

Synthesis of Sansalvamide A Peptidomimetics: Triazole, Oxazole, Thiazole, and Pseudoproline containing compounds

Melinda R. Davis,[†] Hendra Wahyudi,[†] Erinprit K. Singh,[†] Leslie D. Alexander,[†] Lidia A. Nazarova,[†] Joseph B. Kunicki,[†] Kelly A. Fairweather,[‡] Andrew Giltrap,[‡] Katrina A. Jolliffe,[‡] and Shelli R. McAlpine^{δ *}

^δ School of Chemistry, University of New South Wales, Sydney, NSW 2052 Australia

[†] Department of Chemistry and Biochemistry, 5500 Campanile Drive, San Diego State University, San Diego, CA 92182-1030.

[‡] School of Chemistry, University of Sydney, Sydney, NSW 2006 Australia

s.mcalpine@unsw.edu.au

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NMR Dipeptide EtO-Thiazole-Leu-NHBoc	99
NMR Pentapeptide EtO-Thiazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc	100
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Table of compounds with text describing structural variations

Comp #		aa₁	aa₂	aa₃	aa₄	aa₅
1	A-Tri-III	Phe	Leu	Val-Triazole	Leu	Leu
2	B-Tri-III	Phe	Leu	Val-Triazole	Leu	NMe-Leu
3	A-Ox-III	Phe	Leu	Oxazole	Leu	Leu
4	B-Ox-III	Phe	Leu	Oxazole	Leu	NMe-Leu
5	C-Ox-III	Phe	NMe-D-Phe	Oxazole	Leu	Lys(Cbz)
6	D-Ox-III	(2R,3R)- β -Benzoxy-Phe	Leu	Oxazole	D-Leu	D-Phe
7	D-Ox-II	(2R,3R)- β -Benzoxy-Phe	Oxazole	NMe-Val	D-Leu	D-Phe
8	D-Ox-I	Phenyl-Oxazole	Leu	NMe-Val	D-Leu	D-Phe
9	A-Th-III	Phe	Leu	Thiazole	Leu	Leu
10	B-Th-III	Phe	Leu	Thiazole	Leu	NMe-Leu
11	C-Th-III	Phe	NMe-D-Phe	Thiazole	Leu	Lys(Cbz)
12	A-PP-II	Phe	Thr(Ψ Me,Me-Pro)	Val	Leu	Leu
13	A-PP-III	Phe	Leu	Thr(Ψ Me,Me-Pro)	Leu	Leu

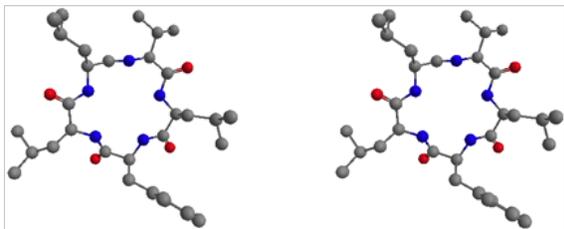
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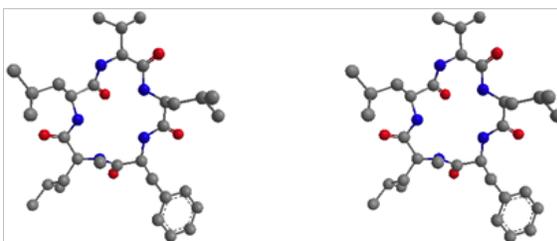
Table of cytotoxicity of additional compounds

Compound		PGI at 25μM	Error
B		86%	$\pm 0.3\%$
C		78.8%	$\pm 1.4\%$
D		47.5%	$\pm 5.1\%$
2	B-Tri-III	60.9%	$\pm 3.7\%$
4	B-Ox-III	23.4%	$\pm 6.0\%$
5	C-Ox-III	42.2%	$\pm 0.8\%$
6	D-Ox-III	2.3%	$\pm 1.3\%$
7	D-Ox-II	4.6%	$\pm 2.5\%$
8	D-Ox-I	2.9%	$\pm 1.6\%$
10	B-Th-III	14.0%	$\pm 5.0\%$
11	C-Th-III	6.1%	$\pm 1.9\%$
12	A-PP-II	7.7%	$\pm 3.3\%$

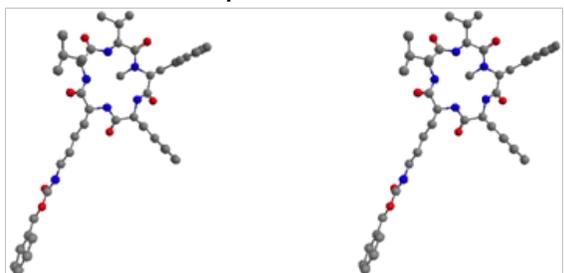
Molecular models of all compounds in stereo



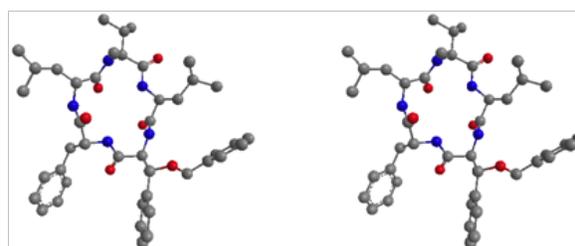
Compound A



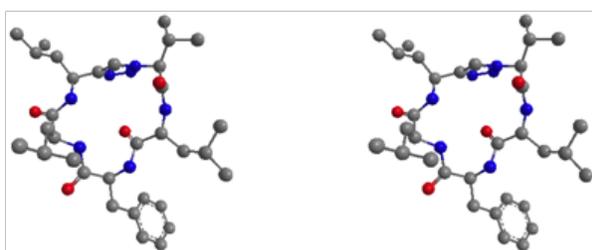
Compound B



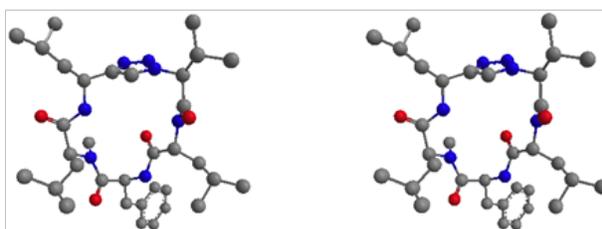
Compound C



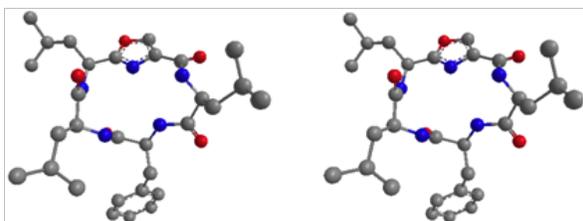
Compound D



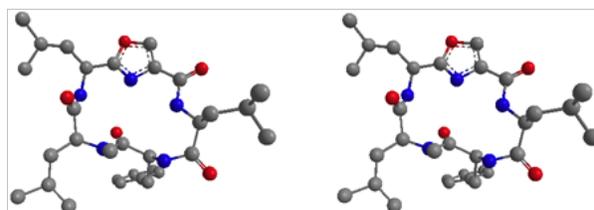
Compound 1



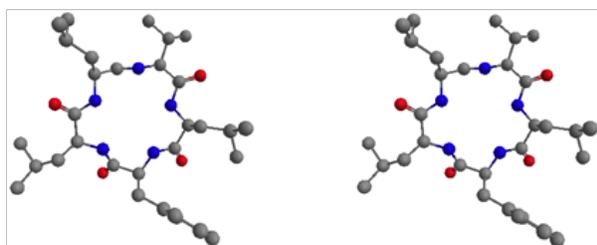
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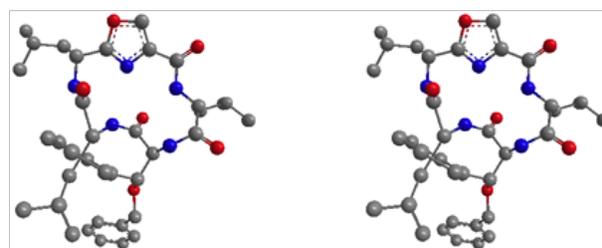
Compound 3



Compound 4



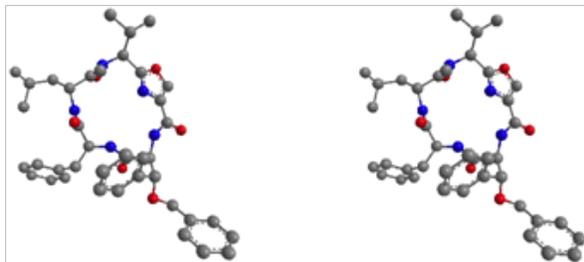
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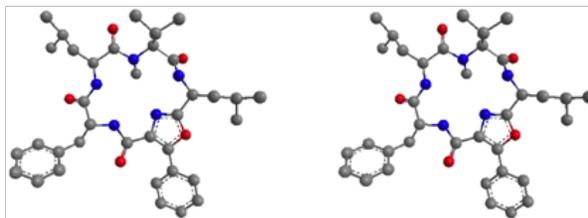
Compound 6

Supplementary Material

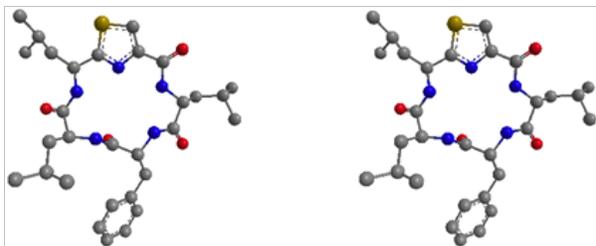
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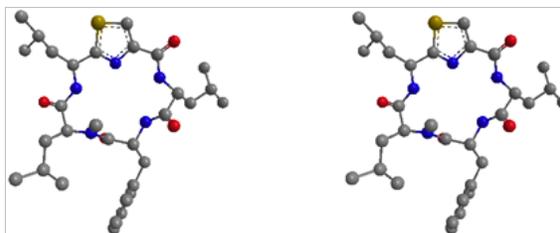
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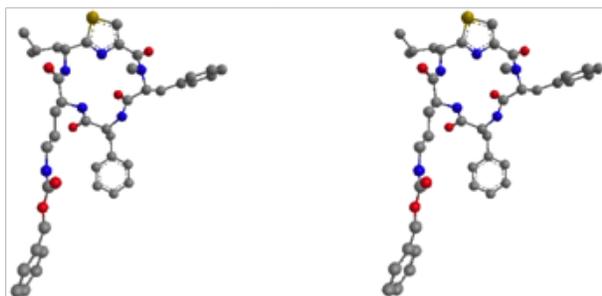
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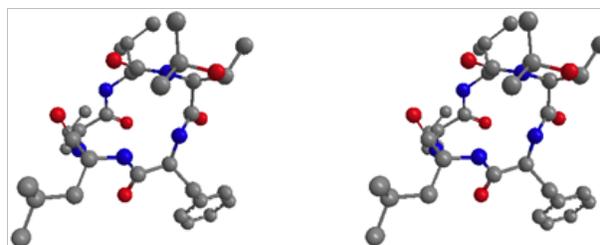
Compound 9



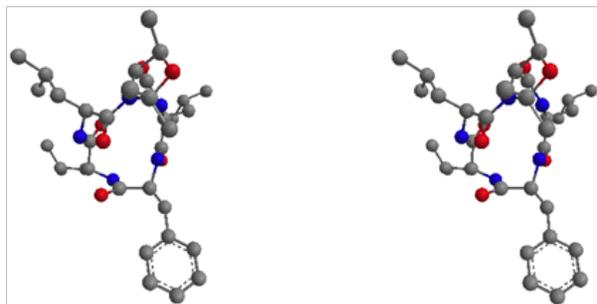
Compound 10



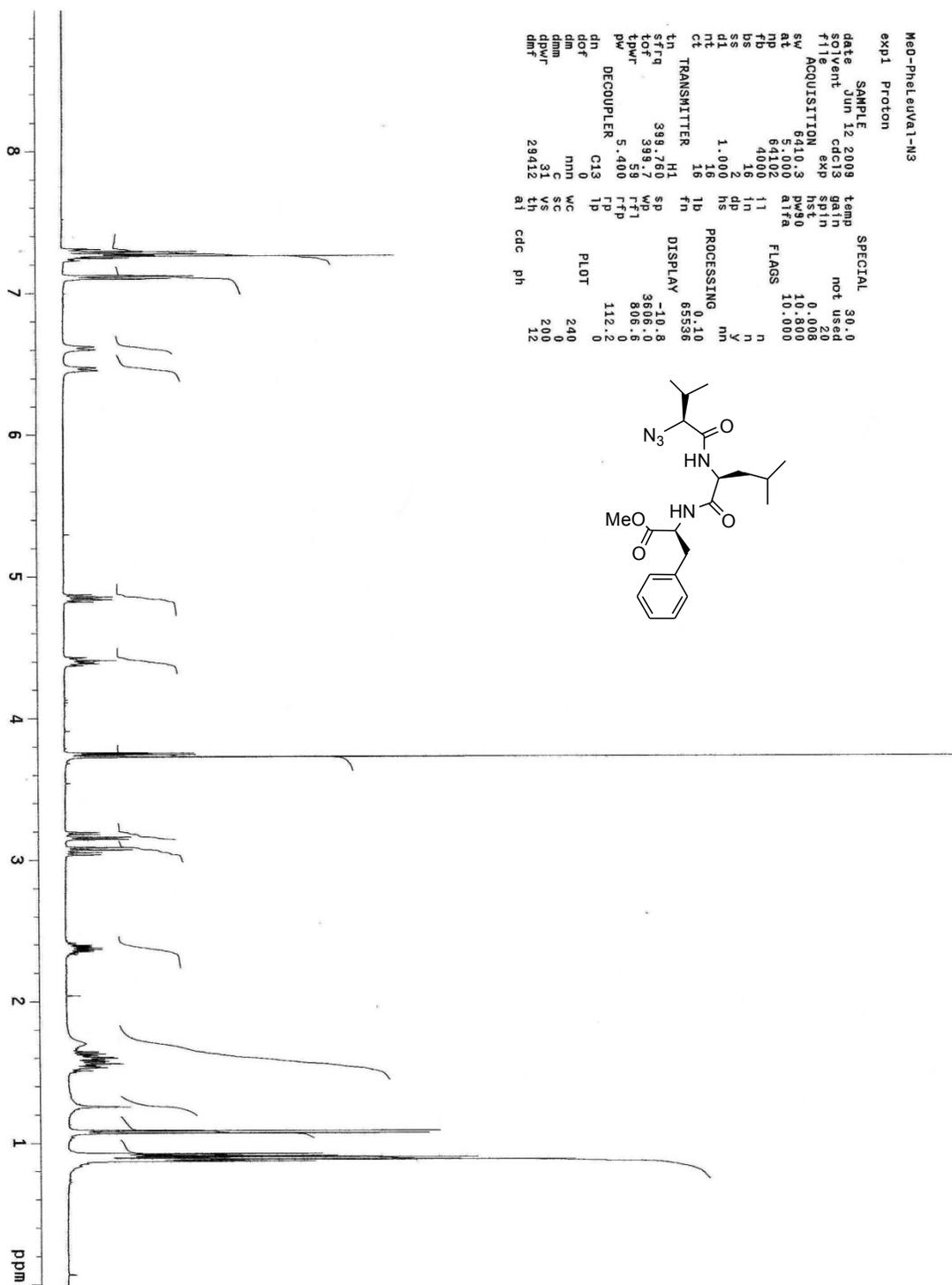
Compound 11



Compound 12

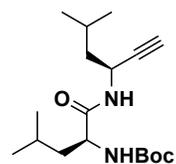
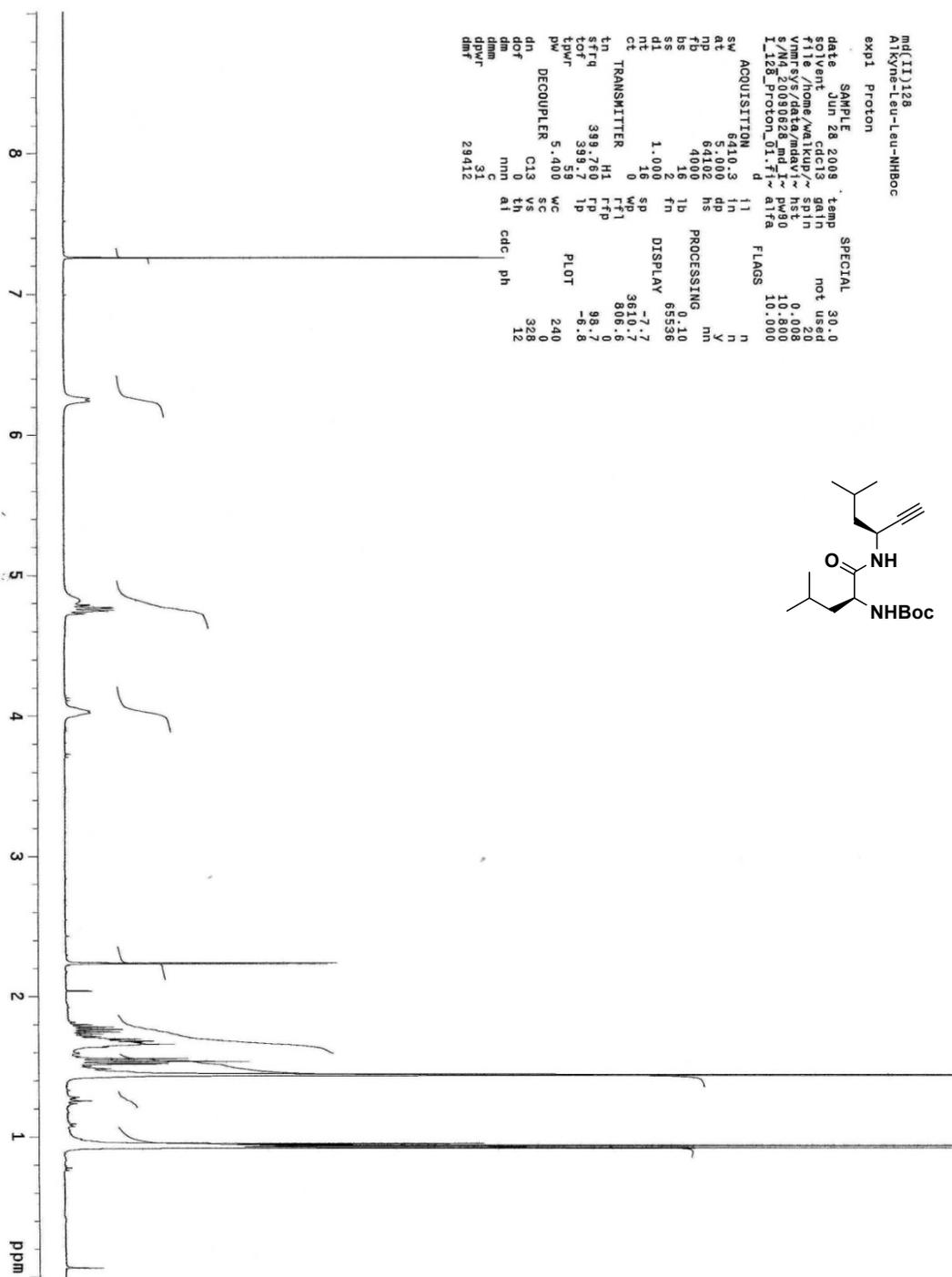


Compound 13



Compound 1: A-Tri-III

NMR Tripeptide MeO-Phe-Leu-Val-N₃ (22)

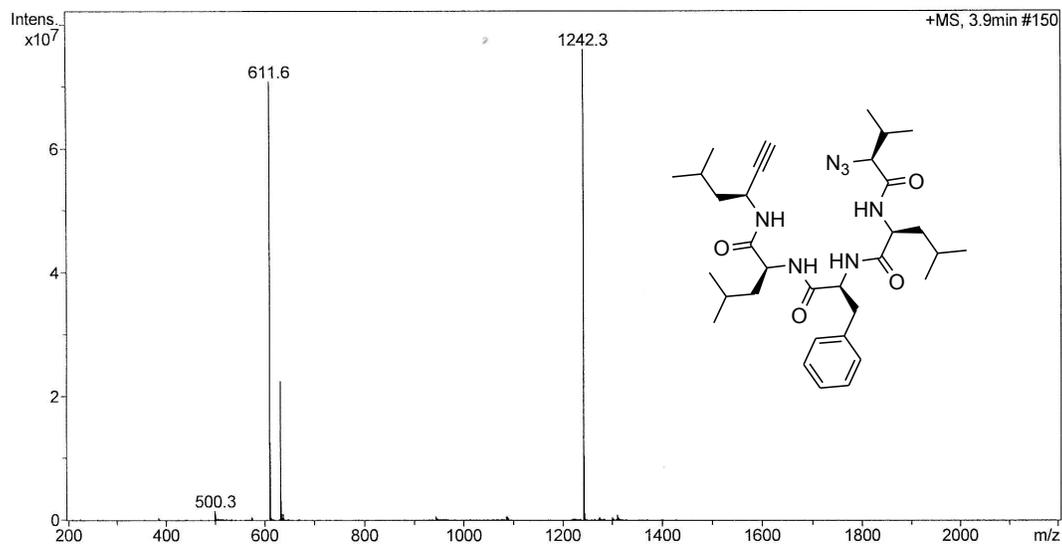
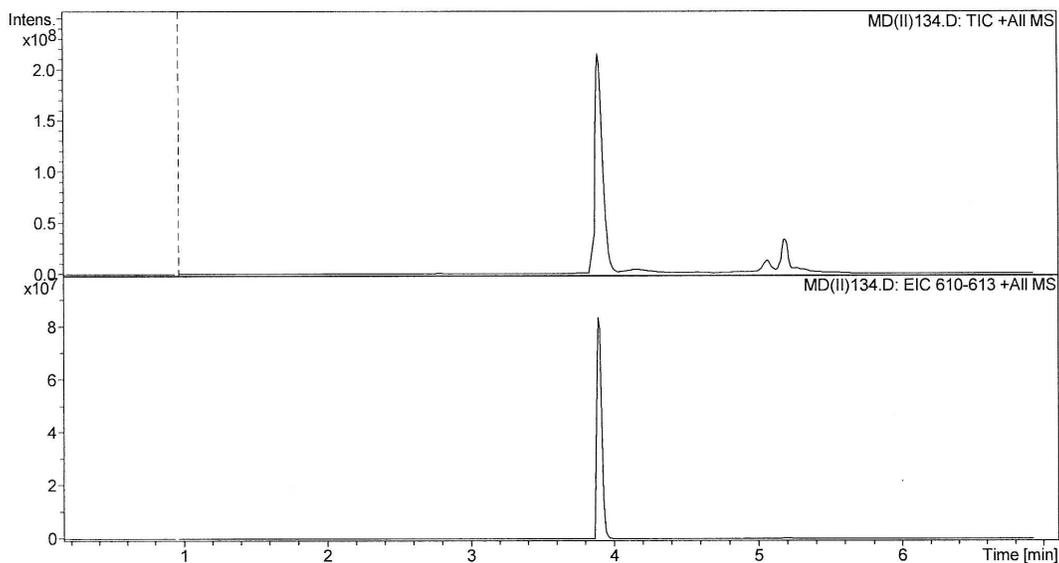


Compound 1: A-Tri-III

NMR Dipeptide Alkyne-Leu-Leu-NHBoc

Display Report - All Windows Selected Analysis

Analysis Name: MD(II)134.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/15/2009 4:50:54 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 7/3/2009 12:29:06 PM
Sample Name: md(II)134
Analysis Info:

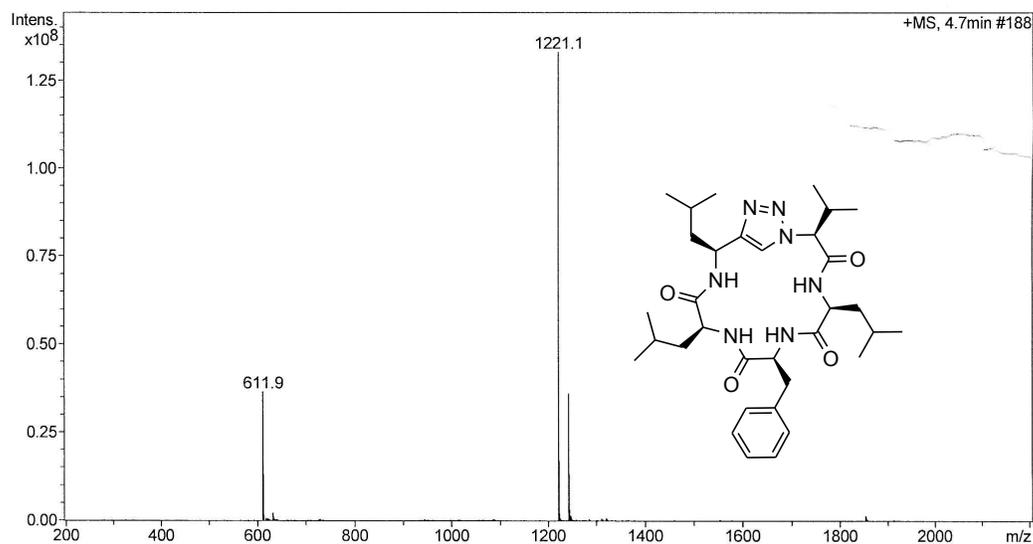
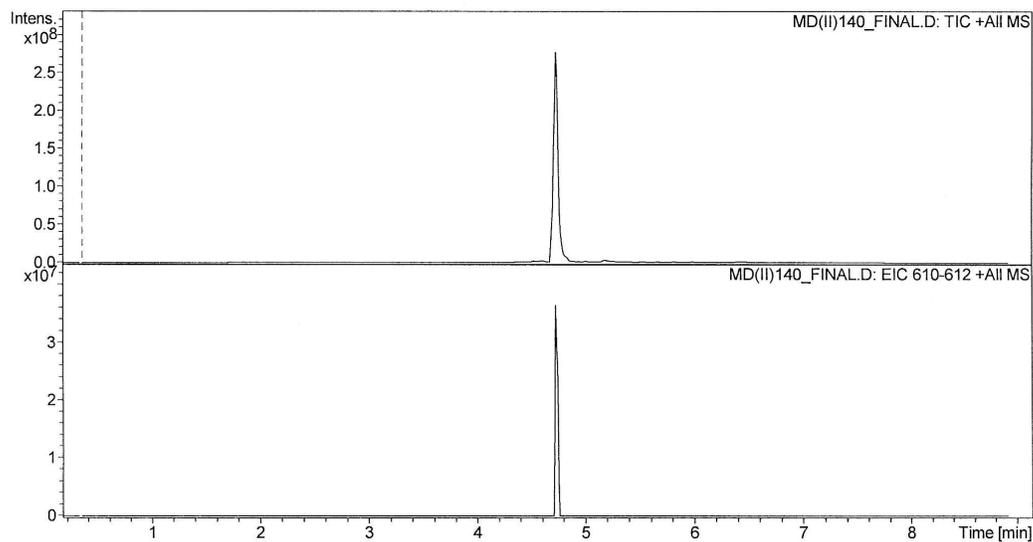


Compound 1: A-Tri-III

LCMS Pentapeptide Alkyne-Leu-Leu-Phe-Leu-Val-N₃ (23) (MW = 611)

Display Report - All Windows Selected Analysis

Analysis Name: MD(II)140_FINAL **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/14/2009 10:24:51 PM
Method: SANA_LCN00.M **Operator:** sdsu **Acq. Date:** 7/14/2009 10:09:44 PM
Sample Name: md(II)140_final
Analysis Info:



Compound 1: A-Tri-III

LCMS Macrocyclic Phe-Leu-Val-Triazole-Leu-Leu (1) (MW = 610)

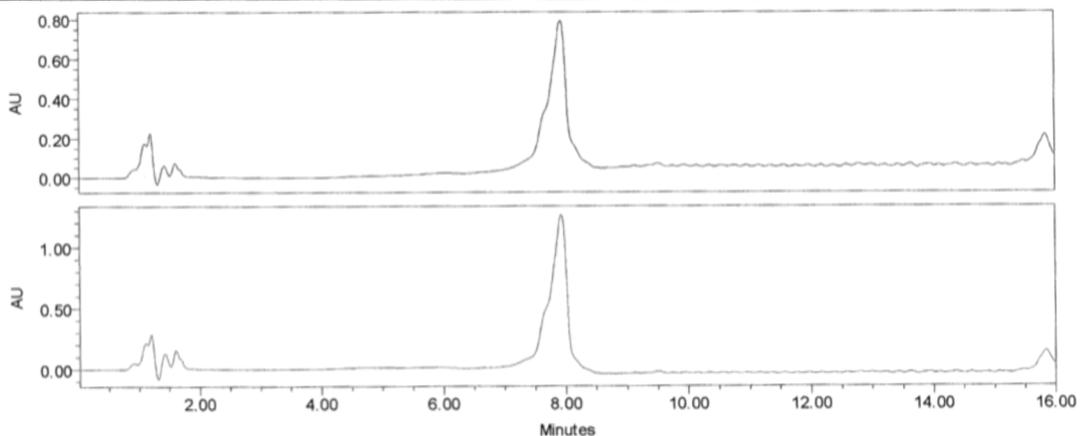
SDSU

Project Name: Defaults
Reported by User: System

Breeze

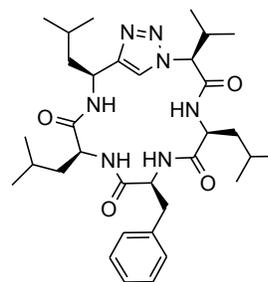
SAMPLE INFORMATION

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Injection #:	30	Date Acquired:	7/14/2009 10:32:58 PM
Run Time:	16.00 Minutes	Injection Volume:	30.00 ul



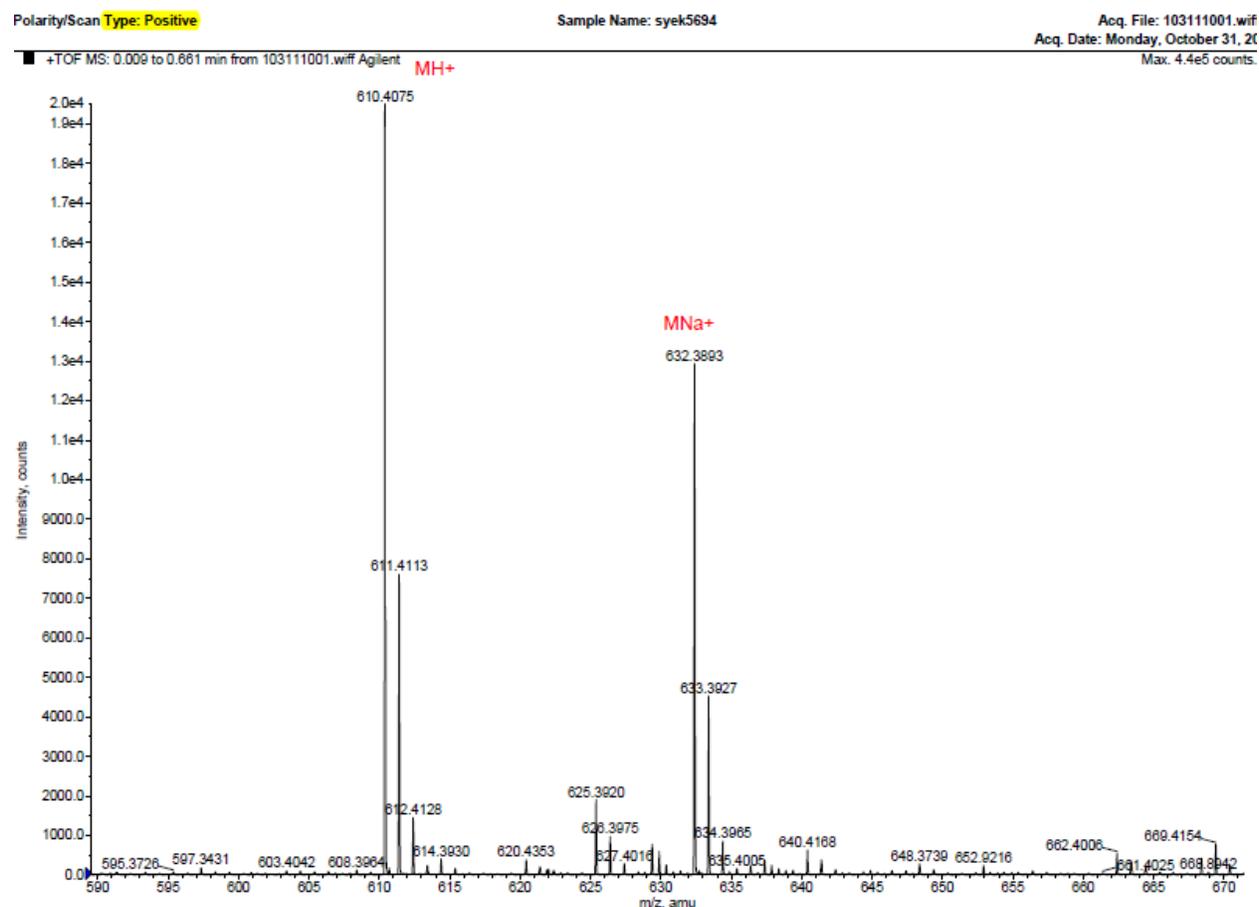
Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
 Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

Peak Name	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	Amount	Units
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2 ****	****	****	****	****	****	****



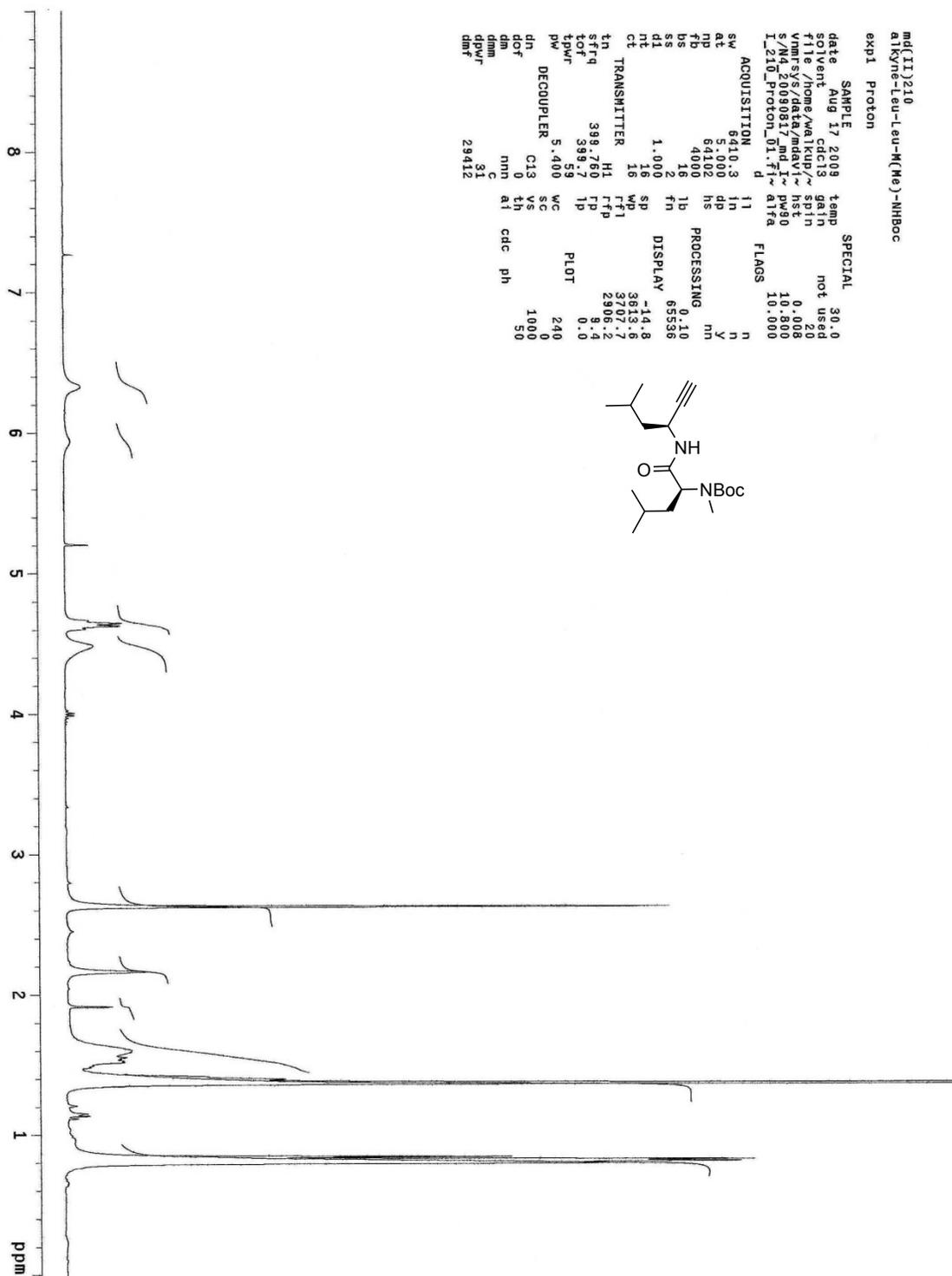
Compound 1: A-Tri-III

HPLC Macrocyclic Phe-Leu-Val-Triazole-Leu-Leu (1)



Compound 1: A-Tri-III

HRMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu (1) (MW = 610.4075)

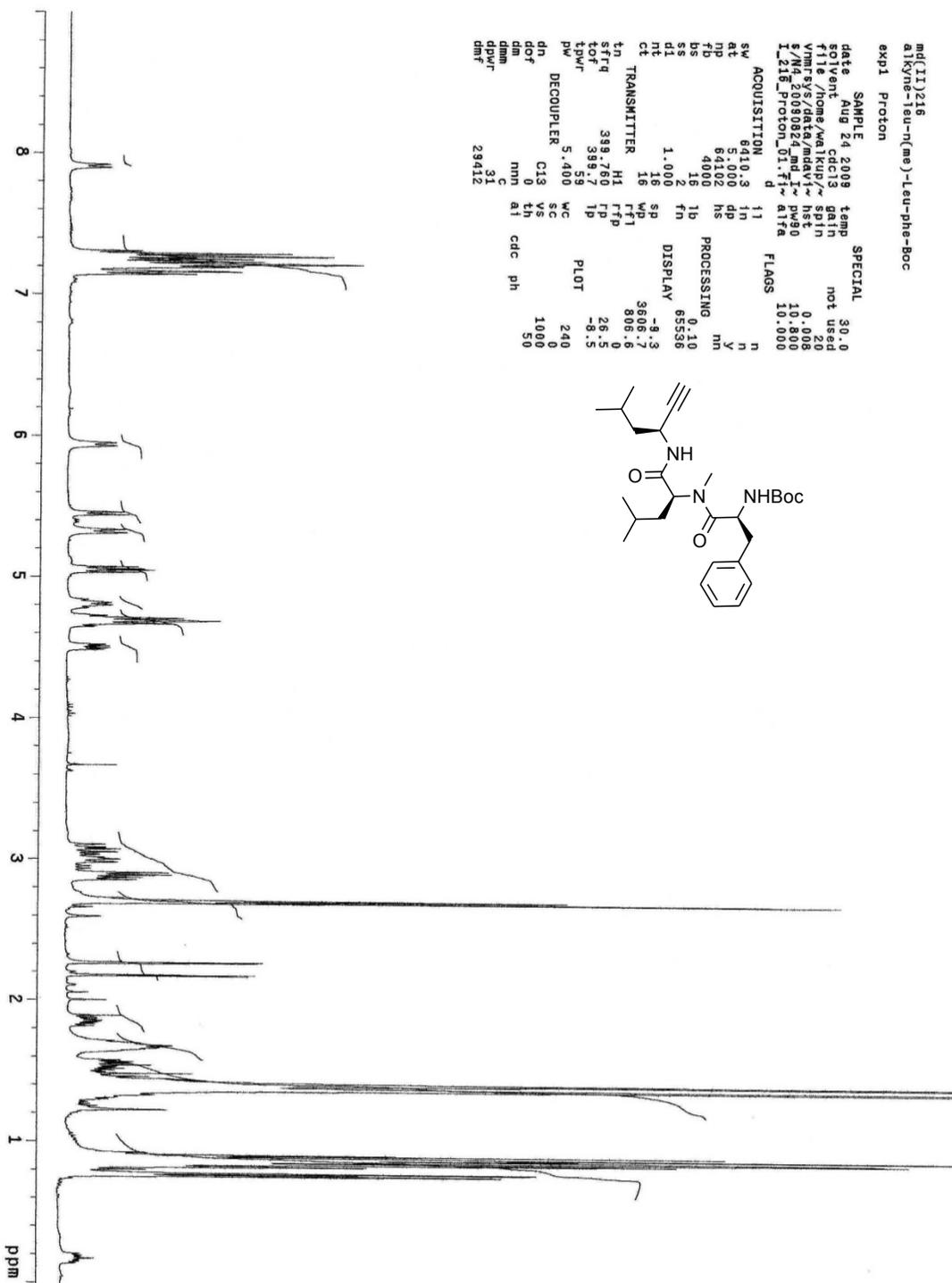


Compound 2: B-Tri-III

NMR Dipeptide Alkyne-Leu-Leu-N(Me)Boc

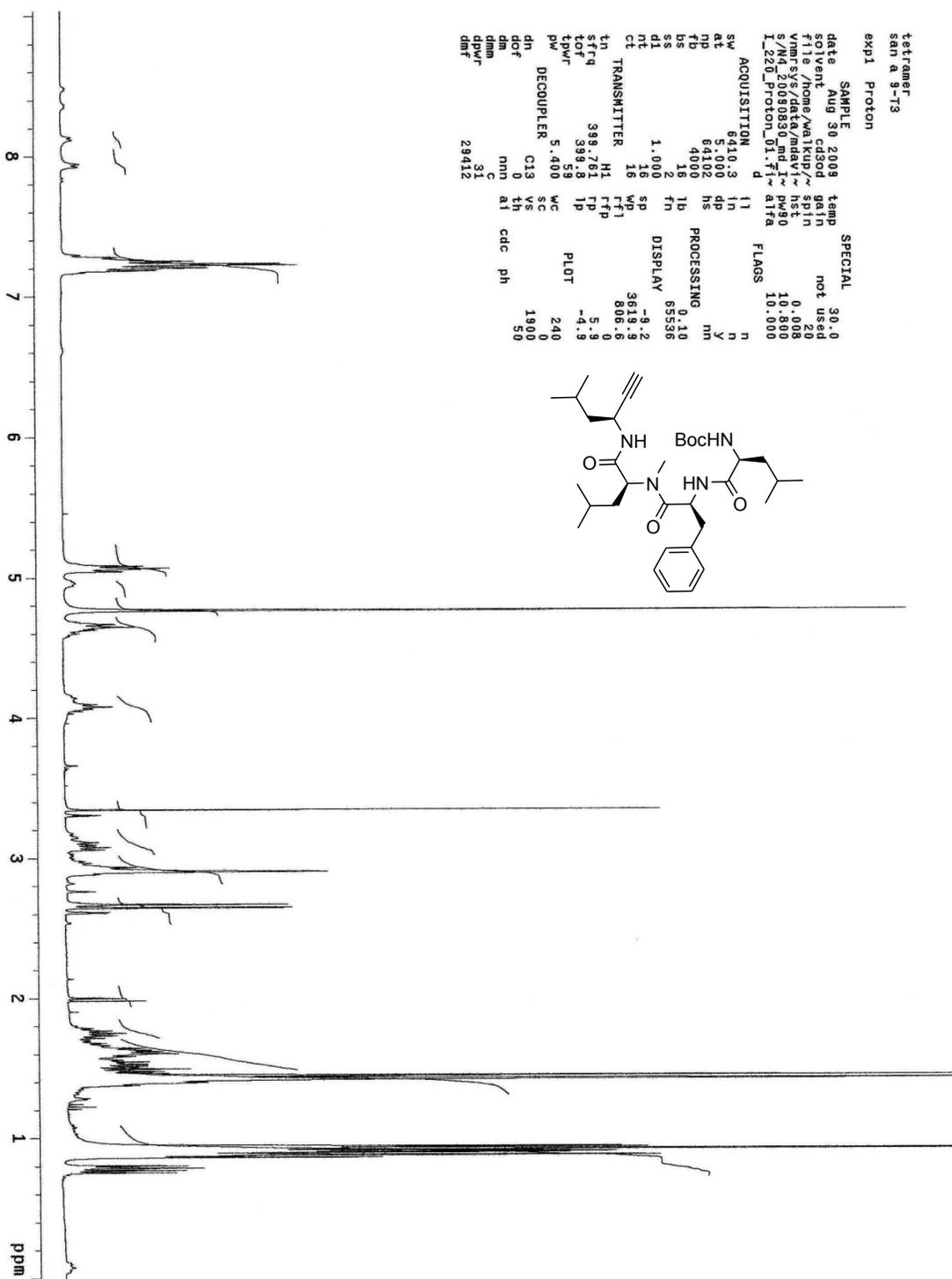
Supplementary Material

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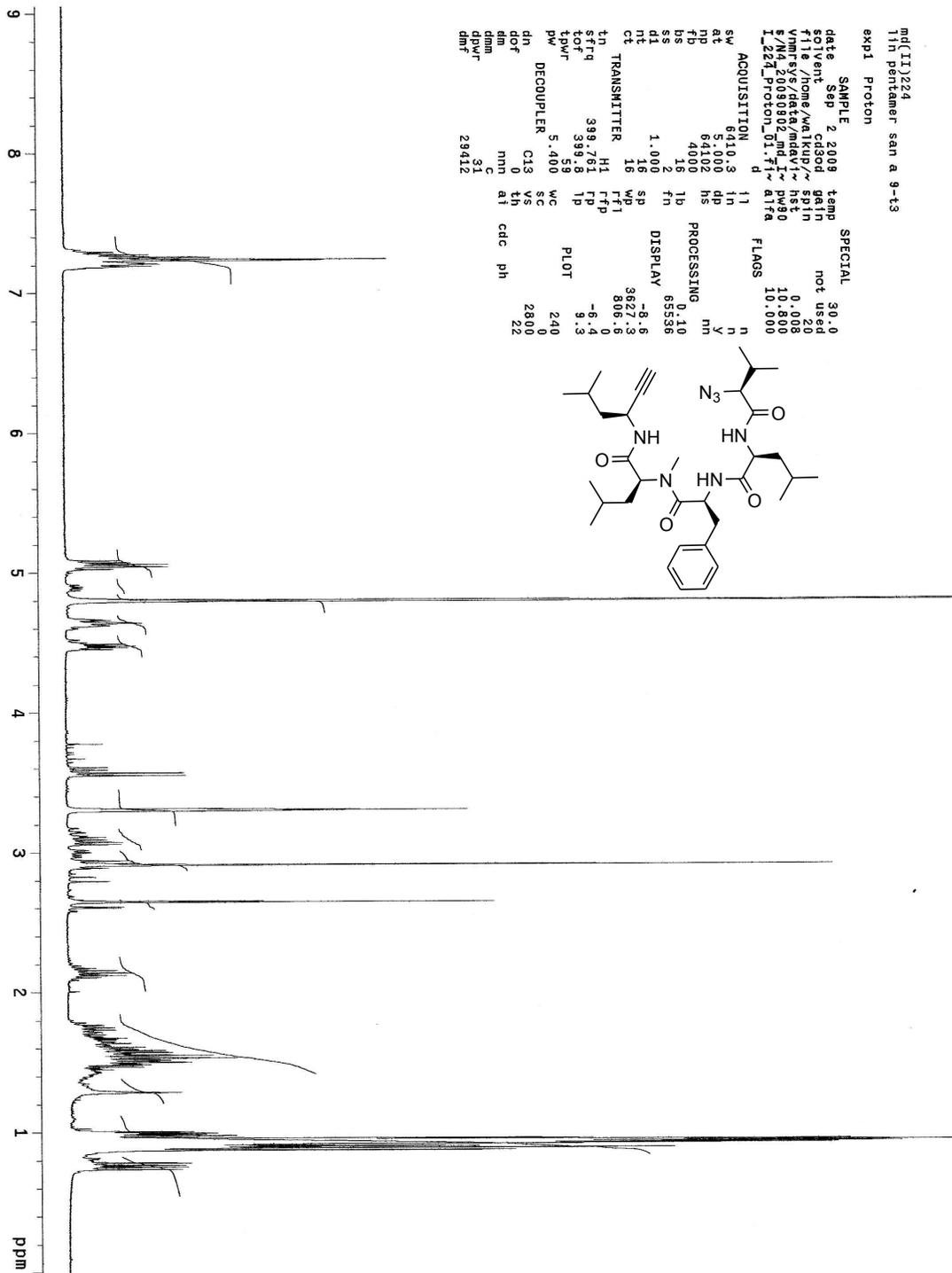
Compound 2: B-Tri-III

NMR Tripeptide Alkyne-Leu-Leu-N(Me)-Phe-NHBoc



Compound 2: B-Tri-III

NMR Tetrapeptide Alkyne-Leu-Leu-N(Me)-Phe-Leu-NHBoc

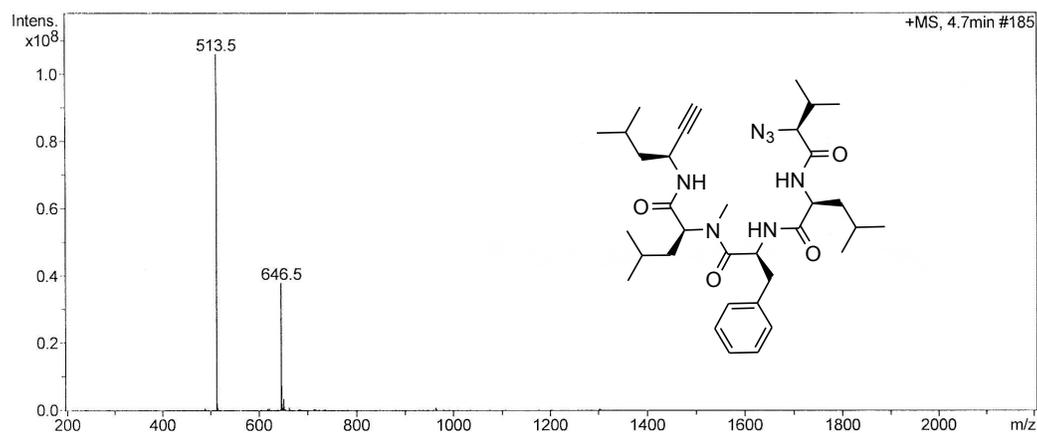
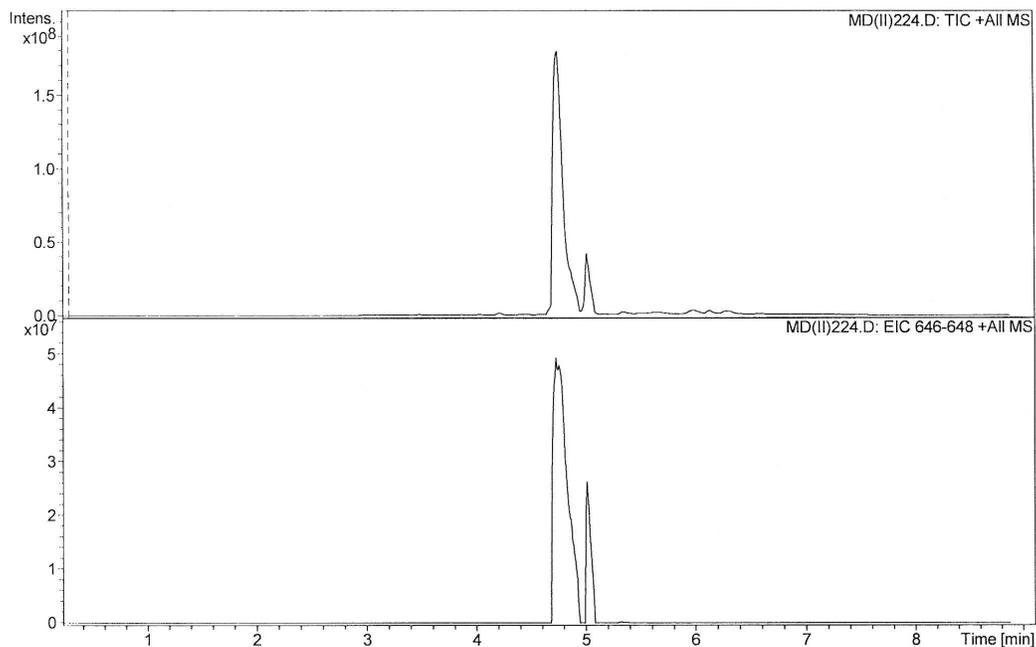


Compound 2: B-Tri-III

NMR Pentapeptide Alkyne-Leu-Leu-N(Me)-Phe-Leu-Val-N₃ (33)

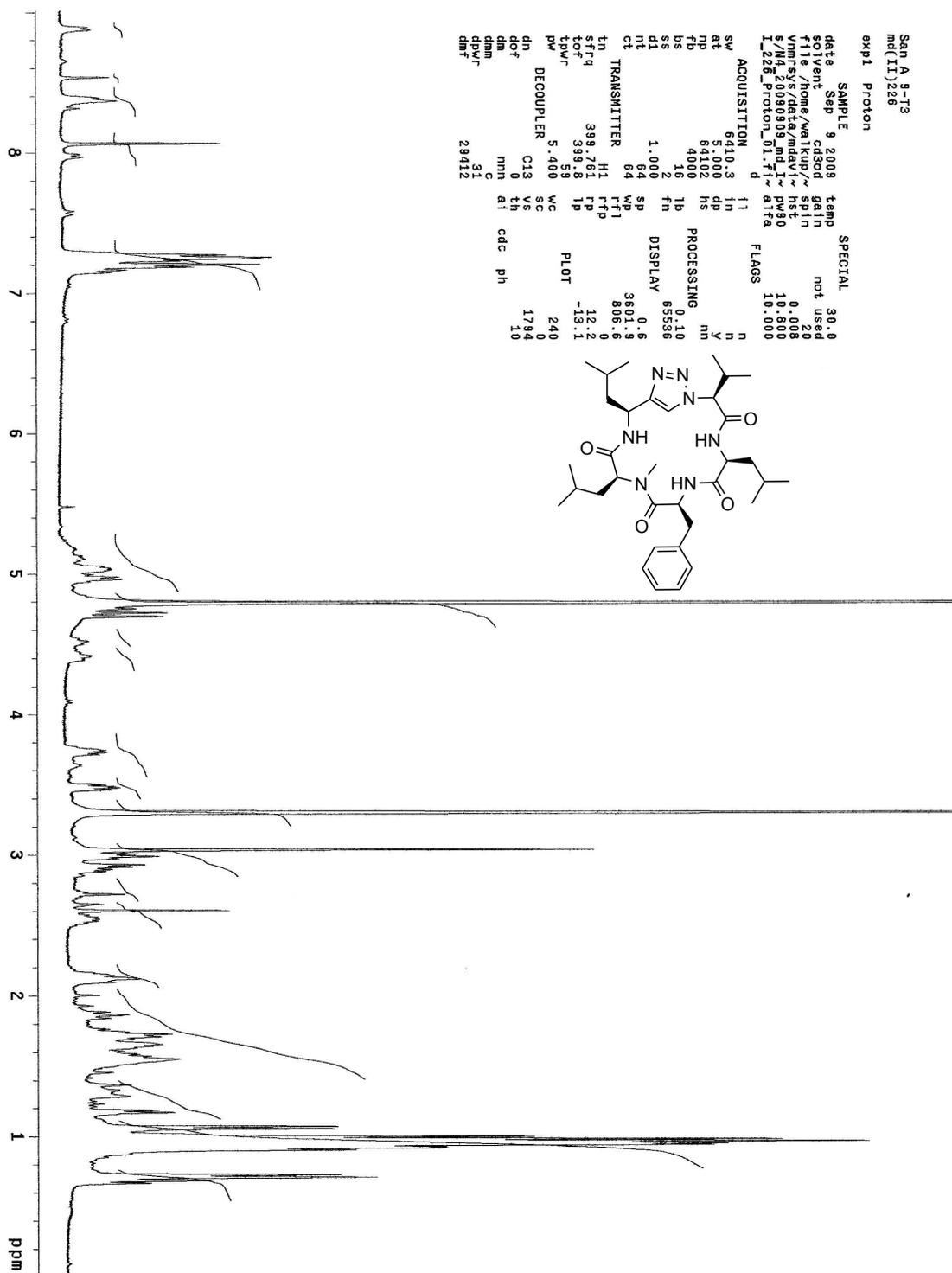
Display Report - All Windows Selected Analysis

Analysis Name: MD(II)224.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/2/2009 8:59:53 PM
Method: SANA_LONG.M **Operator:** sdsu **Acq. Date:** 9/2/2009 8:50:32 PM
Sample Name: md(II)224
Analysis Info:



Compound 2: B-Tri-III

LCMS Pentapeptide Alkyne-Leu-Leu-N(Me)-Phe-Leu-Val-N₃ (33) (MW = 624)

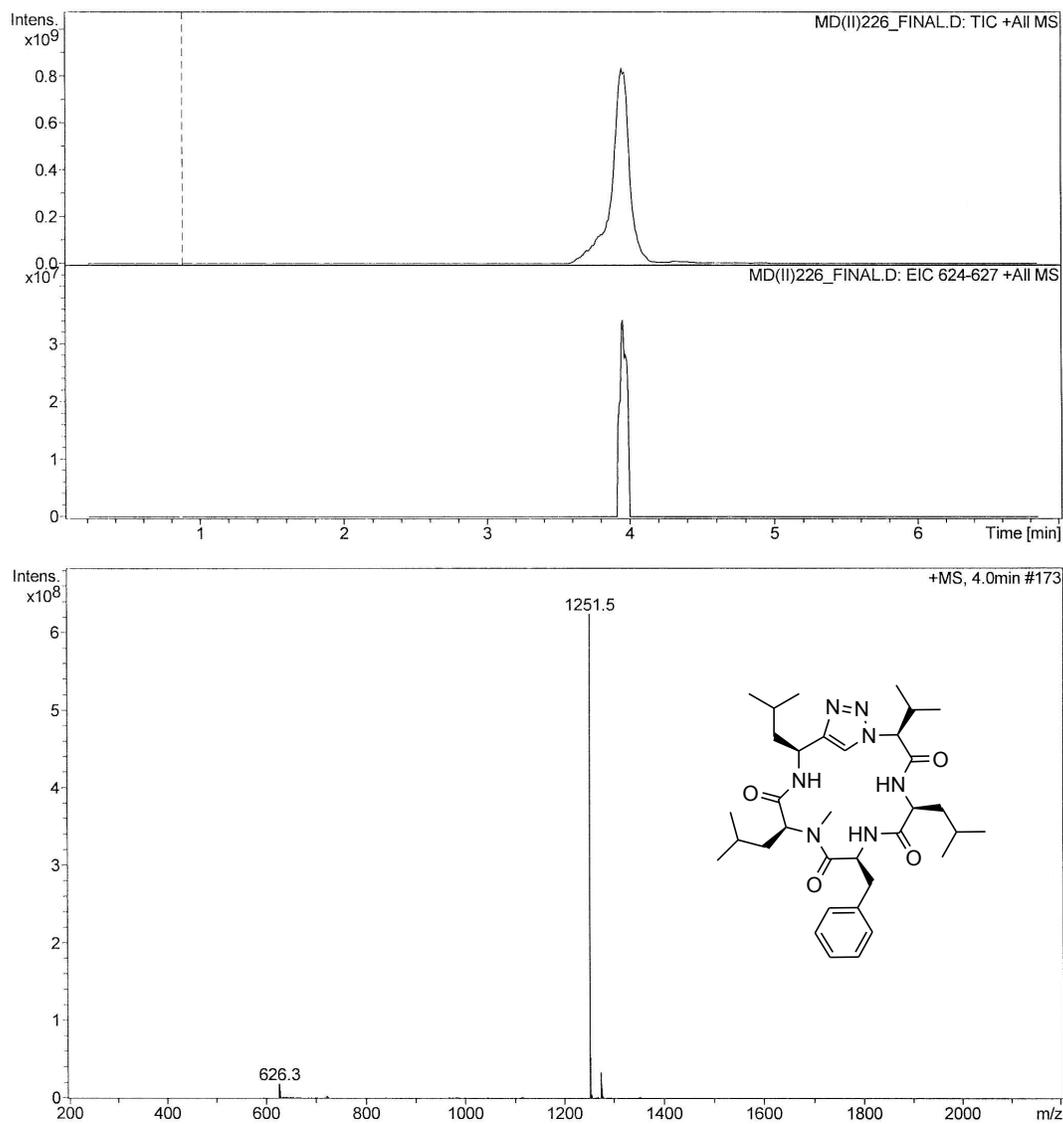


Compound 2: B-Tri-III

NMR Macrocyclic Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2)

Display Report - All Windows Selected Analysis

Analysis Name: MD(II)226_FINAL **Instrument:** Agilent 6330 Ion Trap **Print Date:** 9/9/2009 9:04:20 PM
Method: SANA.M L.D **Operator:** sdsu **Acq. Date:** 9/9/2009 8:56:29 PM
Sample Name: md(II)226_final
Analysis Info:



Compound 2: B-Tri-III

LCMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2) (MW = 624)

Supplementary Material

Davis et al.

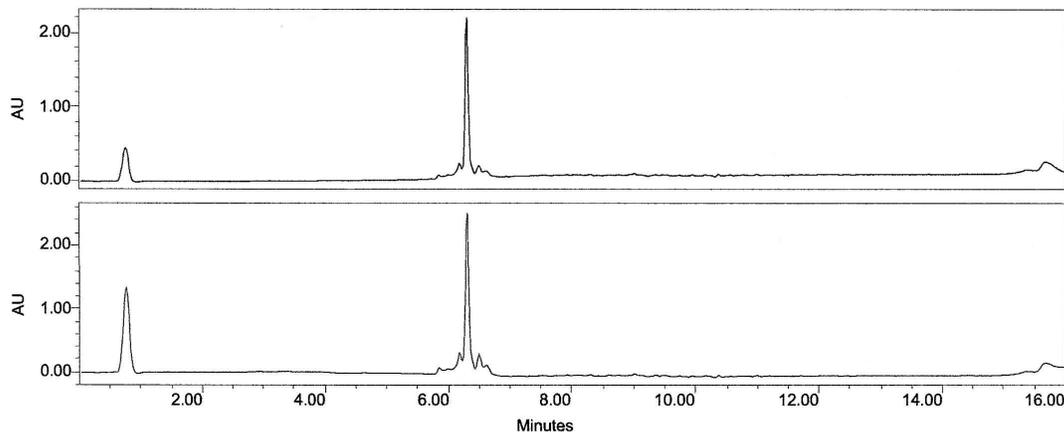
SDSU

Project Name: Defaults
Reported by User: System

1/Breeze

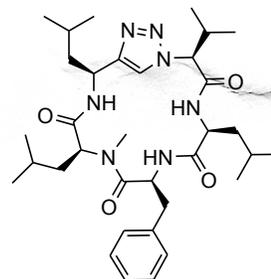
SAMPLE INFORMATION

Sample Name:	md(II)226_f50	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	133	Date Acquired:	9/7/2009 10:43:40 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



Channel: 2487Channel 1 Channel Desc.: Processing Method: *
Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****

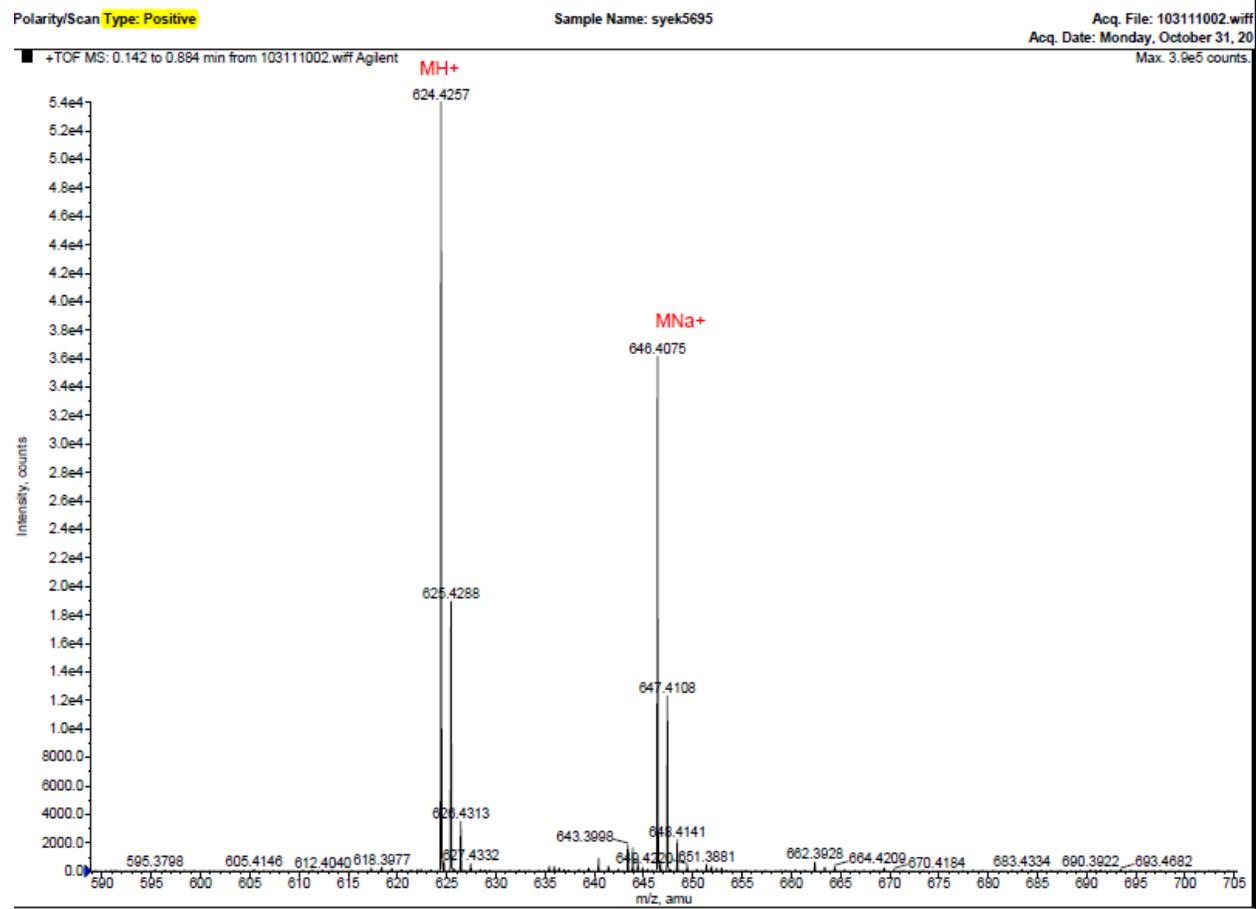


Compound 2: B-Tri-III

HPLC Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2)

Supplementary Material

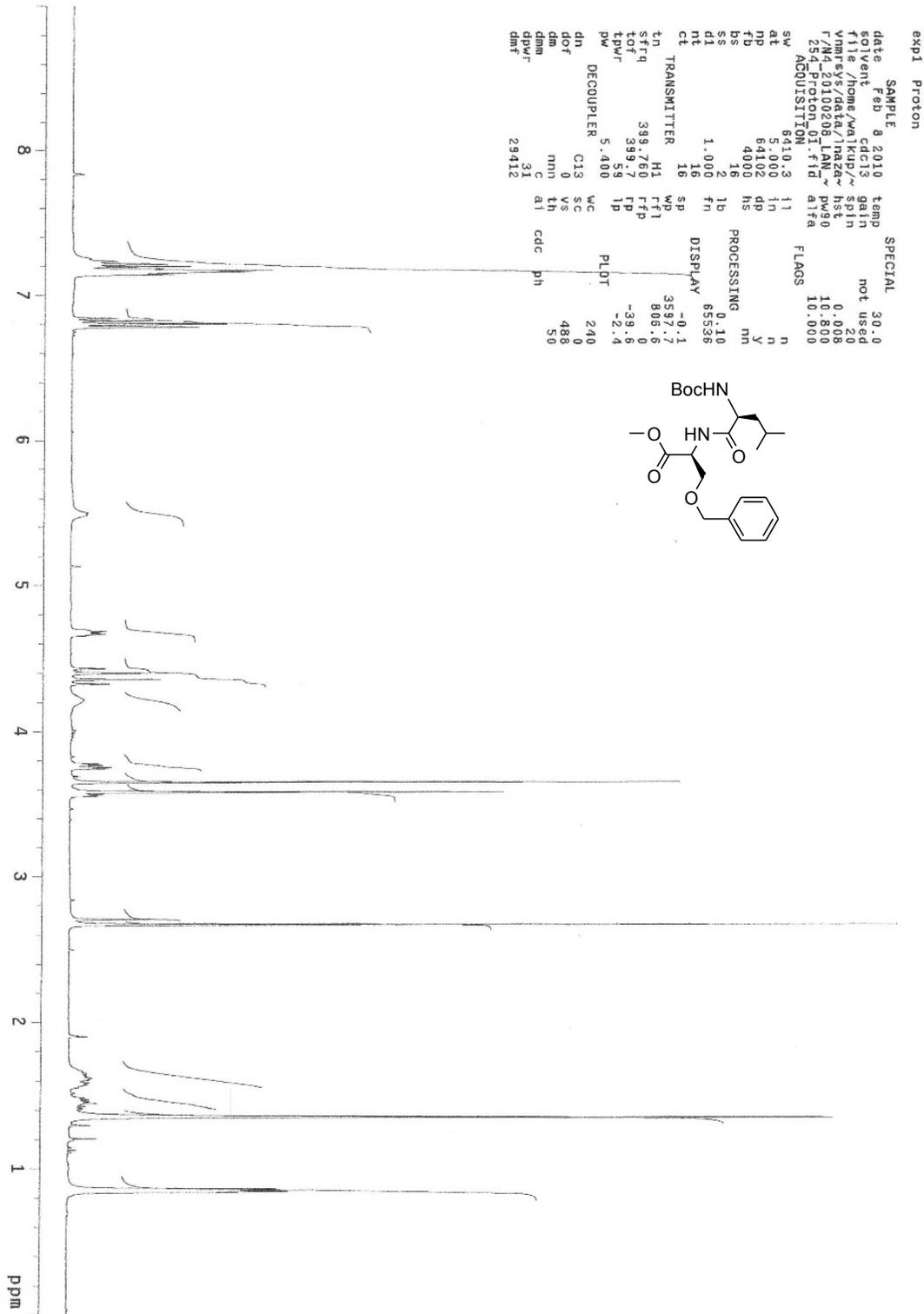
Davis et al.



Compound 2: B-Tri-III

HRMS Macrocycle Phe-Leu-Val-Triazole-Leu-Leu-N(Me) (2) (MW = 624.4257)

Davis et al.

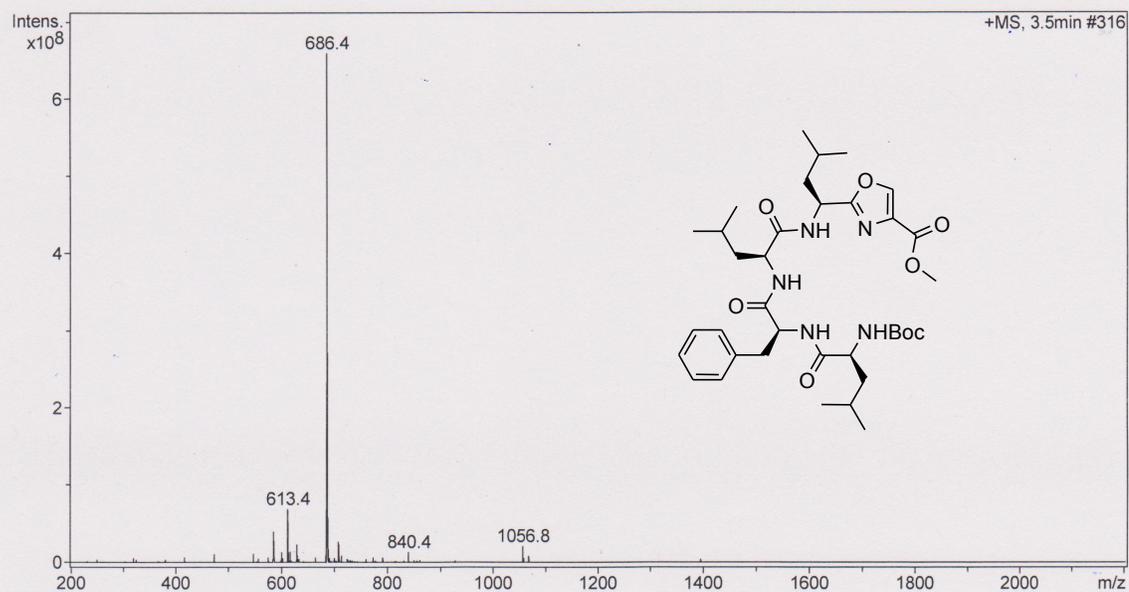
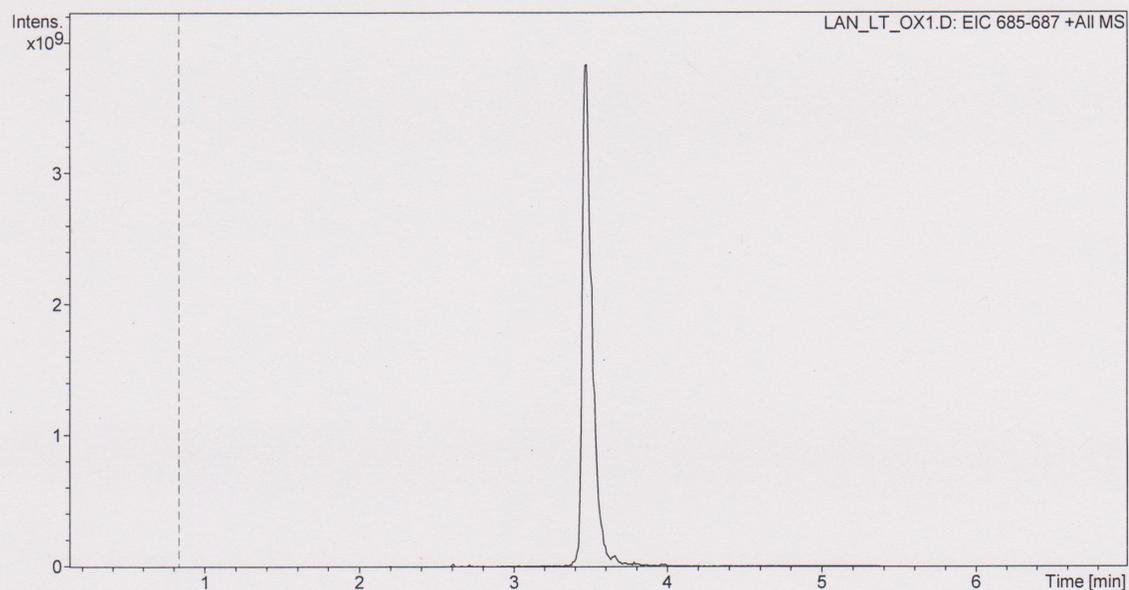


Compound 3: A-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc

Display Report - All Windows Selected Analysis

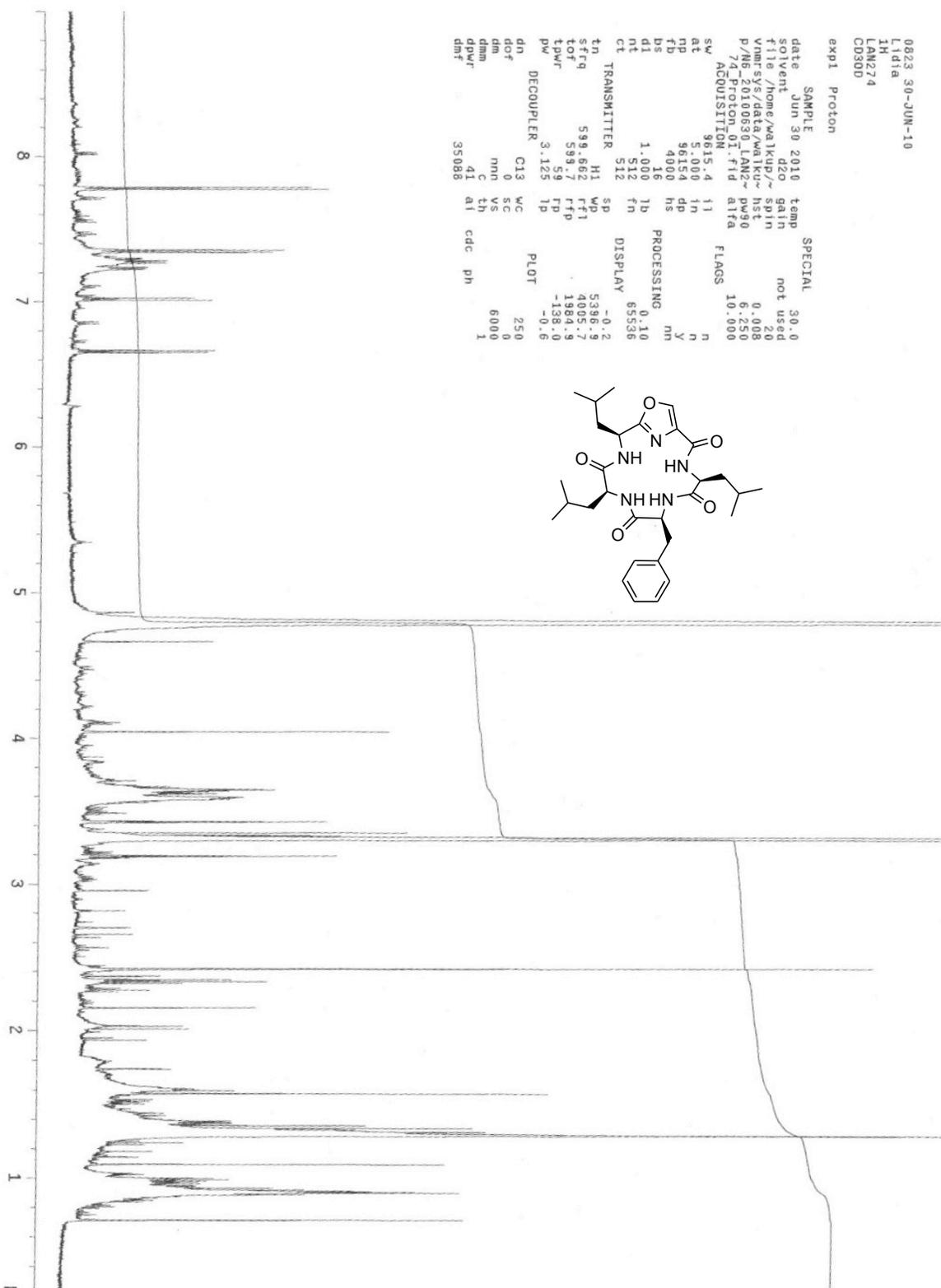
Analysis Name: LAN_LT_OX1.D Instrument: Agilent 6330 Ion Trap Print Date: 6/8/2011 9:35:07 AM
Method: SANA.M Operator: sdsu Acq. Date: 5/11/2010 4:11:04 AM
Sample Name: LAN_LT_Ox1
Analysis Info:



Compound 3: A-Ox-III

LCMS Linear pentapeptide MeO-Oxazole-Leu-Leu-Phe-Leu-NHBoc (43) (MW = 685.85)

Davis et al.



Compound 3: A-Ox-III

NMR Macrocycle Phe-Leu-Oxazole-Leu-Leu (3)

Davis et al.

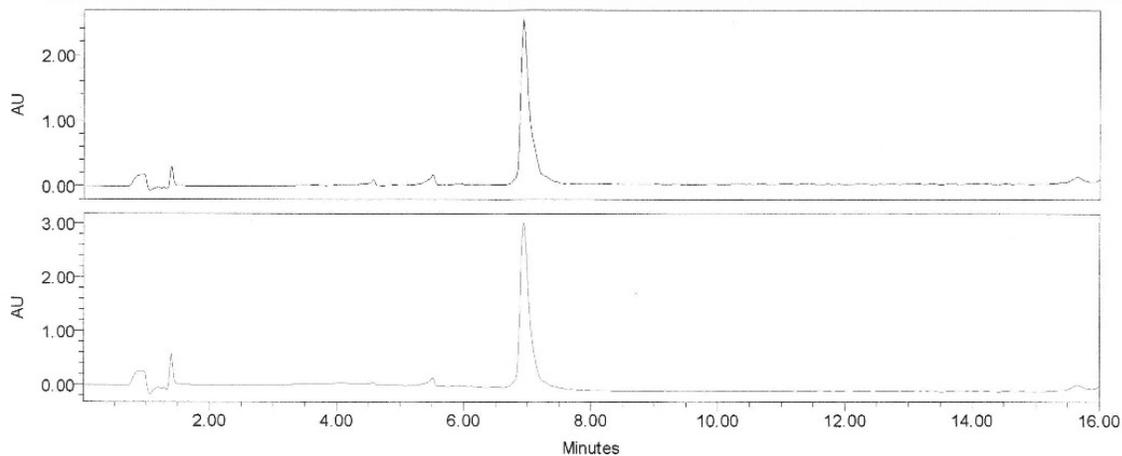
SDSU

Project Name: Defaults
Reported by User: System

Breeze

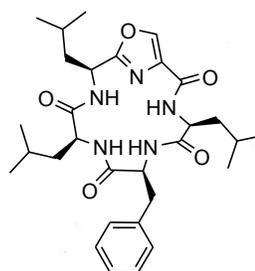
SAMPLE INFORMATION

Sample Name:	oxazole1-Ian	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	299	Date Acquired:	6/28/2010 5:25:18 PM
Run Time:	16.00 Minutes	Injection Volume:	100.00 ul



Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



Compound 3: A-Ox-III

HPLC Macrocycle Phe-Leu-Oxazole-Leu-Leu (3)

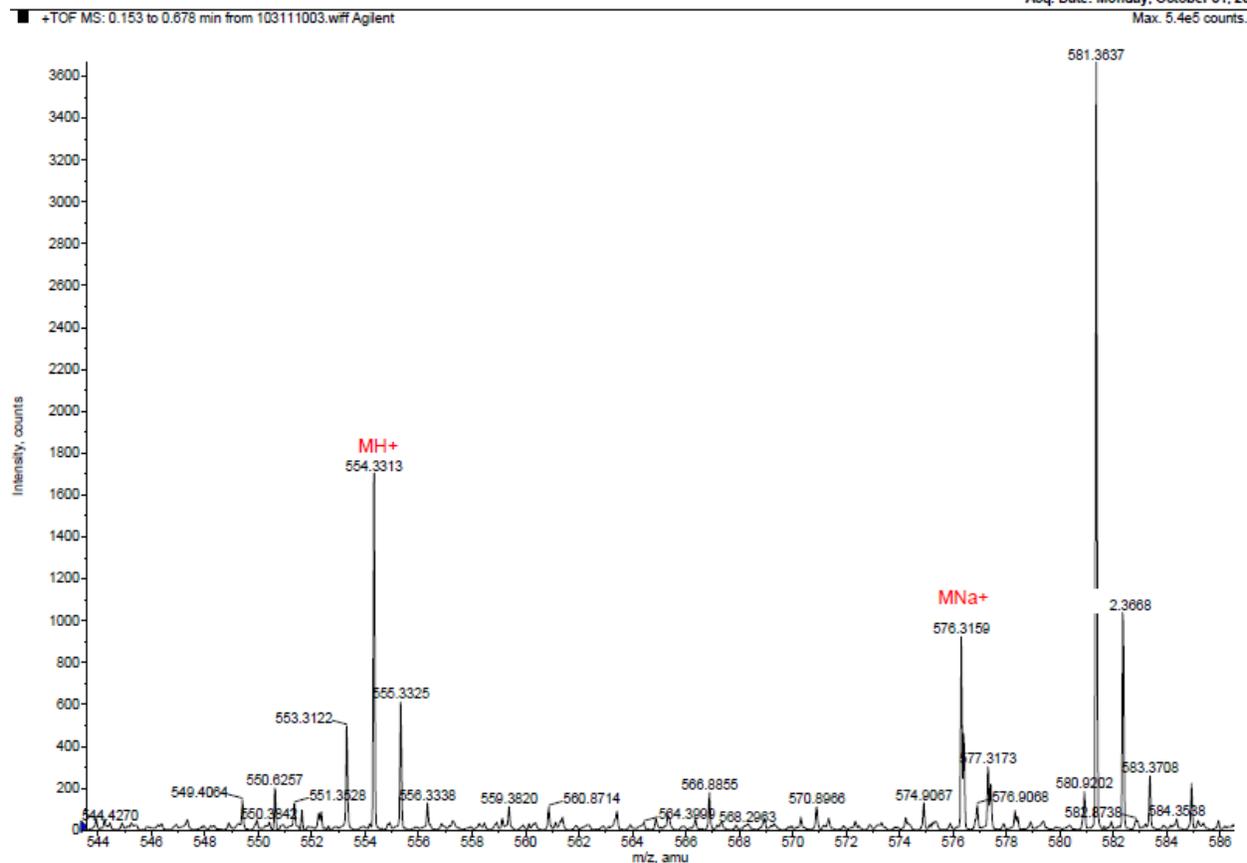
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

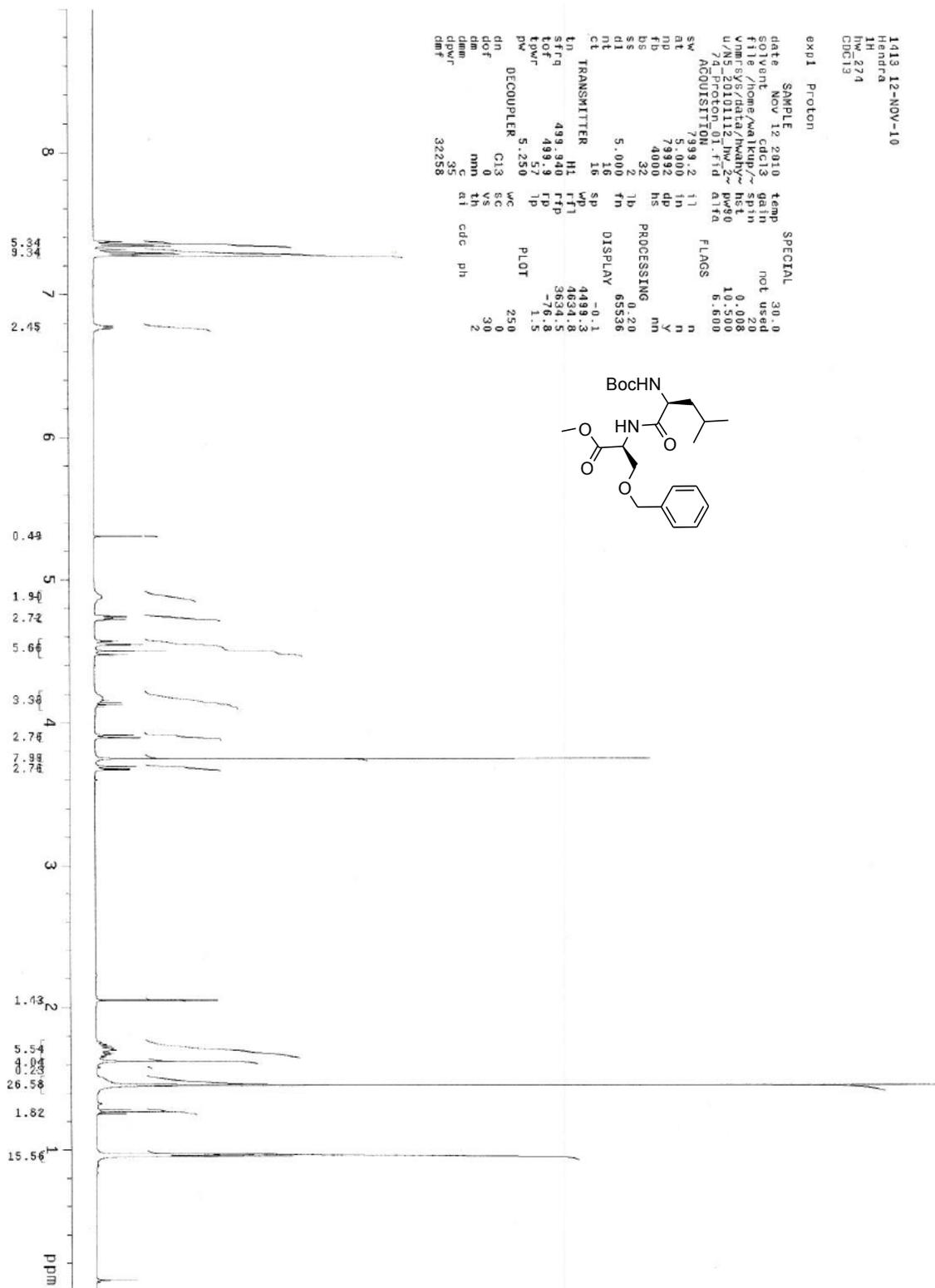
Sample Name: syek5696

Acq. File: 103111003.wiff
Acq. Date: Monday, October 31, 20



Compound 3: A-Ox-III

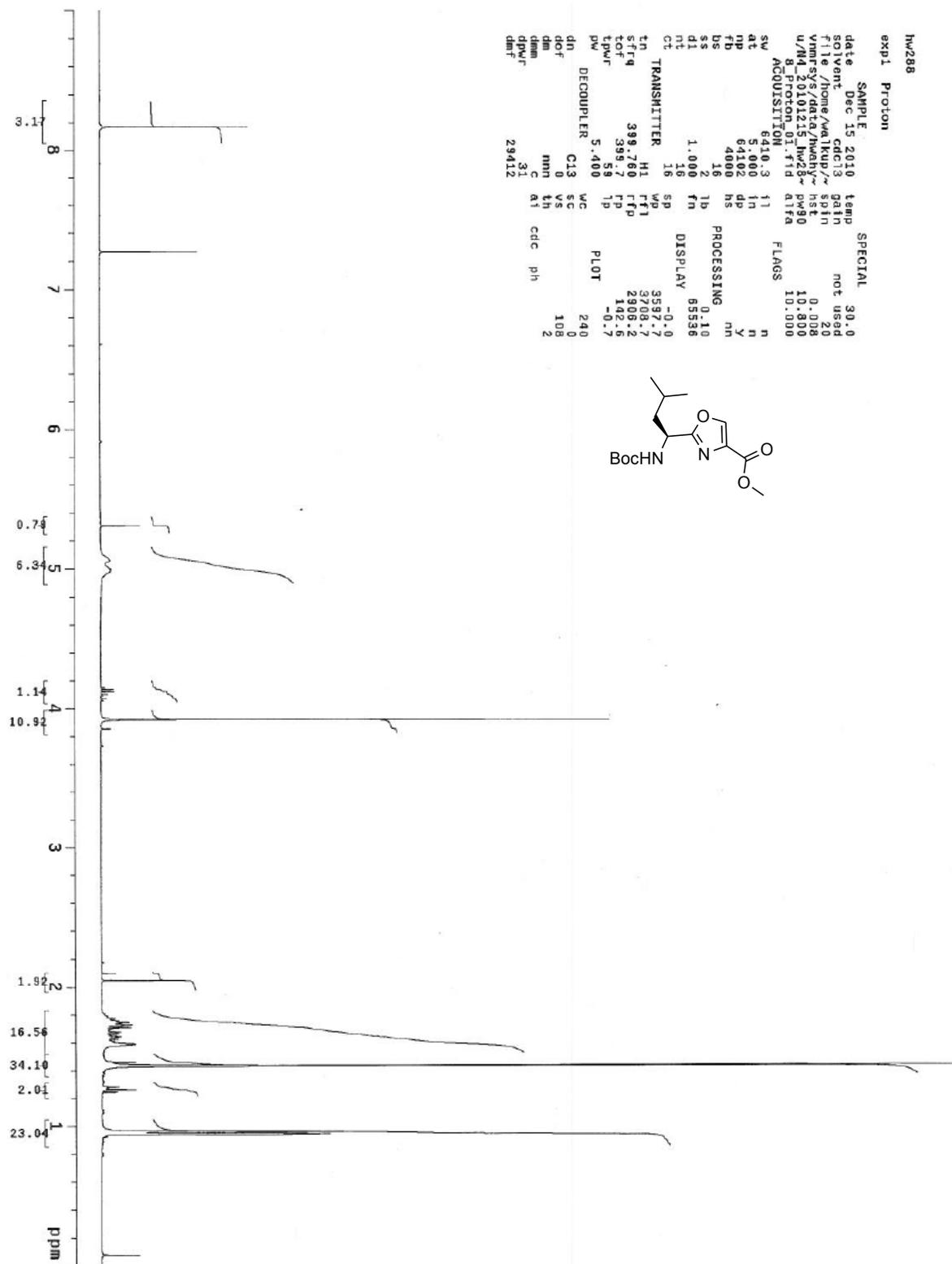
HRMS Macrocycle Phe-Leu-Oxazole-Leu-Leu (3) (MW = 554.3313)



Compound 4: B-Ox-III

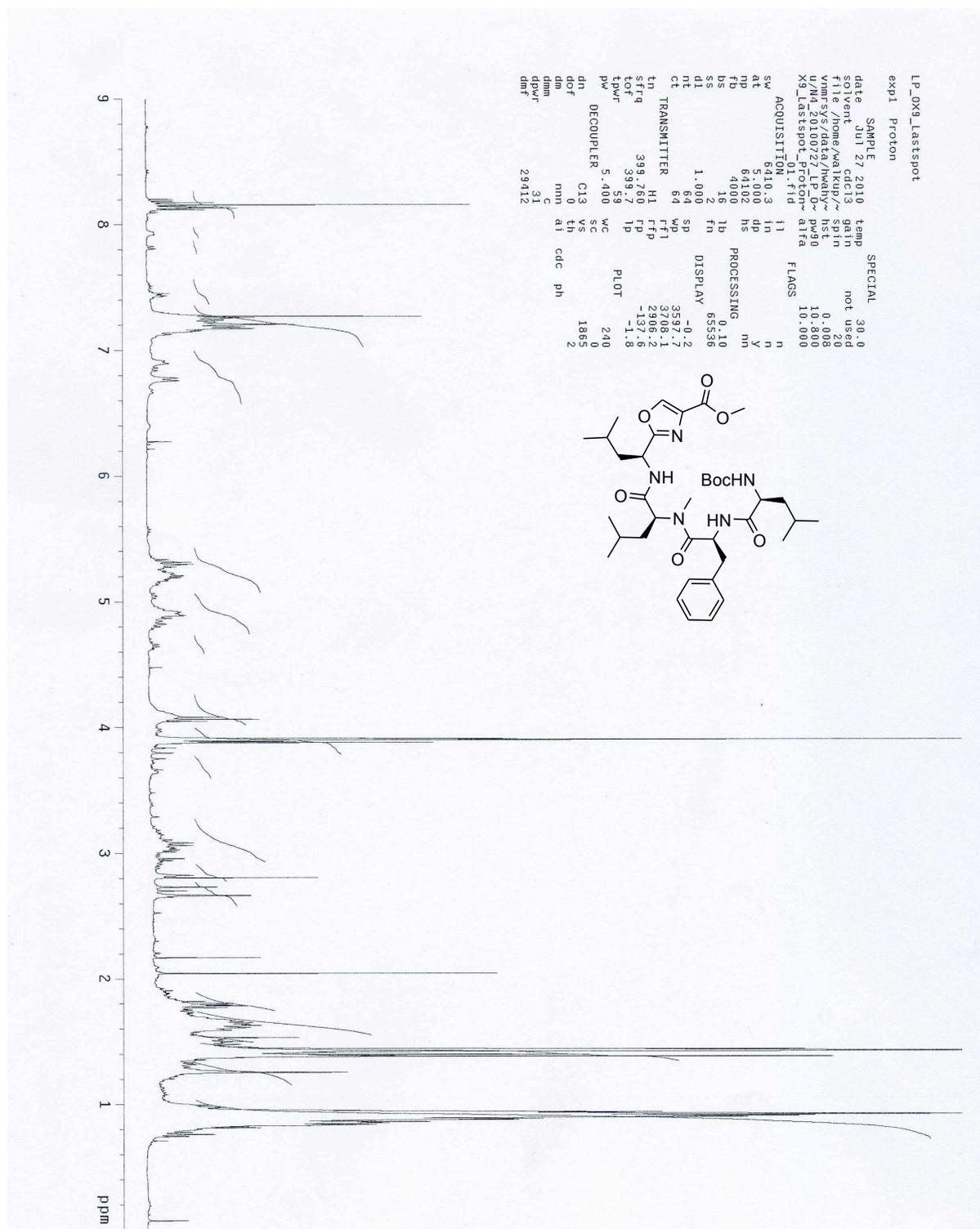
NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc

Davis et al.



Compound 4: B-Ox-III

NMR Dipeptide MeO-Oxazole-Leu-NHBoc

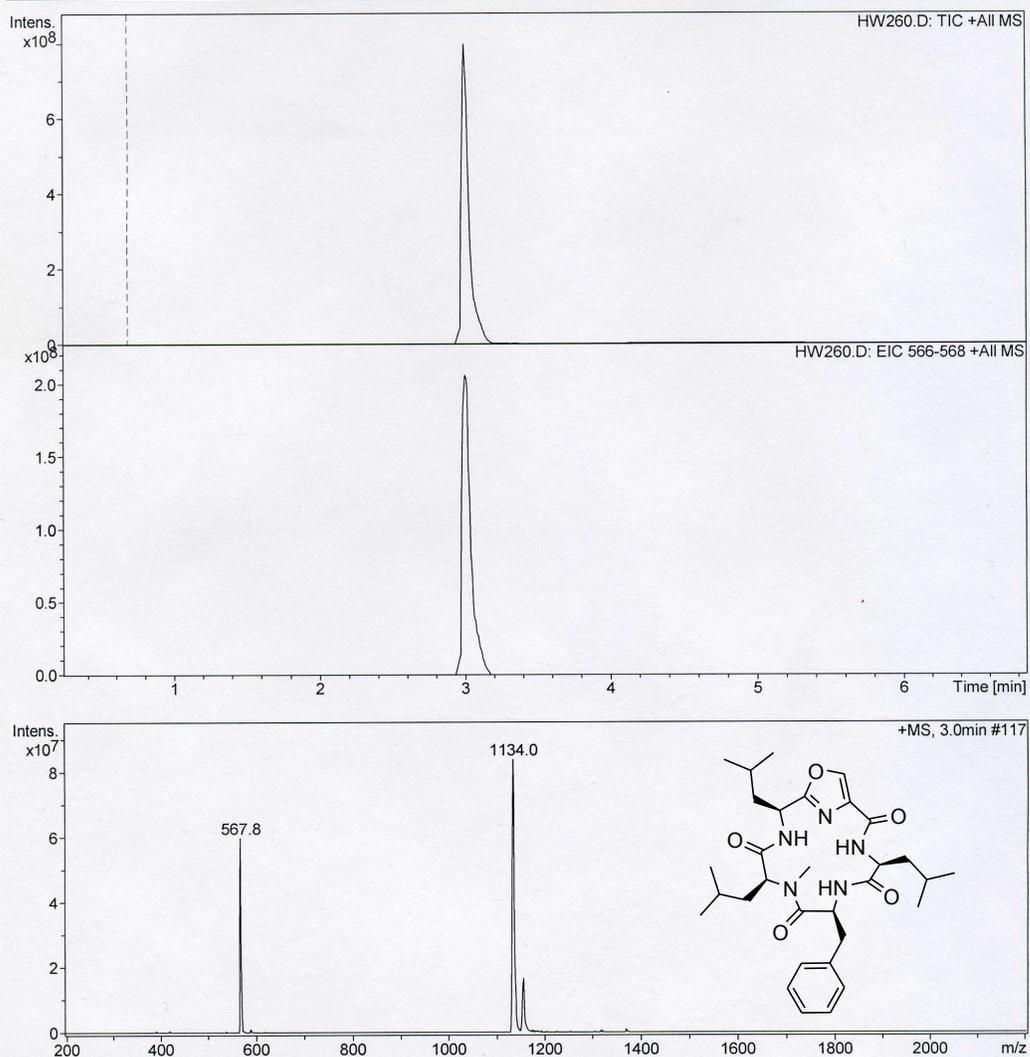


Compound 4: B-Ox-III

NMR Pentapeptide MeO-Oxazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc

Display Report - All Windows Selected Analysis

Analysis Name: HW260.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 11/1/2010 1:38:38 PM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 10/26/2010 4:50:50 PM
Sample Name: hw260
Analysis Info:



Compound 4: B-Ox-III

LCMS Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4) (MW = 567)

Davis et al.

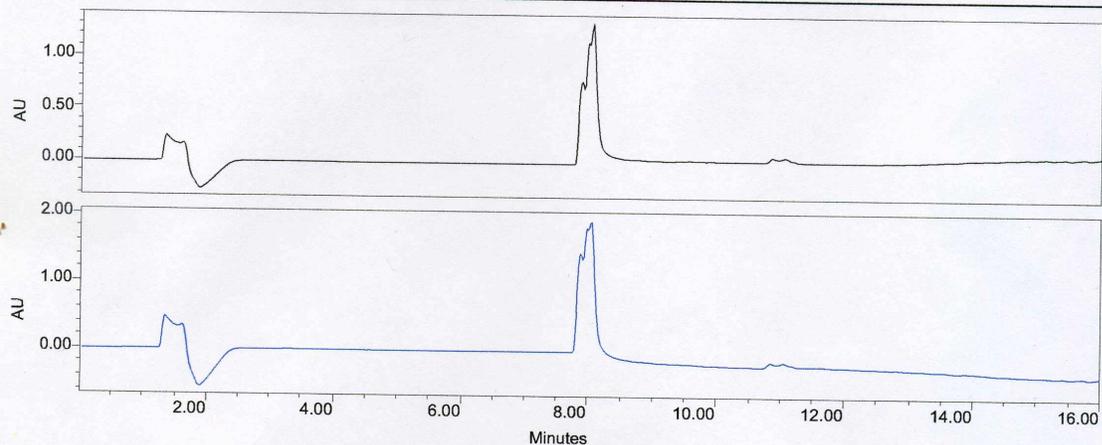
SDSU

Project Name: Defaults
Reported by User: System

Breeze

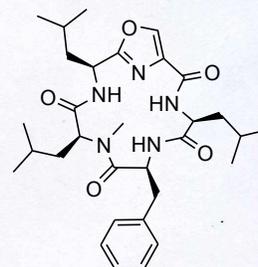
SAMPLE INFORMATION

Sample Name:	hw260	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	852	Date Acquired:	10/27/2010 9:47:35 AM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



Compound 4: B-Ox-III

HPLC Macrocyclic Phe-Leu-Oxazole-Leu-Leu-N(Me) (4)

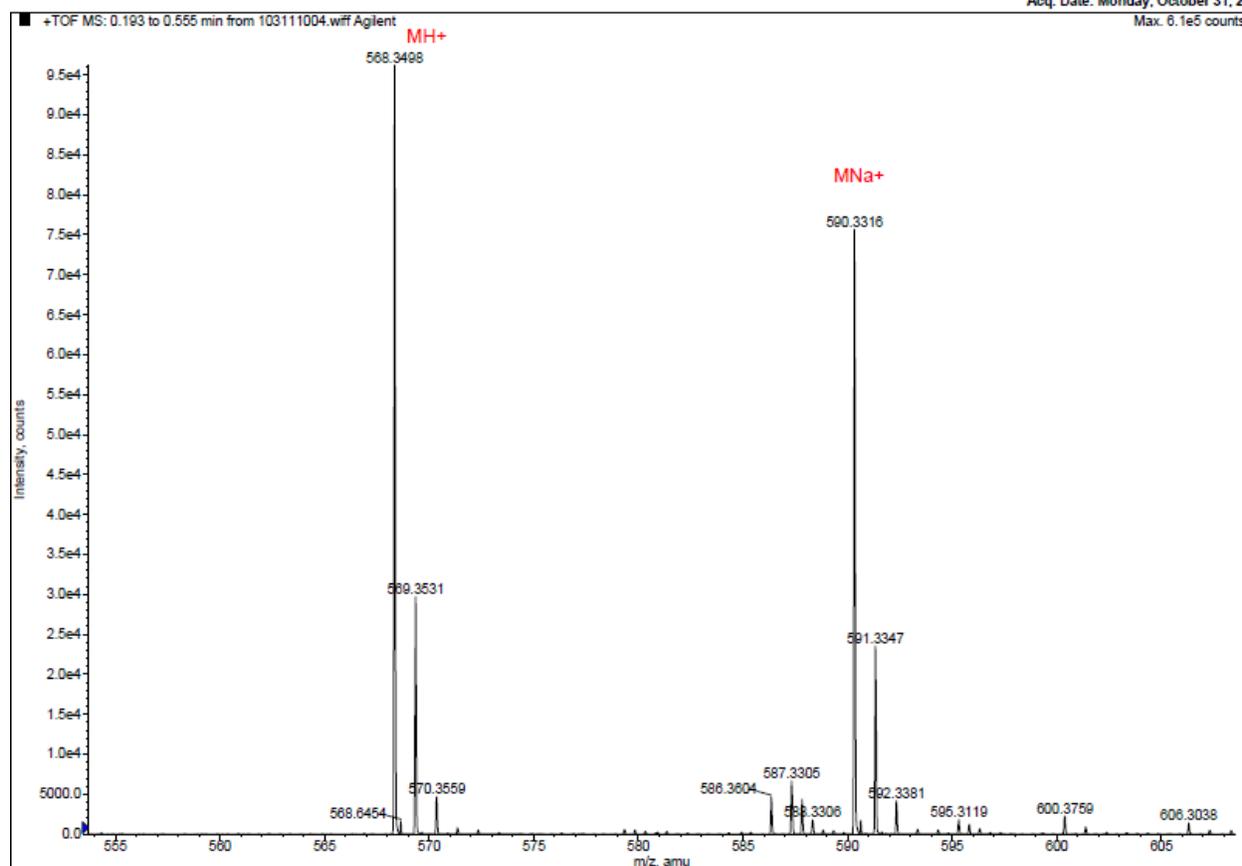
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5697

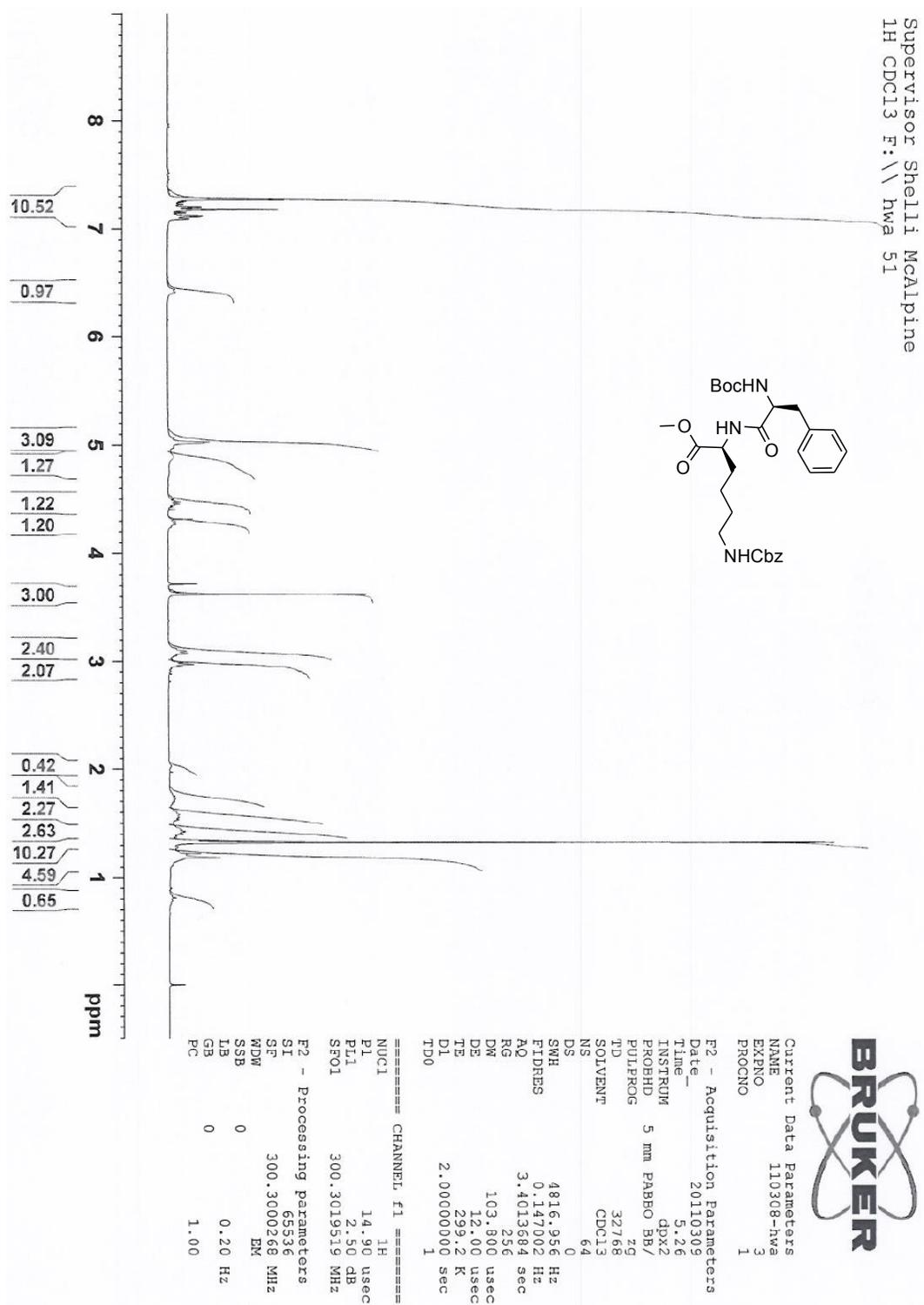
Acq. File: 103111004.wiff
Acq. Date: Monday, October 31, 20



Compound 4: B-Ox-III

HRMS Macrocycle Phe-Leu-Oxazole-Leu-Leu-N(Me) (4) (MW = 568.3520)

Davis et al.

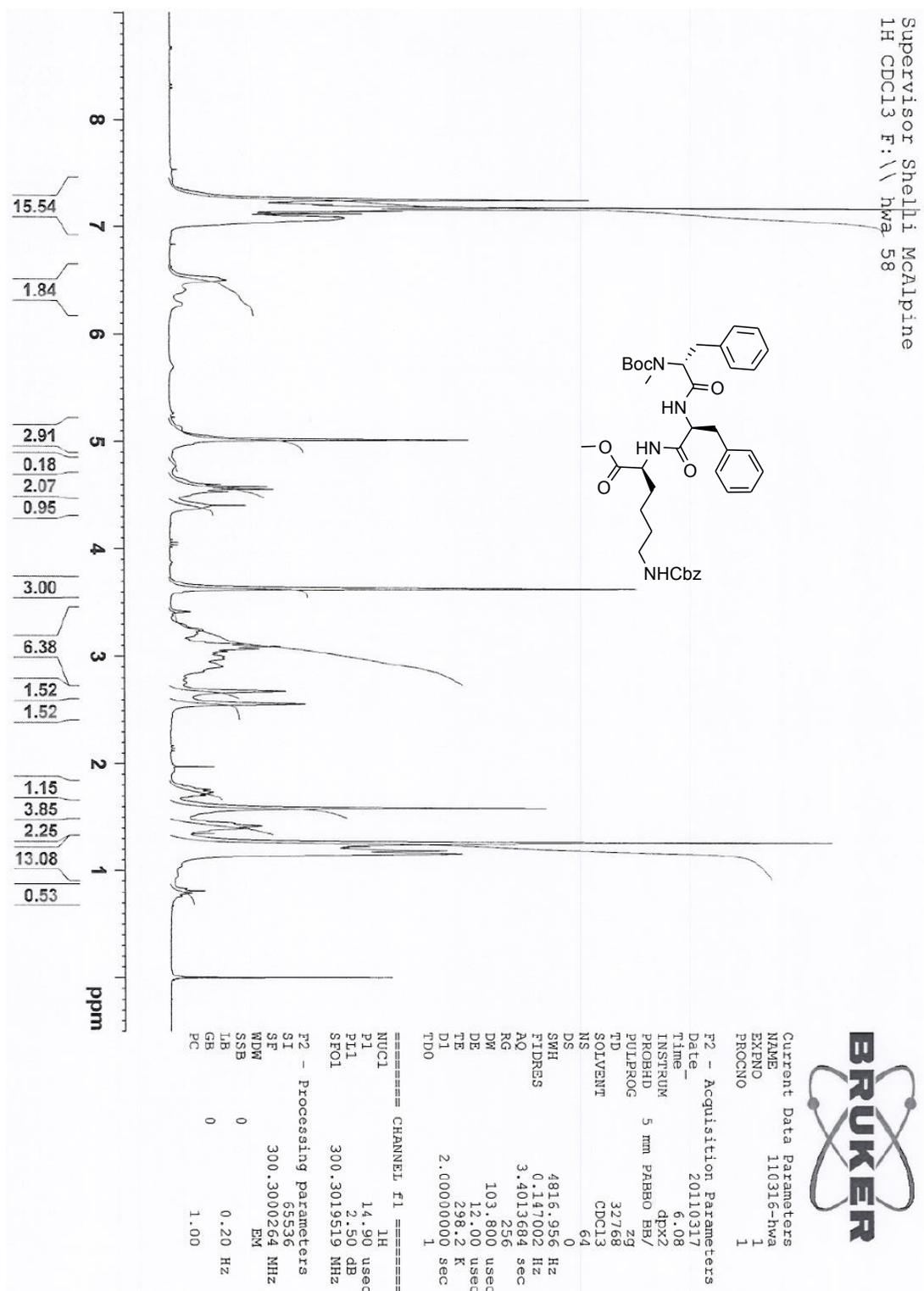


Compound 5: C-Ox-III

NMR Dipeptide MeO-Lys(Cbz)-Phe-NHBoc

Supplementary Material

Davis et al.

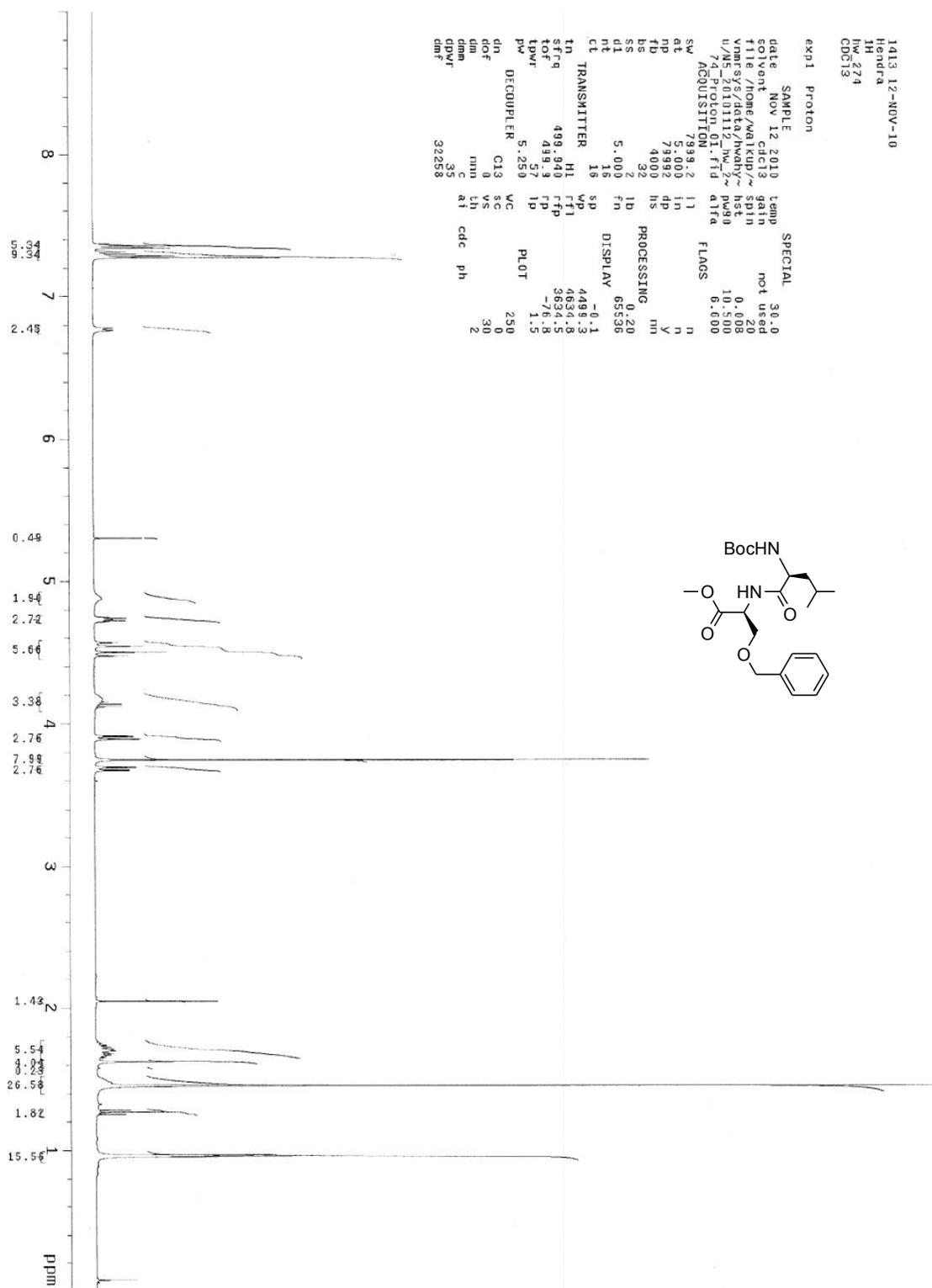


Compound 5: C-Ox-III

NMR Tripeptide MeO-Lys(Cbz)-Phe-D-Phe-N(Me)Boc

Supplementary Material

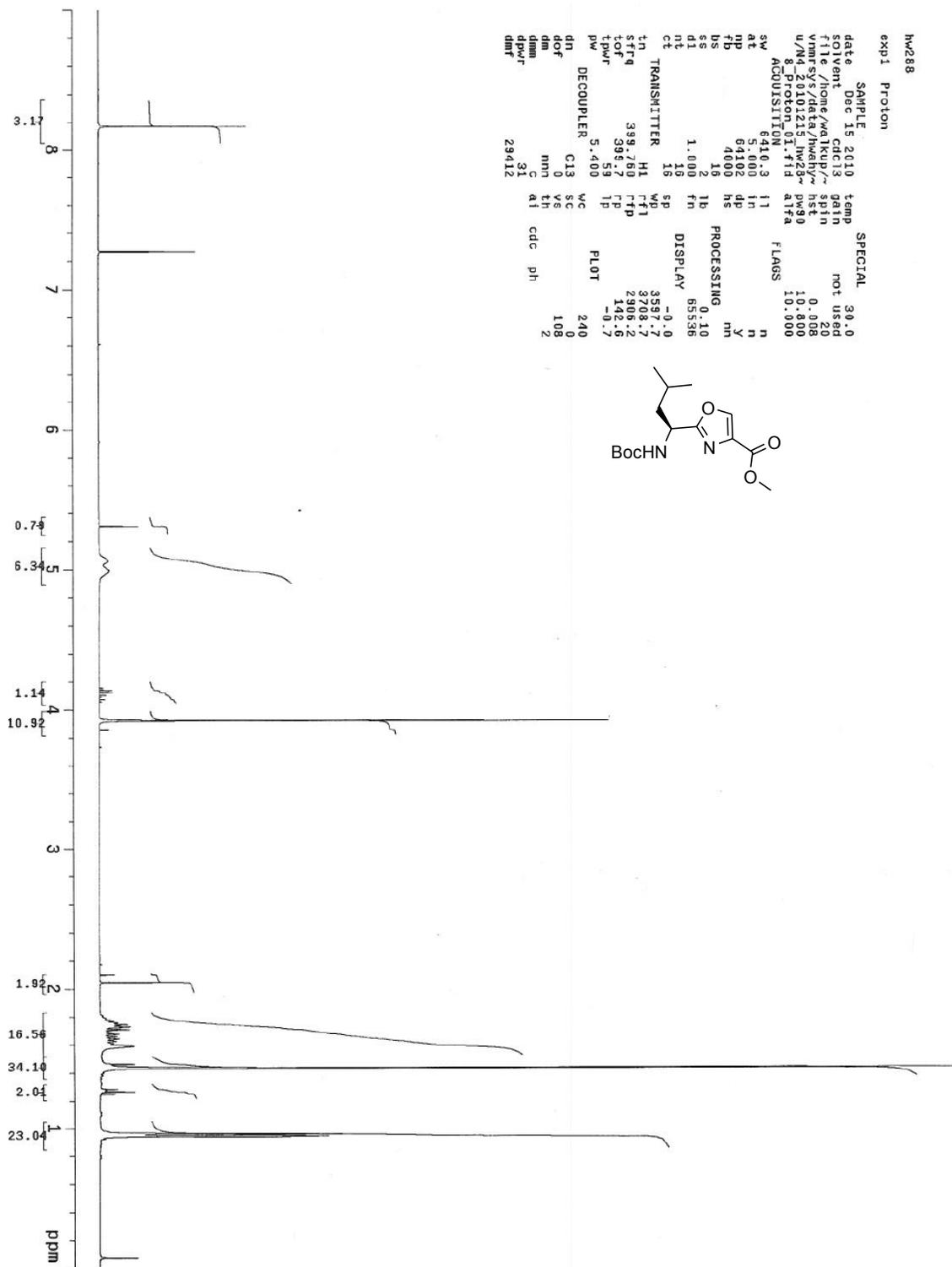
Davis et al.



Compound 5: C-Ox-III

NMR Dipeptide MeO-Ser(Bzl)-Leu-NHBoc

Davis et al.

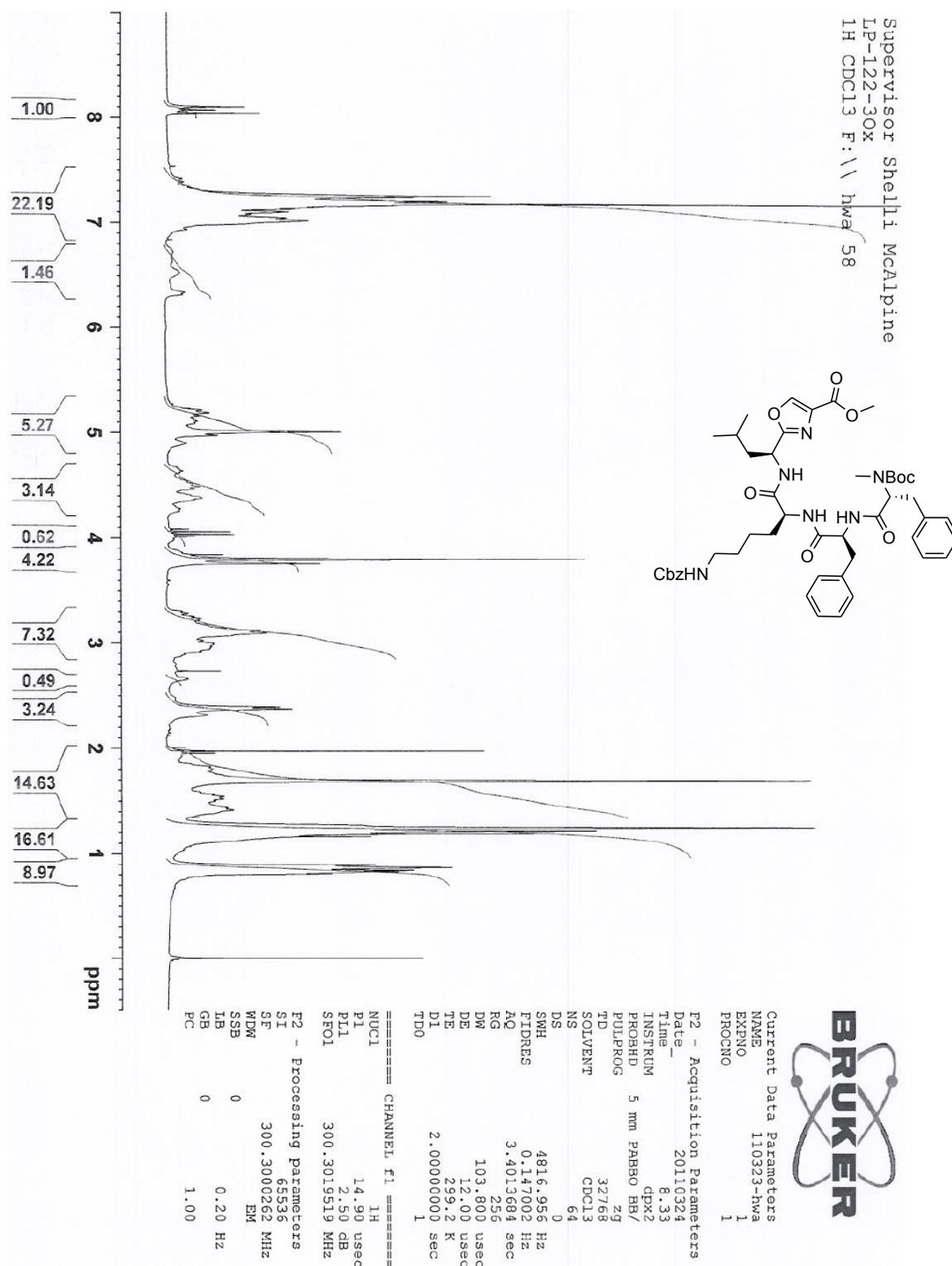


Compound 5: C-Ox-III

NMR Dipeptide MeO-Oxazole-Leu-NHBoc

Supplementary Material

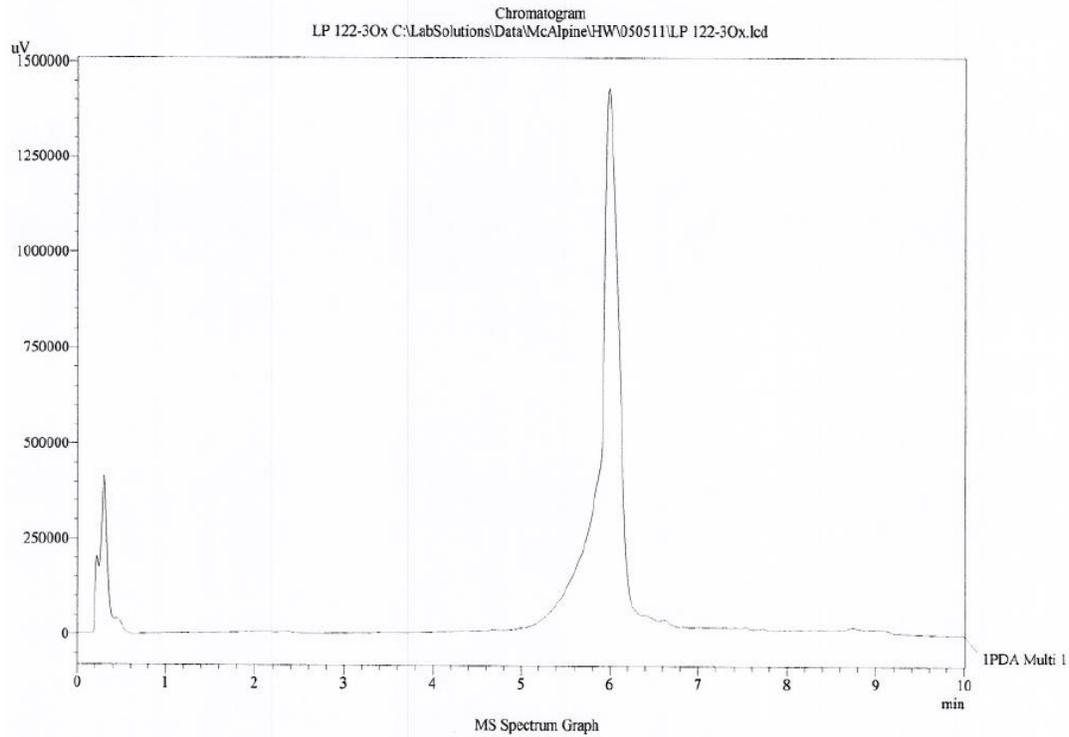
Davis et al.



Compound 5: C-Ox-III

NMR Pentapeptide MeO-Oxazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc

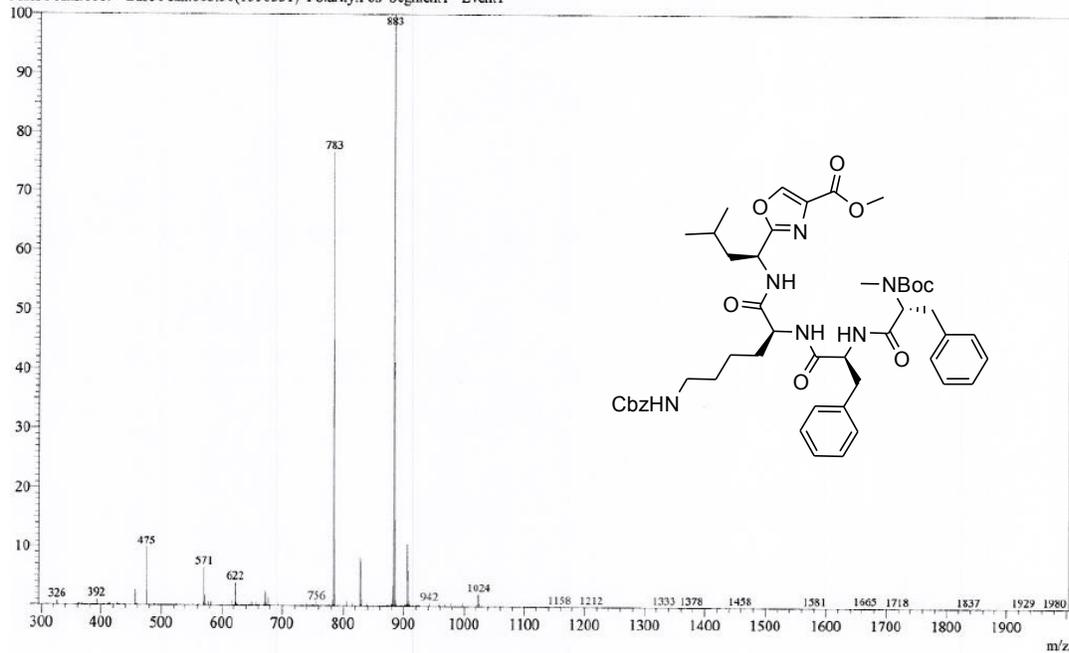
==== Shimadzu LCMSsolution Analysis Report ====



Ret. Time: 6.633(Scan#: 339)

BG Mode: ?

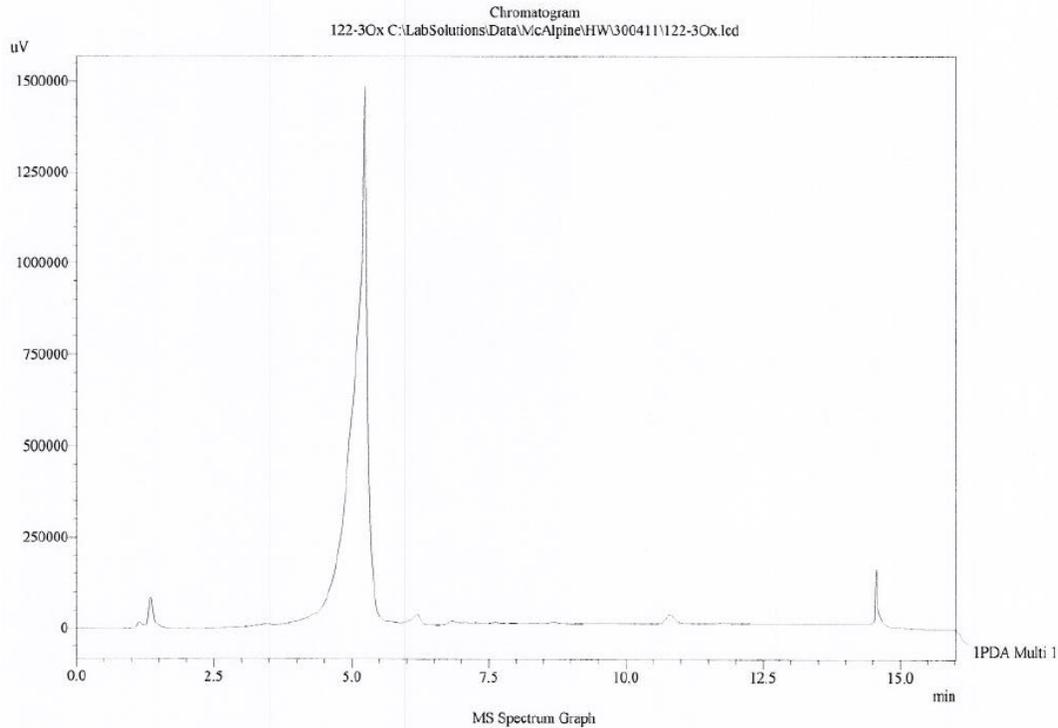
Mass Peaks: 1619 Base Peak: 883.30(1350551) Polarity: Pos Segment: 1 - Event: 1



Compound 5: C-Ox-III

HPLC/LCMS Pentapeptide MeO-Oxazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc (MW = 882)

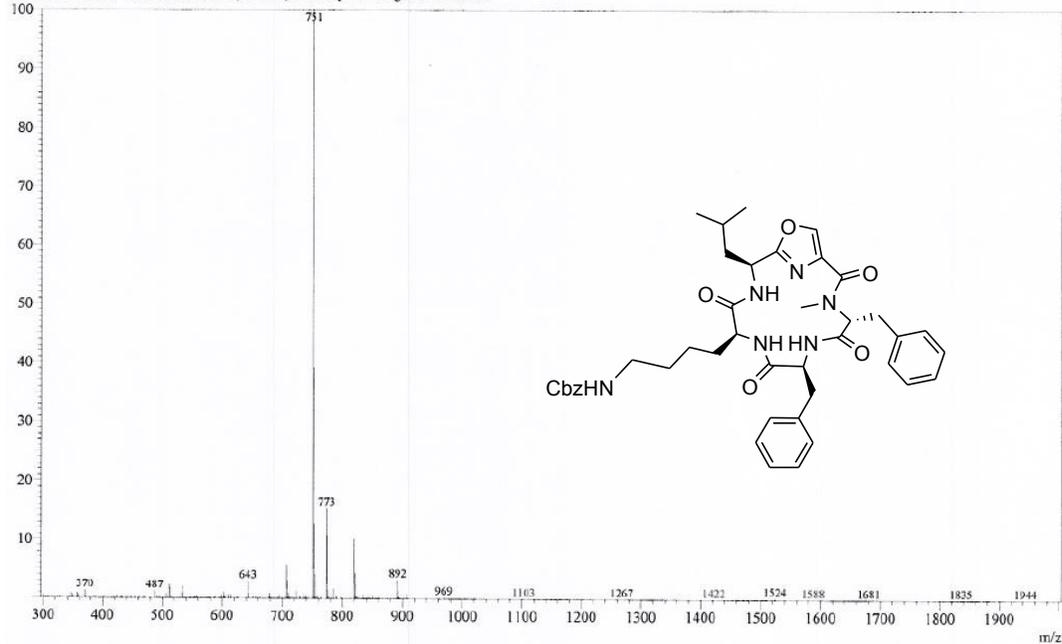
==== Shimadzu LCMSsolution Analysis Report ====



Ret Time: 5.200(Scan#: 253)

BG Mode: ?

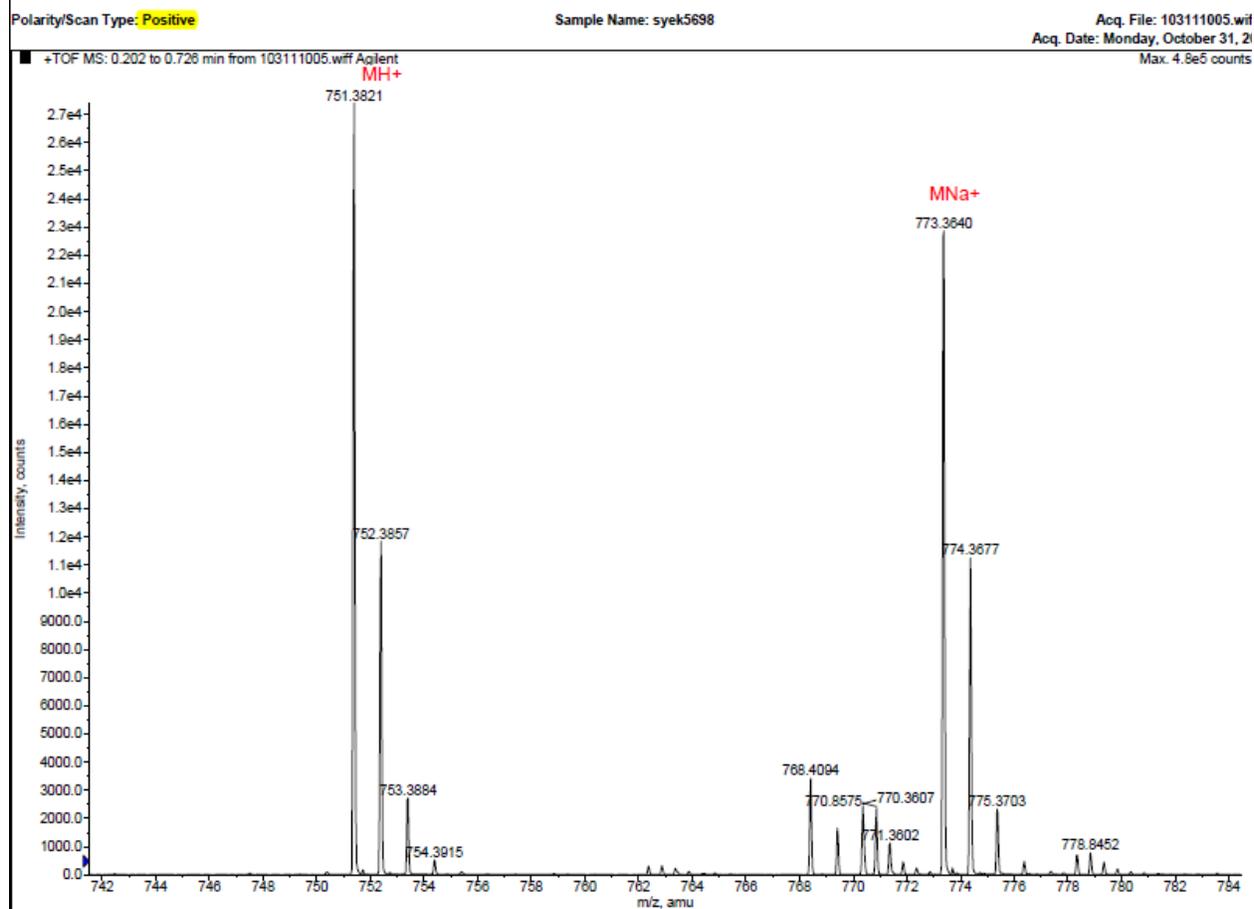
Mass Peaks: 1605 Base Peak: 751.15(881037) Polarity: Pos Segment: 1 - Event: 1



Compound 5: C-Ox-III

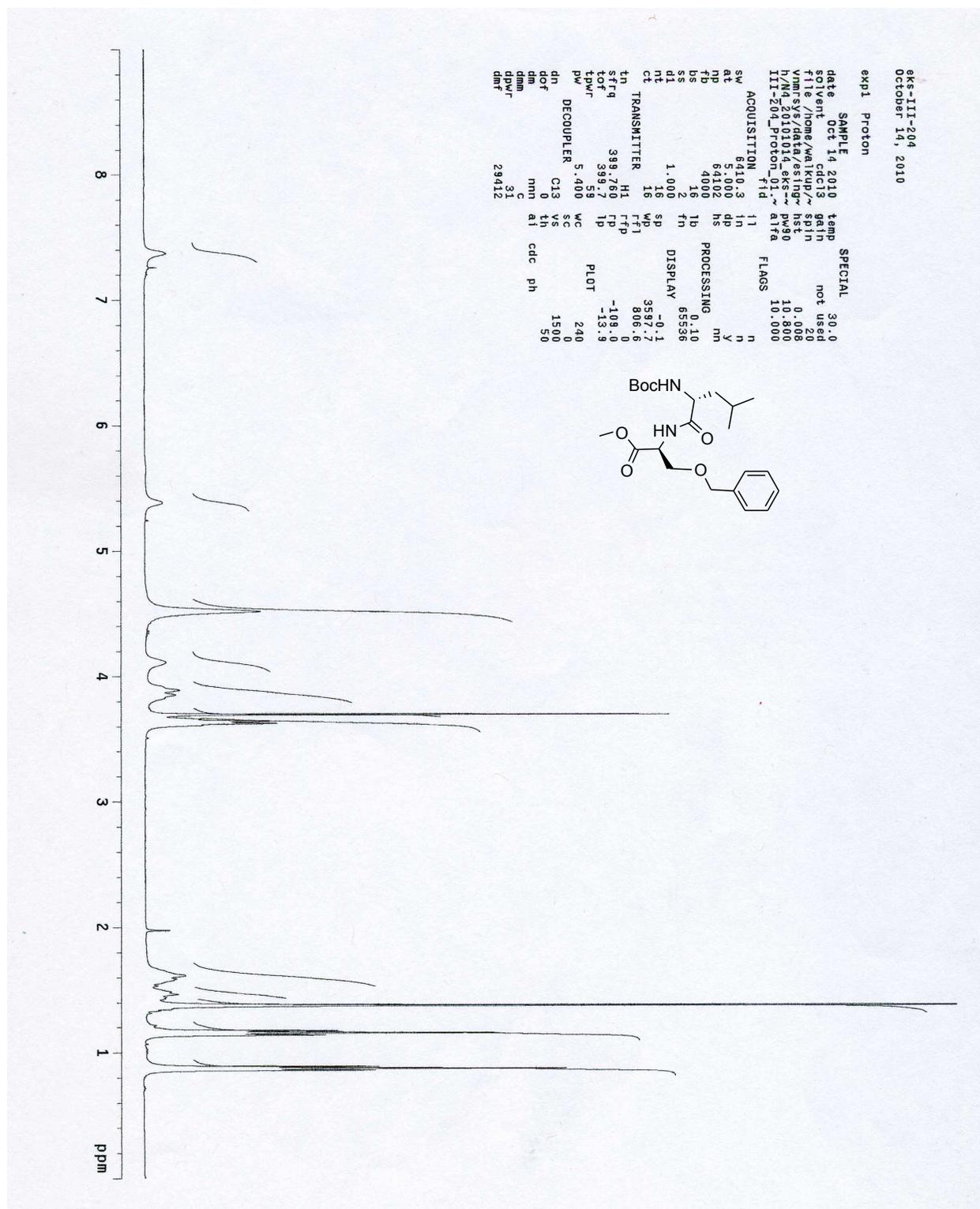
HPLC+LCMS Macrocyclic Phe-D-Phe-N(Me)-Oxazole-Leu-Lys(Cbz) (5) (MW=750)

Davis et al.



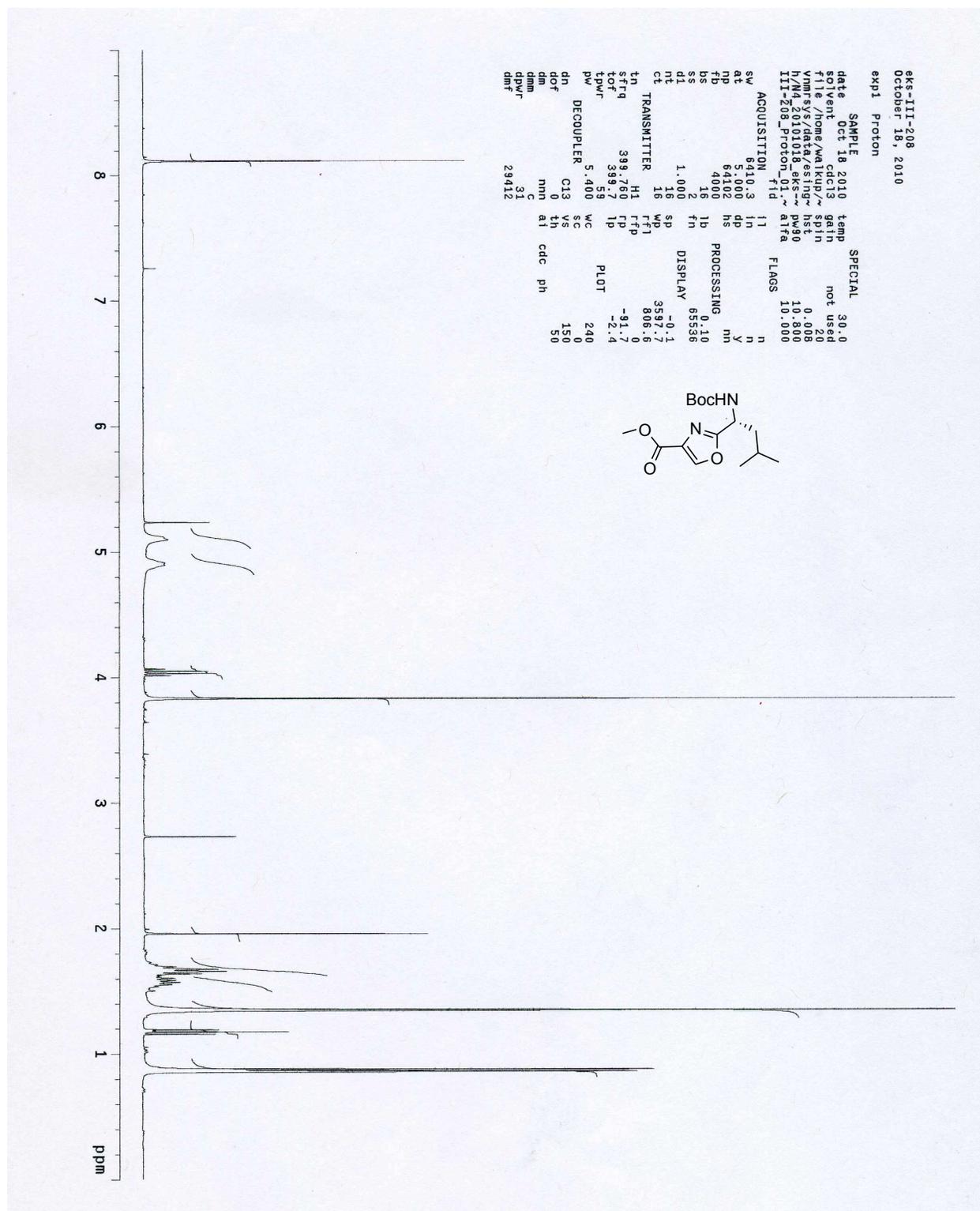
Compound 5: C-Ox-III

HRMS Macrocycle Phe-D-Phe-N(Me)-Oxazole-Leu-Lys(Cbz) (5) (MW= 751.3821)



Compound 6: D-Ox-III

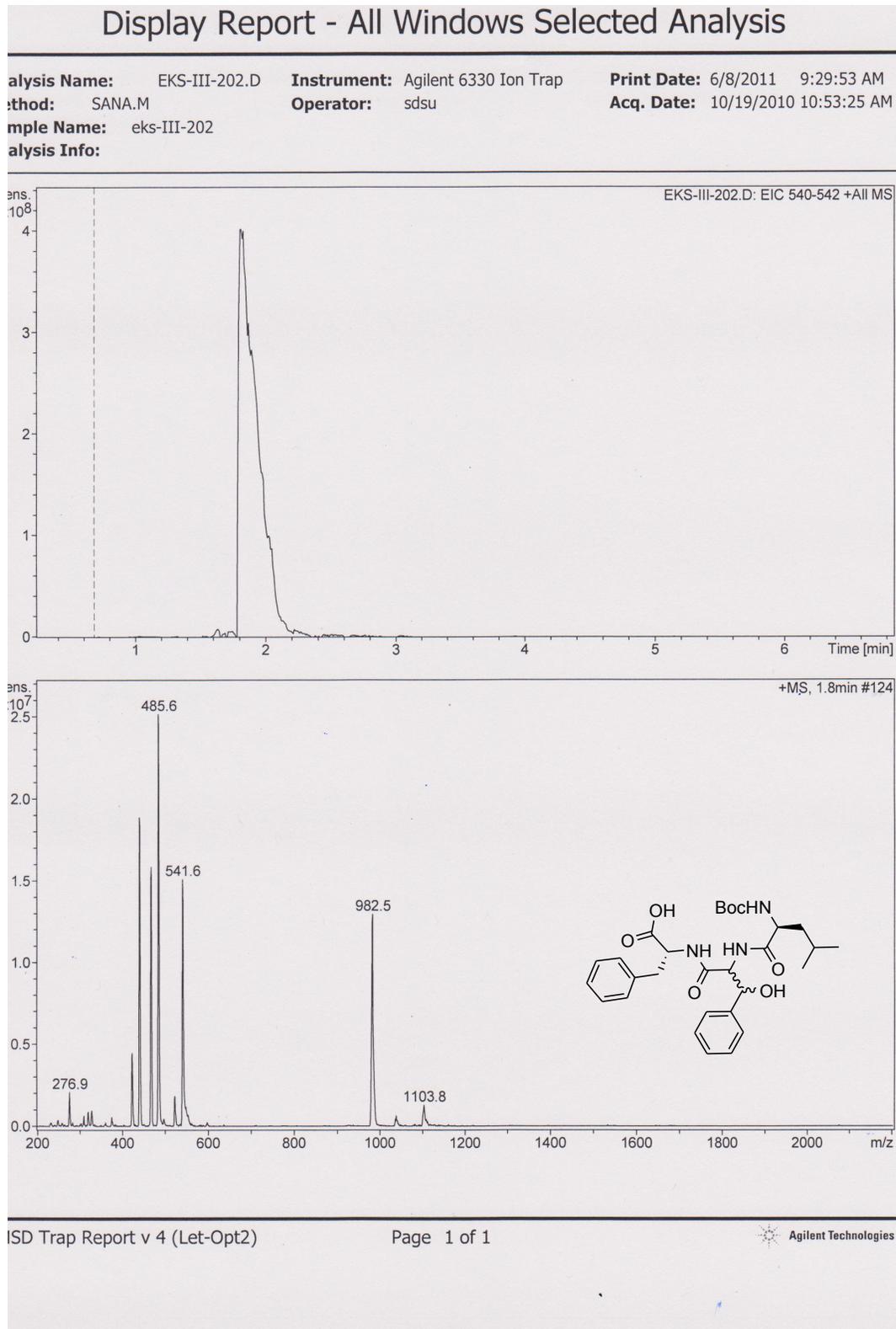
NMR Dipeptide MeO-Ser(Bzl)-D-Leu-NHBoc



Compound 6: D-Ox-III

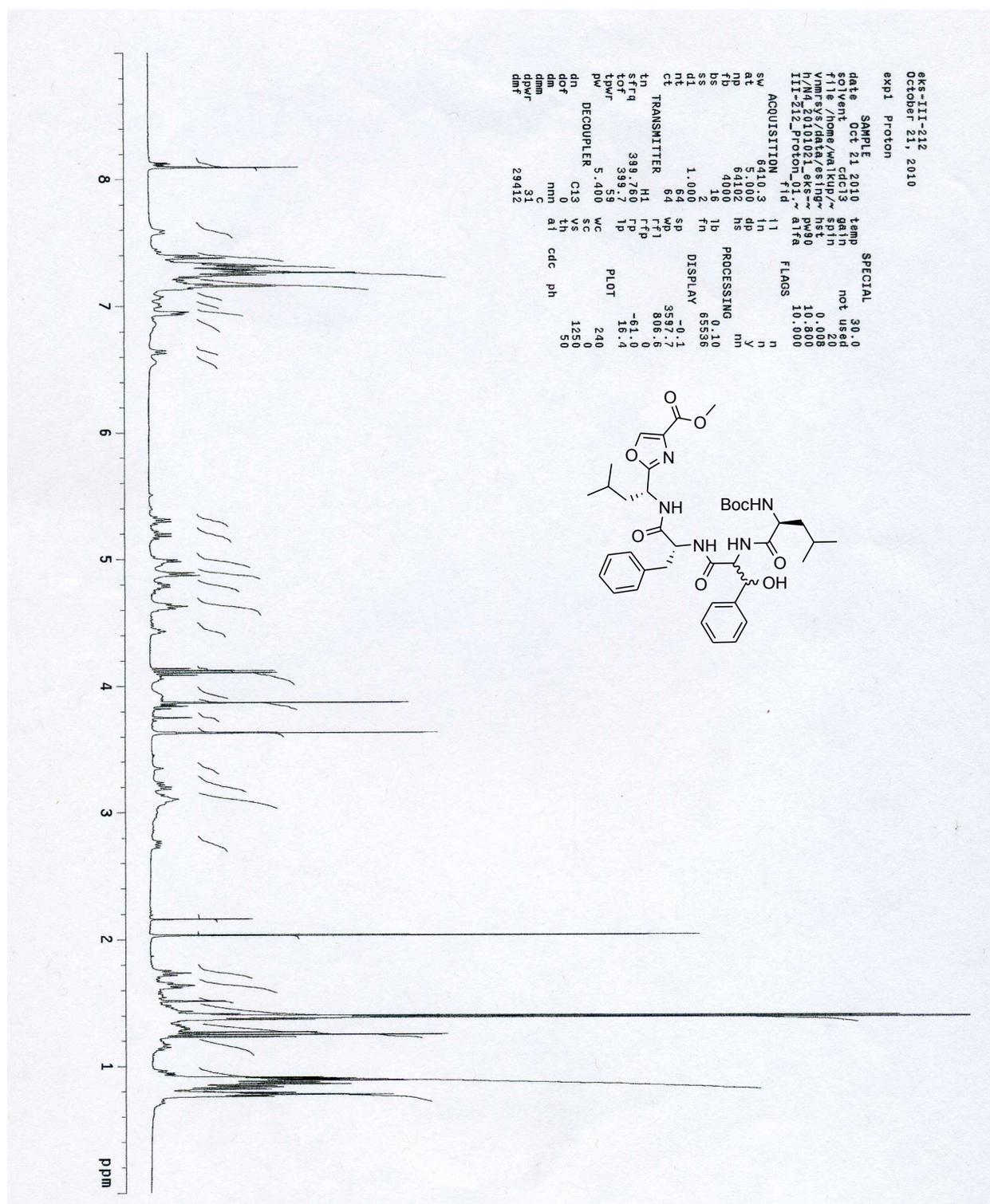
NMR Dipeptide MeO-Oxazole-D-Leu-NHBoc

Davis et al.



Compound 6: D-Ox-III

LCMS Tripeptide HO-D-Phe-Phe-(2R,3R)/(2S,3S)-β-OH-Leu-NHBoc (MW = 541)

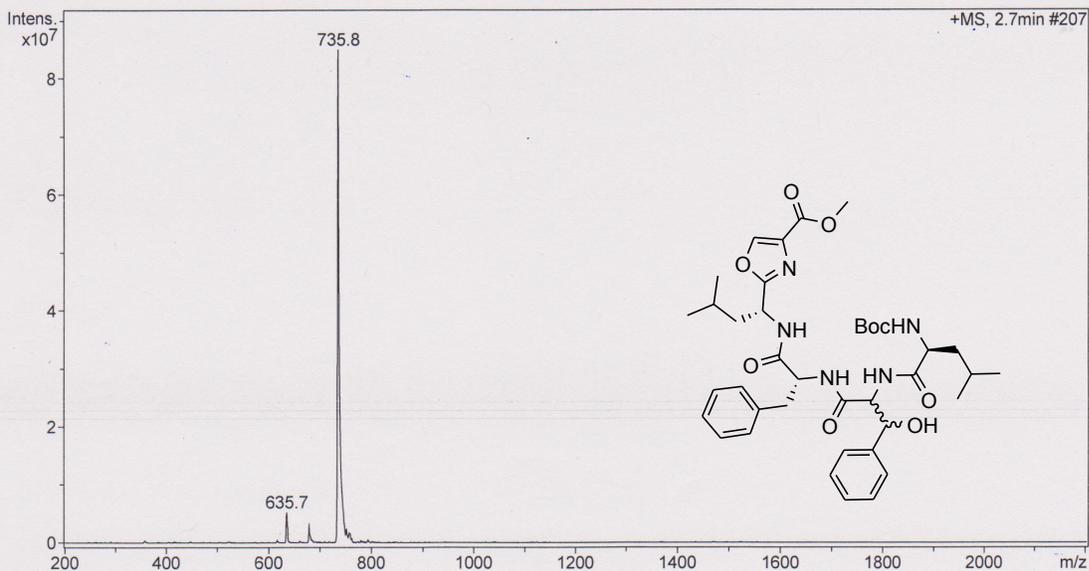
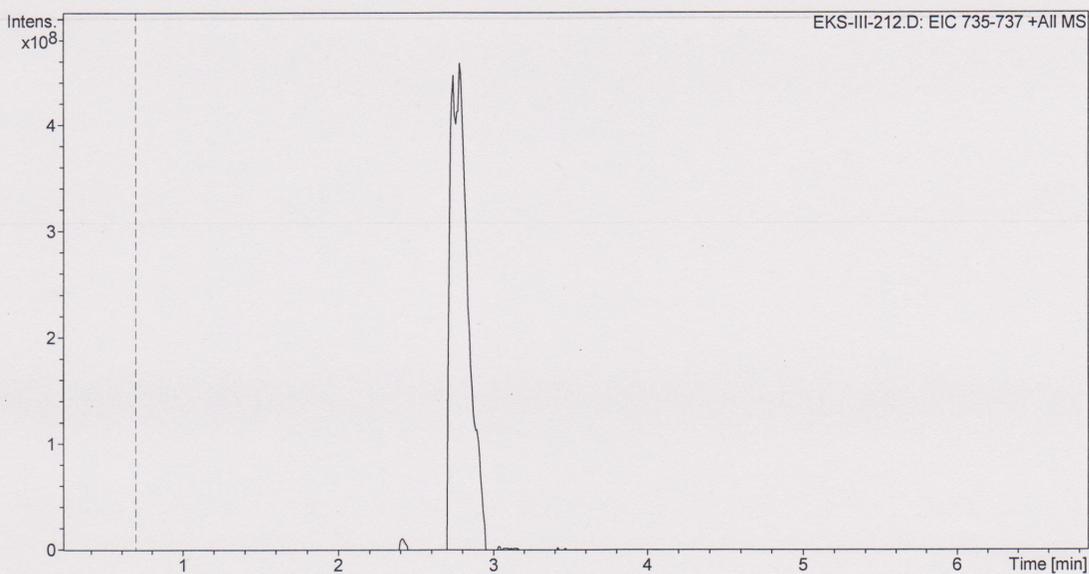


Compound 6: D-Ox-III

NMR Pentapeptide MeO-Oxazole-D-Leu-D-Phe-(2R,3R)/(2S,3S)-β-OH-Phe-Leu-NHBoc

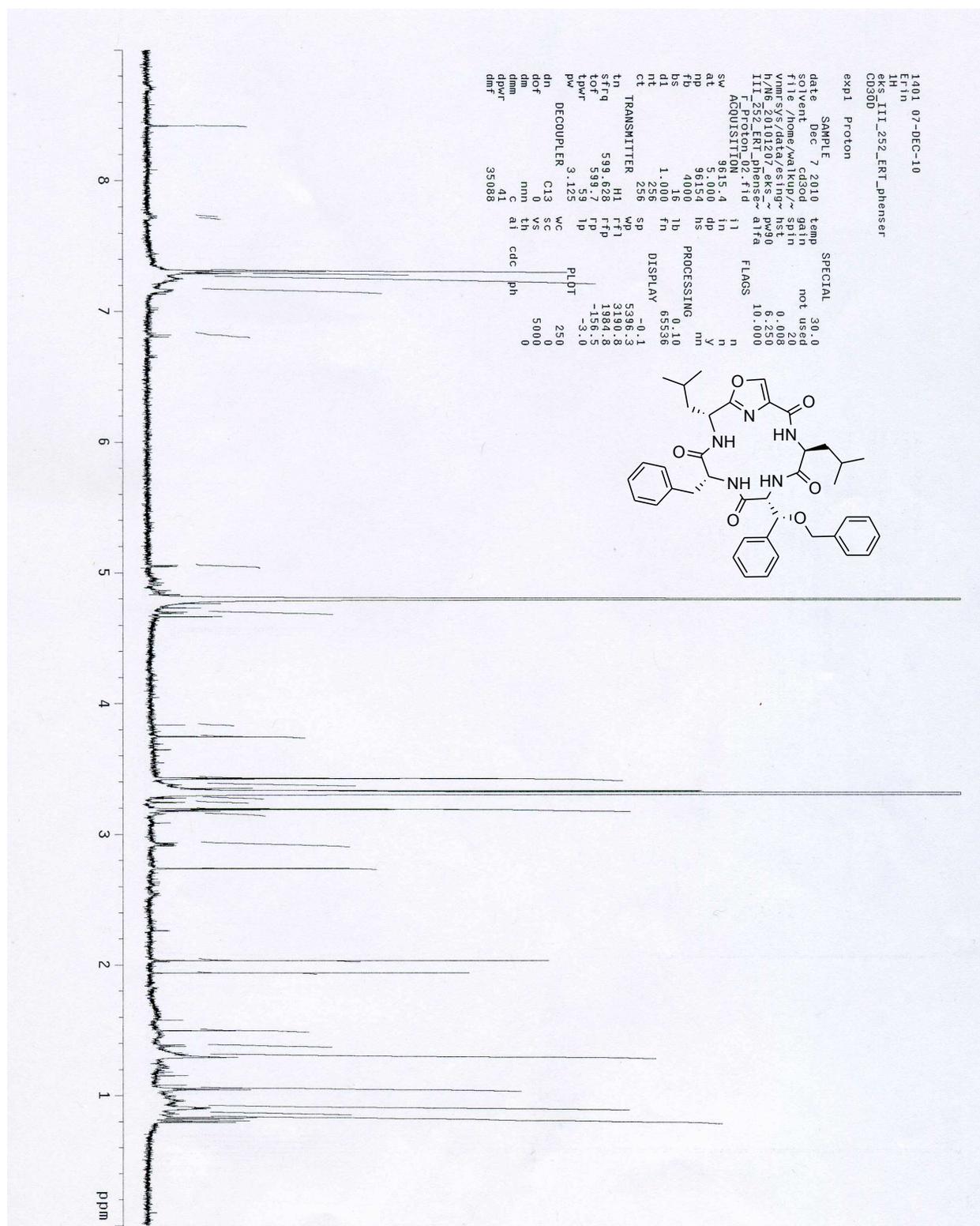
Display Report - All Windows Selected Analysis

Analysis Name: EKS-III-212.D Instrument: Agilent 6330 Ion Trap Print Date: 6/8/2011 9:30:59 AM
Method: SANA.M Operator: sdsu Acq. Date: 10/19/2010 6:46:26 PM
Sample Name: eks-III-212
Analysis Info:



Compound 6: D-Ox-III

LCMS Pentapeptide MeO-Oxazole-D-Leu-D-Phe-(2R,3R)/(2S,3S)- β -OH-Phe-Leu-NHBoc (MW = 736)



Compound 6: D-Ox-III
 NMR Macrocyclic (2R,3R)- β -benzyloxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6)

Davis et al.

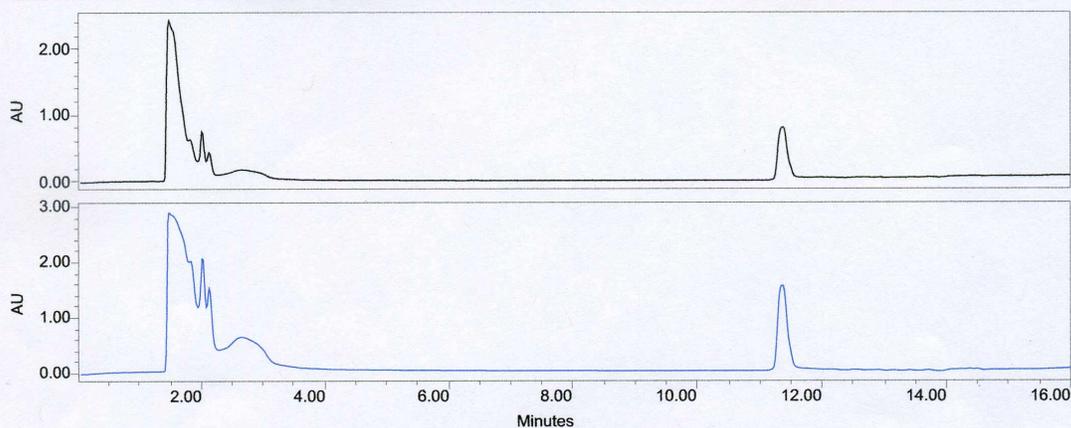
SDSU

Project Name: Defaults
 Reported by User: System

Breeze

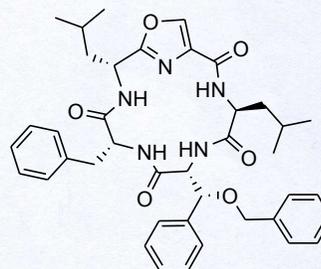
SAMPLE INFORMATION

Sample Name:	eks_comp145_3ox	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	240	Date Acquired:	3/16/2011 1:22:10 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



Compound 6: D-Ox-III

HPLC Macrocycle (2R,3R)- β -benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6)

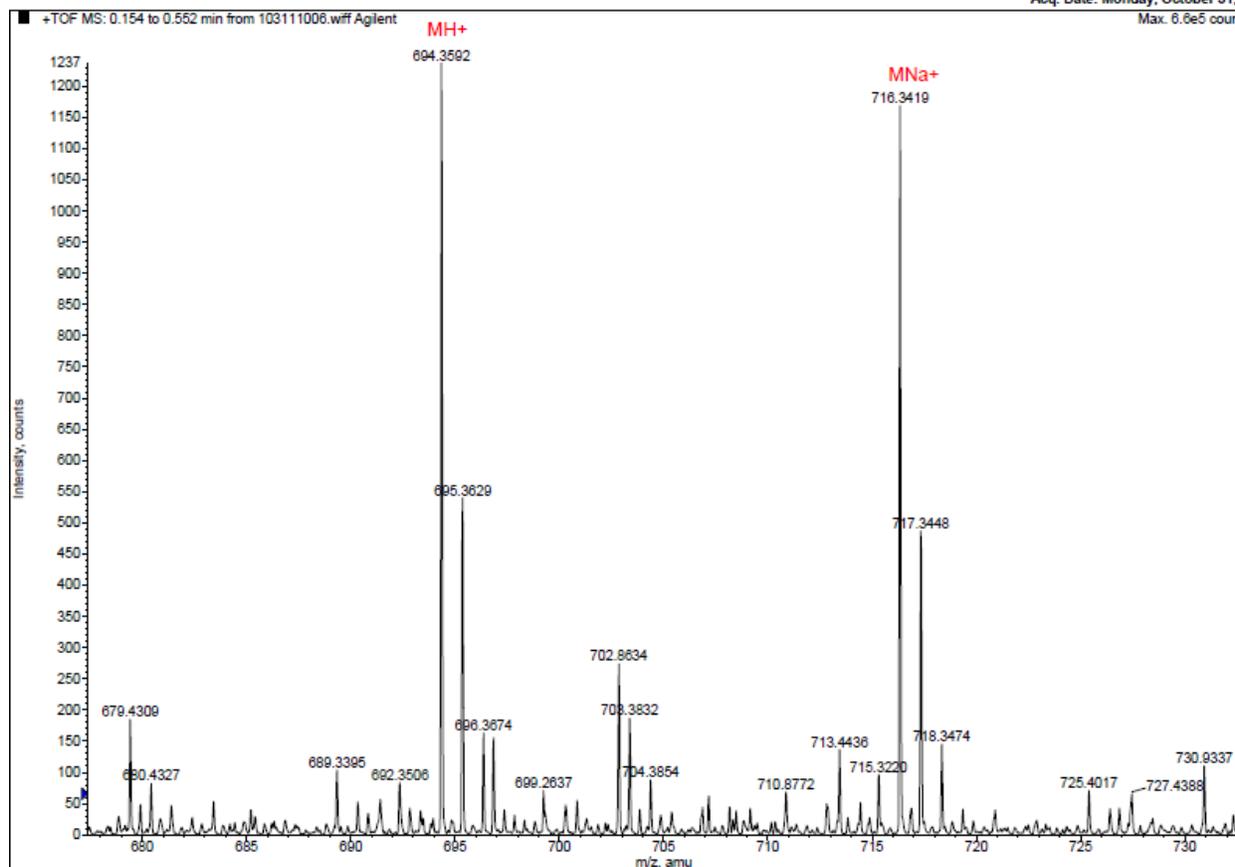
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

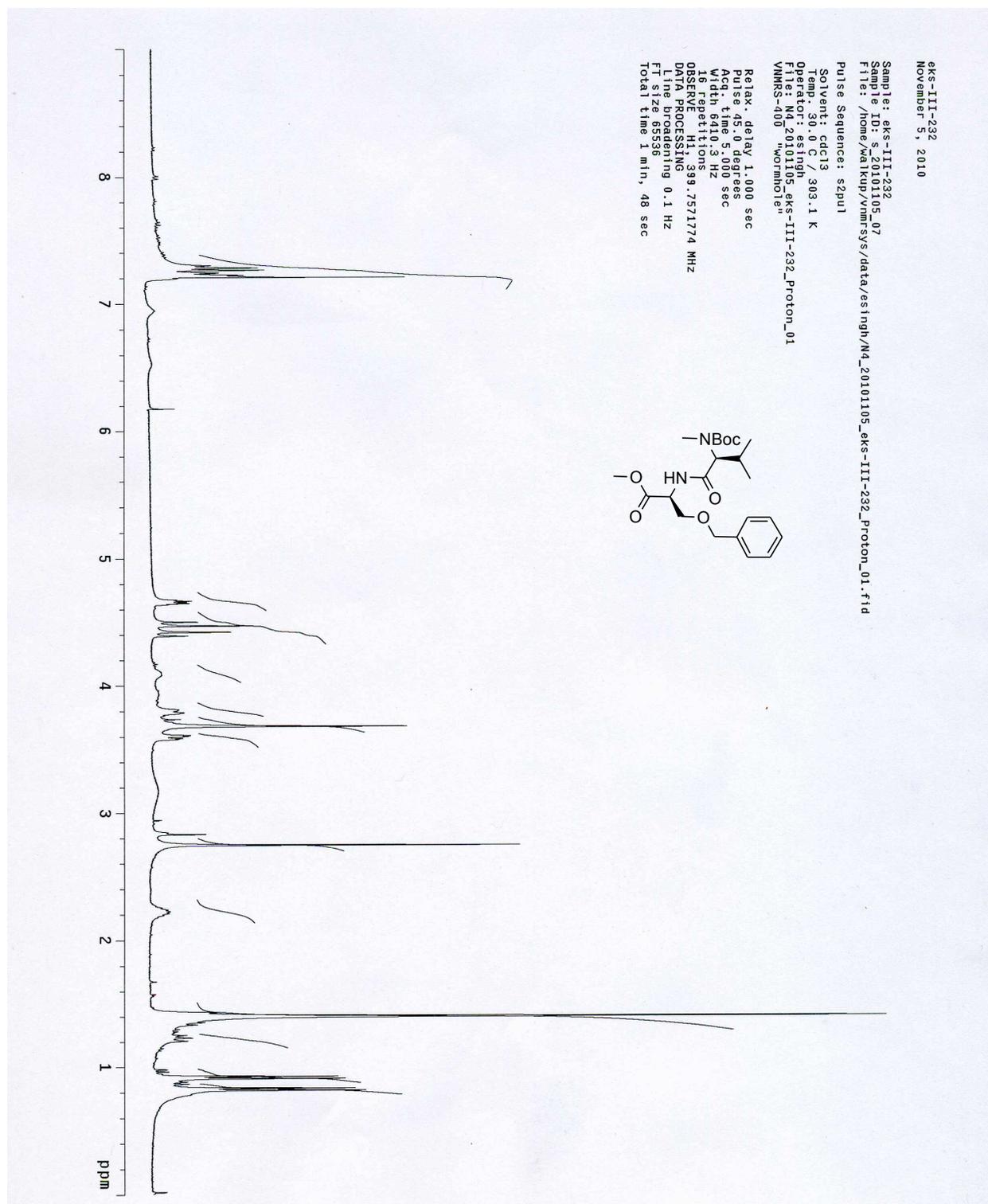
Sample Name: syek5699

Acq. File: 103111006.wil
Acq. Date: Monday, October 31, 2011
Max. 6.6e5 counts



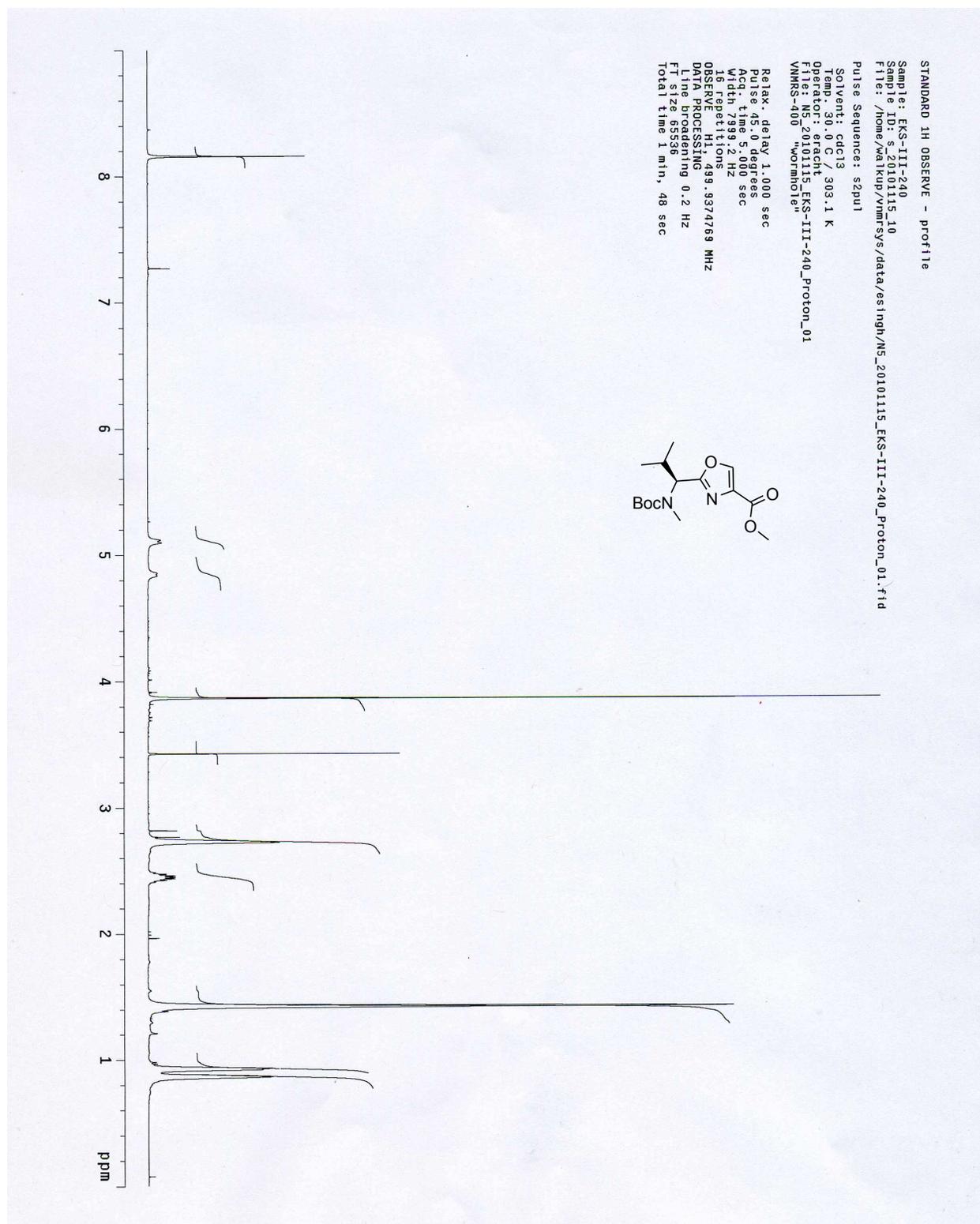
Compound 6: D-Ox-III

HRMS Macrocycle (2R,3R)- β -benzoxy-Phe-Leu-Oxazole-D-Leu-D-Phe (6) (MW = 694.3592)



Compound 7: D-Ox-II

NMR Di-peptide MeO-Ser(Bzl)-Val-N(Me)Boc

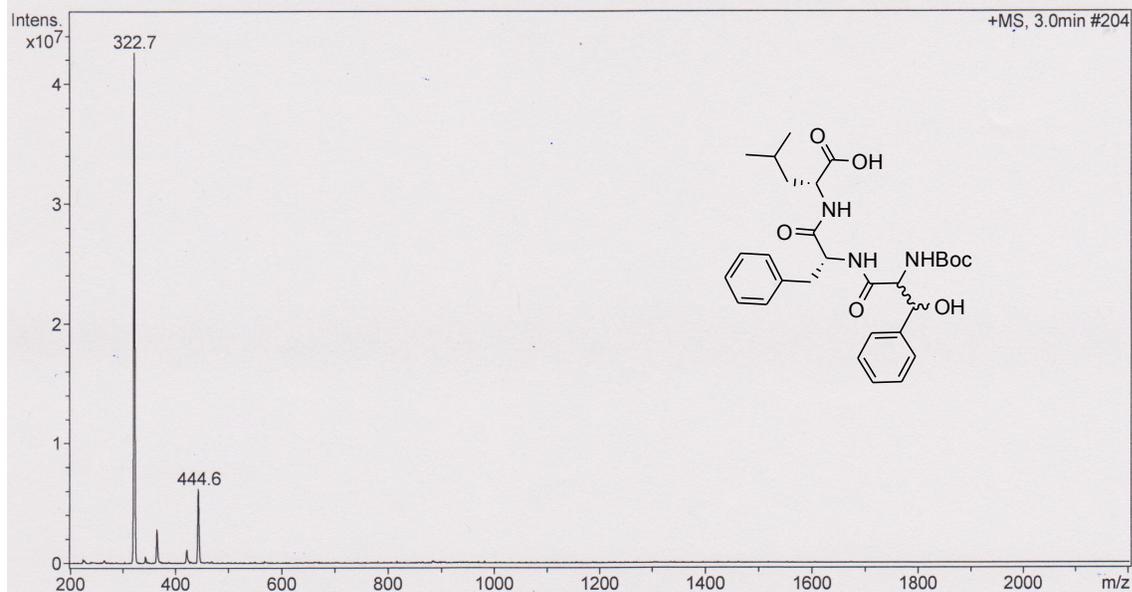
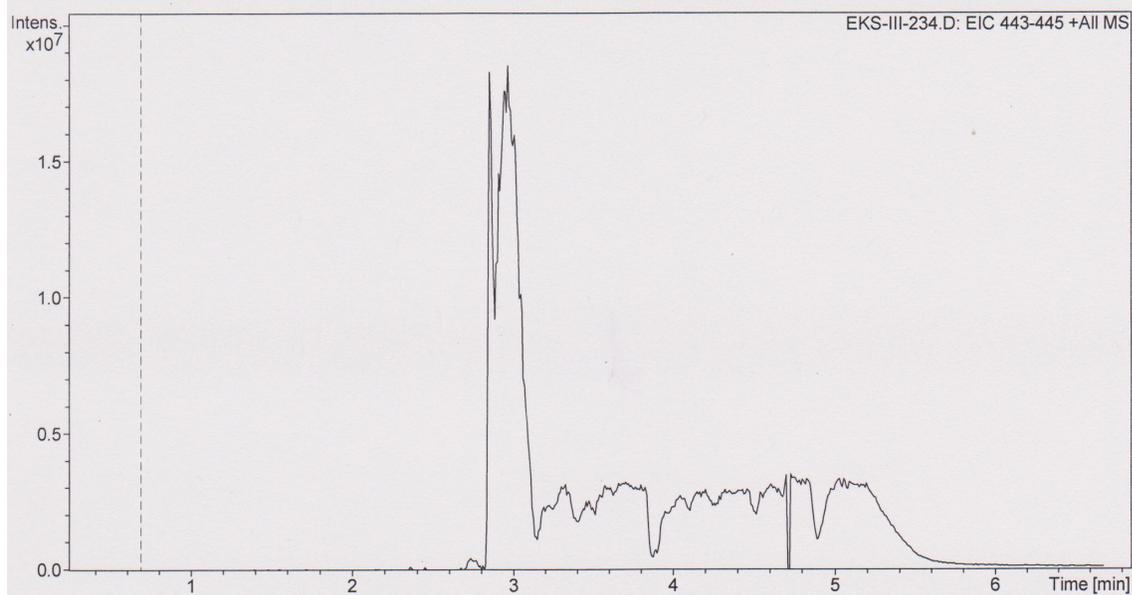


Compound 7: D-Ox-II

NMR Dipeptide MeO-Oxazole-Val-N(Me)Boc

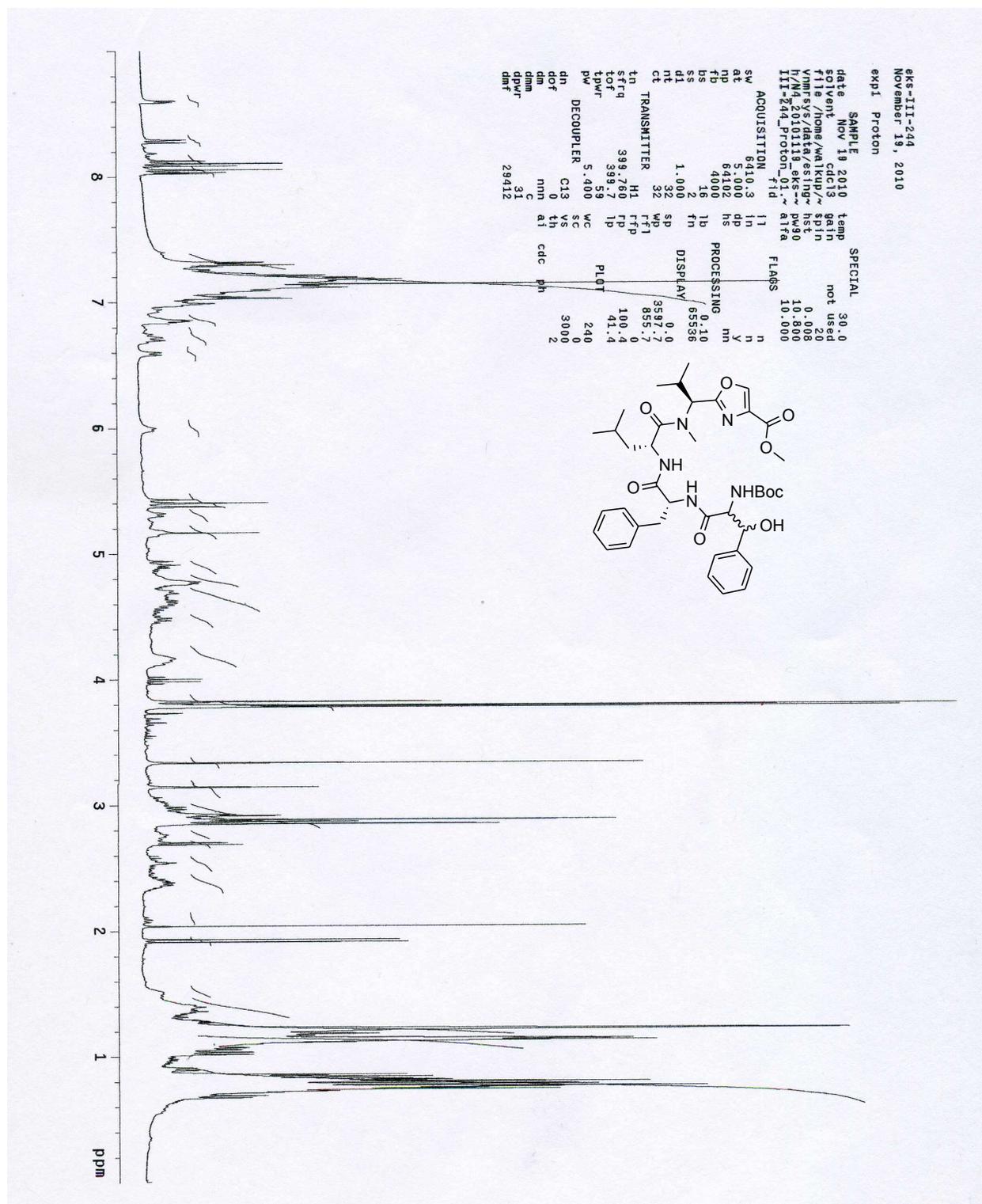
Display Report - All Windows Selected Analysis

Analysis Name: EKS-III-234.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/8/2011 9:22:13 AM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 11/8/2010 12:05:19 PM
Sample Name: eks-III-234
Analysis Info:



Compound 7: D-Ox-II

LCMS Tripeptide HO-D-Leu-D-Phe- β -OH-(2R,3R)/(2S,3S)-NHBOc (MW = 444)

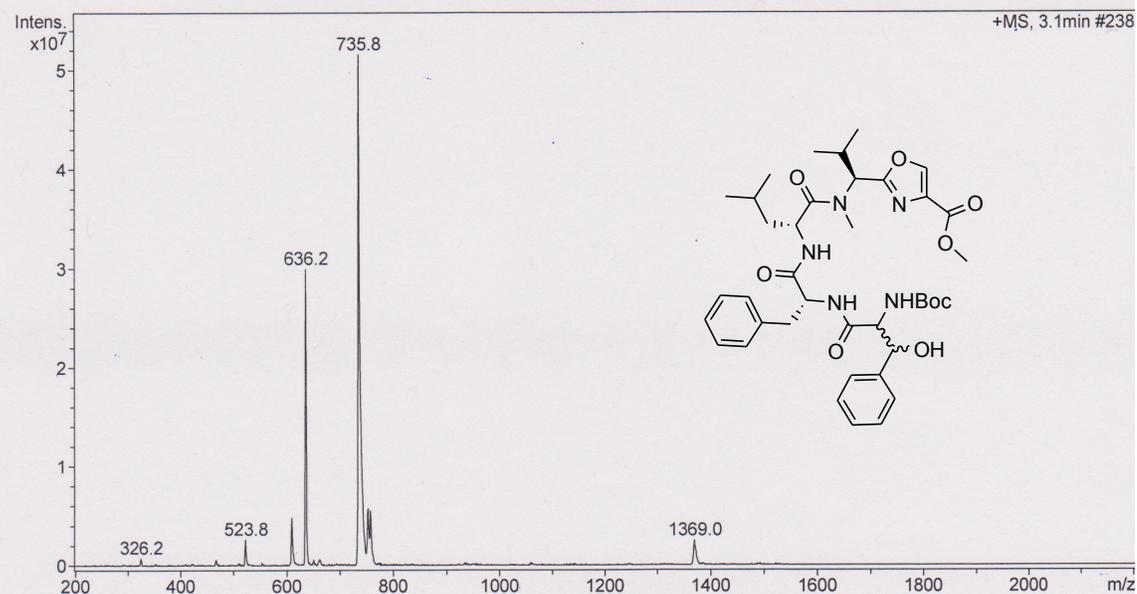
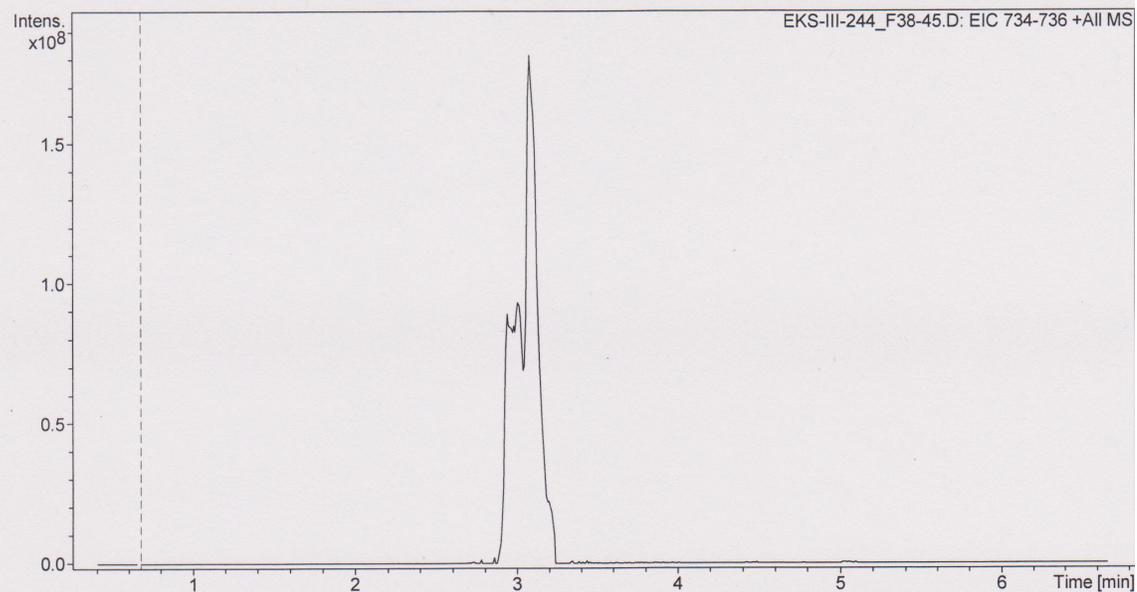


Compound 7: D-Ox-II

NMR Pentapeptide MeO-Oxazole-Val-N(Me)-D-Leu-D-Phe-(2R,3R)/(2S,3S)- β -OH-Phe-NHBoc

Display Report - All Windows Selected Analysis

Analysis Name: EKS-III-244_F38 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/8/2011 9:27:43 AM
Method: SANA.M -45.D **Operator:** sdsu **Acq. Date:** 11/19/2010 4:08:59 AM
Sample Name: eks-III-244_f38-45
Analysis Info:

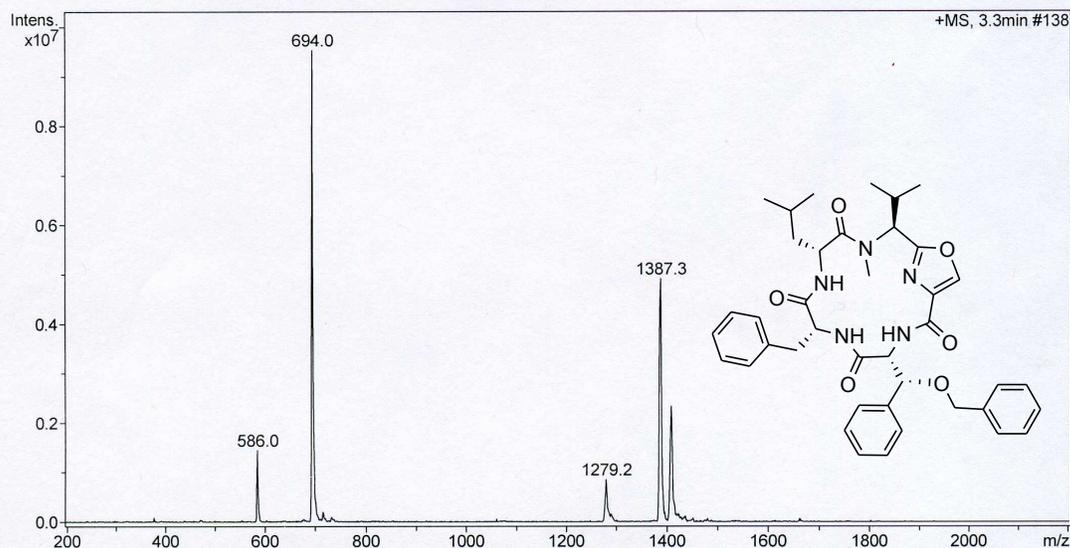
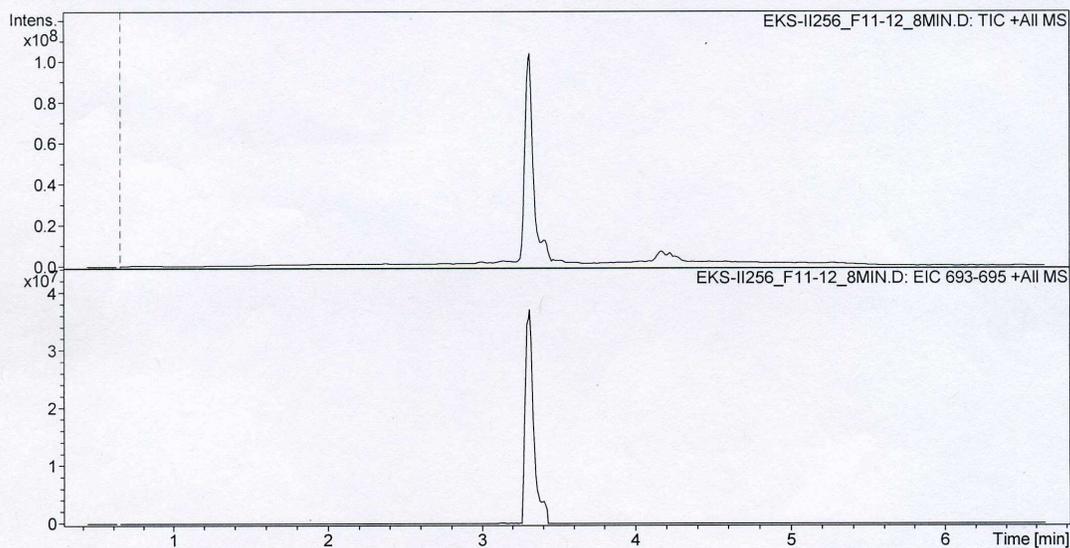


Compound 7: D-Ox-II

LCMS Pentapeptide MeO-oxazole-Val-N(Me)-D-Leu-D-Phe-(2R,3R)/(2S,3S)- β -OH-Phe-NHBoc (MW = 736)

Display Report - All Windows Selected Analysis

Analysis Name: EKS-II256_F11-1 **Instrument:** Agilent 6330 Ion Trap **Print Date:** 12/13/2010 5:30:26 PM
Method: SANA.M 2_8MIN.D **Operator:** sdsu **Acq. Date:** 12/13/2010 4:02:20 PM
Sample Name: eks-II256_f11-12_8min
Analysis Info:



Compound 7: D-Ox-II

LCMS Macrocycle (2R,3R)- β -benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7) (MW = 694)

Davis et al.

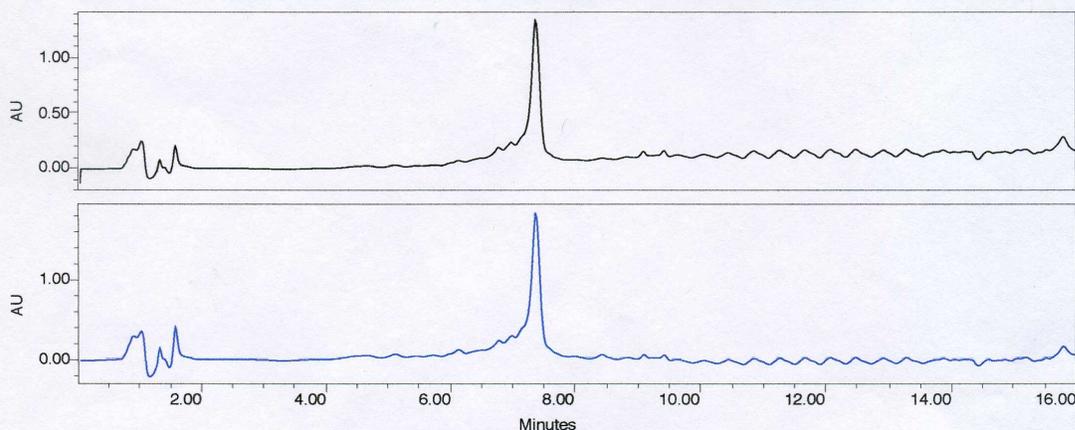
SDSU

Project Name: Defaults
Reported by User: System

Breeze

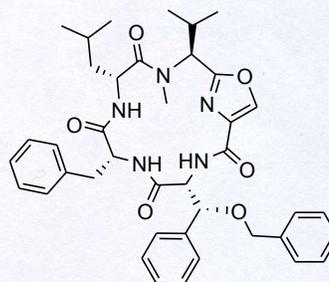
SAMPLE INFORMATION

Sample Name:	eks-III-252_ERT-208	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	42	Date Acquired:	12/7/2010 4:31:57 PM
Run Time:	16.00 Minutes	Injection Volume:	75.00 ul



— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1 ****	****	****	****	****	****	****
2 ****	****	****	****	****	****	****



Compound 7: D-Ox-II

HPLC Macrocycle (2R,3R)-β-benzyloxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7)

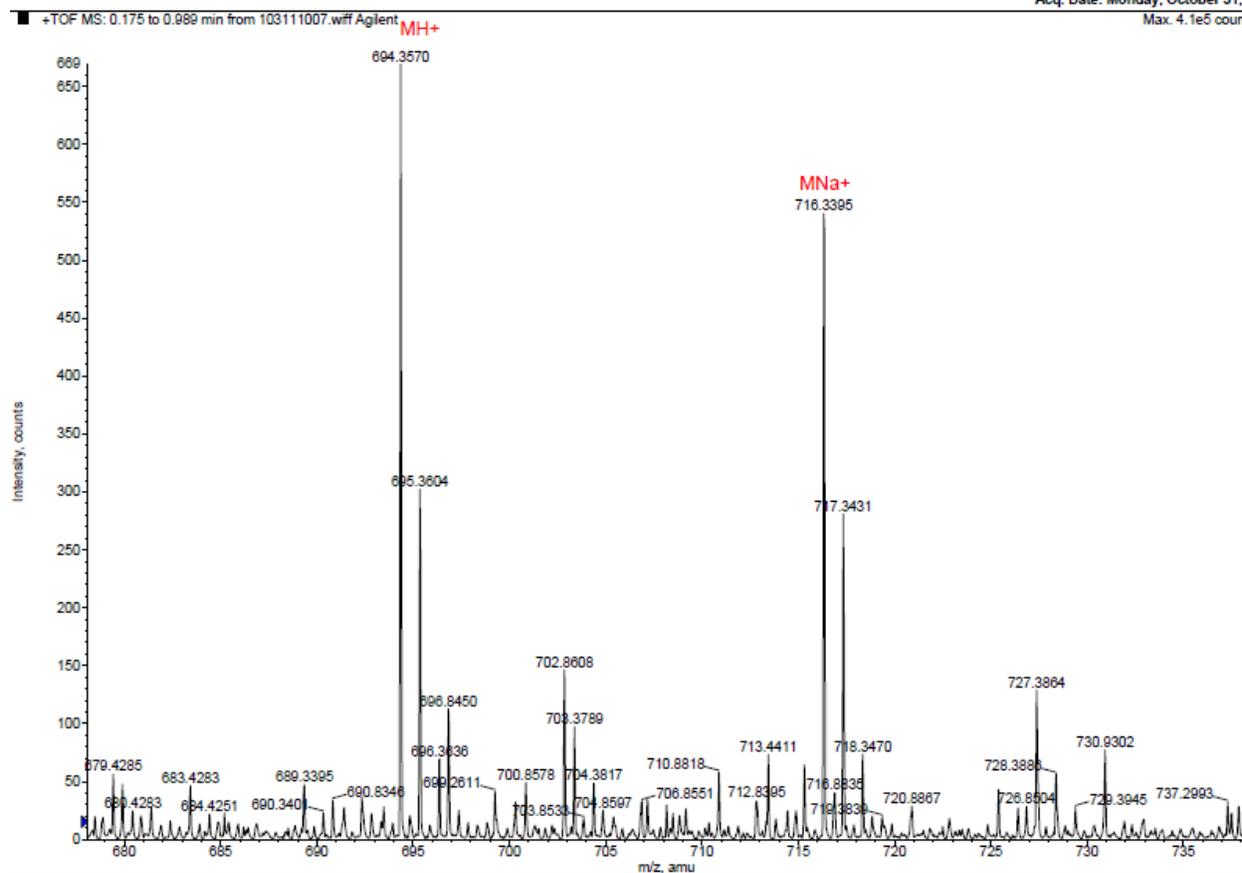
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5700

Acq. File: 103111007.wi
Acq. Date: Monday, October 31, 2011
Max. 4.1e5 counts

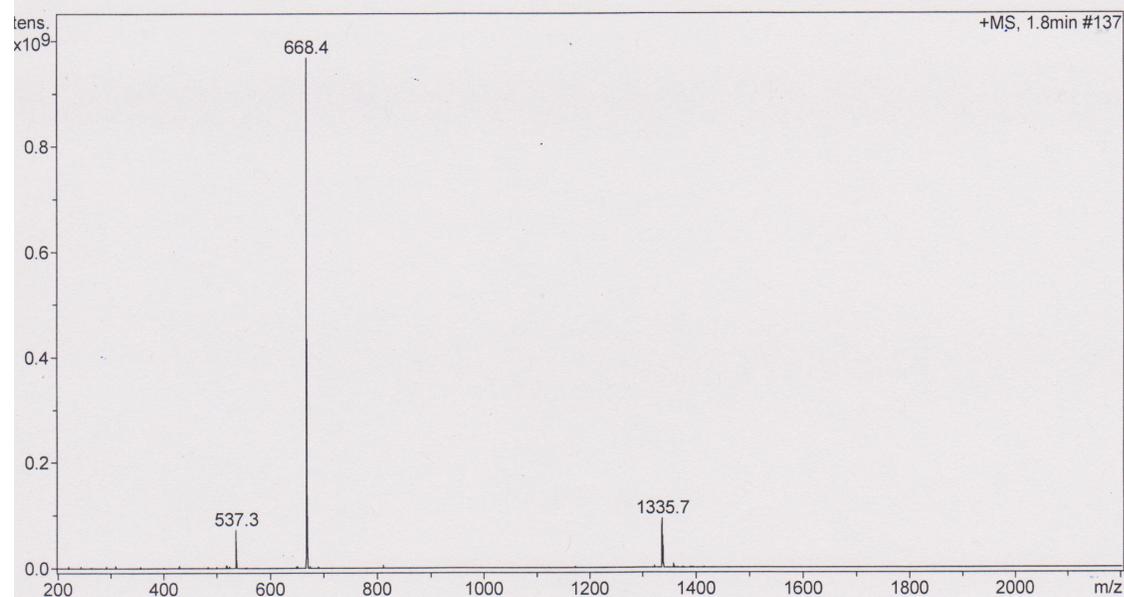
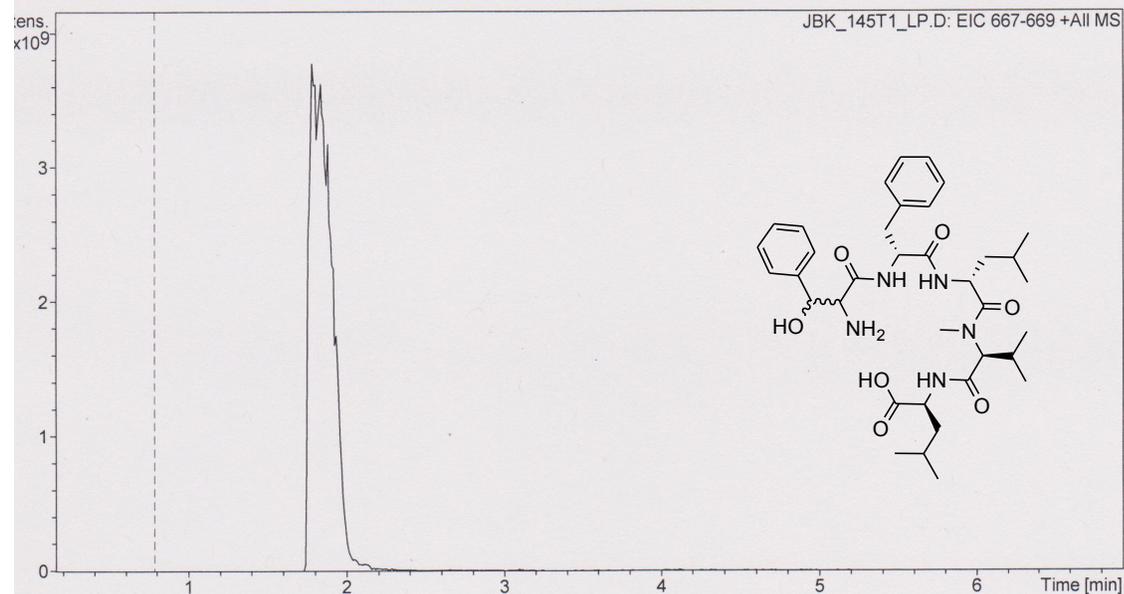


Compound 7: D-Ox-II

HRMS Macrocycle (2R,3R)- β -benzoxy-Phe-oxazole-Val-N(Me)-D-Leu-D-Phe (7) (MW = 694.3570)

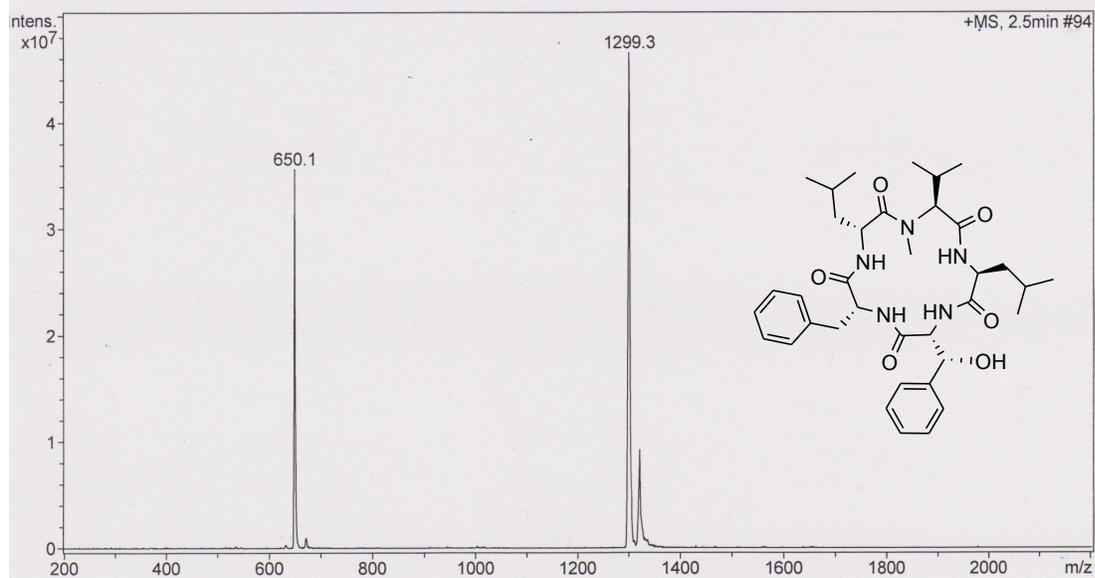
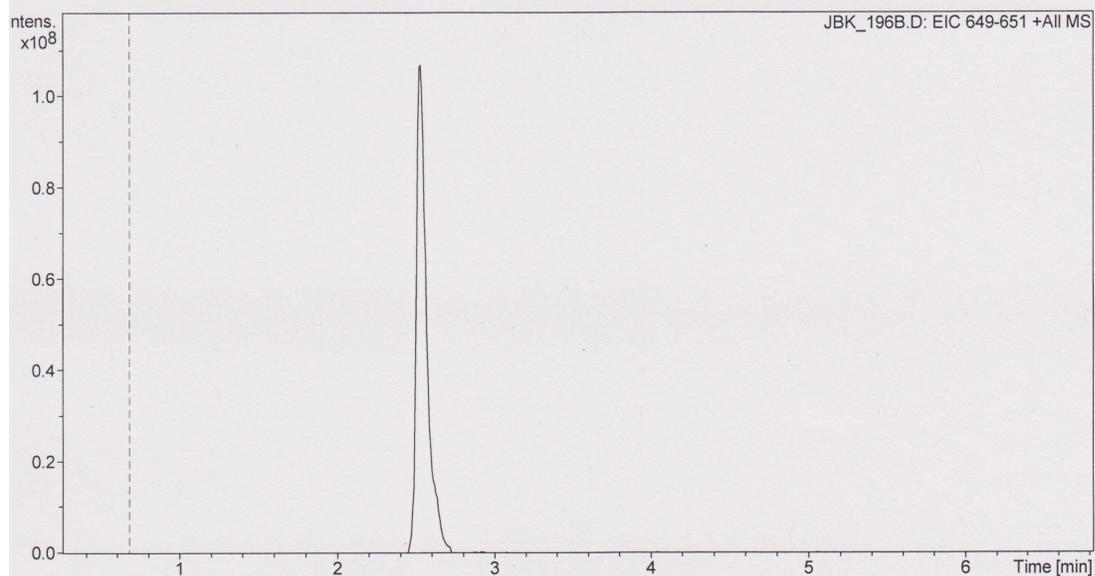
Display Report - All Windows Selected Analysis

Analysis Name: JBK_145T1_LP.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/8/2011 9:18:30 AM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 6/28/2010 10:35:16 AM
Sample Name: jbk_145T1_lp
Analysis Info:



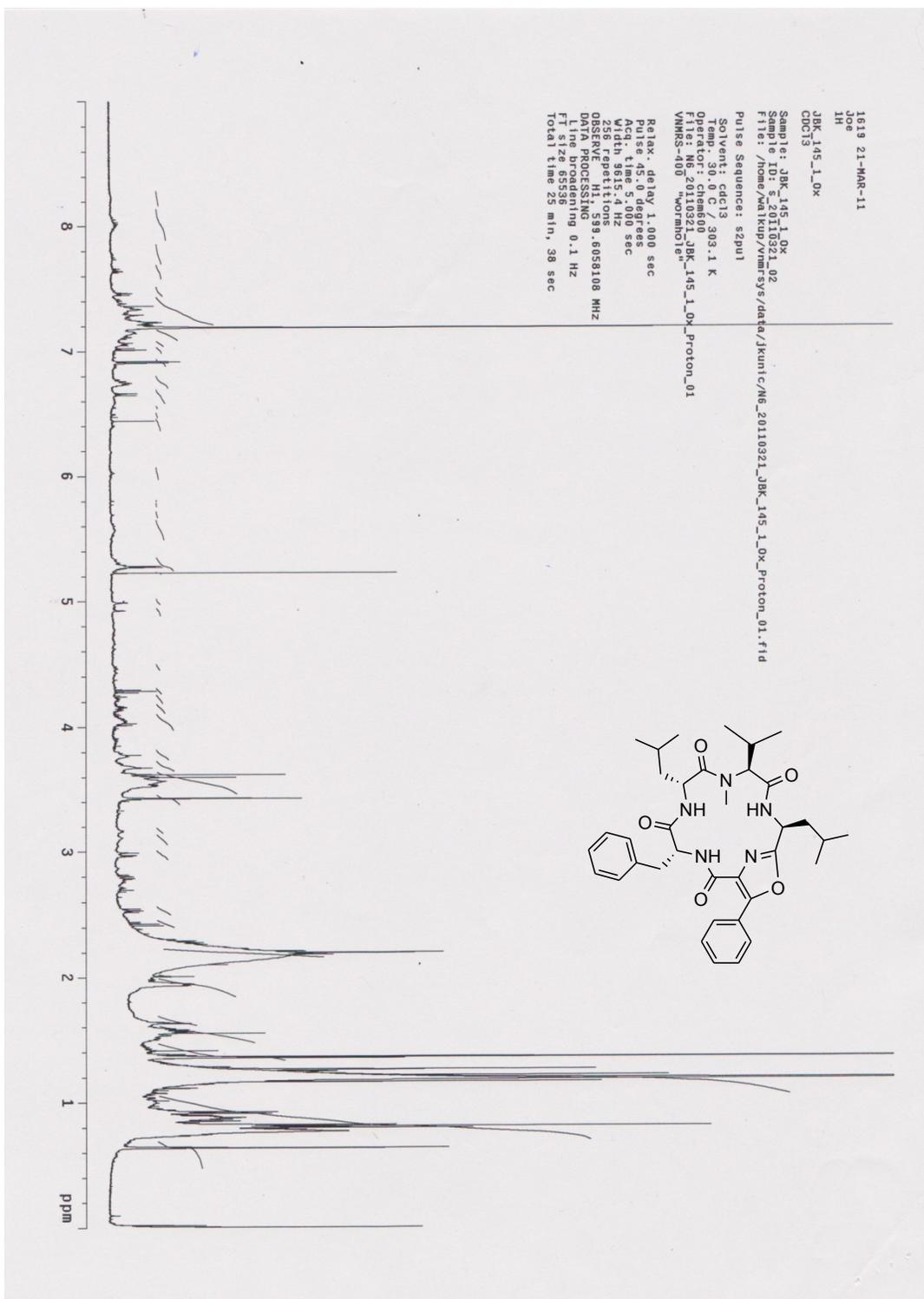
Display Report - All Windows Selected Analysis

Analysis Name: JBK_196B.D Instrument: Agilent 6330 Ion Trap Print Date: 6/8/2011 9:12:14 AM
Method: SANA.M Operator: sdsu Acq. Date: 11/18/2010 4:02:48 AM
Sample Name: jbk_196b
Analysis Info:



Compound 8: D-Ox-I

LCMS Macrocycle β -OH(2R,3R)-Phe-Leu-Val-N(Me)-D-Leu-D-Phe (MW = 649.82)

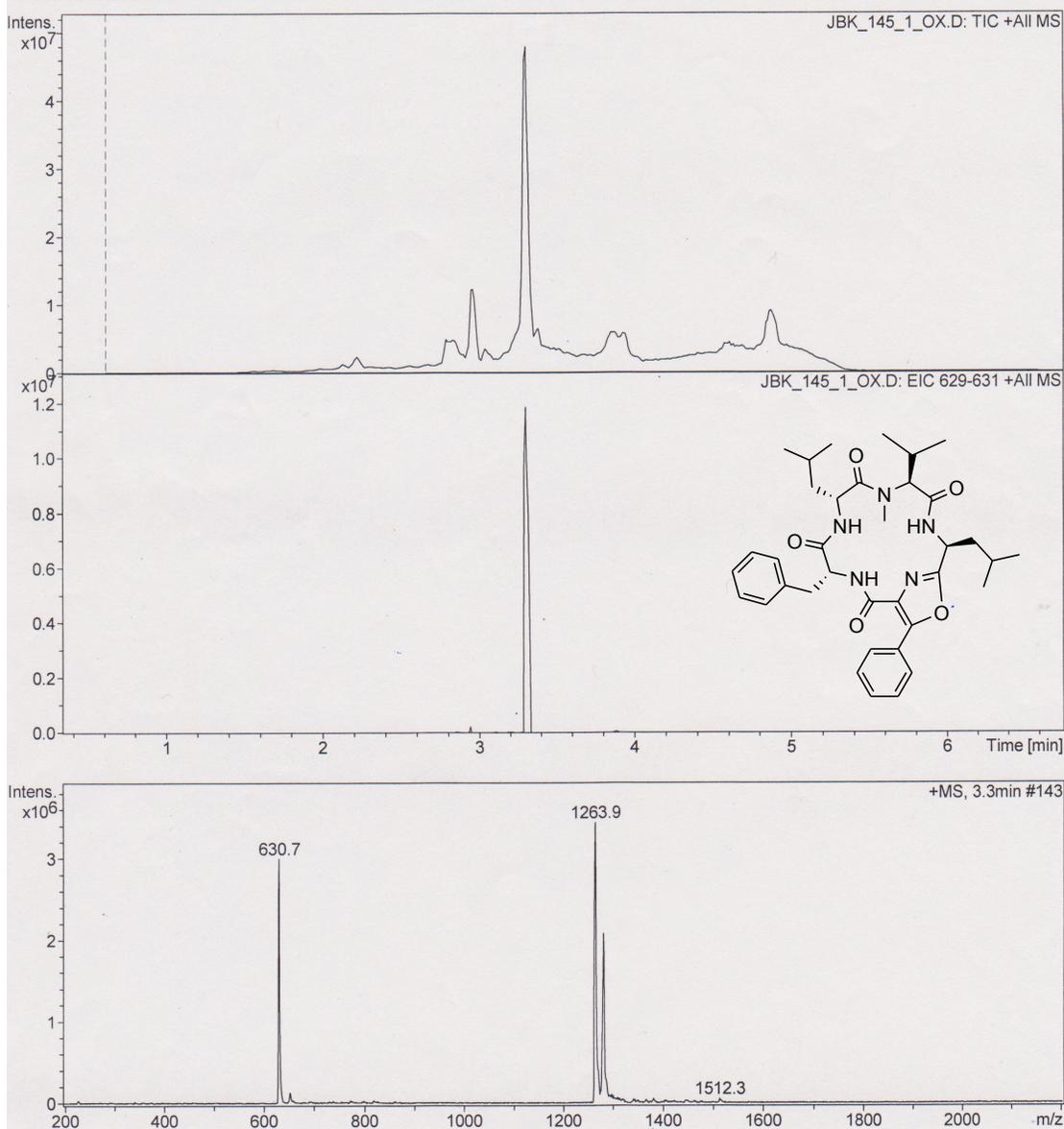


Compound 8: D-Ox-I

NMR Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8)

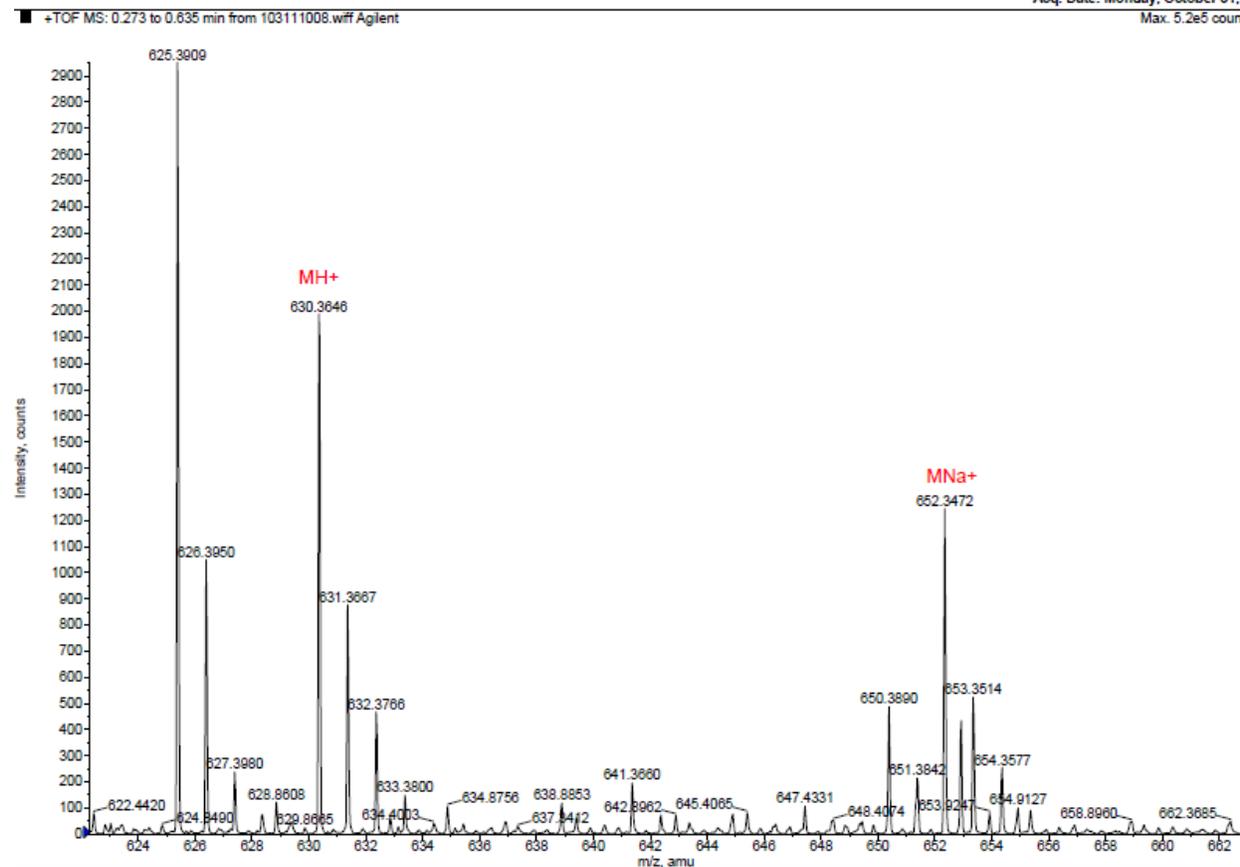
Display Report - All Windows Selected Analysis

Analysis Name: JBK_145_1_OX. Instrument: Agilent 6330 Ion Trap Print Date: 3/20/2011 1:32:40 PM
Method: SANA.M D Operator: sdsu Acq. Date: 3/20/2011 1:24:12 PM
Sample Name: jbk_145_1_Ox
Analysis Info:



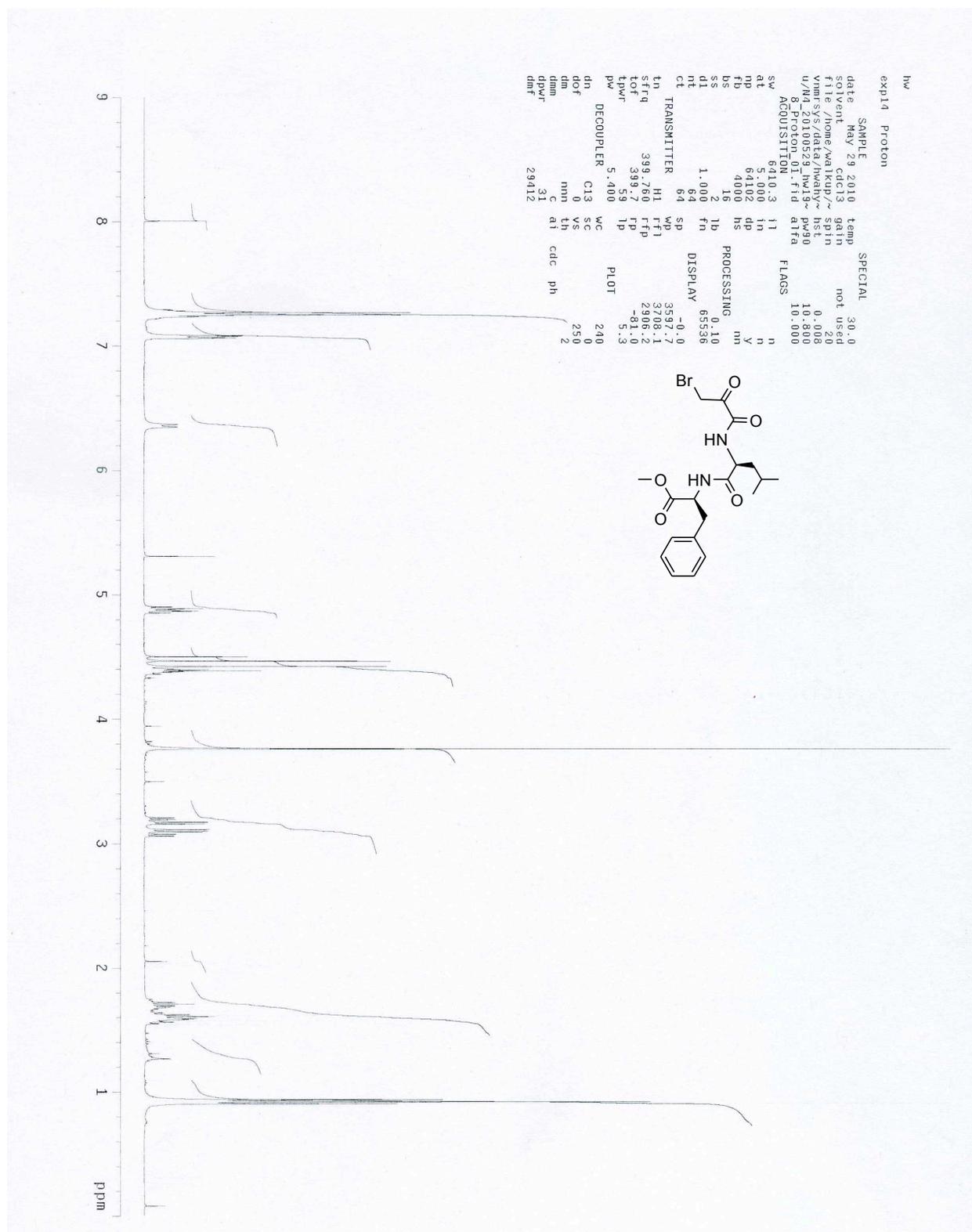
Compound 8: D-Ox-I

LCMS Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8) (MW = 629.79)



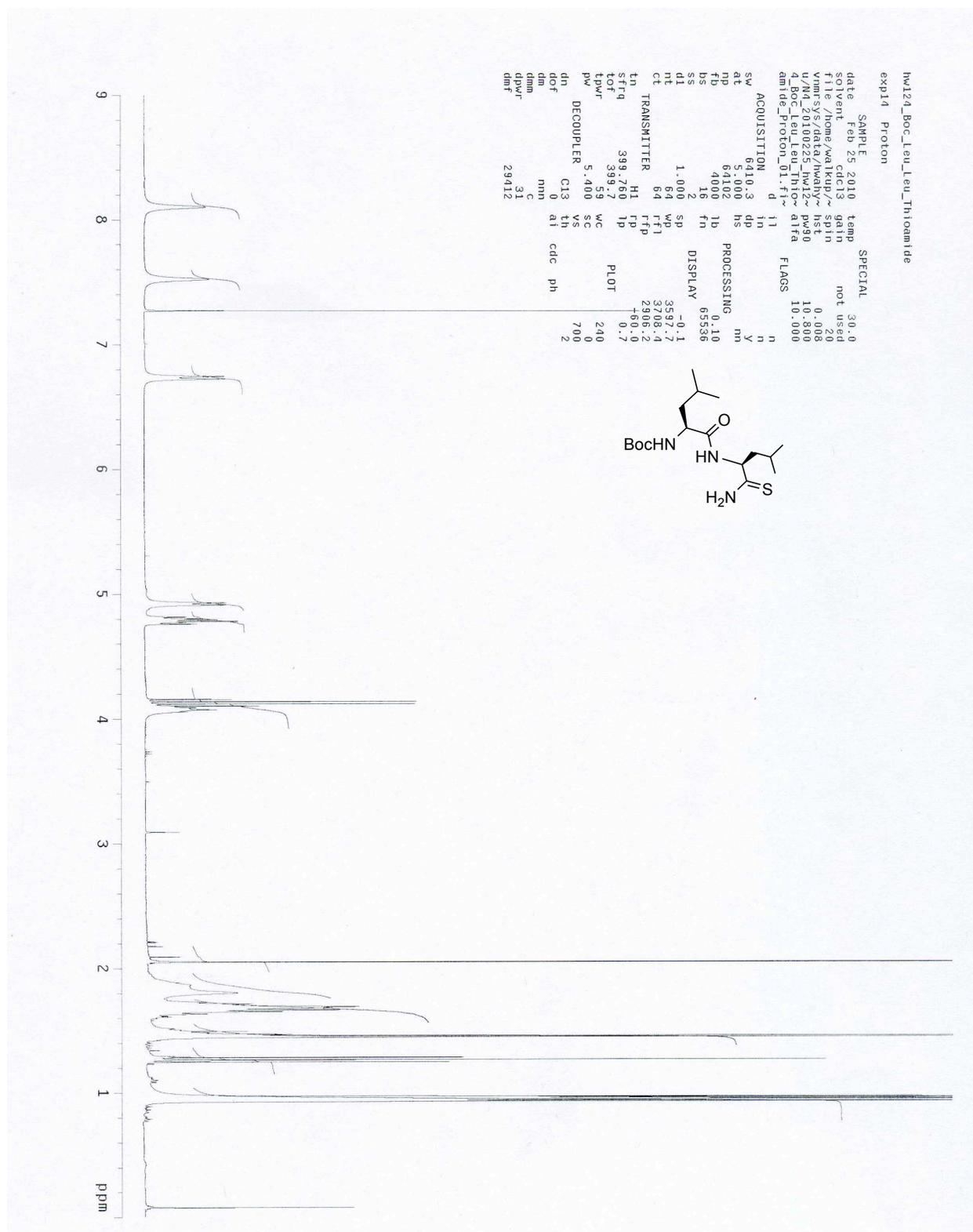
Compound 8: D-Ox-I

HRMS Macrocycle Phe-Oxazole-Leu-Val-N(Me)-D-Leu-D-Phe (8) (MW = 630.3646)



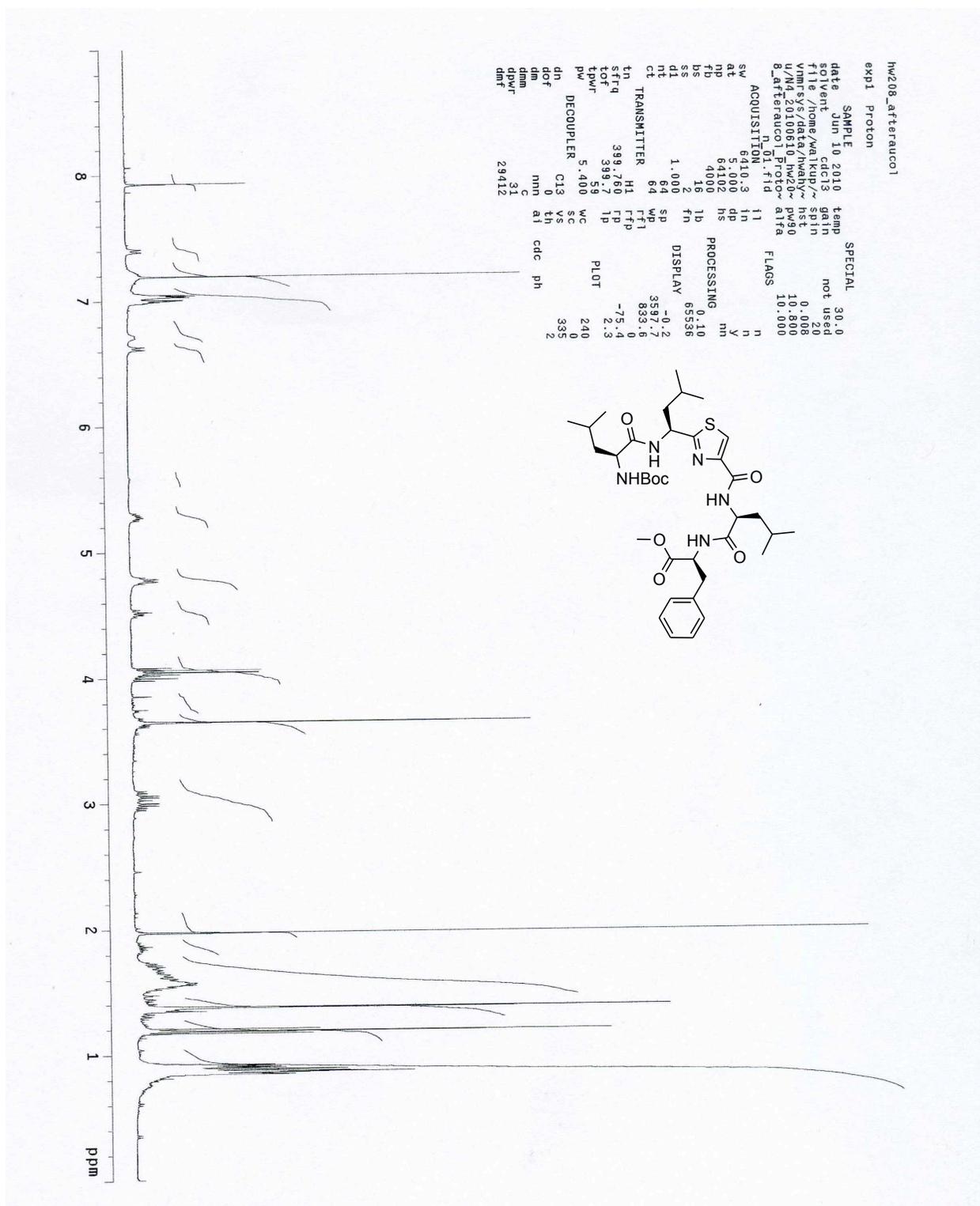
Compound 9: A-Th-III

NMR Tripeptide MeO-Phe-Leu-Ketone-Br (48)



Compound 9: A-Th-III

NMR Diptide Thioamide-Leu-Leu-NHBoc (52)



Compound 9: A-Th-III

NMR Pentapeptide MeO-Phe-Leu-Thiazole-Leu-Leu-NHBoc (53)

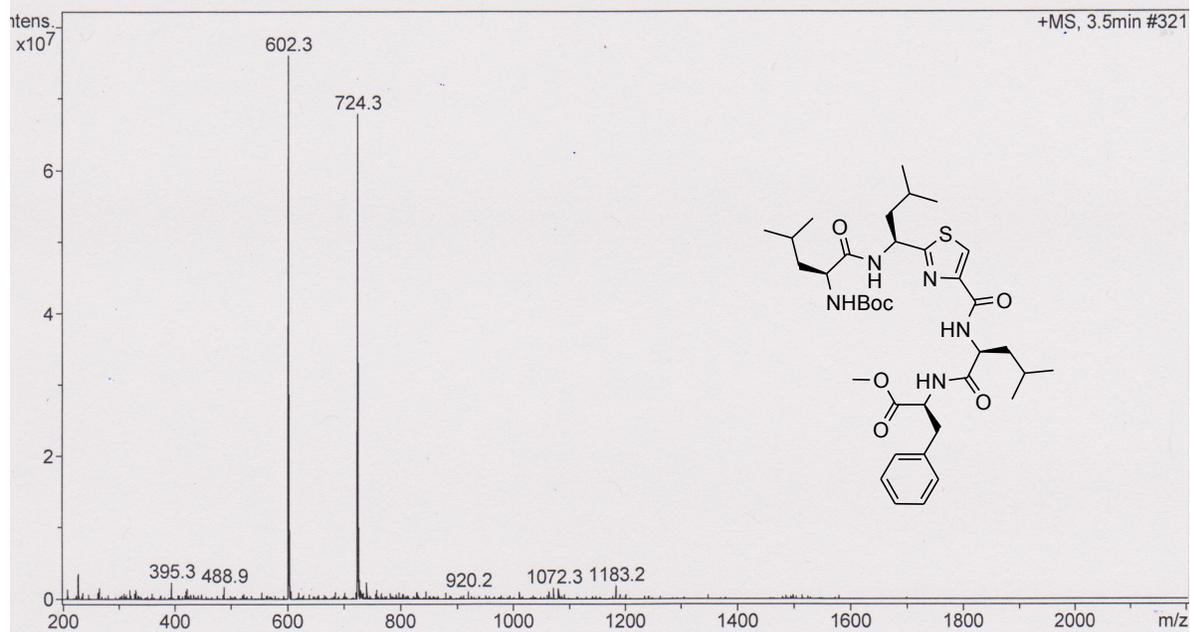
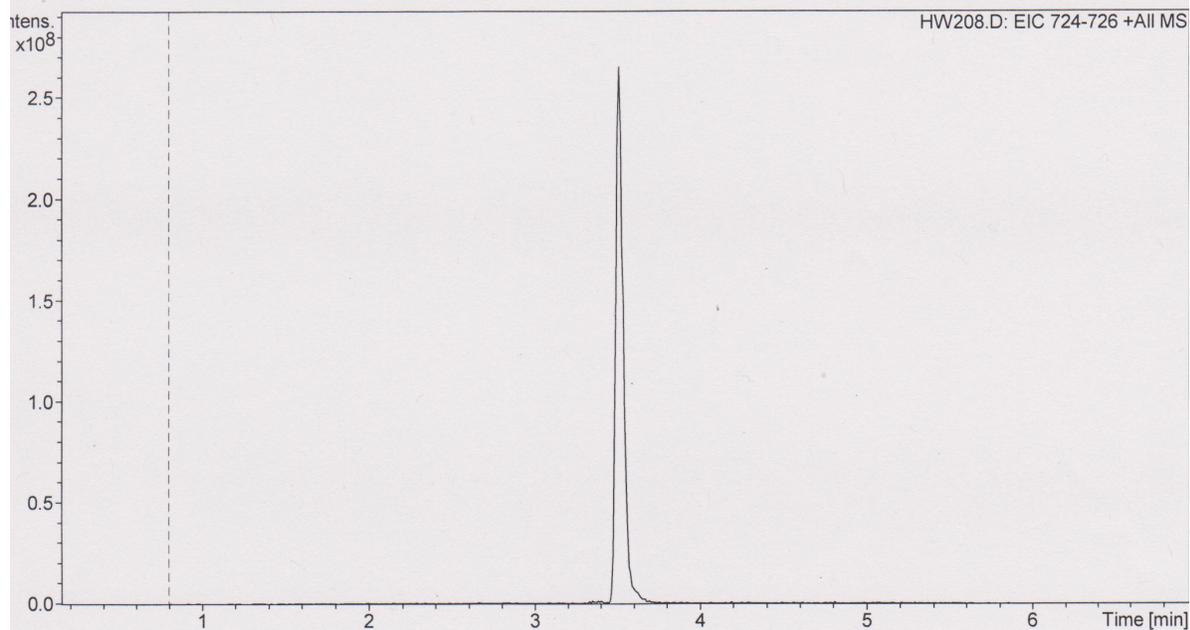
Davis et al.

Display Report - All Windows Selected Analysis

Analysis Name: HW208.D
Method: SANA.M
Sample Name: hw208_aucol35
Analysis Info:

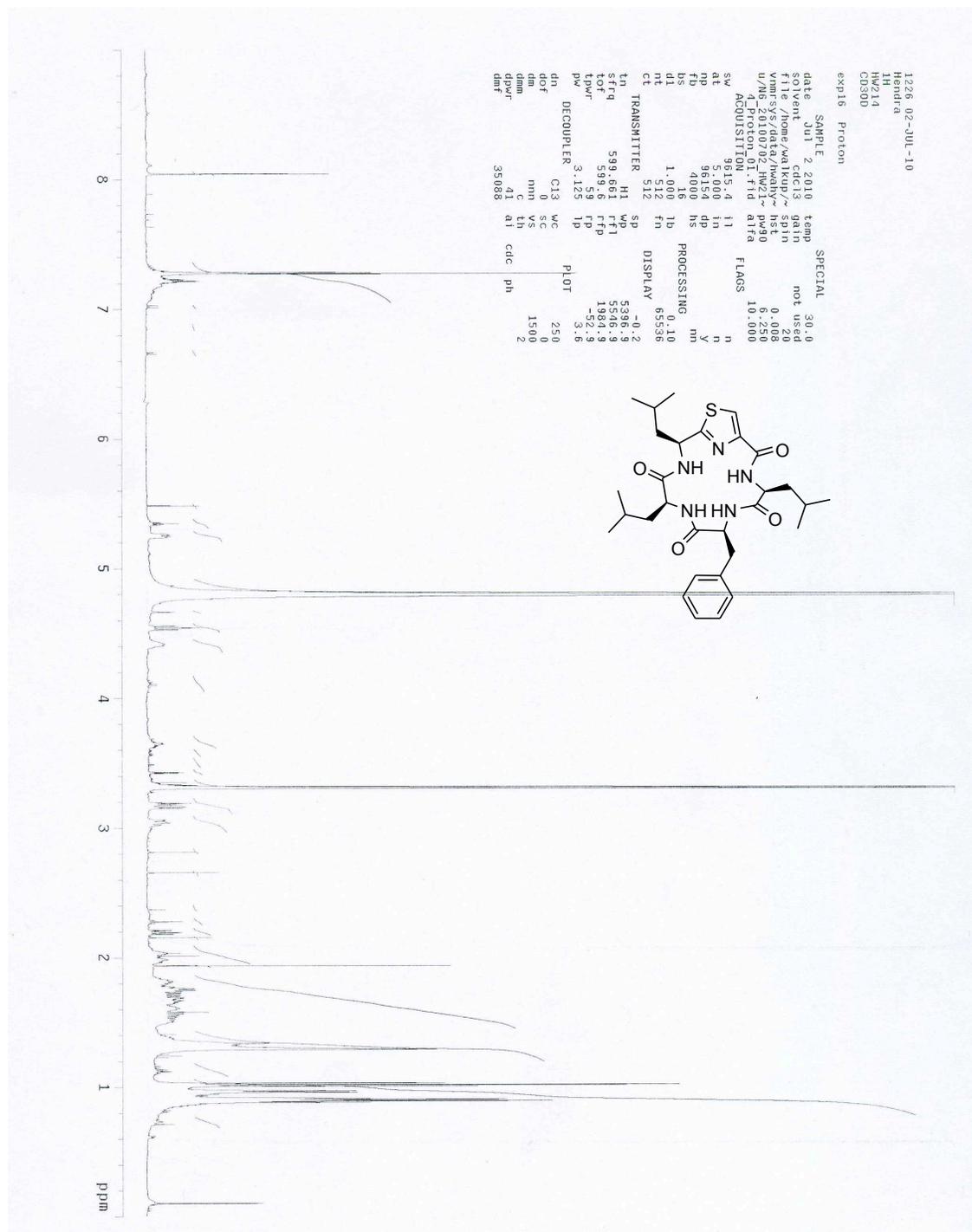
Instrument: Agilent 6330 Ion Trap
Operator: sdsu

Print Date: 6/8/2011 9:14:51 AM
Acq. Date: 6/9/2010 7:21:57 PM



Compound 9: A-Th-III

LCMS Pentapeptide MeO-Phe-Leu-Thiazole-Leu-Leu-NHBoc (53) (MW=701)



Compound 9: A-Th-III

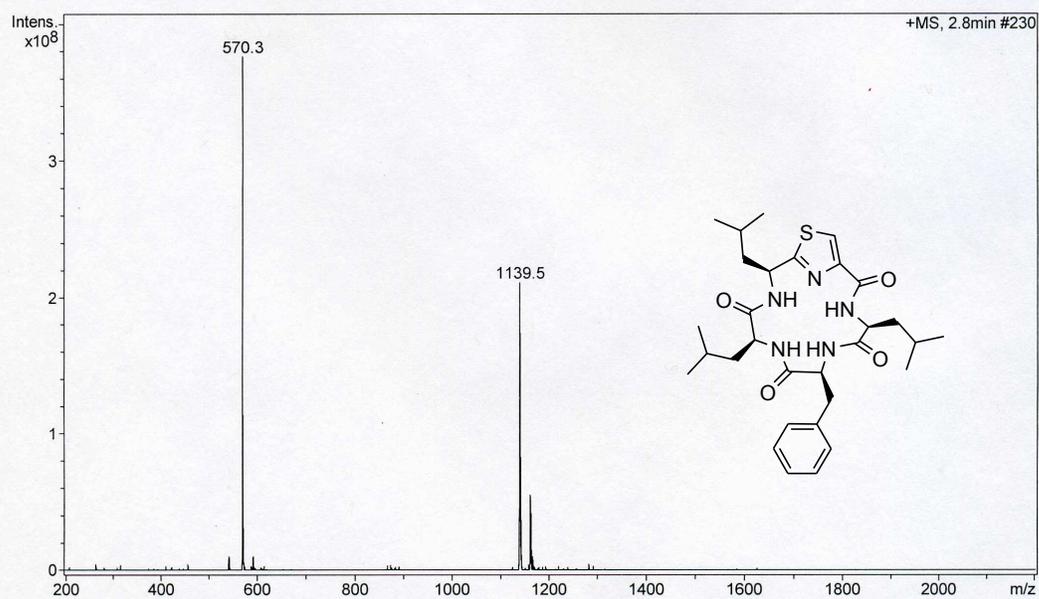
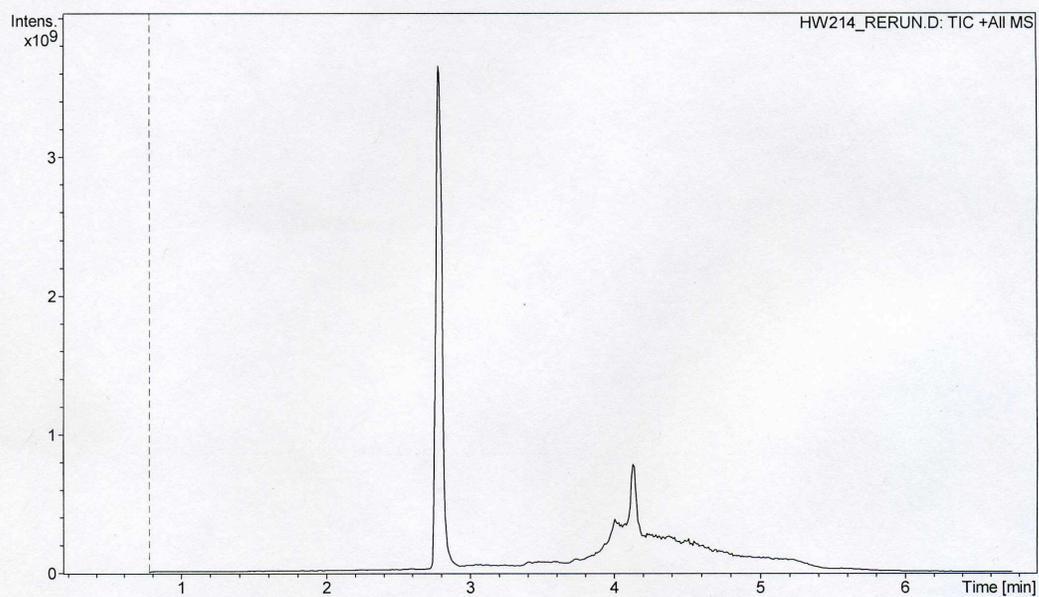
NMR Macrocycle Phe-Leu-Thiazole-Leu-Leu (9)

Display Report - All Windows All Analyses

Operator: sdsu

Instrument: Agilent 6330 Ion Trap

Print Date: 7/13/2010 3:29:17 PM



MSD Trap Report v 4 (Let-Opt2)

Page 1 of 1

Agilent Technologies

Compound 9: A-Th-III

LCMS Macrocycle Phe-Leu-Thiazole-Leu-Leu (9) (MW=569)

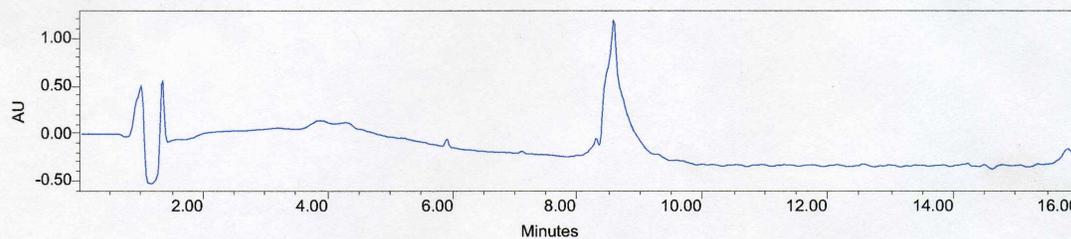
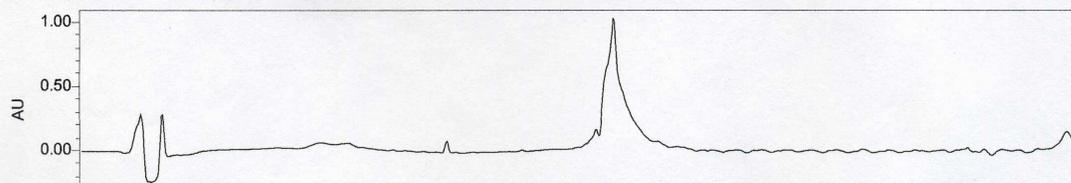
SDSU

Project Name: Defaults
Reported by User: System

Breeze

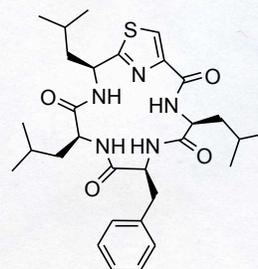
SAMPLE INFORMATION

Sample Name:	hw214	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	377	Date Acquired:	6/30/2010 6:29:30 PM
Run Time:	16.00 Minutes	Injection Volume:	40.00 ul



— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
— Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



Compound 9: A-Th-III

HPLC Macrocyclic Phe-Leu-Thiazole-Leu-Leu (9)

Supplementary Material

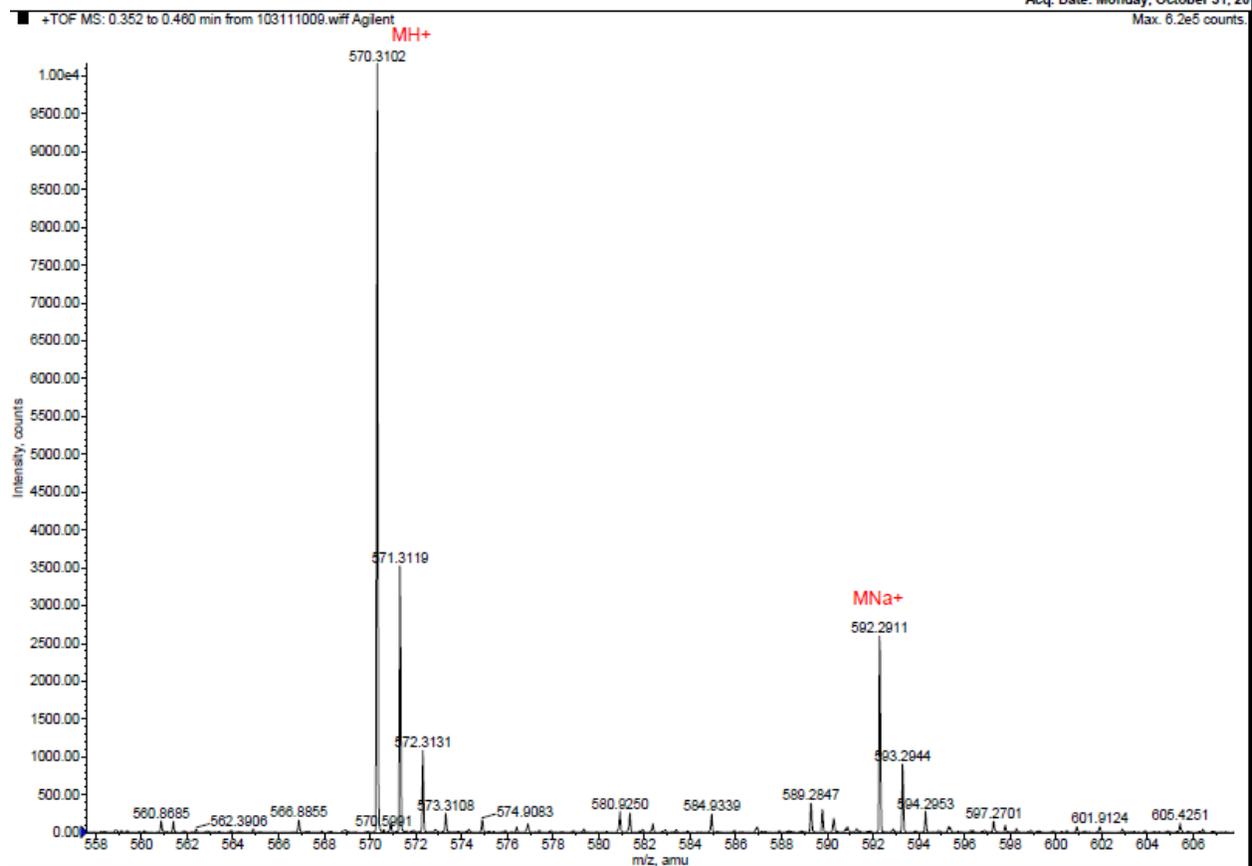
Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5702

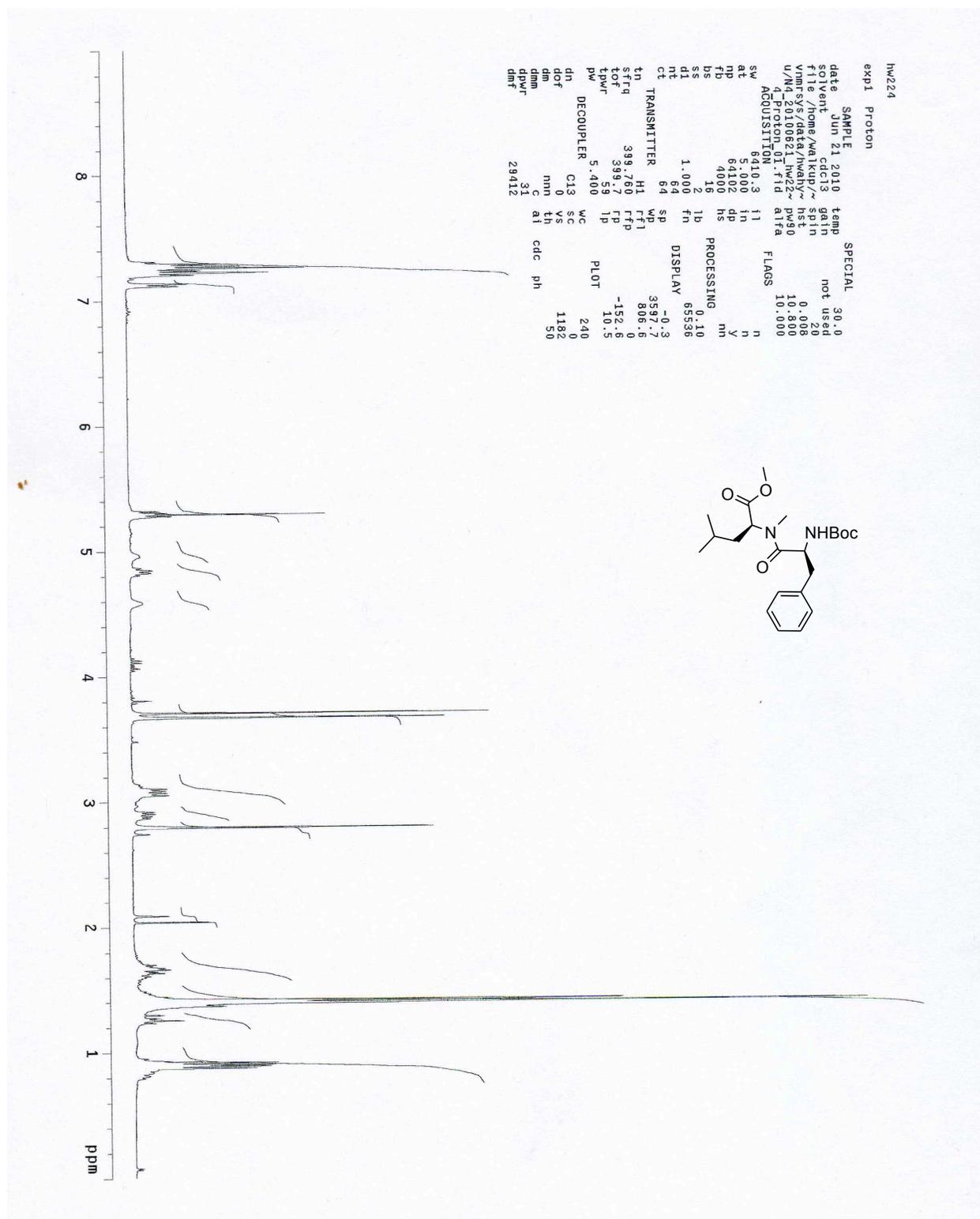
Acq. File: 103111009.wiff

Acq. Date: Monday, October 31, 20



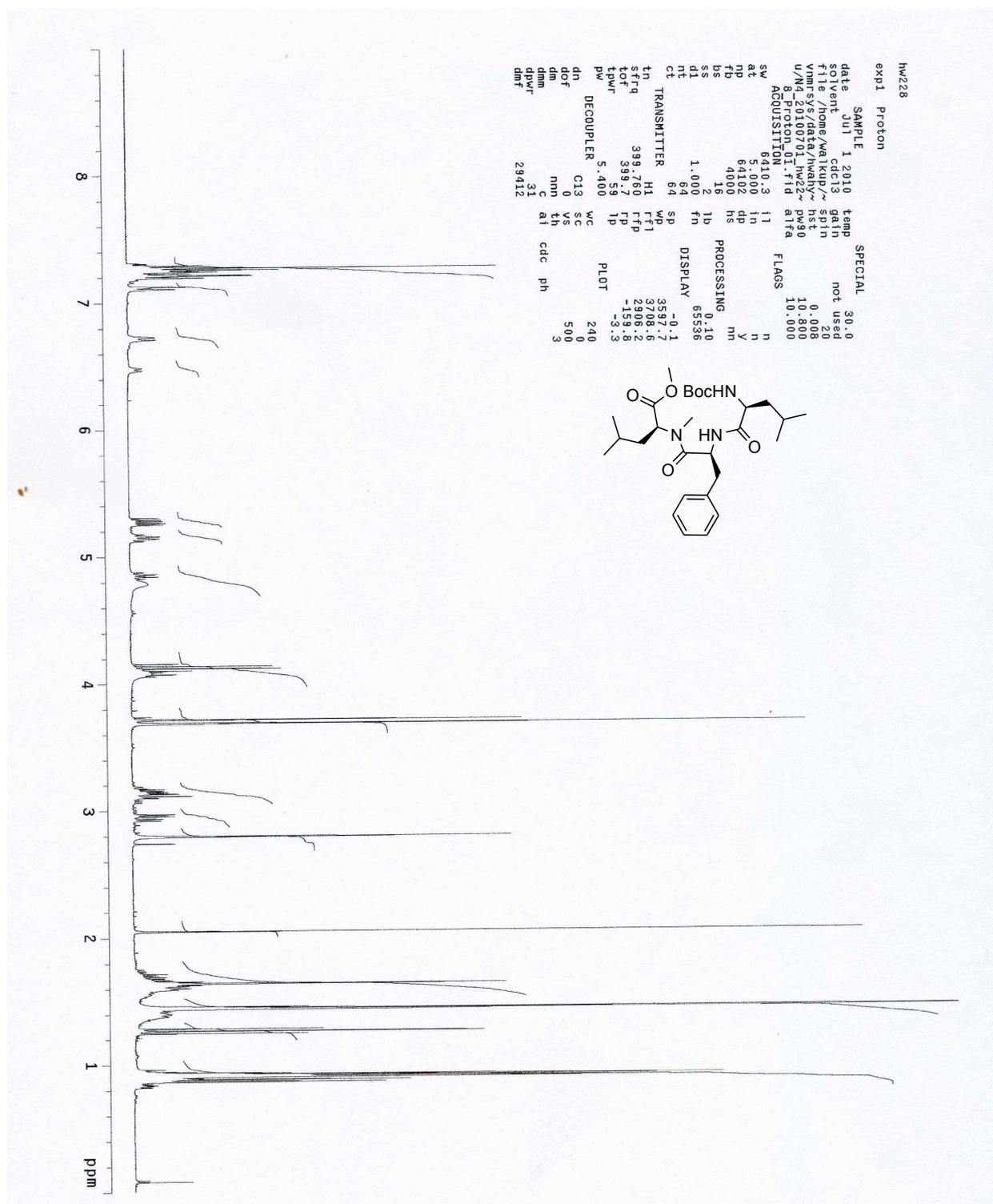
Compound 9: A-Th-III

HRMS Macrocycle Phe-Leu-Thiazole-Leu-Leu (9) (MW= 570.3102)



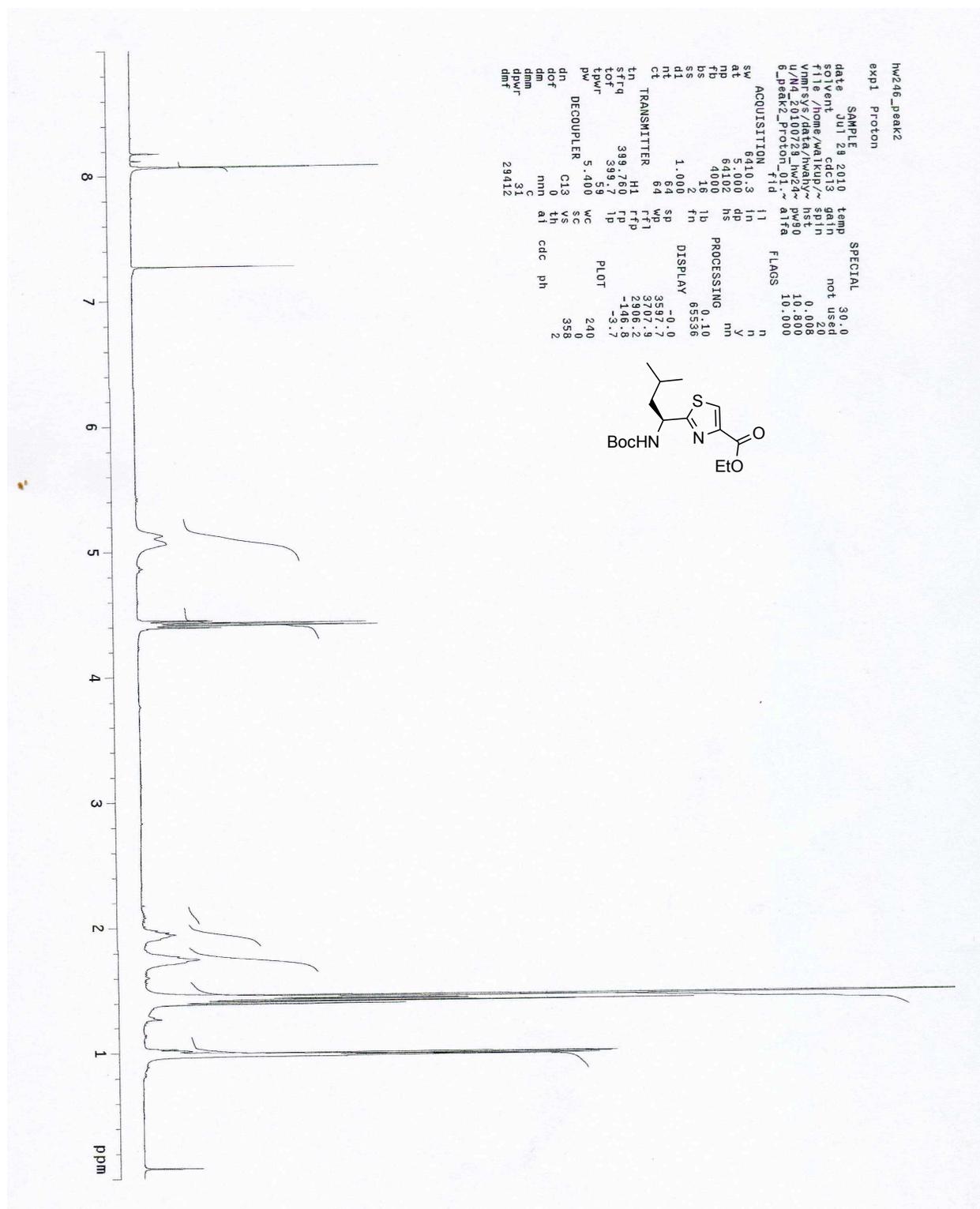
Compound 10: B-Th-III

NMR Dipeptide MeO-Leu-N(Me)-Phe-NHBoc



Compound 10: B-Th-III

NMR Tripeptide MeO-Leu-N(Me)-Phe-Leu-NHBoc

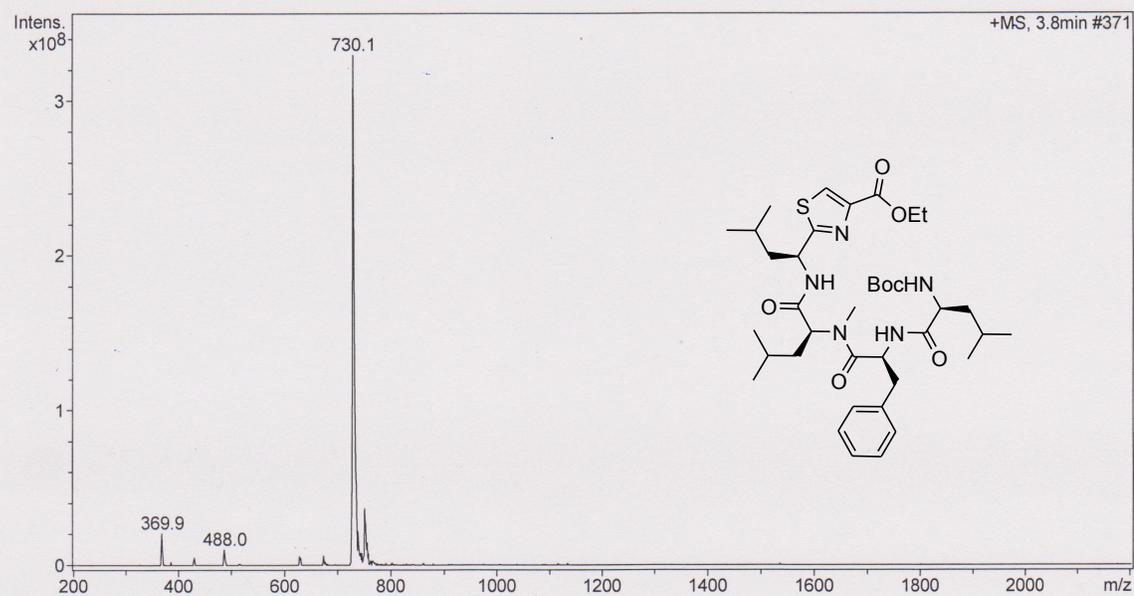
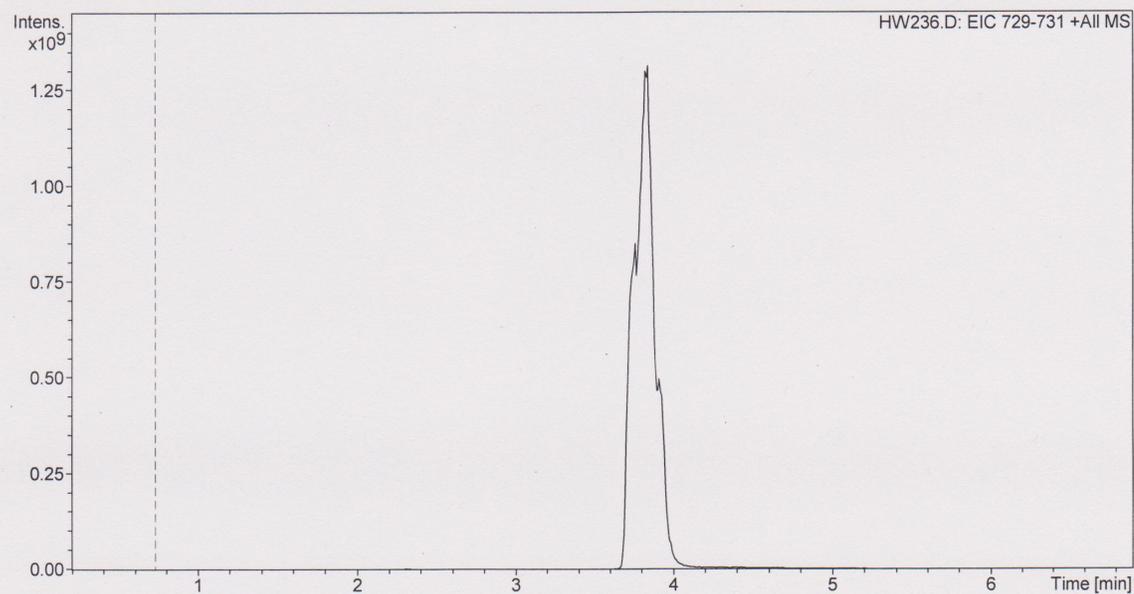


Compound 10: B-Th-III

NMR Di-peptide EtO-Thiazole-Leu-NHBoc (57)

Display Report - All Windows Selected Analysis

Analysis Name: HW236.D **Instrument:** Agilent 6330 Ion Trap **Print Date:** 6/8/2011 9:16:12 AM
Method: SANA.M **Operator:** sdsu **Acq. Date:** 8/12/2010 4:29:06 PM
Sample Name: hw236
Analysis Info:



Compound 10: B-Th-III

LCMS Pentapeptide EtO-Thiazole-Leu-Leu-N(Me)-Phe-Leu-NHBoc (63) (MW = 729)

Davis et al.

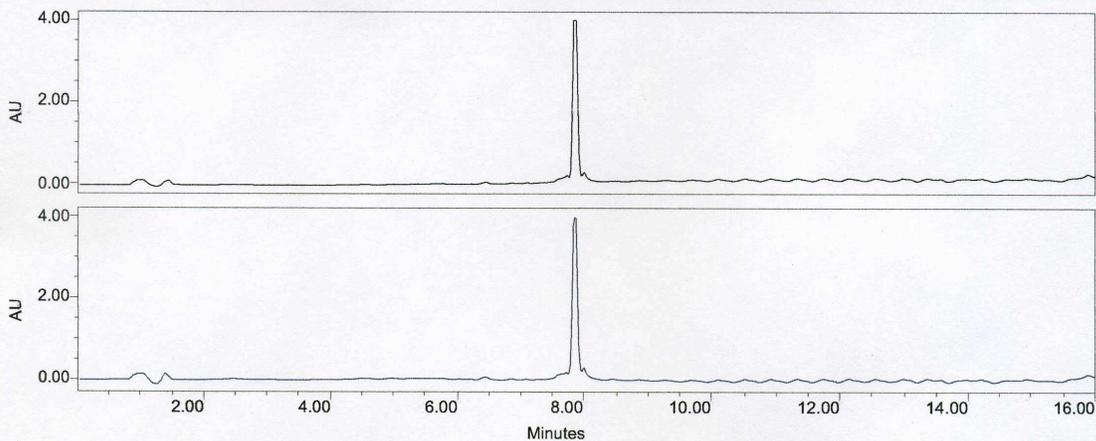
SDSU

Project Name: Defaults
Reported by User: System

Breeze

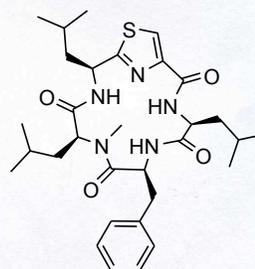
SAMPLE INFORMATION

Sample Name:	hw242	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss
Injection #:	749	Date Acquired:	9/29/2010 11:33:03 AM
Run Time:	16.00 Minutes	Injection Volume:	100.00 ul



— Channel: 2487Channel 1 Channel Desc.: Processing Method: *
 — Channel: 2487Channel 2 Channel Desc.: Processing Method: *

Peak Name	RT (min)	Area (V*sec)	% Area	Height (V)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



Compound 10: B-Th-III

HPLC Macrocyclic Phe-Leu-Thiazole-Leu-Leu-N(Me) (10)

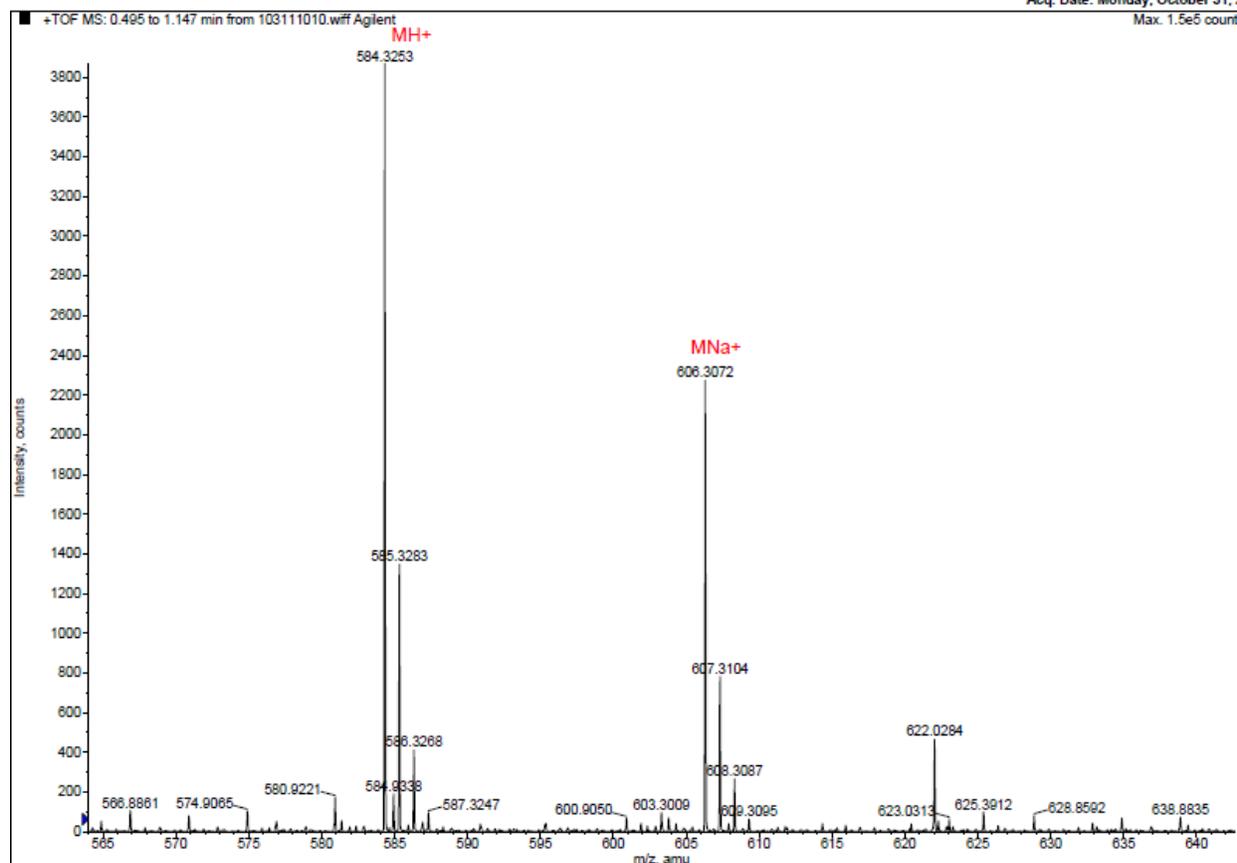
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5703

Acq. File: 103111010.wiff
Acq. Date: Monday, October 31, 20

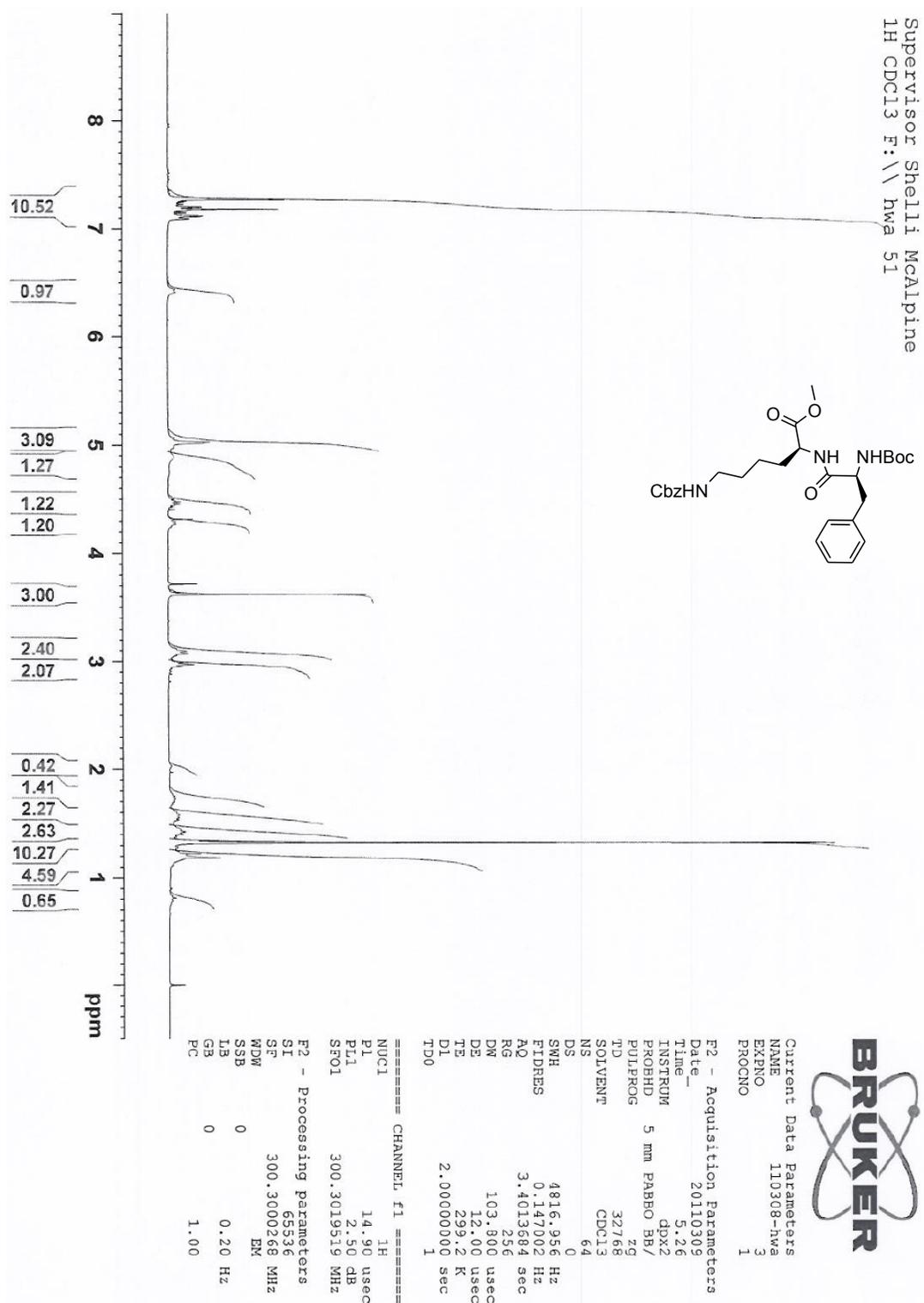


Compound 10: B-Th-III

HRMS Macrocycle Phe-Leu-Thiazole-Leu-Leu-N(Me) (10) (MW = 584.3253)

Supplementary Material

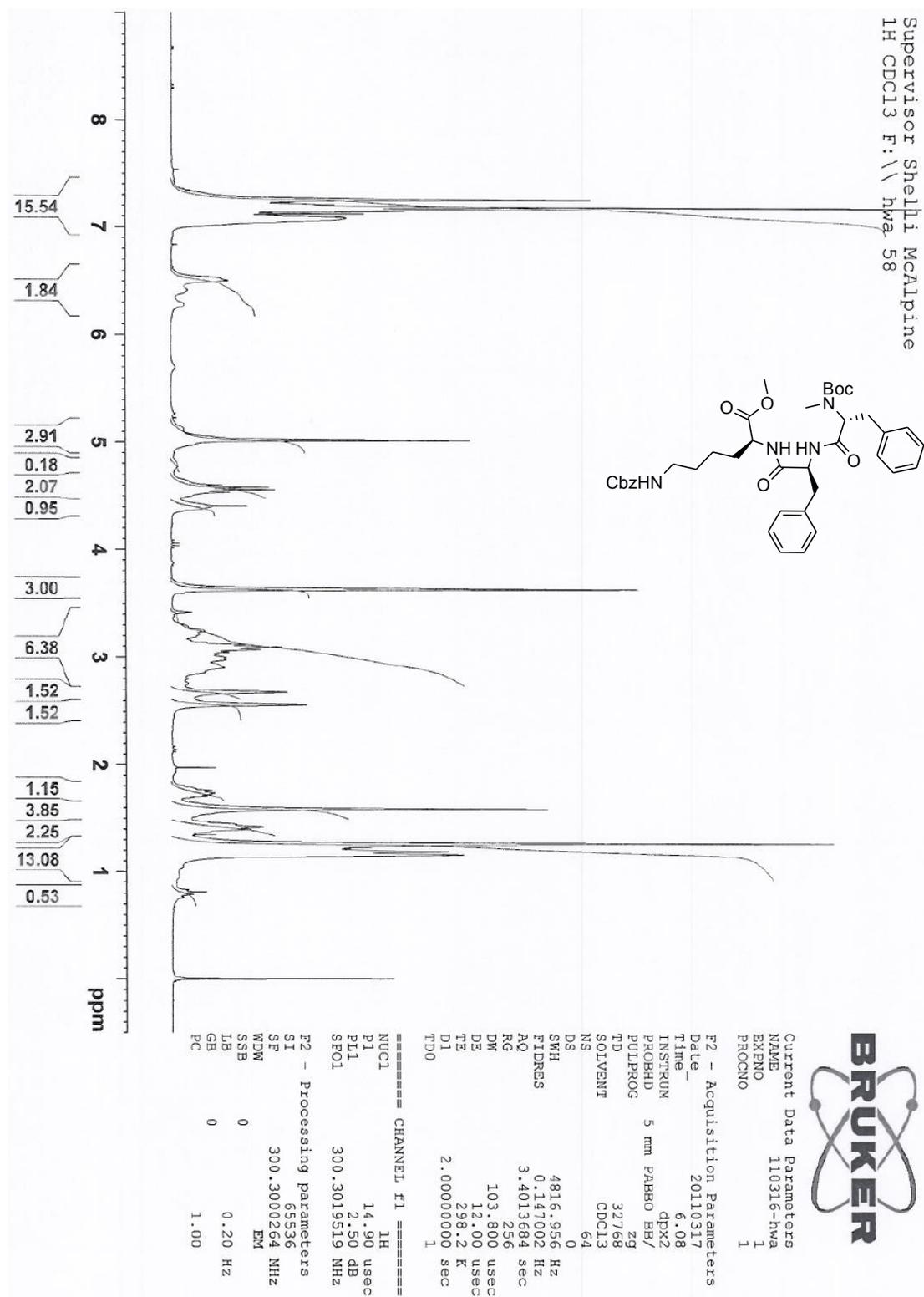
Davis et al.



Compound 11: C-Th-III

NMR Dipeptide MeO-Lys(Cbz)-Phe-NHBoc

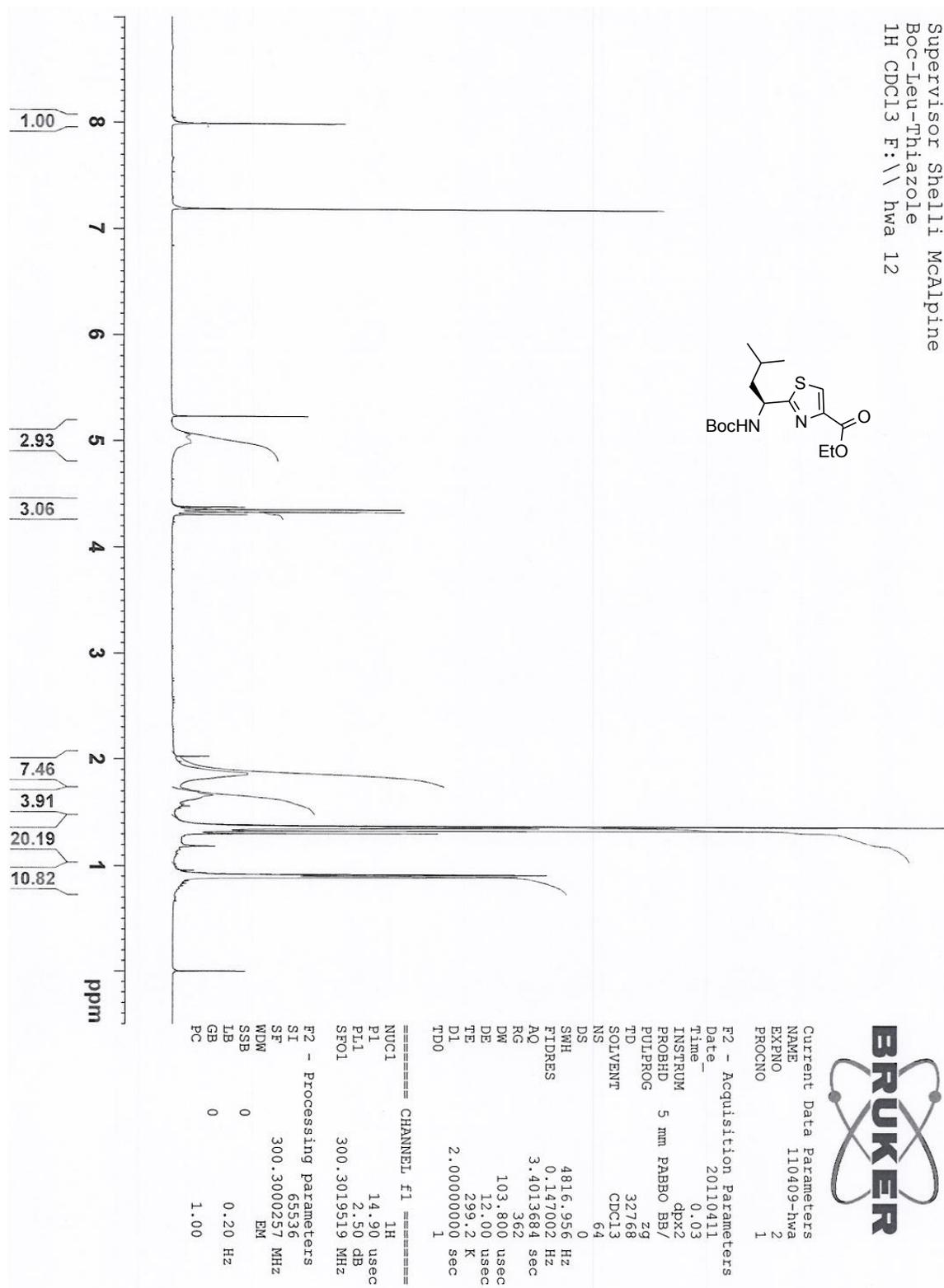
Davis et al.



Compound 11: C-Th-III

NMR Tripeptide MeO-Lys(Cbz)-Phe-D-Phe-N(Me)Boc

Davis et al.

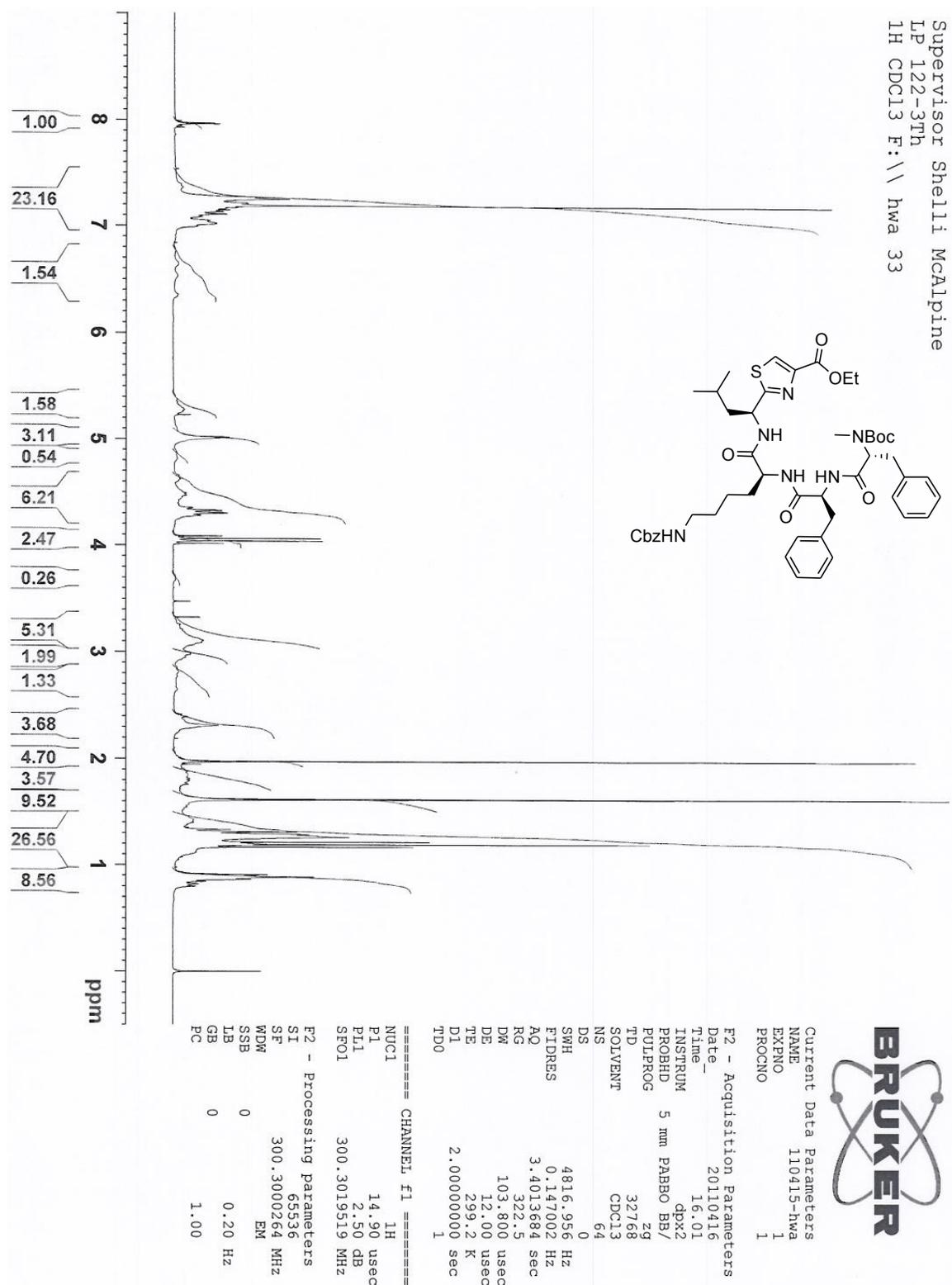


Compound 11: C-Th-III

NMR Dipeptide EtO-Thiazole-Leu-NHBoc

Supplementary Material

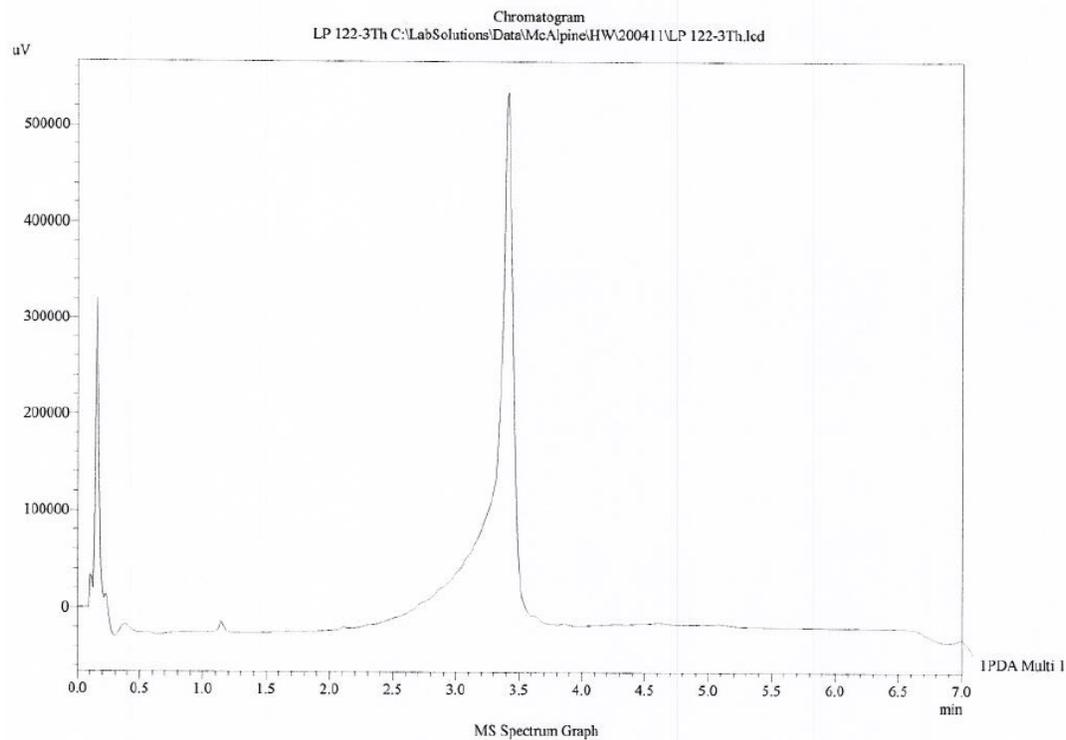
Davis et al.



Compound 11: C-Th-III

NMR Pentapeptide EtO-Thiazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc

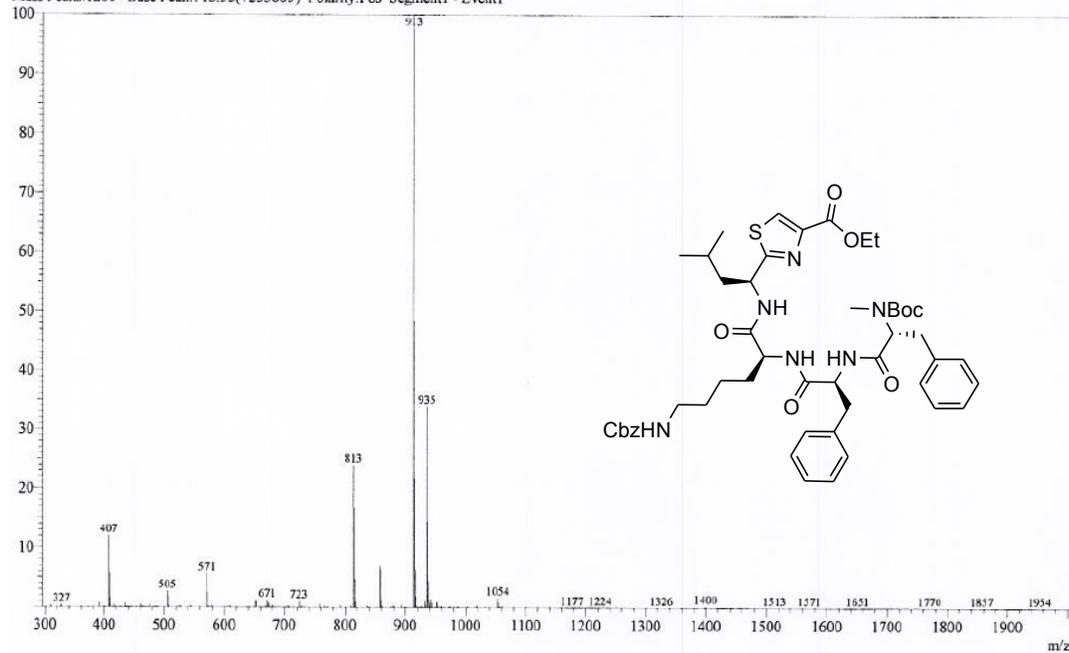
==== Shimadzu LCMSsolution Analysis Report ====



Ret. Time: 3.600 (Scan#: 157)

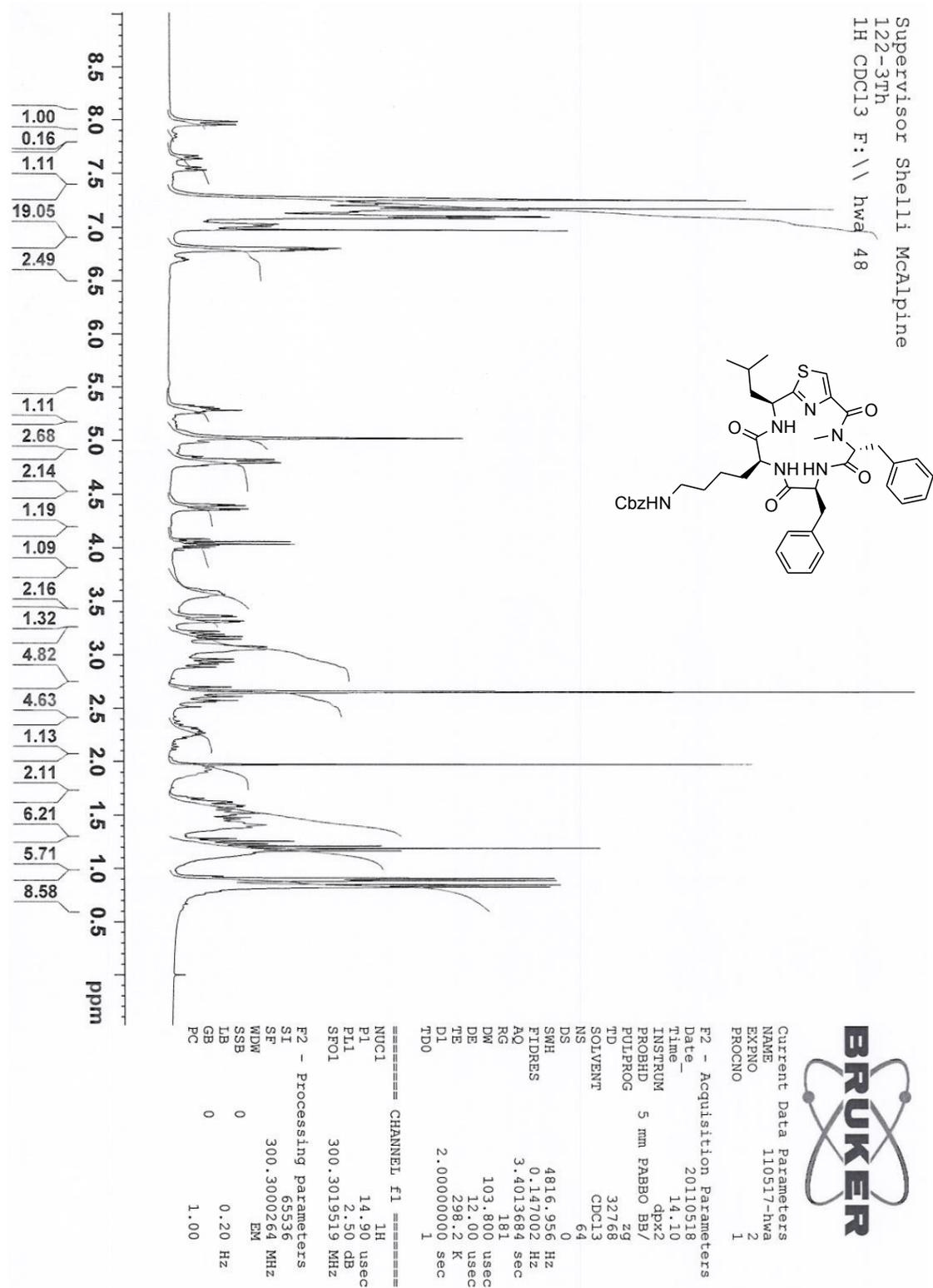
BG Mode: ?

Mass Peaks: 1288 Base Peak: 913.35 (7253665) Polarity: Pos Segment1 - Event1



Compound 11: C-Th-III

HPLC+LCMS Pentapeptide EtO-Thiazole-Leu-Lys(Cbz)-Phe-D-Phe-N(Me)Boc (MW = 912)



Compound 11: C-Th-III

NMR Macrocycle Phe-D-Phe-N(Me)-Thiazole-Leu-Lys(Cbz) (11)

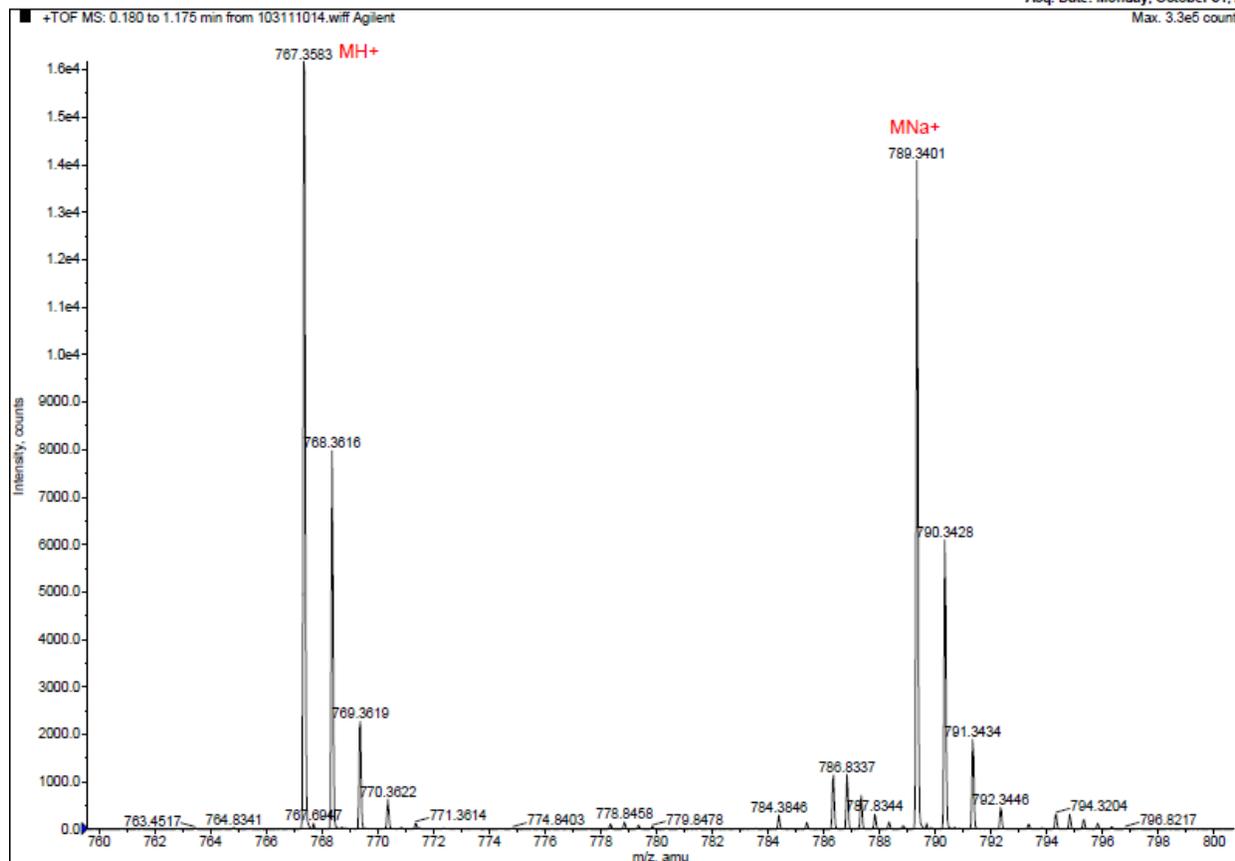
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5711

Acq. File: 103111014.wiff
Acq. Date: Monday, October 31, 20
Max. 3.3e5 counts.



Compound 11: C-Th-III

HRMS Macrocycle Phe-D-Phe-N(Me)-Thiazole-Leu-Lys(Cbz) (11) (MW = 767.3583)

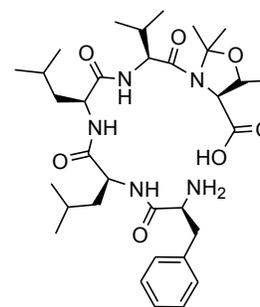
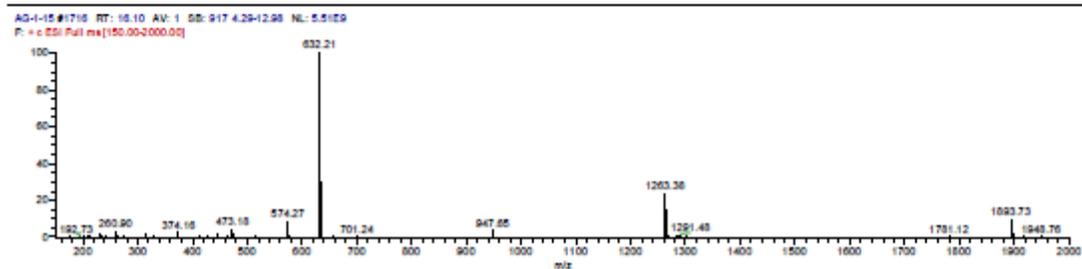
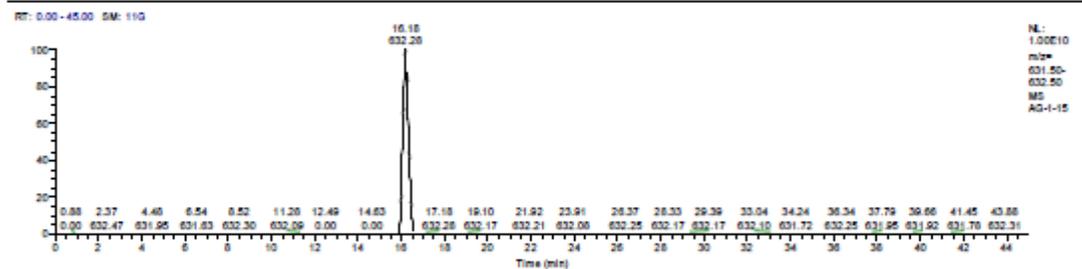
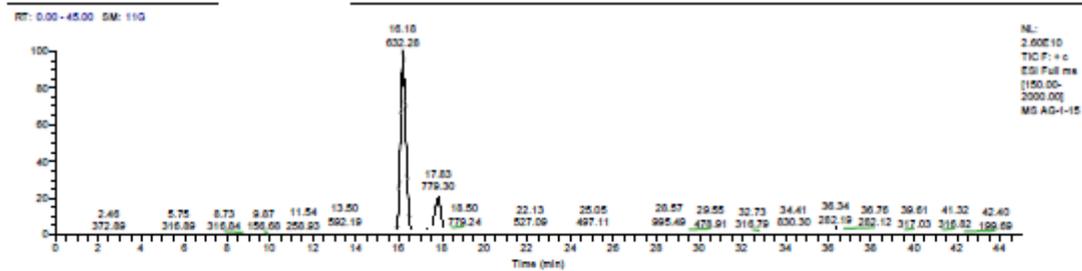
Supplementary Material

Davis et al.

C:\Loliffe\Kelly\AG-1-15

28/05/2010 12:35:41 AM

AG-1-15



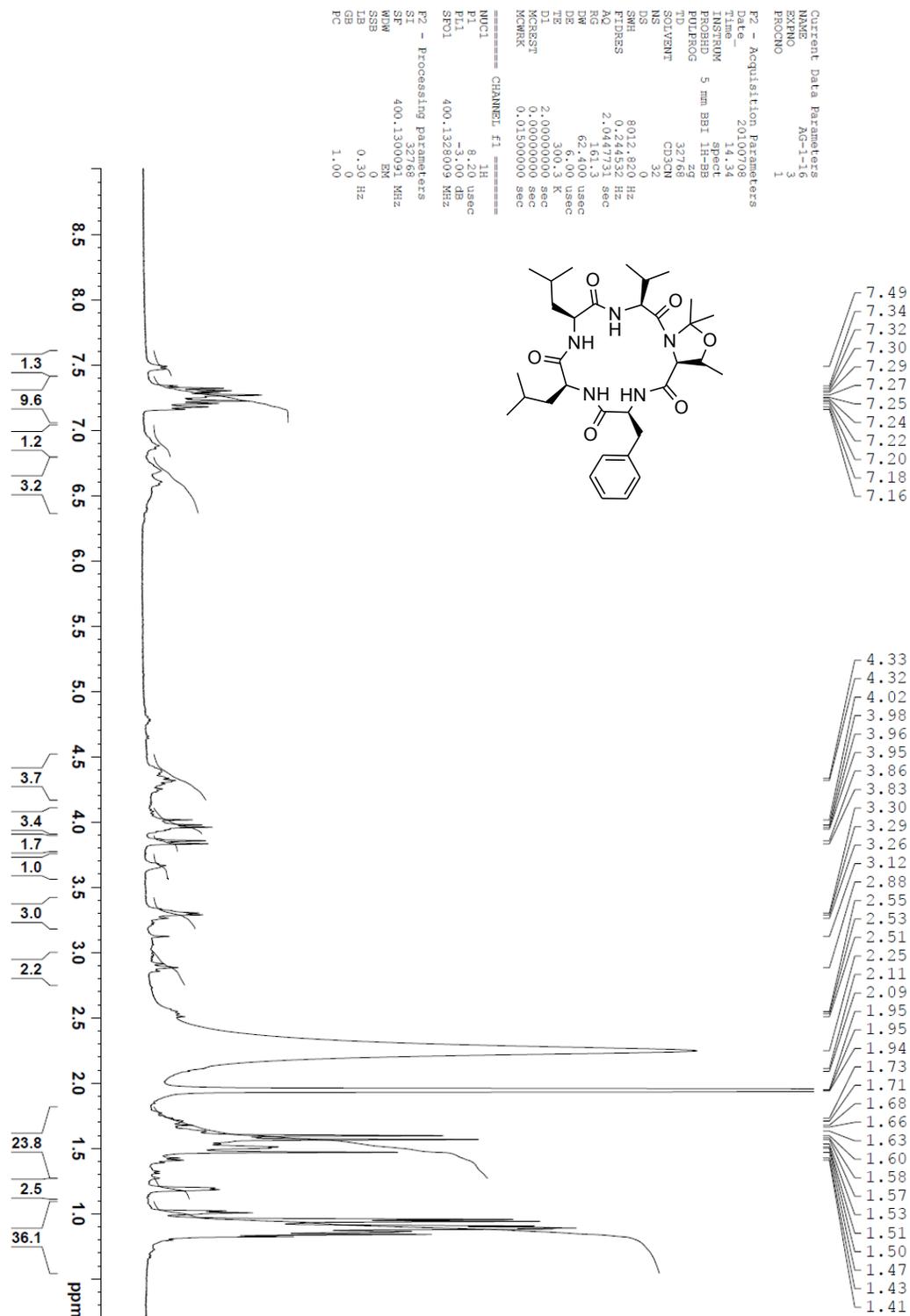
Compound 12: A-PP-II

LCMS Deprotected Pentapeptide HO-Thr(Ψ Me,Me-Pro)-Val-Leu-Leu-Phe-NH₂ (MW = 631)

Supplementary Material

Davis et al.

¹H NMR of Cyclicized Pentapeptide Thr(ψ-Me,Me-Pro)-Val-Leu-Leu-Phe (12-PP)

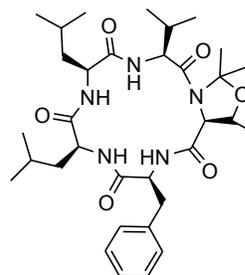
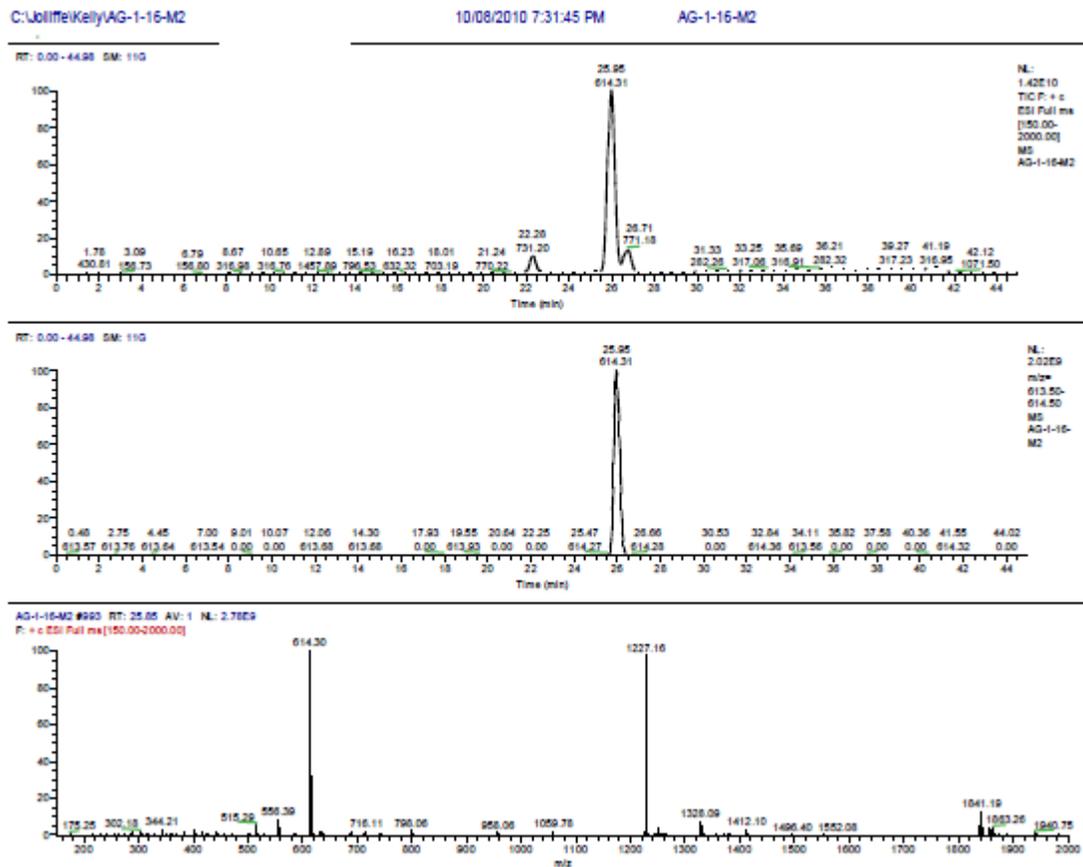


Compound 12: A-PP-II

NMR Macrocycle Phe-Thr(ψMe,Me-Pro)-Val-Leu-Leu (12)

Supplementary Material

Davis et al.



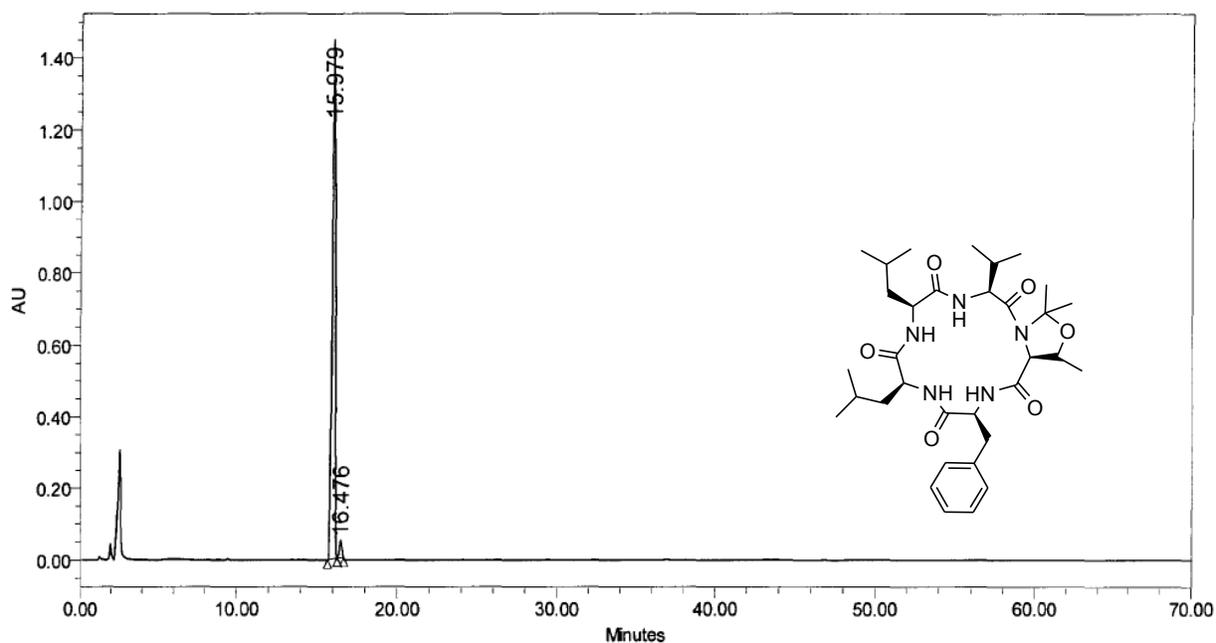
Compound 12: A-PP-II

LCMS Macrocyclic Phe-Thr(ΨMe,Me-Pro)-Val-Leu-Leu (MW = 613)

EmpowerThe University of Sydney, School of Chemistry
Single Channel Report

SAMPLE INFORMATION

Project Name:	Payne	Acq. Method Set:	G_40to100ov30_B_D2ml
Sample Name:	AG-1-16M-2	Sample Set Name:	RJP_AFGPanalyt
Sample Type:	Unknown	Date Acquired:	9/08/2010 9:42:11 PM EST
Vial:	8	Proc. Method:	NoPeaks
Injection #:	1	Date Processed:	13/08/2010 1:49:27 PM EST
Injection Volume:	10.00 ul	Channel Name:	PDA Max Plot 190.0 - 800.0
Run Time:	70.0 Minutes	Proc. Chnl. Descr.:	PDA MaxPlot (190.0 nm to 800.0 nm)
Chromatogram_Info:	0t100%Bover40, A:H2O/TFA 100:0.1, B:ACN/TFA 100:0.1; SunFire C18-106 01;0.2 mL/min		



	RT	Area	% Area	Height
1	15.979	20121855	97.31	1447222
2	16.476	557241	2.69	48631

Compound 12: A-PP-II

HPLC Macrocyclic Phe-Thr(Ψ Me,Me-Pro)-Val-Leu-Leu (12)

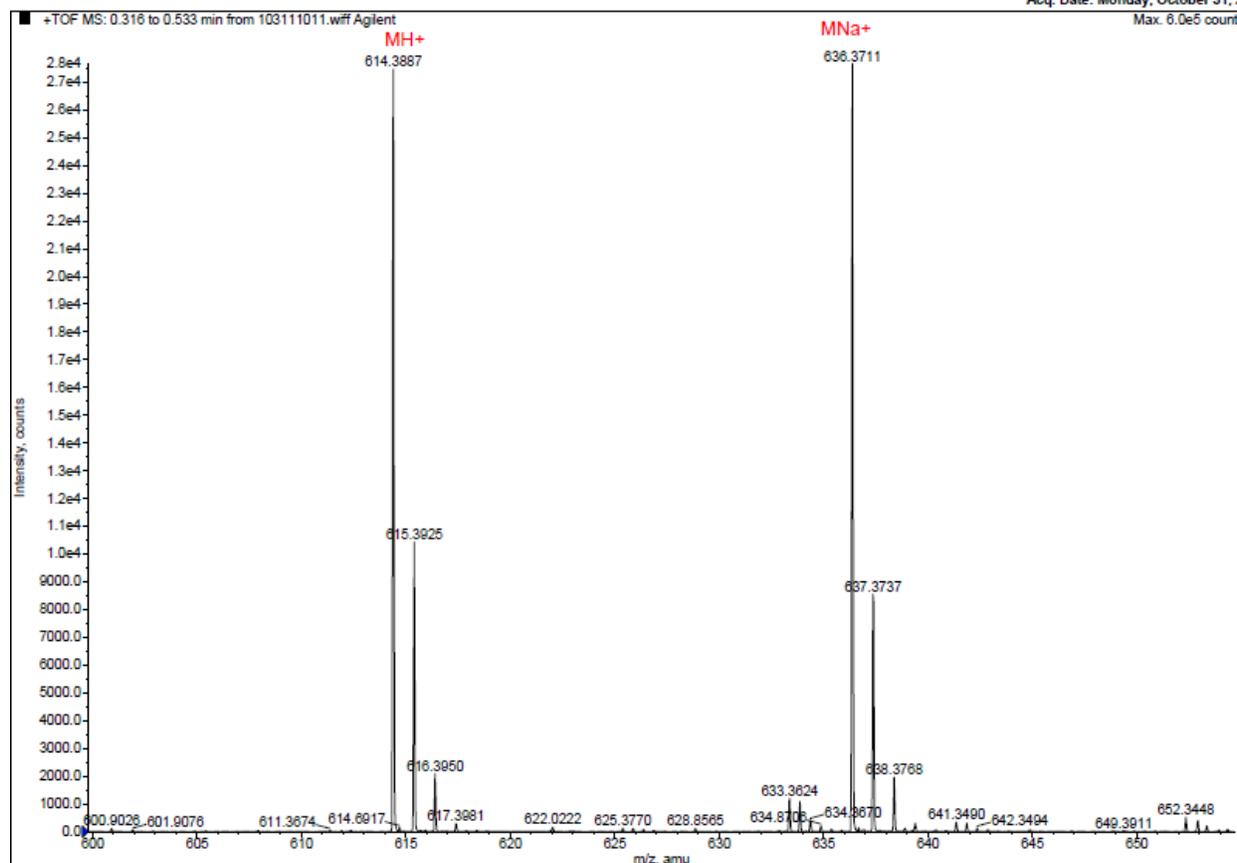
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

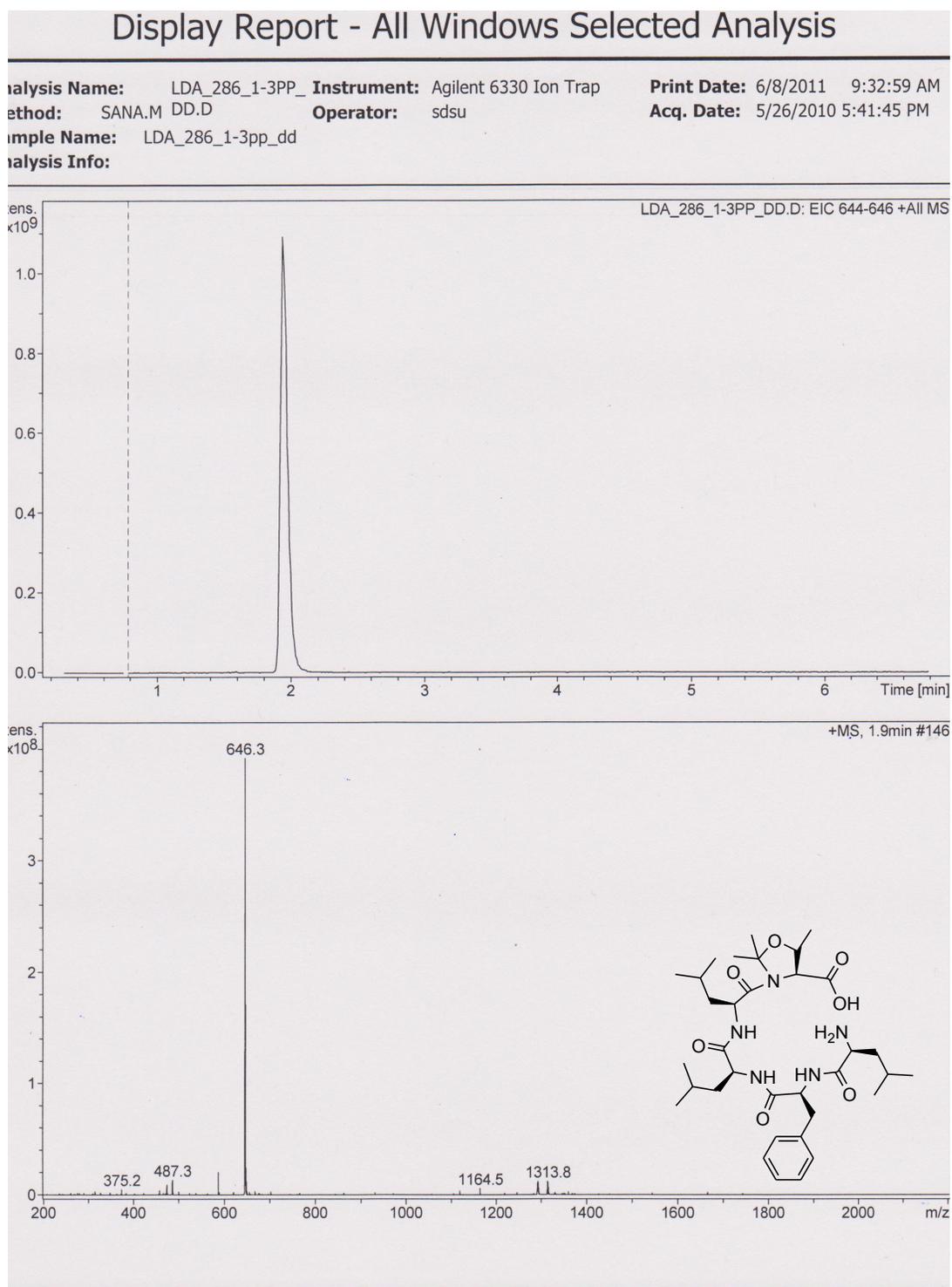
Sample Name: syek5705

Acq. File: 103111011.wiff
Acq. Date: Monday, October 31, 20



Compound 12: A-PP-II

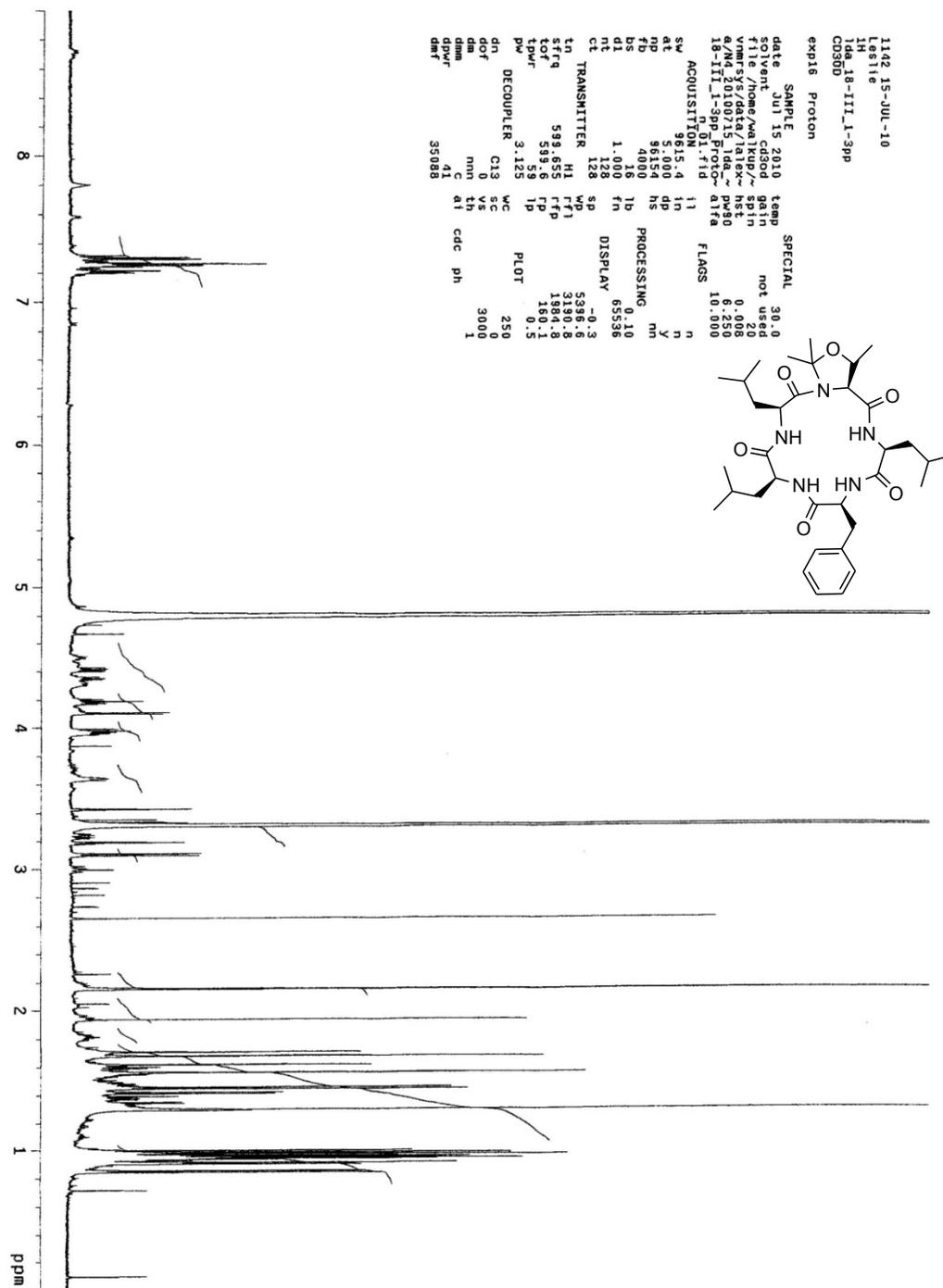
HRMS Macrocycle Phe-Thr(Ψ Me,Me-Pro)-Val-Leu-Leu (MW = 614.3887)



Compound 13: A-PP-III

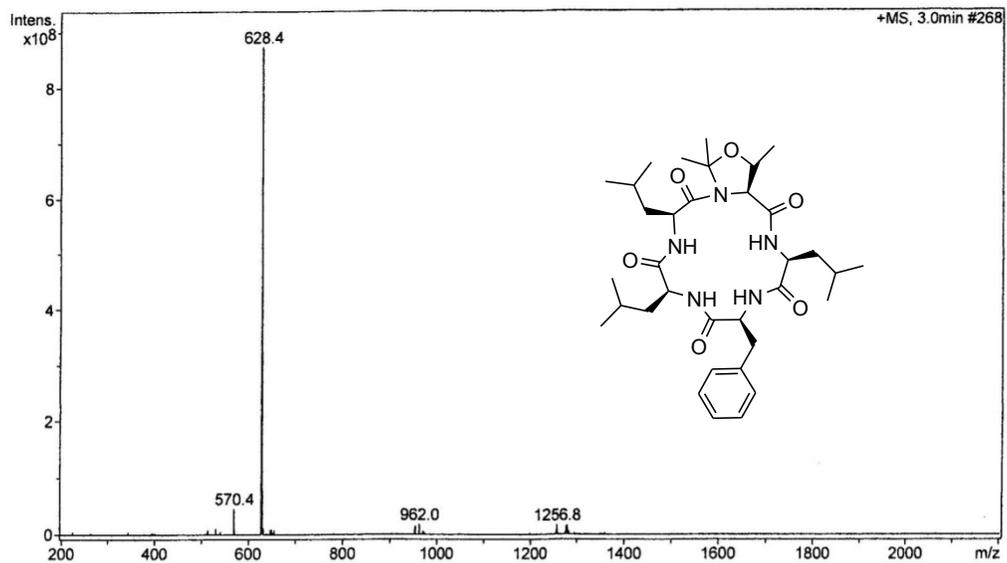
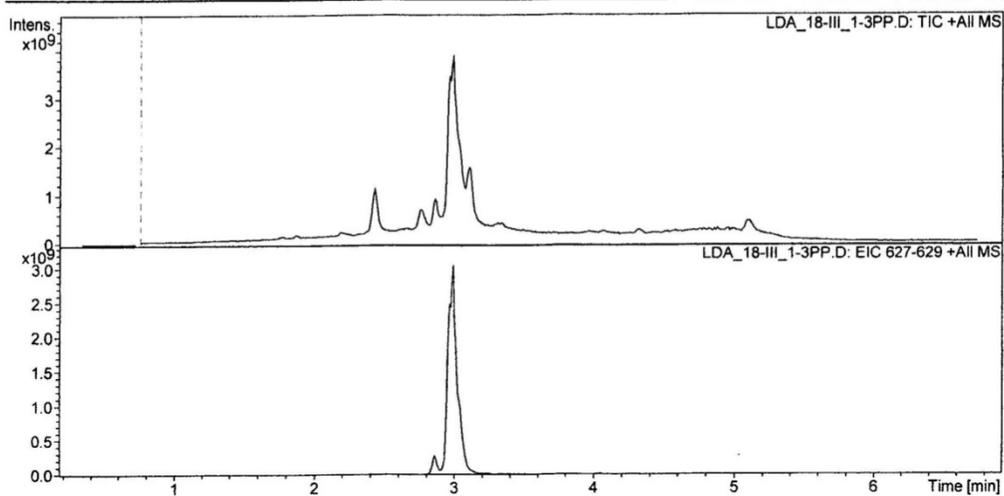
LCMS Deprotected Pentapeptide HO-Thr(Ψ Me,Me-Pro)-Leu-Leu-Phe-Leu-NH₂ (MW=646)

Davis et al.



Display Report - All Windows Selected Analysis

Analysis Name: LDA_18-III_1-3P **Instrument:** Agilent 6330 Ion Trap **Print Date:** 7/29/2010 12:00:31 PM
Method: SANA.M P.D **Operator:** sdsu **Acq. Date:** 7/13/2010 5:53:29 PM
Sample Name: LDA_18-III_1-3pp
Analysis Info:



Compound 13: A-PP-III

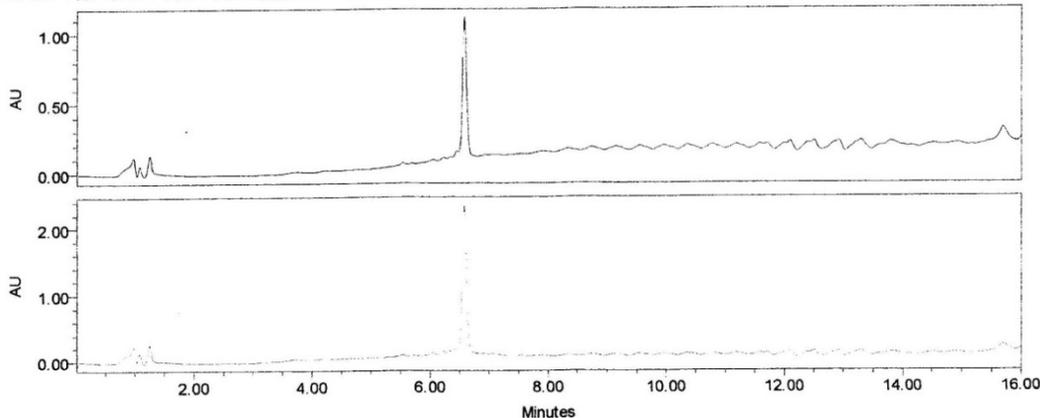
LCMS Macrocycle Phe-Leu-Thr(Ψ Me,Me-Pro)-Leu-Leu (13) (MW= 628)

SDSU

Project Name: Defaults
Reported by User: System

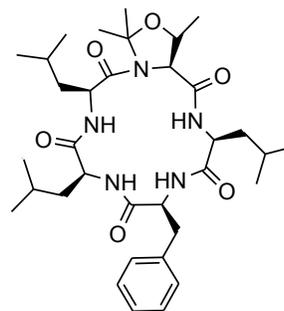
Breeze

SAMPLE INFORMATION			
Sample Name:	LDA_18-III_1-3PP	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method:	primary_sanA_ss_ACN
Injection #:	480	Date Acquired:	7/20/2010 2:25:27 PM
Run Time:	16.00 Minutes	Injection Volume:	50.00 ul



Channel: 2487Channel 1 Channel Desc.: Processing Method: ****
Channel: 2487Channel 2 Channel Desc.: Processing Method: ****

Peak Name	RT (min)	Area (μV*sec)	% Area	Height (μV)	Amount	Units
1	****	****	****	****	****	****
2	****	****	****	****	****	****



Compound 13: A-PP-III

HPLC Macrocycle Phe-Leu-Thr(ΨMe,Me-Pro)-Leu-Leu (13)

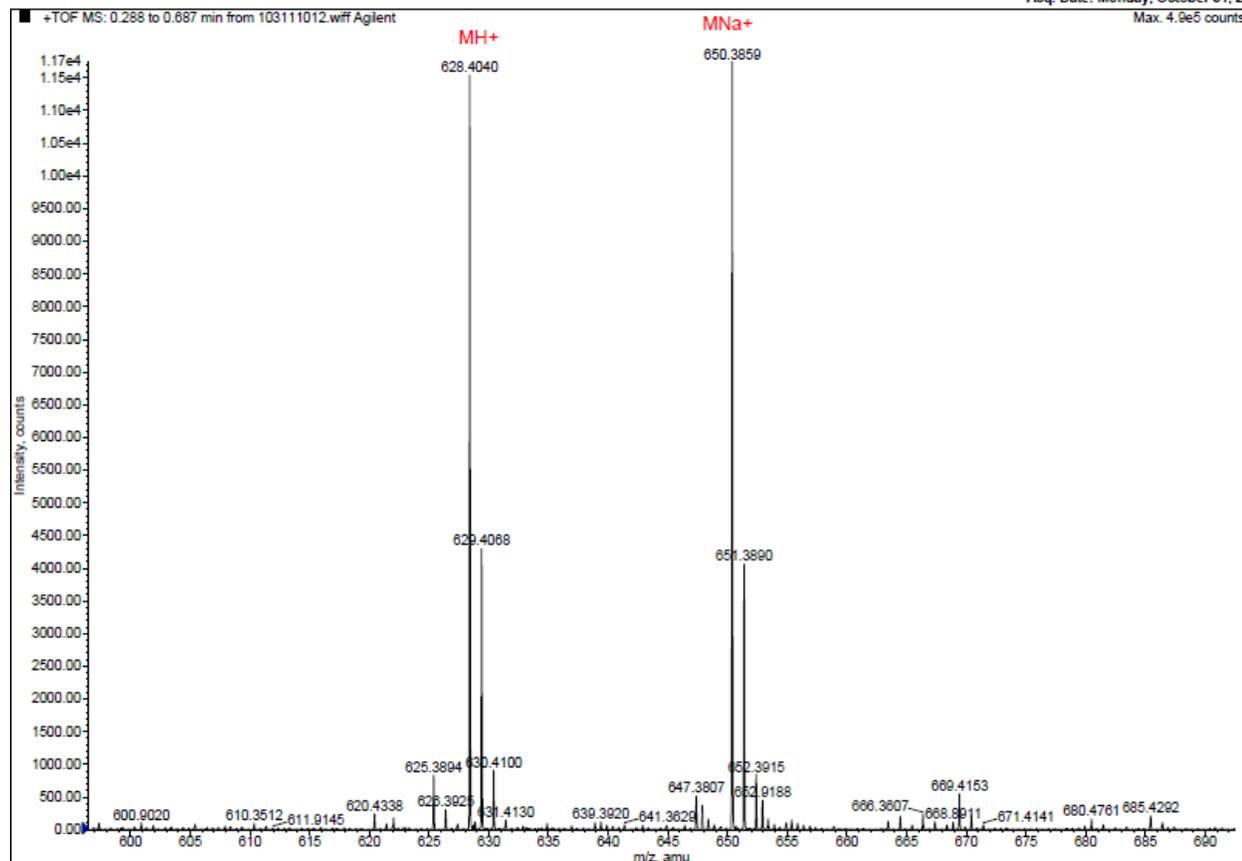
Supplementary Material

Davis et al.

Polarity/Scan Type: Positive

Sample Name: syek5706

Acq. File: 103111012.wiff
Acq. Date: Monday, October 31, 20



Compound 13: A-PP-III

HRMS Macrocycle Phe-Leu-Thr(Ψ Me,Me-Pro)-Leu-Leu (13) (MW= 628.4040)