthew.....	MP 506
Pons, Jaume.....	WP 278	Prasad, Satendra.....	TP 294	Przybylski, Michael.....	ThP 746
Ponts, Nadia.....	ThOF pm 3:30	Prasad, Satendra.....	WP 763	Przybylski, Michael.....	WP 656
Pope, Marshall.....	MOA am 08:50	Prasad, Satendra.....	WP 762	Ptackova, Renata.....	ThP 354
Pope, Matt.....	WP 517	Prasad, Satendra.....	WP 761	Ptitsyn, Andrey.....	ThP 303
Popel, Aleksander S.....	MP 187	Prasad, T. S. Keshava.....	MP 255	Pu, Tsung-Hsien.....	ThP 160
Pophristic, Milan.....	MP 534	Prasad, T. S. Keshava.....	MP 270	Pu, Yi.....	ThOH pm 2:30
Popic, Sasa.....	ThP 043	Prasad, T.S. Keshava.....	ThP 208	Pu, Yi.....	TP 323
Popov, Alexander M.....	ThP 745	Prassas, Ioannis.....	TP 244	Puchades, Cristina.....	ThP 119
Popov, IA.....	TP 449	Praet, Kerri.....	MP 554	Puchowicz, Michelle A.....	WP 603
Popov, Igor.....	ThP 086	Preau, James.....	WP 461	Pudenzi, Marcos.....	TP 584
Popov, Igor.....	TOA pm 4:10	Predel, Reinhard.....	TP 167	Pudenzi, Marcos A.....	TP 586
Popov, Igor.....	TP 325	Préfot, Petra.....	ThP 215	Pudenzi, Marcos A.....	WOA pm 3:30
Popov, Igor.....	TP 409	Prenen, Hans.....	WP 469	Pugh, Coleen.....	TP 784
Popov, Igor.....	WP 724	Prengaman, Linda.....	MP 002	Pugh, Michael.....	TP 491
Popova, Nina N.....	ThP 745	Prenni, Jessica.....	MP 418	Pugmire, Trina.....	ThP 285
Popovici, Andrew.....	TP 304	Prenni, Jessica.....	MP 558	Pulicharla, Rama.....	TP 556
Popovici, Andrew.....	TP 568	Prenni, Jessica.....	ThOG am 08:50	Pullen, Frank.....	WP 695
Popowski, Melissa.....	MP 592	Prenni, Jessica.....	ThP 234	Pulliam, Christopher.....	ThOA am 08:30
Popp, Oliver.....	WP 174	Prenni, Jessica.....	ThP 608	Pulliam, Christopher.....	TP 387
Popp, Robert.....	ThP 262	Prenni, Jessica.....	ThP 607	Puranam, Deva H.....	MP 737
Popp, Robert.....	TOG pm 3:10	Prenni, Jessica.....	WP 550	Puranam, Deva H.....	MP 779
Poppi, Ronei.....	WP 460	Prenni, Jessica.....	WP 550	Purcell, Anthony.....	ThP 342
Porcarì, Andrea.....	WP 709	Prenni, Jessica.....	WP 720	Puri, Neelu.....	WP 481
Porras-Yakushi, Tanya.....	ThP 240	Prentice, Boone.....	ThP 008	Purkayastha, Subhasish.....	ThOC am 08:50
Porta, Tiffany.....	MP 397	Prentice, Boone.....	TP 341	Purves, Randy W.....	ThP 736
Porta, Tiffany.....	WOB am 08:50	Prentice, Boone M.....	TOB am 09:10	Puschner, Birgit.....	TP 765
Porte, Cinta.....	WP 719	Prentice, Boone M.....	TP 340	Putluri, Nagireddy.....	ThP 657
Porter, Forbes D.....	MP 437	Prentice, Boone M.....	TP 339	Putman, Jonathan.....	TP 600
Porter, Ned.....	ThOG pm 2:50	Presler, Marc.....	TP 180	Pyatnitsky, Mikhail.....	ThP 248
Porter, Ned A.....	ThP 485	Press, Randall.....	MP 645	Pyatnitsky, Mikhail A.....	TP 081
Porter, Thomas.....	TP 236	Prest, Harry.....	MP 600	Pyun, Jae-Chul.....	TP 527
Porter, Thomas.....	WP 274	Prest, Harry.....	WP 354	Qamar, Saadia.....	ThP 457

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Qamar, Saadia.....	ThP 519	Quinkert, Zachary T.....	MP 160	Ramakrishnan, Vikram.....	TP 175
Qi, Ming.....	ThP 400	Quinlan, Casey.....	TP 127	Raman, Venu.....	MOH pm 3:50
Qi, Nathan.....	MP 636	Quinn, John.....	MOB am 10:10	Ramanathan, Dil.....	MP 190
Qi, Yue.....	TP 139	Quinn, John P.....	MP 699	Ramanathan, Ragu.....	TP 634
Qi, Yue.....	TP 143	Quinn, Kevin.....	TP 446	Ramanathan, Ragu.....	TP 616
Qi, Yue.....	WP 241	Quinque, Geoffrey.....	TOF pm 4:10	Ramanathan, Ragu.....	TP 633
Qi, Yulin.....	WP 452	Quinton, Loic.....	MOC pm 2:30	Ramaswamy, Subramanian.....	ThP 161
Qi, Yulin.....	WP 554	Quintón, Loic.....	WOE am 09:50	Ramiah, Annapoorani.....	MP 176
Qian, Chen.....	ThP 772	Quintyn, Royston.....	ThOC pm 2:50	Ramireddy, Rajasekhar.....	TP 774
Qian, Fang.....	MP 516	Quintyn, Royston.....	WOD pm 3:50	Ramirez, Sabra.....	ThP 557
Qian, Fang.....	ThP 109	Raab, Andrea.....	WP 342	Ramirez-Correa, Genaro.....	ThOE pm 3:30
Qian, Fang.....	ThP 196	Raab, Michal.....	TP 525	Ramisetty, Sreenivasa.....	MP 156
Qian, Haifeng.....	TP 674	Raab-Traub, Nancy.....	WP 250	Ramkissoon, Kevin.....	ThP 052
Qian, Jiang.....	ThP 133	Raaijmakers, Linsey M.....	ThP 301	Ramkissoon, Kevin R.....	WP 255
Qian, Jie.....	WP 203	Rabaha, Helmy.....	MP 535	Ramon, Jan.....	ThP 022
Qian, Jie.....	WP 264	Rabaha, Helmy.....	ThP 587	Ramos De Jesus, Hugo César.....	ThP 453
Qian, Mark.....	TP 515	Raber, Jacob.....	WOC pm 3:10	Ramp, Thomas.....	MP 639
Qian, Pu.....	ThP 172	Rabuck, Jessica.....	WP 369	Rampersaud, Dianne.....	WP 400
Qian, Weijun.....	WP 088	Rabuck-Gibbons, Jessica.....	ThP 490	Ramsey, J Michael.....	TP 738
Qian, Wei-Jun.....	MP 100	Race, Alan.....	TP 041	Ramsey, J. Michael.....	MOB pm 3:10
Qian, Wei-Jun.....	WOG pm 2:50	Race, Alan M.....	MP 028	Ramsey, J. Michael.....	MP 691
Qian, Wei-Jun.....	WP 513	Rad, Ramin.....	TP 145	Ramsey, J. Michael.....	MP 692
Qian, Wen-Jian.....	MP 189	Raddatz, Christian-Robert.....	MP 388	Ramsey, J. Michael.....	MP 693
Qian, Xiaohong.....	TP 442	Räder, Hans Joachim.....	WP 683	Ramsey, J. Michael.....	MP 694
Qian, Xiaohong.....	WP 166	Radford, Sheena E.....	WP 201	Ramsey, J. Michael.....	TP 739
Qian, Yichao.....	WOC pm 4:10	Radford, Sheena E.....	ThP 106	Ranasinghe, Asoka.....	TP 693
Qian, Yichao.....	WP 561	Radford, Sheena E.....	WOH pm 3:10	Ranasinghe, Asoka.....	WP 725
Qian, Yichao.....	WP 567	Radhakrishnan, Aneasha.....	MP 255	Ranbaduge, Nilini.....	ThP 296
Qiao, Hui.....	MP 339	Radhakrishnan, Sridhar.....	ThP 303	Rand, Kasper D.....	ThP 135
Qiao, Hui.....	ThP 427	Radi, Krisztina.....	ThP 701	Rand, Kasper D.....	TOF am 09:30
Qiao, Hui.....	TP 630	Radi, Krisztina.....	WP 444	Rand, Kasper D.....	TOF pm 2:30
Qiao, Hui.....	WP 558	Radicioni, Giorgia.....	ThP 270	Rand, Scott.....	MP 428
Qiao, Hui.....	WP 648	Radiojac, Predrag.....	WP 038	Randall, Elizabeth C.....	TP 232
Qiao, Jana.....	TOG am 08:30	Radtke, Karl.....	WP 471	Randriamarotia, Martin.....	TP 423
Qiao, Jana W.....	MOG am 08:30	Radu, Lucian G.....	MP 162	Rane, Shailendra.....	TP 496
Qiao, Jana W.....	ThOE am 10:10	Raether, Oliver.....	WP 727	Rane, Shailendra.....	TP 497
Qiao, Jana W.....	ThP 205	Rafiee, Mahmoud-Reza.....	MP 223	Rane, Shailendra.....	TP 498
Qiao, Jana W.....	TP 438	Rafiei, Atefeh.....	TP 657	Rane, Shailendra.....	WP 350
Qiao, Liang.....	TP 389	Raftery, Daniel.....	MP 443	Raney, Kevin.....	ThP 054
Qiao, Lirui.....	ThP 529	Raftery, Daniel.....	ThP 655	Ranganathan, Srivathsan.....	ThP 471
Qin, Guochen.....	WOE pm 3:10	Raftery, Daniel.....	ThP 659	Rangiah, Kannan.....	MP 509
Qin, Hongqiang.....	WP 473	Raftos, David.....	MP 273	Rangiah, Kannan.....	WP 479
Qin, Shanshan.....	WP 736	Rago, Brian.....	WP 272	Rannulu, Nalaka.....	TP 293
Qin, Weijie.....	WP 166	Rahman, A. F. M. Motiur.....	MP 725	Rao, Govind.....	ThP 167
Qing, Lai-Yun.....	WP 053	Rahman, A. F. M. Motiur.....	MP 726	Rao, Mangala.....	ThP 229
Qiu, Difei.....	TP 248	Rahman, Md. Matiur.....	TP 727	Rao, Ramesh.....	MP 338
Qiu, Feng.....	MP 614	Rahman, Mohammad.....	ThP 016	Rao, Ramesh.....	WP 348
Qiu, Feng.....	MP 607	Rahn, Peter.....	WP 640	Rao, Satish.....	TP 491
Qiu, Feng.....	ThP 640	Rainville, Paul.....	MP 714	Rao, Srinivasa.....	TP 337
Qiu, Jinshu.....	WP 606	Rainville, Paul.....	TP 235	Rao, Wei.....	WP 009
Qiu, Ruiqing.....	WP 619	Rainville, Paul.....	TP 629	Rao, Wei.....	WP 741
Qiu, Wen.....	ThP 083	Rainville, Paul.....	TP 693	Rappold, Brian.....	TOG pm 4:10
Qiu, Yu.....	TP 476	Rainville, Paul.....	WP 637	Rappold, Brian.....	WP 427
Qu, Jun.....	MP 224	Rainville, Paul.....	WP 742	Rappold, Eduard.....	WP 140
Qu, Jun.....	ThP 014	Raitakari, Olli.....	WP 504	Raptakis, Emmanuel.....	MP 668
Qu, Jun.....	ThP 013	Raja, Erum.....	WP 121	Rardin, Brent.....	MOB pm 2:30
Qu, Jun.....	TP 245	Raja, Huzefa.....	WP 321	Rardin, Matthew.....	WP 113
Qu, Jun.....	WP 015	Rajagopalan, Pavithra.....	MP 255	Rasam, Pratap.....	TP 496
Qu, Jun.....	WP 193	Rajasekar, Shanmugam.....	TP 669	Rasam, Pratap.....	TP 497
Qu, Jun.....	WP 232	Rajesh, PMN.....	WP 347	Rasam, Pratap.....	TP 498
Qu, Jun.....	WP 598	Rajpal, Arvind Rajpal.....	WP 278	Rasam, Pratap.....	TP 761
Qu, Wenge.....	MP 357	Raju, Rajesh.....	MP 255	Rasam, Pratap.....	TP 762
Qu, Xuewei.....	WP 741	Raju, Rajesh.....	ThP 208	Rasam, Pratap.....	TP 763
Qu, Yi.....	WP 088	Raju, Shruti.....	TP 496	Rasam, Pratap.....	WP 350
Qu, Zhe.....	ThP 302	Raju, Shruti.....	TP 497	Räsänen, Riikka.....	WP 378
Quach, Olivia.....	MP 158	Raju, Shruti.....	TP 498	Rashid, Abdul M.....	WP 684
Qualizza, Brittni A.....	MP 324	Raju, Shruti.....	WP 350	Rashid, Faraz.....	MP 155
Quang, Changyu.....	TP 522	Rakib, Mohammed F.....	TP 563	Raska, Milan.....	ThP 149
Quarmby, Scott.....	MOD pm 4:10	Rakov, Sergey.....	ThP 416	Raska, Milan.....	WP 073
Quast, Matthew.....	TP 776	Rakov, Sergey.....	ThP 581	Raskind, Alexander.....	MP 035
Quazi, Shakey.....	WP 271	Rakowska, Paulina D.....	WP 386	Raskind, Alexander.....	MP 055
Que, Loretta G.....	WOG pm 3:30	Ralph, John.....	WOA am 09:50	Raskind, Sasha.....	MP 597
Queiroz, Nubia C. A.....	WP 711	Ralson-Hooper, Kimberly.....	TP 311	Rasmussen, Matthew.....	MP 568
Quernheim, Martin.....	WP 683	Ramachandran, Sumankalai.....	ThP 423	Rasmussen, Morten.....	TP 144
Quesada Calvo, Florence.....	MP 441	Ramadan, Ahmed A.....	TP 563	Rasoul, Bareza.....	WP 465
Quesada-Calvo, Florence.....	ThP 256	Ramagiri, Suma.....	MP 642	Rassoulpour, Arash.....	ThP 440
Quiason, Cristine.....	WP 005	Ramagiri, Suma.....	ThP 497	Rastogi, Anshu.....	WP 513
Quilliam, Michael.....	MP 353	Ramagiri, Suma.....	WP 186	Rath, Christopher M.....	MOH pm 4:10
Quimby, Bruce.....	TP 582	Ramagiri, Suma.....	WP 268	Rath, Christopher M.....	MP 020

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



Rathahao-Paris, Estelle.....	MP 587	Reimer, Ulf.....	MP 041	Reynolds, James.....	TP 390
Rathahao-Paris, Estelle.....	MP 628	Reimer, Ulf.....	MP 193	Reynolds, James C.....	MP 522
Rathore, Deepali.....	MP 142	Reimer, Ulf.....	ThP 046	Reyzer, Michelle L.....	TP 030
Rathore, Deepali.....	WP 370	Reiner, Eric.....	TP 392	Reyzer, Michelle L.....	TP 042
Ratnayake, Chitra.....	ThP 680	Reiner, Eric.....	WOC pm 2:30	Rezel, Melinda.....	WP 032
Ratnayake, Chitra.....	TP 195	Reiner, Eric J.....	WP 576	Rezenom, Yohannes H.....	MP 563
Ratnayake, Chitra K.....	TP 150	Reiner, Eric J.....	WP 575	Rhea, Patrea.....	ThP 383
Rauch, Jennifer N.....	WP 228	Reiner, Jessica.....	ThP 663	Rhee, David.....	ThP 260
Rauch, Paul J.....	WP 774	Reinhold, Vernon.....	ThOH pm 3:30	Rhim, Johng.....	ThP 392
Raught, Brian.....	MP 258	Reinhold, Vernon.....	TP 332	Rho, Hee-Sool.....	WP 511
Rauniyar, Navin.....	MP 220	Reinhold, Vernon.....	TP 335	Rhoads, Timothy.....	ThP 685
Rauniyar, Navin.....	WP 247	Reinhold, Nico.....	MP 093	Rhoads, Timothy W.....	ThP 068
Ravichandran, Akshaya.....	ThP 681	Reinhold, Nico.....	TP 622	Rhoads, Timothy W.....	WOD am 10:10
Ravikumar, Vaishnavi.....	ThP 080	Reininger, Charlotte.....	MP 379	Ribeiro, Fabio.....	MP 574
Rawat, Vivek.....	ThP 477	Reininger, Charlotte.....	WOB am 10:10	Ribeiro Campos da Silva, Samantha.....	MP 570
Rawlinson, Catherine.....	MP 419	Reisdorph, Nicole.....	TP 446	Ricchiuto, Piero.....	WP 018
Rawlinson, Catherine.....	ThP 653	Reiter, Lukas.....	ThOE pm 2:30	Ricci, Anthony.....	TP 507
Rawlinson, Catherine.....	WP 587	Reiter, Lukas.....	TP 086	Rice-Williams, Samantha.....	TP 107
Ray, Kevin.....	MP 751	Reiter, Lukas.....	WP 722	Rich, Virginia I.....	ThP 555
Ray, Kevin.....	ThP 260	Reitsma, Justin.....	WP 245	Richard, Christian.....	MP 561
Ray, Patricio.....	MP 424	Remes, Philip M.....	MP 672	Richards, Alicia.....	ThP 327
Ray, Phoebe Z.....	MP 555	Remes, Philip M.....	MP 717	Richards, Alicia.....	TP 669
Ray, Steven.....	WOB am 08:30	Remes, Philip M.....	ThP 756	Richards, Don.....	MP 639
Ray, Steven J.....	ThOB pm 4:10	Rempel, Don.....	MP 172	Richards, Matthew.....	TOF pm 3:30
Rayavarapu, Sree.....	MP 424	Rempel, Don.....	MP 173	Richardson, Dominique.....	ThP 492
Rayavarapu, Sree.....	ThOE am 09:50	Rempel, Don L.....	ThP 363	Richardson, Jason L.....	TP 642
Rayavarapu, Sree.....	TP 467	Ren, Bing.....	WOG am 09:50	Richardson, Keith.....	MP 695
Raymond, Kimiyo.....	WP 655	Ren, Da.....	MOE pm 2:50	Richardson, Keith.....	TP 215
Razavi, Morteza.....	TP 462	Ren, Da.....	WP 254	Richardson, Keith.....	TP 722
Razavi, Morteza.....	WP 517	Ren, Da.....	WP 718	Richardson, Keith.....	TP 724
Razavi, Morteza.....	WP 518	Ren, Jia.....	ThP 710	Richardson, Ruth.....	TP 203
Razinkov, Vladimir.....	TP 185	Ren, Jian Min.....	ThP 073	Richardson, Susan.....	WP 562
Razumovskaya, Jane.....	ThP 639	Ren, Jian Min.....	TP 109	Riches, Eleanor.....	WOA pm 2:30
Razunguzwa, Trust.....	MP 380	Ren, Jianhua.....	MP 320	Riches, Eleanor.....	WOA pm 2:50
Read, Howard.....	MP 338	Ren, Jianhua.....	ThP 184	Riches, Zoe.....	MP 214
Read, Howard.....	ThP 749	Ren, Jianmin.....	TP 117	Richter, Bruce.....	MP 784
Reading, Eamonn.....	WOH pm 3:50	Ren, Jian-Min.....	MP 122	Richter, Florian.....	MP 092
Rebane, Riin.....	MP 313	Ren, Jin.....	ThP 259	Ricke, Will.....	MP 448
Reddivari, Lavanya.....	ThP 303	Ren, Ling.....	WP 744	Ricke, Will.....	TP 454
Reddy, Karen.....	ThP 082	Ren, Yan.....	ThP 157	Rickert, Keith.....	MP 536
Reddy, Sharanya.....	ThP 414	Ren, Yan.....	TP 097	Ricky, Akins.....	WOC pm 3:50
Reddy, Sharanya.....	ThP 581	Ren, Yue.....	TOG pm 2:30	Ricky, Alexander.....	WOC pm 3:50
Reddy, Sharanya.....	ThP 582	Ren, Yue.....	WP 747	Ridgeway, Mark.....	ThP 481
Reddy, Sharanya.....	ThP 583	Ren, Zhe.....	WP 016	Ridgeway, Mark.....	WP 663
Reddy, Todime.....	TP 277	Renard, Bernhard.....	ThP 055	Ridgeway, Mark.....	WP 670
Reddy, Todime.....	TP 276	Renard, Pierre-Yves.....	ThOF am 09:10	Ridgeway, Mark.....	WP 664
Redeker, Virginie.....	ThOF am 09:10	Renaud, Justin.....	ThP 700	Ridgeway, Mark.....	WP 690
Redick, Bill.....	ThP 471	Renfrow, Matthew B.....	ThP 149	Ridgeway, Mark.....	WP 686
Redwine, James.....	TP 362	Renfrow, Matthew B.....	WP 073	Riecken, Kristoffer.....	TP 054
Redwine, James G.....	TP 339	Rennie, Emma.....	MP 595	Riedeman, James.....	MOA am 09:50
Reeber, Steven L.....	TP 561	Rennie, Emma.....	MP 585	Riedeman, James.....	MP 574
Reece, Jennifer.....	TP 356	Rensvold, Jarred W.....	ThP 327	Riedeman, James.....	MP 575
Reed, Christopher.....	TP 341	Renuse, Santosh.....	MP 255	Riedeman, James.....	ThP 758
Reed, Jon.....	MP 116	Renuse, Santosh.....	MP 440	Riedeman, James.....	TP 589
Reed, Jon.....	MP 246	Renyer, Kathryn M.....	WP 563	Riemer, Angelika B.....	ThP 343
Reed, Jon.....	MP 266	Repeta, Daniel.....	MP 609	Rienhoff, Hugh.....	WP 512
Reed, Jon.....	WOF am 09:50	Replogle, Randall.....	ThP 758	Rietpietsch, Thomas.....	ThP 317
Reed, Tyler.....	ThP 331	Resar, Linda.....	TP 432	Rigbolt, Kristoffer T.G.....	TP 126
Rees, Jon.....	ThP 382	Reschke, Brent.....	MP 380	Rigdova, Katarina.....	MP 244
Reeser, Matthew.....	TP 238	Reschke, Brent.....	WP 740	Righetti, Laura.....	MP 582
Reeves, Raymond.....	TP 432	Resemann, Anja.....	MOE pm 3:30	Rightmyer, Lisa.....	WOE pm 3:50
Regnier, Fred.....	ThP 766	Resemata, Anja.....	TP 160	Rijkers, Erikjan.....	ThP 239
Regnier, Fred.....	TOB pm 2:30	Resetca, Diana.....	ThP 125	Riley, Nicholas.....	ThP 685
Reichenbach, Stephen.....	MP 600	Ressom, Habtom.....	MP 580	Riley, Nicholas M.....	ThP 068
Reichenbach, Stephen.....	WP 576	Ressom, Habtom.....	ThP 154	Riley, Nicholas M.....	ThP 348
Reichert, Matthew.....	WP 559	Ressom, Habtom.....	TP 756	Rimmer, Catherine.....	ThP 624
Reid, Gavin.....	MP 204	Reuschel, Scott.....	MP 502	Rinaldo, Piero.....	WP 655
Reid, Gavin E.....	ThOG pm 2:30	Reuschel, Scott.....	MP 503	Rinas, Aimee.....	MP 175
Reid, Gavin E.....	ThP 409	Reuter, Klaus.....	ThP 095	Ringe, Dagmar.....	ThP 130
Reid, Michelle.....	MP 408	Rewanwar, Sachin.....	WP 717	Ringeisen, Bradley R.....	MP 278
Reidy, Marie.....	WP 475	Rey, Martial.....	ThP 117	Rinner, Oliver.....	ThOE pm 2:30
Reifschneider, Olga.....	TP 032	Rey, Martial.....	TP 537	Rinner, Oliver.....	TP 086
Reilly, James P.....	ThP 100	Rey, Martial.....	WP 167	Rinner, Oliver.....	WP 722
Reilly, James P.....	ThP 189	Reyes-Garcés, Nathaly.....	MP 770	Rinschen, Markus.....	ThP 314
Reilly, James P.....	WP 038	Reyes-Garcés, Nathaly.....	TP 521	Rippel, Keith.....	MP 749
Reilly, Michael.....	MP 512	Reyes-Garcés, Nathaly.....	WP 750	Riss, Peio.....	MP 665
Reilly, Peter Ta.....	MP 669	Reyes-Soffer, Gisette.....	MP 075	Risticevic, Sanja.....	WOE pm 2:50
Reilly, Peter Ta.....	MP 670	Reynolds, James.....	ThP 500	Ritorto, Maria Stella.....	WP 200
Reimer, Toralf.....	WP 146	Reynolds, James.....	TP 402	Ritter, Reece.....	ThP 127

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Rivera, Elizabeth	MP 512	Rodgers, Wesley	TP 606	Romero, Roman	ThP 610
Rivera, Keith D.	WP 170	Rodgers, Mary T.	TP 322	Romieu, Anthony	ThOF am 09:10
Rix, Uwe	TP 463	Rodin, Igor	WP 423	Romine, Margaret	MP 569
Rizatti, Ana Cecilia	MP 332	Rodin, Igor	WP 713	Romm, Michelle	TP 663
Rizwan, Asif	TP 062	Rodland, Karin	WOG pm 2:50	Romm, Michelle	WP 279
Rizzo, David G.	MP 015	Rodland, Karin D.	TP 169	Römpf, Andreas	TOH pm 2:30
Rizzo, Thomas	ThOD pm 3:10	Rodland, Karin D.	TP 324	Römpf, Andreas	TP 071
Roach, Patrick J.	TP 752	Rodland, Karin D.	WP 513	Ronald, Crystal	MP 579
Roan, Nadia	ThP 511	Rodnin, Mykola	WP 231	Ronald, Hunter	WOC pm 3:50
Robb, Damon	MP 674	Rodríguez, Francisco J.	TP 064	Roncato, Marie-Anne	TP 225
Robb, Damon	MP 675	Rodrigues, Rachel	ThP 174	Rooney, Cathy	ThP 433
Robbins, Phillips W.	TP 223	Rodrigues, Silas P.	MP 103	Root, Daniel	MP 729
Robbins, Winston K.	TP 598	Rodrigues de Souza, Agnelo	MP 159	Roper, Stephen M.	ThP 166
Robbins, Winston K.	WOA am 09:30	Rodríguez, Carlos	TP 188	Roque Martins Silva, Paulo	MP 570
Roberts, Dominic	MP 338	Rodríguez, Henry	ThP 025	Rorabeck, John	WP 307
Roberts, Dominic P T.	WP 348	Rodríguez, Henry	TOG am 08:30	Rorrer, Leonard	MOB pm 2:30
Roberts, Justin	WP 220	Rodríguez, Raquel	WOE am 09:50	Rosa, Paulo	TP 585
Roberts, Mary	ThP 122	Rodríguez, Raymond	TP 258	Rosa, Raymond	ThOE am 09:10
Robertson, Don	ThOE am 08:30	Rodríguez Murillo, Jimmy	MP 159	Rosal, Charlita	WP 579
Robertson, Suzanne	WP 011	Rodríguez-Lafuente, Ángel	MP 770	Rosales, Hernando	TP 416
Robertson, Wesley	WP 744	Rodríguez-Mozaz, Sara	TP 551	Rosati, Sara	TP 237
Robichaud, Guillaume	ThP 007	Rodríguez-Puertas, Rafael	MP 006	Rosati, Sara	WOF am 09:30
Robichaud, Guillaume	TOH am 08:50	Rodriquez, Jaime	WP 141	Roscher, Jörg	TP 555
Robichaud, Guillaume	TP 011	Roede, James	ThP 304	Roschitzki, Bernd	ThP 773
Robichaud, Guillaume	WP 011	Roeder, Martin	MP 356	Roscioli, Kristyn	TOA am 08:50
Robichaud, Guillaume	WP 030	Roehr, Nathan	TP 363	Roscioli, Kristyn M.	MP 654
Robinson, Anthony L.	ThP 614	Roemer, Stephen C.	MP 737	Rose, Christopher	ThP 177
Robinson, Carol	MP 183	Roemer, Stephen C.	MP 779	Rose, Christopher	ThP 685
Robinson, Carol	ThOC pm 2:30	Roemmel, Andreas T.	ThOE pm 3:10	Rose, Christopher M.	ThP 068
Robinson, Carol V.	ThP 501	Roempp, Andreas	TP 020	Rose, Christopher M.	ThP 178
Robinson, Carol V.	WOH pm 3:50	Roenker, Nicole	WP 104	Rose, Christopher M.	WOD am 10:10
Robinson, Errol W.	TOA am 08:50	Roepstorff, Peter	MOH am 09:30	Rose, Kristie	MP 219
Robinson, Errol W.	MP 654	Roeraade, Johan	MP 451	Rose, Kristie	TP 091
Robinson, Errol W.	TOE pm 2:50	Roesli, Christoph	MOF pm 3:50	Rose, Kristie L.	MP 015
Robinson, John H.	ThP 246	Roesli, Christoph	MP 310	Rose, Rebecca	MP 125
Robinson, Michelle	TP 162	Roesli, Christoph	MP 445	Rose, Rebecca	WOH pm 4:10
Robinson, Philip	TP 205	Roesli, Christoph	ThP 343	Rose, Rebecca E.	TP 434
Robinson, Renā	MP 208	Roest, Hannes	MOG pm 3:50	Rose, Rebecca E.	WP 374
Robinson, Renā	ThP 305	Roewer, Claudia	ThP 277	Rosebrock, Adam	TP 638
Robinson, Renā	ThP 344	Roewer, Claudia	WP 715	Rosen, Eli	ThP 007
Robinson, Renā A. S.	ThP 320	Rogers, Chris	WP 083	Rosen, Elias	ThP 006
Robinson, Rena A.S.	WP 117	Rogers, John	ThOF am 09:50	Rosen, Elias	WP 452
Robinson, Rena A.S.	WP 706	Rogers, John	ThOH am 09:10	Rosenbaum, Kevin	MOB pm 2:30
Robinson, Richard	TP 662	Rogers, John	ThP 722	Rosenberger, George	ThP 035
Robinson, Sarah	TP 784	Rogers, John C.	MP 206	Rosenberger, George	TP 181
Robison, Heather	WP 399	Rogers, John C.	ThOH am 09:50	Rosenblatt, Kevin	MP 290
Robotham, Scott	WP 176	Rogers, John C.	ThP 170	Rosenblatt, Michael	MP 188
Roboz, John	WP 116	Rogers, John C.	TP 326	Rosenblatt, Michael	TP 234
Rocconi, Rodney	TP 425	Rogers, John C.	WP 121	Rosenblatt, Mike	ThP 778
Rocha, Rafael	MP 464	Rogers, John C.	WP 481	Rosenfelder, Natalie	WP 577
Rochat, Bertrand	TOG pm 2:50	Rogers, John C.	WP 514	Rosenow, Matthew	TP 440
Rock, Brooke	WP 495	Rogers, John C.	WP 737	Rosol, Thomas J.	MP 229
Rock, Dan	TP 151	Rogers, Richard	TP 152	Rosowski, Kristin	MP 431
Rock, Dan	WP 495	Rogers, Richard	WP 197	Rosowski, Kristin	TP 481
Rocker, Jana	WP 144	Rogers, Richard	WP 196	Ross, Mark M.	ThOA pm 4:10
Rocker, Jana D.	MP 683	Rogowska-Wrzesinska, Adelina	MOH am 09:30	Ross, Robert	MP 392
Rocker, Jana D.	ThP 265	Rohatgi, Nidhi	ThP 199	Ross, Robert	WP 363
Rockwood, Alan L.	WP 035	Rohn, Sascha	TP 054	Røssel Larsen, Martin	ThP 347
Rockwood, Alan L.	WP 439	Rohrer, Jeff	TP 337	Rost, Hannes	ThP 035
Roddy, Thomas	MP 075	Rohrs, Henry W.	ThP 170	Rosu, Frédéric	TOC am 08:50
Roddy, Thomas	ThOE am 09:10	Rojas, Pamela Leal	MP 255	Rotello, Vincent	WP 701
Roddy, Thomas	WP 320	Rojas, Pamela Leal	ThP 208	Rotello, Vincent	WP 723
Roddy, Thomas P.	TP 061	Rojas, Yeny	MP 584	Rotello, Vincent M.	WP 703
Rodgers, M.T.	MP 328	Rojas-Betancourt, Stella	MP 248	Röthlisberger, Ursula	ThOD pm 3:10
Rodgers, Mary T.	MOC am 08:50	Rojasajakul, Teerapat	WP 227	Rouden, Jacques	ThP 499
Rodgers, Ryan	TP 596	Rolando, Christian	MP 083	Rouse, Jason	WP 208
Rodgers, Ryan P.	MOA am 08:30	Rolando, Christian	TP 719	Rouse, Jason	WP 273
Rodgers, Ryan P.	MP 550	Rolando, Christian	WP 729	Rousseaux, Sophie	WOG am 09:50
Rodgers, Ryan P.	MP 555	Roldan, Ariel	WP 230	Rousu, Juho	ThOG am 08:30
Rodgers, Ryan P.	TP 602	Rollet, Marion	ThP 510	Rout, Michael	MOE am 09:30
Rodgers, Ryan P.	TP 595	Rollet, Marion	TP 780	Rout, Michael P.	MP 165
Rodgers, Ryan P.	TP 597	Rollman, Christopher	WP 304	Rout, Michael P.	TP 132
Rodgers, Ryan P.	TP 598	Rollman, Christopher	WP 305	Rout, Michael P.	WP 253
Rodgers, Ryan P.	TP 599	Roman, Gregory	WP 349	Roux, Aurelie	MOH pm 2:50
Rodgers, Ryan P.	TP 601	Romanelli, Anthony	ThP 406	Roux, Aurelie	ThP 387
Rodgers, Ryan P.	TP 600	Romanelli, Anthony	ThP 424	Roux, Aurelie	TP 002
Rodgers, Ryan P.	WOA am 09:30	Romanelli, Anthony	WP 128	Roux, Aurelie	TP 063
Rodgers, Ryan P.	WOA pm 3:50	Romano, Andrea	MP 663	Rowell, Anna Marie	ThP 605
Rodgers, Ryan P.	WOA pm 2:50	Romanov, Vladimir	MP 531	Röwer, Claudia	WP 146

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Rowland, Elden	TP 672	Russell, David H.	TOD pm 3:30	Sakakura, Motoshi	MP 551
Rowland, Steven M.	MOA am 08:30	Russell, David H.	TP 410	Sakakura, Motoshi	TP 383
Rowland, Steven M.	TP 601	Russell, David H.	WP 168	Sakamoto, Taku	WP 143
Rowland, Steven M.	WOA am 09:30	Russell, David H.	WP 670	Sakane, Iwao	MP 196
Roy, Jessie	MP 274	Russell, David H.	WP 662	Sakrikar, Dhananjay	TP 091
Roy, Pascal	ThP 023	Russell, David H.	WP 661	Saksa, Andy	ThOA am 09:10
Roy, René	TP 204	Russell, David H.	WP 660	Sakuma, Takeo	ThP 524
Roy, René	WOF am 08:50	Russell, Jared	ThP 632	Sakuma, Takeo	WP 358
Roy, Sushmita Mimi	TP 445	Russell, Jason	ThP 784	Sakuma, Tomohiro	WP 143
Roy, Sushmita Mimi	WP 138	Russell, Jason	TP 109	Sala, Cecilia	ThP 596
Roy, Sushmita Mimi	WP 137	Russell, Jason	WP 096	Salanoubat, Marcel	MP 617
Roy, Urmi	MP 106	Russell, Peter	ThP 560	Salari, Susan	TP 292
Roy-Lachapelle, Audrey	TP 574	Russell, William K.	ThP 211	Salazar, Carolina	ThP 417
Roy-Lachapelle, Audrey	WP 564	Russell, William K.	WP 168	Salazar, Carolina	TP 643
Rozema, Brent	ThOA pm 3:30	Russell, William K.	WP 670	Salazar, Gary	WP 756
Rozenski, Jef	WP 365	Russo, Paul	TP 188	Saleh, Aljona	MOF pm 2:30
Ruan, Qian	TOA am 09:50	Russo, Paul	TP 440	Salem, Nasser	MP 725
Ruan, Qian	WP 732	Ruttens, Bart	WP 129	Salemi, Michelle	WP 512
Rubakhin, Stanislav	TOA am 09:10	Ruzicka, Josef	MP 242	Salgia, Ravi	WP 141
Rubakhin, Stanislav	TP 001	Ruzicka, Josef	MP 243	Salgueiro, Jéssica Silva	TP 435
Rubakhin, Stanislav	TP 165	Ryabokon, AM	TP 449	Sali, Andrej	TP 132
Rubakhin, Stanislav S.	TP 640	Ryan, Christopher	ThP 676	Salih, Bekir	MP 066
Rucevic, Marijana	ThP 341	Ryan, Jeanne	TP 429	Salih, Bekir	MP 475
Rudaz, Serge	ThP 446	Ryan, Jeanne	WP 457	Salih, Bekir	TP 785
Rudd, Pauline	TP 156	Rybakowska, Iwona	ThP 445	Salisbury, Joseph	TP 546
Rudd, Pauline	WP 023	Rychnovsky, Scott	ThP 462	Sallans, Larry	ThP 627
Ruddy, Brian	ThP 569	Rychnovsky, Scott	ThP 463	Salmi, Jussi	ThP 276
Ruddy, Brian M.	MOA am 08:30	Ryder, Mark	MP 553	Salminen, William	MP 267
Rudelius, Martina	TP 058	Rydevik, Axel	TP 628	Salomon, Arthur	ThP 033
Rudewicz, Patrick	TP 035	Rydin, Emil	ThP 558	Salomon, Karen	MP 720
Rudge, James	WP 640	Ryu, Seung	WP 399	Salomon, Karen	TP 178
Rudney, Joel	ThP 044	Ryumin, Pavel	WP 748	Salovska, Barbora	ThP 201
Rudnick, Paul	MP 219	Ryzhov, Victor	ThP 691	Salter, Tara La Roche	WP 384
Rudolph, Heather L.	WP 555	Ryzhov, Victor	TP 342	Salter, Tara La Roche	WP 386
Rudolph, Samantha	ThP 782	Saalbach, Gerhard	WP 684	Salunkhe, Shardul	WP 717
Ruebel, Oliver	MP 024	Saati, Andrew	WP 208	Salvador, Arnaud	TP 219
Ruesch, Joseph	MP 335	Saavedra-Roman, Luis	ThOE am 08:50	Salvati III, Lawrence	TP 787
Ruffin, Mack T.	MP 446	Saba, Julian	ThOH am 09:50	Samant, Maithilee	MP 716
Ruffolo, Ralph	WP 575	Saba, Julian	ThP 211	Samant, Maithilee	WP 360
Rüger, Christopher	WP 733	Saba, Julian	ThP 722	Samaraweera, Himali	ThP 628
Ruggles, Kelly	ThP 039	Saba, Julian	TP 154	Samavarchi-Tehrani, Payman	MP 258
Ruggles, Kelly	TOG am 08:30	Saba, Julian	TP 337	Samgina, Tatiana	ThP 190
Ruggles, Kelly	TP 082	Saba, Julian	WP 069	Samii, Kaveh	MP 148
Ruggles, Kelly	TP 433	Saba, Julian	WP 065	Samii, Kaveh	WP 156
Ruggles, Kelly V.	MOG am 08:30	Sabala, Lucia	ThP 101	Samir, Parimal	WP 243
Ruggles, Kelly V.	TP 173	Sabari, Benjamin R.	WOG am 09:50	Sampaio, Julio	TP 298
Ruggles, Kelly V.	TP 438	Sabatini, Robert	MOC am 09:10	Samra, Stephanie	MP 591
Ruggles, Kelly V.	WOG pm 3:50	Sabia, Rocchina	WP 087	Samson, Kevin	TP 292
Ruhaak, L. Renee	ThP 153	Sabidó, Eduard	ThP 220	Samson-Thibault, François	MP 490
Ruhaak, L. Renee	ThP 729	Sabol, Jenny K.	ThP 724	Samuelson, John	ThP 159
Ruhaak, Renee	ThP 155	Sabra, Ramzi	ThP 297	Samuelson, John	TP 223
Ruijken, Marco	TP 613	Sachsenberg, Timo	MP 052	Samuelsson, Kristin	TP 618
Rumbelow, Stephen	ThP 532	Sachsenberg, Timo	ThP 459	Samulak, Billy	ThP 454
Runoldsdottir, Hrafnhildur L.	WP 448	Sachsenberg, Timo	ThP 457	Samulak, Billy	ThP 487
Ruotolo, Brandon	ThP 487	Sachsenberg, Timo	ThP 458	San Francisco, Susan	WP 615
Ruotolo, Brandon	ThP 488	Sachsenberg, Timo	ThP 519	Sana, Theodore R.	WP 591
Ruotolo, Brandon	ThP 489	Sacktor, Ned	TP 468	Sanchez, Laura	MP 020
Ruotolo, Brandon	ThP 490	Sadagopan, Nalini	WP 133	Sanchez, Laura	MP 056
Ruotolo, Brandon	TOC am 09:30	Sadeghi, Kambiz	MP 552	Sanchez, Laura	ThOA pm 2:50
Ruotolo, Brandon	TOC pm 3:10	Sadilek, Martin	WP 443	Sancho, Renata	WP 406
Ruotolo, Brandon	TOF pm 3:50	Sadowsky, Michael	WOE pm 4:10	Sanda, Miloslav	ThP 139
Ruotolo, Brandon	WP 369	Saepoo, Brooke	WP 459	Sanda, Miloslav	WP 089
Ruotolo, Brandon	WP 675	Saffaj, Taoufiq	WP 549	Sanda, Miloslav	WP 075
Ruparelia, Frenny	TP 521	Sagawa, Takehito	ThP 620	Sander, Chris	MP 215
Rupérez, Francisco J.	MP 582	Saha, Anumita	WOB am 08:30	Sanders, David J.	WP 082
Ruppert, Thomas	ThP 343	Saha, Krishnendu	WP 703	Sanders, Mark	MP 623
Ruprecht, Benjamin	ThOB am 09:30	Saha, Shyamasree	MOG am 09:10	Sanders, Mark	WP 203
Ruprecht, Benjamin	ThOB pm 3:50	Sahadevan, Sonu	ThP 161	Sanders, Nathan	ThP 484
Ruprecht, Benjamin	WP 095	Sahasrabuddhe, Nandini	MP 440	Sanders, Nathan	ThP 759
Rush, John	ThOF pm 2:30	Sahasrabuddhe, Nandini A.	MP 255	Sanders, Rogier	TOF am 08:50
Rush, John	ThP 219	Sahu, Alexandria	WP 113	Sandlers, Yana	WP 438
Rush, Michael	WP 332	Sahu, Apeksha	MP 255	Sandonato, Beatriz	TP 231
Rush, Michael	WP 331	Sahyouni, Fatima	WP 233	Sandonato, Beatriz	TP 415
Ruskiewicz, Dorota	TP 402	Saidi, Wissam A.	WP 706	Sandoval, Wendy	ThP 357
Russ, Manuela	WP 715	Saito, Kazuki	MP 621	Sandoval, Wendy	WP 048
Russell, Claire	ThP 163	Saito, Kazunori	MP 062	Sandoval-Calderon, Mario	MP 056
Russell, David H.	WP 700	Saito, Mak	MP 275	Sandra, Koen	ThP 389
Russell, David H.	MOC pm 2:50	Saito, Mak	WP 112	Sandra, Pat	ThP 389
Russell, David H.	MP 563	Saito, Yutaka	WP 143	Sandri, Brian	MP 429

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Sang, Yongqi	MP 357	Scalabrin, Matteo	ThP 468	Schalz, Hans-Günter	TP 338
Sangaraju, Dewakar	ThP 522	Scalf, Mark	MOG am 08:50	Schmerberg, Claire	WOE am 09:10
Sanjib Meitei, Ningombam	MP 238	Scalf, Mark	ThP 221	Schmid, Kara E.	ThP 306
Santa, Cátia	ThP 315	Scarfe, Graeme	MP 645	Schmid, Rainer	WP 136
Santamaria, Raphaël	ThP 678	Schaab, Christoph	ThP 019	Schmid, Sandra	ThP 136
Santasania, Carmen	MP 774	Schachterle, Steven	MP 720	Schmidt, Carla	ThOC pm 2:30
Santasania, Carmen T.	TP 534	Schaefer, Mathias	TP 338	Schmidt, Eduardo	TP 584
Santiago, Brandon	WP 770	Schaer, Martin	WOB pm 3:50	Schmidt, Eduardo	WP 709
Santiago, Brandon	WP 768	Schafer, Barry	WP 120	Schmidt, Eduardo M.	TP 586
Santini, Robert E.	TOB am 09:10	Schafer, Barry	WP 110	Schmidt, Eduardo M.	WOA pm 3:30
Santoro, Massimo	TP 754	Schaffer, Jean E.	WP 520	Schmidt, Frauke	MP 549
Santoro, Massimo	TP 755	Schambeau, Lindsay	TP 425	Schmidt, Michael	MP 690
Santos, Dora	ThOC am 09:10	Schambeau, Lindsay	WP 144	Schmidt, Tannin	WP 072
Santos, Jandyson M.	WOA pm 3:30	Schänzer, Wilhelm	WP 301	Schmit, Pierre-Olivier	ThP 253
Santos, Joana	TP 101	Schappler, Julie	ThP 446	Schmit, Pierre-Olivier	TP 178
Santos, Marcia	TP 149	Scharf, Annette	ThP 343	Schmit, Pierre-Olivier	WP 076
Santos, Marcia R.	WP 065	Schatz, Philipp	WP 592	Schmitt, Manfred	MP 004
Santos, Marcia R.	TOC pm 2:30	Scheerlinck, Ellen	ThP 776	Schmitt, Manfred	TP 052
Santos, Vanessa	TP 231	Scheerlinck, Ellen	WP 294	Schmitt, Pierre-Olivier	MP 157
Santos, Vanessa	TP 584	Scheffler, Kai	MP 186	Schmitt, Thomas	MP 267
Santos-Neto, Alvaro	TP 576	Scheibner, Olaf	TOG pm 2:50	Schmitter, Jean-Marie	MP 241
Santos-Silva, Alan	WP 460	Scheibner, Olaf	TP 280	Schmitz, Oliver	WP 592
Sap, Karen	ThP 239	Scheibner, Olaf	WP 568	Schnackenberg, Laura	MP 267
Sapkota, Shraddha	MP 594	Scheidweiler, Karl	TP 045	Schnatbaum, Karsten	MP 041
Saradjian, Peter	TOF pm 3:30	Scheltema, Richard Alexander	ThP 762	Schnatbaum, Karsten	MP 193
Saraf, Anita	ThOF pm 3:30	Schenerman, Mark	WP 194	Schnatbaum, Karsten	ThP 046
Sarajlic, E	MP 507	Schenk, Emily	MP 249	Schneider, André	TP 134
Saraswat, Suraj	ThP 100	Schenk, Emily	ThP 481	Schneider, Birgit	MP 294
Saraswat, Suraj	WP 038	Schenkel, John	TP 233	Schneider, Brad	WP 696
Sarathy, Jansy	TP 026	Schenone, Monica	WOG am 08:50	Schneider, Brad	WP 771
Sarathy, Jansy	WP 553	Schepmoes, Athena	WOE am 08:30	Schneider, Bradley	WP 772
Sardiu, Mihaela	MP 156	Schepmoes, Athena A.	TP 169	Schneider, Marilyn	ThOC am 09:50
Sardiu, Mihaela	ThOF pm 3:30	Schepmoes, Athena A.	WP 513	Schneider, Richard	TP 627
Šardzik, Robert	ThP 492	Scherer, Alexander	TP 589	Schneider, Richard	WP 616
Sarg, Bettina	ThP 226	Scherer, Alexander	TP 588	Schneider, Sallie S.	MP 423
Sarg, Bettina	ThP 242	Scherl, Alexander	MP 148	Schnell, Gilles	MP 450
Sarkar, Amalendu	TP 791	Scherl, Alexander	TP 093	Schnier, Paul	WP 225
Sarkar, Depanjan	TP 398	Scherl, Alexander	WP 156	Schnier, Paul D.	MP 184
Sarkar, Depanjan	WP 412	Schey, Kevin	TP 070	Schnoelzer, Martina	ThP 343
Sarpe, Vladimir	MOF am 09:10	Schey, Kevin L.	MP 022	Schnur, Joel	TP 188
Sarracino, David	ThP 450	Schey, Kevin L.	TP 039	Schock, Tracey	ThP 647
Sarsby, Joscelyn	TP 041	Schey, Kevin L.	TP 091	Schoen, Alan	WOC am 09:30
Sartain, Mark	ThOA pm 3:50	Schicklberger, Marcus	ThP 649	Schoene, Cedrik	MP 004
Sartain, Mark J.	MP 589	Schiel, John	MOE am 09:10	Schoene, Cedrik	TP 052
Sartain, Mark J.	WP 290	Schiel, John	MOE pm 4:10	Schoenherr, Regine	ThP 218
Sasaki, Jennifer	TOH am 08:30	Schiel, John	TP 252	Scholl, Peter	ThP 610
Sasseti, Christopher	WOF pm 3:10	Schiel, John	TP 266	Scholten, Arjen	ThP 212
Satake, Hiroyuki	MP 661	Schiel, John	WP 214	Scholten, Arjen	ThP 301
Sathe, Gajanan J.	MP 255	Schieltz, David M.	ThP 382	Schommer, Vanessa	TP 057
Satoh, Ryo	WP 131	Schiffer, Jamie	ThP 118	Schöneich, Christian	WP 503
Satoh, Takaya	MP 005	Schiffler, Stefan	MP 021	Schonthal, Axel H.	ThP 680
Satpayev, Dau	TP 206	Schilders, Karin	TP 482	Schoofs, Liliane	WP 469
Satulovsky, Javier	MP 716	Schiller, Juergen	WP 284	Schorr, Pascal	WP 452
Sauter, Denise	TP 171	Schiller, Jürgen	MP 252	Schrader, Wolfgang	TP 592
Sauter, Drew	MP 392	Schilling, Birgit	WP 118	Schrader, Wolfgang	TP 593
Sauter, Drew	MP 659	Schilling, Oliver	TP 172	Schrader, Wolfgang	WOA am 08:30
Sauter, Drew	WP 363	Schinazi, Raymond F.	ThP 679	Schraen, Susanna	WP 447
Sauter III, Andrew	MP 659	Schintu, Nicoletta	TP 016	Schraen-Maschke, Susanna	TP 472
Sauter III, Andrew D.	MP 392	Schintu, Nicoletta	TP 047	Schreiber, Andre	ThP 524
Sauvagnat, Berengere	TOF pm 3:30	Schioppa, Enrico	TOH pm 3:10	Schreiber, Andre	WP 357
Sauvé, Sébastien	ThP 566	Schirm, Michael	TP 423	Schreiber, Andre	WP 358
Sauvé, Sébastien	WP 296	Schirm, Michael	WP 137	Schreiber, Stuart L.	ThP 512
Sauvé, Sébastien	WP 565	Schlaak, Joerg	MP 431	Schriemer, David	MOF am 09:10
Savant, Ishani	WP 636	Schlapbach, Ralph	ThP 329	Schriemer, David	ThP 117
Savas, Jeffrey	MP 220	Schlapbach, Ralph	ThP 773	Schriemer, David	ThP 400
Savas, Jeffrey	ThOC pm 3:10	Schlapbach, Ralph	WP 154	Schriemer, David	TP 536
Saveliev, Sergei	ThP 778	Schlatzer, Daniela M.	WP 603	Schriemer, David	TP 538
Savidor, Alon	ThP 015	Schlegl, Judith	MP 041	Schriemer, David	WP 167
Savidor, Alon	ThP 197	Schlegl, Judith	ThP 046	Schriemer, David C.	ThOF am 09:50
Savitski, Mikhail	MP 041	Schleuder, Detlev	MP 344	Schriemer, David C.	TP 537
Savitski, Mikhail	ThP 046	Schleuder, Detlev	TP 565	Schroeder, John T.	MP 255
Savtchenko, Serguei	TP 374	Schlicht, Kari	ThOC am 09:10	Schroeder, Tara	MP 195
Sawant, Durvesh	TP 763	Schlicht, Kari	WP 437	Schroeder, Tara	WP 192
Sawant, Durvesh	TP 761	Schlörger, Nils	TP 338	Schroeder, Tara	WP 515
Sawant, Durvesh	TP 762	Schluessener, Michael P.	TP 565	Schröter, Christian	WOD am 09:30
Sawhney, Ashish	TP 499	Schlüter, Hartmut	TP 054	Schubert, Sören	TP 212
Saylor, Sarah	TP 570	Schlüter, Hartmut	WP 744	Schueller, Michael	TP 552
Scalabrin, Matteo	ThP 460	Schmainda, Kathleen	MP 428	Schuerenberg, Martin	TP 051

Program code: M,T,W, Th = Day    O = Oral, P = Poster    Time or poster number

# INDEX OF AUTHORS



Schug, Kevin	MP 076	Seeley, Erin H.	MP 014	Seyer, Alexandre	MP 581
Schug, Kevin	ThP 066	Seeley, Erin H.	MP 002	Seyer, Alexandre	ThP 391
Schug, Kevin	ThP 430	Seeley, Erin H.	TP 218	Seyer, Alexandre	WP 281
Schug, Kevin	ThP 557	Seeley, Erin H.	WP 002	Seyfert, Sonja	TP 447
Schug, Kevin	TP 505	Seib, Larry	MP 474	Seyfried, Nicholas	MP 216
Schug, Kevin A.	TP 490	Seiman, Andrus	MP 210	Seyfried, Nicholas	WP 178
Schuhmann, Kai	ThOG pm 3:30	Seipert, Richard	MOG pm 2:50	Seyfried, Nicholas	WP 237
Schuhmann, Kai	TP 298	Seipert, Richard	WP 041	Seymour, Sean	TP 184
Schuler, Benjamin	ThOD pm 2:30	Seipert, Richard	WP 049	Seymour, Sean L.	MOE pm 2:30
Schulman, Howard	TP 445	Seiser, Christian	MP 228	Seymour, Sean L.	ThP 316
Schultz, Brian	TP 066	Sekhar Nirujogi, Raja	ThP 077	Seymour, Sean L.	TP 085
Schultz, J Albert	TP 002	Seki, Toshio	MP 005	Seymour, Sean L.	WP 029
Schultz, J Albert	TP 063	Sekimoto, Kanako	TP 383	Seyoum, Berhane	TP 143
Schultz, J. Albert	MOH pm 2:50	Sekiya, Sadanori	TP 166	Seyoum, Berhane	TP 139
Schultz, Jo El	ThP 210	Selby, Timothy	ThP 758	Seyoum, Berhane	TP 248
Schultz, Melissa M.	TP 550	Selevsek, Nathalie	MP 152	Seyoum, Berhane	WP 441
Schultze, Kevin	MOB pm 3:10	Selevsek, Nathalie	ThP 329	Sha, Jiahao	ThP 238
Schulz, Angela	WP 656	Selevsek, Nathalie	WP 154	Sha, Jiahao	WP 149
Schulz, Jacqueline	TP 031	Selimov, Renat	MP 340	Shabanowitz, Jeffrey	MOE am 08:30
Schulz, Michael	WP 284	Sellami, Lyna	ThP 351	Shabanowitz, Jeffrey	MOH am 10:10
Schulze, Kerry	WP 511	Selvan, Lakshmi Dhevi N.	MP 255	Shabanowitz, Jeffrey	MP 146
Schulze, Waltraud X.	ThP 075	Semis, Rita	WP 472	Shabanowitz, Jeffrey	ThP 686
Schunter, Alissa	ThP 207	Sempos, Christopher	WP 453	Shabanowitz, Jeffrey	TOG am 08:50
Schurmann, Claudia	ThP 250	Semyonov, Alexander	ThP 571	Shabanowitz, Jeffrey	TP 188
Schuster, Stephanie	TP 110	Semyonov, Alexander	TP 755	Shaffer, Christopher	WOD pm 3:30
Schütz, Frédéric	TOG pm 2:50	Semyonov, Alexander	TP 754	Shaffer, Ian	TP 373
Schuurman, Janine	TP 237	Semyonov, Alexander	WP 359	Shaffer, Ian	TP 404
Schwab, Nicolas	MP 390	Sena Esteves, Miguel	ThP 403	Shaffer, Ian	TP 405
Schwamborn, Kristina	TP 058	Seneviratne, Chinthaka A.	TOH pm 3:30	Shaffer, Scott A.	MP 134
Schwämmle, Veit	WOG am 08:30	Seneviratne, Chinthaka A.	TP 748	Shaffer, Scott A.	MP 219
Schwartz, Jae	ThP 743	Sengupta, Shantanu	TP 436	Shaffer, Scott A.	ThP 403
Schwartz, Michael	WP 652	Sengupta, Srana	ThP 082	Shaffer, Scott A.	ThP 402
Schwartz, Steven	ThOA pm 3:10	Senior, Adam	MP 341	Shaffer, Scott A.	WOF pm 3:10
Schwarz, Rico	ThOF am 08:30	Senior, Adam	MP 756	Shah, Bhavana	TP 642
Schwarzenberg, Adrian	ThP 696	Senior, Adam	MP 783	Shah, Dimple	MP 350
Schwarzenberg, Adrian	TP 369	Senior, Adam	MP 761	Shah, Dimple	WP 347
Schwarzenberg, Adrián	TP 524	Senior, Adam	MP 760	Shah, Dimple	WP 349
Schwarzinger, Clemens	MOA pm 3:50	Senior, Adam	MP 759	Shah, Hardik	WP 609
Schwarzinger, Clemens	TP 417	Senior, Adam	MP 757	Shah, Harshil	ThP 021
Schweiger-Hufnagel, Ulrike	WP 076	Senior, Adam	MP 758	Shah, Manesh B.	ThP 555
Schweikhard, Lutz	MOB am 08:30	Senior, Adam	ThP 589	Shah, Punit	ThOH am 10:10
Schwemer, Theo	WP 733	Senko, Michael W.	MP 672	Shah, Punit	ThP 156
Schweppe, Devin	ThP 464	Senko, Michael W.	MP 717	Shah, Punit	TP 003
Schweppe, Devin	ThP 465	Senko, Michael W.	ThP 753	Shah, Punit	TP 477
Schweppe, Devin	WOF pm 3:30	Senko, Michael W.	ThP 756	Shah, Sumit	WP 717
Schwerdtle, Tanja	TP 031	Senko, Michael W.	WP 737	Shah, Sumit	TP 663
Schwitulla, Elke	TP 153	Seo, Jong Bok	ThP 271	Shah, Sumit	WP 279
Schymanski, Emma	TP 667	Seo, Jungju	TP 048	Shah, Sumit	WP 590
Scigocki, David	WP 047	Seo, Youjin	MOC pm 3:50	Shah, Vinit	ThOE am 09:10
Sciuto, Stephen	MOC am 09:50	Seo, Youjin	MP 101	Shah, Vinit	TP 061
Scott, Alison	ThP 337	Seo, Youjin	ThP 724	Shah, Vishal	ThP 675
Scott, C. Ronald	WP 443	Seo, Youngsook	TP 257	Shah, Vishal	TP 657
Scott, Garry	TP 724	Seo, Youngsuk	WP 066	Shaheed, Sadr-ul	WP 491
Scott, Nichollas	TP 131	Seok, Ae Eun	TP 441	Shahidi-Latham, Sheerin K.	WP 005
Scott, Nichollas	TP 137	Seol, Haeri	MP 163	Shaikh, Shifa M	TP 563
Scott, Nichollas	WP 069	Seol, Haeri	ThOE am 09:50	Shain, Kenneth	ThOE am 08:50
Scott Carnell, Lisa	TOA pm 2:50	Sepehr, Estatira	TP 499	Shaked, Yuval	MP 433
Scrivens, James	ThP 120	Sepulveda, Jorge	WP 426	Shalender, Bhasin	MP 735
Scrivens, James	ThP 701	Sequeria, Carita	WP 611	Shalender, Bhasin	WP 432
Scrivens, James	ThP 712	Serang, Oliver	WP 033	Shaler, Thomas A.	WP 213
Scrivens, James	WP 444	Serpa, Jason	ThP 049	Shambaugh, Joe	TP 661
Seage III, George	WOF pm 4:10	Serpa, Jason	ThP 455	Shambaugh, Joe	WP 050
Seah, Martin P.	WP 386	Serrano, Mahalia	TP 774	Shamji, Alykhan F.	ThP 512
Sealey Voyksner, Jennifer	ThP 630	Sertamo, Katriina	ThP 254	Shams-Ud-Doha, Km	ThP 099
Searcy, Louis	TP 044	Servage, Kelly A.	MOC pm 2:50	Shan, Baozhen	MP 434
Searle, Brian C.	MP 219	Servage, Kelly A.	WP 661	Shan, Baozhen	ThP 016
Searle, Brian C.	ThP 076	Serys-Kubertavicius, Martynas	ThP 645	Shan, Baozhen	ThP 017
Sebastian, Alan	MP 302	Sessler, Nicole	ThP 360	Shan, Guomin	WP 110
Sebastianelli, Chiara	ThP 595	Seth Chhabra, Ekta	ThP 134	Shan, Guomin	WP 120
Sebban, Muriel	TP 775	Sethi, Atul	MP 432	Shanaiah, Narasimhamurthy	ThP 655
Šebela, Marek	TP 490	Seto, Carmal	ThP 497	Shandilya, Devkant	TP 532
Sebree, Joshua	ThP 364	Seto, Yasuo	MP 525	Shane, Erica	WP 190
Sederoff, Ronald	MP 209	Seto, Yasuo	MP 526	Shang, Jackie X.	TP 632
Sedin, Dana	ThP 608	Settineri, Tina	ThOE pm 2:50	Shang, Sufen	ThP 103
Sedin, Dana	ThP 607	Seulen, Sarah	MP 326	Shanmugam, Avinash	WP 045
Seeberger, Peter H.	TP 160	Severinsen, Robert D.	ThP 285	Shao, Chun	ThP 771
Seegers, Susan	ThP 618	Seward, Robert J.	ThP 536	Shao, Chun	WP 007
Seeholzer, Steven H.	ThP 018	Seyer, Alexandre	MP 528	Shao, Chun	WP 008

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Shao, Wenguang.....	TP 226	Sheng, Quanhu.....	ThP 014	Shion, Henry.....	TP 156
Shao, Yuan.....	TP 068	Sheng, Quanhu.....	WP 044	Shion, Henry.....	TP 236
Shao, Yuan.....	TP 069	Shepard, Jason.....	MP 385	Shion, Henry.....	WP 274
Shapiro, Adam.....	MP 153	Shepard, Jason.....	ThP 413	Shiota, Teruhisa.....	MP 476
Shapiro, Charles L.....	MP 229	Shepard, Jason.....	ThP 415	Shiota, Teruhisa.....	MP 551
Shapiro, Michael.....	ThP 502	Shepson, Paul B.....	MP 554	Shiota, Teruhisa.....	ThP 633
Shariatgorji, Mohammadreza.....	MP 026	Sherman, David H.....	WP 335	Shiota, Teruhisa.....	TP 383
Shariatgorji, Mohammadreza.....	TP 012	Sherman, Nicholas.....	WP 460	Shiota, Teruhisa.....	TP 782
Shariatgorji, Mohammadreza.....	TP 013	Sherrod, Stacy D.....	TOB pm 2:50	Shipkova, Petia.....	ThOE am 08:30
Shariatgorji, Mohammadreza.....	TP 016	Sherwood, Robert.....	TP 203	Shipkova, Petia.....	WP 487
Shariatgorji, Mohammadreza.....	TP 047	Shestov, Alexander.....	WP 584	Shipps, Jr., Gerald W.....	MP 131
Sharma, Dhananjay.....	WP 531	Sheth, Sunil.....	MP 444	Shirey, Robert.....	WP 642
Sharma, Isha.....	MP 410	Shevchenko, Andrej.....	ThOG pm 3:30	Shirkhan, Hamid.....	WP 571
Sharma, Jyoti.....	MP 255	Shevchenko, Andrej.....	ThP 611	Shirodkar, Apurva.....	MP 233
Sharma, Kirti.....	WP 257	Shevchenko, Andrej.....	TP 298	Shisheva, Assia.....	TP 143
Sharma, Kumar.....	TOH am 09:10	Shevchenko, Anna.....	ThP 611	Shisheva, Assia.....	WP 241
Sharma, Kundan.....	ThP 458	Shevchenko, Ganna.....	WP 489	Shively, Carol A.....	WP 148
Sharma, Praveen Kumar.....	TP 274	Shevchenko, Valeriy.....	WP 207	Shively, Christian.....	WP 258
Sharma, Sandeep.....	WP 531	Sheynkman, Gloria.....	TP 077	Shockcor, John.....	TP 061
Sharma, Vagisha.....	MP 219	Sheynkman, Gloria M.....	MOG am 08:50	Shockcor, John.....	WP 022
Sharma, Vagisha.....	ThP 025	Sheynkman, Gloria M.....	ThP 221	Shoeib, Ahmed Sayed.....	MP 067
Sharon, Michal.....	WP 757	Shi, Fengjian.....	TP 407	Shofstahl, Jim.....	WP 029
Sharopov, Alex.....	ThP 564	Shi, Fengjian.....	WOB pm 3:30	Shomar, Basem.....	TP 563
Sharp, Joshua S.....	ThP 726	Shi, Honglan.....	TP 575	Shomo, Ronald.....	TP 767
Sharp, Joshua.....	MP 176	Shi, Honglan.....	WP 569	Shon, Hyun Kyong.....	TP 199
Sharp, Joshua S.....	MP 177	Shi, Lei.....	ThP 080	Short, Tim.....	MP 553
Sharp, Joshua S.....	ThP 723	Shi, Longkai.....	TP 474	Short, Tim.....	TP 712
Sharp, Joshua S.....	TP 320	Shi, Shengjing.....	ThP 649	Shortreed, Michael.....	TP 077
Shaughnessy, Conner.....	MP 424	Shi, Stone D.-H.....	ThP 246	Shortreed, Michael R.....	MOG am 08:50
Shaughnessy, Conner.....	TP 467	Shi, Tujin.....	WOG pm 2:50	Shortreed, Michael R.....	ThP 221
Shaul, Nellie J.....	TP 549	Shi, Tujin.....	WP 513	Shou, Wilson.....	MP 639
Shavkunov, Alexander.....	TP 072	Shi, Wuxian.....	TP 233	Shou, Wilson.....	ThP 666
Shavkunov, Alexander S.....	MP 427	Shi, Xiaodong.....	MP 329	Showalter, Hollis.....	ThP 454
Shaw, Jared B.....	MP 654	Shi, Xiaofeng.....	ThP 730	Showalter, Julie.....	ThP 668
Shaw, Jared B.....	TOE pm 2:50	Shi, Xiaojin.....	WP 629	Shpigun, Oleg.....	WP 423
Shaw, Patrick.....	TOG am 09:10	Shi, Yi.....	TP 132	Shpigun, Oleg.....	WP 713
Shaw, Patrick G.....	MP 255	Shi, Yifan.....	MP 514	Shrestha, Bindesh.....	ThOB am 09:10
Shaw, Tanya.....	WP 405	Shi, Yifan.....	WP 106	Shrestha, Bindesh.....	TP 378
She, Yi-Min.....	WOE pm 3:10	Shi, Yujun.....	TP 721	Shrestha, Bindesh.....	WOB pm 2:50
Shearer, Todd.....	ThP 539	Shiao, Tze Chieh.....	TP 204	Shteynberg, David D.....	ThP 031
Shedden, Kerby A.....	MP 446	Shiao, Tze Chieh.....	WOF am 08:50	Shu, Qin.....	WP 217
Sheehan, Terry.....	WP 566	Shida, Yasuo.....	MOA pm 3:10	Shu, Yue-Zhong.....	MP 643
Sheff, Joey.....	TP 536	Shiea, Christopher.....	TP 399	Shu, Yue-Zhong.....	WOF am 08:30
Shei, Paul.....	ThP 266	Shiea, Christopher.....	WP 346	Shuford, Christopher.....	MP 287
Shellie, Robert A.....	ThP 783	Shiea, Jentaie.....	MP 402	Shuford, Christopher.....	TOG pm 4:10
Shelton, David Shelton.....	WP 278	Shiea, Jentaie.....	MP 389	Shuford, Christopher.....	WP 134
Shen, Angela Qi.....	WP 484	Shiea, Jentaie.....	MP 384	Shuford, Christopher.....	WP 428
Shen, Helen.....	TP 634	Shiea, Jentaie.....	MP 382	Shuford, Christopher.....	WP 429
Shen, Helen.....	TP 616	Shiea, Jentaie.....	TP 382	Shuford, Christopher M.....	MP 532
Shen, Helen.....	TP 633	Shiea, Jentaie.....	WP 415	Shui, Wenqing.....	WP 736
Shen, Hong.....	WP 639	Shiea, Jentaie.....	WP 422	Shukla, Anil.....	WP 516
Shen, Hongwu.....	WP 543	Shieh, Michael.....	TP 681	Shukla, Anil.....	WP 745
Shen, Huibin.....	ThOG am 08:30	Shields, David.....	ThP 294	Shukla, Anil K.....	TP 324
Shen, Jenny.....	WP 546	Shields, Jefry.....	ThP 424	Shukla, Arun.....	ThP 133
Shen, Jiaqi.....	MP 662	Shields, Jefry.....	ThP 473	Shulaev, Vladimir.....	ThP 393
Shen, Jim.....	ThP 768	Shih, Hsi-Chang.....	MP 425	Shulaev, Vladimir.....	ThP 417
Shen, Jim.....	TP 501	Shih, Ie-Ming.....	ThP 295	Shulaev, Vladimir.....	TP 643
shen, jim.....	WP 188	Shih, Jean Chen.....	WP 246	Shulman, Nick.....	WOG pm 4:10
Shen, Jim.....	WP 543	Shih, Norrapat.....	WP 101	Shuman, Nicholas.....	MOD am 08:30
Shen, Li.....	WP 575	Shiki, Shigetomo.....	ThP 761	Shuttleworth, Steve.....	WP 508
Shen, Min.....	WP 225	Shilo, Konstantin.....	MP 442	Shvartsburg, Alexandre A.....	WP 767
Shen, Sean.....	MP 467	Shilov, Ignat.....	TP 085	Shyong, BaoJen.....	ThOE am 09:30
Shen, Sean.....	TP 471	Shilov, Ignat V.....	MOE pm 2:30	Shyong, BaoJen.....	ThP 546
Shen, Shichen.....	MP 224	Shima, Masahide.....	MP 005	Shyong, Bao-Jen.....	TOE am 08:50
Shen, Shichen.....	WP 015	Shima, Noriaki.....	ThP 592	Shyr, Yu.....	WP 044
Shen, Shichen.....	WP 232	Shimada, Haruo.....	MOA pm 3:10	Shyti, Reinald.....	MP 027
shen, xiaohang.....	TP 523	Shimada, Kenichi.....	ThP 512	Shyti, Reinald.....	TP 005
Shen, Xiaohang.....	TP 520	Shimbo, Kazutaka.....	WP 102	Sica, Vincent.....	WP 321
Shen, Xiaomeng.....	MP 224	Shimelis, Olga.....	MP 732	Sichilongo, Kwenga.....	WP 542
Shen, Xiaomeng.....	ThP 013	Shimelis, Olga.....	MP 773	Sickmann, Albert.....	MP 087
Shen, Xiaomeng.....	WP 232	Shimelis, Olga.....	MP 774	Sickmann, Albert.....	MP 452
Shen, Xingyu.....	MOA am 09:50	Shimizu, Hiroshi.....	WP 130	Sickmann, Albert.....	ThP 224
Shen, Yuanyuan.....	ThP 194	Shimizu, Takao.....	ThP 398	Sickmann, Albert.....	TP 105
Shen, Yufeng.....	TOA am 08:50	Shin, Hye-Seoung.....	MP 360	Siddhar, K Rangasamy.....	WP 328
Shen, Yufeng.....	WOE am 08:30	Shin, Hyun-Cheol Shin.....	ThOB pm 2:50	Sidhu, Rohini.....	WP 520
Sheng, Huaming.....	MOA am 09:50	Shin, Yong-Seoung.....	TP 441	Sidoli, Simone.....	MP 034
Sheng, Huaming.....	MP 577	Shinholt, Deven.....	MP 698	Sidoli, Simone.....	TP 144
Sheng, Huaming.....	TP 358	Shin-ichi, Kawano.....	WP 629	Sidoli, Simone.....	WOG am 08:30
Sheng, Huaming.....	TP 360	Shion, Henry.....	TP 061	Siegel, David.....	TOA am 10:10

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Siegel, Donald.....	WP 303	Singh, Rajesh.....	ThP 235	Smargiasso, Nicolas.....	ThP 256
Siegel, Marshall M.....	MP 622	Singh, Ravinder.....	WP 726	Smargiasso, Nicolas.....	TP 176
Siegel, Marshall M.....	WP 052	Singh, Sasha.....	WP 018	Smart, Brian.....	MP 716
Siegel, Marshall M.....	WP 732	Singh, Sasha A.....	WP 070	Smeal, Tod.....	TP 028
Siegel, Paul D.....	ThP 309	Singh, Sheo.....	WP 320	Smeekens, Johanna.....	ThP 230
Siehnell, Richard.....	WOH pm 2:50	Singh, Shivendra.....	TP 615	Smeekens, Johanna.....	TP 191
Siek, Kevin.....	MP 660	Singhania, Akul.....	ThP 439	Smelkinson, Margery.....	TOG am 09:30
Siek, Kevin.....	WOA pm 3:10	Sinisalo, Juha.....	TP 443	Smilowitz, Jennifer.....	WOE am 08:50
Siems, Bill.....	TOC am 09:10	Sinnis, Photini.....	ThP 278	Smilowitz, Jennifer T.....	MP 071
Siems, Bill.....	WP 693	Sinotte, Marc.....	WP 564	Smirnova, Lena.....	WP 581
Siems, William.....	TP 432	Sinz, Andrea.....	ThOF am 08:30	Smit, Marjon A.....	MP 263
Siems, William.....	WP 673	Sipe, David.....	TP 133	Smit, Vincent.....	MP 004
Siems, William.....	WP 774	Siple, Joseph.....	MP 781	Smith, Archer.....	TP 234
Siems, William F.....	ThP 480	Sirdeshmukh, Ravi.....	MP 255	Smith, Archer D.....	ThP 144
Siems, William F.....	WP 692	Sisco, Edward.....	ThP 601	Smith, Cornelia.....	TP 634
Sierra, Cesar.....	TP 416	Sisco, Edward.....	WP 302	Smith, Cornelia.....	TP 633
Sierra-Ávila, César A.....	TP 588	Sisco, Edward.....	WP 291	Smith, Cornelia.....	TP 616
Sighart, Stefanie.....	ThP 019	Sitek, Barbara.....	MP 431	Smith, Derek.....	ThP 026
Sigurdson, Wendy.....	TP 448	Sitek, Barbara.....	TP 481	Smith, Derek.....	TP 255
Sigurðsson, Baldur Bragi.....	MP 578	Sitnikov, Dmitri.....	MP 633	Smith, Desmond.....	WP 516
Sikorski, Patricia.....	ThP 283	Sivagnanam, Kumaran.....	MP 102	Smith, Donald.....	WOC am 09:50
Silberring, Jerzy.....	MP 620	Sivaraman, Lakshmi.....	MP 366	Smith, Donald F.....	TP 597
Silcock, Paul.....	ThP 571	Sivaraman, lakshmi.....	WP 543	Smith, Dr. Conor.....	MP 777
Silcock, Paul.....	WP 359	Siwick, Deborah A.....	MP 120	Smith, Geoffrey T.....	ThP 147
Silivra, Oleg.....	ThP 750	Siwik, Deborah A.....	MP 465	Smith, Glenn.....	ThP 675
Silivra, Oleg.....	TP 755	Sizykh, Vadim.....	WP 689	Smith, Jacquelyn.....	WP 273
Sillevis Smitt, P.A.E.....	TP 444	Sjöberg, Per J R.....	ThP 558	Smith, James.....	ThP 681
Silva, Elisângela.....	MP 464	Sjoelund, Virginia.....	MP 261	Smith, Jennifer.....	TP 072
Silva, Jeffrey C.....	MP 122	Sjoelund, Virginia.....	MP 269	Smith, Jeremy P.....	MP 480
Silva, Jeffrey C.....	ThP 073	Sjoelund, Virginia.....	ThP 074	Smith, Josie M.....	ThP 605
Silva, Jeffrey C.....	TP 109	Sjoelund, Virginia.....	TOG am 09:30	Smith, Julia.....	ThP 701
Silva, Jeffrey C.....	TP 117	Sjoelund, Virginia.....	WP 256	Smith, Kate.....	ThP 777
Silva, Manori.....	WP 461	Skaar, Eric P.....	TP 073	Smith, Lloyd.....	TP 077
Silva Salgueiro, Jessica.....	WP 434	Skaltsounis, Alexios Leandros.....	WP 600	Smith, Lloyd.....	WP 239
Silva-Sanchez, Cecilia.....	WP 062	Skende, Estela.....	WP 537	Smith, Lloyd M.....	MOG am 08:50
Silveira, Joshua.....	WP 663	Skerritt, Jen.....	MP 738	Smith, Lloyd M.....	ThP 221
Silveira, Joshua.....	WP 664	Skerritt, Jen.....	TP 769	Smith, Martin B.....	MP 522
Silveira, Joshua.....	WP 686	Skerritt, Jen.....	TP 768	Smith, Nadia.....	MP 490
Silveira, Joshua.....	WP 690	Skiba, Nikolai.....	TP 147	Smith, Philip.....	ThOA am 10:10
Silveira, Joshua A.....	MOC pm 2:50	Skilton, St John.....	WP 270	Smith, Richard.....	MOC pm 3:10
Silveira, Joshua A.....	WP 661	Skinner, Owen.....	ThP 088	Smith, Richard.....	MP 421
Sim, Jeffrey.....	ThP 764	Skinner, Owen.....	WOH pm 3:30	Smith, Richard.....	WOE am 08:30
Sim, Kae Hwan.....	ThP 038	Skinner, Owen S.....	WP 157	Smith, Richard.....	WOG pm 2:50
Simell, Olli.....	WP 028	Skipp, Paul.....	ThP 060	Smith, Richard.....	WP 322
Simell, Tuula.....	WP 028	Skipp, Paul.....	ThP 249	Smith, Richard D.....	MOG pm 3:30
Simeone, Diane M.....	MP 446	Skipp, Paul.....	WP 468	Smith, Richard D.....	MP 100
Smithy, Johayra.....	WP 324	Skipp, Paul J.....	ThP 439	Smith, Richard D.....	MP 569
Simmons, Doug.....	MP 721	Sklorz, Martin.....	WP 715	Smith, Richard D.....	MP 677
Simmons, Jane Ellen.....	WP 562	Sklorz, Martin.....	WP 733	Smith, Richard D.....	ThOB am 10:10
Simmons, Larry P.....	ThP 306	Skoblin, Michael.....	ThP 751	Smith, Richard D.....	ThOG pm 4:10
Simolin, Helena.....	TP 443	Skold, Karl.....	MP 426	Smith, Richard D.....	ThP 741
Simon, John.....	MP 738	Sköld, Olof.....	WP 012	Smith, Richard D.....	TOB am 09:50
Simon, John.....	TP 768	Skopec, Mary.....	TP 552	Smith, Richard D.....	TOB pm 4:10
Simon, Kathryn.....	TP 249	Skouta, Rachid.....	ThP 512	Smith, Richard D.....	TOC am 08:30
Simon, Romain.....	TP 484	Škrášková, Karolina.....	TP 015	Smith, Richard D.....	TP 083
Simon, Romain.....	WOG pm 3:10	Skubitz, Amy.....	TP 428	Smith, Richard D.....	TP 169
Simon, Stéphanie.....	MP 527	Slade, Dea.....	TP 096	Smith, Richard D.....	TP 324
Simonian, Margaret.....	TP 461	Slade, Peter.....	WP 198	Smith, Richard D.....	TP 715
Simonis, Frank.....	MP 477	Slade, William.....	MP 114	Smith, Richard D.....	TP 716
Simón-Manso, Yamil.....	MP 604	Slagel, Joseph.....	ThP 031	Smith, Richard D.....	TP 714
Simons, Brigitte.....	ThP 287	Slamnoi, Stefan.....	ThP 746	Smith, Richard D.....	TP 717
Simons, Brigitte.....	WP 271	Slater, Peter.....	TP 589	Smith, Richard D.....	WP 513
Simons, Brigitte.....	WP 602	Slavov, Svetoslav.....	MP 267	Smith, Richard D.....	WP 516
Simons, Kai.....	TP 298	Sleczka, Bogdan.....	TP 693	Smith, Richard D.....	WP 698
Simonyi, Agnes.....	ThP 302	Sleno, Lekha.....	TP 204	Smith, Richard D.....	WP 745
Simpson, David.....	MP 091	Sleno, Lekha.....	TP 631	Smith, Richard D.....	WP 767
Simpson, John T.....	MP 469	Sleno, Lekha.....	TP 657	Smith, Rob.....	ThP 030
Sims, Paul F. G.....	MP 272	Sleno, Lekha.....	WOF am 08:50	Smith, Rob.....	ThP 029
Sinatra, Francy.....	WP 769	Sliva, Jeffrey.....	TP 457	Smith, Rob.....	WP 036
Sindona, Giovanni.....	MP 014	Sloan, Angela.....	TP 213	Smith, Robert.....	ThOC am 09:10
Sindona, Giovanni.....	TP 511	Slovin, Janet P.....	MP 611	Smith, Robert.....	WP 760
Sindt, Nathan.....	MP 558	Slysz, Gordon.....	WOF am 08:30	Smith, Whitney.....	TP 665
Singer, Thomas.....	TP 171	Slysz, Gordon W.....	TP 169	Smithgall, Thomas.....	WP 220
Singewald, Nicolas.....	ThP 242	Slysz, Gordon W.....	TP 324	Smithgall, Thomas E.....	ThP 132
Singh, Daljeet.....	WP 117	Smallegan, Michael.....	MP 121	Smolenski, Ryszard.....	ThP 445
Singh, Karam.....	MP 419	Smárason, Sigurður V.....	MP 578	Smoluch, Marek.....	MP 620
Singh, Pradeep.....	WOH pm 2:50	Smarcaro Cunha, Valnei.....	MP 570	Smotrov, Nadya.....	TOF pm 3:30
Singh, Pradeep K.....	ThP 464	Smargiasso, Nicolas.....	MP 441	Snedecor, June.....	MP 043
Singh, Pragya.....	TP 175			Sneekes-Vriese, Eveline.....	ThP 119

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Snider, Elise.....	ThP 435	Song, Yuling .....	WP 629	Sprung, Robert.....	ThOE am 08:50
Snider, Jacqueline .....	TP 173	Song, Yu-Qiao .....	WP 413	Squina, Fabio .....	MP 562
Snider, Jacqueline .....	WOG pm 3:50	Sonnenburg, Justin S.....	ThP 334	Sreedasyam, Avinash.....	TP 680
Snijder, Joost.....	TP 136	Sonnett, Matthew.....	TP 180	Sreekumar, Arun.....	ThP 658
Snovida, Sergei.....	ThOH am 09:50	Sonomura, Kazuhiro.....	MP 755	Sreenivasamurthy, Sreelakshmi.....	MP 255
Snovida, Sergei.....	ThOH am 09:10	Soon-U Lee, Lawrence.....	WP 449	Sreenivasamurthy, Sreelakshmi.....	MP 270
Snovida, Sergei.....	ThP 211	Soper, Molly.....	ThP 488	Srinivasan, Saipraveen.....	ThP 136
Snovida, Sergei.....	ThP 722	Sorensen, Dylan J.....	WP 118	Sripathi Prakash, Harischandra.....	TP 647
Snovida, Sergei.....	TP 326	Soriano, Brian D.....	ThP 246	SriRamaratnam, Rohitha.....	ThP 512
Snovida, Sergei.....	WP 121	Sosnoff, Connie.....	TP 476	Srivastava, Praveen.....	WP 646
Snow, Gregory.....	WP 638	Sosnoff, Connie.....	WOC pm 3:50	Srivastava, Sanjeeva.....	WP 235
Snow, Nicholas.....	WP 720	Sottas, Pierre-Edouard.....	TOG pm 2:50	Srivastava, Shiv.....	WP 513
Snyder, A. Peter.....	ThP 077	Soufi, Boumediene.....	MP 215	Srivastava, Sudhir.....	WP 513
Snyder, A. Peter.....	ThP 333	Soufi, Boumediene.....	WP 242	Srzentic, Kristina.....	MOE am 08:50
Snyder, Lawrence.....	MP 643	Soulby, Andrew.....	WP 729	Srzentić, Kristina.....	WP 172
Snyder, Melissa.....	ThP 345	Sousa, Ilza M. O.....	WP 711	St. John - Williams, Lisa.....	TP 470
Snyder, Nathaniel.....	WP 499	Sousa, Mirta M. L.....	TP 175	Staals, Raymond.....	ThP 458
Snyder, Nathaniel W.....	TP 310	Sousou, Nigel.....	MP 666	Stacey, Catherine.....	ThP 612
Snyder, Nathaniel W.....	WOH am 08:50	Sousou, Nigel.....	TP 277	Stacey, Gary.....	WOC pm 4:10
Snyder, Shane A.....	WP 340	Southard, Adrian.....	TP 711	Stachl, Christiane N.....	MOC pm 3:30
Soares, Fernando.....	MP 464	Southworth, Daniel.....	ThP 454	Stachl, Christiane N.....	WP 669
Sobott, F.....	WP 229	Souza, Sandra.....	TP 460	Stacy, Tina.....	MP 691
Sobott, Frank.....	ThP 191	Souza, Wanderley.....	ThOA am 09:30	Stacy, Tina.....	TP 738
Sobott, Frank.....	TOC pm 3:50	Sovocool, Wayne.....	WP 579	Stadlmann, Johannes.....	TP 096
Sobott, Frank.....	WP 031	Sowa, Mathew.....	TP 145	Staes, An.....	WP 129
Sobsey, Constance.....	WP 471	Sowole, Modupeola.....	ThP 124	Stafford, George.....	MOC pm 3:10
Sobus, Jon.....	TP 476	Soya, Naoto.....	WP 230	Stafford, George.....	MP 716
Soderblom, Erik J.....	WOG pm 3:30	Spahr, Christopher S.....	ThP 246	Stafford, George.....	ThP 472
Soderblom, Erik J.....	TP 457	Spangler, Glenn E.....	ThP 479	Stafford, George.....	ThP 483
Soderblom, Erik J.....	TP 470	Sparbier, Katrin.....	TP 212	Stafford, George.....	WP 681
Söderquist, Marcus.....	MP 426	Sparling, Richard.....	TP 183	Stafford, George C.....	ThP 482
Söderquist, Marcus.....	MP 786	Spaulding, Susan.....	TP 660	Stafford, George C.....	ThP 484
Sodeyama, Manabu.....	MP 525	Spector, Neil.....	TP 457	Stahl-Zeng, Jianru.....	MP 344
Soellner, Matthew.....	ThP 490	Spector, Neil.....	TP 470	Stahl-Zeng, Jianru.....	TP 565
Soilis, Nicolaos.....	WP 525	Spector, Tim D.....	ThP 257	Stampella, Alessandra.....	ThP 594
Sojo, Luis.....	MP 311	Speer, Jennifer.....	WP 309	Stangl, Chris.....	ThP 367
Sokolowska, Izabela.....	MP 106	Speir, J. Paul.....	MP 140	Stanley, Bruce.....	MP 517
Sokolowska, Izabela.....	MP 162	Speller, Abigail.....	MOH pm 3:10	Stanley, Scott.....	TP 628
Sokolowska, Izabela.....	WP 457	Speller, Abigail.....	TOG pm 3:30	Stapels, Martha.....	WP 506
Sokolowski, Bernd.....	TP 140	Speller, Abigail.....	TP 375	Staples, Gregory.....	WP 066
Solano, Maria.....	TP 155	Speller, Abigail V. M.....	WP 020	Staples, Gregory.....	WP 205
Solari, Fiorella.....	TP 105	Spellman, Daniel.....	WP 184	Stapleton, Donald S.....	WOD am 10:10
Solis, Nestor.....	TP 131	Spence, Dana M.....	WP 632	Stapleton, Heather.....	ThP 570
Sollenberg, Ulla.....	MP 426	Spencer, David.....	WP 194	Star, Alexander.....	WP 706
Solliec, Morgan.....	TP 574	Spencer, Jean.....	ThP 057	Stark, Ann-Katherine Stark.....	WP 757
Solliec, Morgan.....	WP 564	Spencer, Jean L.....	MP 120	Stark, Harald.....	TOA pm 3:10
Solouki, Touradj.....	MP 047	Spencer, Jean L.....	MP 465	Stark, James.....	ThOA pm 3:30
Solouki, Touradj.....	MP 296	Spencer, Jean L.....	TP 095	Starodubtceva, Natalia.....	TP 409
Solouki, Touradj.....	ThP 514	Spencer, Sandra.....	MP 327	Starodubtceva, NL.....	TP 449
Solouki, Touradj.....	TP 347	Spencer, Sandra.....	TP 349	Starodubtseva, Natalia.....	TOA pm 4:10
Solouki, Touradj.....	WP 657	Spengler, Bernhard.....	TOH pm 2:30	Stashenko, Elena.....	TP 679
Solouki, Touradj.....	WP 658	Spengler, Bernhard.....	TP 020	Stauber, Jonathan.....	MP 025
Som, Anirban.....	TP 398	Spengler, Bernhard.....	TP 071	Stauber, Jonathan.....	TOH am 09:10
Soma, Lawrence.....	ThP 593	Spengler, Bernhard.....	WP 300	Stauber, Jonathan.....	TP 009
Somani, Sandeep.....	WP 717	Sperling, Michael.....	MP 007	Stauber, Jonathan.....	TP 034
Somerville, Stephen.....	ThP 377	Sperling, Michael.....	MP 667	Stauber, Jonathan.....	TP 050
Son, Jin Gyeong.....	TP 199	Sperling, Michael.....	MP 709	Stauber, Jonathan.....	TP 249
Song, Benben.....	WP 465	Sperling, Michael.....	TP 031	Staunton, Lisa.....	WP 475
Song, Botao.....	MP 307	Sperling, Michael.....	TP 032	Stavrianidi, Andrey.....	WP 423
Song, Ehwang.....	TP 107	Sperling, Michael.....	WP 442	Stavrianidi, Andrey.....	WP 713
Song, Haowei.....	ThP 199	Sperry, Sam.....	ThOC am 09:10	Staykova, Doroteya.....	WP 468
Song, Jaewoo.....	ThP 554	Sperry, Sam.....	WP 620	Staymates, Matthew.....	WP 380
Song, Jing.....	TP 118	Spetman, Brian D.....	ThOF pm 3:10	Stead, Sara.....	MP 338
Song, Junghan.....	ThP 591	Spetman, Brian D.....	TOE pm 4:10	Stecker, Kelly.....	MP 406
Song, Liguó.....	TP 743	Spicer, Vic.....	TP 183	Stedwell, Corey.....	ThP 227
Song, Liguó.....	WP 377	Splendore, Maurizio.....	MP 720	Stedwell, Corey.....	TP 363
Song, Lihui.....	WOC pm 4:10	Splendore, Maurizio.....	ThP 266	Steen, Hanno.....	MP 457
Song, Peiming.....	WP 752	Splendore, Maurizio.....	TP 178	Steen, Hanno.....	MP 680
Song, Qingyu.....	ThP 753	Spooner, Neil.....	WP 640	Steen, Hanno.....	MP 747
Song, Seounghee.....	MP 537	Spraggins, Jeffrey.....	MOB am 09:50	Steen, Hanno.....	ThOE pm 4:10
Song, Ting.....	TP 119	Spraggins, Jeffrey.....	MOH pm 2:30	Steen, Hanno.....	ThP 279
Song, Ting.....	TP 259	Spraggins, Jeffrey.....	MP 023	Steen, Hanno.....	TP 187
Song, Ting.....	TP 333	Spraggins, Jeffrey.....	TP 039	Steen, Judith.....	MP 457
Song, Wei.....	TP 028	Spraggins, Jeffrey.....	TP 042	Steenwyk, Rick.....	MOC pm 4:10
Song, Xiaoling.....	ThP 274	Spraggins, Jeffrey.....	TP 070	Steenwyk, Rick.....	ThP 677
Song, Xiaomin.....	TP 327	Spraggins, Jeffrey.....	TP 073	Steere, Allen C.....	WOF pm 2:30
Song, Yang.....	WOD pm 3:50	Spraggins, Jeffrey M.....	MP 015	Stein, Stephen.....	MP 048
Song, Yue.....	ThP 528	Springer, Michael.....	MP 680	Stein, Stephen.....	MP 051
Song, Yue.....	WP 356	Spruce, Lynn.....	ThP 018	Stein, Stephen.....	ThOG am 10:10

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Stein, Stephen.....	WP 051	Strickland, Erin C.....	MP 480	Sugiyama, Naoki.....	ThP 667
Stein, Stephen.....	WP 119	Strickland, Erin C.....	MP 479	Suh, Jeffrey.....	MP 250
Stein, Stephen E.....	MP 604	Strickland, Erin C.....	ThP 359	Suh, Joo Woon.....	ThP 628
Steinberger, Birgit.....	MP 135	Strittmatter, Nicole.....	MOH pm 3:10	Suh, Joon Hyuk.....	TP 509
Steiner, Douglas.....	MP 167	Strittmatter, Nicole.....	ThP 379	Suh, Jung-Keun.....	WP 206
Steinhorst, Klaus.....	MP 021	Strittmatter, Nicole.....	TOG pm 3:30	Suh, Moo-Jin.....	ThP 284
Steiniger, David.....	ThP 571	Strittmatter, Nicole.....	TP 215	Suh, Moo-Jin.....	ThP 283
Steininger, Harald.....	TOA pm 2:30	Strittmatter, Nicole.....	TP 375	Suh, Sunglll.....	ThP 591
Steinkamp, F. Lucas.....	WP 401	Strizki, Julie M.....	MP 131	Suhitha, S.....	WP 328
Steinmetz, Vincent.....	TP 372	Stroble, Carol.....	ThP 155	Suita, Hiroshi.....	MP 067
Stellacci, Francesco.....	ThP 495	Stroh, Fred.....	TP 736	Sukhishvili, Svetlana A.....	WP 552
Stelter, Andreas.....	ThP 573	Stroh, Justin.....	ThP 502	Sukumar, Saraswati.....	MP 440
Steltgens, Sascha.....	TP 141	Stroh, Justin.....	TP 028	Sulc, Miroslav.....	ThP 354
Stemmler, Elizabeth A.....	MP 568	Strop, Pavel.....	WP 278	Suleiman, Shadeah L.....	ThOE pm 4:10
Stemmler, Elizabeth A.....	ThP 150	Strouse, Robert.....	TP 243	Sullivan, Leslie.....	ThP 583
Stenken, Julie A.....	ThP 346	Strupat, Kerstin.....	TP 035	Sullivan, Leslie.....	WP 408
Stennicke, Vibeke.....	ThP 103	Struwe, Weston.....	ThP 712	Sullivan, Sarah.....	ThP 665
Stenzel-Poore, Mary.....	MOH pm 3:30	Stuani, Lucille.....	MP 617	Sulman, Erik.....	ThP 041
Stephan, Müller.....	TP 742	Stuart, Scott.....	ThP 193	Sulman, Erik Philip.....	MP 427
Stephens, Daren.....	WP 480	Stuchlova Horynova, Milada.....	WP 073	Sulyok, Michael.....	MP 344
Stephenson, Tesia N.....	ThP 084	Studnicka, Michael.....	WP 153	Sulzer, Philipp.....	MP 663
Stephenson, William.....	MOC am 08:30	Stuff, John.....	MP 772	Sulzer, Philipp.....	ThP 738
Sterling, Harry.....	ThP 102	Stühler, Kai.....	WP 248	Sumerlin, Brent S.....	TP 786
Steuer, Andrea E.....	ThOE pm 3:10	Stulik, Jiri.....	ThP 201	Summers, Ryan.....	MOA am 08:50
Steven, Rory T.....	MP 001	Stumbaum, Mihaela.....	ThP 746	Sumner, Lloyd.....	ThP 636
Stevens, Douglas.....	TP 392	Sturgeon, Susan R.....	MP 423	Sumner, Lloyd.....	WP 720
Stevens, Douglas.....	WOC pm 2:30	Sturm, Robert.....	WP 644	Sumner, Lloyd W.....	MP 614
Stevens, Douglas.....	WP 348	Sturtevant, Drew.....	ThP 393	Sumner, Lloyd W.....	MP 607
Stevens, Jan F.....	MP 598	Sturtevant, Drew.....	TOH pm 4:10	Sumner, Lloyd W.....	ThP 640
Stevens, Jan F.....	ThP 643	Sturtevant, Drew.....	TP 037	Sumner, Lloyd W.....	WP 589
Stevens, Susan.....	MOH pm 3:30	Stutts, Whitney L.....	MP 354	Sun, Difei.....	TP 648
Steward, Sandy.....	TP 662	Stutzman, John.....	MP 248	Sun, Frank.....	ThP 405
Stewart, Alastair G.....	ThP 501	Styles, Iain B.....	MP 028	Sun, Grace Y.....	ThP 302
Stewart, Tyler.....	WP 073	Styles, Iain B.....	MP 253	Sun, Haidan.....	WP 016
Steyaert, Sandra.....	TP 078	Styles, Iain B.....	TP 232	Sun, Hao.....	TP 625
St-Germain, Jonathan R.....	WP 181	Su, Bin.....	MP 508	Sun, Helen.....	MP 512
Stickle, Dawn.....	TP 427	Su, Dian.....	MP 100	Sun, Helen (Qingyu).....	MP 363
Stickle, Dawn.....	WP 327	Su, Dian.....	WP 277	Sun, Helen Qingyu.....	TP 278
Stiles, Charles D.....	TP 007	Su, Hung.....	MP 384	Sun, Huadong.....	ThP 441
Stiles, Charles D.....	TP 055	Su, Hung.....	WP 422	Sun, Jianghao.....	WP 338
Stinson, Craig.....	ThOD am 08:50	Su, Lijuan.....	TP 553	Sun, Jianghao.....	WP 337
Stinson, Craig.....	TP 290	Su, Wan-Chih.....	ThP 714	Sun, Jinchun.....	MP 267
Stirm, Brian.....	MP 554	Su, Wan-Chih.....	ThP 713	Sun, Jing.....	MP 269
Stites, Ryan.....	TP 543	Su, Xiaomeng.....	ThOH am 08:30	Sun, Jin-Lan.....	WP 356
Stites, Wesley.....	ThP 127	Su, Xiaoyang.....	MP 118	Sun, Li.....	WP 108
Stock, Daniela.....	ThP 501	Su, Xuan.....	TP 283	Sun, Liangliang.....	MP 080
Stock, Naomi.....	TP 673	Su, Yijin.....	MP 329	Sun, Liangliang.....	ThP 198
Stockmann, Henning.....	MOE pm 4:10	Su, Yuan.....	ThOG pm 3:50	Sun, Liangliang.....	ThP 731
Stocks, Bradley.....	TOF am 09:10	Su, Yuan.....	WP 388	Sun, Liangliang.....	TOB pm 3:50
Stockwell, Brent R.....	ThP 512	Su, Zhiduan.....	WP 044	Sun, Liangliang.....	TP 194
Stoermer, Carsten.....	MP 148	Subbannayya, Tejaswini.....	MP 255	Sun, Lulu.....	ThP 574
Stojko, Johann.....	WP 265	Subbannayya, Yashwanth.....	MP 255	Sun, Michael Xin.....	WP 086
Stokes, Matthew P.....	TP 109	Subbannayya, Yashwanth.....	ThP 208	Sun, Qian.....	TP 281
Stolee, Jessica.....	MP 439	Subbotin, Roman.....	TOC pm 4:10	Sun, Qian.....	TP 757
Stoll, Maria S.K.....	WP 595	Subhedar, Nivedita.....	TP 763	Sun, Qian.....	WP 393
Stolowitz, Mark.....	MP 019	Subramanian, Aravind.....	WOG pm 2:30	Sun, Qian.....	WP 629
Stoop, Marcel.....	ThP 209	Subramanian, Kanagaraj.....	WP 247	Sun, Qian.....	WP 739
Stopka, Sylwia.....	TP 408	Subramanian, Mani.....	MOA am 08:50	Sun, Rachel.....	MP 510
Stopka, Sylwia.....	WOB pm 2:50	Subramanian, Murali.....	ThP 673	Sun, Rui-Xiang.....	ThP 051
Stout, Steven.....	ThOE am 09:10	Subramaniyan, Saravanan.....	TP 528	Sun, Rui-Xiang.....	WP 054
Stover, Eric.....	MP 742	Subramaniyan, Saravanan.....	TP 529	Sun, Rui-Xiang.....	WP 053
Stover, Michele L.....	MP 319	Subramaniyan, Saravanan.....	WP 539	Sun, Shisheng.....	ThP 040
Stow, Sarah M.....	ThP 484	Such-Sanmartin, Gerard.....	MP 034	Sun, Shisheng.....	WOF pm 4:10
Stow, Sarah M.....	TOC am 09:50	Such-Sanmartin, Gerard.....	ThP 258	Sun, Su.....	ThP 123
Stowers, Sarah.....	TP 503	Suckau, Detlef.....	TP 160	Sun, Wenjian.....	MP 662
Stranzl, Thomas.....	TP 075	Suckau, Detlev.....	MOE pm 3:30	Sun, Wenjian.....	ThP 574
Stratton, Tim.....	MP 472	Suckau, Detlev.....	TP 008	Sun, Wenjian.....	TP 396
Stratton, Tim.....	MP 641	Suckau, Detlev.....	TP 057	Sun, Wenjian.....	WP 393
Stratton, Tim.....	ThP 639	Suckau, Detlev.....	TP 051	Sun, Xin.....	TP 168
Stratton, Tim.....	TP 530	Suckau, Detlev.....	TP 056	Sun, Xue-Long.....	ThP 720
Stratton, Tim.....	TP 526	Suckau, Detlev.....	WP 517	Sun, Yanchun.....	WP 731
Stratton, Tim.....	WP 603	Suckau, Detlev.....	WP 518	Sun, Yaping.....	TP 336
Stratton, Tim.....	WP 650	Suder, Piotr.....	MP 620	Sun, Yulin.....	WP 152
Stratton, Tim.....	WP 728	Suematsu, Makoto.....	ThP 111	Sun, Zhe.....	MP 535
Straus, Rita.....	TP 343	Suematsu, Makoto.....	TP 017	Sun, Zhe.....	ThP 587
Strauss, Ethan.....	MP 188	Suflita, Joseph M.....	TP 665	Sundström, Mira.....	MP 289
Strauss, Ethan.....	ThP 778	Suflita, Joseph M.....	TP 666	Sunner, Jan.....	ThP 010
Strauss, Megan.....	MP 413	Suga, Masao.....	MP 661	Sunner, Jan.....	TP 665
Streibel, Thorsten.....	MOD pm 2:50	Sugiyama, Masuyuki.....	TP 744	Sunner, Jan.....	TP 666

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Suoniemi, Matti.....	TP 443	Sze, Siu Kwan.....	ThP 038	Tan, Minjia.....	TP 112
Sura, Srinivas.....	TP 554	Sze, Siu Kwan.....	ThP 157	Tan, Minjia.....	TP 106
Surampalli, Rao Y.....	TP 556	Sze, Siu Kwan.....	TP 097	Tan, Peng.....	WP 653
Surratt, Gordon.....	WP 548	Szewc, Mark.....	MP 195	Tan, Shyh-Han.....	WP 513
Surratt, Jason.....	TOA pm 3:10	Szewczuk, Larry.....	TOF pm 4:10	Tan, Suejane.....	TP 373
Susan, Fanayan.....	WP 079	Szidat, Soenke.....	WP 756	Tan, Suejane.....	TP 404
Sussman, Michael.....	MP 406	Szopa, Cyril.....	ThP 369	Tan, Suejane.....	TP 405
Sussman, Michael.....	ThOG pm 3:10	Szpyt, John.....	TP 145	Tan, Xiaoli.....	TP 588
Sussman, Michael.....	TP 669	Tabet, Jean-Claude.....	MP 581	Tan, Xiaoli.....	TP 589
Suttle, Blake.....	TP 660	Tabet, Jean-Claude.....	MP 587	Tan, Yanglan.....	ThP 717
Sutton, Chris.....	WP 491	Tabet, Jean-Claude.....	MP 617	Tan, Zhijing.....	MP 446
Sutton, Jennifer.....	WP 196	Tabet, Jean-Claude.....	ThP 513	Tan, Zhijing.....	TP 421
Sutton, Jennifer.....	WP 197	Tabet, Jean-Claude.....	ThP 696	Tan, Zhijing.....	WP 458
Suzuki, Koichi.....	ThP 592	Tabet, Jean-Claude.....	TP 524	Tan, Zhijing.....	WP 500
Suzuki, Nobuhiro.....	ThP 417	Tabet, Jean-Claude.....	TP 577	Tanaka, Kaori.....	ThP 397
Suzuki, Nobuhiro.....	TP 643	Tabisz, Stephanie.....	TP 067	Tanaka, Kazuki.....	TP 744
Svan, Alfred.....	TP 566	Tachikawa, Hiroshi.....	MP 740	Tanaka, Kazuo.....	ThP 721
Svane, Simon.....	TP 355	Tacio Teixeira, Gleber.....	TP 586	Tanaka, Kenichiro.....	MP 739
Svatoš, Aleš.....	MP 030	Tackett, Phil.....	MOA am 10:10	Tanaka, Kenichiro.....	WP 182
Svenningsson, Per.....	TP 013	Tadano, Jun.....	TP 027	Tanaka, Koichi.....	MP 130
Svenningsson, Per.....	TP 016	Tadesse, Mahlet.....	MP 580	Tanaka, Koichi.....	TP 166
Svenningsson, Per.....	TP 047	Tadesse, Mahlet.....	TP 756	Tanaka, Nobuo.....	TOB pm 3:30
Svenson, Karen L.....	MOG pm 2:30	Tadjimukhamedov, Fatkhulla K.....	MP 469	Tandon, Kawaljit.....	ThOA pm 3:50
Svinkina, Tanya.....	ThP 205	Tagett, Rebecca Tagett.....	TP 488	Tang, Donald.....	ThP 567
Svinkina, Tanya.....	WOG am 08:50	Taguchi, Kaori.....	ThP 378	Tang, Gang.....	MP 765
Svitel, George.....	MP 184	Taguchi, Vince.....	WP 579	Tang, Haixu.....	ThP 165
Svoboda, Michal.....	WP 293	Taguchi, Vince Y.....	WP 575	Tang, Haixu.....	WP 038
Svobodova, Helena.....	MP 710	Tai, Akihiro.....	MP 613	Tang, Haixu.....	WP 064
Svobodova, Helena.....	MP 747	Tai, Susan.....	WP 453	Tang, Hui.....	MP 231
Svobodova, Helena.....	ThP 445	Taipov, Marat.....	WP 207	Tang, Hui.....	ThOF pm 4:10
Svobodova, Helena.....	WP 754	Takabayashi, Yu.....	MP 551	Tang, Jason X.....	MP 213
Swales, John.....	TOH am 08:30	Takach, Edward.....	TP 024	Tang, Jason X.....	TOG am 10:10
Swaney, Danielle.....	ThP 236	Takagi, Yuta.....	MP 476	Tang, Kai.....	ThP 126
Swanson, Raymond.....	MP 444	Takahashi, Atsuko.....	ThP 621	Tang, Kai.....	WP 390
Swearingen, Kristian E.....	WP 766	Takahashi, Katsutoshi.....	MP 062	Tang, Keqi.....	MP 677
Sweedler, Jonathan.....	TOA am 09:10	Takahashi, Katsutoshi.....	TP 021	Tang, Keqi.....	ThOB am 10:10
Sweedler, Jonathan.....	TP 001	Takahashi, Kazuo.....	WP 073	Tang, Keqi.....	ThOG pm 4:10
Sweedler, Jonathan.....	TP 165	Takahashi, Masakazu.....	MP 766	Tang, Keqi.....	TOB pm 4:10
Sweedler, Jonathan V.....	TP 640	Takahashi, Nobuhiro.....	WP 372	Tang, Keqi.....	TP 324
Sweeney, Colin.....	ThP 313	Takahashi, Ryan.....	ThP 357	Tang, Keqi.....	TP 715
Sweet, Robert A.....	ThP 042	Takahashi, Ryo.....	MP 105	Tang, Keqi.....	TP 714
Swenberg, James.....	ThP 523	Takakusa, Hideo.....	MOF pm 3:10	Tang, Keqi.....	TP 716
Swenson, Andrew.....	TP 494	Takama, Kazuyuki.....	MOA pm 3:10	Tang, Keqi.....	WP 745
Swenson, Tami.....	TP 660	Takats, Zoltan.....	MOH pm 3:10	Tang, Lina.....	WP 533
Swentko, Nathan.....	ThP 781	Takats, Zoltan.....	MP 404	Tang, Ning.....	MP 085
Sweredoski, Michael.....	ThOF pm 2:50	Takats, Zoltan.....	ThP 379	Tang, Ning.....	MP 139
Sweredoski, Michael.....	ThP 147	Takats, Zoltan.....	ThP 664	Tang, Ning.....	TP 246
Sweredoski, Michael.....	ThP 310	Takats, Zoltan.....	TOG pm 3:30	Tang, Ning.....	TP 262
Sweredoski, Michael J.....	MP 226	Takats, Zoltan.....	TP 215	Tang, Ning.....	WP 133
Sweredoski, Michael J.....	MP 225	Takats, Zoltan.....	TP 375	Tang, Ning.....	WP 204
Sweredoski, Michael J.....	ThP 240	Takats, Zoltan.....	WP 020	Tang, Sandra.....	WP 681
Swiderski, Piotr.....	ThP 526	Takats, Zoltan.....	WP 424	Tang, Shaojun.....	MP 680
Swift, Barb.....	MP 512	Takayama, Mitsuo.....	TP 383	Tang, Wanjin.....	ThP 681
Swift, Christopher.....	TP 354	Takei, Makoto.....	MOF pm 3:10	Tang, Wei.....	TP 469
Swiontek, Alex.....	ThP 586	Takeuchi, Kohei.....	MP 606	Tang, Weijuan.....	MP 577
Syage, Jack.....	MP 686	Takigami, Shoji.....	MP 476	Tang, Weijuan.....	TP 358
Syed, Nazia.....	MP 255	Takyi-Williams, John.....	WP 390	Tang, Weijuan.....	TP 360
Syed, Sarfaraz.....	WOC am 09:50	Tallman, Keri A.....	ThP 485	Tang, Wen.....	TP 253
Syka, John E. P.....	MP 084	Tam, James.....	TP 097	Tang, Wilfred.....	MOE am 09:10
Syka, John E. P.....	MP 146	Tam, Maggie.....	MP 531	Tang, Wilfred.....	ThP 222
Syka, John E. P.....	ThP 686	Tam, Sidney.....	MP 593	Tang, Wilfred.....	TP 074
Sykes, Craig.....	ThP 006	Tam, Stanley.....	TP 145	Tang, Wilfred.....	TP 091
Sykes, Craig.....	TOH am 08:50	Tammsalu, Triin.....	ThP 241	Tang, Xiaoting.....	ThP 103
Sykes, Craig.....	TP 011	Tamura-Wells, Jessica.....	ThP 252	Tang, Zuojian.....	TP 082
Sykes, Craig.....	WP 011	Tan, Aimin.....	WP 549	Tanga, Mary J.....	WP 465
Sylvestersen, Kathrine.....	ThP 243	Tan, Bo.....	ThP 530	Tanimoto, Akiko.....	ThOF am 09:30
Symonds, Josh M.....	TP 729	Tan, Fengji.....	ThP 323	Tanner, Greg.....	WOE pm 2:30
Syvänen, Stina.....	TP 059	Tan, Haiyan.....	MP 217	Tanner, Meghan.....	TP 425
Szakacs, Gergely.....	ThP 379	Tan, Jing.....	MP 330	Tanphaichitr, Nongnuj.....	MP 250
Szalay, Dániel.....	MP 404	Tan, Kar-Chun.....	MP 419	Tao, Dingyin.....	WP 446
Szapacs, Matthew.....	TOE am 08:30	Tan, Kar-Chun.....	ThP 653	Tao, Lei.....	WP 354
Szapacs, Matthew.....	TOE am 09:50	Tan, Lei.....	ThP 187	Tao, Li.....	MOE pm 3:10
Szapacs, Matthew.....	TP 465	Tan, Lei.....	ThP 192	Tao, Nannan.....	TP 008
Szapacs, Matthew.....	TP 466	Tan, Lei.....	TP 353	Tao, Qingping.....	MP 600
Szarka, Szabolcs.....	WP 233	Tan, Lin.....	ThP 383	Tao, Qingping.....	WP 576
Szczesniewski, Andre.....	MP 291	Tan, Melvin.....	WP 524	Tao, Shujuan.....	TP 331
Szczesniewski, Andre.....	MP 754	Tan, Min.....	ThP 199	Tao, Shujuan.....	WP 080
Szczesniewski, Andre.....	ThP 603	Tan, Ming.....	ThP 098	Tao, Sijia.....	ThP 679
Sze, Siu Kwan.....	ThOF pm 3:50	Tan, Minjia.....	ThP 091	Tao, Weiguo.....	WP 163

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Tao, Weiguo Andy.....	MOH am 08:30	Termopoli, Veronica.....	MP 722	Thompson, Corbin.....	WP 011
Tao, Weiguo Andy.....	ThP 079	Termopoli, Veronica.....	TP 764	Thompson, Emma.....	MP 273
Tao, Weiguo Andy.....	TP 670	Ternes, Thomas A.....	TP 565	Thompson, J. Will.....	ThP 267
Tao, Xiaolu.....	WP 636	Ternette, Nicola.....	ThP 342	Thompson, J. Will.....	TOA pm 2:50
Tao, Yeqing.....	ThP 129	Terry, Alvin.....	MP 170	Thompson, J. Will.....	TP 457
Tao, Yi.....	ThP 436	Teruaki, Nakatsuji.....	MOH pm 4:10	Thompson, J. Will.....	WOG pm 3:30
Tao, Yi.....	ThP 538	Tessaro, Elias.....	TP 584	Thompson, J. Will.....	WP 586
Tao, Yuanqi.....	TP 129	Tessaro, Elias.....	TP 586	Thompson, Jenny Heidbrink.....	MP 063
Taoka, Masato.....	ThP 520	Teuber Seger, Signe.....	ThP 135	Thompson, Mary.....	MOE am 09:30
Taoka, Masato.....	WP 372	Teubl, Jennifer.....	ThP 039	Thompson, Patricia A.....	ThP 656
Tarafdar, Sreya.....	WP 220	Teubl, Jennifer.....	TP 082	Thompson, Steve.....	ThP 002
Taranto, Adam.....	ThP 045	Teutenberg, Thorsten.....	TP 581	Thomsen, Ditte.....	TP 356
Tarasova, Irina A.....	WP 164	Thakolwiboon, Smathorn.....	ThP 289	Thomson, Bruce A.....	WOD pm 2:50
Taremi, Shane.....	MP 131	Thannhauser, Theodore W.....	ThP 173	Thorsteinsdottir, Margret.....	ThP 401
Tarr, Matthew.....	ThP 353	Thanos, Panayotis K.....	MOH pm 2:50	Thorsteinsdottir, Margret.....	WP 448
Tarr, Matthew A.....	MP 555	Thanos, Panayotis K.....	ThP 387	Threadgill, Graham J.....	WP 497
Tartiere, Aude.....	WP 138	Tharakan, Ravi.....	ThP 273	Thulin, Craig.....	MP 239
Tarui, Naoki.....	MOF pm 3:10	Tharakan, Ravi.....	TP 146	Thulin, Craig.....	WOE am 09:30
Tasoglu, Cagdas.....	ThP 185	Tharakan, Ravi.....	WP 602	Thurlow, Sophie.....	TOE pm 3:50
Tata, Alessandra.....	WP 709	Thaysen-Andersen, Morten.....	WP 079	Thyagarajan, Arvind.....	TP 529
Tate, Stephen.....	TP 181	Thayumanavan, Sankaran.....	TP 774	Thyagarajan, Arvind.....	WP 539
Tate, Stephen.....	TP 186	Theberge, Marie-Claude.....	MP 490	Thyagarajan, Janani.....	TP 528
Tate, Stephen A.....	ThP 330	Theberge, Marie-Claude.....	MP 493	Thyparambil, Sheeno.....	WP 141
Tate, Stephen A.....	TP 087	Theberge, Marie-Claude.....	MP 496	Tian, Geng.....	TOF am 09:10
Tate, Stephen A.....	TP 085	Theberge, Roger.....	ThP 057	Tian, Qingguo.....	ThP 496
Tate, Stephen A.....	TP 182	Theberge, Roger.....	WP 445	Tian, Qingguo.....	WP 100
Tatham, Michael H.....	ThP 241	Thein, Moe.....	MP 453	Tian, Qingguo.....	WP 526
Tatlay, Jaspaul.....	TP 655	Theis, Jason D.....	ThP 272	Tian, Yongfeng.....	TP 475
Tattersal, Peter.....	MP 765	Theret, Alain.....	TP 219	Tian, Yuan.....	MP 706
Tauler, Romà.....	TP 639	Therrien, Daniel.....	MP 167	Tian, Yuan.....	MP 707
Tauler, Romà.....	TP 637	Theurillat, Jean-Philippe.....	WOG am 08:50	Tian, Yuan.....	ThP 040
Tauler, Romà.....	WP 719	Thévenot, Etienne.....	MP 581	Tian, Yuan.....	ThP 156
Taumer, Christoph.....	ThP 043	Thevis, Mario.....	TP 628	Tian, Yuan.....	ThP 184
Taus, Thomas.....	TP 096	Thevis, Mario.....	WP 301	Tian, Zhixin.....	ThP 063
Taus, Thomas.....	TP 098	Thibault, Pierre.....	ThOC am 08:30	Tice, Joe.....	MP 386
Tautenhahn, Ralf.....	MP 596	Thibault, Pierre.....	TP 113	Tice, Joseph.....	MP 523
Tautenhahn, Ralf.....	ThP 639	Thibault, Pierre.....	TP 130	Tichy, Ales.....	ThP 201
Tautges, Stephanie.....	MP 431	Thibault, Pierre.....	TP 108	Tie, Liu.....	TP 243
Tautges, Stephanie.....	TP 481	Thiele, Herbert.....	MP 021	Tiedje, James.....	MP 564
Tavares, Clint.....	ThP 350	Thiemann, Joachim.....	MP 356	Tiers, Laurent.....	WP 447
Taverna, Domenico.....	MP 014	Thienpont, Linda.....	WP 453	Tietel, Zipora.....	MP 606
Taverna, Domenico.....	TP 511	Thiniou, Marco.....	TP 733	Tikhonov, George.....	MP 660
Tavşanlı, Burak.....	MP 066	Thomas, Andreas.....	WP 301	Tikhonov, George.....	WOA pm 3:10
Tawfall, Amanda.....	WP 720	Thomas, Andrew L.....	ThP 302	Tillement, Olivier.....	MP 731
Taylor, Adrian.....	WP 295	Thomas, Aurelien.....	TOH pm 3:50	Timmons, Michael D.....	MP 292
Taylor, Adrian.....	WP 308	Thomas, Brian.....	TP 660	Timpe, Leslie.....	MP 453
Taylor, Alan W.....	WP 436	Thomas, Corinne.....	ThP 247	Tinaztepe, Emir.....	WP 111
Taylor, Alastair.....	WP 760	Thomas, Daniel.....	MP 095	Ting, Edwin Zhi Wei.....	WP 449
Taylor, Amber.....	ThP 733	Thomas, Derek.....	ThP 076	Ting, Lily.....	TP 145
Taylor, Jordan.....	WOG pm 2:30	Thomas, Joji K.....	MP 255	Ting, Ying Sonia.....	MOG am 09:50
Taylor, Martin S.....	WP 253	Thomas, May-Lin.....	MP 377	Ting, Ying Sonia.....	ThP 763
Taylor, Nicholas M. I.....	ThP 072	Thomas, Michael.....	TP 295	Ting, Ying Sonia.....	TP 083
Taylor, Ryan.....	MP 059	Thomas, Paul.....	ThP 058	Ting, Ying Sonia.....	WP 115
Taylor, Ryan.....	MP 060	Thomas, Paul.....	ThP 059	Ting, Ying Sonia.....	WP 737
Taylor, Stephen.....	MP 521	Thomas, Paul.....	TOE pm 3:30	Ting, Zhi Wei.....	MP 342
Tchernyshyov, Irina.....	TP 188	Thomas, Paul.....	TP 234	Ting, Zhi Wei.....	MP 351
Teague, Matt.....	TP 028	Thomas, Paul.....	TP 402	Ting, Zhi Wei.....	TP 275
Tebbe, Andreas.....	ThP 019	Thomas, Paul.....	WOH pm 3:30	Tintaru, Aura.....	TP 781
Technau, Martin.....	ThP 781	Thomas, Paul.....	WP 157	Tipple, Christopher A.....	ThP 579
Tee, Ting Yee.....	TP 303	Thomas, Powers.....	TP 068	Tipple, Christopher A.....	ThP 580
Tegeler, Tony.....	TP 440	Thomas, Rebecca.....	WP 425	Tischler, Marc.....	WP 354
Telenga, Eef.....	ThP 389	Thomas, Stefani.....	ThP 295	Tisdale, Evgenia.....	WP 755
Telepchak, Michael.....	MP 349	Thomas, Stefani.....	ThP 339	Titsch, Craig.....	MP 074
Telles, Guilherme.....	WP 460	Thomas, Tiffany.....	MP 075	Titus, Mark.....	ThP 423
Tellström, Verena.....	ThP 637	Thomas, Tiffany.....	WP 426	Tiwari, Neil.....	MP 468
Tellström, Verena.....	TP 750	Thomas-Ahner, Jennifer M.....	ThP 292	Tjoe, Elina.....	TP 132
Telu, Kelly H.....	MP 604	Thompson, Alex.....	WP 775	t'Kindt, Ruben.....	ThP 389
Temel, Hamdi.....	WP 556	Thompson, Andrew.....	ThP 215	Tobias, Herbert.....	MP 335
ten Hacken, Nick.....	ThP 389	Thompson, Charles.....	ThOE am 09:30	Tobolkina, Elena.....	TP 389
Tender, Leonard.....	MP 279	Thompson, Charles.....	ThP 546	Todd, Daniel.....	WP 476
Teng, Pang-Ning.....	ThP 202	Thompson, Charles D.....	ThP 521	Todd, Daniel A.....	MP 312
Tennichi, Yoshika.....	TP 604	Thompson, Christopher.....	MP 249	Todd, John F.J.....	WOC am 08:50
Tenzer, Stefan.....	ThP 015	Thompson, Christopher.....	TP 209	Todua, Nino G.....	MP 295
Tenzer, Stefan.....	TP 084	Thompson, Christopher.....	TP 299	Todua, Nino G.....	TP 569
Tep, Samnang.....	WP 191	Thompson, Christopher J.....	MP 140	Toelgyesi, László.....	MP 702
Terada, Hidetoshi.....	MP 739	Thompson, Christopher J.....	MP 141	Toghi Eshghi, Shadi.....	ThOH am 10:10
Terada, Naoki.....	TP 166	Thompson, Christopher J.....	ThP 693	Toghi Eshghi, Shadi.....	TP 003
Terasaki, Tetsuya.....	MP 447	Thompson, Corbin.....	ThP 006	Tokarski, Caroline.....	MP 068
Terhune, Scott.....	WP 245	Thompson, Corbin.....	TOH am 08:50	Tokarski, Caroline.....	MP 083

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Tokarski, Caroline.....	TP 719	Tran, Bao Quoc.....	TP 437	Tsien, Roger.....	ThOC pm 3:10
Tokmina-Lukaszewska, Monika.....	TP 656	Tran, Janessa L.....	MP 563	Tsim, Karl, W. K.....	ThP 619
Tokunaga, Ayaka.....	WP 102	Tran, john.....	MP 676	Tsirigotaki, Alexandra.....	WP 229
Tokuoka, Suzumi.....	ThP 398	Tran, John C.....	TP 196	Tsirigotaki, Alexandra.....	WP 219
Toledo-Sherman, Leticia.....	WP 480	Tran, Tran.....	TP 655	Tso, Patrick.....	WP 673
Tolentino-Cortez, Tarson.....	MP 006	Trapa, Patrick.....	MP 126	Tsou, Chih-Chiang.....	MP 035
Toler, Strawn.....	MP 553	Traub, Angelica.....	ThP 602	Tsou, Chih-Chiang.....	ThP 028
Tölgyesi, László.....	WP 560	Trauger, Sunia.....	WP 339	Tsou, Chih-Chiang.....	WOD am 09:10
Tolic, Nikola.....	MOG pm 3:30	Trede, Dennis.....	MP 021	Tsou, Chih-Chiang.....	WP 045
Tolic, Nikola.....	ThP 062	Trede, Dennis.....	TP 047	Tsuchihashi, Hitoshi.....	ThP 592
Tolic, Nikola.....	ThP 064	Trelle, M.B.....	WP 229	Tsugawa, Hiroshi.....	WP 604
Tolic, Nikola.....	TOA am 08:50	Trelle, Morten B.....	WP 219	Tsuge, Koichiro.....	MP 526
Tolic, Nikola.....	TP 169	Tremblay, Michel.....	MP 262	Tsuge, Kouichiro.....	MP 525
Tolic, Nikola.....	WOE am 08:30	Tremintin, Guillaume.....	WP 076	Tsukamoto, Taku.....	MP 755
Tolic, Nikola.....	WP 088	Trengove, Naomi.....	WP 587	Tsunoi, Yoshimasa.....	WP 354
Tollefson, Julie.....	WP 537	Trengove, Robert.....	MP 419	Tsybin, Oleg Yu.....	MP 700
Tollenaar, Rob.....	MP 004	Trengove, Robert.....	ThP 653	Tsybin, Yury O.....	WP 156
Tollervey, James R.....	ThP 450	Trengove, Robert.....	WP 587	Tsybin, Yury O.....	MOB am 09:30
Tolley, Dennis.....	MP 696	Trengrove, Robert.....	ThP 614	Tsybin, Yury O.....	MOE am 08:50
Tolmachev, Aleksey.....	ThOB am 10:10	Trent, Tyler.....	TP 564	Tsybin, Yury O.....	MP 700
Tolmachev, Aleksey.....	TOC am 08:30	Tretter, Kelly.....	ThP 607	Tsybin, Yury O.....	MP 701
Tolmachev, Aleksey.....	WP 698	Treyakov, Kirill V.....	MP 295	Tsybin, Yury O.....	ThP 687
Tolmachev, Aleksey V.....	MP 654	Treyakov, Kirill V.....	TP 569	Tsybin, Yury O.....	WP 172
Tolmachev, Aleksey V.....	MP 677	Treyakova, Natalia.....	ThP 522	Tsybin, Yury O.....	WP 418
Tolmachev, Aleksey V.....	TOB am 09:50	Treuheit, Michael.....	TOF am 10:10	Tu, Aye.....	TP 258
Tolmachev, Aleksey V.....	TP 716	Trevitt, Adam.....	ThOD am 10:10	Tu, Chengjian.....	ThP 014
Tolmachev, Aleksey V.....	TP 717	Trevitt, Adam J.....	TP 371	Tu, Chengjian.....	TP 488
Tolner, Else.....	MP 027	Trevitt, Adam J.....	TP 355	Tu, Chengjian.....	WP 015
Tolstikh, Tatiana.....	ThP 405	Trexler, Heather.....	ThOE am 09:30	Tu, Patricia.....	MP 065
Toman, Blaza.....	WP 453	Trimpin, Sarah.....	MP 301	Tu, Peijun.....	ThP 550
Tomazela, Daniela.....	WP 184	Trimpin, Sarah.....	MP 538	Tu, Qiang.....	MP 484
Tomczyk, Nick.....	TP 724	Trimpin, Sarah.....	ThP 732	Tu, Zhijian.....	MP 270
Tomer, Kenneth B.....	MP 072	Trimpin, Sarah.....	TP 163	Tubbs, Kemmons.....	WP 192
Tomer, Kenneth B.....	ThP 404	Trimpin, Sarah.....	TP 198	Tubbs, Kemmons.....	WP 266
Tomezyk, Aurore.....	TP 249	Trimpin, Sarah.....	TP 288	Tucholska, Monika.....	TP 087
Tomita, Atsumi.....	WP 130	Trimpin, Sarah.....	TP 319	Tucker, Bryan S.....	TP 786
Tomko, Jonathan.....	WP 459	Trimpin, Sarah.....	TP 790	Tudor, Andrew.....	TP 157
Tomlinson, Ronaldo.....	ThP 405	Trimpin, Sarah.....	WOB am 09:50	Tudor, Greg.....	TP 437
Toms, Andrew.....	MP 333	Trimpin, Sarah.....	WP 702	Tudor, Gregory.....	ThP 642
Toms, Andrew.....	MP 665	Trimpin, Sarah.....	WP 755	Tudor, Gregory.....	TP 299
Tonge, Robert.....	ThP 036	Trinh, Hung.....	ThP 229	Tudor, Gregory.....	TP 688
Tonillo, Jason.....	TP 141	Trinh, Hung.....	TP 146	Tudor, Gregory.....	WP 601
Topolcan, Ondrej.....	ThP 139	Trinidad, Jonathan.....	ThP 233	Tuerk, Jochen.....	TP 581
Topolyan, Artyom.....	WP 027	Tripet, Brian P.....	MP 276	Tuerk, Jochen.....	WP 568
Toppari, Jorma.....	WP 028	Triquigneaux, Mathilde.....	MP 588	Tufariello, Jessica.....	WP 774
Torget González, Gabriela Desireé.....	ThP 453	Trivedi, Geetika.....	TP 680	Tufariello, Joann.....	WP 111
Törnqvist, Margareta.....	WP 456	Trivett, Ian.....	ThP 749	Tump, Cornelis.....	WP 651
Torres, Eduardo.....	ThP 319	Trnka, Michael.....	ThP 037	Turchetta, Renato.....	ThP 002
Torres, Oscar B.....	WP 211	Trnka, Michael.....	ThP 048	Turchin, Howard.....	TP 238
Tortella, Frank C.....	ThP 306	Trolard, Ron.....	MP 216	Turck, Chris.....	WP 583
Tortorelli, Silvia.....	WP 655	Trost, Matthias.....	ThP 338	Turecek, Frantisek.....	MP 192
Tosin, Manuela.....	WP 329	Trost, Matthias.....	WP 200	Turecek, Frantisek.....	ThOD am 08:30
Toth, Laszlo.....	WP 424	Troyer, Dean.....	TP 069	Turecek, Frantisek.....	WOD pm 3:30
Toth, Steven.....	MP 088	Trucksis, Michele.....	WP 652	Turecek, Frantisek.....	WP 443
Totten, Sarah.....	ThP 729	Trudgian, David.....	MP 254	Tureček, Frantisek.....	TP 353
Totten, Sarah M.....	ThOH am 08:50	Trufanov, Andrew.....	ThP 690	Tureček, František.....	TOD pm 2:50
Touré, Momar.....	WP 682	Truillet, Charles.....	MP 731	Turesky, Robert.....	WP 485
Toutoungi, Danielle.....	ThOC am 09:10	Tsai, Alice.....	WP 620	Turgeon, Coleman.....	WP 655
Toutoungi, Danielle.....	WP 760	Tsai, Cheng-Han.....	WP 493	Turiak, Lilla.....	ThP 771
Towers, Mark.....	ThP 001	Tsai, Chia-Wei.....	ThP 579	Turiák, Lilla.....	WP 007
Towers, Mark.....	TP 004	Tsai, Chia-Wei.....	ThP 580	Turiák, Lilla.....	WP 008
Townsend, R. Reid.....	ThP 039	Tsai, Cindy.....	MP 518	Turino, Gerard.....	ThP 448
Townsend, R. Reid.....	ThP 170	Tsai, Ping-Ju.....	ThP 388	Turino, Gerard.....	TP 450
Townsend, R. Reid.....	TP 082	Tsai, Sheng-Ta.....	WP 246	Turk, John.....	ThP 199
Townsend, R. Reid.....	TP 173	Tsai, Tsung-Heng.....	ThP 154	Turko, Illarion.....	MP 234
Townsend, R. Reid.....	TP 433	Tsai, Yu-Hsuan.....	MP 240	Turko, Illarion.....	TP 689
Townsend, R. Reid.....	WOG pm 3:50	Tsaparikos, Konstantinos.....	TP 028	Turley, Wesley.....	WP 636
Townsend, Reid.....	ThP 205	Tsarbopoulos, Anthony.....	ThP 087	Turner, Matthew.....	TP 402
Townsend, Reid.....	TOG am 08:30	Tsarbopoulos, Anthony.....	WP 600	Turner, Matthew.....	TP 390
Townsend, Reid.....	TP 169	Tschismarov, Roland.....	MP 228	Turner, Meredith E.....	TP 470
Townsend, Dave.....	WP 482	Tse, Eric.....	ThP 454	Turunen, Brandon.....	TP 201
Toyama, Brandon.....	ThOC pm 3:10	Tse, Francis.....	WP 528	Turvey, Stuart.....	ThP 222
Toyoda, Michisato.....	ThP 012	Tse, Francis.....	WP 645	Turvey, Stuart.....	WP 150
Trabelsi, Fethi.....	WP 549	Tse-Dinh, Yuk-Ching.....	MP 249	Tuskan, Gerald.....	TP 675
Trachsel, Christian.....	ThP 329	Tseng, Cheng-Ming.....	MP 306	Tusky, Steve.....	TOF am 09:50
Tracy, Mark.....	WP 262	Tseng, Cheng-Ming.....	MP 307	Twaddle, Nathan C.....	TP 499
Trainer, Melissa.....	ThP 364	Tseng, Chiao-Li.....	MP 593	Twaddle, Nathan C.....	TP 624
Tran, Bao.....	ThP 325	Tseng, Chiao-Li.....	TP 650	Tyagi, Aman.....	MP 164
Tran, Bao Q.....	MP 039	Tseng, Chiao-Li.....	TP 655	Tyan, Yu-Chang.....	TP 200

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Tyan, Yu-Chang.....	WP 462	Uthayakumar, Rampriya.....	TP 528	van de Ven, Stephanie.....	MP 019
Tyburski, John B.....	TP 659	Uthayakumar, Rampriya.....	TP 529	Van De Waterbeemd, Michiel.....	WOG am 09:30
Tykesson, Emil.....	ThP 730	Uthayakumar, Rampriya.....	WP 328	van den Anker, John N.....	MP 424
Tykwinski, Rik.....	TP 589	Uthayakumar, Rampriya.....	WP 539	van den Berg, Albert.....	TP 611
Tykwinski, Rik R.....	TP 588	Uwakweh, Agbo-Oma.....	MP 312	van den Bremer, Ewald T. J.....	TP 237
Tyldesley-Worster, Richard.....	WP 586	Uygun, Basak.....	WP 239	van den Brink, Floris T.G.....	TP 611
Tyler, Andrew.....	ThP 536	Uzuner, Ugur.....	ThP 123	van den Broek, Irene.....	WP 518
Tyler, Chelsea.....	TP 349	Vaccaro, Nicholas.....	TP 301	van den Maagdenberg, Arn.....	TP 005
Tymchenko, Oleksii.....	WOG pm 4:10	Vachet, Richard.....	MOF am 09:50	van den Maagdenberg, Arn M.J.M.....	MP 027
Tymiak, Adrienne.....	MP 172	Vachet, Richard.....	MP 185	van den Waterbeemd, Michiel.....	TP 136
Tymiak, Adrienne.....	MP 180	Vachet, Richard.....	ThP 115	van der Burgt, Yuri E.M.....	TP 161
Tymiak, Adrienne.....	ThP 441	Vachet, Richard.....	ThP 114	van der Burgt, Yuri E.M.....	WP 518
Tymiak, Adrienne.....	TP 541	Vachet, Richard.....	TP 774	van der Gugten, J Grace.....	TOG pm 3:10
Tymiak, Adrienne.....	WP 487	Vachet, Richard.....	WP 701	Van Der Hart, Marieke.....	ThP 440
Tymiak, Adrienne A.....	MOE pm 3:10	Vachet, Richard.....	WP 723	Van Der Kroft, Claartje.....	TP 658
Tyner, Jeffrey.....	ThP 219	Vachet, Richard W.....	WP 703	Van der Oost, John.....	ThP 458
Tyson, Gene W.....	ThP 555	Vacratis, Panayiotis.....	TOD am 10:10	van der Plas-Duivesteijn, Suzanne.....	MP 037
Yaesoontrachoon, Kitipong.....	MP 424	Vadali, Gouri.....	ThP 450	van der Post, Sjoerd.....	MP 210
Yaesoontrachoon, Kitipong.....	TP 467	Vadi, Alessandro.....	WP 187	Van Der Post, Sjoerd.....	MP 211
Ubaida Mohien, Ceereena.....	ThP 273	Vahidi, Siavash.....	MOF am 10:10	Van der Rest, Guillaume.....	ThOF am 09:10
Ubaida Mohien, Ceereena.....	TP 146	Vaikkinen, Anu.....	TP 401	van der Zee, Ate.....	WP 147
Ubaida Mohien, Ceereena.....	TP 468	Valaskovic, Gary.....	ThP 445	Van Dorsseleer, Alain.....	MOE am 09:50
Ubaida Mohien, Ceereena.....	WP 602	Valaskovic, Gary.....	WP 158	Van Dorsseleer, Alain.....	MP 157
Ubhayasekera, Kumari.....	TP 455	Valaskovic, Gary A.....	MP 710	Van Dorsseleer, Alain.....	ThP 095
Ubhi, Baljit.....	MP 578	Valaskovic, Gary A.....	MP 747	Van Dorsseleer, Alain.....	WP 265
Ubhi, Baljit.....	ThP 406	Valaskovic, Gary A.....	WP 159	van Els, Cecile A.C.M.....	WOE am 10:10
Ubhi, Baljit.....	TP 661	Valaskovic, Gary A.....	WP 754	Van Eyk, Jennifer.....	ThOE pm 3:30
Uboh, Cornelius.....	ThP 593	Valeja, Santosh G.....	ThP 065	Van Eyk, Jennifer.....	ThP 300
Ubukata, Masaaki.....	WP 576	Valeja, Santosh G.....	ThP 078	Van Eyk, Jennifer.....	TP 188
Uckert, Kyle.....	ThP 366	Valeja, Santosh G.....	WP 162	Van Eyk, Jennifer E.....	WP 497
Uclés Duque, Samanta.....	WP 360	Valentine, Stephen.....	MP 590	van Eyk, Jennifer E.....	TP 477
Udeshi, Namrata.....	ThP 205	Valentine, Stephen.....	TP 540	van Gaans-van den Brink, J.....	WOE am 10:10
Udeshi, Namrata.....	WOG am 08:50	Valentine, Stephen.....	WP 672	van Herpen, Laurens.....	WOF am 10:10
Ueberheide, Beatrix.....	MP 149	Valentine, Stephen.....	WP 699	Van Hoek, Monique.....	TP 188
Ueberheide, Beatrix.....	WP 111	Valentine, Stephen J.....	ThP 105	Van Natta, Kristine.....	MP 282
Uechi, Guy.....	TP 615	Valenzano, Kenneth.....	WOH am 10:10	Van Natta, Kristine.....	MP 283
Ueckert, Torsten.....	ThP 222	Valkenburg, Dirk.....	MOG pm 3:10	van Natta, Kristine.....	MP 285
Ueckert, Torsten.....	ThP 317	Valkenburg, Dirk.....	MP 032	van Oosterhout, Antoon.....	ThP 389
Ueda, Morio.....	TP 604	Valkenburg, Dirk.....	MP 682	van Oostrum, Jan.....	ThP 442
Ugarov, Michael.....	MP 702	Valkenburg, Dirk.....	ThP 191	Van Orden, Steve L.....	TOE pm 3:10
Ugarov, Michael.....	ThP 744	Valkenburg, Dirk.....	TOC pm 3:50	Van Riper, Susan K.....	TP 076
Uher, Josef.....	TOH pm 3:10	Valkenburg, Dirk.....	TP 482	van Soest, Remco.....	MP 221
Ukibe, Masahiro.....	ThP 761	Valkenburg, Dirk.....	WP 031	van Soest, Remco.....	MP 748
Ulasi, Gloria N.....	WP 765	Valkenburg, Dirk.....	WP 035	van Soest, Remco.....	ThOE pm 2:50
Ulbrich, Arne.....	WOA am 09:50	Valkenburg, Dirk.....	WP 042	Van Soest, Remco.....	ThP 067
Ulmer, Candice.....	MP 785	Valkenburg, Dirk.....	WP 469	Van Soest, Remco.....	ThP 425
Ulmer, Candice.....	WP 397	Vallabhaneni, Prashanthi.....	WOF am 09:50	Van Steendam, Katleen.....	ThP 776
Ulrich, Robert.....	MOB pm 3:50	Vallance, Claire.....	ThP 002	Van Steendam, Katleen.....	WP 294
Umlauf, Ellen.....	WP 140	Vallur, Raghavan.....	ThP 301	Van Stipdonk, Michael J.....	ThOD pm 3:50
Ungaro, Rémi.....	TP 781	Van, Anh.....	MP 010	Van Stipdonk, Michael J.....	TP 364
Unger, Mark.....	TP 216	van Aghoven, Maria.....	WP 729	van Tilborg, Marcel.....	WP 055
Unger, Steve.....	TP 493	Van Amerom, Friso H.W.....	ThP 369	van Veelen, Peter.....	TP 005
Unger, Steve.....	WP 524	Van Amerom, Friso H.W.....	TOA pm 2:30	Van Veldhoven, Paul P.....	TP 015
Uno, Shohai.....	MP 525	van Amerom, Friso H.W.....	TP 710	van Wijk, Klaas.....	TP 672
Untiedt, Steve.....	MP 553	Van Amerom, Friso H.W.....	TP 712	van Wijk, Klaas J.....	ThP 075
Uplekar, Shaunak.....	ThP 167	Van Amerom, Friso H.W.....	WP 345	van Zeijl, René J. M.....	MP 027
Uppal, Annu.....	MP 155	van Bavel, Bert.....	ThP 544	Vanamala, Jairam.....	ThP 303
Upton, Mark.....	ThP 612	van Bavel, Bert.....	ThP 551	vandell, Victor.....	MP 341
Urbach, Dieter.....	WP 300	Van Berkel, Gary J.....	ThOB am 08:30	Vandell, Victor.....	MP 757
Urban, Jan.....	TOD pm 2:50	Van Berkel, Gary J.....	ThP 004	Vandell, Victor.....	MP 758
Urdahl, Randall.....	TP 752	Van Berkel, Gary J.....	ThP 005	Vandell, Victor.....	MP 759
Urh, Marjeta.....	MP 188	Van Berkel, Gary J.....	ThP 670	Vandell, Victor.....	MP 760
Urh, Marjeta.....	ThP 778	van Bodegom, Diederik.....	ThP 219	Vandell, Victor.....	MP 761
Urh, Marjeta.....	ThP 779	van Breemen, Richard.....	WP 332	Vandell, Victor.....	MP 769
Urh, Marjeta.....	TP 234	van Breemen, Richard B.....	MP 644	Vandell, Victor.....	MP 783
Urisman, Anatoly.....	ThP 027	van Breemen, Richard B.....	ThP 654	Vandell, Victor.....	MP 756
Urlaub, Henning.....	MP 198	van Breemen, Richard B.....	WP 325	Vandell, Victor.....	ThP 589
Urlaub, Henning.....	ThP 203	van Breemen, Richard B.....	WP 331	Vandenberg, Albert.....	ThP 736
Urlaub, Henning.....	ThP 456	van Dam, Annie.....	MP 298	Vandergrift, Gregory W.....	MP 556
Urlaub, Henning.....	ThP 457	Van Damme, Petra.....	TP 078	Vandergrift, Gregory W.....	WP 746
Urlaub, Henning.....	ThP 459	Van De Goor, Tom.....	TP 192	Vanduijn, Martijn.....	ThP 064
Urlaub, Henning.....	ThP 458	van de Goor, Tom A.....	MP 715	Vanduijn, Martijn M.....	ThP 062
Urlaub, Henning.....	ThP 519	van de Merbel, Nico.....	TOE am 09:10	Vanek, Ondrej.....	MP 183
Usmanov, Dilshadbek.....	TP 726	Van De Plas, Raf.....	MOB am 09:50	vanHoor, Elmar.....	ThP 209
Usmanov, Dilshadbek.....	TP 725	Van De Plas, Raf.....	MOH pm 2:30	Vaniya, Arpana.....	MP 616
Ustinov, Alexey.....	WP 027	Van de Plas, Raf.....	MP 014	Vantangoli, Marguerite.....	WP 581
Usui, Fumihiko.....	TP 383	Van de Plas, Raf.....	MP 029	Vantongeren, Sean.....	WP 010
Usui, Kiyotaka.....	ThP 592	Van de Plas, Raf.....	MP 022	Varberg, Joseph.....	ThOF pm 3:30
Usuki, Toyonobu.....	ThP 448	Van de Plas, Raf.....	MP 023	Varesio, Emmanuel.....	MP 057

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Varesio, Emmanuel	MP 629	Vertes, Akos	WOB pm 2:50	Voelz, David G.	ThP 366
Varesio, Emmanuel	MP 632	Vertes, Akos	WP 740	Voets, Olaf	ThP 239
Varesio, Emmanuel	WP 614	Veselkov, Kirill	ThP 379	Vogel, Horst	TP 389
Varfolomeev, SD	TP 449	Veselkov, Kirill	TOG pm 3:30	Vogelsang, Maryann S.	ThP 450
Varfolomeev, Sergey	TOA pm 4:10	Veselkov, Kirill	TP 375	Voggu, Ramakrishna Reddy	MP 508
Varga, János	TP 263	Veselkov, Kirill	WP 020	Voglmeir, Josef	ThP 492
Varga, Peter	WP 424	Vestal, Marvin	ThP 009	Vogt, Bruno	WP 671
Varghese, Rency	MP 580	Vetere, Alessandro	TP 593	Voigt, Emily A.	ThP 179
Varghese, Rency	TP 756	Veжина, Chad	MP 448	Voinov, Valery	ThP 689
Vargo, John	TP 552	Veжина, Chad	TP 454	Voinov, Valery G.	ThP 688
Varma, Vijayalakshmi	WP 249	Via, Laura E.	TP 030	Völker, Uwe	ThP 250
Varshney, Brajesh	WP 717	Vialaret, Jérôme	WP 245	Volkin, David	WP 417
Vashishth, Deepak	ThP 247	Vickery, Lillian	ThP 260	Volkman, Brian F.	WP 212
Vasicek, Lisa A.	ThP 202	Vidal de Miguel, Guillermo	ThP 476	Volkow, Nora D.	MOH pm 2:50
Vass, Andrea	WP 362	Vidal de Miguel, Guillermo	ThP 477	Volkow, Nora D.	ThP 387
Vassallo, Jose	MP 464	Vidić, Jana	WP 135	Volland, Hervé	MP 528
Vaudel, Marc	MP 033	Viehland, Larry	ThP 480	Volland, Hervé	MP 527
Vaudel, Marc	TP 105	Viehoff, Maria	MP 477	Volmer, Dietrich	WP 452
Vavrova, Jirina	ThP 201	Veira da Costa Monteiro, Thays	MP 570	Volmer, Dietrich	WP 554
Vayn, Patrick	WP 047	Viel, François	MP 496	Volmer, Dietrich	WP 697
Vaz, Boniek G.	TP 594	Viel, François	MP 486	Volmer, Dietrich A.	MP 556
Vázquez, Jesús	ThP 336	Viel, François	MP 489	Vom Eysler, Claudia	TP 581
Vedder, Sven	TP 583	Viel, François	MP 485	von Helden, Gert	TOC am 10:10
Veenstra, Timothy D.	WP 236	Viel, François	MP 494	von Stedingk, Hans	WP 456
Vegvari, Akos	WP 032	Viel, François	MP 488	von Sydow, Lena	MP 205
Veijola, Riitta	WP 028	Viel, François	MP 495	Vonderach, Matthias	WP 056
Veitinger, Michael	WP 140	Viel, François	TP 517	Vora, Gary	MP 279
Velásquez, Erika	TP 686	Viel, Stéphane	TP 780	Vora, Gary J.	MP 278
Velmurugan, Devadasan	WP 328	Viel, Stéphane	WP 682	Vorobyev, Aleksey	ThP 690
Velmurugan, Devadasan	WP 539	Viggiano, Al	MOD am 08:30	Vorweg, Lars	MOE pm 3:30
Venâncio, Tiago	TP 614	Vila, Maria Candida	TP 467	Voss, Bradley J.	MP 123
Vendramini, Pedro Henrique	TP 584	Vilanova, Mar	ThP 746	Voss, Don Marvin	TP 481
Venkatakrishnan, Vinod Kumar	MP 575	Vilaseca, Marta	ThP 746	Voss, Marvin	MP 431
Venkataramanan, Keerthi	MP 572	Villalta, Peter	ThP 522	Votta, Bart	MP 512
Venkateshwaran, Muthusubramanian	MP 405	Villanova Bridi, Aline	ThP 138	Vouros, Paul	WP 373
Venkatramn, Vidya	ThP 300	Villard, Claude	ThP 351	Vouros, Paul	WP 775
Venne, Saskia	ThP 224	Villen, Judit	ThP 236	Vouros, Paul	WP 776
Venne, Saskia	TP 105	Villeneuve, Dan	TP 311	Vowcicefski, Rachel	WP 395
Venot, Andre	TP 320	Villeneuve, Daniel	WP 132	Vowcicefski, Rachel	WP 741
Venter, Andre	MP 316	Villiers, Florent	ThOB am 09:10	Voyksner, Robert	ThP 630
Venter, Andre	ThP 629	Vincenzi Oliveira, Regina	TP 621	Voyksner, Robert D.	MP 686
Ventura, Dan	ThP 029	Viner, Rosa	ThP 160	Voyksner, Robert D.	TP 636
Ventura, Dan	WP 036	Viner, Rosa	ThP 170	Voytovich, Julia	ThP 218
Ventura-Espejo, Estela	MP 034	Viner, Rosa	ThP 222	Vrana, Julie A.	ThP 272
Ventura-Espejo, Estela	ThP 258	Viner, Rosa	TOC pm 2:30	Vrána, David	ThP 396
Venturini, Gabriela	MP 459	Viner, Rosa	TP 149	Vrkoslav, Vladimir	MP 030
Venturini, Gabriela	ThP 651	Viner, Rosa	TP 326	Vu, Trung Nghia	WP 042
Venturini, Gabriela	TP 435	Viner, Rosa	TP 337	Vuckovic, Dajana	MP 588
Venugopalan, Abhilash	ThP 204	Viner, Rosa	WP 065	Vuckovic, Dajana	MP 633
Verani, Claudio	WP 702	Viner, Rosa	WP 150	Vujaskovic, Zeljko	ThP 390
Verano-Braga, Thiago	MP 719	Viner, Rosa	WP 481	Vujaskovic, Zeljko	ThP 642
Verano-Braga, Thiago	MP 718	Viner, Rosa	WP 510	Vujaskovic, Zeljko	TP 067
Verbeck, Guido	TOH pm 4:10	Viner, Rosa	WP 738	Vujaskovic, Zeljko	TP 299
Verbeck, Guido	WOH am 09:50	Vinueza, Nelson	TP 535	Vujaskovic, Zeljko	TP 688
Verbeeck, Nico	MP 022	Vinueza, Nelson	WP 306	Vukoti, Krishna	ThP 298
Verbeeck, Nico	MP 029	Visa, Neus	TOF pm 3:10	Vyatkin, Kira	ThP 064
Verberkmoes, Nathan C.	ThP 555	Visser, Jan	TOH pm 3:10	Vyatkin, Kira	ThP 062
Vercruyse, Nicholas	ThP 578	Vissers, Johannes P.C.	MP 265	Waaijer, Cathelijm	MP 368
Verdenaud, Marion	WOE am 09:50	Vissers, Johannes PC	ThOB pm 3:50	Wachsmuth, Christian	TP 750
Verdin, Eric	WP 113	Vissers, Johannes Pc	ThP 036	Wada, Hiroo	TP 193
Verenchikov, Anatoly	MP 651	Vissers, Johannes Pc	TP 004	Wada, Shun	ThP 633
Verenchikov, Anatoly	ThOB pm 3:10	Vissers, Johannes Pc	WP 126	Waddell, Keith	ThP 569
Verenchikov, Anatoly	ThP 690	Viswanathan, Rajesh	ThP 646	Waddell, Keith	WP 144
Verenchikov, Anatoly	WOA pm 3:10	Viswanathan, Vasanthi S.	ThP 512	Waddell, Keith A.	WP 264
Verenchikov, Anatoly N.	WP 164	Vitek, Olga	MOG pm 3:50	Wade, Mary	ThP 077
Verhaert, Peter D.	MP 434	Vitek, Olga	MP 019	Wade, Mary Margaret	ThP 333
Verhaert, Peter D.	WOF am 10:10	Vitek, Olga	ThP 257	Wadsworth, John	MP 182
Verhaert, Peter D.	WP 478	Vitha, Mark	WP 720	Waelkens, Etienne	MP 022
Veri, Vinicius	ThOA am 09:30	Vitko, Dijana	MP 228	Waelkens, Etienne	MP 029
Verma, Archana	WP 717	Vitko, Dijana	WOF pm 2:50	Wager-Miller, James	TP 198
Vermillion, Katie	MP 049	Vlad, Camelia	ThP 746	Wager-Miller, James	TP 288
Verreault, Alain	TP 113	Vladimirov, Gleb	MOB am 08:50	Waggoner, Derek	MP 573
Verrijzer, Peter	ThP 239	Vladimirov, Gleb	MP 704	Waghmare, Sakham	ThP 525
Vertes, Akos	MP 398	Vliet, Kent	TP 188	Wagner, Craig	TP 201
Vertes, Akos	MP 439	Vo Duy, Sung	ThP 566	Wagner, David	ThP 675
Vertes, Akos	ThOB am 09:10	Vo Duy, Sung	WP 296	Wagner, David	TP 635
Vertes, Akos	TP 135	Vo Duy, Sung	WP 565	Wagner, Elizabeth	WP 562
Vertes, Akos	TP 378	Voelger, Hans Rainer	WP 049	Wagner-Roussel, Elsa	MOE am 09:50
Vertes, Akos	TP 408	Voelker, Sarah E.	ThP 626	Wahlander, Asa	MP 152

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Wahlander, Asa .....	WP 154	Wang, Daojing .....	TP 740	Wang, Miao .....	ThP 399
Wahlig, Taylor .....	ThOG pm 3:10	Wang, Deping .....	WP 659	Wang, Miao .....	WOH am 09:30
Waidelich, Dietmar .....	MP 238	Wang, Deven .....	TP 681	Wang, Minglin .....	ThP 527
Waidelich, Dietmar .....	MP 310	Wang, Di .....	WP 345	Wang, Mingxun .....	MOH pm 4:10
Waite, Randy .....	MP 696	Wang, Dong .....	MP 427	Wang, Mingxun .....	MP 043
Waitt, Greg .....	ThP 539	Wang, Evelyn .....	ThP 066	Wang, Mingxun .....	MP 056
Waitt, Greg .....	ThP 675	Wang, Evelyn .....	ThP 430	Wang, Mingyi .....	ThP 300
Waitt, Greg .....	WP 105	Wang, Fan .....	TP 469	Wang, Minkun .....	ThP 154
Wakabayashi, Masaki .....	TOB pm 3:30	Wang, Fang .....	ThP 648	Wang, Ning .....	WOD pm 4:10
Walch, Axel .....	MP 004	Wang, Fangjun .....	WP 068	Wang, Nu .....	WP 721
Walch, Axel .....	MP 021	Wang, Feng .....	ThP 675	Wang, Pei .....	ThOE am 10:10
Walch, Axel .....	TP 052	Wang, Gehua .....	TP 213	Wang, Pei .....	TOG am 08:30
Waldera-Lupa, Daniel M. ....	WP 248	Wang, Guanbo .....	TP 237	Wang, Pei .....	TP 433
Waldman, Frederic .....	ThP 655	Wang, Guanghui .....	ThP 052	Wang, Pengcheng .....	TP 670
Waldron, Karen .....	TP 530	Wang, Guanghui .....	WP 255	Wang, Peter .....	WP 159
Waldron, Michael .....	MP 505	Wang, Guisong .....	ThP 202	Wang, Peter .....	WP 754
Waldron, Michael .....	TP 501	Wang, Hanliu .....	WP 217	Wang, Phillip .....	WP 644
Waldron, Michael P. ....	MP 764	Wang, Haopeng .....	ThOB am 08:50	Wang, Qi .....	ThP 771
Wales, Thomas .....	WP 220	Wang, Haopeng .....	WP 749	Wang, Qi .....	WOF pm 2:30
Wales, Thomas E. ....	ThP 132	Wang, Hay-Yan J. ....	ThP 388	Wang, Qi .....	WP 007
Wales, Thomas E. ....	WP 221	Wang, Heng .....	WP 530	Wang, Qi .....	WP 008
Walker, Angela .....	ThP 454	Wang, Hoau-Yan .....	WP 148	Wang, Qian .....	TP 221
Walker, Dale .....	ThP 615	Wang, Hong .....	MP 217	Wang, Qian .....	WP 563
Walker, Douglas .....	ThP 304	Wang, Hongmei .....	ThP 436	Wang, Qianghu .....	MP 427
Walker, Gary .....	MP 622	Wang, Hongxia .....	WP 262	Wang, Qianghu .....	ThP 041
Walker, Gary .....	WP 052	Wang, Hongxia (Jessica) .....	ThP 765	Wang, Qinggang .....	MP 765
Walker, Gary .....	WP 732	Wang, Hongxia (Jessica) .....	WP 202	Wang, Qinghe .....	TP 562
Walker, Hunter .....	ThP 733	Wang, Hongxia (Jessica) .....	WP 732	Wang, Qingjun .....	TP 132
Walker, L. DeEtte .....	MP 599	Wang, Hsueh-Chun .....	ThP 444	Wang, Qingqing .....	MP 509
Walker, Larry .....	ThP 426	Wang, Hui .....	TP 028	Wang, Qingqing .....	WP 479
Walla, Michael D. ....	MP 506	Wang, Jack .....	MP 209	Wang, Quanhui .....	ThP 323
Walmsley, Scott .....	WP 119	Wang, Jerry .....	MP 487	Wang, Quanhui .....	WP 016
Walpurgis, Katja .....	WP 301	Wang, Jia .....	TP 284	Wang, Quanhui .....	WP 152
Walsh, Callee .....	MP 380	Wang, Jian .....	MP 366	Wang, Renxue .....	WP 610
Walsh, Callee .....	TOH am 09:50	Wang, Jian .....	TP 087	Wang, Renzhi .....	ThP 669
Walsh, Callee .....	TP 218	Wang, Jian .....	TP 182	Wang, Rong .....	MP 516
Walsh, Callee .....	WP 405	Wang, Jian .....	TP 730	Wang, Rong .....	ThP 196
Walsh, Callee M. ....	TP 038	Wang, Jian .....	WP 534	Wang, Rong .....	TP 458
Walter, Jasmin .....	ThP 773	Wang, Jianqi .....	TP 115	Wang, Rong .....	WP 752
Walter, Ulrich .....	TP 105	Wang, Jianshuang .....	ThP 428	Wang, Ronghua .....	TP 616
Walters, Benjamin .....	MOF am 08:30	Wang, Jianshuang .....	ThP 702	Wang, Ruyi .....	WP 624
Walters, Benjamin .....	WP 218	Wang, Jie .....	WP 638	Wang, Sean .....	TOG am 08:30
Walther, Dirk .....	ThP 075	Wang, Jihong .....	WP 194	Wang, Shao-Zhen .....	MP 346
Walton, Anthony .....	WP 751	Wang, Jinglan .....	MP 072	Wang, Shao-Zhen .....	ThP 528
Walton, Barbara .....	TOH pm 4:10	Wang, Jingqiang .....	TP 142	Wang, Shao-Zhen .....	WP 356
Walton, Jayme .....	ThP 557	Wang, Jingxin .....	TP 168	Wang, Sheng-Ping .....	ThOE am 09:10
Wamhoff, Eike .....	TP 160	Wang, Jingxin .....	TP 422	Wang, Sheng-Ping .....	TP 061
Wan, Terence S.M. ....	WP 582	Wang, Jinhua .....	ThP 527	Wang, Sheng-Ping .....	TP 459
Wan, Xuelian .....	TP 106	Wang, Jinwei .....	TP 028	Wang, Shih-Hao .....	ThP 152
Wan Jamaluddin, Wan Noor Faradalila .....	MP 358	Wang, Jinyuan .....	ThP 406	Wang, Shou-Ze .....	WP 389
Wan Jamaluddin, Wan Noor Faradalila .....	ThP 623	Wang, Jinyuan .....	WP 128	Wang, Shunhai .....	TOE am 10:10
Wanagat, Jonathan .....	TP 692	Wang, John .....	ThP 660	Wang, Tiffany .....	ThP 270
Wang, Alexandre .....	MP 293	Wang, Junhua .....	MP 596	Wang, Tsung-Min .....	WP 462
Wang, Amy .....	MP 514	Wang, Junhua .....	MP 634	Wang, Tzu-Fan .....	ThP 152
Wang, An .....	TP 475	Wang, Junhua .....	WP 287	Wang, Wan .....	MP 487
Wang, An .....	TP 474	Wang, Junhua .....	WP 603	Wang, Wei .....	WP 567
Wang, Baixin .....	MP 563	Wang, Kai-Yi .....	WP 492	Wang, Weihai .....	MOE am 08:30
wang, Beibei .....	TP 306	Wang, Kefei .....	MP 363	Wang, Weihai .....	MOH am 10:10
wang, Beibei .....	WP 653	Wang, Kefei .....	TP 562	Wang, Weixun .....	TP 460
Wang, Beixi .....	MP 301	Wang, Kelly .....	MP 641	WANG, Wenwen .....	TP 758
Wang, Beixi .....	MP 538	Wang, Kevin K.W. ....	ThP 449	Wang, Xianglong .....	ThOE am 10:10
Wang, Beixi .....	TP 198	Wang, Laixin .....	MP 502	Wang, Xianzhe .....	TOB pm 3:10
Wang, Beixi .....	TP 319	Wang, Laixin .....	MP 503	Wang, Xianzhe .....	TP 089
Wang, Beixi .....	WOB am 09:50	Wang, Laixin .....	ThP 438	WANG, Xiao .....	MOB pm 2:50
Wang, Beixi .....	WP 755	Wang, Lanqing .....	WOC pm 3:50	Wang, Xiaodong .....	TP 014
Wang, Benlian .....	TP 118	Wang, Leo .....	MP 743	Wang, Xiaoli .....	MP 500
Wang, Bin .....	WP 413	Wang, Li .....	ThP 206	Wang, Xiaoli .....	WP 116
Wang, Bin .....	WP 629	Wang, Liang .....	MP 670	Wang, Xiaoshi .....	WP 067
Wang, Bruce .....	ThP 472	Wang, Liang .....	MP 669	Wang, Xiaoyan .....	MP 349
Wang, Bruce .....	ThP 483	Wang, Lifei .....	MP 366	Wang, Xinyi .....	WP 343
Wang, Bruce .....	WP 681	Wang, Lin .....	MP 511	Wang, Xu .....	MP 251
Wang, Changsui .....	ThP 611	Wang, Linan .....	MP 442	Wang, Xu .....	ThP 407
Wang, Chao .....	ThP 498	Wang, Linna .....	MOH am 08:30	Wang, Xu .....	WP 633
Wang, Charles .....	MP 270	Wang, Linna .....	ThP 079	Wang, Xu .....	WP 635
Wang, Chengcheng .....	TOB pm 4:10	Wang, Lintao .....	WP 210	Wang, Xuya .....	ThP 170
Wang, Chin-Hsiung .....	WP 415	Wang, Li-Quan .....	WP 630	Wang, Yan .....	ThP 235
Wang, Chunyan .....	ThP 399	Wang, Lusheng .....	WP 046	Wang, Yang .....	WP 390
Wang, Chunyan .....	WOH am 09:30	Wang, Meiyao .....	MOE pm 4:10	Wang, Yen-Chieh .....	ThP 275
Wang, Dan .....	ThP 720	Wang, Meiyao .....	TP 689	Wang, Yi .....	ThP 770

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS

Wang, Yi Sheng.....	MP 393	Webb, Ian.....	ThOB am 10:10	Wells, Mitch.....	MOA am 10:10
Wang, Yingfeng.....	MP 627	Webb, Ian.....	TOC am 08:30	Wells, Mitch.....	MOB pm 2:30
Wang, Yingfeng.....	TP 125	Webb, Ian K.....	MP 677	Wells, Mitch.....	MP 530
Wang, Yinsheng.....	MOC am 09:10	Webb, Ian K.....	TOB am 09:50	Welsch, Matthew E.....	ThP 512
Wang, Yinsheng.....	MP 113	Webb, Ian K.....	TP 716	Wemmer, David.....	ThP 649
Wang, Yinsheng.....	TP 685	Webb, Ian K.....	TP 717	Wen, Bo.....	ThP 323
Wang, Yinsheng.....	WP 251	Webb, Ian K.....	TP 714	Wen, Bo.....	WP 016
Wang, Yinsheng.....	WP 367	Webb, Rebecca.....	MP 381	Wen, Dingyi.....	ThP 109
Wang, Yinsheng.....	WP 366	Webb, Rebecca.....	WP 385	Wen, Dingyi.....	TP 336
Wang, Yi-Sheng.....	MP 309	Webborn, Peter.....	TOH am 08:30	Wen, Jianzhong.....	WP 226
Wang, Yi-Sheng.....	ThP 742	Weber, Darren.....	MP 071	Wen, Zhihui.....	MP 044
Wang, Yi-Sheng.....	WP 691	Weber, Frank.....	MP 431	Wen, Zhihui.....	ThOF pm 3:30
Wang, Yongdon.....	TP 755	Weber, Rolf.....	MP 332	Wendel, Sarah.....	WOF pm 4:10
Wang, Yongdong.....	MP 666	Weber, Wolfgang.....	MP 356	Wendl, Michael C.....	TP 433
Wang, Yongdong.....	TP 248	Wecksler, Aaron.....	TP 159	Wendling, Karen S.....	ThP 609
Wang, Yongdong.....	TP 547	Weckwerth, Wolfram.....	ThP 721	Wendt, Chris.....	MP 424
Wang, Yongdong.....	TP 572	Wedel, Michael.....	WP 519	Wendt, Juergen.....	ThP 609
Wang, Yongdong.....	WP 352	Weekes, Michael.....	MP 133	Wendt, Karin.....	MP 289
Wang, Yongdong.....	WP 719	Wegstein, Jo.....	WP 191	Wendt, Katharyn.....	ThP 471
Wang, Yongqiang.....	MP 222	Wehe, Christoph.....	WP 442	Weng, Guofeng.....	TP 352
Wang, Yunzhu.....	ThP 552	Wehe, Christoph A.....	MP 709	Weng, Hanrong.....	WP 486
Wang, Yuqin.....	MP 244	Wehe, Christoph Alexander.....	MP 007	Weng, Rueyhung.....	TP 120
Wang, Yuzhuo.....	MP 650	Wei, Cong.....	ThP 421	Wenger, Craig D.....	ThP 221
Wang, Yuzhuo.....	MP 649	Wei, Gary.....	TP 545	Wenhai, Jin.....	WP 068
Wang, Yuzhuo.....	TP 351	Wei, Hui.....	MOE pm 3:10	Wenkel, Norbert.....	TP 581
Wang, Ze.....	ThP 151	Wei, Hui.....	MP 172	Wennblom, Trevor.....	MOG pm 4:10
Wang, Zhechen.....	TOA pm 3:50	Wei, Hui.....	MP 180	Wennblom, Trevor.....	MP 033
Wang, Zheng.....	MP 279	Wei, Hui.....	TP 541	Wenschuh, Holger.....	MP 041
Wang, Zhengfang.....	WP 026	Wei, Juan.....	MOB am 09:10	Wenschuh, Holger.....	MP 193
Wang, Zhenghe.....	TP 118	Wei, Juan.....	WP 329	Wenschuh, Holger.....	ThP 046
Wang, Zhenzhen.....	TOA am 08:30	Wei, Juan.....	WP 729	Wentker, Kristina.....	WP 442
Wang, Zhenzhen.....	WP 612	Wei, Michael.....	TP 769	Wentzel, Daria.....	WP 480
Wang, Zuya.....	TP 082	Wei, Pu.....	MP 394	Werb, Zena.....	MP 436
Wanigasekara, Maheshika.....	ThP 244	Wei, Qing.....	ThP 149	Werlich, Mark.....	ThP 759
Wanner, Ina.....	TP 471	Wei, Ru.....	ThP 781	Werth, Emily.....	MP 103
Wanniarachchi, Indika.....	MP 302	Wei, Ru.....	ThP 780	Wesdemiotis, Chrys.....	MOA pm 2:30
Want, Elizabeth J.....	MP 583	Wei, Wei.....	ThP 724	Wesdemiotis, Chrys.....	ThP 509
Ward, Malcolm.....	MP 244	Wei, Xianrong (Jenny).....	WP 433	Wesdemiotis, Chrys.....	TP 253
Ward, Malcolm.....	ThP 163	Wei, Xian-Yong.....	WP 389	Wesdemiotis, Chrys.....	TP 785
Ward, Weslyn.....	WP 480	Wei, Xin.....	ThP 206	Wesdemiotis, Chrys.....	TP 784
Wariishi, Hiroyuki.....	WP 282	Wei, Ziping.....	WP 190	Wesdemiotis, Chrys.....	TP 776
Warkentin, Thomas D.....	ThP 736	Weidner, Steffen M.....	MOA pm 3:50	West, Andy.....	WP 013
Wartner, Isiah M.....	MP 780	Weidner, Steffen M.....	TP 417	West, Graham M.....	WOH pm 2:30
Warnick, Karl.....	MP 696	Weimer, Bart.....	TP 333	West, Graham M.....	ThP 335
Warnke, Stephan.....	TOC am 10:10	Wein, Samuel.....	ThOF pm 2:30	West, Graham M.....	TP 094
Warnken, Uwe.....	ThP 343	Wein, Samuel.....	ThP 237	West, Keith P.....	WP 511
Warrander, John.....	TP 285	Weinman, Marcus.....	ThP 286	West, Raymond.....	MOD pm 3:30
Warren, Daniel.....	WP 128	Weinman, Marcus.....	WOD am 08:30	West, Raymond.....	WP 392
Warren, Daniel.....	WP 505	Weinmann, Wolfgang.....	ThP 590	West, Tiffanie.....	ThP 618
Warren, William.....	MP 185	Weinmann, Wolfgang.....	WP 293	Westermann, Benoit.....	MP 450
Warscheid, Bettina.....	TP 134	Weinreb, Paul.....	ThP 109	Westland, Jessica.....	TP 582
Washabaugh, Michael.....	WP 199	Weinstock, David.....	ThP 219	Westmacott, Garrett.....	TP 213
Washburn, Michael.....	MP 044	Weintraub, Susan T.....	ThP 076	Westmacott, Garrett R.....	TP 216
Washburn, Michael.....	MP 154	Weintraub, Susan T.....	ThP 385	Westphall, Michael.....	ThOG pm 3:10
Washburn, Michael.....	MP 156	Weis, David.....	MOF am 08:50	Westphall, Michael.....	ThP 177
Washburn, Michael.....	ThOF pm 3:30	Weis, David.....	ThP 362	Westphall, Michael.....	ThP 685
Wassif, Christopher A.....	MP 437	Weis, David.....	WP 215	Westphall, Michael.....	TP 669
Watanabe, Hiromitsu.....	ThP 621	Weisbecker, Carl.....	MP 050	Westphall, Michael S.....	ThP 068
Watanabe, Jun.....	MP 476	Weisbecker, Carl.....	MP 331	Westphall, Michael S.....	ThP 179
Watanabe, Jun.....	MP 551	Weisbrod, Chad.....	MOB am 10:10	Westphall, Michael S.....	ThP 178
Watanabe, Jun.....	ThP 633	Weisbrod, Chad.....	WP 734	Westphall, Michael S.....	ThP 327
Watanabe, Jun.....	TP 510	Weisbrod, Chad R.....	MP 084	Westphall, Michael S.....	ThP 348
Watanabe, Jun.....	TP 782	Weisbrod, Chad R.....	MP 699	Westphall, Michael S.....	WOA am 09:50
Watanabe, Kenichi.....	TP 027	Weisbrod, Chad R.....	TP 599	Westphall, Michael W.....	WOD am 10:10
Watanabe, Kyoko.....	WP 614	Weiser, Thomas.....	TP 171	Westrup, Sebastian.....	TP 280
Watanabe, Miki.....	ThP 647	Weismann, Cara M.....	ThP 403	Westrup, Sebastian.....	WP 568
Watanabe, Susumu.....	MP 526	Weisser, Juliane.....	TP 172	Wetie, Armand G. Ngounou.....	WP 457
Watkins, Amanda.....	TP 464	Weisz, Daniel A.....	MP 111	Wetzel, Collin.....	ThP 516
Watkins, Rachel H.....	MP 272	Weitz, Karl.....	ThOG pm 4:10	Wey, Emmanuel.....	TP 222
Watkinson, Tom G.....	WOH pm 3:10	Weitz, Karl.....	TP 676	Wheat, Thomas E.....	MP 729
Watrous, Jeramie.....	MP 056	Weitzel, Douglas H.....	ThP 084	Wheat, Thomas E.....	MP 728
Watson, Bonnie.....	ThP 636	Welch, Emmet.....	WP 640	Wheelan, Patricia.....	WP 480
Watson, Caroline.....	MP 194	Welham, Nathan.....	WP 239	Whelan, Stephen.....	WP 195
Watson, Clifford.....	TP 759	Welling, Stuart.....	ThP 274	Whelan, Stephen A.....	MP 120
Watson, William.....	ThP 433	Wellman, Sydney M.J.....	TP 370	Whelan, Stephen A.....	MP 465
Watson, William.....	WP 475	Wells, Carrow.....	TP 201	Whelan, Stephen A.....	TP 095
Wattenberg, Andreas.....	TP 153	Wells, Edward.....	TP 506	Wheritt, Daniel J.....	ThP 640
Waybright, Timothy J.....	WP 236	Wells, Edward.....	TP 493	Whetton, Anthony.....	WP 114
Waybright, Veronica.....	MP 076	Wells, Edward.....	WP 524	Whetton, Anthony D.....	ThP 036

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



# INDEX OF AUTHORS



White, Kami K.....	WP 485	Williams, Gary .....	ThP 682	Wirth, Mary.....	WP 169
White, Melanie.....	TP 131	Williams, Gordon Harold.....	WP 432	Wiseman, Alexander.....	TP 359
White, Nathan.....	ThP 770	Williams, Grace.....	TP 128	Wiseman, Justin.....	TP 026
White, Thomas.....	ThP 559	Williams, Jeffrey T.....	TP 600	Wiseman, Justin.....	TP 023
White, Thomas.....	TP 267	Williams, Jon.....	ThP 675	Wiseman, Justin.....	WP 400
Whiteaker, Jeff.....	ThP 025	Williams, Jon.....	TP 201	Wishart, David.....	ThP 269
Whiteaker, Jeff.....	ThP 218	Williams, Jon D.....	ThP 539	Wisniewski Junior, Alberto.....	TP 586
Whitehouse, Craig.....	ThP 414	Williams, Jon D.....	WP 105	Wissdorf, Walter.....	TP 735
Whitehouse, Craig M.....	ThP 416	Williams, Jonathan P.....	MP 181	Wissdorf, Walter.....	TP 733
Whitehouse, Craig M.....	TP 267	Williams, Jonathan P.....	TOC pm 3:50	Wissdorf, Walter.....	TP 732
Whitehouse, Craig M.....	WP 408	Williams, Jonathan P.....	WP 586	Wissdorf, Walter.....	TP 731
Whitehurst, Charles E.....	MP 131	Williams, Katherine.....	MP 436	Wistuba, Ignacio.....	WP 141
Whitelegge, Julian.....	ThP 676	Williams, Lee.....	MP 341	Witkowska, H. Ewa.....	ThP 511
Whiteley, Gordon.....	MP 132	Williams, Lee.....	MP 757	Witt, Matthias.....	MOB am 08:50
Whitmarsh, Samuel.....	TP 390	Williams, Lee.....	MP 758	Witt, Matthias.....	MP 549
Whitney, Richard.....	ThP 641	Williams, Lee.....	MP 759	Witt, Matthias.....	TP 610
Wholtman, Mary.....	ThP 199	Williams, Lee.....	MP 760	Witt, Matthias.....	TP 609
Whyatt, Kate.....	ThP 749	Williams, Lee.....	MP 761	Wittrig, Ashley.....	ThOD am 09:50
Wiangnon, Kanjana.....	TP 420	Williams, Lee.....	MP 783	Wittrig, Ashley.....	TP 360
Wickens, Leanne.....	ThP 439	Williams, Lee.....	MP 756	Wleklinski, Michael.....	TP 741
Wickramasekara, Samantha.....	ThP 277	Williams, Lee.....	ThP 589	Wo, Xingde.....	TP 619
Wickramasekara, Samantha I.....	ThP 286	Williams, Michael.....	TP 432	Woenker, Tim.....	TOB pm 2:30
Wickramasinghe, Lanka.....	WP 702	Williams, Pamela.....	MP 380	Wohlfarth, Ariane.....	TP 045
Wider, Gerhard.....	WOF am 09:10	Williams, Preston.....	WP 251	Wojcik, Lisa.....	MP 131
Widjaja, Fanny.....	MP 358	Williams, Spencer J.....	ThOD am 09:10	Wojcik, Roza.....	MP 660
Widjaja, Fanny.....	ThP 623	Williams, Todd.....	MP 474	Wojcik, Roza.....	WP 753
Widmalm, Goran.....	ThP 492	Williams, Tracie.....	TP 155	Wojdyla, Katarzyna.....	MOH am 09:30
Wiechmann, Anja.....	MP 157	Williams, Vaughan.....	MP 699	Wolf, Jan-Christoph.....	WOB pm 3:50
Wiederkehr, Andreas.....	WP 510	Williamson, Andrew.....	WP 114	Wolf, Jean-Pierre.....	MOD am 09:10
Wiederschain, Dmitri.....	ThP 405	Williamson, Catherine.....	MP 583	Wolf, Roland.....	MP 214
Wieghaus, Andreas.....	MP 653	Williamson, James.....	MOH am 09:30	Wolfe, Benjamin.....	ThOA pm 2:50
Wieghaus, Andreas.....	TOB am 10:10	Williamson, James.....	MP 718	Wolfe, Lisa.....	MP 418
Wieland, Jamie.....	WP 310	Williamson, James.....	MP 719	Wolfe, Lisa.....	WP 550
Wiesner, Jan.....	MOE pm 3:30	Williamson, Yulanda.....	TP 155	Wolfe, Lisa M.....	ThP 234
Wigger, Tina.....	TP 612	Willingale, Richard.....	TP 487	Wolff, Jeremy.....	TOE pm 3:10
Wigmore, Cassandra.....	MP 434	Willingham, David.....	WP 299	Wolff, Jeremy J.....	MP 141
Wijeratne, Aruna.....	ThP 210	Willis, Judith.....	ThP 331	Wolff, Jeremy J.....	MP 140
Wijeratne, Neloni.....	TP 195	Willison, Stuart.....	MP 520	Wolff, Suzanne.....	MP 218
Wijeratne, Neloni R.....	ThP 680	Willson, Tim.....	TP 201	Wolf-Yadlin, Alejandro.....	WOH pm 2:50
Wikfors, Rick.....	MP 715	Wilmers, Klaus.....	WP 360	Wolle, Mesay Mulugeta.....	ThP 447
Wikoff, William.....	WP 286	Wilmott, Audrey.....	MP 495	Wolscheid, Bernd.....	MP 432
Wikswow, John.....	MP 585	Wilson, Andrew.....	WP 311	Wolski, Witold.....	MP 260
Wikswow, John P.....	TOB pm 2:50	Wilson, Derek.....	MP 531	Wong, David L.....	WP 680
Wilcock, Brandon.....	MP 502	Wilson, Derek.....	ThP 125	Wong, Judi.....	MP 453
Wildburger, Norelle.....	WP 238	Wilson, Derek.....	WP 757	Wongkongkathep, Piriya.....	MP 145
Wildgoose, Jason L.....	TP 722	Wilson, Derek J.....	WP 779	Wongkongkathep, Piriya.....	TOD am 08:50
Wildgoose, Jason L.....	TP 723	Wilson, Ian.....	TOF am 08:50	Wongkongkathep, Piriya.....	TOE pm 3:10
Wildgruber, Moritz.....	MP 021	Wilson, Ian.....	WP 596	Woo, Jongmin.....	MP 128
Wiley, Steven.....	WOG pm 2:50	Wilson, John P.....	ThP 032	Woo, Jongmin.....	WP 014
Wilhelm, Mathias.....	MP 041	Wilson, John P.....	WP 170	Wood, Elizabeth.....	ThOE am 08:50
Wilhelm, Mathias.....	ThP 046	Wilson, Landon.....	MP 586	Wood, Elizabeth.....	TP 463
Wilhelm, Mathias.....	TP 683	Wilson, Landon.....	TP 680	Wood, Karen.....	TP 227
Wilhelm, Randy.....	MP 736	Wilson, Michael.....	TP 403	Wood, Troy.....	ThP 737
Wilhide, Joshua.....	MP 403	Wilson, Michael.....	WOB pm 4:10	Wood, Troy.....	TP 066
Wilhide, Joshua.....	ThP 167	Wilson, Michael.....	WP 720	Wood, Troy.....	WP 555
Wilhide, Joshua.....	TP 373	Wilson, Michael C.....	MP 039	Wood, William W.....	ThP 178
Wilhide, Joshua.....	TP 404	Wilson, Michael C.....	TP 286	Woodall, Daniel.....	MP 538
Wilhide, Joshua.....	TP 405	Wilson, Richard.....	MP 600	Woodall, Daniel.....	WOB am 09:50
Wilkins, Lynne R.....	WP 485	Wilson, Robin.....	MP 517	Woodard, Jonathan.....	TP 185
Wilkerson, Emily M.....	ThP 348	Wilson, Tracey.....	TP 684	Woodcroft, Ben J.....	ThP 555
Wilkey, Daniel.....	WP 494	Wiltfang, Jens.....	MP 451	Woodling, Kellie.....	MP 769
Wilkey, Daniel W.....	TP 305	Wiltshire, Steven.....	WP 484	Woods, Alisa.....	MP 106
Wilkins, Charles L.....	WP 755	Winck, Flavia.....	WP 460	Woods, Alisa.....	WP 457
Wilkins, John.....	TP 183	Windisch, Janet.....	TOA am 09:30	Woods, Alisa G.....	MP 162
Willard, Stephanie.....	ThP 282	Winget, Jason M.....	WP 766	Woods, Alisa G.....	TP 429
Willard, Stephanie L.....	WP 148	Winkler, Paul C.....	ThOC am 09:50	Woods, Amina S.....	TP 063
Willets, Matt.....	MP 639	Winkler, Paul C.....	WP 777	Woods, Amina S.....	MOH pm 2:50
Willets, Matt.....	MP 008	Winkler, Stephan.....	TP 075	Woods, Amina S.....	ThP 387
Williams, Brad.....	TP 235	Winnike, Jason.....	MP 601	Woods, Amina S.....	TP 002
Williams, Brad J.....	ThP 274	Winter, Benjamin.....	ThP 002	Woods, Jeremy.....	WP 074
Williams, Christopher.....	ThP 394	Winter, Greg.....	MP 403	Woody, Nathaniel.....	WP 618
Williams, Clay E.....	WOD am 10:10	Winter, Greg.....	TP 404	Woody, Nathaniel.....	TP 625
Williams, Cynthia.....	ThP 153	Winter, Greg.....	TP 405	Woolf, Eric.....	WP 108
Williams, Cynthia.....	TP 333	Winter, Gregory.....	TP 373	Woolf, Eric.....	WP 652
Williams, Darrell.....	TP 724	Winter, Michael.....	WP 760	Woolley, G. Andrew.....	MP 202
Williams, Emily.....	TP 228	Wintrode, Patrick.....	ThP 122	Wooster, Luke.....	WP 759
Williams, Evan.....	MP 260	Wintrode, Patrick.....	ThP 121	Wooten, Mark.....	TP 292
Williams, Evan R.....	TP 745	Wirth, Christopher.....	MP 554	Wootton, Christopher.....	WP 729
Williams, Evan R.....	WOB am 09:10	Wirth, Hans-Jürgen.....	ThP 783	Wopperer, Samuel.....	TP 245

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Wormwood, Kelly.....	TP 429	Wu, Xia.....	ThOC pm 3:50	Xiaotun, Guo.....	MP 357
Wormwood, Kelly.....	WP 457	Wu, Xia.....	ThP 465	Xiaoying, Jia.....	MP 122
Worsnop, Douglas.....	TOA pm 3:10	Wu, Xia.....	ThP 464	Xie, Boer.....	MP 171
Worth, Andrew J.....	TP 310	Wu, Xinyan.....	MP 255	Xie, Dan.....	ThOE am 09:10
Worth, Andrew J.....	WOH am 08:50	Wu, Xinyan.....	MP 440	Xie, Dan.....	TP 459
Worthington, Kenneth.....	ThP 748	Wu, Xinyan.....	ThP 082	Xie, Dianlin.....	TP 541
Wouters, Eloy R.....	TP 740	Wu, Xinyan.....	ThP 219	Xie, Fang.....	TP 169
Wright, David.....	MP 058	Wu, Xinyan.....	TOG am 09:10	Xie, Fang.....	WOE am 08:30
Wright, Katherine.....	TP 251	Wu, Xiongwu.....	ThP 314	Xie, Fang.....	WP 495
Wright, Katherine.....	WP 271	Wu, Xudong.....	WOG am 08:30	Xie, Hongwei.....	ThP 775
Wright, Michael.....	WP 425	Wu, Yibo.....	MP 260	Xie, Hongwei.....	WP 209
Wright, Phillip C.....	ThP 083	Wu, Yiman.....	MP 593	Xie, Huizhi.....	WP 652
Wright, Phillip C.....	ThP 645	Wu, Yiman.....	TP 655	Xie, Jianping.....	TP 122
Wright, Yvonne.....	MP 287	Wu, Yingnian.....	MP 626	Xie, Ling.....	ThP 290
Wright, Yvonne.....	TOG pm 4:10	Wu, Yue.....	ThP 553	Xie, Michael.....	WP 074
Wright, Yvonne.....	WP 429	Wu, Yunqi.....	WP 234	Xie, Peng.....	MP 232
Wright, Zachary.....	TP 138	Wu, Yuxi.....	ThP 308	Xie, Peng.....	TP 123
Wrobel, John.....	ThP 025	Wu, Zhanpin.....	MP 600	XIE, Shengkai.....	MP 330
Wrobel, John.....	TP 433	Wu, Zhanpin.....	WP 576	Xie, Wei.....	WP 652
Wrobel, John A.....	ThP 290	Wu, Zhaoxiang (Sean).....	MP 293	Xie, Xiaolei.....	TP 445
Wrobel, John A.....	TP 173	Wu, Zhen.....	WP 169	Xie, Xiaolei.....	WP 137
Wrobel, John A.....	WOG pm 3:50	Wu, Zhiping.....	MP 217	Xie, Xiaolei.....	WP 218
Wrona, Mark.....	MP 714	Wu, Zhixiang.....	TP 106	Xie, Zhongyu.....	TP 112
Wrona, Mark.....	TP 629	Wu, Zhongtao.....	WP 638	Xin, Baozhong.....	WP 530
Wrona, Mark.....	WP 637	Wu, Kuen-Yuh.....	TP 312	Xin, Lei.....	ThP 016
Wu, Chaochao.....	TP 169	Wuehr, Martin.....	MP 259	Xing, Jie.....	MP 342
Wu, Chaochao.....	WOE am 08:30	Wuest, Bernhard.....	WP 355	Xing, Jie.....	MP 351
Wu, Chaochao.....	WOG pm 2:50	Wuest, Bernhard.....	WP 560	Xing, Jie.....	MP 535
Wu, Chaochao.....	WP 513	Wühr, Martin.....	TP 180	Xing, Jie.....	ThP 587
Wu, Charlene.....	TP 312	Wurch, Louie L.....	MP 129	Xing, Jie.....	TP 275
Wu, Chih-Ching.....	ThP 291	Wurlitzer, Marcus.....	WP 744	Xing, Jie.....	WP 449
Wu, Chih-Hsing.....	ThP 152	Wurtele, Eve Syrkin.....	ThP 652	Xing, Jinsong.....	TP 520
Wu, Ching.....	MP 386	Wüthrich, Thomas.....	ThP 590	Xing, Jinsong.....	TP 523
Wu, Ching.....	ThP 507	Wyatt, Shane.....	MP 364	Xing, Weiman.....	ThP 470
Wu, Ching.....	WP 758	Wyczalkowski, Matthew A.....	TP 433	Xiong, Bob.....	WP 040
Wu, Christine.....	WOG pm 4:10	Wylie, Philip.....	MP 347	Xiong, Caiqiao.....	MP 400
Wu, Christine.....	WP 017	Wynne, Kieran.....	WP 475	Xiong, Lei.....	WP 124
Wu, Christine.....	WP 037	Wynne, Paul.....	MP 419	Xiong, Weili.....	ThP 332
Wu, Cong.....	TP 165	Wynne, Paul.....	WP 625	Xiong, Zhichao.....	WP 473
Wu, Fengqi.....	WP 416	Wypych, Jette.....	TP 239	Xiu, Lichen.....	WP 162
Wu, Herren.....	TP 431	Wysocki, Vicki.....	MP 138	Xu, April.....	TP 236
Wu, Houdini.....	ThP 394	Wysocki, Vicki.....	ThOA pm 3:10	Xu, April.....	WP 274
Wu, Hsuan-Wen.....	ThP 388	Wysocki, Vicki.....	ThOC pm 2:50	Xu, Dong.....	TP 125
Wu, Jason Boyang.....	WP 246	Wysocki, Vicki.....	ThOF am 09:30	Xu, Dunming.....	MP 348
Wu, Jikang.....	ThOF am 09:30	Wysocki, Vicki.....	ThP 113	Xu, Fuxing.....	WOD pm 2:30
Wu, Jing.....	MP 446	Wysocki, Vicki.....	ThP 259	Xu, Hongliang (Leo).....	TP 547
Wu, Jing.....	WP 060	Wysocki, Vicki.....	ThP 296	Xu, Hongliang (Leo).....	WP 352
Wu, Jing.....	WP 458	Wysocki, Vicki.....	TOD am 09:10	Xu, Keyang.....	WP 277
Wu, Jing.....	WP 501	Wysocki, Vicki.....	WOD pm 3:50	Xu, Libin.....	ThOG pm 2:50
Wu, Jinn.....	WP 488	Wysocki, Vicki H.....	MP 229	Xu, Libin.....	ThP 485
Wu, Jinn.....	WP 529	Wysocki, Vicki H.....	TP 227	Xu, Meng.....	WP 527
Wu, Jinn.....	WP 630	Wytenbach, Thomas.....	MOC pm 4:10	Xu, Min.....	WP 673
Wu, Kuan-Jung.....	ThP 501	Xia, Hanxue.....	MP 050	Xu, Mingguo.....	TP 655
Wu, Kuen-Yuh.....	ThP 434	Xia, Shijing.....	MP 325	Xu, Ping.....	WP 016
Wu, Lauren.....	WOE am 08:50	Xia, Wenle.....	TP 457	Xu, Pu-Ting.....	ThP 390
Wu, Lauren D.....	ThP 729	Xia, Wenle.....	TP 470	Xu, Pu-Ting.....	ThP 642
Wu, Lianming.....	TP 394	Xia, Yu.....	MP 323	Xu, Pu-Ting.....	TP 688
Wu, Long.....	ThP 051	Xia, Yu.....	ThOD am 08:50	Xu, Qun.....	MP 469
Wu, Long.....	WP 053	Xia, Yu.....	ThOG pm 3:50	Xu, Shaohang.....	WP 016
Wu, Long.....	WP 054	Xia, Yu.....	ThP 187	Xu, Shengsheng.....	ThP 090
Wu, Minghuo.....	WOC pm 4:10	Xia, Yu.....	ThP 192	Xu, Sihang.....	MP 478
Wu, Minghuo.....	WP 561	Xia, Yu.....	ThP 734	Xu, Sophia (Xiaohui).....	TP 024
Wu, Qihua.....	WP 569	Xia, Yu.....	TP 290	Xu, Tao.....	WP 021
Wu, Qinghao.....	MOD pm 3:50	Xia, Yu.....	TP 353	Xu, Wei.....	MP 649
Wu, Qinghao.....	ThP 365	Xia, Yu.....	WP 021	Xu, Wei.....	MP 650
Wu, Quan.....	TP 100	Xia, Yu.....	WP 388	Xu, Wei.....	ThP 531
Wu, Ronghu.....	ThP 230	Xia, Yuan-qing.....	MP 197	Xu, Wei.....	ThP 757
Wu, Ronghu.....	TP 191	Xiao, Chunying.....	WP 700	Xu, Wei.....	TP 351
Wu, Shari.....	TP 502	Xiao, Gang.....	MOE pm 2:50	Xu, Wei.....	TP 720
Wu, Shiao-Lin.....	TP 154	Xiao, Gang.....	WP 254	Xu, Weifeng.....	MP 074
Wu, Shiao-Lin.....	TP 264	Xiao, Hua.....	MP 456	Xu, Wenfeng.....	ThP 103
Wu, Si.....	MOG pm 3:30	Xiao, kaijie.....	ThP 063	Xu, Xiaobin.....	ThP 109
Wu, Si.....	ThP 064	Xiao, Kunhong.....	MP 082	Xu, Xiaoyan.....	TP 619
Wu, Si.....	ThP 062	Xiao, Kunhong.....	ThP 133	Xu, Xiaoyan.....	WP 731
Wu, Si.....	TOE pm 2:50	Xiao, Saijin.....	TP 388	Xu, Xin.....	MP 514
Wu, Si.....	WP 088	Xiao, Xifeng.....	ThP 366	Xu, Yang.....	WP 108
Wu, Sz-Wei.....	ThP 160	Xiao, Yongsheng.....	TP 685	Xu, Yang.....	WP 652
Wu, Wei.....	MP 610	Xiao, Yu.....	TP 718	Xu, Yaolin.....	ThP 709
Wu, Weidong.....	WP 416	Xiaorong, Wang.....	ThP 463	Xu, Yingrong.....	ThP 359

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS

Xu, Yuan.....	MP 605	Yang, Jingzhi.....	WP 715	Yao, Jingwen.....	TP 166
Xu, Zangwei.....	TOF pm 3:30	Yang, Jonathan.....	ThP 223	Yao, Jinting.....	TP 281
Xu, Zhe.....	TP 169	Yang, Julie.....	ThP 044	Yao, Jinting.....	WP 629
Xu, Zhe.....	WOE am 08:30	Yang, Jun.....	MP 430	Yao, Ming.....	WP 639
Xuan, Yue.....	MP 186	Yang, Juncong.....	ThP 252	Yao, Qiuming.....	TP 125
Xuan, Yue.....	WP 265	Yang, Juncong.....	TP 014	Yao, Tso-Pang.....	WP 259
Xue, Baiyi.....	MP 587	Yang, Juncong.....	TP 484	Yao, Xiao Jie.....	ThP 133
Xue, Bing.....	ThP 574	Yang, Juncong.....	WP 654	Yao, Xiaojie.....	MP 082
Xue, Chang.....	MP 192	Yang, Junhai.....	MOB am 09:50	Yao, Xudong.....	MP 251
Xue, Chang.....	TOD pm 2:50	Yang, Junhai.....	MP 017	Yao, Xudong.....	ThP 194
Xue, Changhu.....	ThP 718	Yang, Junhai.....	MP 023	Yao, Xudong.....	TP 486
Xue, Liang.....	TP 670	Yang, Junhai.....	MP 029	Yao, Xudong.....	WP 502
Xue, Lingling.....	WP 652	Yang, Junhai.....	ThP 009	Yao, Yuyu.....	ThP 099
Yabannavar, Asha.....	ThP 103	Yang, Junhai.....	WP 001	Yao, Zhiping.....	MP 131
Yabuki, Masashi.....	TP 027	Yang, Lili.....	MP 592	Yao, Zhongping.....	WP 375
Yabusaki, Katsumi.....	WP 018	Yang, Linan.....	MP 574	Yarasheski, Kevin.....	TP 651
Yadavalli, Sivaramakrishna.....	MP 254	Yang, Menglin.....	TP 537	Yariwake, J. H.....	WP 668
Yager, James D.....	WP 581	Yang, Ming-Hui.....	TP 200	Yaron, Avraham.....	ThP 197
Yagnik, Gargey.....	MP 473	Yang, Ming-Hui.....	WP 462	Yates, John.....	ThOC pm 3:10
Yagnik, Gargey.....	TP 043	Yang, Ning.....	TP 165	Yates, John.....	ThP 021
Yagnik, Gargey.....	TP 022	Yang, Paul.....	ThP 565	Yates, John R.....	WP 247
Yalcin, Talat.....	ThP 185	Yang, Paul.....	TP 578	Yates, Nathan.....	ThP 042
Yamabe, Keiko.....	MP 755	Yang, Peiyong.....	ThP 383	Yates, Nathan.....	TP 460
Yamada, Iwao.....	WP 018	Yang, Pengxiang.....	ThP 569	Yates, Nathan.....	TP 615
Yamada, Iwao.....	WP 070	Yang, Ping.....	MP 429	Yates, Nathan.....	WOG pm 4:10
Yamada, Masaki.....	ThP 398	Yang, Seo-Yun.....	WP 224	Yates, Nathan.....	WP 017
Yamada, Naoyuki.....	WP 102	Yang, Shuang.....	TP 003	Yates, Nathan.....	WP 037
Yamada, Takayuki.....	ThP 375	Yang, Shuang.....	TP 478	Yates, Nathan.....	WP 158
Yamada, Tesshi.....	WP 143	Yang, Shuang.....	TP 477	Yates, Sandy.....	MP 614
Yamada, Toichiro.....	TP 027	Yang, Shuiping.....	TP 388	Yates III, John.....	TP 483
Yamada, Yoshihiro.....	TP 166	Yang, Sophia.....	WOE pm 3:50	Yates III, John R.....	MP 065
Yamamoto, Tatsuya.....	ThP 111	Yang, Tianjiao.....	ThP 148	Yates III, John R.....	MP 220
Yamashita, Masami.....	WOG am 09:30	Yang, Wan Seok.....	ThP 512	Yates III, John R.....	WP 730
Yamauchi, Yoshio.....	ThP 520	Yang, Weiming.....	ThOH am 10:10	Yates, III, John R.....	TP 091
Yamauchi, Yoshio.....	WP 372	Yang, Weiming.....	WOF pm 4:10	Yau, Natalie.....	TP 260
Yan, Bo.....	WP 703	Yang, Xi.....	MP 267	Yavor, Mikhail.....	ThOB pm 3:10
Yan, Jing.....	ThOC pm 2:50	Yang, Xian.....	WP 468	Yaworsky, Dustin.....	ThP 274
Yan, Ping.....	ThOE am 10:10	Yang, Xianshu.....	MP 131	Yazawa, Itaru.....	MP 740
Yan, Ping.....	ThP 025	Yang, Xianshu.....	TOF pm 3:30	Yazawa, Itaru.....	TP 510
Yan, Ping.....	ThP 218	Yang, Xiaohan.....	TP 675	Ye, Gene F.....	ThP 505
Yan, Ping.....	TOG am 08:30	Yang, Xiaoyu.....	MP 051	Ye, Hongping.....	ThP 143
Yan, Xiaojing.....	TOB pm 3:50	Yang, Xingye.....	WP 488	Ye, Joshua Sha.....	TP 630
Yan, Xiaojing.....	TP 194	Yang, Xu.....	TP 079	Ye, Joshua Sha.....	WP 558
Yan, Xin.....	TP 387	Yang, Yanan.....	MP 518	Ye, Kai.....	TP 433
Yan, Xinjian.....	MP 604	Yang, Yanan.....	TP 179	Ye, Mingliang.....	TP 694
Yan, Xinjian.....	WP 051	Yang, Yanan.....	WOG am 10:10	Ye, Mingliang.....	WP 068
Yan, Xinjian.....	WP 119	Yang, Yanan.....	WP 290	Ye, Mingliang.....	WP 473
Yan, Xiuping.....	WP 473	Yang, Yang.....	TP 353	Ye, Sha Joshua.....	MP 339
Yan, Yuetian.....	MP 172	Yang, Yanling.....	MP 217	Ye, Sha Joshua.....	ThP 217
Yan, Yuetian.....	ThP 107	Yang, Yanou.....	WP 622	Ye, Sha Joshua.....	TP 558
Yanes Santos, Enrique.....	ThP 692	Yang, Yijie.....	TP 366	Ye, Sha Joshua.....	WP 648
Yang, Bing.....	ThP 051	Yang, Yimin.....	ThP 131	Ye, Xiaoying.....	MP 132
Yang, Bo.....	MP 328	Yang, Yinghang.....	ThP 061	Ye, Xiaoyun.....	WP 461
Yang, Bo.....	ThP 718	Yang, Yingying.....	ThP 463	Yefremova, Yelena.....	ThP 107
Yang, Charles.....	ThP 565	Yang, Yong.....	ThP 173	Yeh, Lee-Chuan Caroline.....	ThP 385
Yang, Charles.....	TP 578	Yang, Zamin.....	MP 129	Yeh, Suzie.....	TOE am 08:50
Yang, Charles.....	TP 579	Yang, Zhao.....	TP 143	Yelamanchi, Soujanya D.....	MP 255
Yang, Charles R.....	TP 469	Yang, Zhao.....	TP 139	Yen, Roger.....	MP 453
Yang, Charles T.....	TP 284	Yang, Zhao.....	WP 241	Yen, Ten-Yang.....	MP 453
Yang, Charles T.....	TP 280	Yang, Zhibo.....	WOB pm 3:10	Yergey, Alfred L.....	MP 437
Yang, Charles T.....	TP 580	Yang, Zhibo.....	WP 009	Yergey, Alfred L.....	ThP 491
Yang, Cheng.....	ThP 530	Yang, Zhibo.....	WP 395	Yi, Pan.....	ThOE am 09:10
Yang, Cheng.....	WP 736	Yang, Zhibo.....	WP 741	Yi, Yi MP 626.....	
Yang, Chenxi.....	MP 460	Yang, Zhicheng.....	TP 322	Yi, Zhengping.....	TP 139
Yang, Cuiping.....	WP 739	Yang, Zicheng.....	MP 689	Yi, Zhengping.....	TP 143
Yang, Dorothy.....	TP 571	Yang, Zicheng.....	MP 720	Yi, Zhengping.....	TP 488
Yang, Dorothy.....	WP 355	Yang, Zong.....	MP 378	Yi, Zhengping.....	WP 241
Yang, Dorothy.....	WP 560	Yang, Zong.....	WP 416	Yigit, Mehmet.....	MP 385
Yang, Fukang.....	MP 643	Yang, Zong.....	WP 413	Yildirim, Funda.....	MP 066
Yang, Fuquan.....	MP 222	Yang, Zong.....	WP 414	Yilmaz, Mustafa.....	WP 556
Yang, Guixiang.....	WP 739	Yang, Zong.....	WP 407	Yi-Ming, Yang.....	WP 159
Yang, Han-Yin.....	ThP 326	Yang, Zong.....	WP 404	Yin, Feng.....	TP 494
Yang, Hao.....	MP 221	Yano, Ikuko.....	ThP 672	Yin, Haidi.....	TP 421
Yang, Hao.....	MP 748	Yao, Bella.....	TP 632	Yin, Haidi.....	WP 060
Yang, Hao.....	ThOE pm 2:50	Yao, Chunxiang.....	MP 120	Yin, Haidi.....	WP 458
Yang, Heyi.....	WP 303	Yao, Chunxiang.....	MP 465	Yin, Haidi.....	WP 500
Yang, Hongbing.....	ThP 342	Yao, Chunxiang.....	WOF pm 2:30	Yin, Haidi.....	WP 501
Yang, Jane.....	MP 207	Yao, Chunxiang.....	WP 195	Yin, Hengfu.....	TP 675
Yang, Jiange.....	TP 142	Yao, Guocan.....	TP 391	Yin, Hongfeng.....	TP 334

Program code: M,T,W, Th = Day

O = Oral, P = Poster

Time or poster number



# INDEX OF AUTHORS

Yin, Hongfeng.....	WP 205	Yu, Qing.....	TP 168	Zamora, Ismael.....	WP 618
Yin, John.....	ThP 179	Yu, Sean.....	WP 659	Zampronio, Cleidiane G.....	WP 082
Yin, Lihui.....	WP 414	Yu, X. Christopher.....	WP 049	Zampronio, Cleidiane G.....	WP 765
Ying, Wantao.....	TP 442	Yu, Xiang.....	ThP 058	Zandkarimi, Fereshteh.....	ThP 380
Yocum, Anastasia.....	WP 045	Yu, Xiang.....	ThP 144	Zandkarimi, Fereshteh.....	ThP 606
Yoda, Akinori.....	ThP 219	Yu, Xiang.....	ThP 698	Zang, Alex.....	TP 634
Yokoi, Yasuto.....	WP 287	Yu, Xiang.....	TP 323	Zang, Li.....	WP 081
Yokomizo, Takehiko.....	WOH am 09:10	Yu, Yanbao.....	ThP 283	Zang, Qingce.....	ThP 669
Yokoo, Sami.....	WP 460	Yu, Yanbao.....	ThP 284	Zang, Tuo.....	MP 214
Yokota, Ryo.....	MP 107	Yu, Yaping.....	ThP 117	Zang, Xiaoling.....	MP 599
Yonemori, Kim.....	WP 485	Yu, Yi-Kuo.....	MP 042	Zanon, Stephen.....	TP 178
Yong, Huiyee.....	ThP 126	Yu, Yi-Kuo.....	ThP 195	Zanotelli, Vito.....	TP 086
Yong, Wei.....	WP 407	Yu, Ying Qing.....	TP 157	Zaragoza, William J.....	TP 210
Yonggang, Liu.....	WP 653	Yu, Ying Qing.....	TP 158	Zare, Richard.....	MOD pm 3:50
Yoo, Jong Shin.....	TP 257	Yu, Ying Qing.....	TP 265	Zare, Richard.....	ThP 365
Yoo, Yejin.....	MP 453	Yu, Ying-Qing.....	TP 156	Zarraga, Gabriela.....	TP 145
Yoon, Seongho.....	TP 604	Yu, Ying-Qing.....	TP 541	Zarrine-Afsar, Arash.....	ThOD pm 2:30
Yoon, Sohee.....	TP 199	Yu, Ying-Qing.....	WP 023	Zaslaver, Olga.....	TP 638
Yoon, Sung Hwan.....	TP 286	Yu, Yonghao.....	TP 115	Zatz, Mayana.....	MP 459
Yoon, Sung Hwan.....	TP 377	Yu, Zhihao.....	WP 692	Zavalin, Andre.....	ThP 009
Yoon, Sung Hwan.....	TP 400	Yuan, Hang.....	ThP 715	Zavalin, Andre.....	WP 001
Yoon, Sung Hwan.....	TP 403	Yuan, Haodan.....	ThP 496	Zdaril, Peter.....	ThP 764
Yoon, Sung Hwan.....	TP 386	Yuan, Joshua.....	ThP 123	Zeidan, Asad.....	ThP 297
Yorke, Selwyn.....	MP 514	Yuan, Joshua.....	TP 678	Zeilinger, Katrin.....	MP 585
Yoshida, Hideo.....	WP 070	Yuan, Long.....	MOF pm 3:30	Zekavat, Behrooz.....	MP 296
Yoshida, Masaru.....	ThP 375	Yuan, Min.....	WOD am 09:50	Zekavat, Behrooz.....	TP 347
Yost, Richard A.....	MP 011	Yuan, Min.....	WP 608	Zekavat, Behrooz.....	WP 658
Yost, Richard A.....	MP 240	Yuan, Moucun.....	WP 127	Zekavat, Behrooz.....	WP 657
Yost, Richard A.....	MP 376	Yuan, Wenlin.....	WP 484	Zelesky, Veronica.....	MP 639
Yost, Richard A.....	MP 408	Yuan, Zuofei.....	ThP 070	Zelesky, Veronica.....	TP 625
Yost, Richard A.....	MP 631	Yuan, Zuofei.....	TP 099	Zelesky, Veronica.....	TP 627
Yost, Richard A.....	MP 785	Yuan, Zuofei.....	WP 097	Zelesky, Veronica.....	WP 618
Yost, Richard A.....	Special	Yuan, Zuo-Fei.....	TP 184	Zelesky, Veronica.....	WP 627
Yost, Richard A.....	ThP 449	Yuan, Zuo-Fei.....	WP 053	Zeller, Martin.....	WP 301
Yost, Richard A.....	ThP 579	Yue, Hongfei.....	WP 527	Zellner, Maria.....	WP 140
Yost, Richard A.....	TP 044	Yue, Xiaofei.....	ThP 669	Zemla, Marcin.....	TP 381
Yost, Richard A.....	WOC am 08:30	Yue, Xiaoshan.....	ThP 200	Zen, Nobuyuki.....	ThP 761
Yost, Richard A.....	WP 397	Yue, Xiaoshan.....	ThP 207	Zeneyedpour, Lona.....	ThP 209
Yost, Richard A.....	WP 647	Yue, Zhenfeng.....	WP 416	Zeneyedpour, Lona.....	WP 151
Yost, Richard A.....	WP 680	Yueshuai, Guo.....	WP 149	Zeng, Hang.....	ThP 677
You, Han-Pin.....	TP 200	Yui, Yuko.....	MP 766	Zeng, Jianing.....	MP 074
You, Ximeng.....	MP 575	Yuill, Elizabeth.....	WOB am 08:30	Zeng, Jianing.....	TOE am 09:30
Youhnovski, Nikolay.....	WP 535	Yuki, Hashi.....	WP 629	Zeng, Jianing.....	WP 636
Young, Andrew.....	ThP 092	Yukihira, Daichi.....	MP 062	Zeng, Lingfei.....	WP 163
Young, Holly.....	TP 304	Yukihira, Daichi.....	WP 282	Zeng, Lixia.....	ThP 395
Young, Holly C.....	TP 568	Yun, Tatyana.....	TP 072	Zeng, Lu.....	MP 713
Young, Lydia M.....	ThP 106	Yurong, Guo.....	MOH pm 4:10	Zeng, Rong.....	WP 044
Young, Michelle E.....	MP 233	Zabet Moghaddam, Masoud.....	WP 234	Zeng, Rong.....	WP 090
Young, Nicolas L.....	MP 230	Zabet Moghaddam, Masoud.....	WP 615	Zeng, Shang.....	WP 704
Young, Nicolas L.....	ThOF pm 3:10	Zabrouskov, Vlad.....	MP 717	Zeng, Wen-Feng.....	WP 054
Young, Nicolas L.....	ThP 129	Zabrouskov, Vlad.....	WP 737	Zeng, Wen-Feng.....	WP 053
Young, Nicolas L.....	TOE pm 4:10	Zacca, Jorge.....	ThOA am 09:30	Zeng, Yi.....	MP 020
Young, Nicolas L.....	TP 456	Zachara, Natasha.....	ThP 082	Zenka, Roman.....	ThP 272
Young, Nicolas L.....	WP 735	Zacharos, Athanasios.....	MP 668	Zenobi, Renato.....	MP 303
Young, Ryland.....	MP 563	Zachova, Katerina.....	ThP 149	Zenobi, Renato.....	TP 742
Young, Sydney.....	MP 239	Zahari, Muhammad.....	MP 440	Zenobi, Renato.....	WOB pm 3:50
Youngmin, Hong.....	ThP 554	Zahari, Muhammad S.....	MP 255	Zenobi, Renato.....	WOF am 09:10
Yoveva, Aneliya.....	MP 092	Zahari, Sadiq.....	TOG am 09:10	Zequi, Stenio.....	MP 464
Yu, Chi Li.....	MOA am 08:50	Zahedi, René.....	ThP 224	Zerweck, Johannes.....	MP 193
Yu, Chuan-Yih.....	ThP 165	Zahedi, René.....	ThP 225	Zgoda, Victor.....	ThP 248
Yu, Chuan-Yih.....	WP 064	Zahedi, René.....	TP 105	ZHA, Cheng.....	WP 413
Yu, Clinton.....	ThP 463	Zaher, Ahmed M.....	WP 319	Zhai, Bo.....	WOG am 09:10
Yu, Clinton.....	ThP 462	Zaia, Joseph.....	ThOH pm 4:10	Zhai, Yanbing.....	MP 649
Yu, Haoying.....	TP 245	Zaia, Joseph.....	ThP 711	Zhan, Dongliang.....	WP 127
Yu, Haoying.....	WP 598	Zaia, Joseph.....	ThP 734	Zhan, Song.....	TP 281
Yu, Jau-Song.....	ThP 291	Zaia, Joseph.....	ThP 730	Zhan, Zhaoqi.....	MP 351
Yu, Jau-Song.....	WP 493	Zaia, Joseph.....	ThP 771	Zhan, Zhaoqi.....	MP 342
Yu, Jian.....	TP 633	Zaia, Joseph.....	WP 007	Zhan, Zhaoqi.....	MP 535
Yu, Jianshi.....	ThP 638	Zaia, Joseph.....	WP 008	Zhan, Zhaoqi.....	ThP 587
Yu, Jianshi.....	ThP 642	Zaia, Joseph.....	WP 085	Zhan, Zhaoqi.....	TP 275
Yu, John.....	MP 515	Zaia, Joseph.....	WP 674	Zhan, Zhaoqi.....	WP 449
Yu, Kate.....	ThP 529	Zajac, Matt.....	TOF pm 4:10	Zhang, Aiping.....	MP 424
Yu, Kenneth.....	WP 499	Zakharov, Florence.....	MP 347	Zhang, Aiping.....	ThOE am 09:50
Yu, Li-Rong.....	WP 249	Zaknoun, Hafid.....	MP 531	Zhang, Aiping.....	TP 467
Yu, Li-Rong.....	WP 470	Zalko, Daniel.....	TP 309	Zhang, Aming.....	TP 240
Yu, Lu.....	WP 160	Zaman, Uzma.....	ThP 459	Zhang, Anna.....	TP 154
Yu, Peng.....	MP 611	Zambardi, Gilles.....	TP 219	Zhang, Bai.....	ThP 156
Yu, Qing.....	MOH am 09:10	Zamora, Ismael.....	MP 639	Zhang, Bailin.....	ThP 405
Yu, Qing.....	ThP 493	Zamora, Ismael.....	TP 625	Zhang, Bo.....	MOG am 10:10

Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number

# INDEX OF AUTHORS



Zhang, Bo.....	TOF pm 3:10	Zhang, Qian.....	WP 184	Zhang, Zhen.....	ThP 040
Zhang, Boyan.....	MOG pm 2:50	Zhang, Qibin.....	ThOG pm 4:10	Zhang, Zhen.....	ThP 156
Zhang, Boyu.....	TP 790	Zhang, Qibin.....	WP 088	Zhang, Zhen.....	ThP 295
Zhang, Chao.....	TP 296	Zhang, Qinghe.....	WP 404	Zhang, Zheng-Xiang.....	ThP 533
Zhang, Chen.....	ThP 660	Zhang, Rena.....	TOE am 08:50	Zhang, Zheng-Xiang.....	TP 533
Zhang, Chenghong.....	WP 712	Zhang, Rong.....	ThP 527	Zhang, Zhenqing.....	WP 739
Zhang, Chi.....	MP 580	Zhang, Rui.....	MP 550	Zhang, Zhibin.....	ThP 537
Zhang, Chi.....	TP 756	Zhang, Rui.....	ThP 123	Zhang, Zhiping.....	TP 385
Zhang, Chunchao.....	ThP 454	ZHANG, Ruiping.....	ThP 669	Zhang, Zhongqi.....	TP 240
Zhang, Dongdong.....	MP 357	Zhang, Sheng.....	MP 118	Zhang, Zhongqi.....	TP 642
Zhang, Fan.....	TP 264	Zhang, Sheng.....	ThP 173	Zhang, Zhongqi.....	WP 718
Zhang, Fantong.....	TP 355	Zhang, Sheng.....	TP 203	Zhang, Zhichuan.....	MP 009
Zhang, Guangnong.....	TP 494	Zhang, Shenyan.....	ThP 323	Zhao, Hanwei.....	ThP 116
Zhang, Hailong.....	ThOH pm 3:30	Zhang, Shunsheng.....	MP 357	Zhao, Hanwei.....	TOE am 10:10
Zhang, Hailong.....	TP 332	Zhang, Suhong.....	ThP 282	Zhao, Hongyan.....	WP 764
Zhang, Hailong.....	TP 335	Zhang, Suping.....	TP 544	Zhao, Hui.....	ThOA pm 3:30
Zhang, Haiying.....	WOF am 08:30	Zhang, Terry.....	WP 228	Zhao, Lei.....	ThP 218
Zhang, Hao.....	MP 111	Zhang, Terry.....	WP 263	Zhao, Liang.....	WP 581
Zhang, Hao.....	MP 173	Zhang, Tianhong.....	WP 739	Zhao, Matthew M.....	WP 710
Zhang, Hao.....	ThOF am 10:10	Zhang, Tong.....	ThP 723	Zhao, Ning.....	TP 367
Zhang, Hao.....	ThP 362	Zhang, Wanjun.....	WP 166	Zhao, Qihong.....	ThP 441
Zhang, Hao.....	ThP 461	Zhang, Wei.....	ThP 324	Zhao, Rui.....	TOA am 08:50
Zhang, Huaizhong.....	ThP 034	Zhang, Weiyi.....	ThOD pm 4:10	Zhao, Rui.....	TP 324
Zhang, Hui.....	MP 432	Zhang, Wen.....	WP 683	Zhao, Rui.....	WOG pm 2:50
Zhang, Hui.....	ThOH am 10:10	Zhang, Wenhao.....	MP 378	Zhao, Rui.....	WP 088
Zhang, Hui.....	ThP 040	Zhang, Wenzhu.....	MP 165	Zhao, Shuai Sherry.....	MP 079
Zhang, Hui.....	ThP 156	Zhang, Xiang.....	MP 601	Zhao, Shuang.....	TP 306
Zhang, Hui.....	ThP 295	Zhang, Xiangmin.....	TP 139	Zhao, Shuang.....	WP 653
Zhang, Hui.....	ThP 451	Zhang, Xiangmin.....	TP 143	Zhao, Weiping.....	WP 639
Zhang, Hui.....	TP 003	Zhang, Xiangmin.....	TP 488	Zhao, Xiaohang.....	WP 152
Zhang, Hui.....	TP 478	Zhang, Xiangmin.....	WP 241	Zhao, Yimeng.....	MP 080
Zhang, Hui.....	TP 477	Zhang, Xiao.....	ThP 433	Zhao, Yingming.....	TP 106
Zhang, Hui.....	WOF pm 4:10	Zhang, Xiaohua.....	MP 649	Zhao, Yingming.....	TP 112
Zhang, Hui.....	WP 616	Zhang, Xiaohua.....	MP 650	Zhao, Yingming.....	WOG am 09:50
Zhang, Hui.....	WP 635	Zhang, Xiaoqun.....	TP 013	Zhao, Yingming.....	WP 259
Zhang, Jennifer.....	WP 218	Zhang, Xiaoqun.....	TP 016	Zhao, Yu fen.....	ThP 715
Zhang, Jennifer.....	WP 276	Zhang, Xiaotao.....	TP 474	Zhao, Yue.....	ThP 768
Zhang, Ji.....	MP 513	Zhang, Xiaotao.....	TP 475	Zhao, Yue.....	WP 188
Zhang, Jiang.....	ThP 092	Zhang, Xiaoxi.....	TP 250	Zhao, Yue.....	WP 543
Zhang, Jiang.....	TOD am 08:50	Zhang, Xin.....	MP 782	Zhao, Yuejie.....	ThP 725
Zhang, Jiazhen.....	ThP 079	Zhang, Xin.....	ThP 436	Zhao, Yun-Peng.....	WP 389
Zhang, Jie.....	TP 523	Zhang, Xin.....	ThP 538	Zhao, Yuwen.....	TP 504
Zhang, Jing.....	ThP 300	Zhang, Xing.....	MP 145	Zhao, Yu.....	WP 414
Zhang, Jiyang.....	WOF pm 2:30	Zhang, Xing.....	TOD pm 3:10	Zheng, Ai-Li.....	WP 389
Zhang, Jun.....	ThP 666	Zhang, Xing.....	TP 432	Zheng, Chunxiang.....	ThOC pm 3:50
Zhang, Jun.....	TOF am 10:10	Zhang, Xing.....	WP 673	Zheng, Chunxiang.....	ThP 464
Zhang, Junmei.....	TP 104	Zhang, Xing.....	WP 692	Zheng, Chunxiang.....	ThP 465
Zhang, Junmei.....	WP 058	Zhang, Xinrong.....	TP 379	Zheng, Chunxiang.....	ThP 466
Zhang, Kai.....	ThP 091	Zhang, Xinrong.....	TP 385	Zheng, Jie.....	ThP 126
Zhang, Kangling.....	MP 231	Zhang, Xinyu.....	MP 677	Zheng, Jie.....	WP 333
Zhang, Kangling.....	ThOF pm 4:10	Zhang, Xinyu.....	ThOB am 10:10	Zheng, Naiyu.....	WP 636
Zhang, Kate.....	WP 506	Zhang, Xinyu.....	TOB am 09:50	Zheng, Nancy.....	MP 505
Zhang, Kerong.....	ThP 530	Zhang, Xinyu.....	TOC am 08:30	Zheng, Ning.....	ThP 462
Zhang, Kerong.....	TP 619	Zhang, Xinyu.....	TP 714	Zheng, Ning.....	ThP 470
Zhang, Kun.....	ThP 051	Zhang, Xinyu.....	TP 717	Zheng, Qiuling.....	ThP 461
Zhang, Kun.....	WP 053	Zhang, Xu.....	ThP 204	Zheng, Shirui.....	MP 519
Zhang, Li.....	MP 597	Zhang, Yajie.....	TP 115	Zheng, Suping.....	TP 261
Zhang, Lichao.....	MOE am 08:30	Zhang, Yanlin.....	WP 064	Zheng, X. Long.....	ThP 128
Zhang, Lichao.....	TOG am 08:50	Zhang, Yi.....	ThP 091	Zheng, Yajun.....	TP 385
Zhang, Li-Kang.....	MP 640	Zhang, Yi.....	TP 106	Zheng, Yi.....	ThP 739
Zhang, Lingjuan.....	MOH pm 4:10	Zhang, Yi.....	TP 112	Zheng, Yun.....	TP 712
Zhang, Linwen.....	ThOB am 09:10	Zhang, Yiming.....	MP 400	Zheng, Yupeng.....	MP 676
Zhang, Linwen.....	TP 378	Zhang, Ying.....	MP 044	Zheng, Zhi-Fu.....	ThP 388
Zhang, Liwen.....	ThP 263	Zhang, Ying.....	ThP 363	Zhong, Chengli.....	ThOH pm 4:10
Zhang, Lixin.....	MP 056	Zhang, Ying.....	TP 159	Zhong, Fan.....	WP 016
Zhang, Liya.....	WP 407	Zhang, Ying.....	TP 638	Zhong, Feng.....	MP 721
Zhang, Man-Yu.....	ThP 528	Zhang, Yinna.....	ThP 531	Zhong, Hongying.....	TP 116
Zhang, Man-Yu.....	WP 356	Zhang, Yixiang.....	TP 678	Zhong, Jun.....	MP 255
Zhang, Mengliang.....	ThP 561	Zhang, Yixin.....	MP 445	Zhong, Jun.....	ThP 082
Zhang, Mengliang.....	WP 026	Zhang, Yuesheng.....	WP 373	Zhong, Jun.....	ThP 219
Zhang, Michael.....	MP 514	Zhang, Yuling.....	TP 152	Zhong, Wendy.....	MP 484
Zhang, Min.....	TP 226	Zhang, Yun.....	MP 138	Zhong, Wendy.....	ThP 698
Zhang, Ming.....	ThP 014	Zhang, Yun.....	ThP 259	Zhong, Wendy Hengwen.....	MP 736
Zhang, Ming.....	TP 245	Zhang, Yun.....	TOD am 09:10	Zhong, Wenwan.....	WP 704
Zhang, Ming.....	WP 193	Zhang, Yun.....	WOD pm 3:50	Zhong, Xiaojin.....	TP 389
Zhang, ming.....	WP 598	Zhang, Yuzheng.....	ThOE am 10:10	Zhong, Xuefei.....	ThOH am 09:10
Zhang, Mingzuan.....	MP 131	Zhang, Yuzheng.....	TOG am 08:30	Zhou, Aimin.....	WP 530
Zhang, Ning.....	MP 400	Zhang, Zhaorui.....	WP 088	Zhou, Aiming.....	ThP 720
Zhang, Pingbo.....	ThP 300	Zhang, Zhe.....	MOF am 09:50	Zhou, An.....	TP 439

Program code: M,T,W, Th = Day

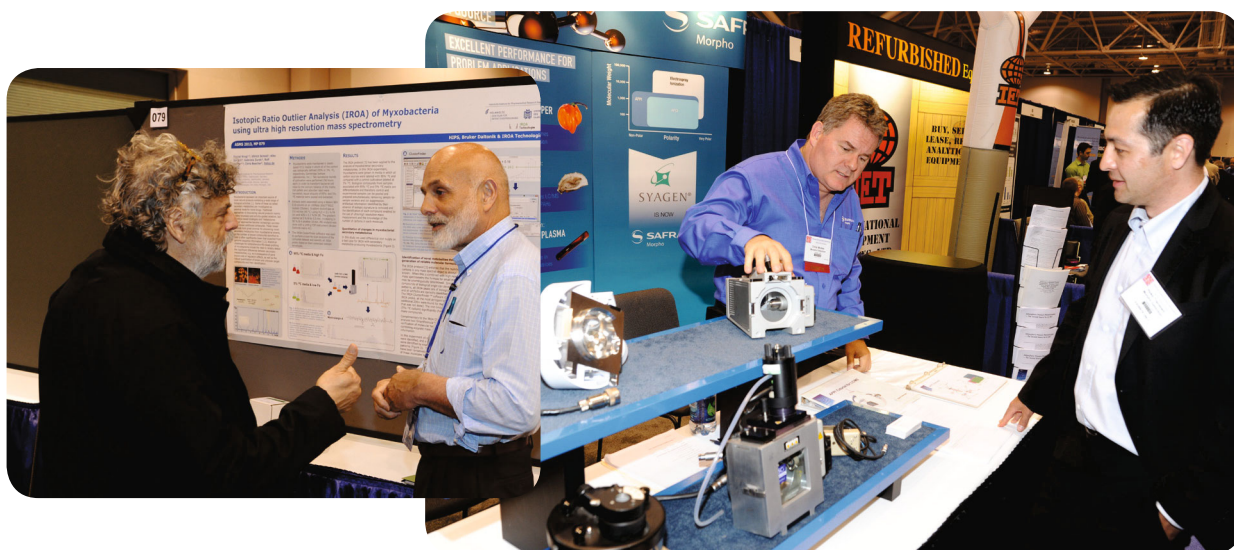
O = Oral, P = Poster

Time or poster number



# INDEX OF AUTHORS

Zhou, Baojin	ThP 323	Zhou, Zuomin	ThP 238	Zhukova, Daria	ThP 223
Zhou, Bo	WP 303	Zhou, Zuomin	WP 149	Zhuo, Xiaoliang	MP 643
Zhou, Dandan	TP 320	Zhu, Yizhun	ThP 530	Zhurov, Konstantin O.	WP 418
Zhou, Dawei	MP 487	Zhu, Aiping	ThP 435	Zi, Jin	ThP 323
Zhou, Dawei	WP 488	Zhu, Alex	TP 179	Zi, Jin	WP 016
Zhou, Dawei	WP 529	Zhu, Feifei	ThP 233	Zi, Jin	WP 152
Zhou, Guangchun	WP 104	Zhu, Guijie	TOB pm 3:50	Zich, David	WP 476
Zhou, Haihong	MP 075	Zhu, Guijie	TP 194	Ziebell, Michael	MP 131
Zhou, Hui	ThP 302	Zhu, Hanyu	MP 775	Ziebell, Michael	TOF pm 3:30
Zhou, Hui	TP 190	Zhu, Hong-Wen	WP 090	Ziegler, Emanuel	MP 041
Zhou, Huiyu	ThP 767	Zhu, Hongying	MP 399	Ziegler, Emanuel	ThP 046
Zhou, Jianying	ThP 040	Zhu, Jiangjiang	MP 443	Ziegler, Steven	ThP 219
Zhou, Jian-Ying	ThP 451	Zhu, Jiangjiang	ThP 659	Zimmerman, Carl	ThP 576
Zhou, Jian-Ying	WOF pm 4:10	Zhu, Jianhui	MP 446	Zimmerman, Lisa	ThP 025
Zhou, Keyu	TP 562	Zhu, Jianhui	ThP 289	Zimmerman, Matthew	TP 026
Zhou, Li	MP 400	Zhu, Jianhui	TP 421	Zimmerman, Matthew	WP 553
Zhou, Ling	TP 520	Zhu, Jianhui	WP 060	Zimmerman, Tyler A.	ThP 144
Zhou, Longhu	ThP 679	Zhu, Jianhui	WP 458	Zimmermann, Ralf	MOD pm 2:50
Zhou, Manshui	MP 599	Zhu, Jianhui	WP 501	Zimmermann, Ralf	ThP 609
Zhou, Min	ThOC pm 2:30	Zhu, Jian-Kang	TP 670	Zimmermann, Ralf	WP 715
Zhou, Min	ThP 501	Zhu, Jie	TP 431	Zimmermann, Ralf	WP 733
Zhou, Mowei	MOE pm 3:50	Zhu, Jinghua	MP 752	Zimmermann, Stefan	MP 388
Zhou, Mowei	WOD pm 3:50	Zhu, Jun	WP 068	Zinck, Nicholas	WP 757
Zhou, Rong	WP 003	Zhu, Liang	TP 388	Zink, Erika	WP 088
Zhou, Ruo	ThP 323	Zhu, Min	TP 243	Zinnel, Nathanael F.	WP 168
Zhou, Ruo	WP 016	Zhu, Mingshe	MP 197	Zivkovic, Angela	ThP 729
Zhou, Shan	MP 348	Zhu, Mingshe	TOA am 09:50	Znaty, David	WP 047
Zhou, Shaoman	ThP 679	Zhu, Mingshe	TP 045	Zong, Chengli	TP 320
Zhou, Shiyue	ThOH am 09:50	Zhu, Mingshe	WP 639	Zong, Zhi-Min	WP 389
Zhou, Shiyue	ThOH pm 2:50	Zhu, Mingzhi	MP 610	Zonja, Bozo	TP 551
Zhou, Shiyue	ThP 148	Zhu, Nick	WP 357	Zordan, Christopher	MOA am 09:10
Zhou, Shiyue	ThP 154	Zhu, Qiuying	TP 519	Zosel, Franziska	ThOD pm 2:30
Zhou, Tao	ThP 238	Zhu, Rong	ThP 739	Zou, Hanfa	TP 694
Zhou, Tao	WP 149	Zhu, Rui	ThP 297	Zou, Hanfa	WP 068
Zhou, Wei	ThOF am 09:30	Zhu, Shaolong	WP 779	Zou, Hanfa	WP 473
Zhou, Xiang	MP 508	Zhu, Wei	TP 431	Zounemat Kermani, Nazanin	WP 020
Zhou, Xiang	WP 530	Zhu, Xiang	ThP 067	Zu, Chengli	MP 325
Zhou, Xiaoyu	ThP 760	Zhu, Xiang	ThP 425	Zubair, Faizan	MP 017
Zhou, Xiaoyu	TOB am 09:30	Zhu, Xiaodong	TP 506	Zubarev, Roman	MOG am 10:10
Zhou, Yafei	TP 388	Zhu, Xiaodong	TP 493	Zubarev, Roman	TOF pm 3:10
Zhou, Yihong	ThP 331	Zhu, Xin	WP 133	Zucchetti, Massimo	TP 029
Zhou, Ying	TP 300	Zhu, Yanlong	MOC am 08:50	Zuck, Paul	MP 536
Zhou, Yiyong	TP 423	Zhu, Yixin	WP 752	Zuckermann, Ronald	ThP 184
Zhou, Yiyong	TP 445	Zhu, Yongxin	ThP 441	Zucki, Fernanda	MP 461
Zhou, Yiyong	WP 137	Zhu, Yue	ThP 619	Zucki, Fernanda	ThP 307
Zhou, Yiyong	WP 138	Zhu, Zhengjiang	ThP 634	Zuppa, Athena	WP 646
Zhou, Yu	MP 348	Zhu, Zhenqian	TP 743	Zuzheng, Luo	WOC pm 3:50
Zhou, Yueming	MP 400	Zhu, Zhenqian	WP 377	Zweigenbaum, Jerry	ThP 614
Zhou, Zhaohui	MP 168	Zhu, Zhikai	ThOH am 08:30	Zweigenbaum, Jerry	ThP 630
Zhou, Zhaohui Sunny	WP 718	Zhu, Zhikai	WP 260	Zwier, Timothy	TP 362
Zhou, Zhen	ThP 574	Zhuk, Eugene	ThP 743	Zybailov, Boris	ThP 054
Zhou, Zinan	WOH am 08:50	Zhuk, Iryna	WP 552		



Program code: M,T,W, Th = Day      O = Oral, P = Poster      Time or poster number



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