SUPPLEMENT

NATURE METHODS
LipidBlast - in-silico tandem mass spectrometry database for lipid identification

Tobias Kind, Kwang-Hyeon Liu, Do Yup Lee, Brian DeFelice, John K. Meissen and Oliver Fiehn

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Supplementary Figure 1: Compound structure examples from all 26 lipid classes covered in LipidBlast. File type is MS PowerPoint.

Supplementary Figure 2: Investigation of fragmentations and rearrangements of different phospholipid classes from authentic reference compounds using electrospray ion trap tandem mass spectrometry. File type is MS PowerPoint

Supplementary Figure 3: Custom modeling of *m/z* fragments and abundances shown for phosphatidylcholine. The candidate PC 36:2 cannot be identified with the standard LipidBlast libraries. A custom created library allows the subsequent identification of MS/MS spectra obtained from a quadrupole time-of-flight (Q-TOF) instruments. File type is MS PowerPoint.

Supplementary Figure 4: Detailed search results of all 134 MS/MS spectra from forty different platforms containing screenshots of pictures from NIST MS Search GUI program. All raw mass spectral files and search statistics are supplied together with the LipidBlast software. File type is MS PowerPoint.

Supplementary Figure 5: Validation of LipidBlast with MS/MS spectra obtained from a quadrupole time-of-flight (Q-TOF) instrument. All raw mass spectral files are supplied with the LipidBlast software. File type is MS PowerPoint.

Supplementary Note 1: Complete literature reference collection used for LipidBlast development, covering ~300 external literature references. References were used to develop or validate known fragmentations and to manually extract high-resolution tandem mass spectra. File type is MS DOC.

Supplementary Table 1: Detailed statistics of the LipidBlast MS/MS libraries with detailed lipid compound numbers, MS/MS spectra numbers, covered adduct types ($[M+H]^+$; $[M+Na]^+$; $[M+NH_4]^+$; $[M-H]^-$; $[M-2H]^{(2-)}$; $[M+NH_4-CO]^+$; $[M+2Na-H]^+$; $[M]^+$; $[M-H+Na]^+$; $[M+Li]^+$) and histogram statistics of accurate mass values and peak numbers in library. File type is XLS and stored externally.

Supplementary Table 2: Complete table of mass spectrometry platforms that can be used with the LipidBlast libraries. Forty different mass spectrometer types from seven major vendors can be used with LipidBlast. The table shows cross-platform independence and the ability of the LipidBlast libraries to identify compounds from different MS platforms. File type is XLS and stored externally.

Online Supplement LipidBlast:

The LipidBlast software itself and all MS/MS in-silico spectra, all references spectra, compound structure examples as well as all statistical evaluations can be found under:

http://fiehnlab.ucdavis.edu/projects/LipidBlast

Questions regarding LipidBlast and software should be directed to:
Dr. Tobias Kind (tkind@ucdavis.edu)
http://fiehnlab.ucdavis.edu/staff/kind/

Davis, May15 2013

LipidBlast - In silico created MS/MS libraries for lipid profiling

Supplement of covered structures
The structure drawing files (*.mrv) MarvinSketch
can be found under:

http://fiehnlab.ucdavis.edu/projects/LipidBlast

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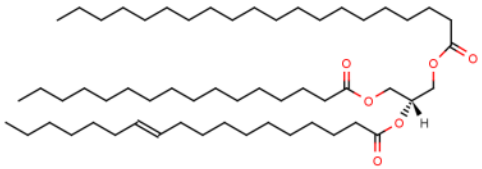
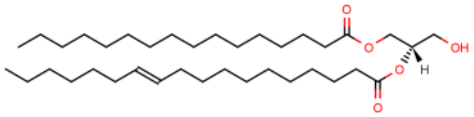
Created: October 2012; Kind/FiehnLab

Covered structures and MS/MS spectra in LipidBlast

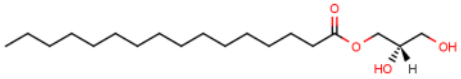
Num	Lipid class	PIC	Short Name	Number compounds	Number MS/MS spectra	Number MS/MS libraries
1	Phosphatidylcholines	ok	PC	5,476	10,952	2
2	Lysophosphatidylcholines	ok	lysoPC	80	160	2
3	Plasmenylphosphatidylcholines	ok	plasmenyl-PC	222	444	2
4	Phosphatidylethanolamines	ok	PE	5,476	16,428	3
5	Lysophosphatidylethanolamines	ok	lysoPE	80	240	3
6	Plasmenylphosphatidylethanolamines	ok	plasmenyl-PE	222	666	3
7	Phosphatidylserines	ok	PS	5,123	15,369	3
8	Sphingomyelines	ok	SM	168	336	2
9	Phosphatidic acids	ok	PA	5,476	16,428	3
10	Phosphatidylinositols	ok	PI	5,476	5,476	1
11	Phosphatidylglycerols	ok	PG	5,476	5,476	1
12	Cardiolipins	ok	CL	25,426	50,852	2
13	Ceramide-1-phosphates	ok	CerP	168	336	2
14	Sulfatides	ok	ST	168	168	1
15	Gangliosides	ok	[glycan]-Cer	880	880	1
16	Monoacylglycerols	ok	MG	74	148	2
17	Diacylglycerols	ok	DG	1,764	3,528	2
18	Triacylglycerols	ok	TG	2,640	7,920	3
19	Monogalactosyldiacylglycerols	ok	MGDG	5,476	21,904	4
20	Digalactosyldiacylglycerols	ok	DGDG	5,476	10,952	2
21	Sulfoquinovosyldiacylglycerols	ok	SQDG	5,476	5,476	1
22	Diacylated phosphatidylinositol monomannoside	ok	Ac2PIM1	144	144	1
23	Diacylated phosphatidylinositol dimannoside	ok	Ac2PIM2	144	144	1
24	Triacylated phosphatidylinositol dimannoside	ok	Ac3PIM2	1,728	1,728	1
25	Tetraacylated phosphatidylinositol dimannoside	ok	Ac4PIM2	20,736	20,736	1
26	Diphosphorylated hexaacyl Lipid A	ok	LipidA-PP	15,625	15,625	1
Total	**All libraries**			**119,200**	**212,516**	**50**



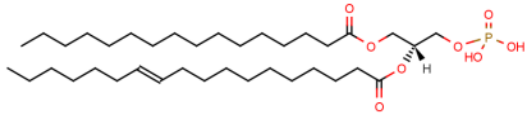
Abbreviation TG(16:0/18:1(11E)/20:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-3-eicosanoyl-sn-glycerol
Formula C57H108O6
Mass 888.81



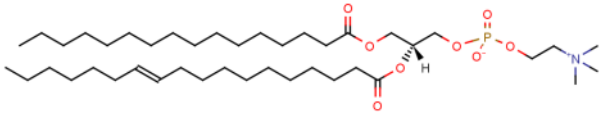
Abbreviation DG(16:0/18:1(11E)/0:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycerol
Formula C37H70O5
Mass 594.52



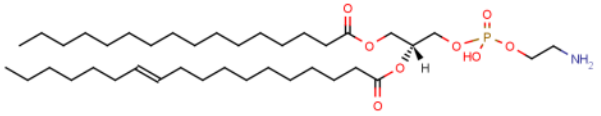
Abbreviation MG(16:0/0:0/0:0)
Systematic Name 1-hexadecanoyl-sn-glycerol
Formula C19H38O4
Mass 330.28



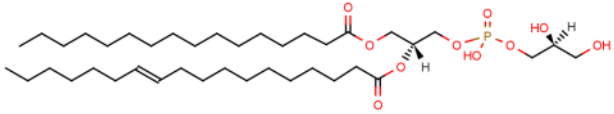
Abbreviation PA(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphate
Formula C37H71O8P
Mass 674.49



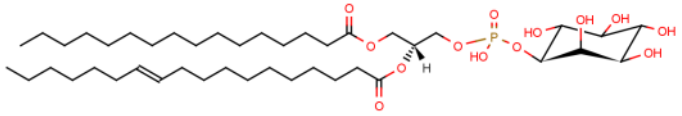
Abbreviation PC(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphocholine
Formula C42H82NO8P
Mass 759.58



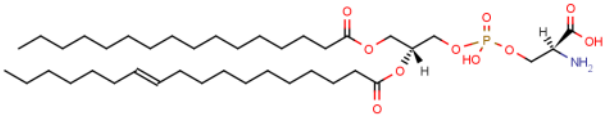
Abbreviation PE(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoethanolamine
Formula C39H76NO8P
Mass 717.53



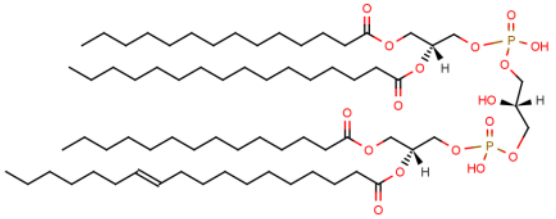
Abbreviation PG(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-sn-glycerol)
Formula C40H77O10P
Mass 748.53



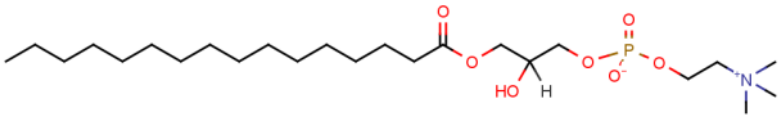
Abbreviation PI(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-myo-inositol)
Formula C43H81O13P
Mass 836.54



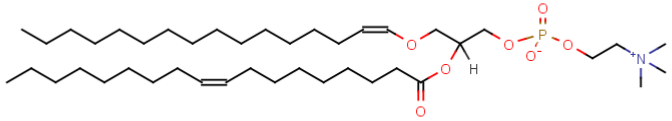
Abbreviation	**PS(16:0/18:1(11E))**
Systematic Name	**1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoserine**
Formula	**C40H76NO10P**
Mass	**761.52**



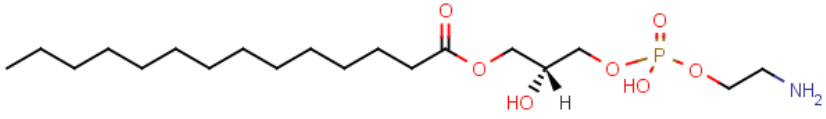
Abbreviation	**CL(1'-[14:0/16:0],3'-[14:0/18:1(11E)])**
Systematic Name	**1'-[1-tetradecanoyl-2-hexadecanoyl-sn-glycero-3-phospho],3'-[1-tetradecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho]-sn-glycerol**
Formula	**C71H136O17P2**
Mass	**1322.93**



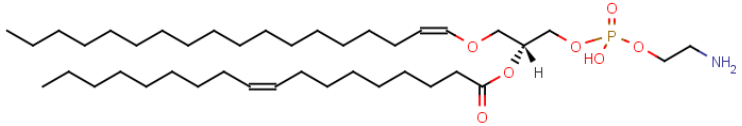
Common Name	**PC(16:0/0:0)[U] (lysoPC)**
Systematic Name	**1-hexadecanoyl-sn-glycero-3-phosphocholine**
Exact Mass	**495.33**
Formula	**C24H50NO7P**



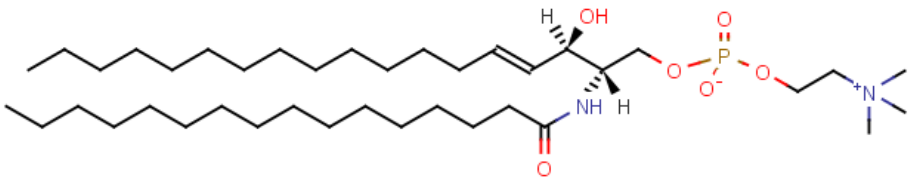
LM ID	**LMGP01030007 (plasmenyl-PC)**
Common Name	**PC(P-16:0/18:1(9Z))[U]**
Exact Mass	**743.58**
Formula	**C42H82NO7P**



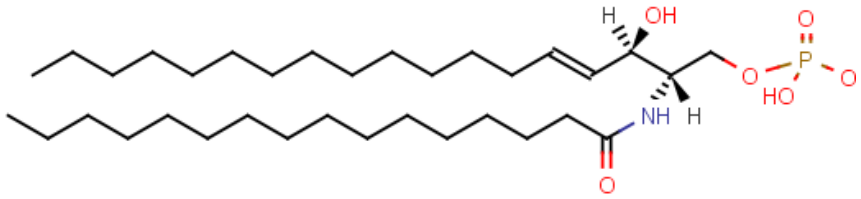
LM ID	**LMGP02050003 (lysoPE)**
Common Name	**PE(14:0/0:0)**
Exact Mass	**425.25**
Formula	**C19H40NO7P**



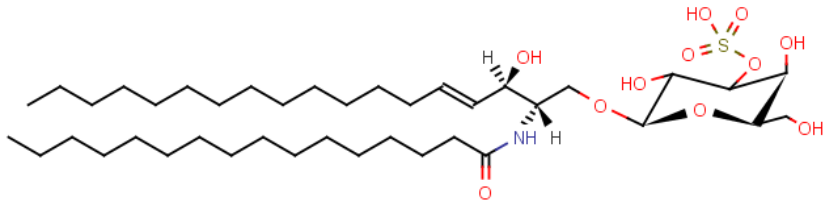
LM ID	**LMGP02030004 (plasmenyl-PE)**
Common Name	**PE(P-18:0/18:1(9Z))**
Exact Mass	**729.57**
Formula	**C41H80NO7P**



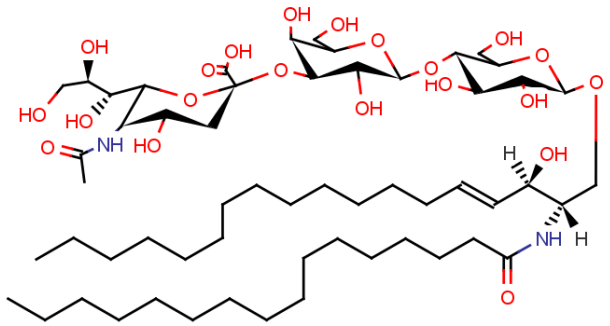
LM ID	**LMSP03010003**
Common Name	**SM(d18:1/16:0)**
Systematic Name	**N-(hexadecanoyl)-sphing-4-enine-1-phosphocholine**
Synonyms	**C16 Sphingomyelin**
Exact Mass	**702.57**
Formula	**C39H79N2O6P**



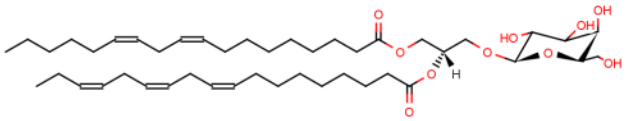
LM ID	**LMSP02050002 (Ceramide-phosphate)**
Common Name	**CerP(d18:1/16:0)**
Systematic Name	**N-(hexadecanoyl)-sphing-4-enine-1-phosphate**
Synonyms	**C16 CerP**
Exact Mass	**617.48**
Formula	**C34H68NO6P**



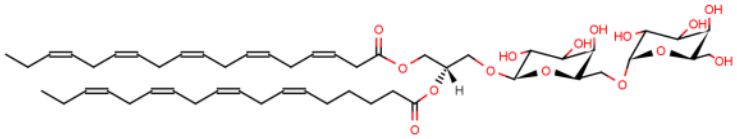
LM ID	**LMSP06020002**
Common Name	**C16 Sulfatide**
Systematic Name	**(3'-sulfo)Galß-Cer(d18:1/16:0)**
Synonyms	**C16 Sulfatide**
Exact Mass	**779.52**
Formula	**C40H77NO11S**



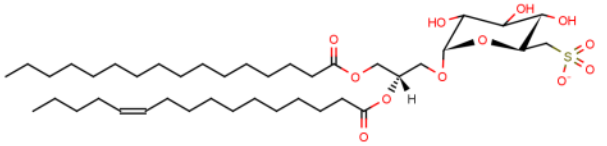
LM ID	**LMSP0601AJ01 (GM3 ganglioside)**
Common Name	**-**
Systematic Name	**NeuAca2-3Galß1-4Glcß-Cer(d18:1/16:0)**
Synonyms	**-**
Exact Mass	**1152.71**
Formula	**C57H104N2O21**



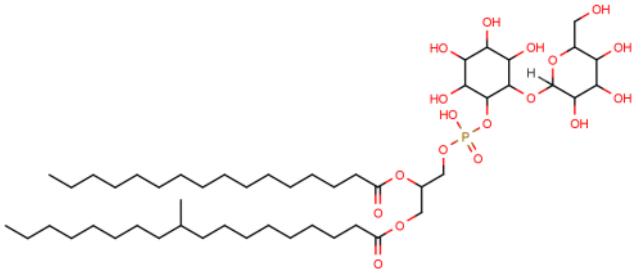
LM ID LMGL05010024
Common Name MGDG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Systematic Name 1-(9Z,12Z-octadecadienoyl)-2-(9Z,12Z,15Z-octadecatrienoyl)-3-O-ß-D-galactosyl-sn-glycerol
Synonyms Monogalactosyldiacylglycerol(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Exact Mass 776.54
Formula C45H76O10



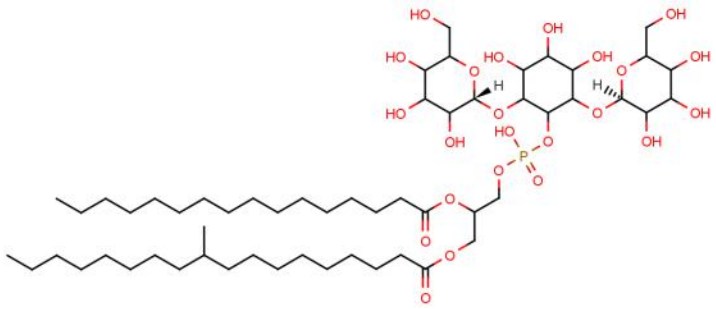
LM ID LMGL05010010
Common Name DGDG(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))
Systematic Name 1-(3Z,6Z,9Z,12Z,15Z-octadecapentaenoyl)-2-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-3-O-(6'-O-a-D-galactosyl-ß-D-galactosyl)-sn-glycerol
Synonyms Digalactosyldiacylglycerol(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))
Exact Mass 930.53
Formula C51H78O15



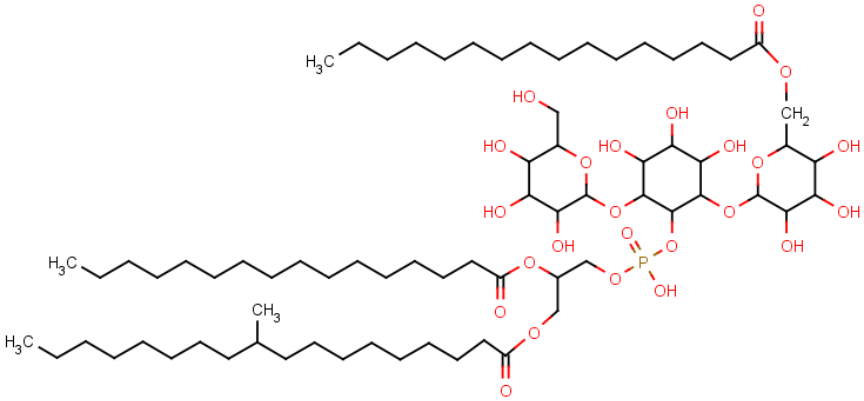
LM ID LMGL05010007
Common Name SQDG(16:0/16:1(11Z))
Systematic Name 1-hexadecanoyl-2-(11Z-hexadecenoyl)-3-(6'-sulfo-a-D-quinovosyl)-sn-glycerol
Synonyms sulfoquinovosyldiacylglycerols; SQDG(16:0/16:1)
Exact Mass 791.50
Formula C41H75O12S



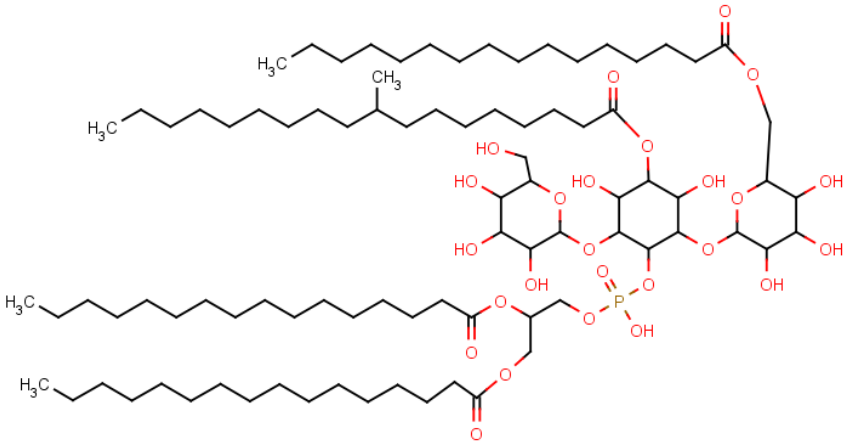
Diacylated phosphatidylinositol monomannoside **Ac2PIM1**
Ac2PIM1(16:0/methyl-18:0)
C50H95O18P
1014.625603



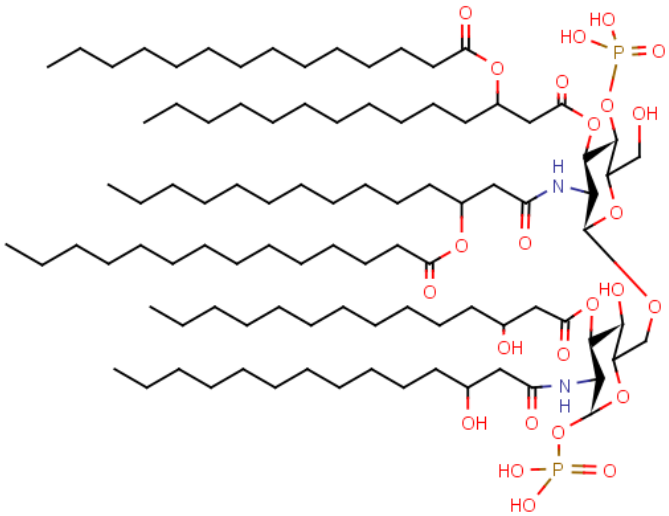
Diacylated phosphatidylinositol dimannoside **Ac2PIM2**
Ac2PIM2(16:0/methyl-18:0)
C56H105O23P
Mass: 1176.678426



Triacylated phosphatidylinositol dimannoside
Ac3PIM2(16:0/methyl-18:0/16:0)
C72H135O24P 1414.908092



Tetraacylated phosphatidylinositol dimannoside
C88H165O25P 1653.137757
Ac4PIM2(16:0/16:0/16:0/methyl-18:0)



Diphosphorylated hexaacyl Lipid A
1825.250692 C96H182N2O25P2
LipidA-PP [14/14/14/14/3O-(14)/3O-(14)]

LipidBlast - In silico created MS/MS libraries for lipid profiling

Supplement of fragmentation modeling from
standard reference compounds.
Raw MS/MS Spectra can be found under:

http://fiehnlab.ucdavis.edu/projects/LipidBlast

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Brian DeFelice, John K. Meissen and Oliver Fiehn
FiehnLab – Metabolomics
UC Davis Genome Center, Davis, USA

Created: October 2010; Liu/FiehnLab

Phospholipids ID Collection A

Dr. KH LIU
UC Davis Metabolomics

LipidBlast

Fragmentation Pattern of Phospholipid on LTQ MS

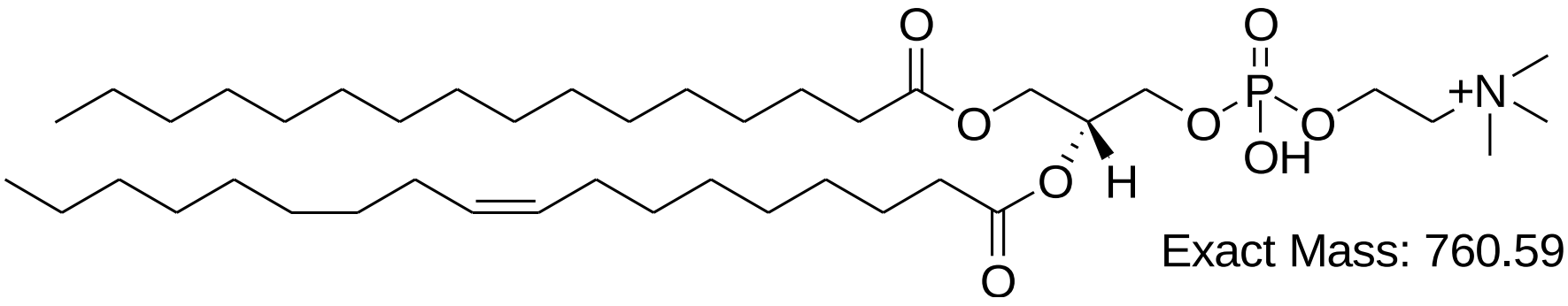
PL	(+)	(+)			(-)	(-)	(-) FFA	Formed Adduct
PC	-18 (H^+)	-59 (both)	-183 (both)		-74 (Ac^-)		No	H^+, Na^+ Ac^-
PE	-43 (Na^+)	-141 (both)					Yes	H^+, Na^+ $-H^+$
PS	-87	-185 (both)			-87 ($-H^+$)		Yes	H^+, Na^+ $-H^+$
SM	-18 (H^+)	-59 (Na^+)	-183 (Na^+)		-74 (Ac^-)	-145 (Ac^-)	No	H^+, Na^+ Ac^-
PI	No signal				-162 ($-H^+$)	241*	Yes	$-H^+$
PG	No signal				-74 ($-H^+$)	227*	Yes	$-H^+$
PA	-98 (Na^+)	-120 (Na^+)					Yes	Na^+ $-H^+$

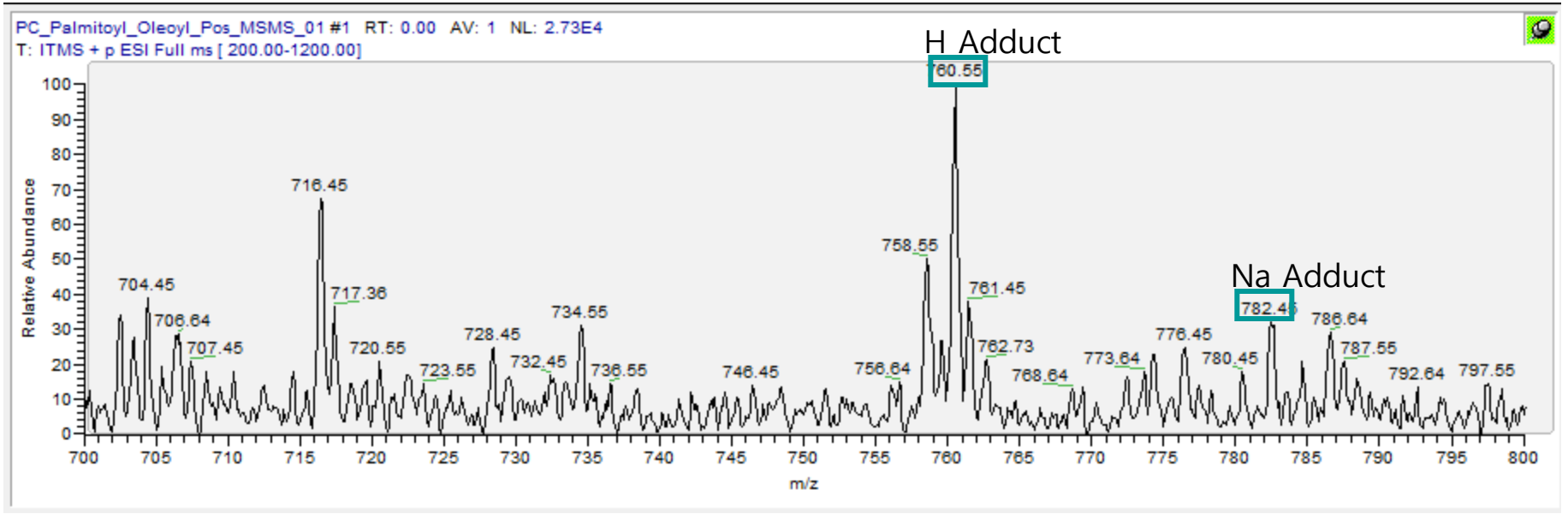
(Na^+), (H^+), (Ac^-): Adduct Ion, Both: (Na^+) or (H^+)
*** Characteristic Fragment Ion**

Phosphatidylcholine ID

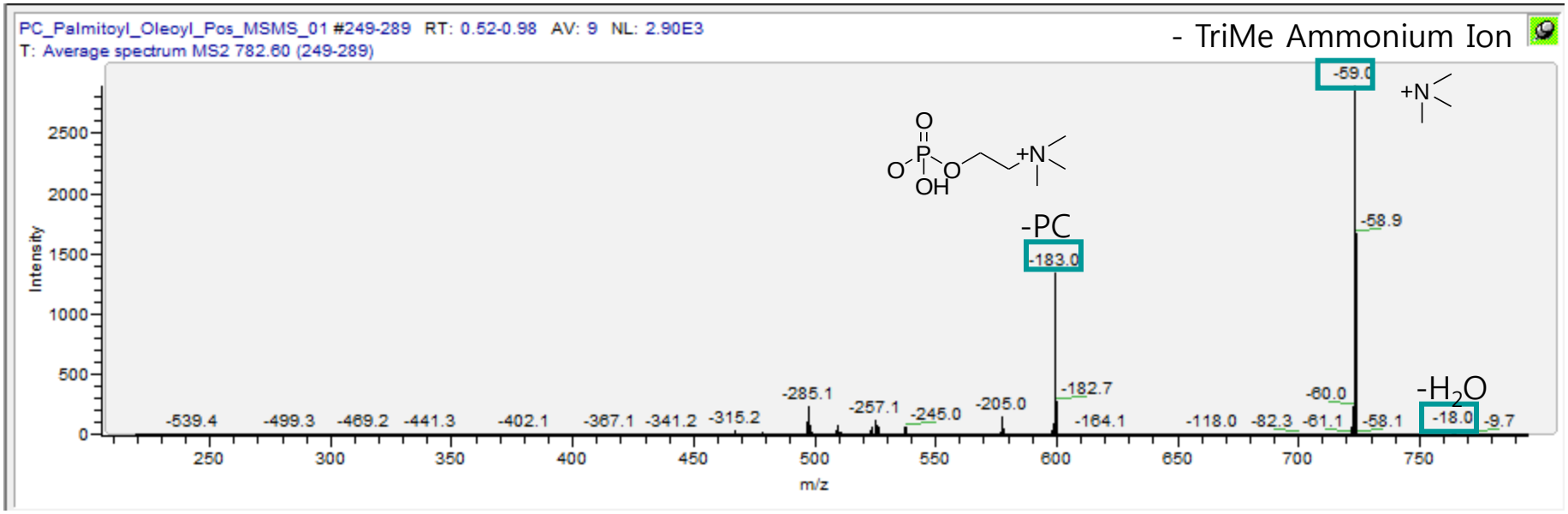
m/z 760.6 (PC 34:1 (16:0, 18:1))

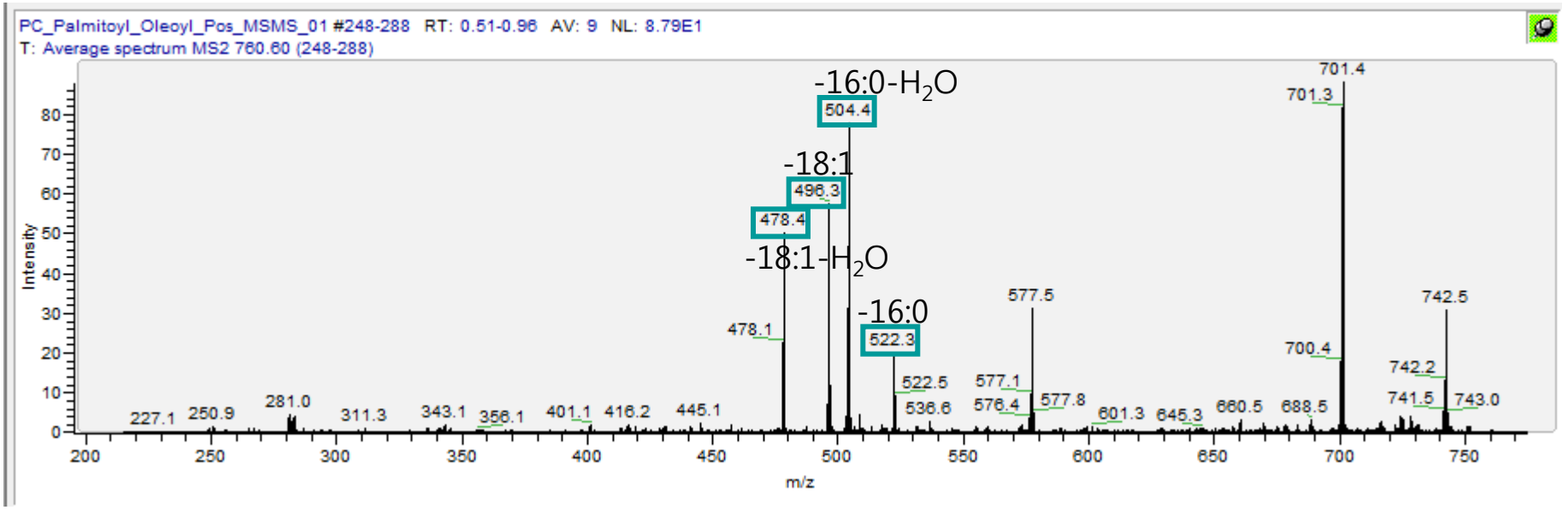
Pos. Mode



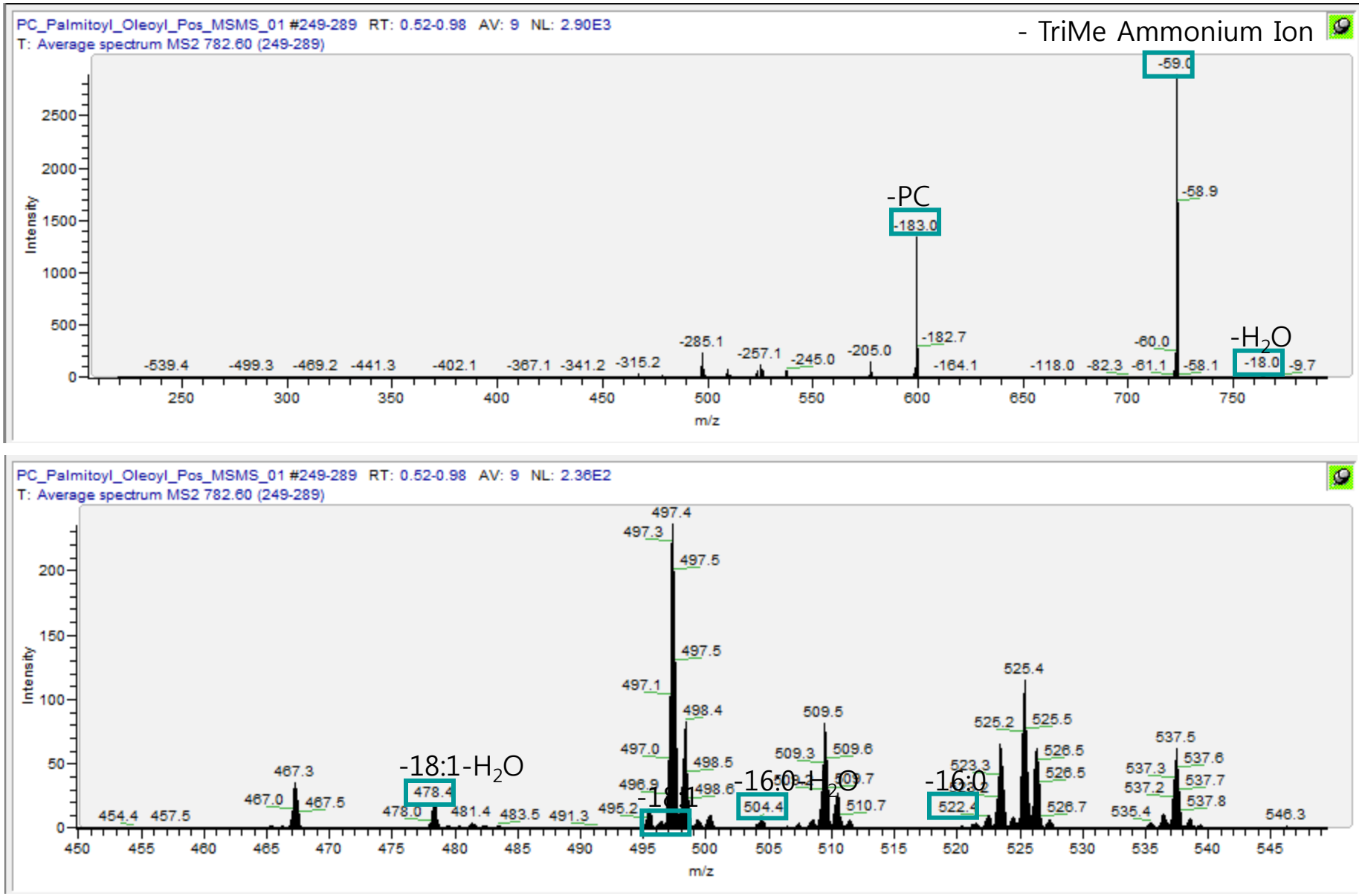


m/z 782.6 (PC 34:1, Sodium Adduct (16:0, 18:1)) Pos. Mode

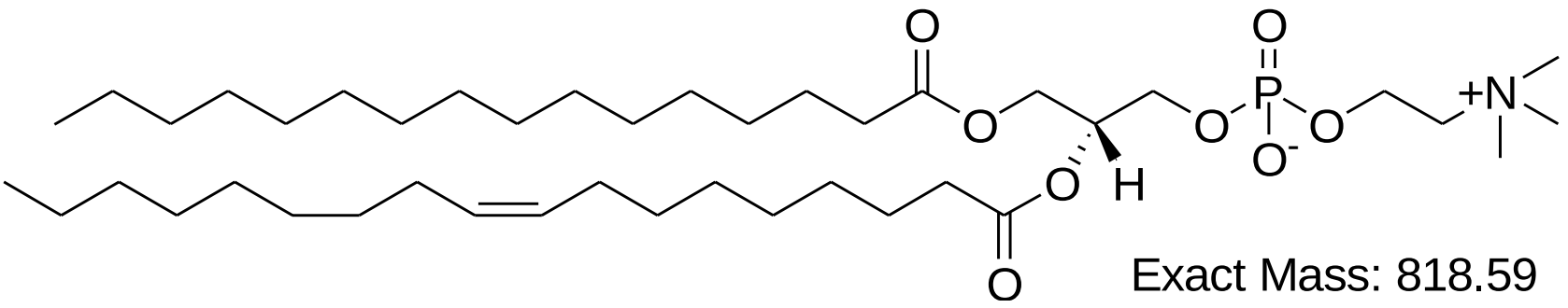


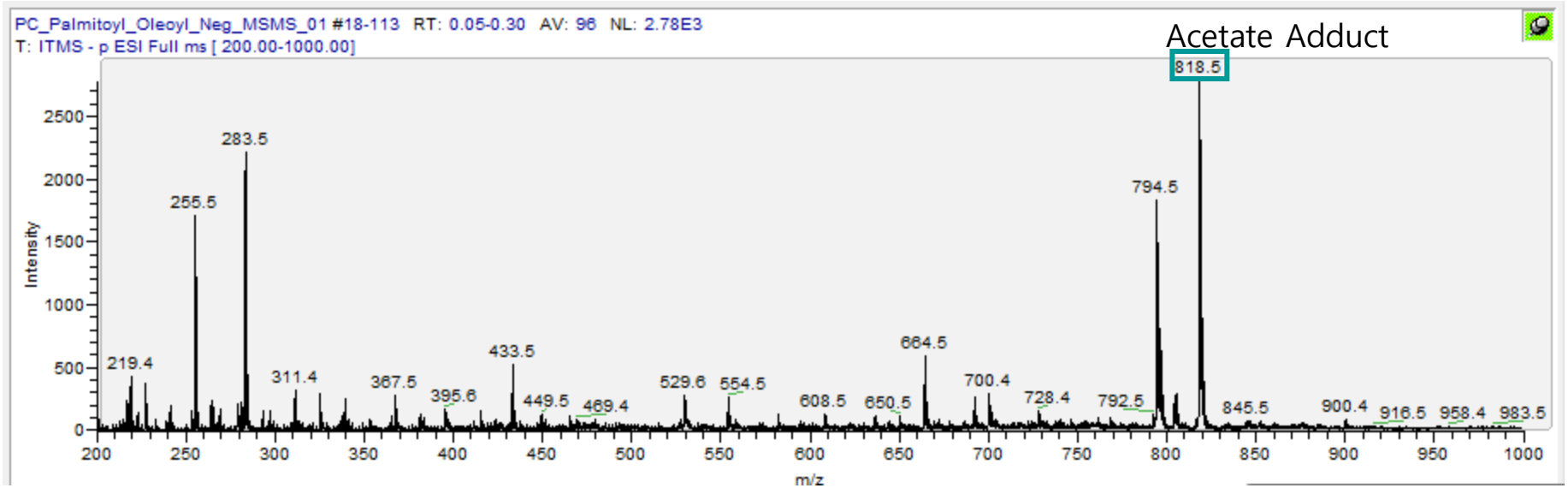


m/z 782.6 (PC 34:1, Sodium Adduct (16:0, 18:1)) Pos. Mode

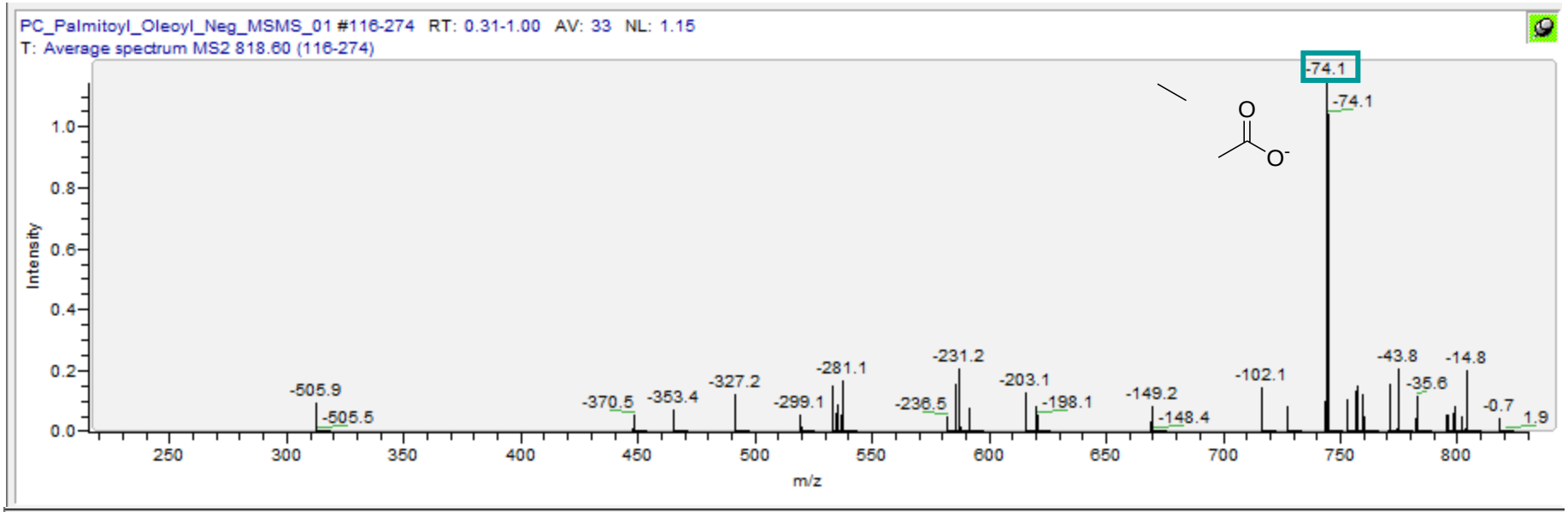


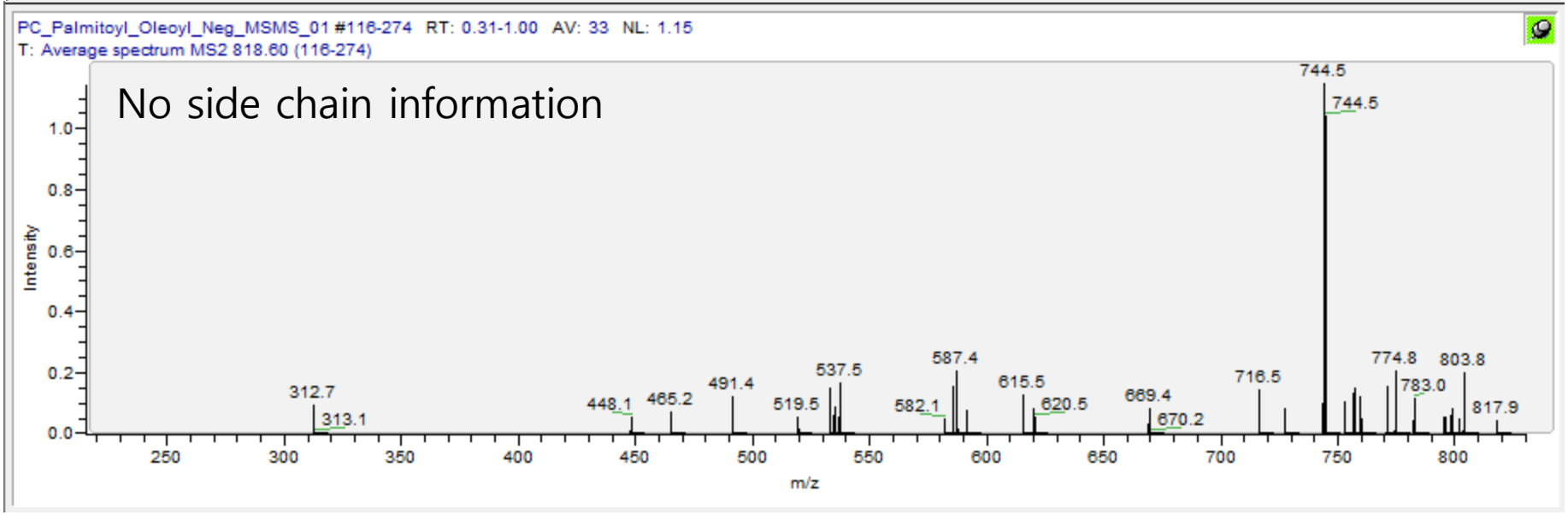
m/z 818.6 (PC 34:1, Acetate Adduct (16:0, 18:1)) Neg. Mode





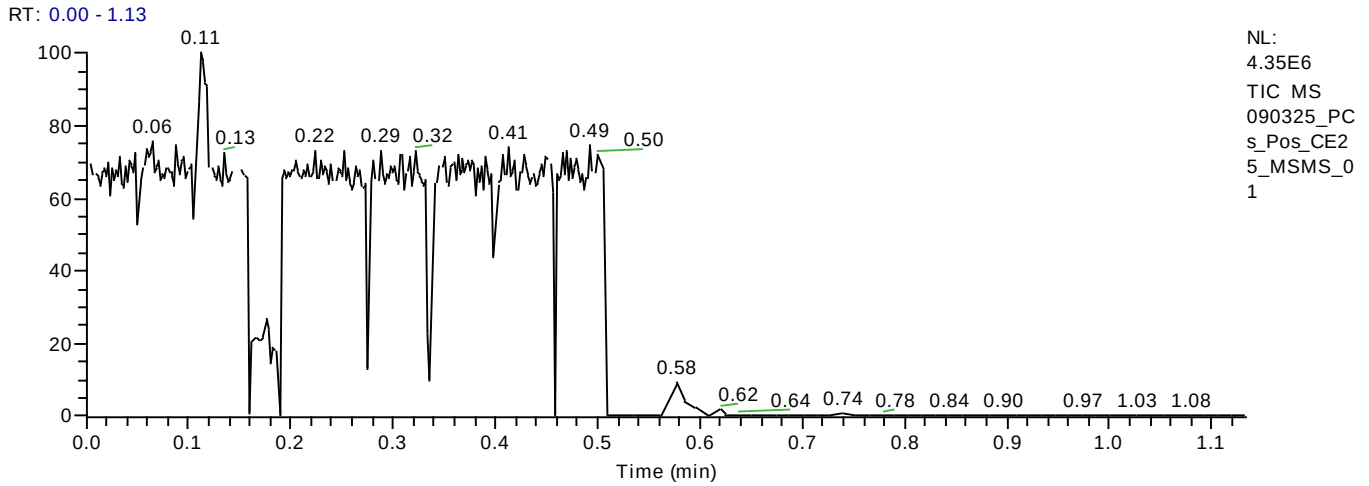
m/z 818.6 (PC 34:1, Acetate Adduct (16:0, 18:1)) Neg. Mode



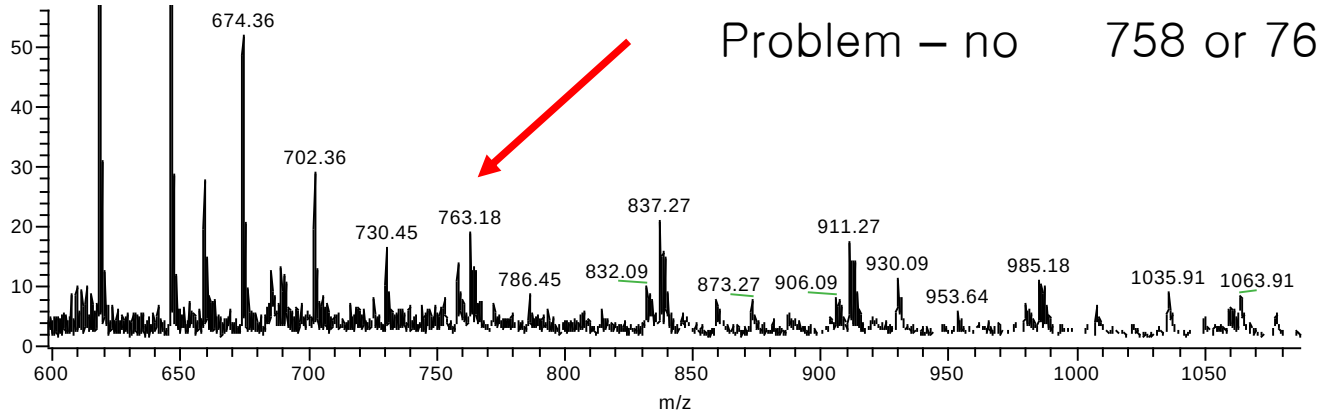


PC – Bovine brain

090325_PCs_Pos_CE25_MSMS_01 3/25/2009 10:44:40 AM PL Standard

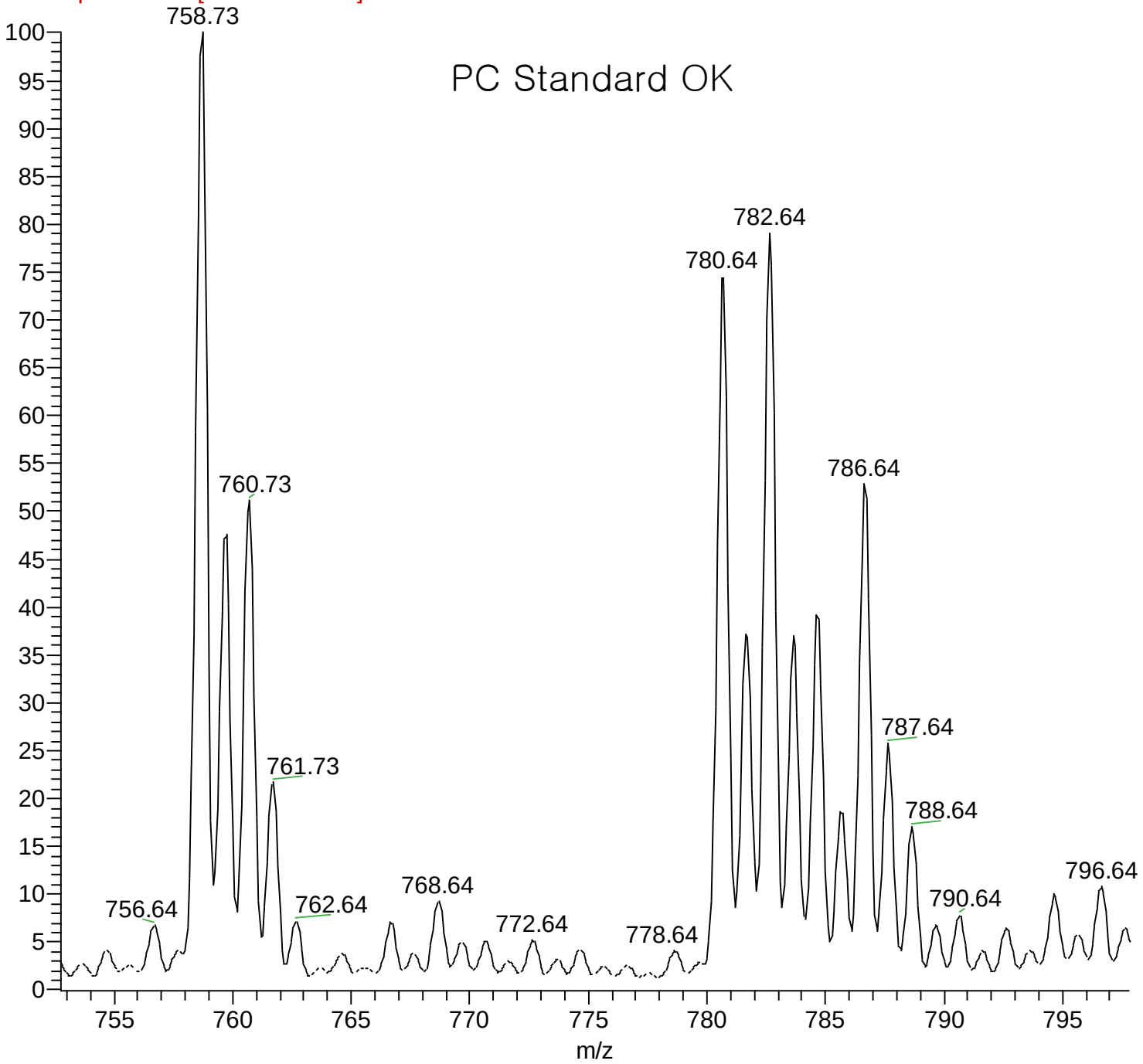


090325_PCs_Pos_CE25_MSMS_01 #45-214 RT: 0.09-0.43 AV: 170 NL: 5.20E3
T: ITMS + p ESI Full ms [300.00-1100.00]



Problem – no 758 or 760

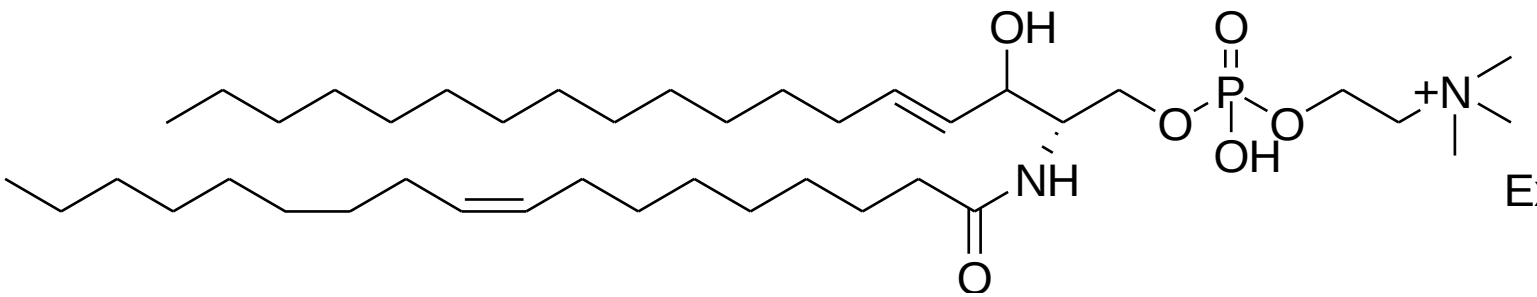
Plasma_ZoomScan_CE45_Pos_01 #54-347 RT: 0.06-0.35 AV: 294 NL: 9.26E4
F: ITMS + p ESI Z ms [700.00-800.00]



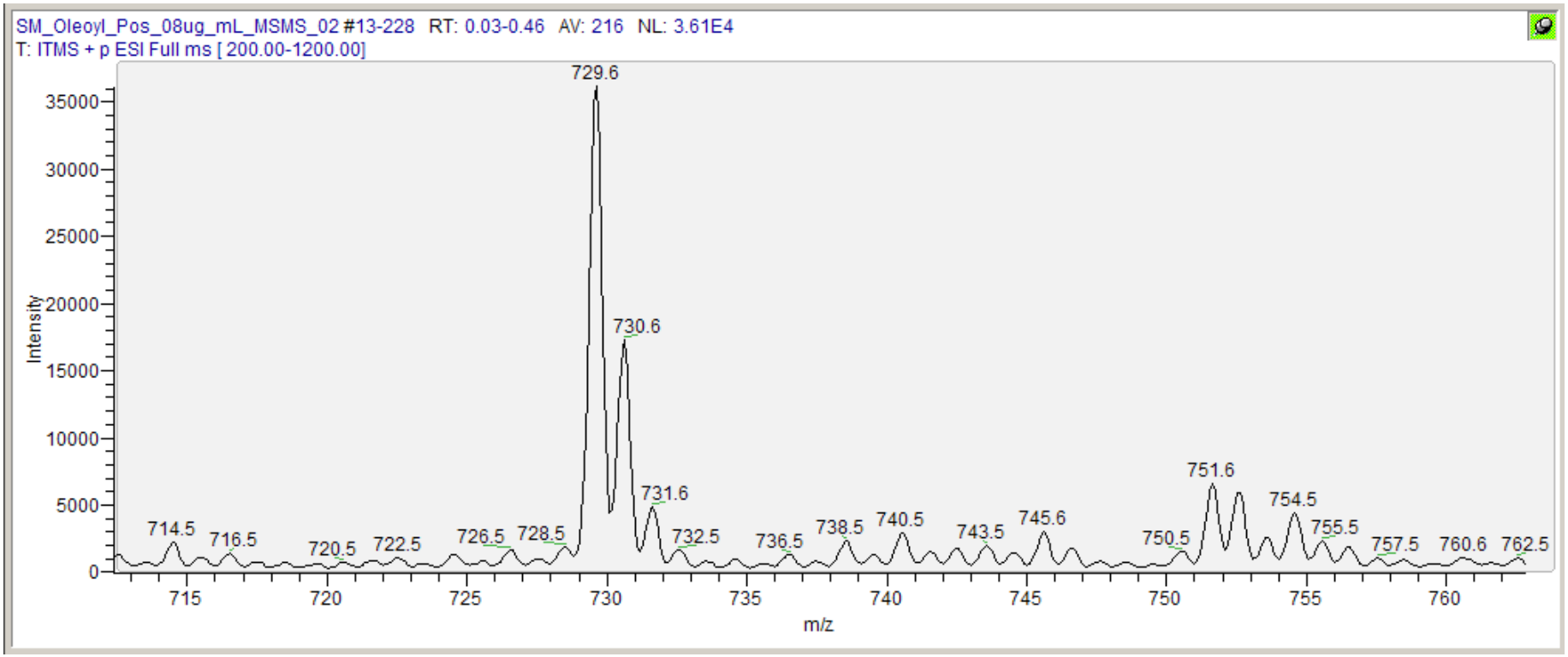
Sphingomyelin ID

m/z 729.6 (SM 36:1 (18:1))

Pos. Mode

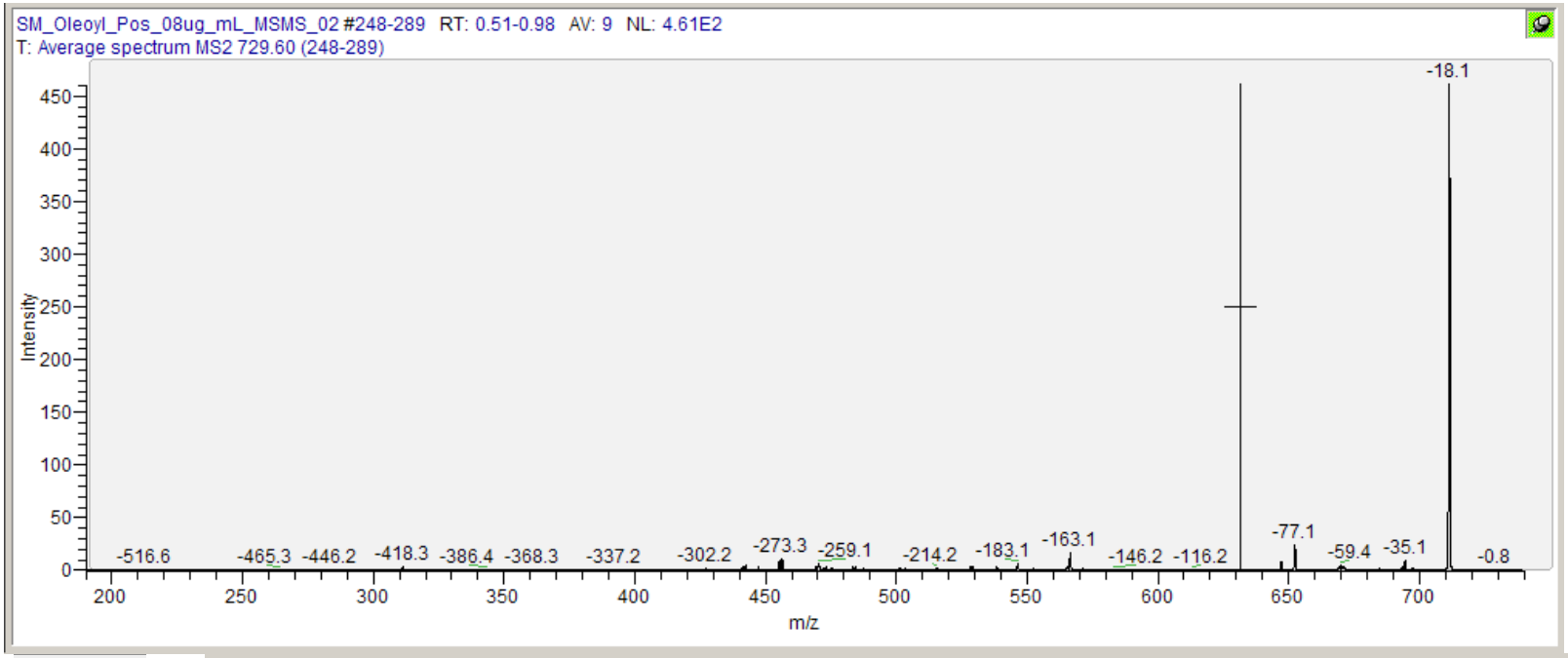


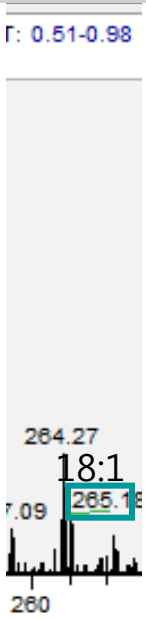
Exact Mass: 729.59

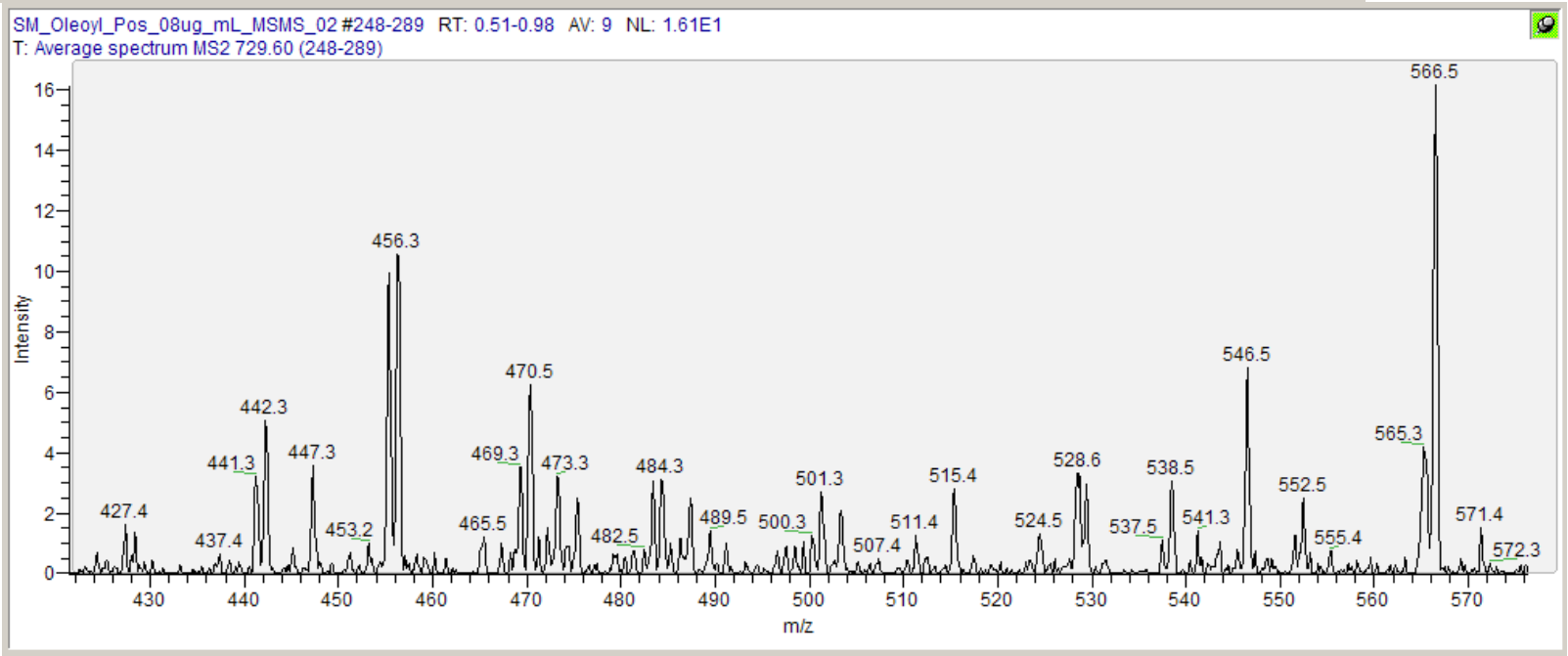


m/z 729.6 (SM 36:1 (18:1))

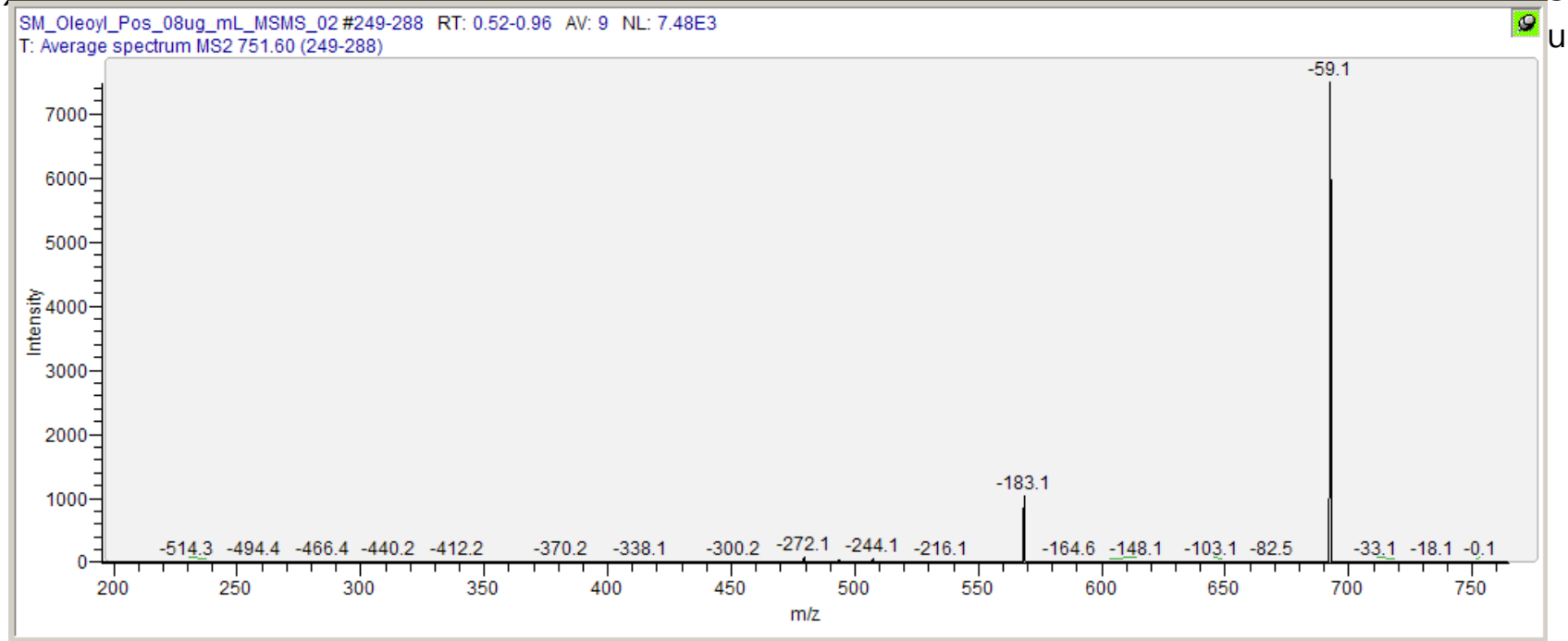
Pos. Mode

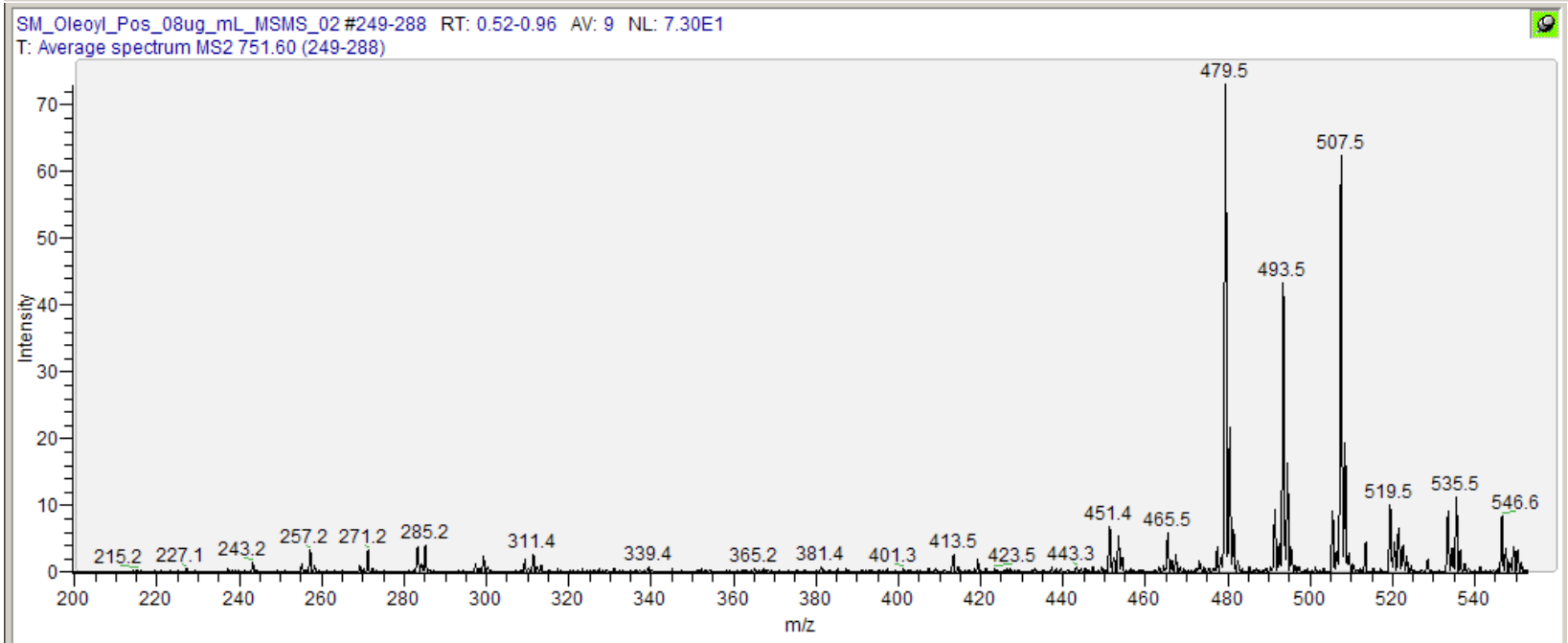






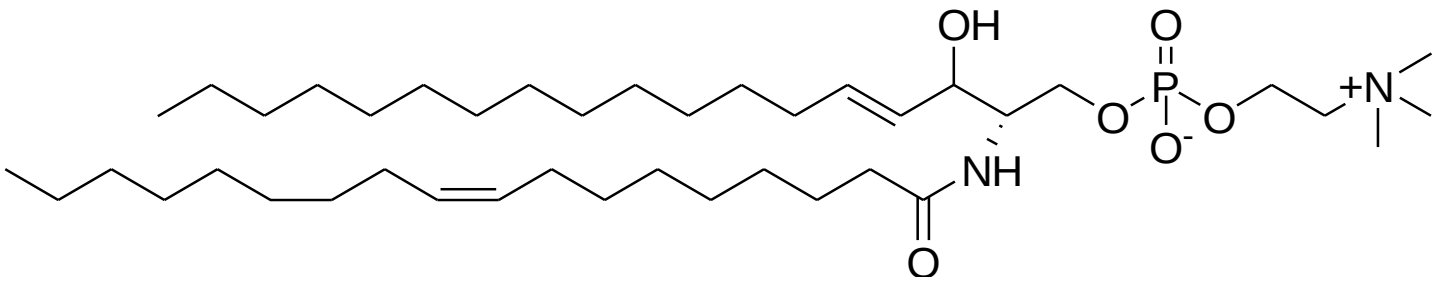
m/z 751.6 (SM 36:1, Sodium Adduct (18:1)) Pos. Mode

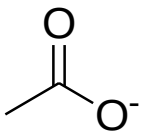




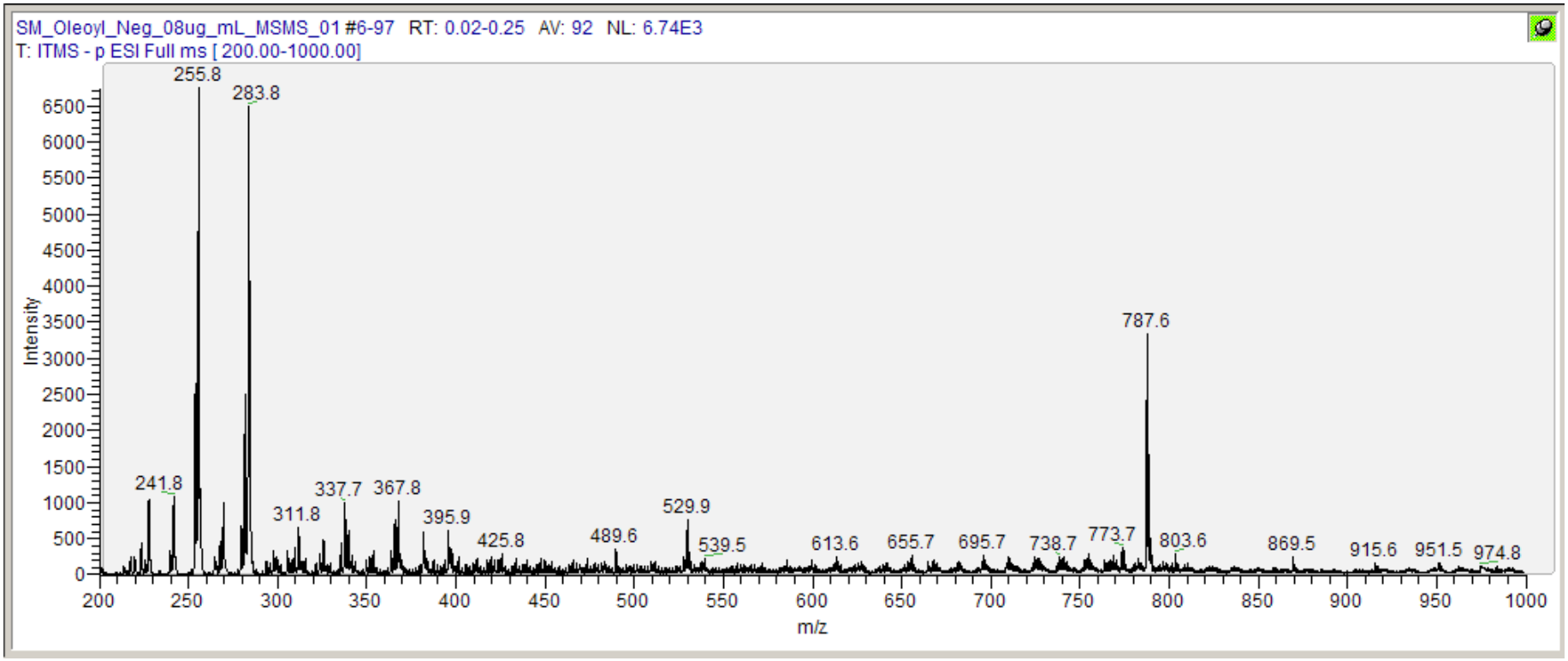
m/z 787.6 (SM 36:1, Acetate Adduct (18:1))

Neg. Mode

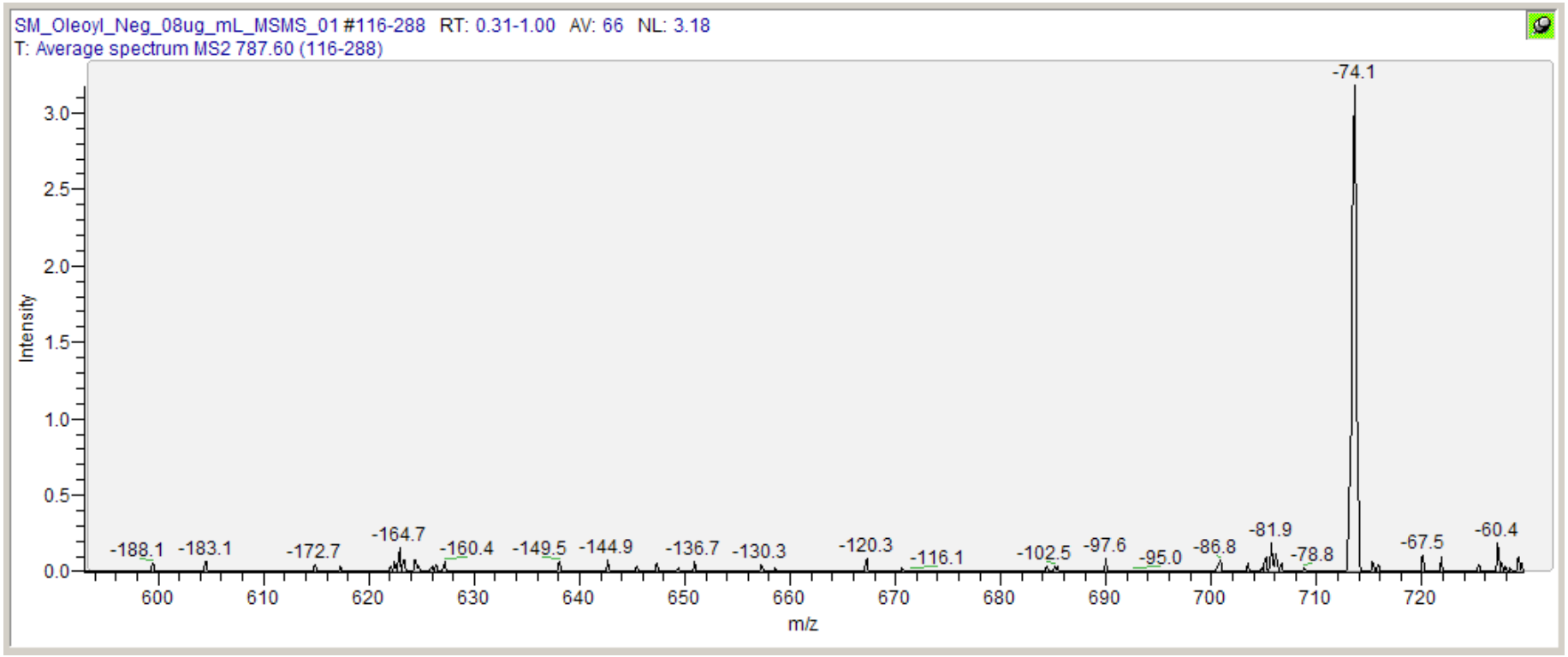




Exact Mass: 787.60



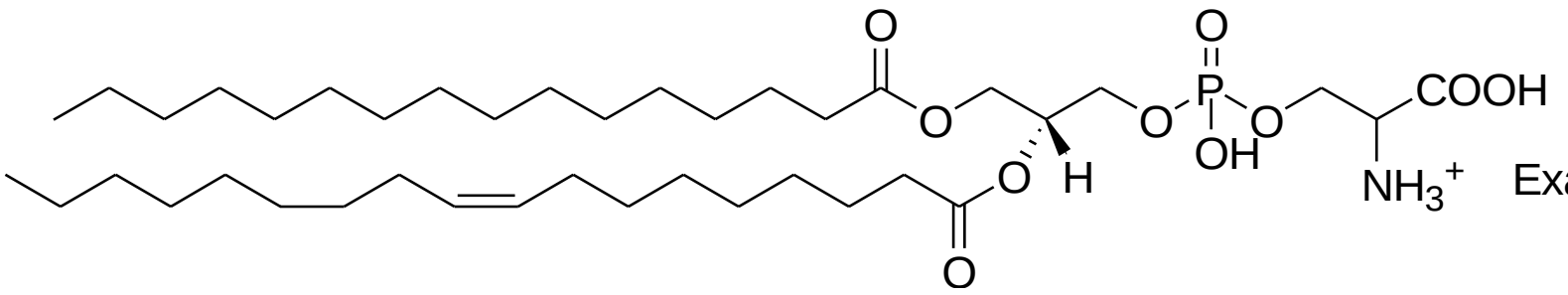
m/z 787.6 (SM 36:1, Acetate Adduct (18:1)) Neg. Mode



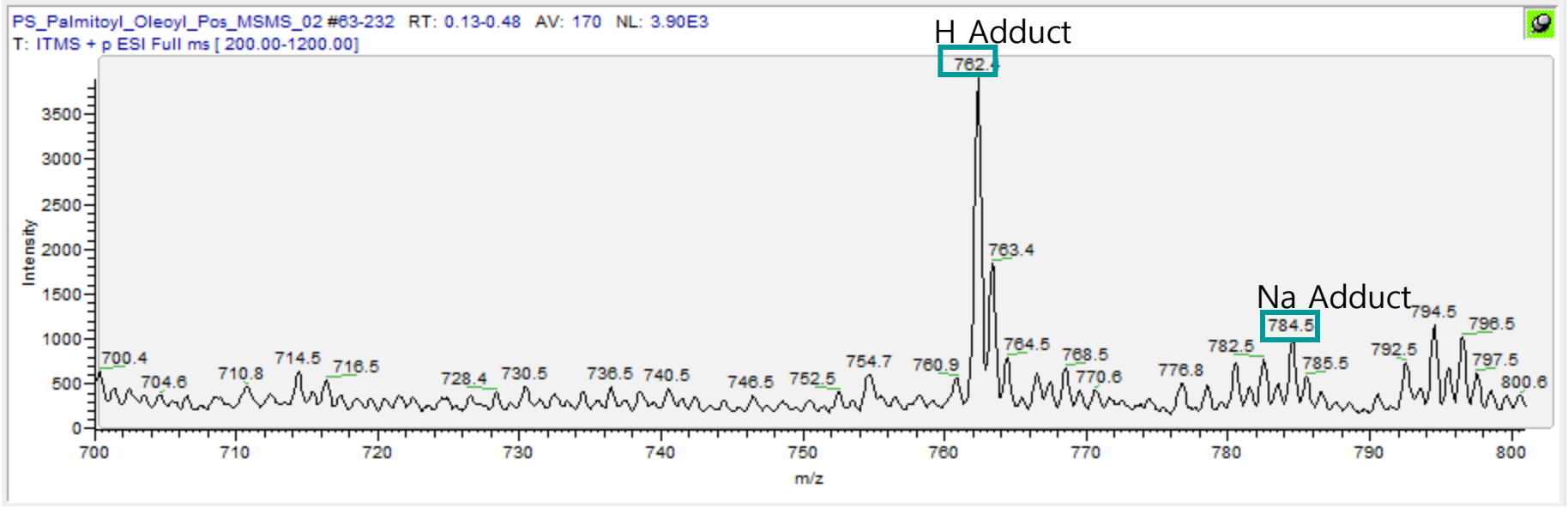
Phosphatidylserine ID

m/z 762.6 (PS 34:1 (16:0, 18:1))

Pos. Mode

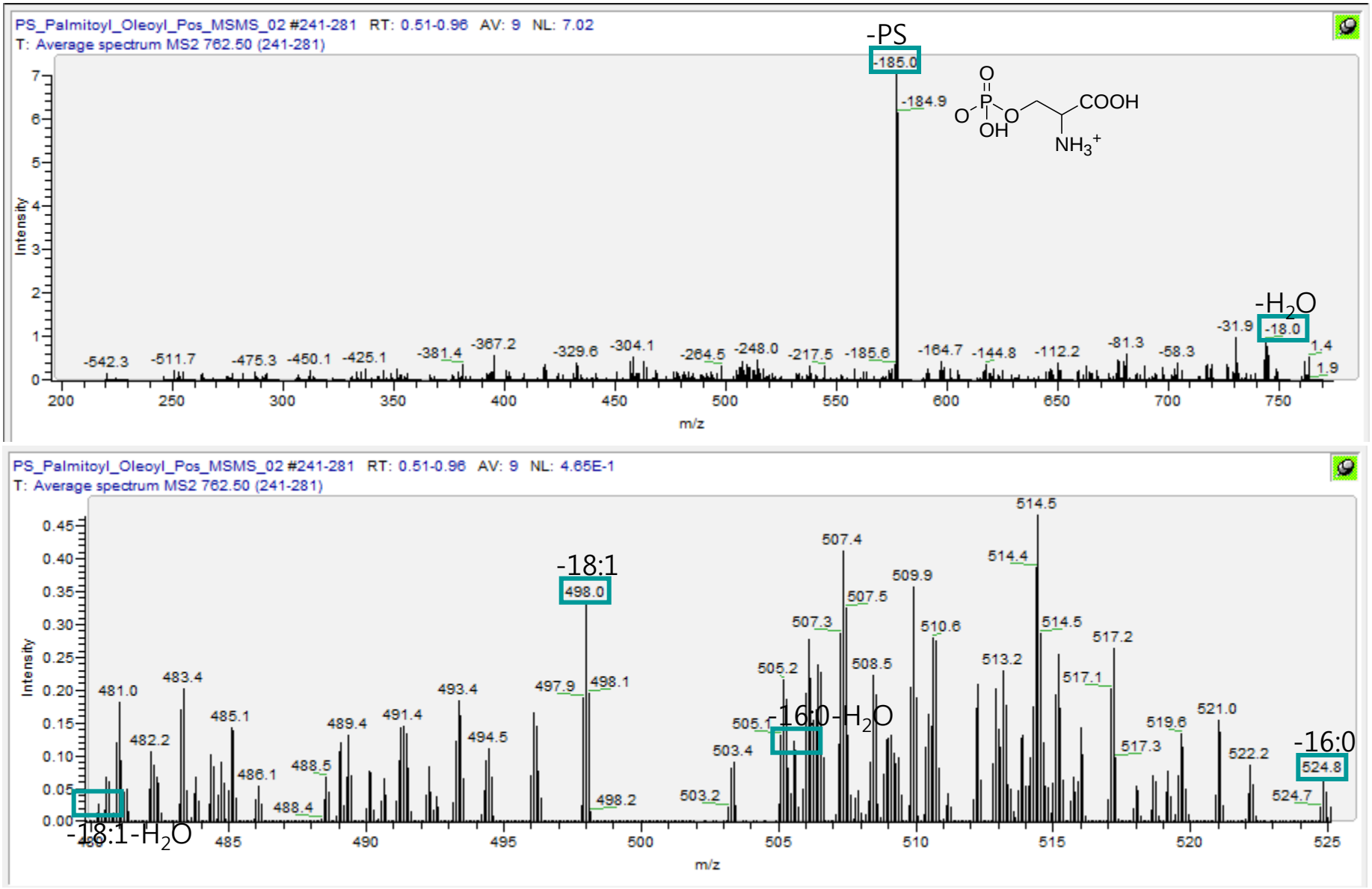


Exact Mass: 762.53

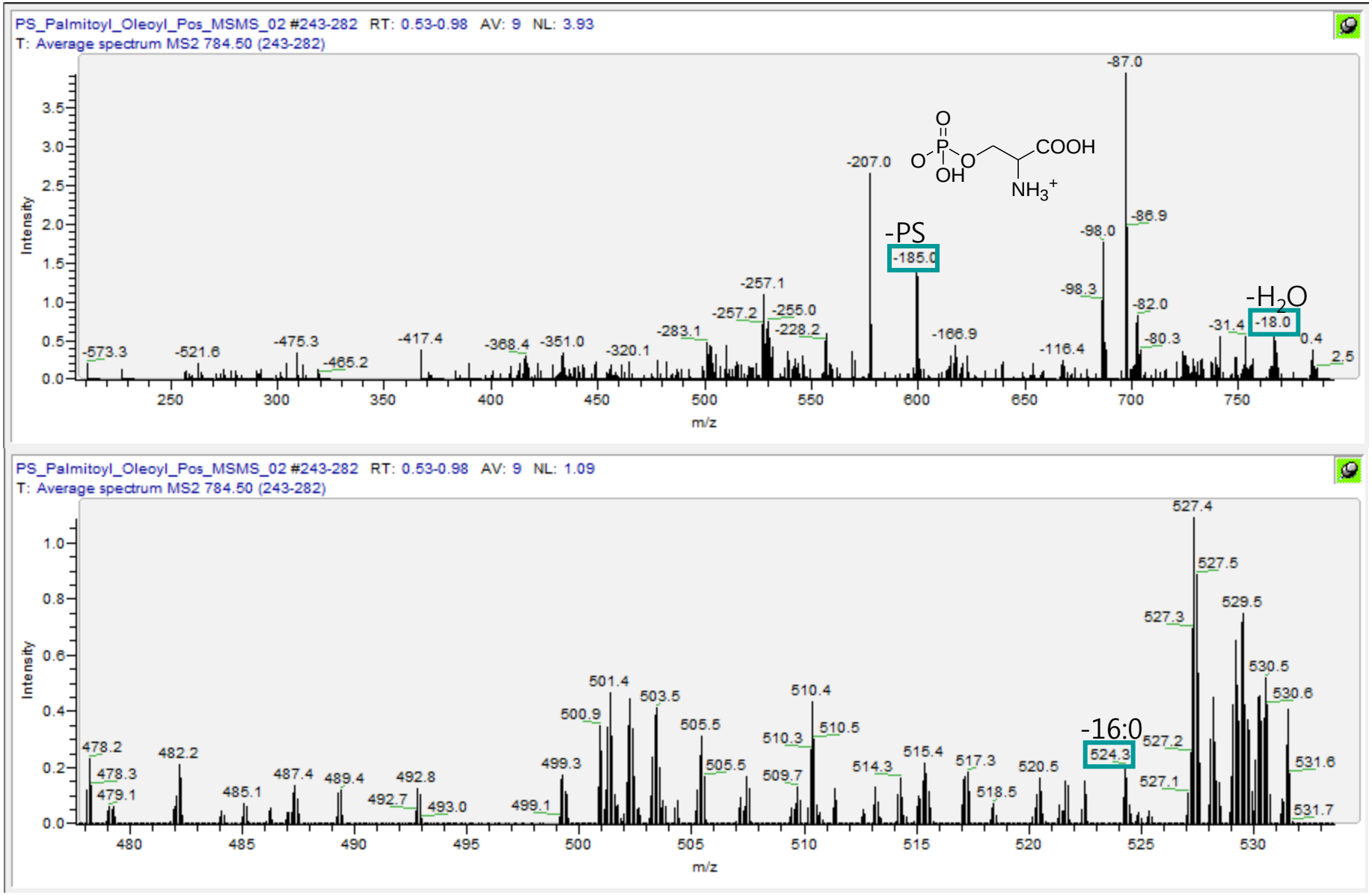


m/z 762.6 (PS 34:1 (16:0, 18:1))

Pos. Mode

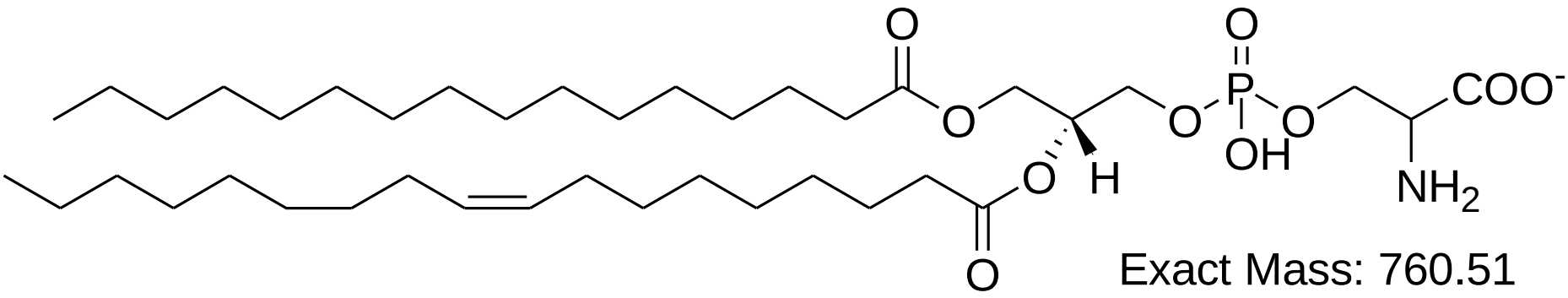


m/z 784.5 (PS 34:1, Sodium Adduct (16:0, 18:1)) Pos. Mode

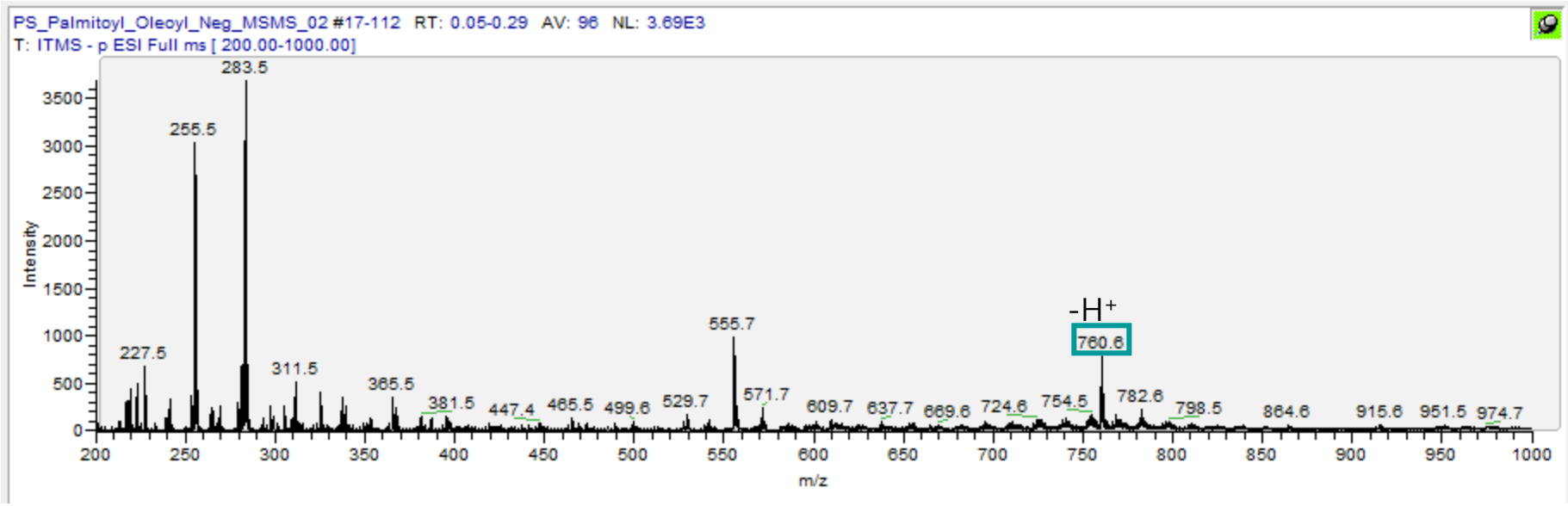


m/z 760.6 (PS 34:1 (16:0, 18:1))

Neg. Mode

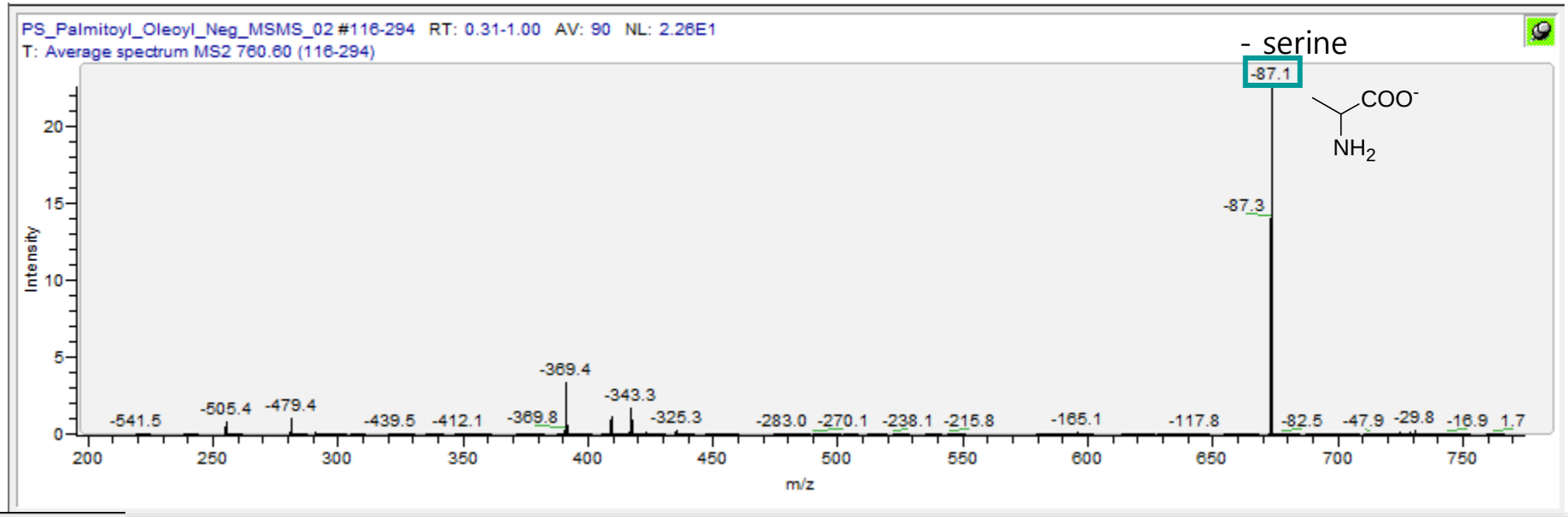


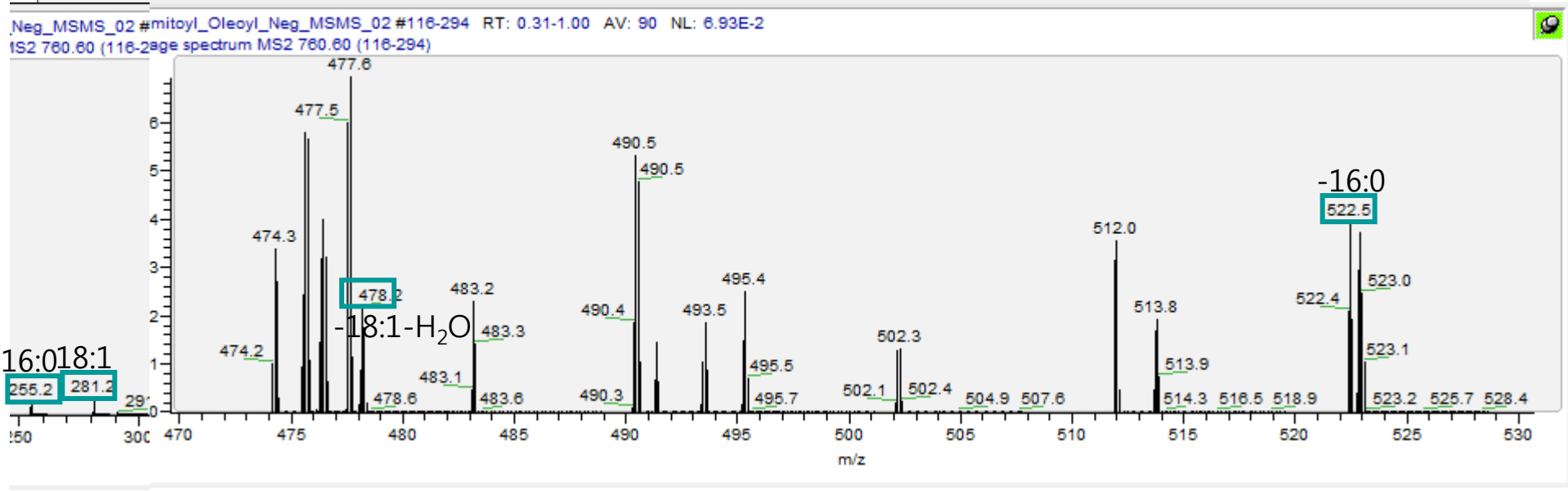
Exact Mass: 760.51



m/z 760.6 (PS 34:1 (16:0, 18:1))

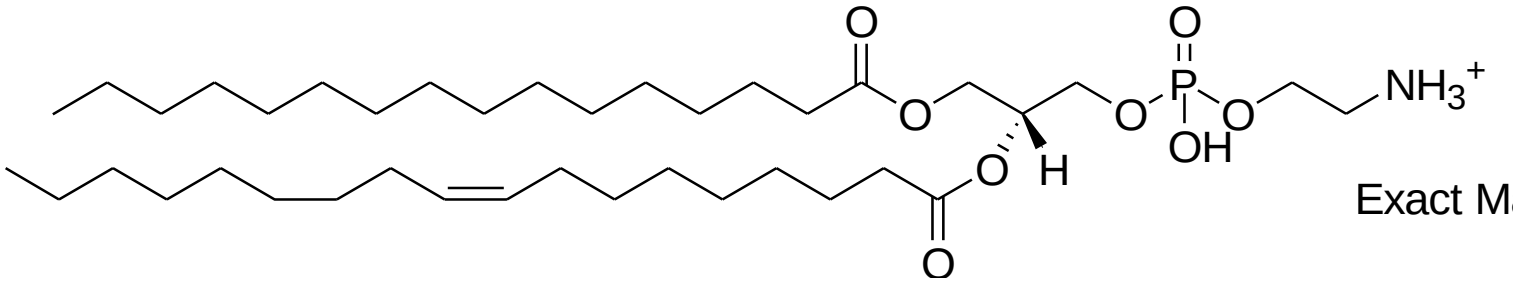
Neg. Mode



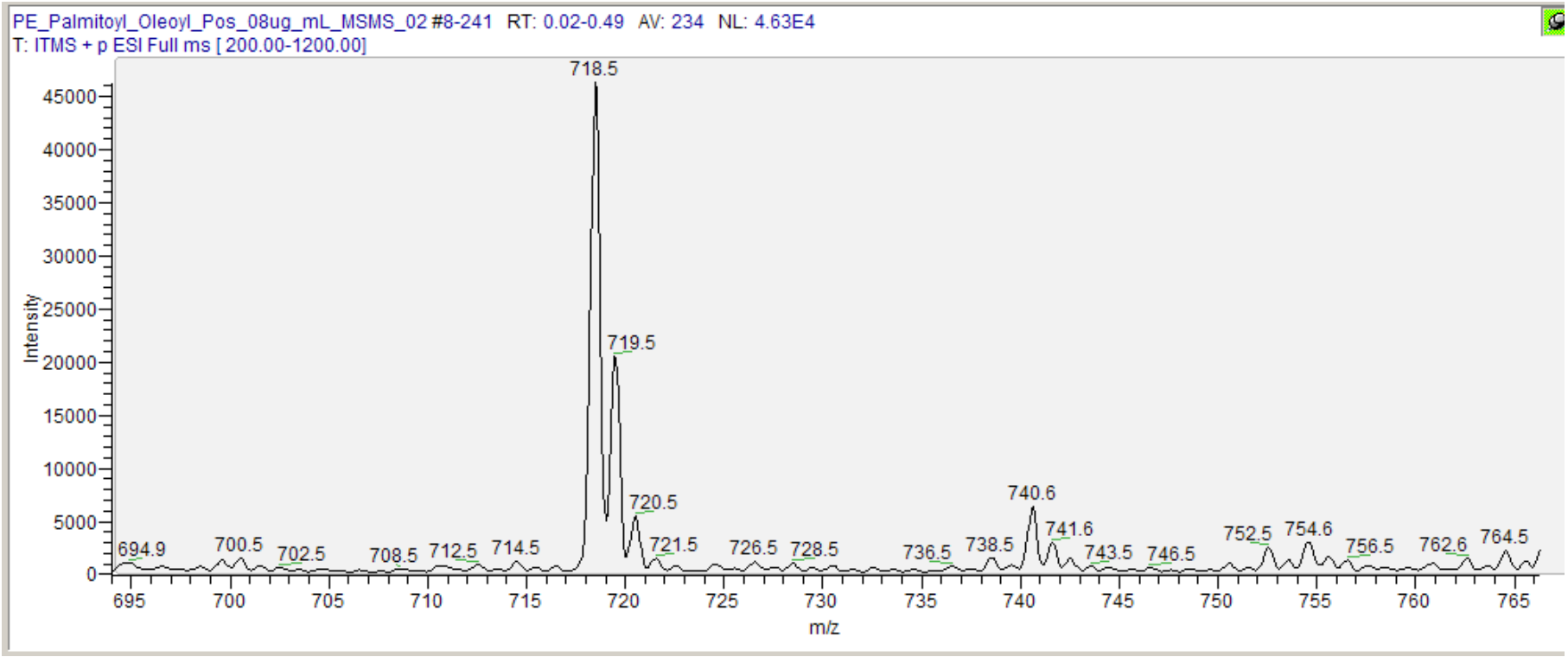


Phosphatidylethanolamine ID

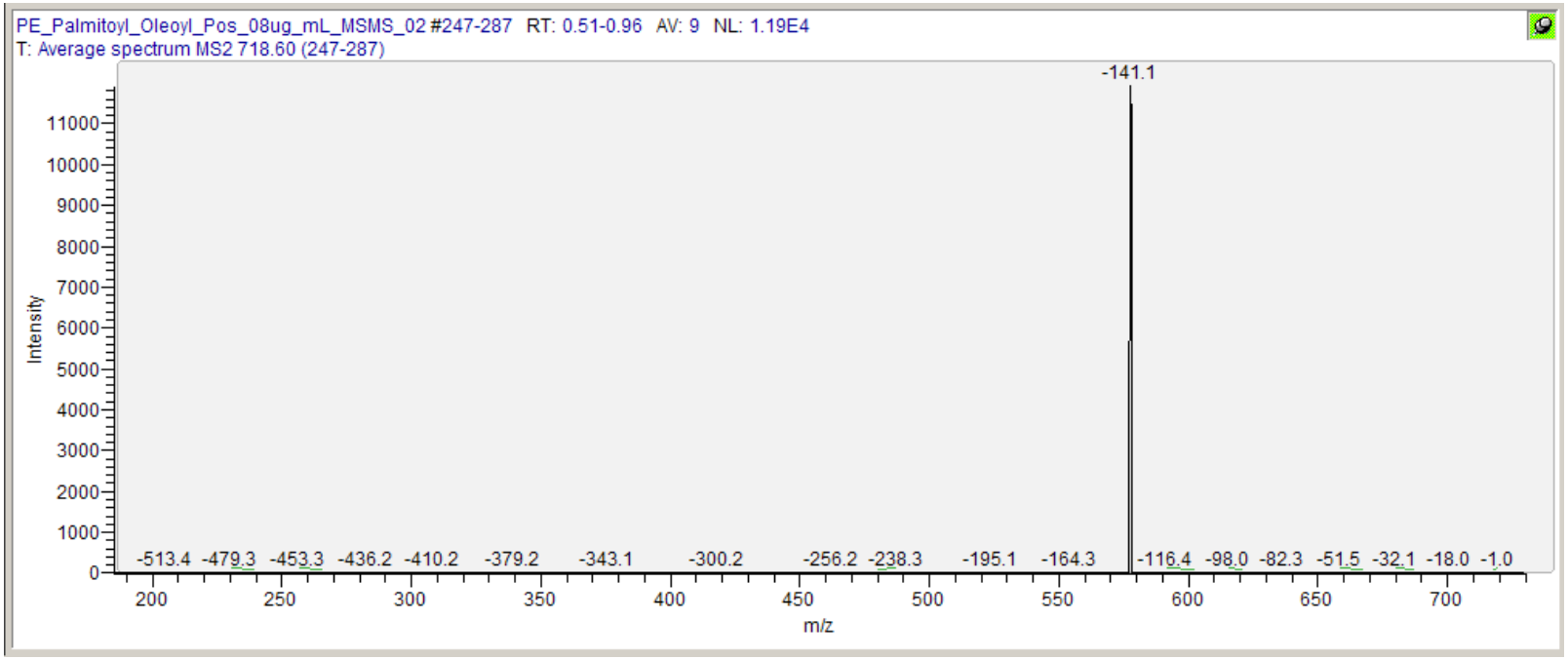
m/z 718.6 (PE 34:1 (16:0, 18:1))

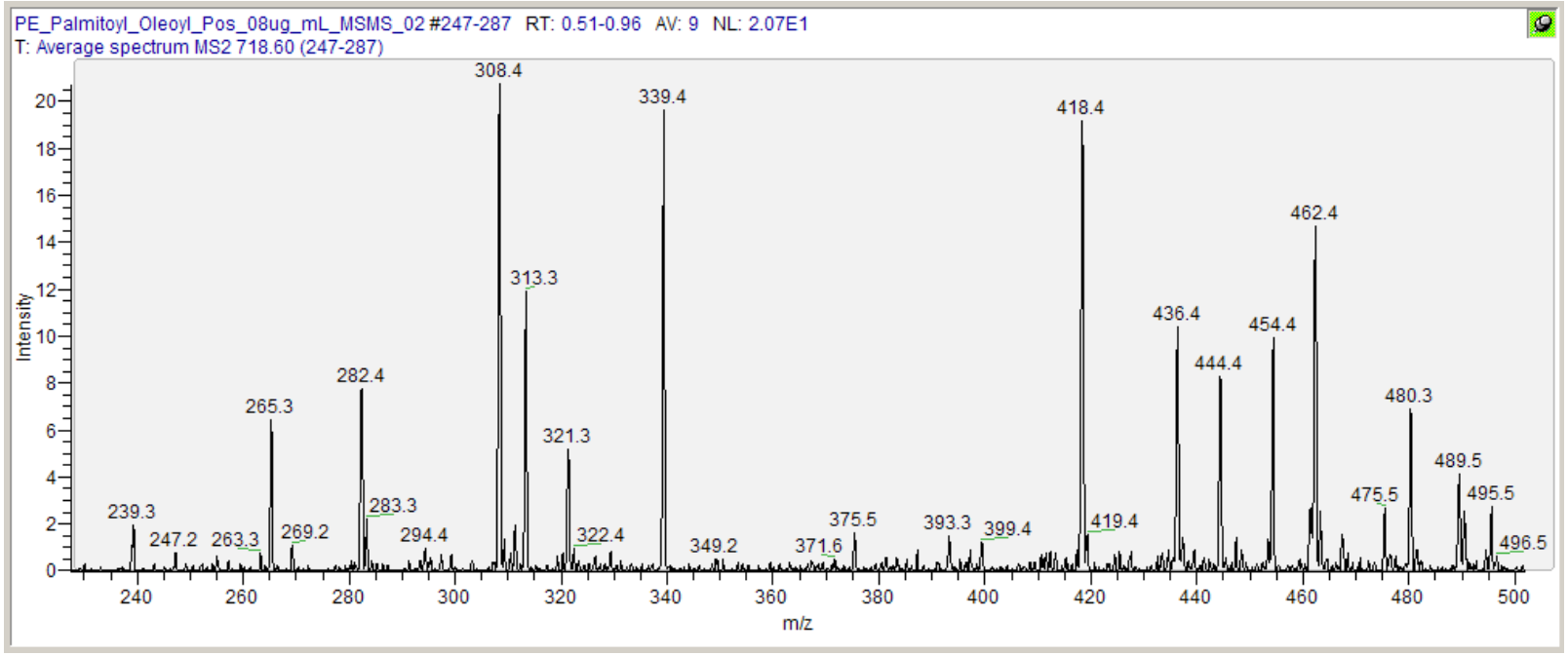


Exact Mass: 718.54

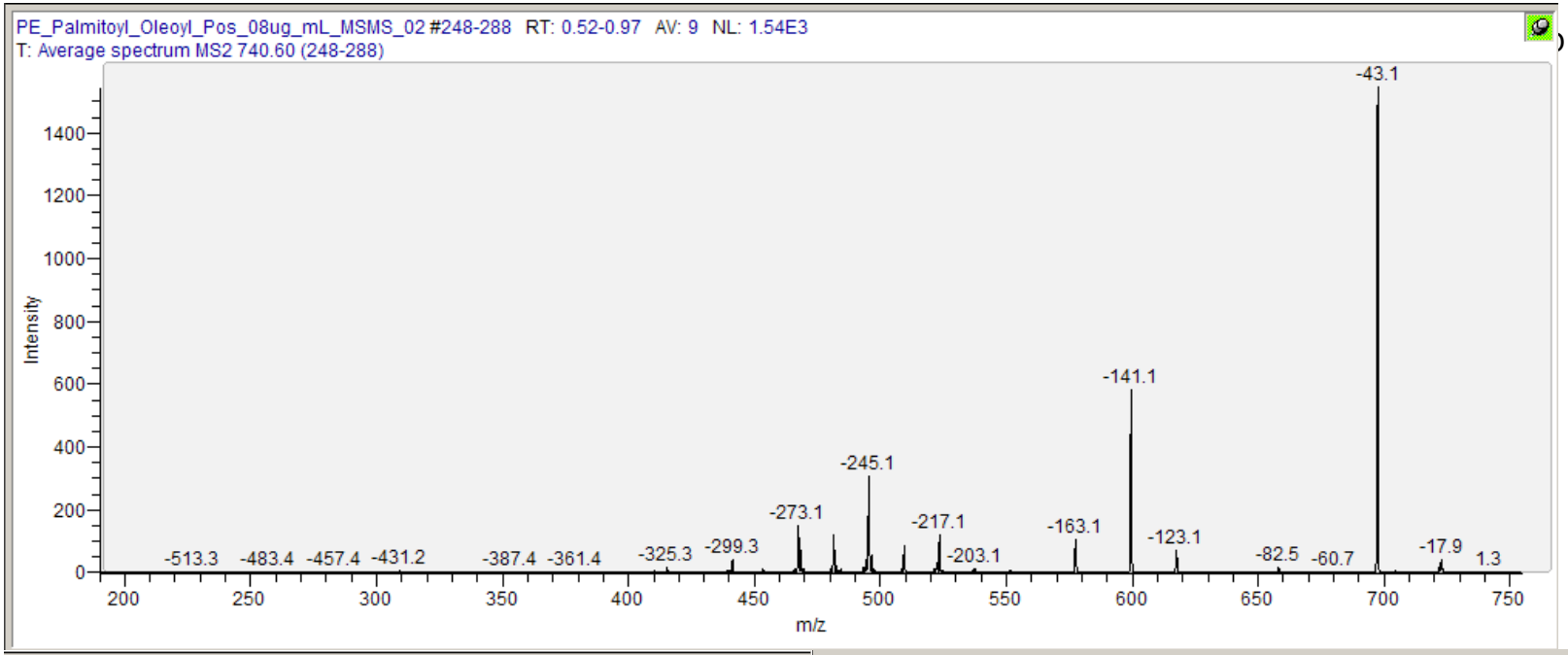


m/z 718.6 (PE 34:1 (16:0, 18:1))

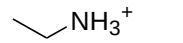


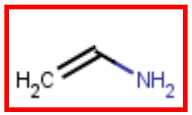


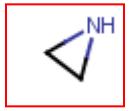
m/z 740.6 (PE 34:1, sodium adduct (16:0, 18:1))

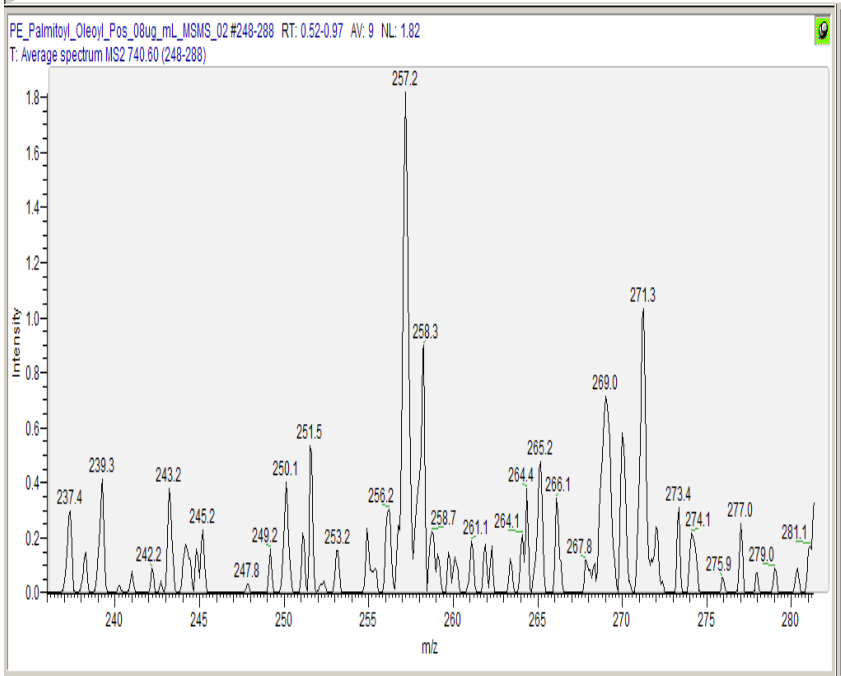


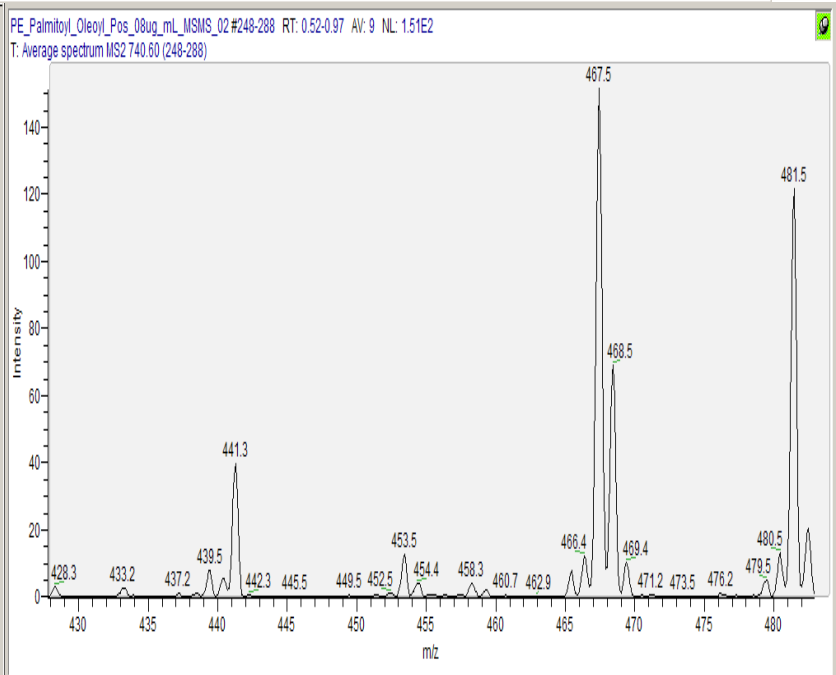
onium ion





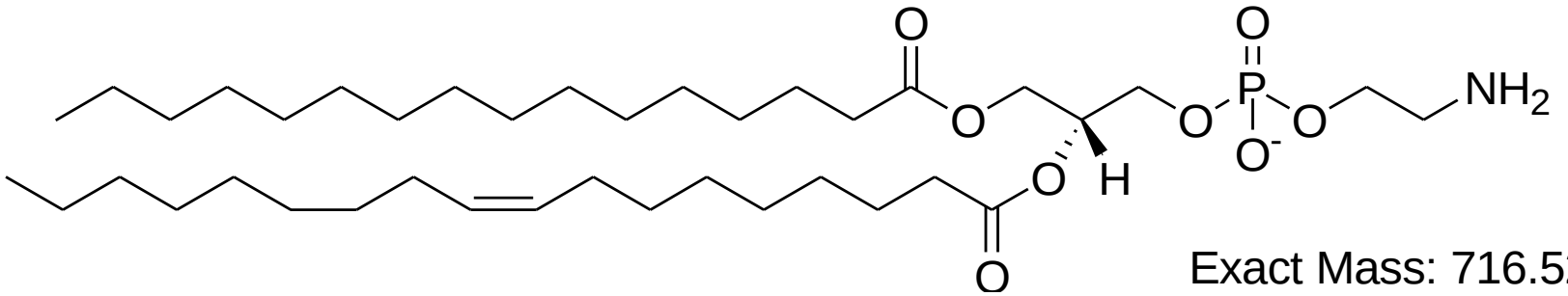




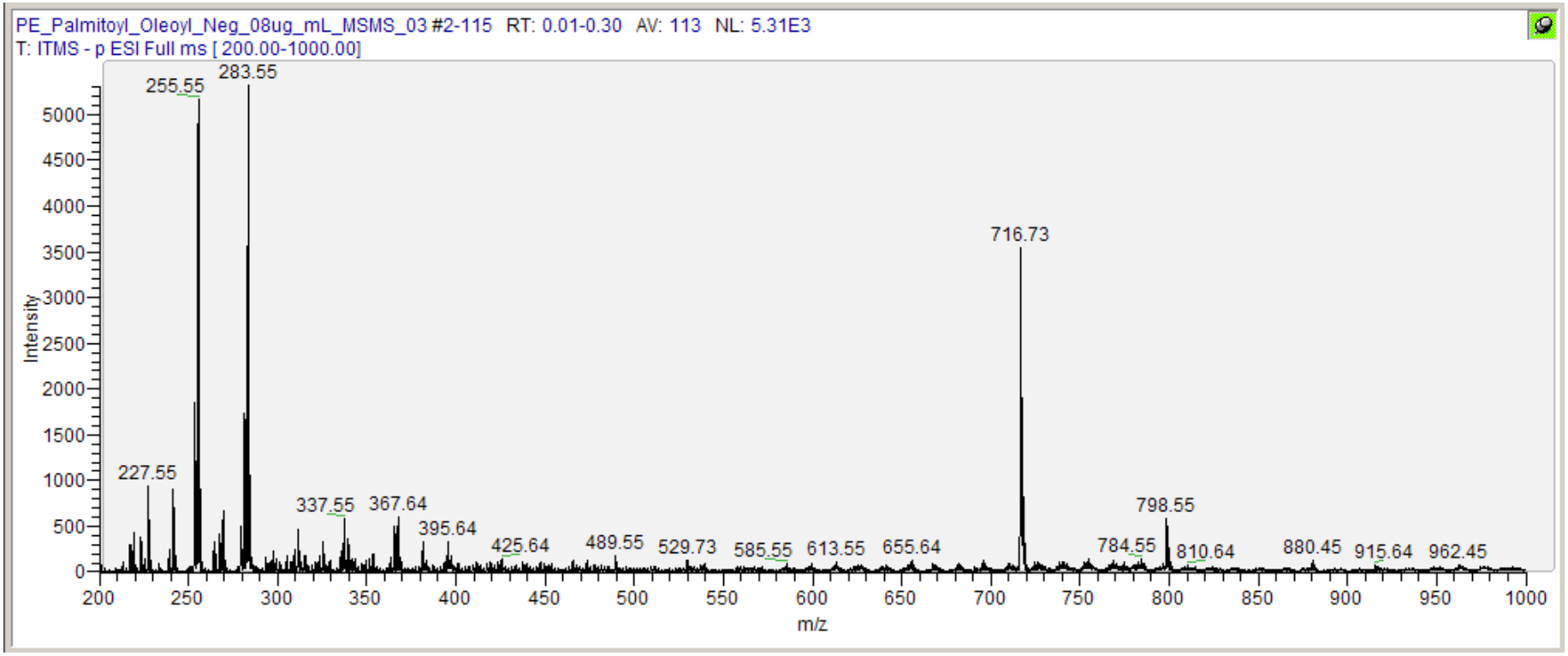


m/z 716.7 (PE 34:1 (16:0, 18:1))

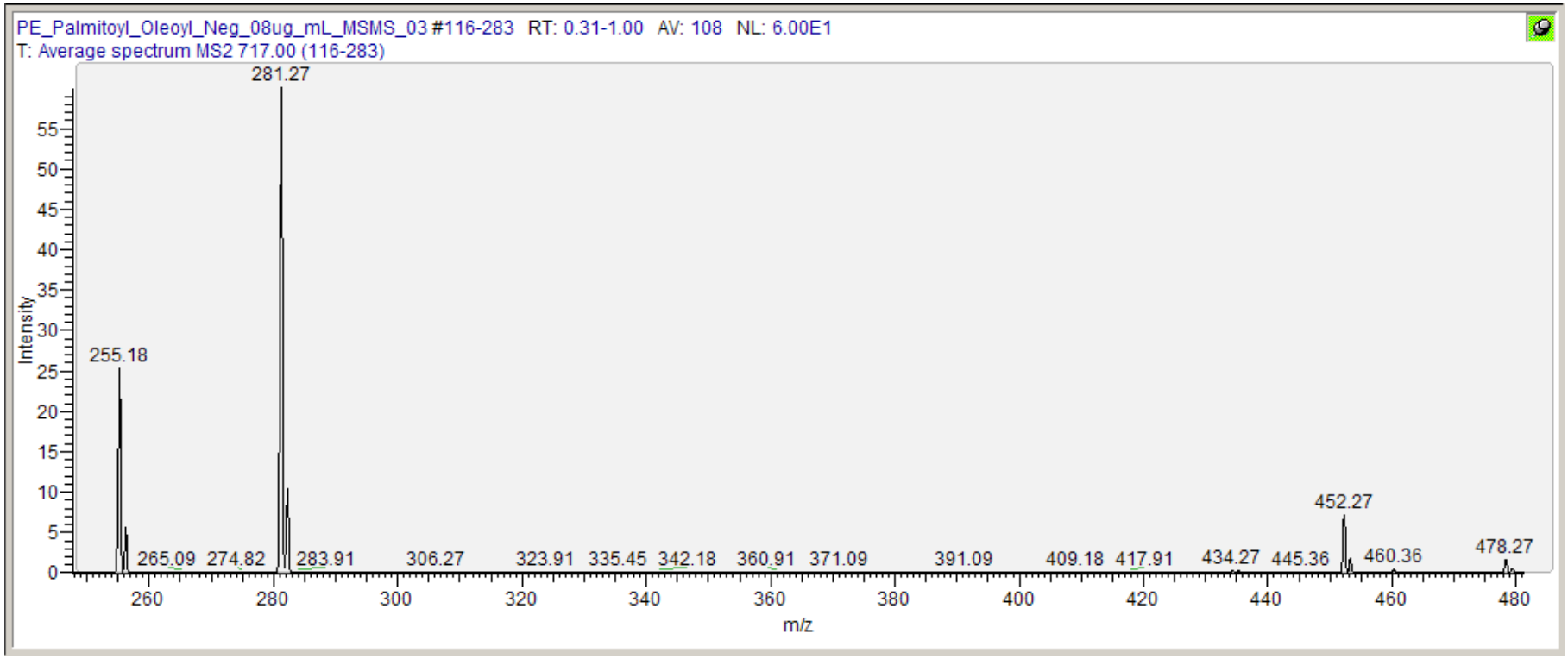
Neg. Mode



Exact Mass: 716.52



m/z 716.7 (PE 34:1 (16:0, 18:1)) Neg. Mode

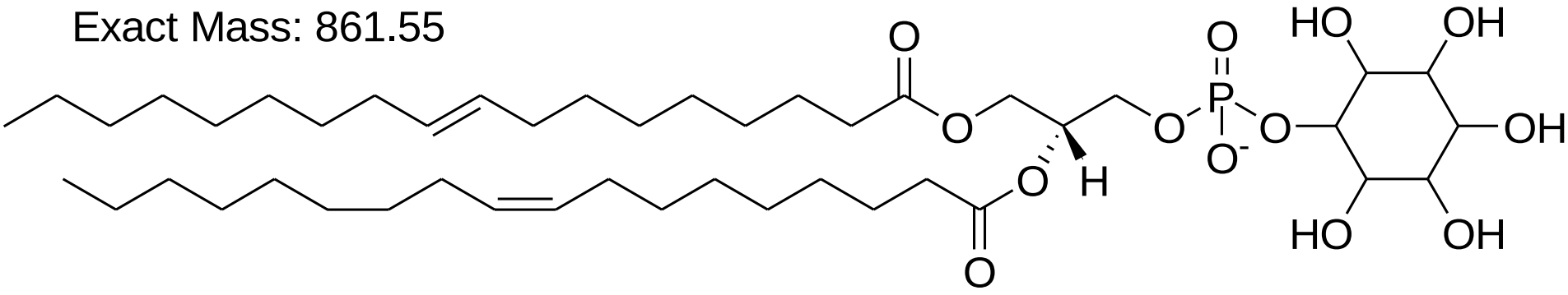


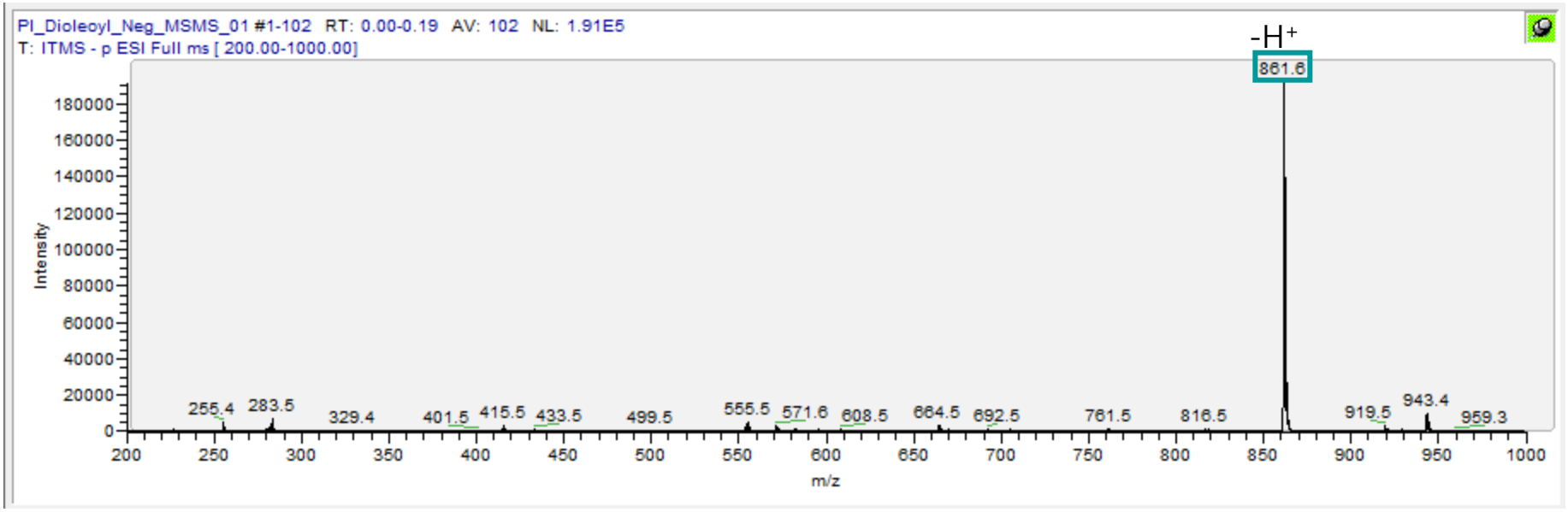
Phosphatidylinositol ID

m/z 861.6 (PI 36:1 (18:1, 18:1))

Neg. Mode

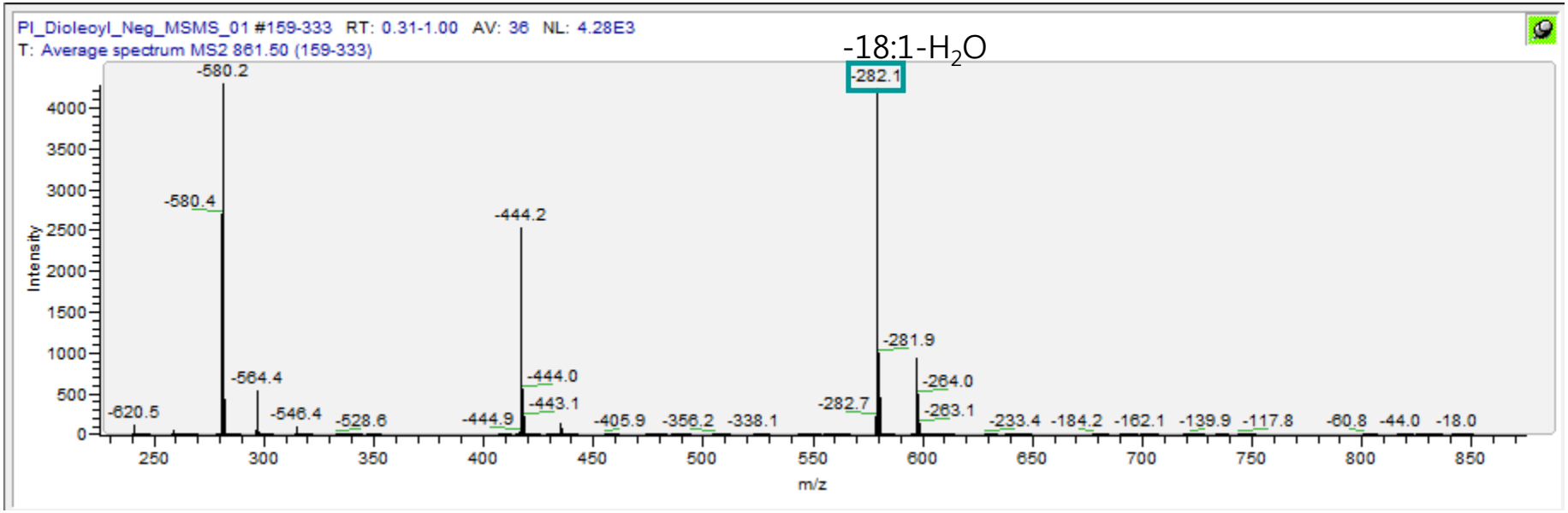
Exact Mass: 861.55

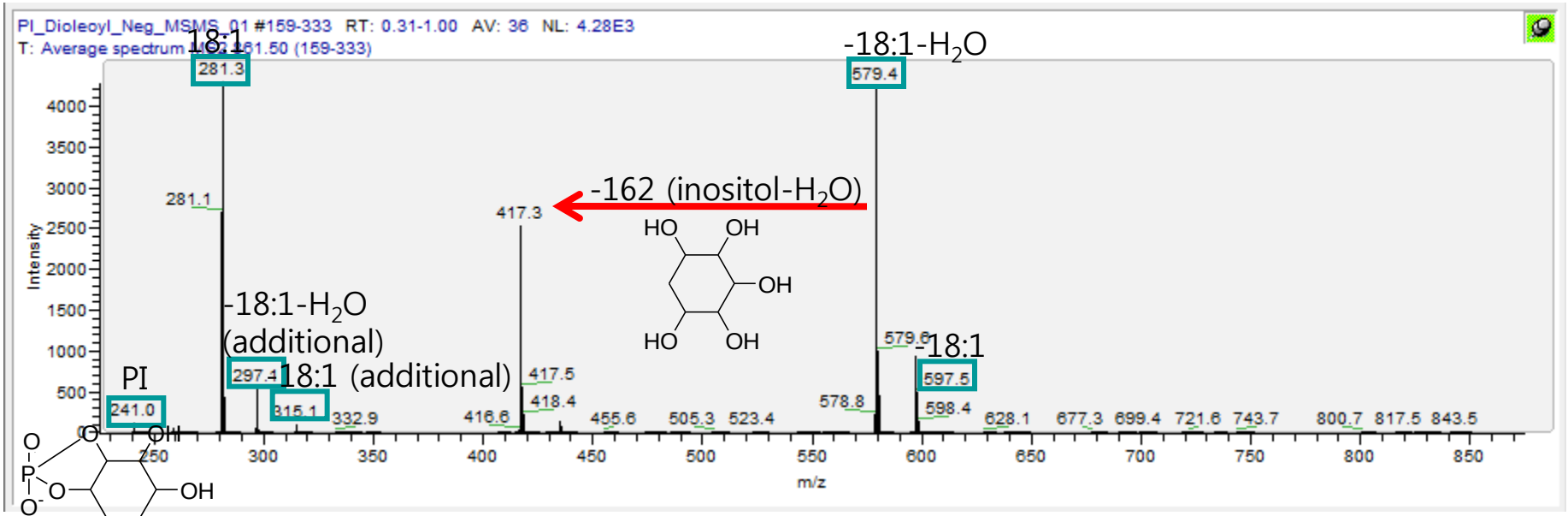




m/z 861.6 (PI 36:2 (18:1, 18:1))

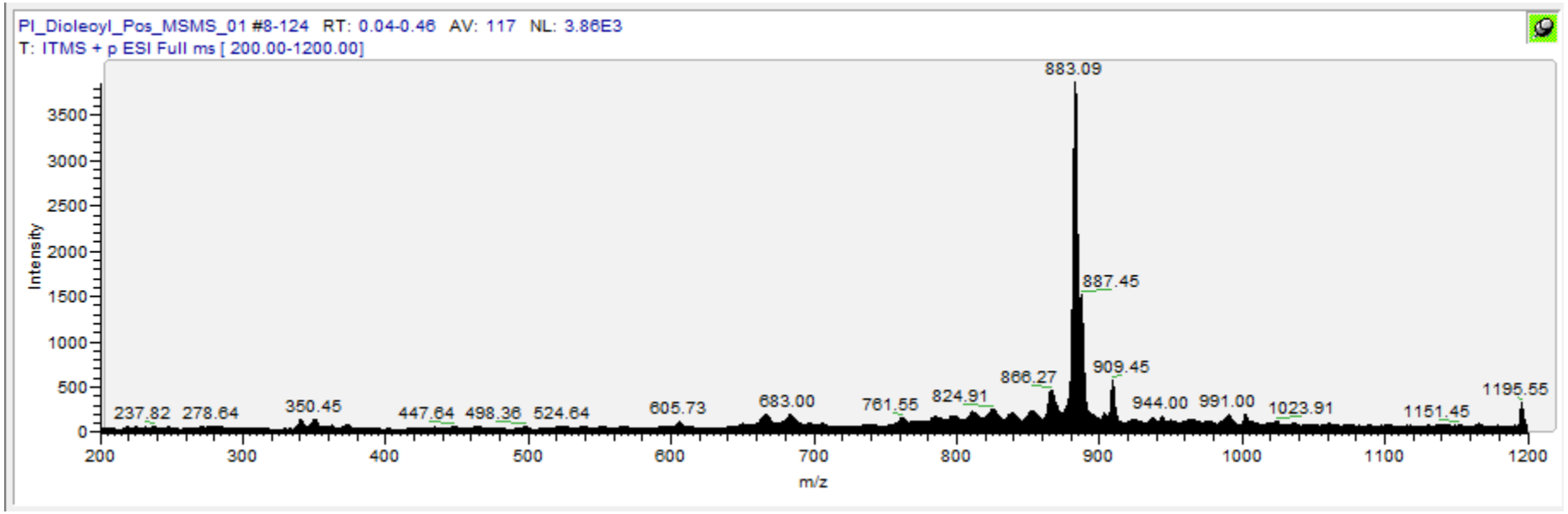
Neg. Mode





Exact Mass: 241.01

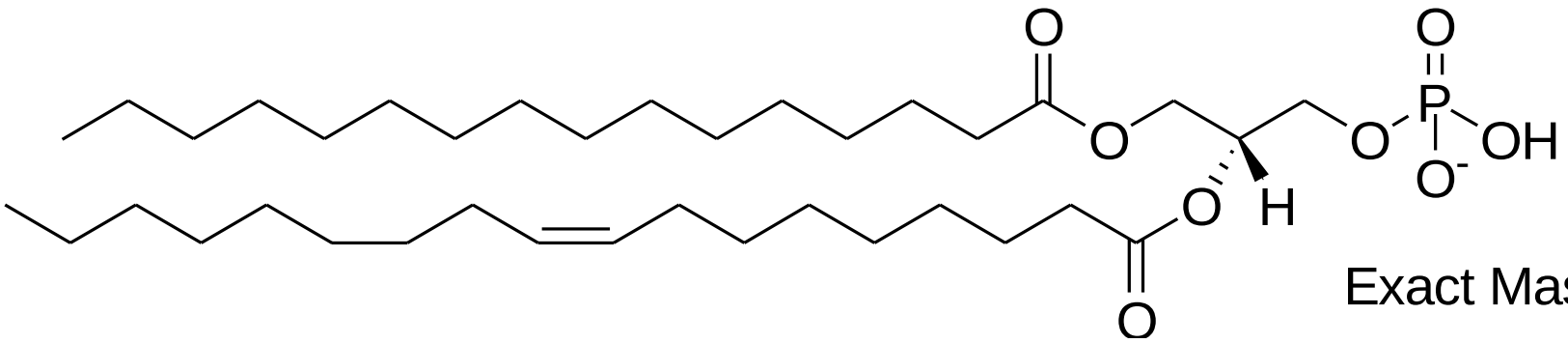
m/z 883.1 ?? (PI 36:1 (18:1, 18:1)) Pos. Mode



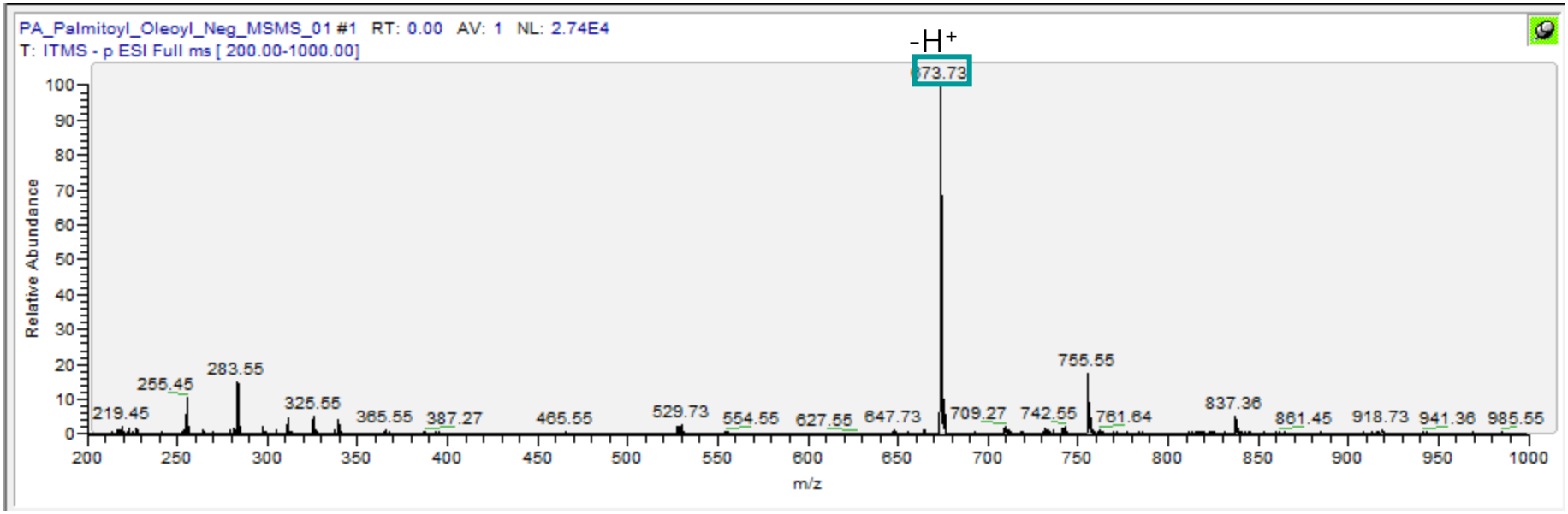
Phosphatidic acid ID

m/z 673.7 (PA 34:1 (16:0, 18:1))

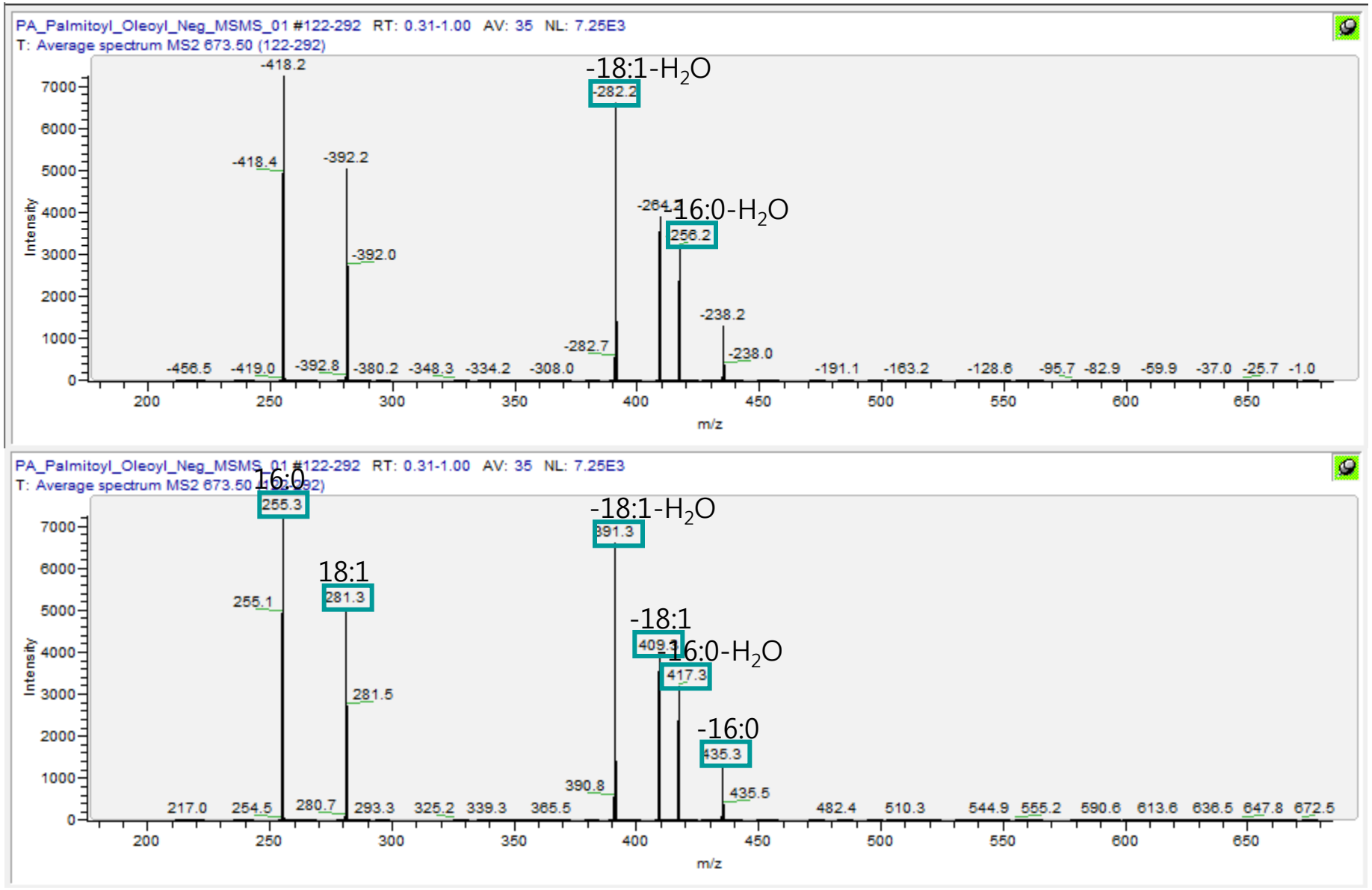
Neg. Mode



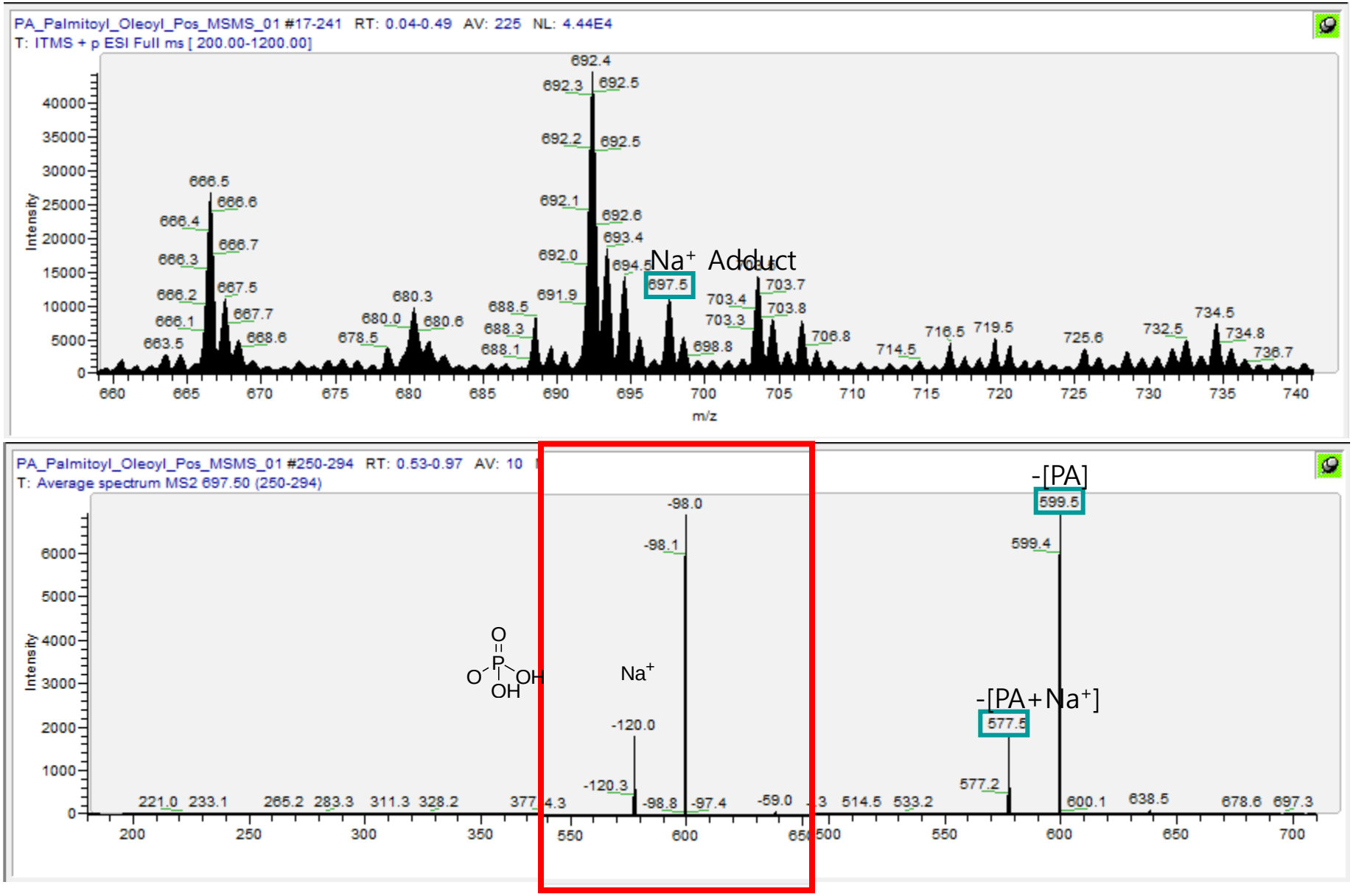
Exact Mass: 673.48



m/z 673.7 (PA 34:1 (16:0, 18:1)) Neg. Mode



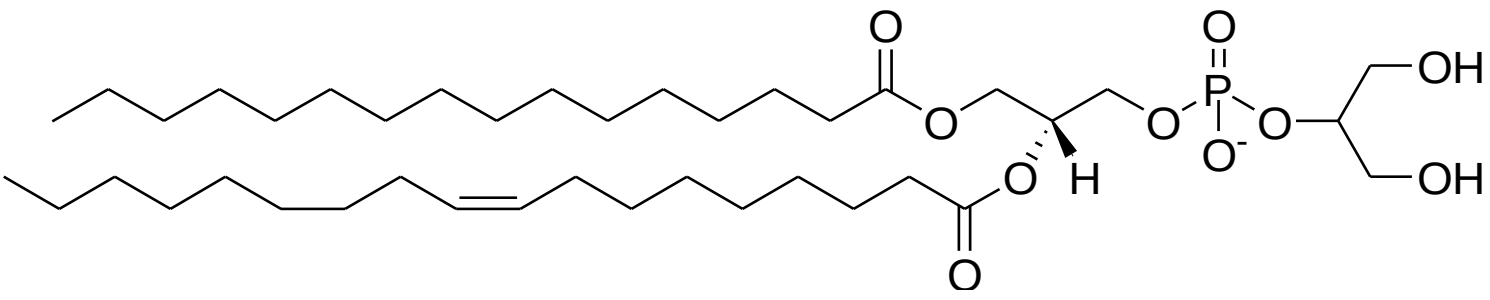
m/z 697.5 (PA 34:1, Sodium Adduct (16:0, 18:1)) Pos. Mode



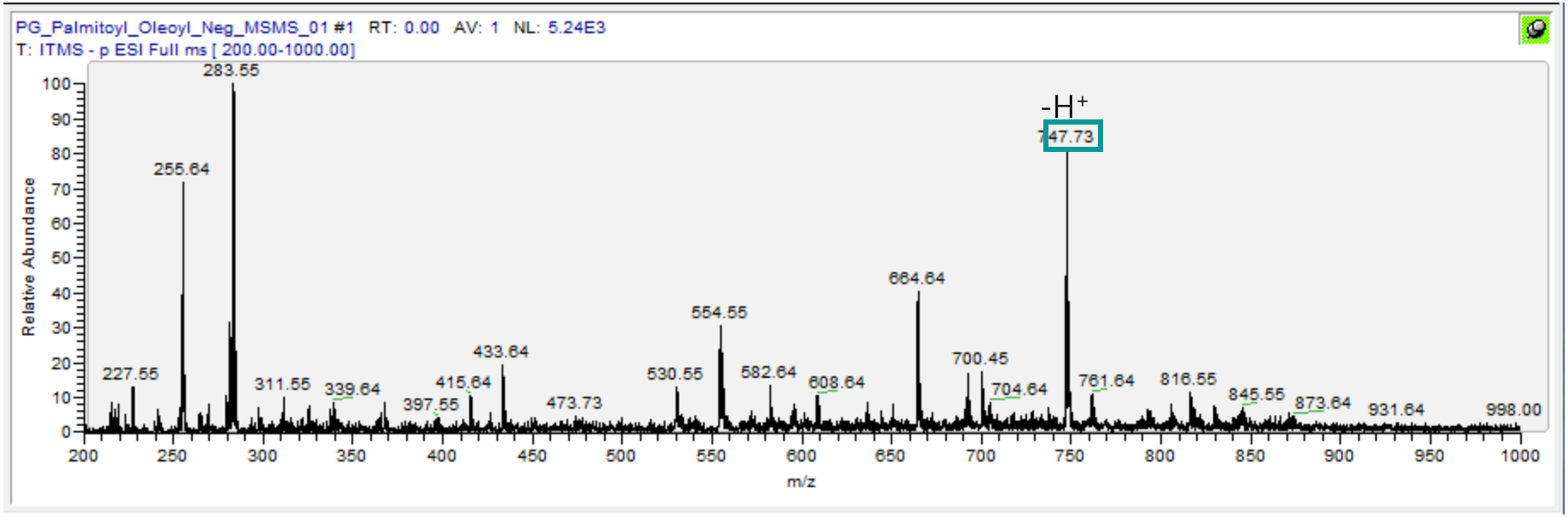
PhosphatidylIglycerol ID

m/z 747.7 (PG 34:1 (16:0, 18:1))

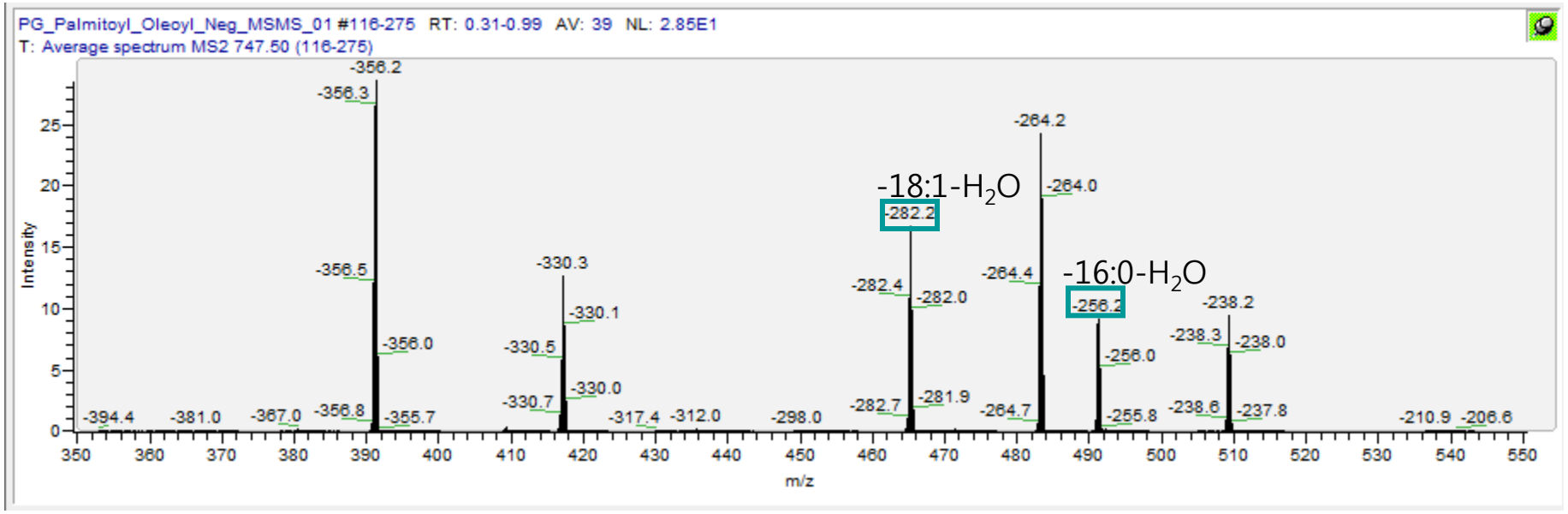
Neg. Mode

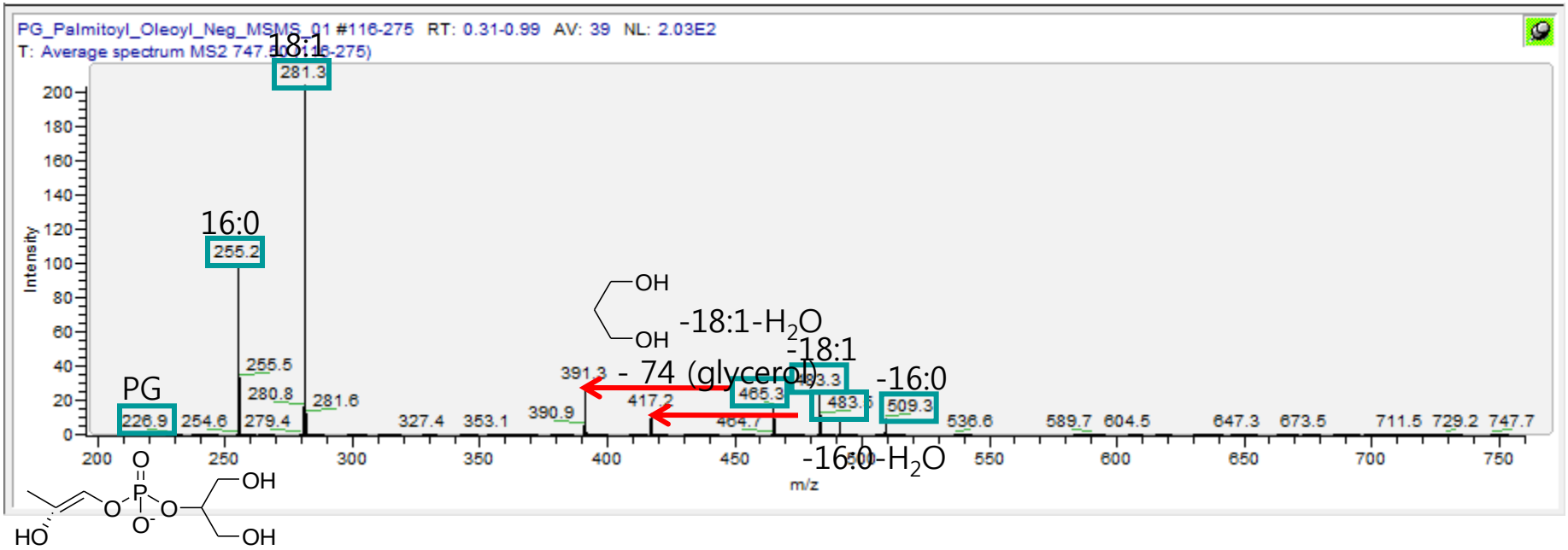


Exact Mass: 747.52



m/z 747.7 (PG 34:1 (16:0, 18:1)) Neg. Mode

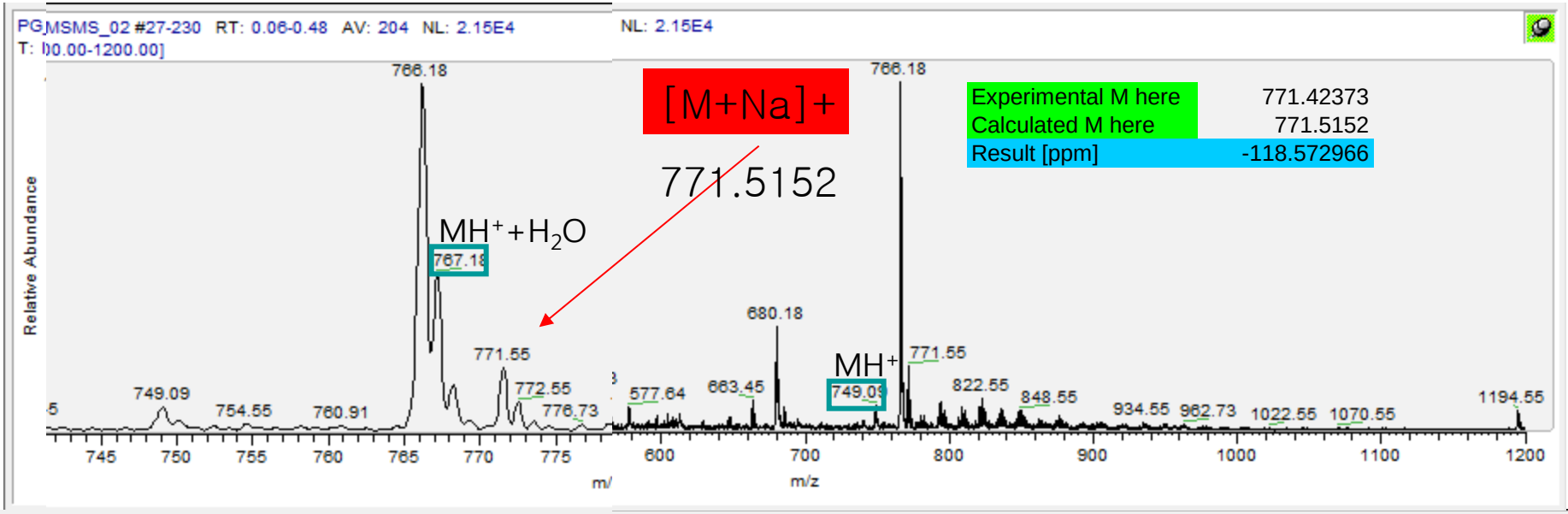


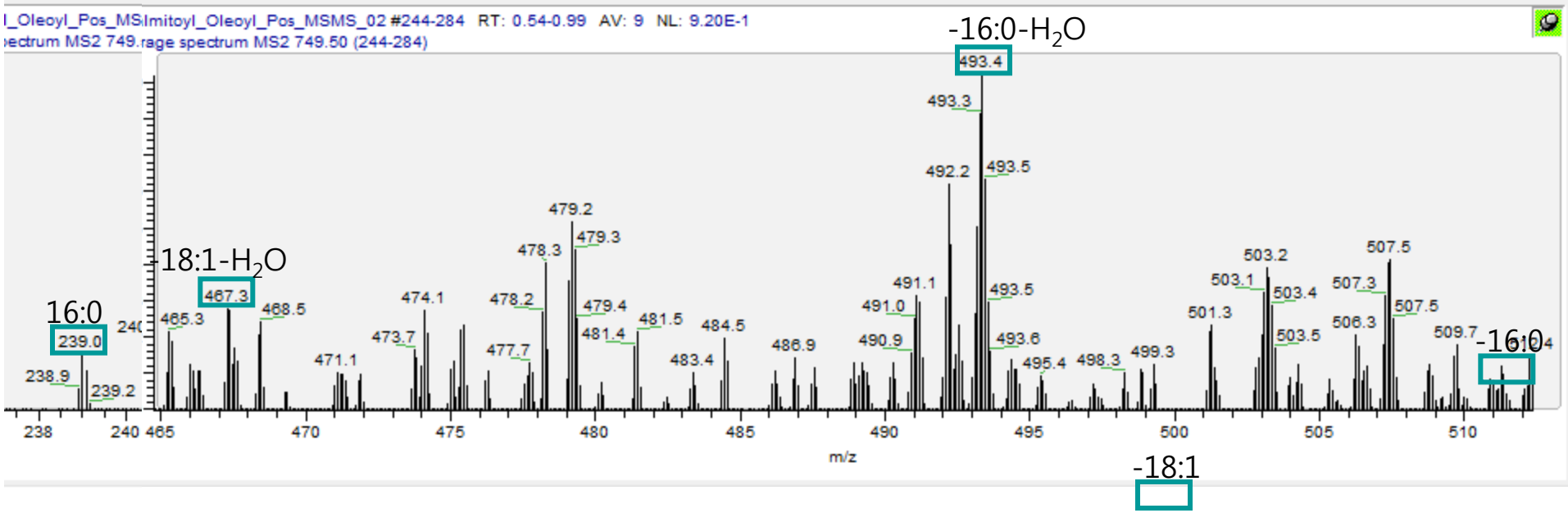


Exact Mass: 227.03

m/z 749.7 (PG 34:1 (16:0, 18:1)) M+H

Pos. Mode

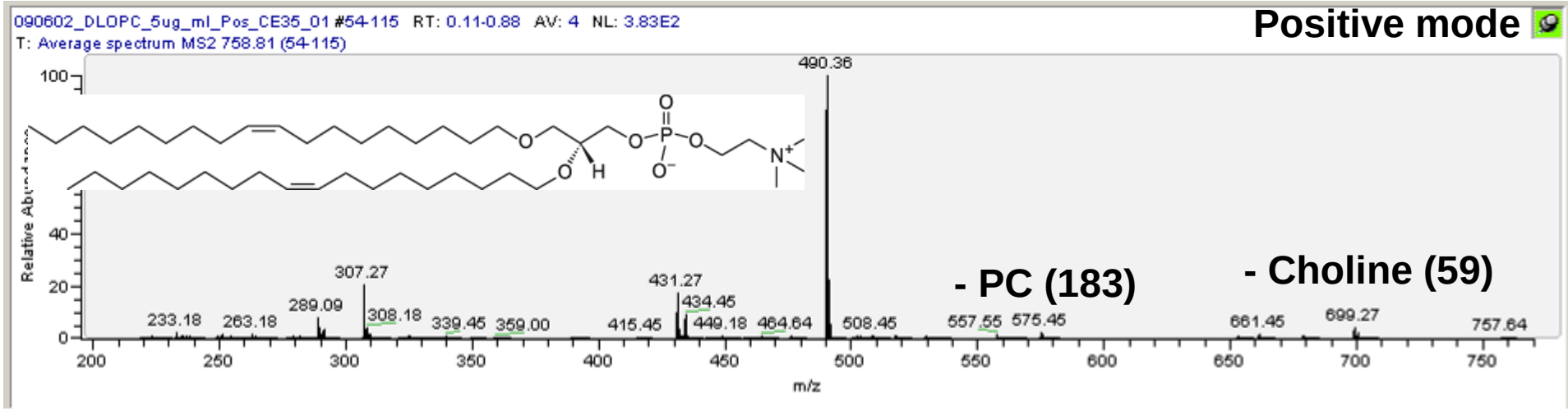




Phospholipids ID Collection B

Dr. KH LIU
UC Davis Metabolomics
LipidBlast

DLOPC (18:1, 18:1, diether form, *m/z* 758.8 [M+H]+)



Exact Mass: 758.6

18:1 Diether PC (1,2-di-O-(9Z-octadecenyl)-sn-glycero-3-phosphocholine)

Exact Mass: 508.4

Exact Mass: 490.4

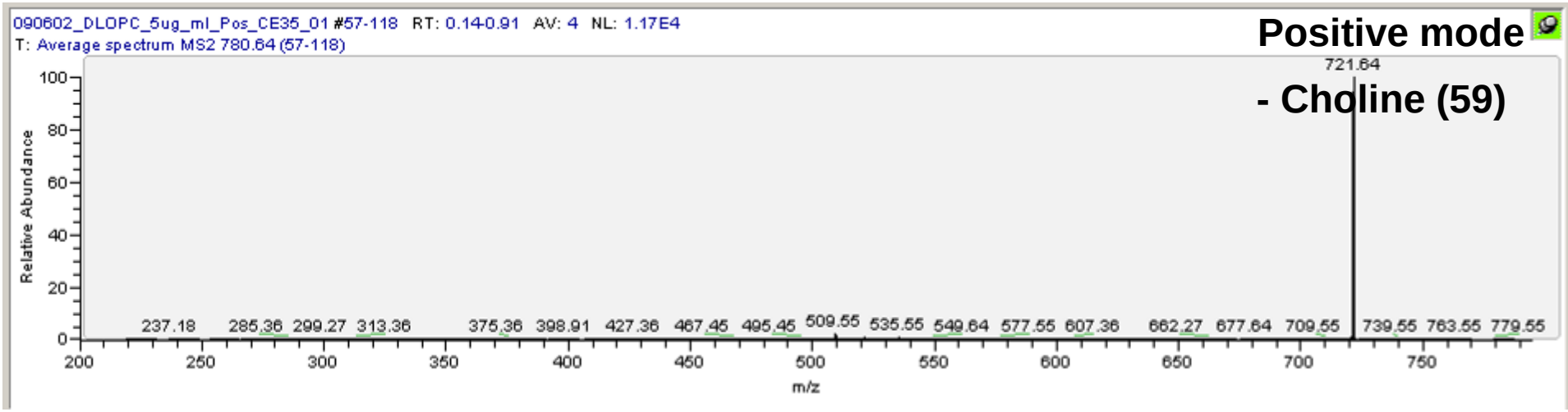
Exact Mass: 431.3

Exact Mass: 307.3

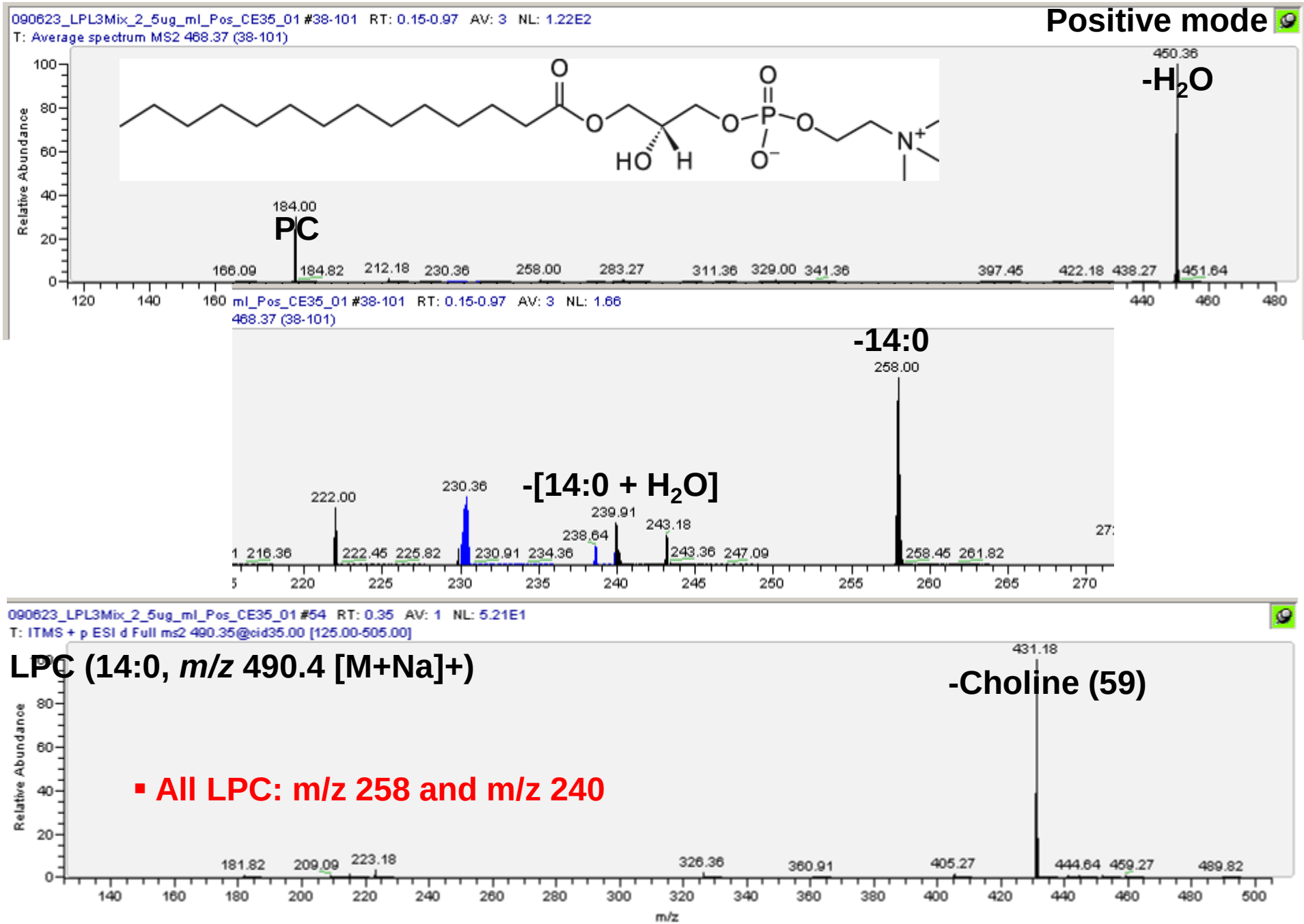
Exact Mass: 699.6

Exact Mass: 575.6

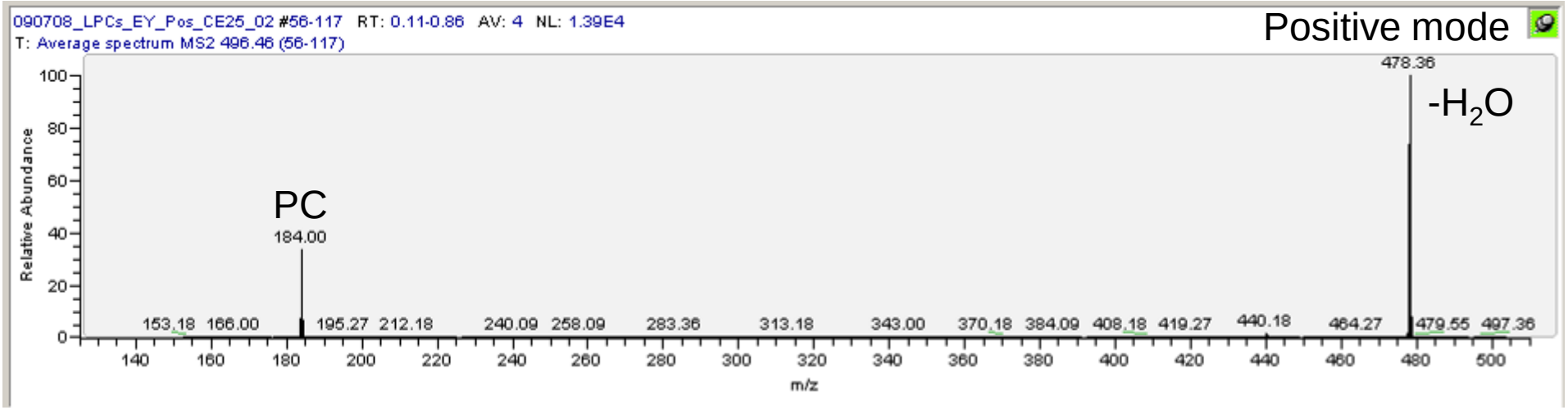
DLOPC (18:1, 18:1, diether form, *m/z* 780.8 [M+Na]+)

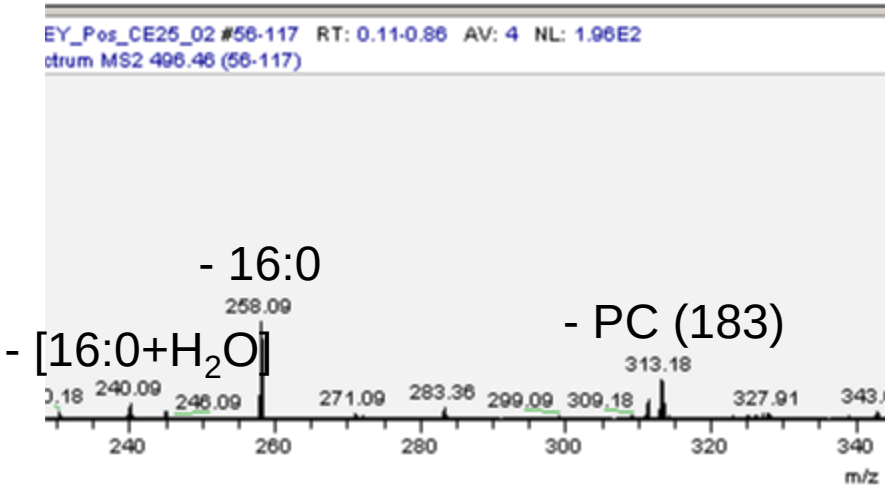


LPC (14:0, *m/z* 468.6 [M+H]+)

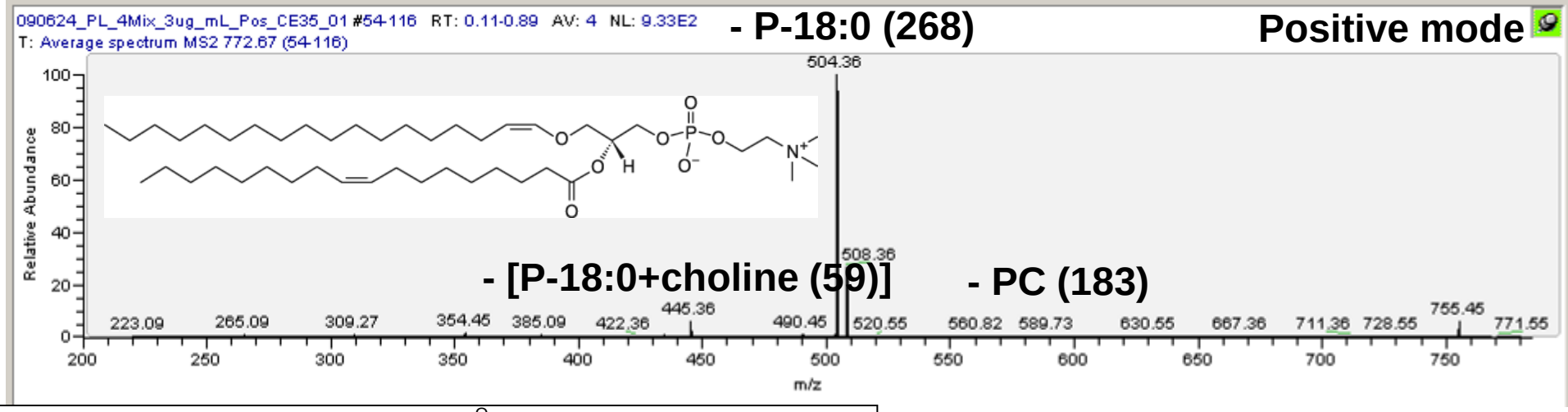


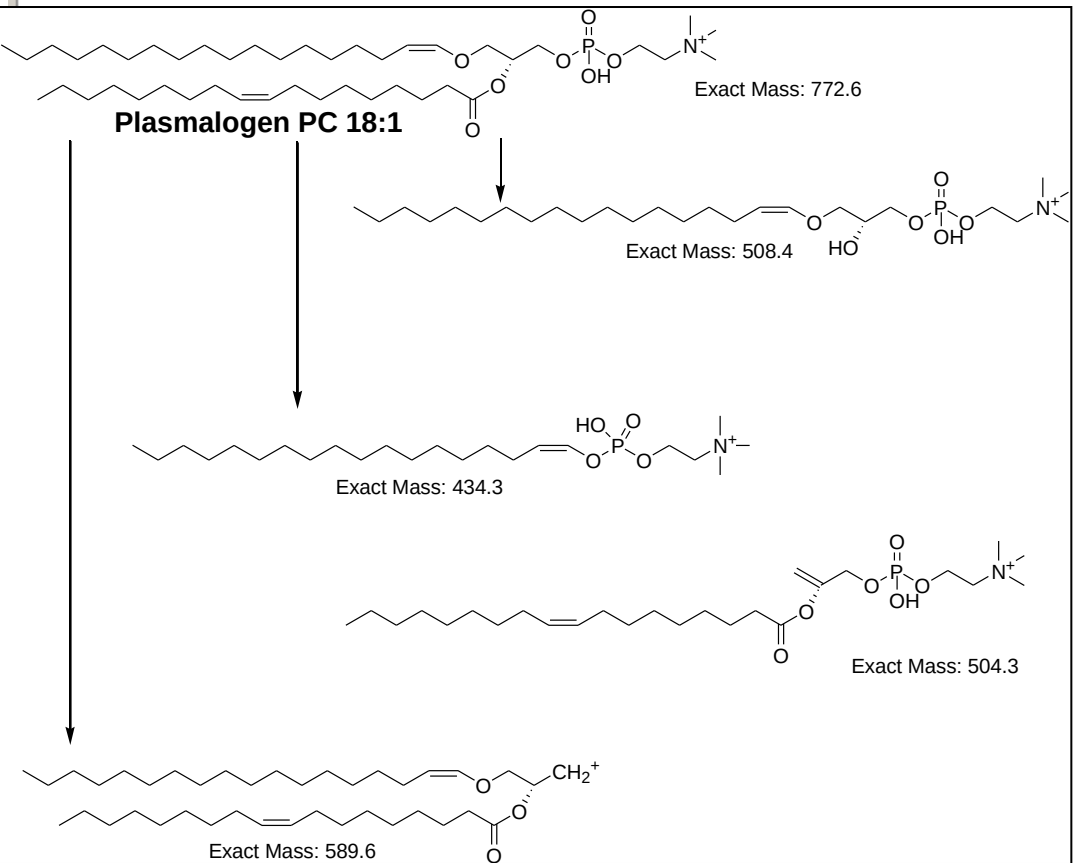
LPC 16:0 (m/z 496.4, [M+H]+)





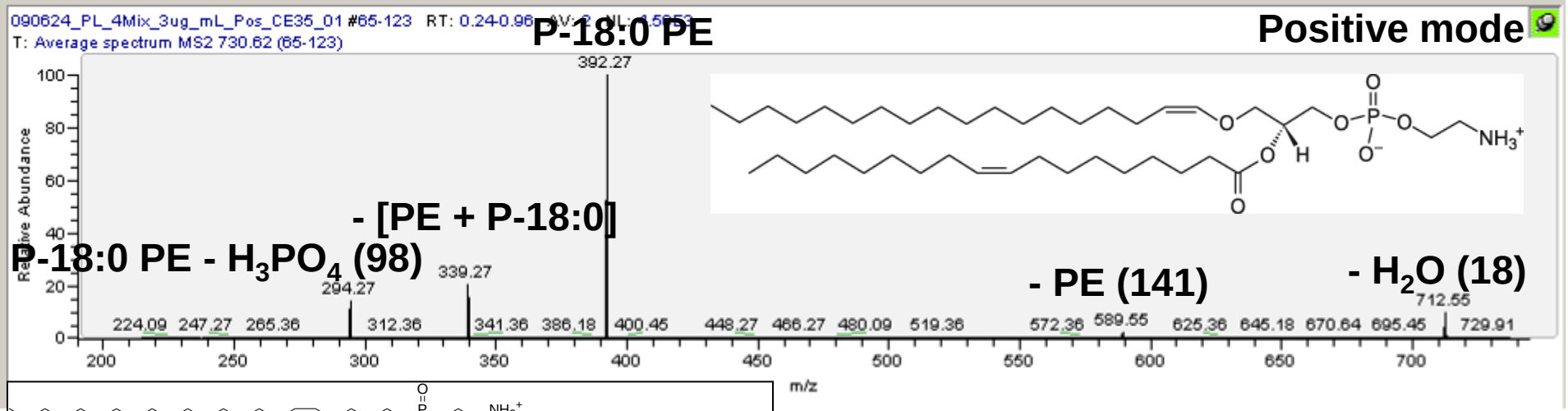
Plasmalogen PC (P-18:0, 18:1, *m/z* 772.7 [M+H]+)

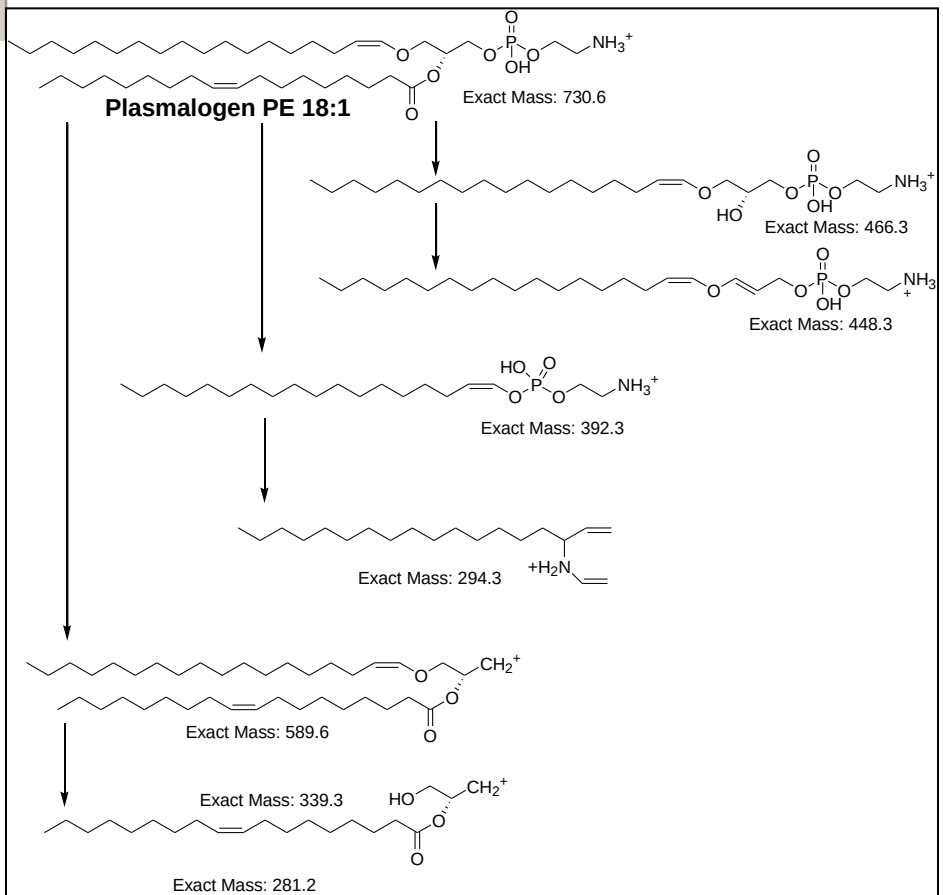




- Positive mode
- Characteristic ion of plasmalogen PC
  - P-18:0: loss of m/z 268 from MH^+
  - P-18:1: loss of m/z 266 from MH^+
  - P-16:0: loss of m/z 240 from MH^+
  - P-16:1: loss of m/z 238 from MH^+
  -

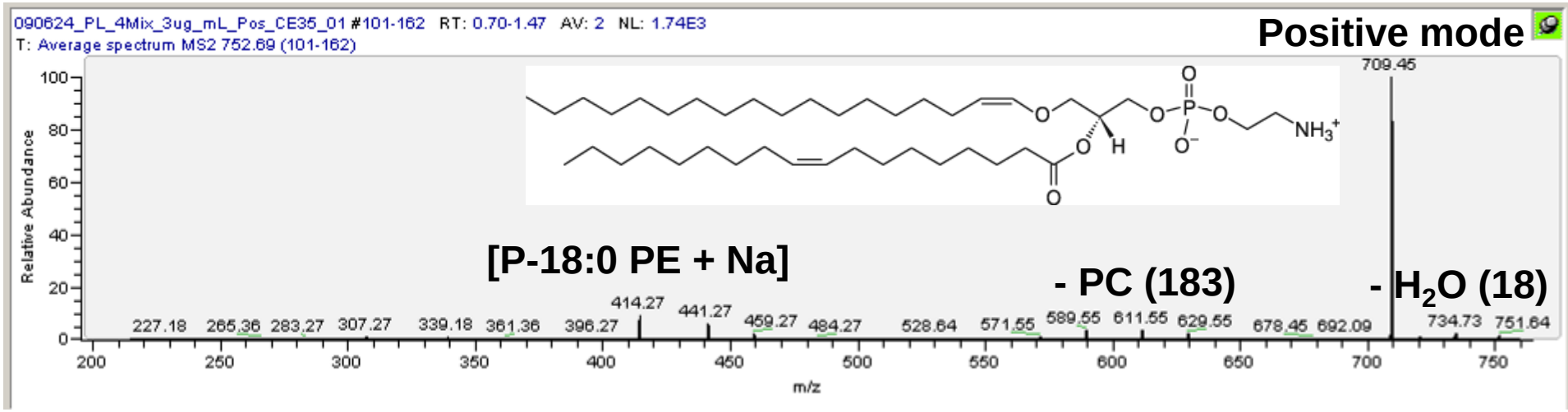
Plasmalogen PE (P-18:0, 18:1, *m/z* 730.7 [M+H]+)





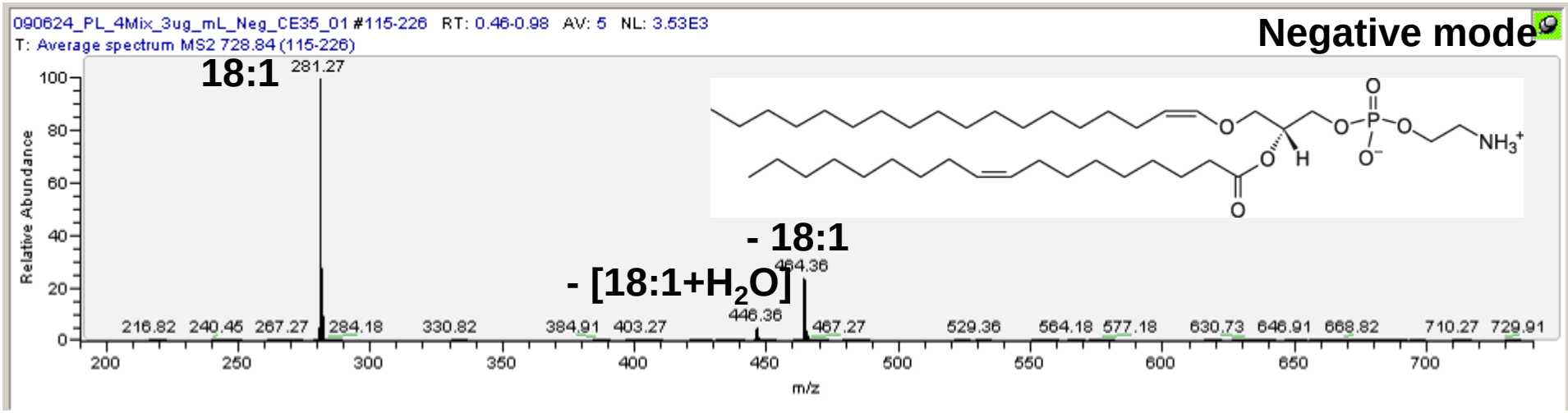
- Positive mode
- Characteristic ion of plasmalogen PE
  - P-20:0: m/z 420
  - P-20:1: m/z 418
  - P-18:0: m/z 392
  - P-18:1: m/z 390
  - P-16:0: m/z 364
  - P-16:1: m/z 362
  -

Plasmalogen PE (P-18:0, 18:1, *m/z* 752.7 [M+Na]+)

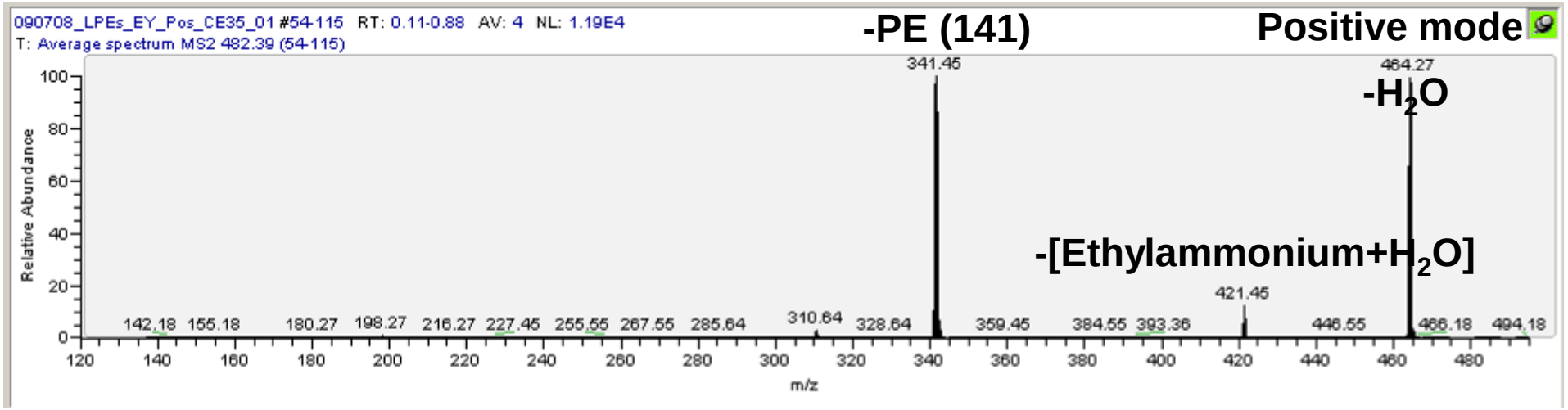


- Positive mode
- Characteristic ion of plasmalogen PE
  - P-20:0: m/z 442
  - P-20:1: m/z 440
  - P-18:0: m/z 414
  - P-18:1: m/z 412
  - P-16:0: m/z 386
  - P-16:1: m/z 384
  -

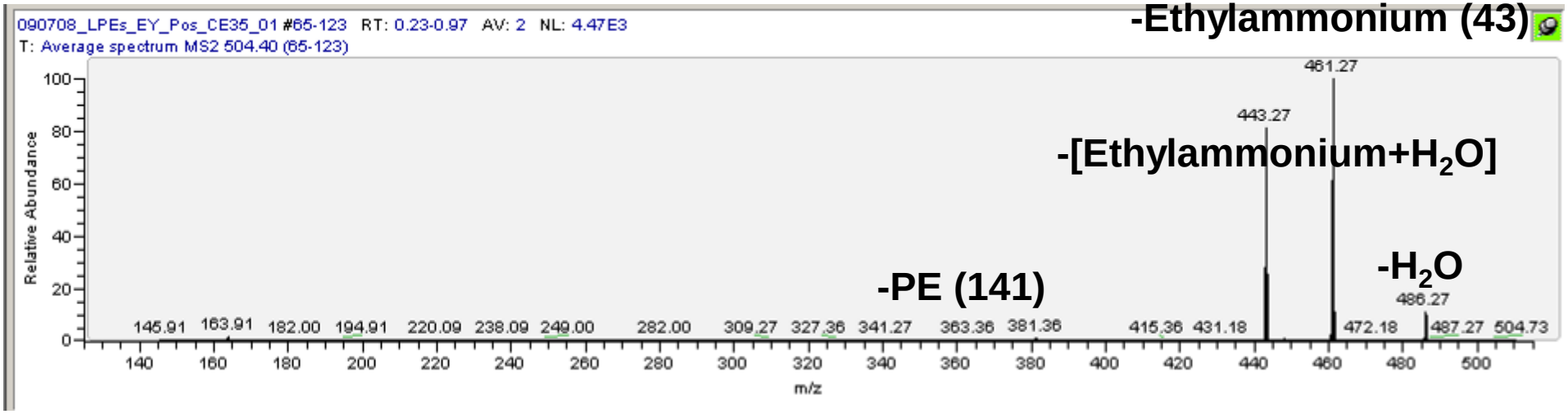
Plasmalogen PE (P-18:0, 18:1, *m/z* 728.6 [M-H]-)



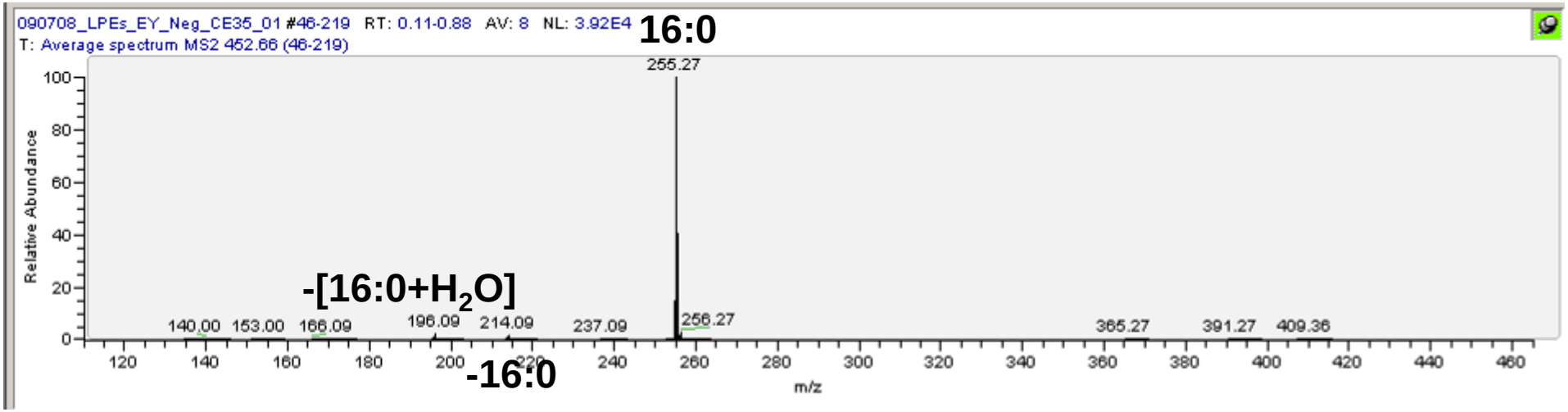
LPE (18:0, *m/z* 482.4 [M+H]+)



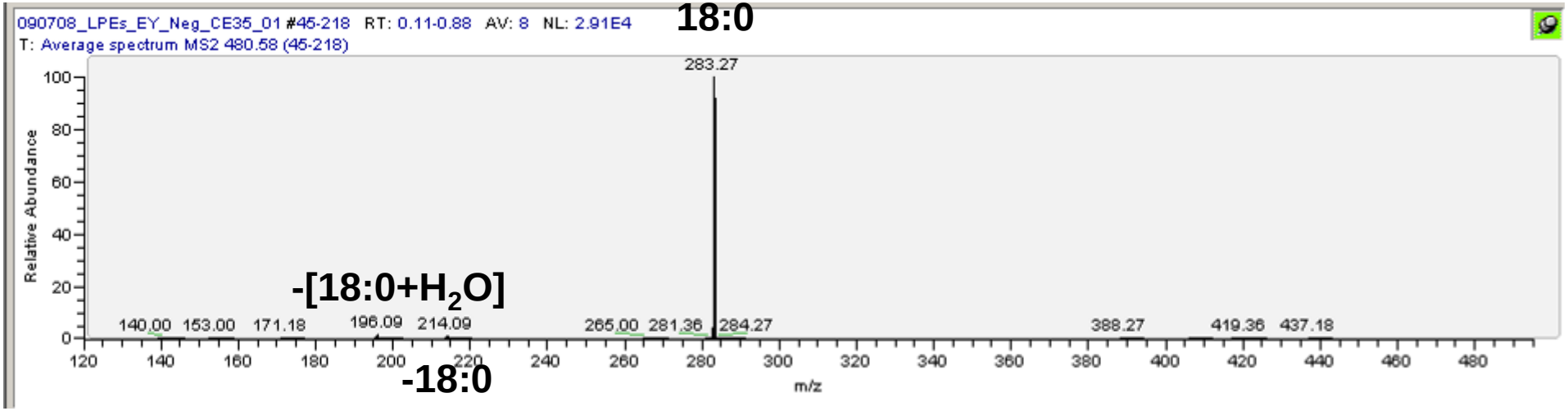
LPE (18:0, *m/z* 504.4 [M+Na]+)



LPE (16:0, *m/z* 452.3 [M-H]-)

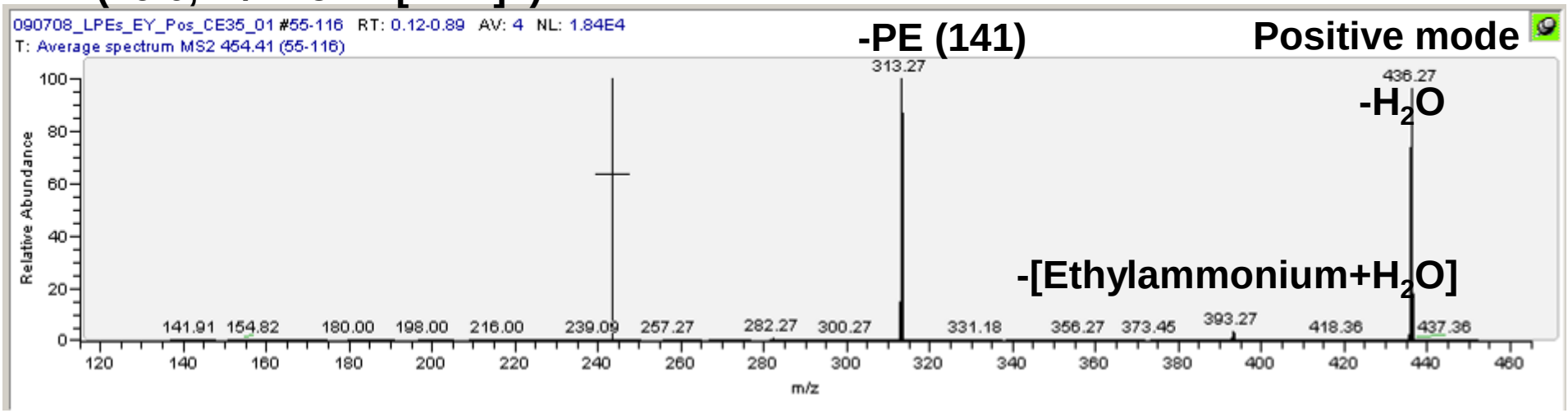


LPE (18:0, *m/z* 480.5 [M-H]-)

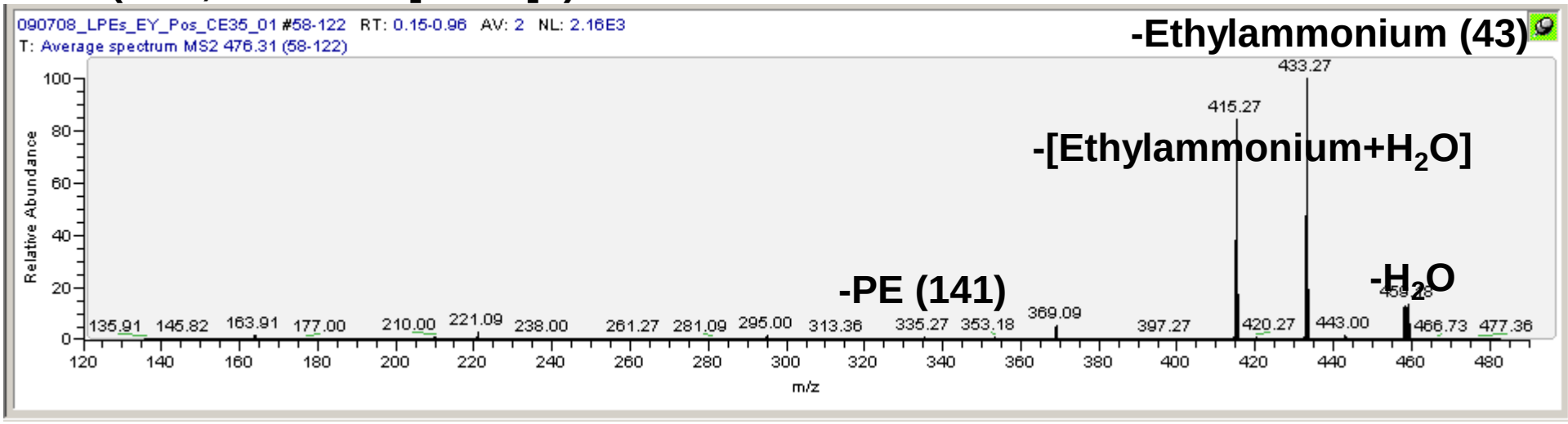


- All LPE: m/z 196 and m/z 214

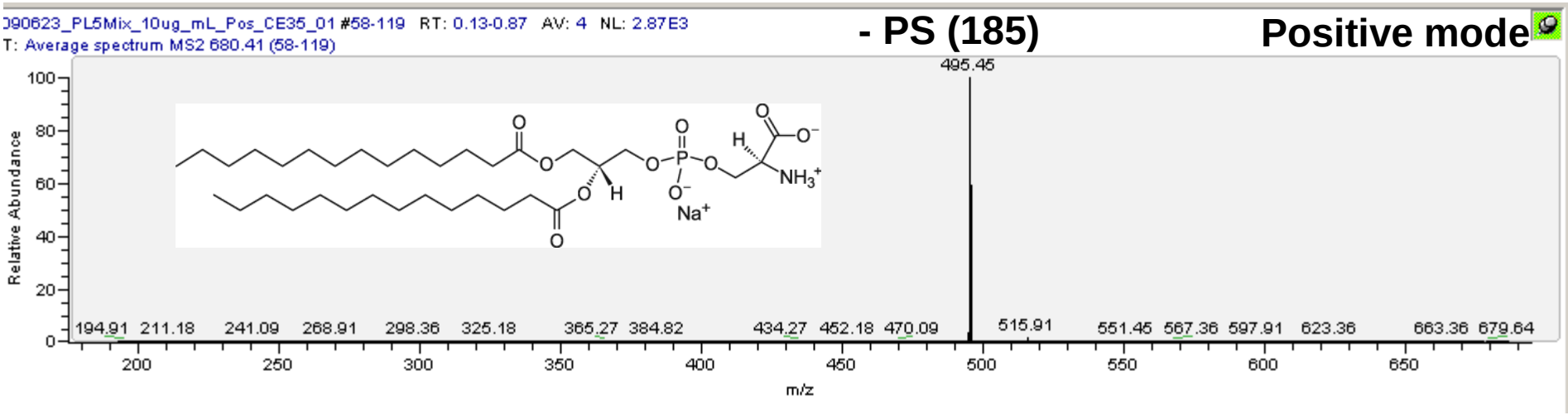
LPE (16:0, *m/z* 454.4 [M+H]+)



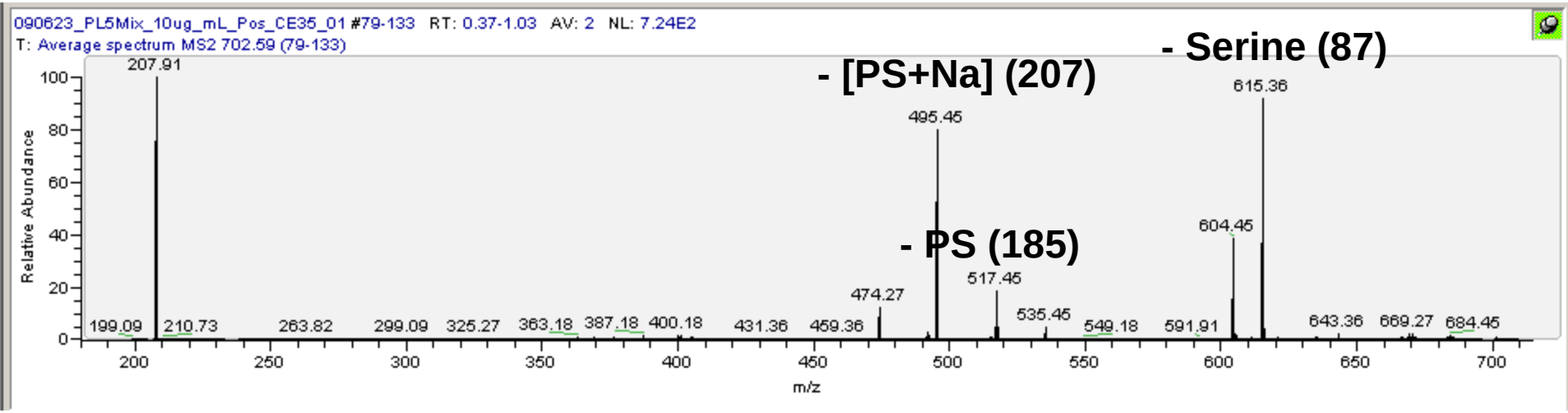
LPE (16:0, *m/z* 476.4 [M+Na]+)



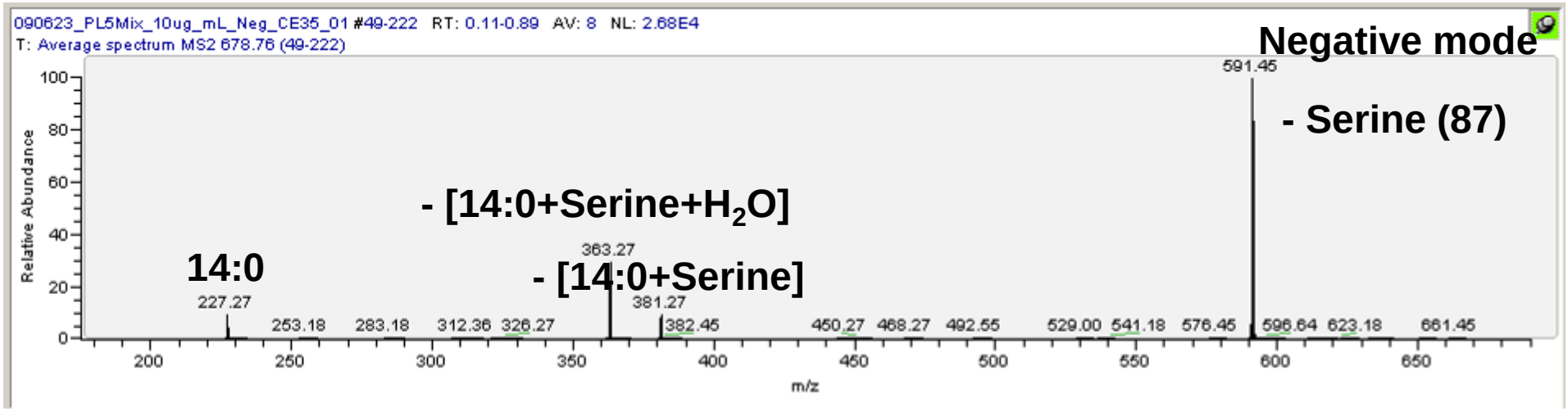
DMPS (14:0, 14:0, *m/z* 680.6 [M+H]+)

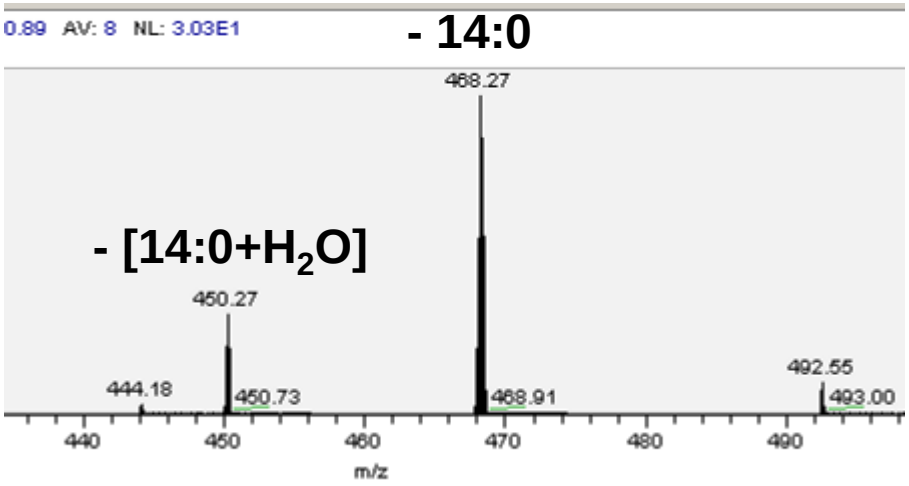


DMPS (14:0, 14:0, *m/z* 702.6 [M+Na]+)

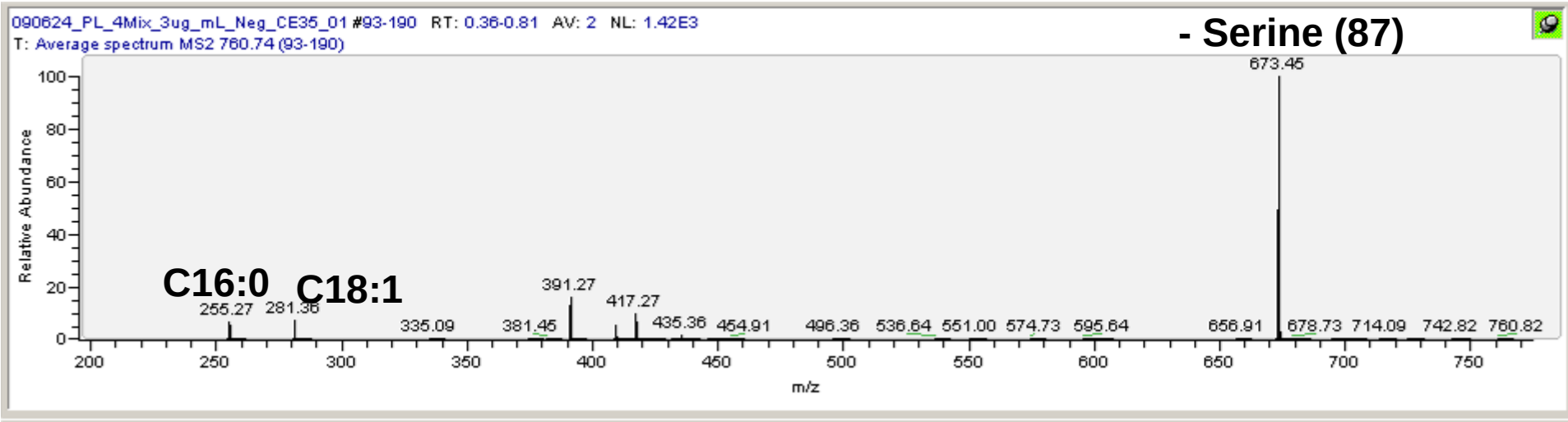


DMPS (14:0, 14:0, *m/z* 678.6 [M-H]-)

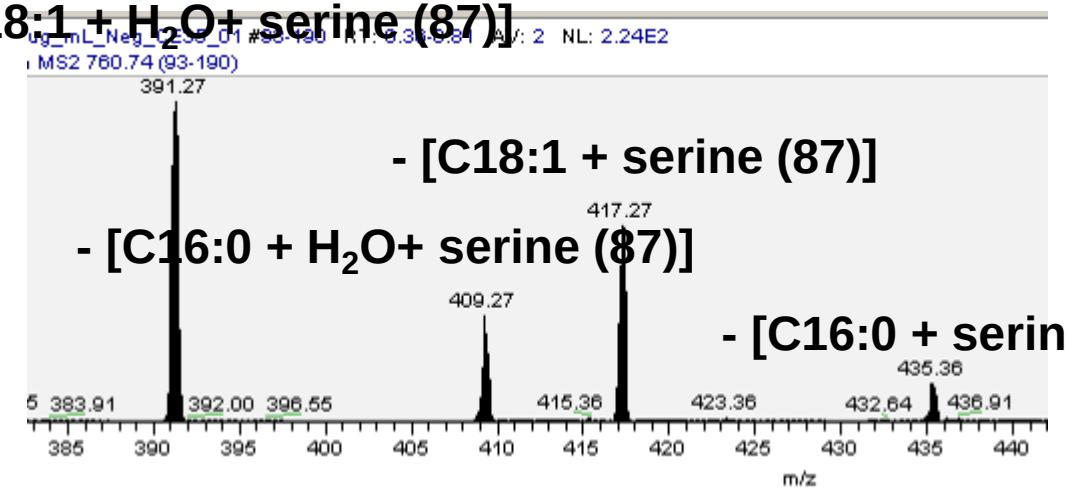




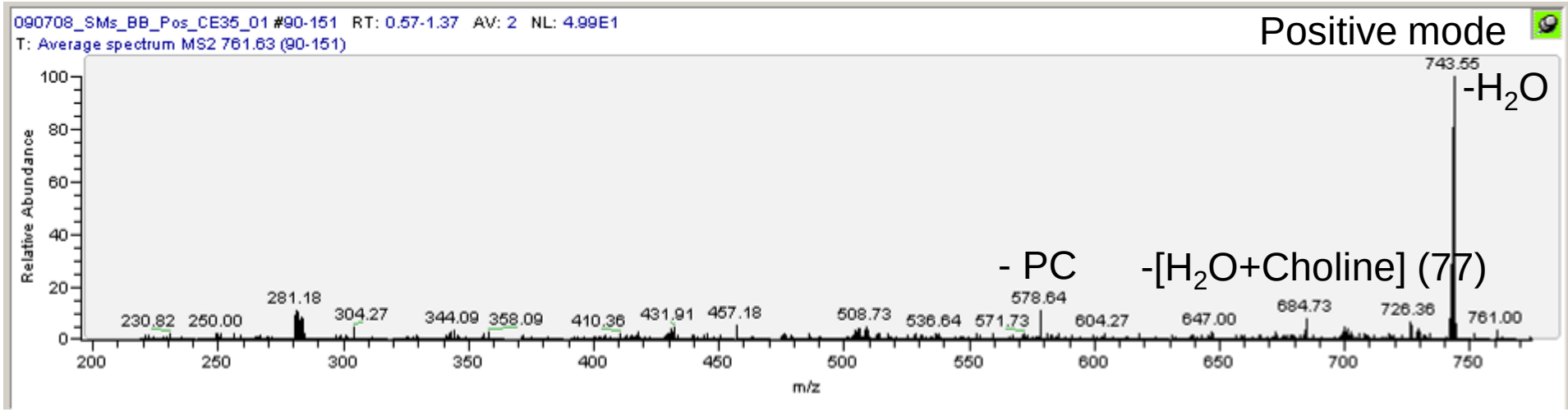
POPS (16:0, 18:1, *m/z* 760.7 [M-H]-)



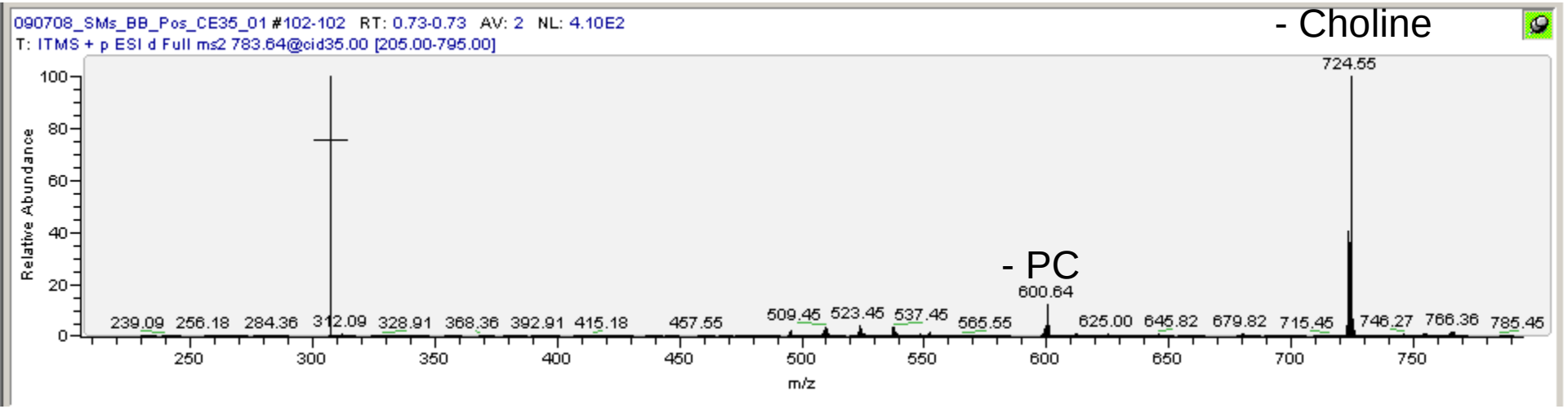
- [C18:1 + H_2O+ serine (87)]



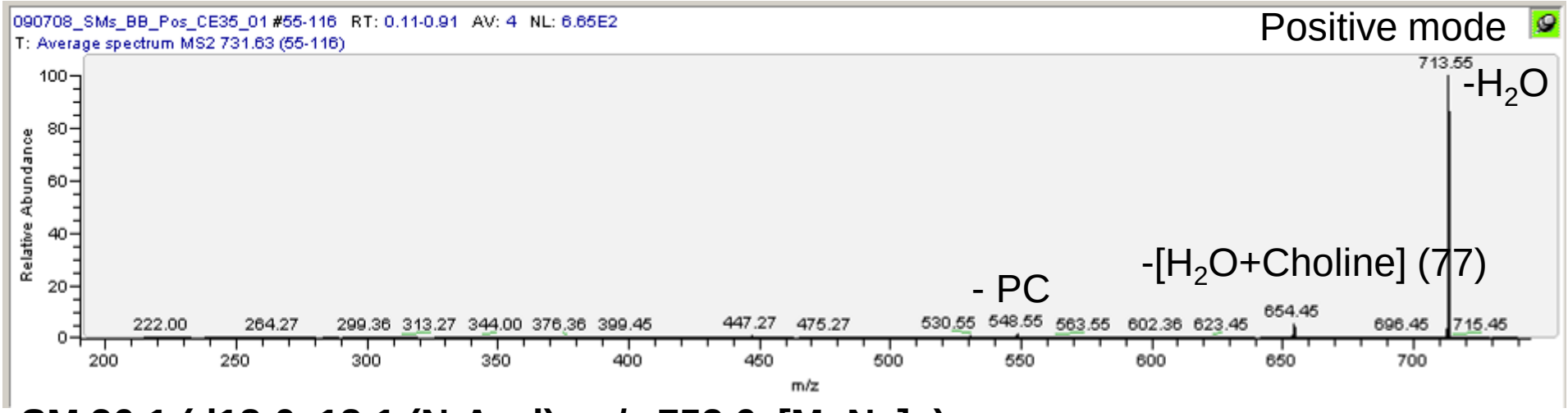
SM 38:0 (d18:0, 20:0 (N-Acyl), m/z 761.7, [M+H]+)



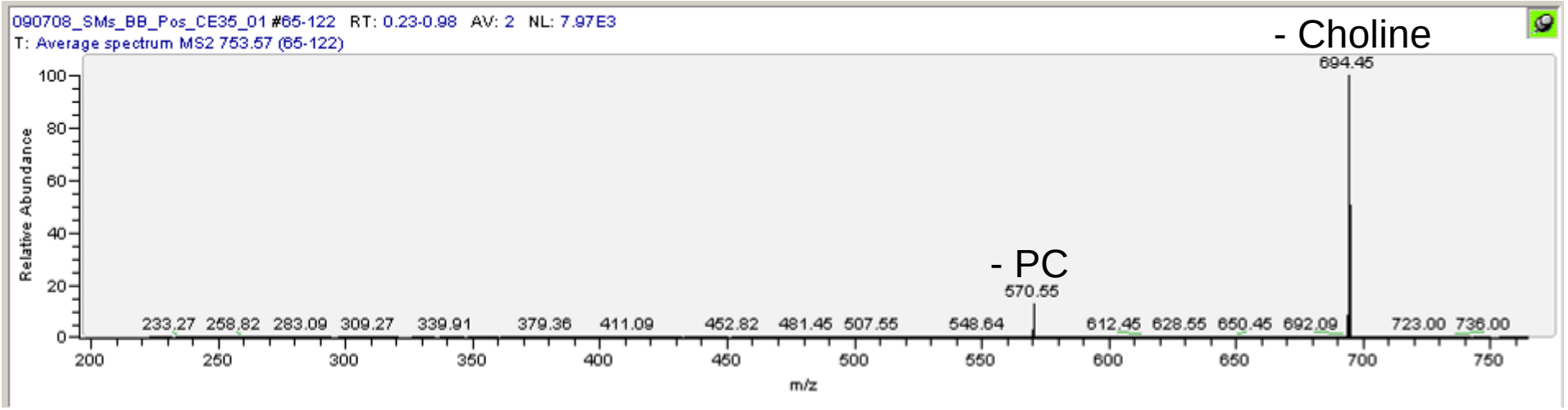
SM 38:0 (d18:0, 20:0 (N-Acyl), m/z 783.6, [M+Na]+)

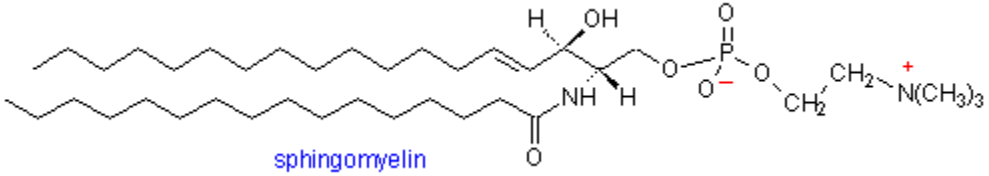


SM 36:1 (d18:0, 18:1 (N-Acyl), m/z 731.6, [M+H]+)



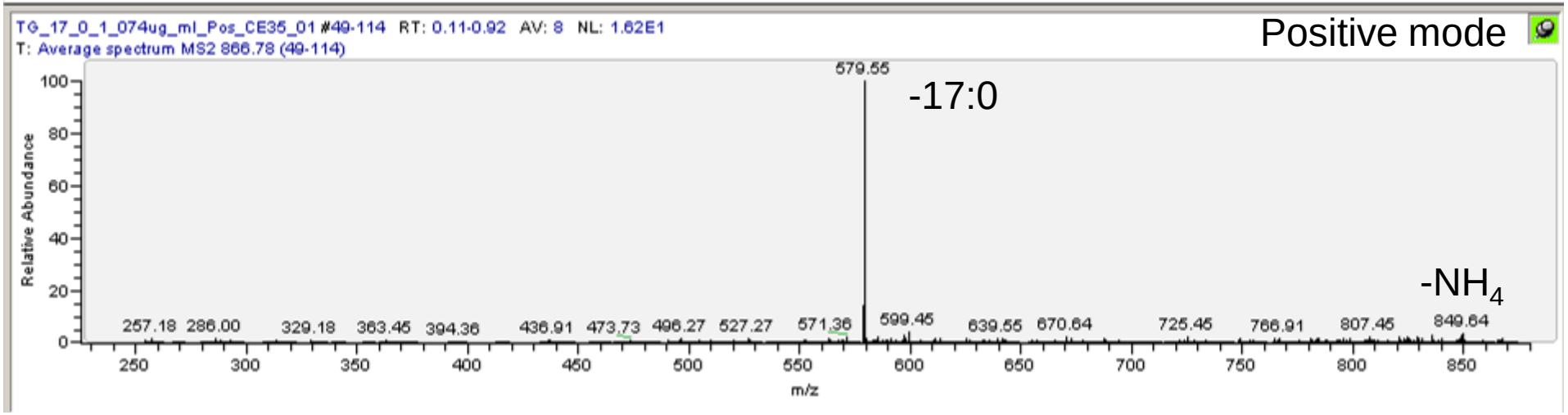
SM 36:1 (d18:0, 18:1 (N-Acyl), m/z 753.6, [M+Na]+)



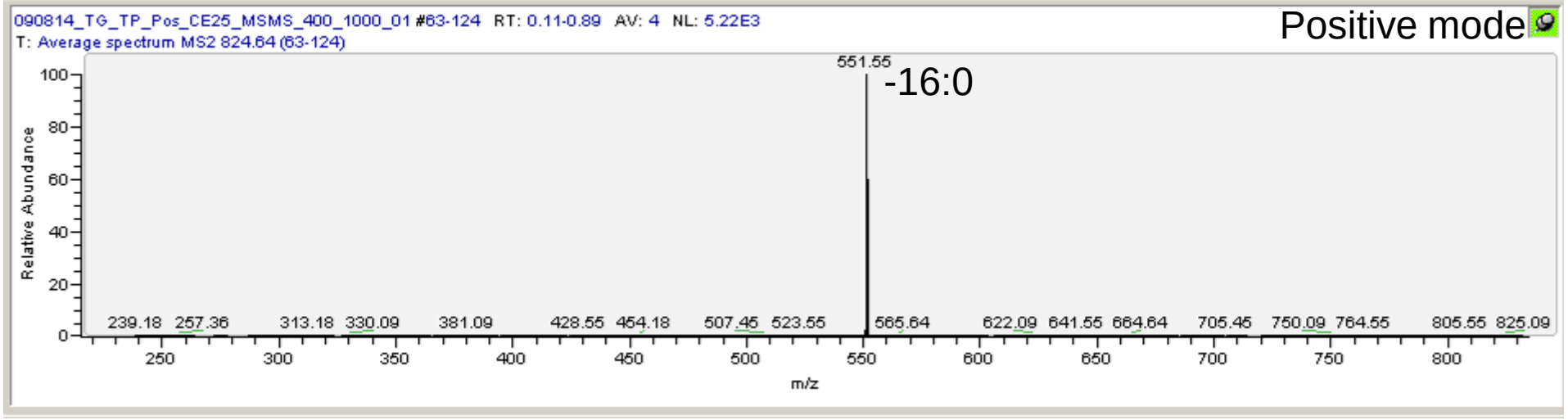


SM 34:1 (d18:1, 16:0)

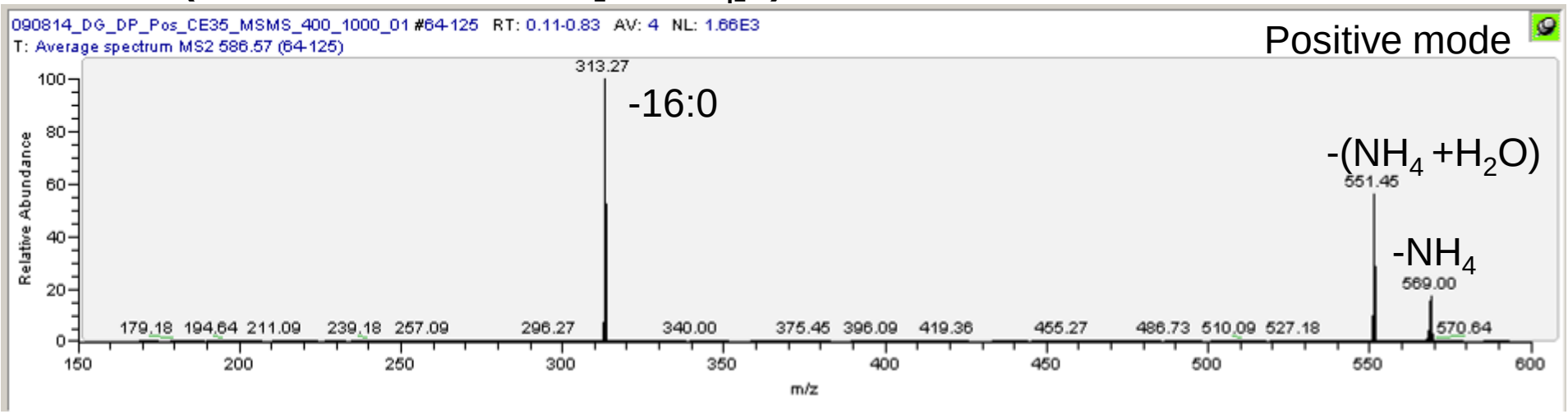
TG 54:0 (17:0, 17:0, 17:0, m/z 866.8, $[M+NH_4]+$)



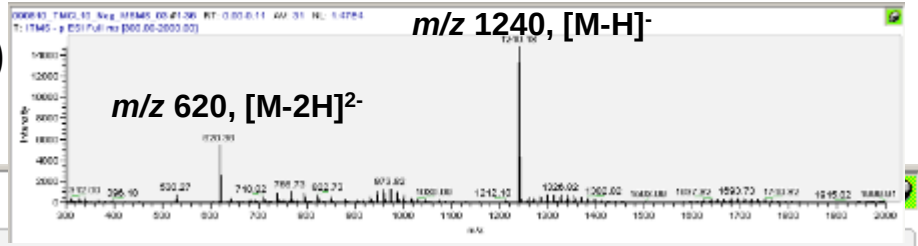
TG 48:0 (16:0, 16:0, 16:0, m/z 824.7, $[M+NH_4]+$)

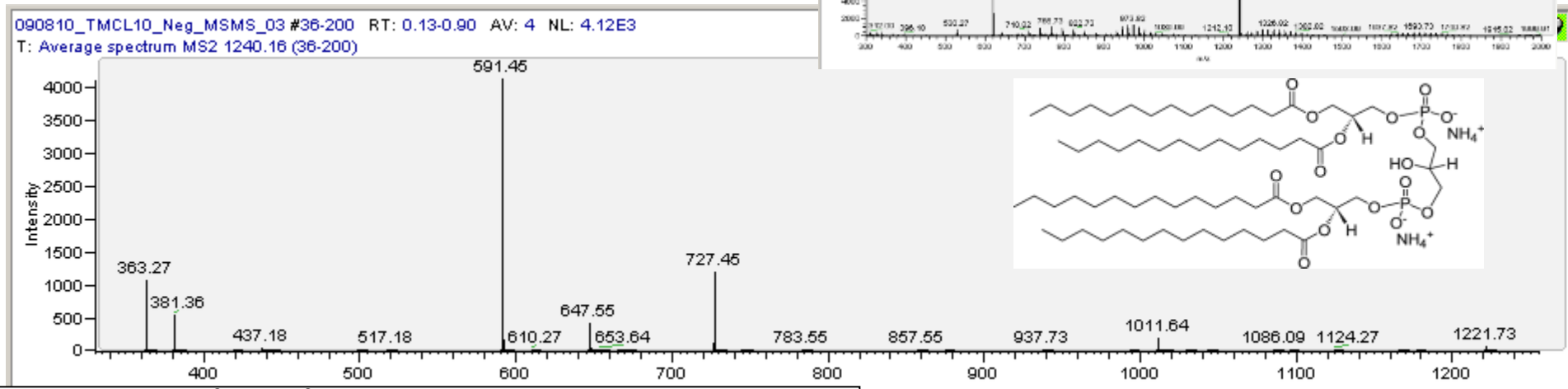


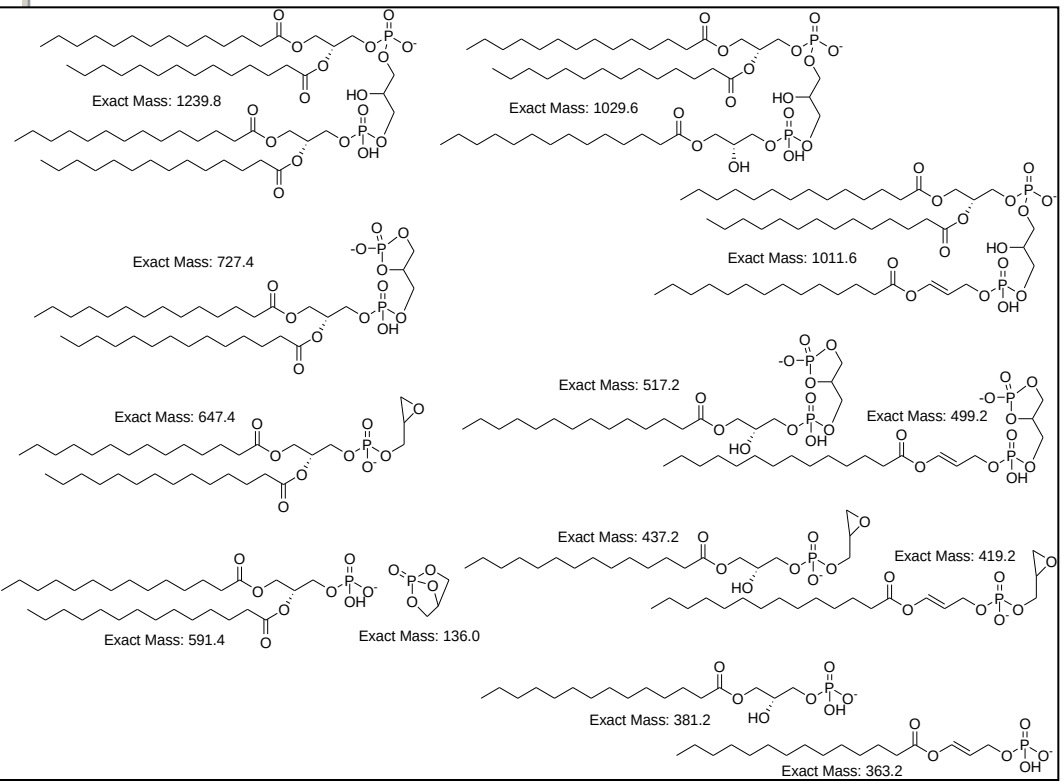
DG 32.0 (16:0, 16:0, m/z 586.6, [M+NH_4]+)



Cardiolipin 14:0 (CL 14:0, m/z 1240, [M-H]-)

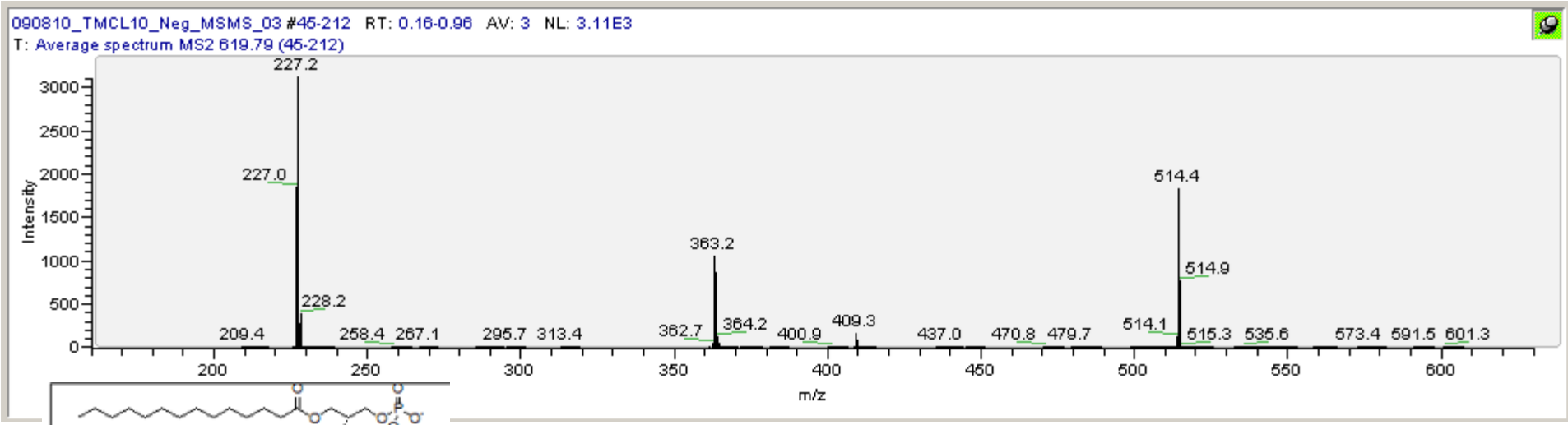


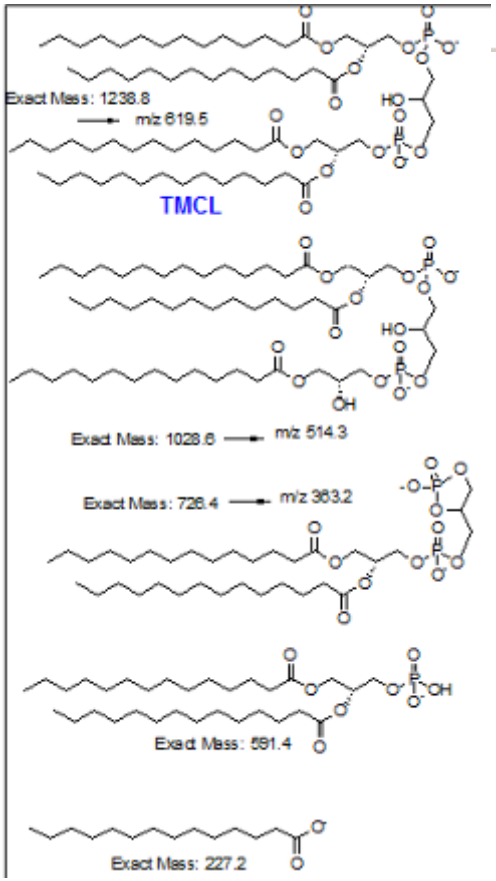




- Negative mode
- Characteristic ion
  - m/z 1240: [M-H]-
  - m/z 727.5: loss of diacyl group
  - m/z 647.6: loss of diacyl + 80
  - m/z 591.5: loss of diacyl + 136
  - m/z 381.4: acyl chain information
  - m/z 363.3: acyl chain information

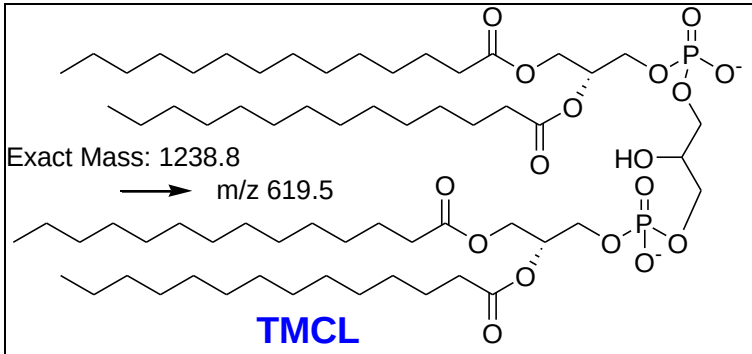
Cardiolipin 14:0 (CL 14:0, m/z 620, [M-2H]2-)



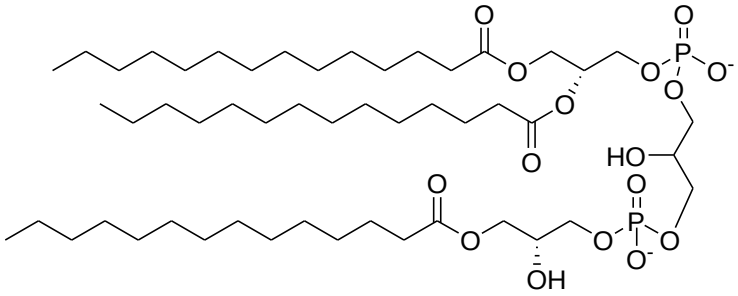


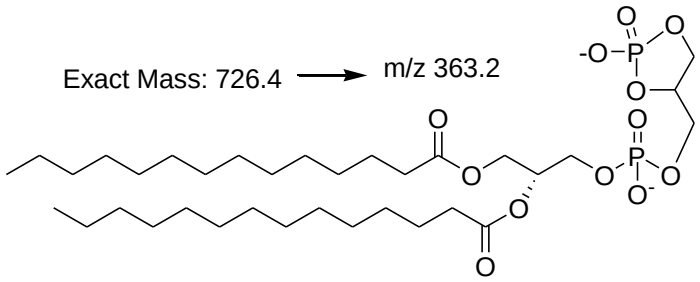
- Negative mode
- Characteristic ion
  - m/z 620: [M-2H]2-
  - m/z 514.4: loss of monoacyl group
  - m/z 363.2: loss of diacyl group
  - m/z 227.2: 14:0

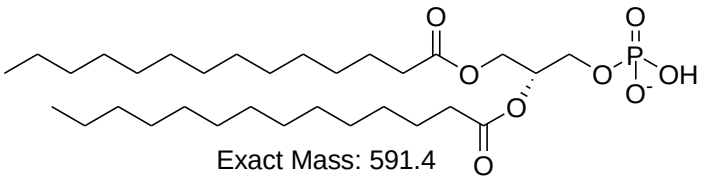
✓ **Positive mode: No signal**

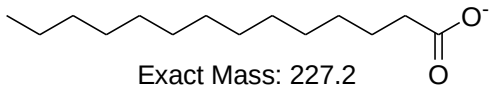

Exact Mass: 1238.8
m/z 619.5

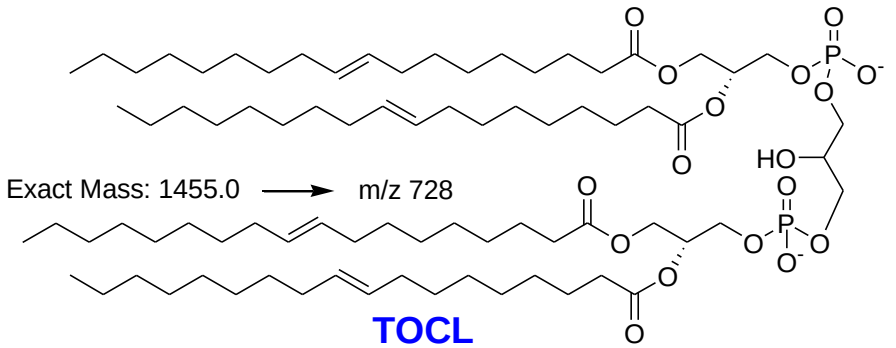
TMCL


Exact Mass: 1028.6
m/z 514.3

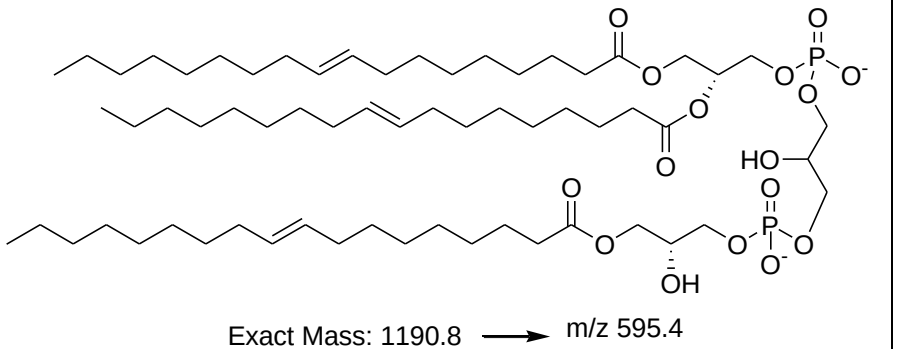

Exact Mass: 726.4
m/z 363.2

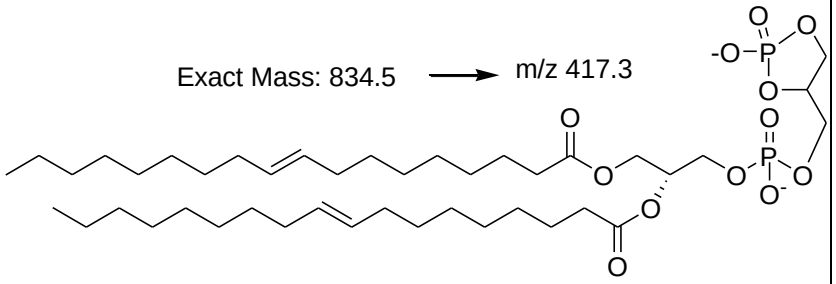

Exact Mass: 591.4

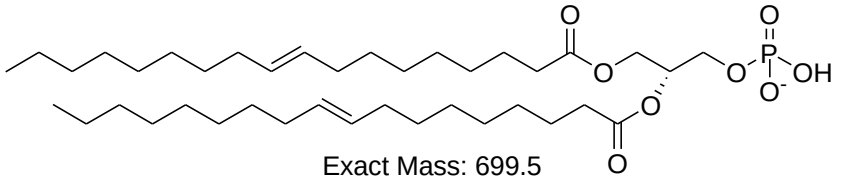

Exact Mass: 227.2

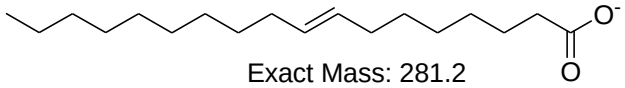

Exact Mass: 1455.0
m/z 728

TOCL

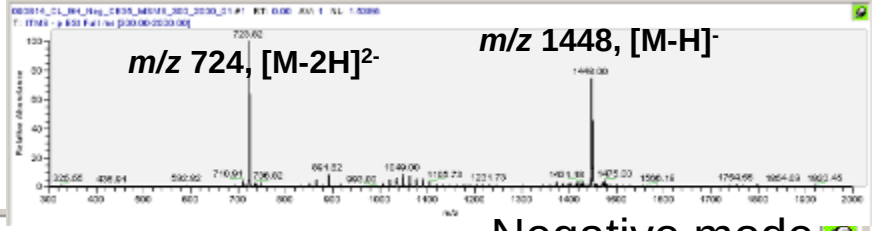

Exact Mass: 1190.8
m/z 595.4


Exact Mass: 834.5
m/z 417.3

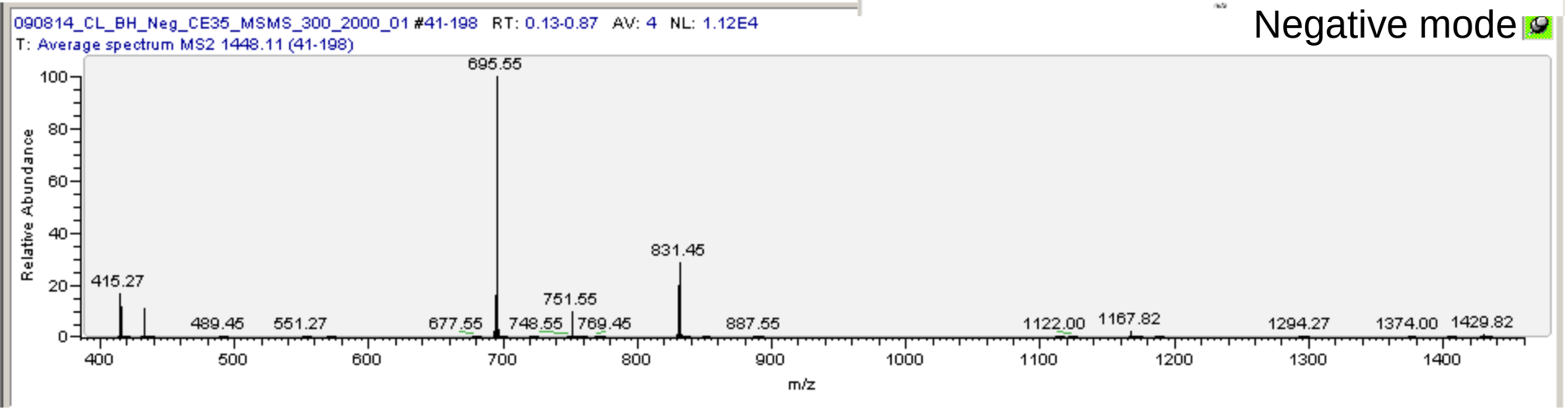

Exact Mass: 699.5


Exact Mass: 281.2

Cardiolipin 18:2 (CL 18:2, m/z 1448, [M-H]-)



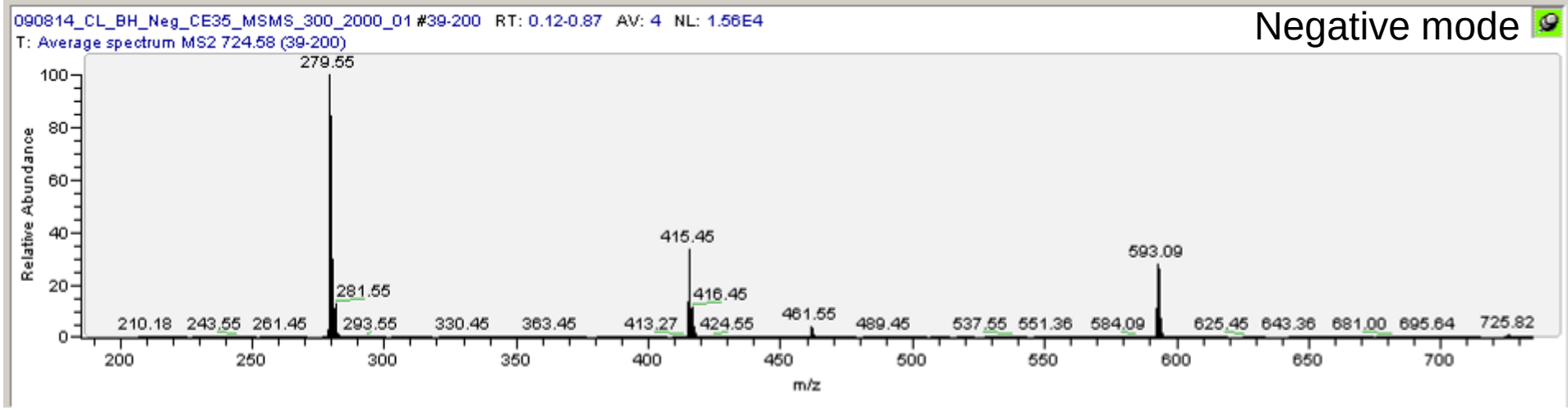
Negative mode



- Negative mode
- Characteristic ion
  - m/z 1448: [M-H]-
  - m/z 831.5: loss of diacyl group
  - m/z 751.6: loss of diacyl + 80
  - m/z 695.6: loss of diacyl + 136
  - m/z 433.3: acyl chain information
  - m/z 415.3: acyl chain information

✓ **Positive mode: No signal**

Cardiolipin 18:2 (CL 18:2, m/z 724, [M-2H]2-)

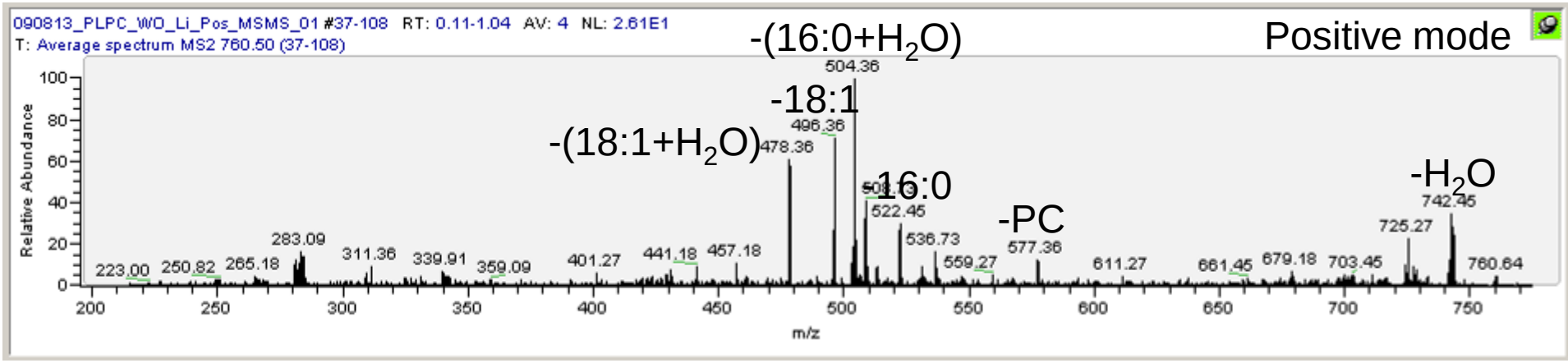


- Negative mode
- Characteristic ion
  - m/z 724: [M-2H]2-
  - m/z 695.4
  - m/z 593.1: loss of monoacyl group
  - m/z 415.5: loss of diacyl group
  - m/z 279.6: 18:2

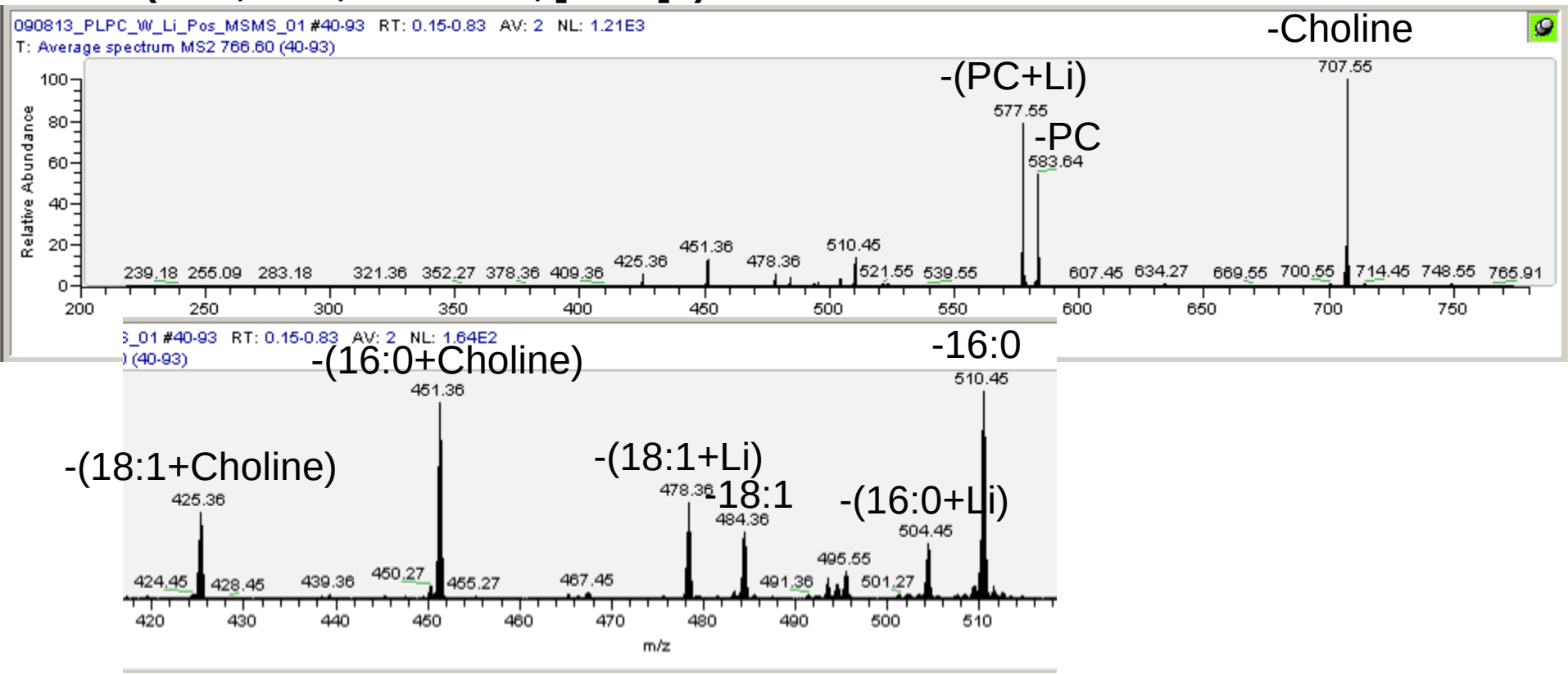
Li Adduct

By adding LiOH in reconstitution solvent
(Final concentration of Li: 2 mM)

PLPC (16:0, 18:1, m/z 760.6, [M+H]+)



PLPC (16:0, 18:1, m/z 766.6, [M+Li]+)



Identified Lithium Adduct of Phosphatidylcholine

- **Lithium adduct: Acyl chain information**
- **Sodium adduct: no acyl chain information**

PL	Acyl chain	[MH]+	[M+Li]+	PL	Acyl chain	[MH]+	[M+Li]+
PC 34:2	16:0, 18:2	758.7	764.7	PC 36:2	18:0, 18:2	786.7	792.7
PC 34:1	16:0, 18:1	760.7	766.7	PC 36:1	18:0, 18:1	788.7	794.7
PC 34:0	16:0, 18:0	762.7	768.7	PC 38:7	16:1, 22:6	804.6	810.6
PC 36:6	16:1, 20:5	778.7	784.7	PC 38:6	16:0, 22:6	806.6	812.6
PC 36:5	16:0, 20:5	780.7	786.7	PC 38:5	18:1, 20:4	808.6	814.6
PC 36:4	18:2, 18:2	782.7	788.7	PC 38:4	18:0, 20:4	810.6	816.6
PC 36:3	18:1, 18:2	784.7	790.7	PC 38:3	18:0, 20:3	812.6	818.6

Identification of major PL and NL from standard blood

m/z	PL/TG	m/z	PL/TG	m/z	PL/TG	m/z	PL/TG	m/z	PL/TG
468.5	LPC 14:0	614.5	DG 34:0 NH4+	780.7	PC 34:2 Na	850.6	TG 50:1 NH4+	904.6	TG 54:2 NH4+
480.5	LPC P-16:0	638.5	DG 36:2 NH4+	782.7	PC 34:1 Na	852.6	PC 39:1 Na	906.5	TG 54:1 NH4+
482.5	LPC 15:0	640.5	DG 36:1 NH4+	784.7	PC 34:0 Na	854.6	PC 39:0 Na	908.6	TG 54:0 NH4+
494.7	LPC 16:1	642.5	DG 36:0 NH4+	786.7	PC 36:2	856.6	PC 40:6 Na	916.5	TG 56:10 NH4+
496.6	LPC 16:0	666.5	DG 38:2 NH4+	788.7	PC 36:1	858.6	PC 40:5 Na	918.5	TG 56:9 NH4+
508.7	LPC P-18:0	668.5	DG 38:1 NH4+	794.6	PC 35:2 Na	860.6	PC 40:4 Na	920.6	TG 56:8 NH4+
510.6	LPC 17:0	669.4	SM 30:1 Na	796.6	PC 35:1 Na	862.6	PC 40:3 Na	922.6	TG 56:7 NH4+
518.5	LPC 18:3	670.5	DG 38:0 NH4+	798.6	PC 35:0 Na	864.6	PC 40:2 Na	924.6	TG 56:6 NH4+
520.6	LPC 18:2	671.6	SM 30:1 Na	800.7	PC 36:6 Na	866.6	PC 40:1 Na	926.6	TG 56:5 NH4+
522.6	LPC 18:1	675.6	SM 32:1	802.7	PC 36:5 Na	868.6	PC 40:0 Na	928.6	TG 56:4 NH4+
524.6	LPC 18:0	677.5	SM 32:0	804.7	PC 36:4 Na	870.6	TG 52:5 $NH4^+$	930.6	TG 56:3 NH4+
526.6	LPE 22:6	697.4	SM 32:1 Na	806.6	PC 36:3 Na	872.7	TG 52:4 NH4+	932.6	TG 56:2 NH4+
536.7	LPC P-20:0	699.4	SM 32:0 Na	808.7	PC 36:2 Na	874.6	TG 52:3 NH4+	934.6	TG 56:1 NH4+
538.6	LPC 19:0	703.7	SM 34:1	810.7	PC 36:1 Na	876.6	TG 52:2 NH4+	936.6	TG 56:0 NH4+
542.5	LPC 20:5	705.8	SM 34:0	812.7	PC 36:0 Na	878.6	TG 52:1 NH4+	938.6	TG 58:12 NH4+
544.6	LPC 20:4	725.5	SM 34:1 Na	814.7	PC 37:6 Na	880.6	TG 52:0 NH4+	940.6	TG 58:11 NH4+
546.6	LPC 20:3	727.5	SM 34:0 Na	820.6	PC 37:3 Na	886.6	TG 53:4 NH4+	942.6	TG 58:10 NH4+
548.6	LPC 20:2	753.3	SM 36:1 Na	822.6	PC 37:2 Na	888.5	TG 53:3 NH4+	946.6	TG 58:9 NH4+
550.9	LPC 20:1	755.1	SM 36:0 Na	824.6	PC 38:8 Na	890.6	TG 54:9 NH4+	952.6	TG 58:6 NH4+
552.9	LPC 20:0	756.5	PC 34:3	826.6	PC 38:7 Na	892.6	TG 54:8 NH4+	954.6	TG 58:5 NH4+
568.6	LPC 22:6	758.7	PC 34:2	832.6	PC 38:4 Na	894.6	TG 54:7 NH4+	956.6	TG 58:4 NH4+
570.6	LPC 22:5	760.7	PC 34:1	834.7	PC 38:3 Na	896.6	TG 54:6 NH4+	958.6	TG 58:3 NH4+
578.6	LPC 22:1	762.7	PC 34:0,	836.7	PC 38:2 Na	898.7	TG 54:5 NH4+	960.6	TG 58:2 NH4+
610.5	DG 34:2 NH4+	768.7	PE 38:4	846.6	TG 50:3 NH4+	900.7	TG 54:4 NH4+	986.6	TG 60:3 NH4+
612.5	DG 34:1 NH4+	774.6	PE 32:1	848.7	TG 50:2 NH4+	902.7	TG 54:3 NH4+		

Reconstitution solvent: Chloroform/Methanol (1/9) containing 7.5 mM ammonium acetate

LipidBlast - In silico created MS/MS libraries for lipid profiling

Custom modeling for other instruments

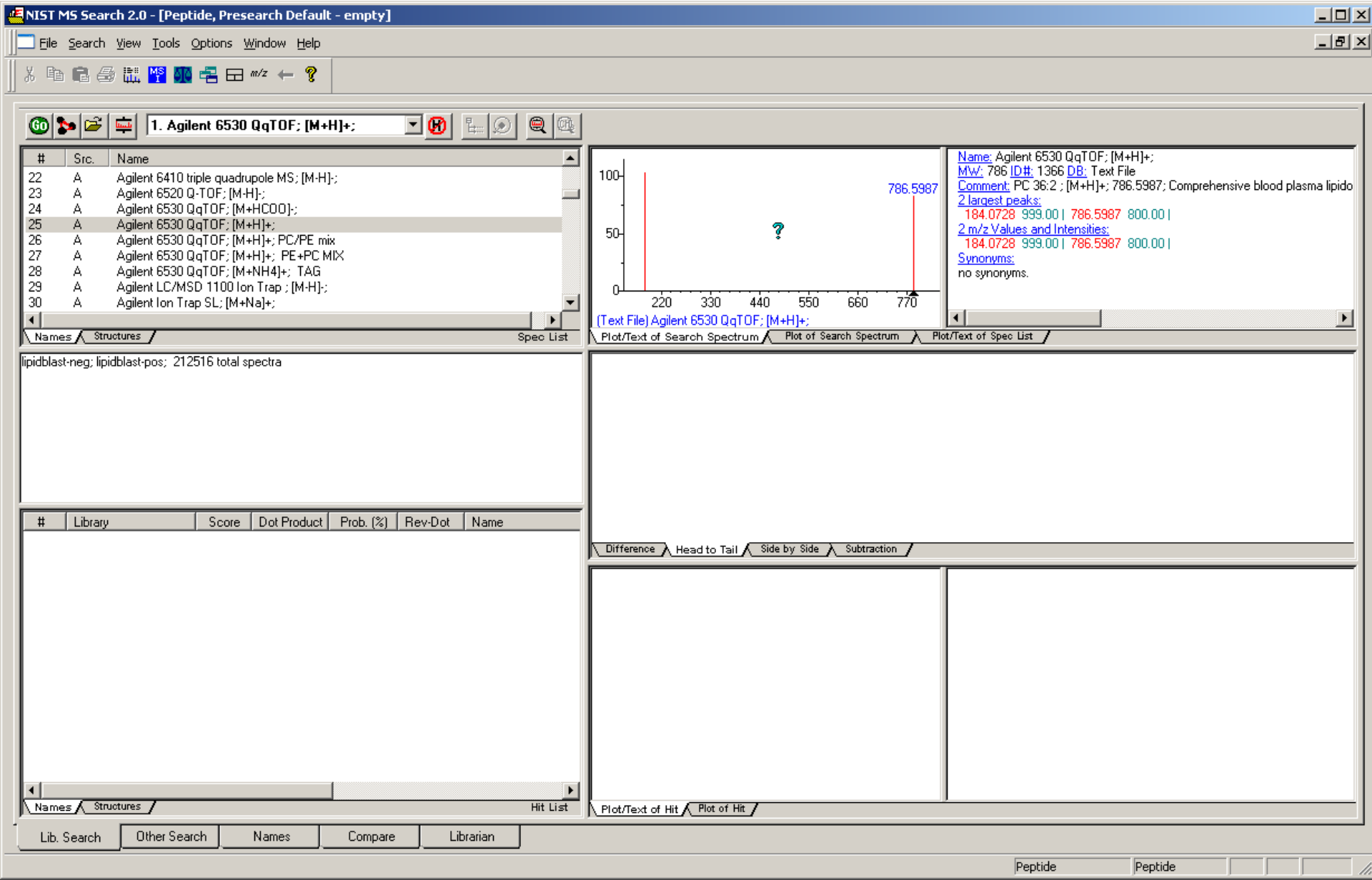
http://fiehnlab.ucdavis.edu/projects/LipidBlast

Tobias Kind, Oliver Fiehn
FiehnLab – Metabolomics
UC Davis Genome Center, Davis, USA

Supplement: Custom creation of LipidBlast libraries
New PC library for QTOF
Time to create new library <10 min using EXCEL templates.

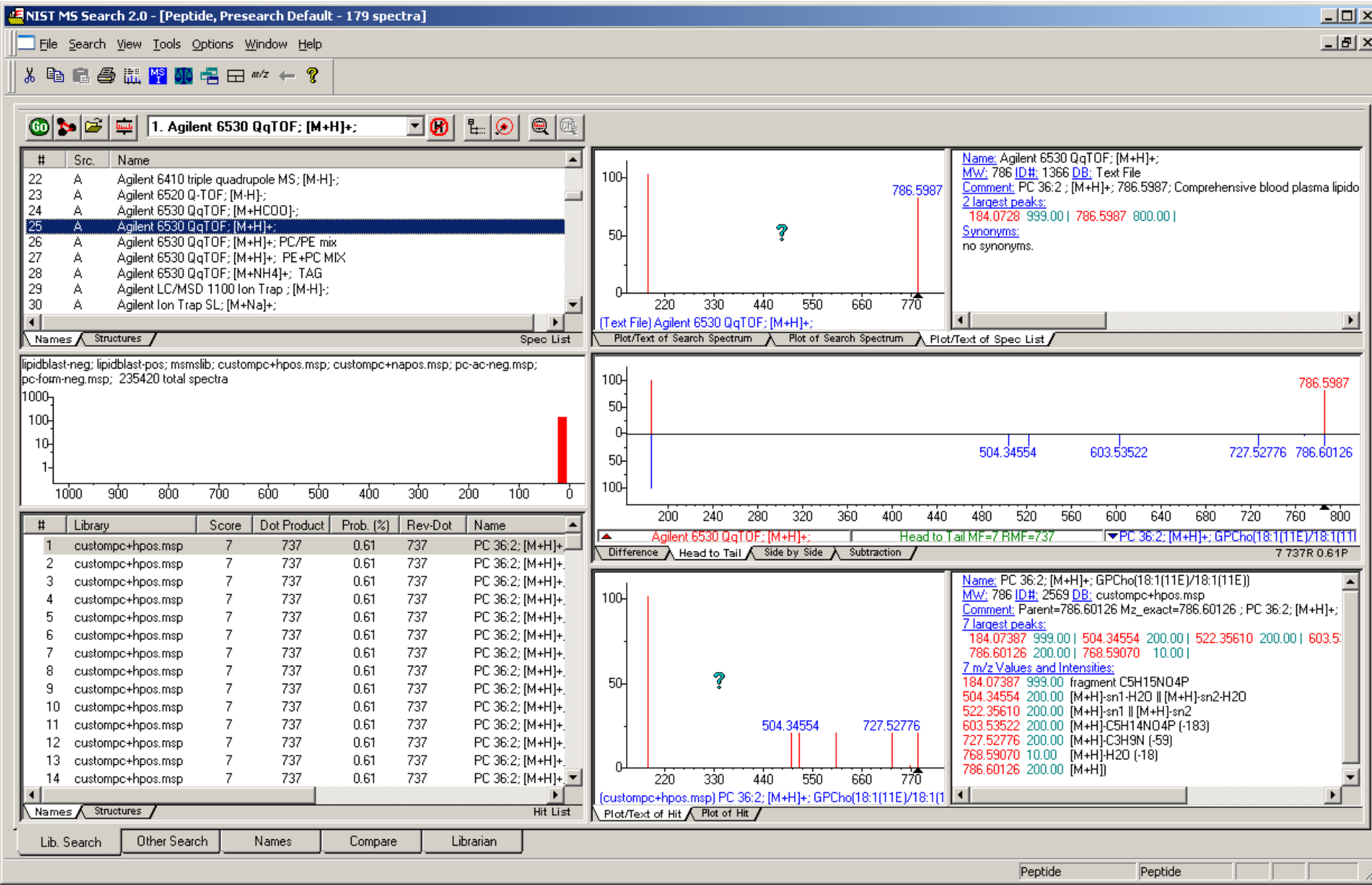
Q-TOF spectrum of PC 36:2 ; [M+H]+; 786.5987 can not be found in standard LipidBlast library, due to missing fragments in the spectrum. A custom library can be created to model specific m/z values (next slide).

Source MS/MS data Agilent 6530 QqTOF; [M+H]+;
Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry;
Sandra K, Pereira Ados S, Vanhoenacker G, David F, Sandra P.; Journal of Chromatography A, 1217 (2010) 4087-4099



The custom LipidBlast library correctly identifies PC 36:2 from MS/MS data of a Q-TOF mass spectrometer.
For QTOFs at selected voltage only precursor and product ion m/z 184 are oberved.

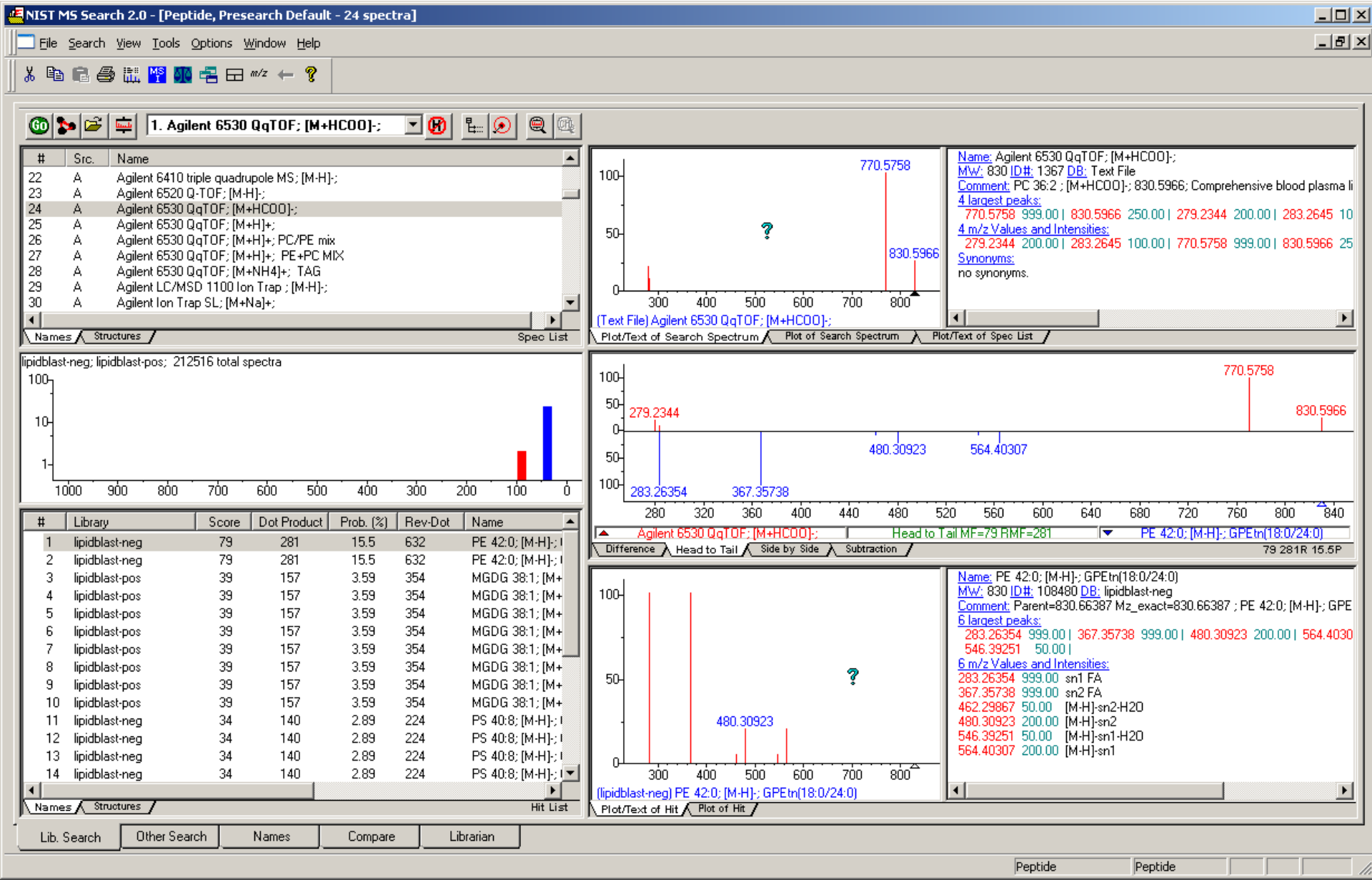
Source MS/MS data:
Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry;
Sandra K, Pereira Ados S, Vanhoenacker G, David F, Sandra P.; Journal of Chromatography A, 1217 (2010) 4087-4099



Supplement: Custom creation of LipidBlast libraries
New formate adduct library [M+HCOO]-
Time to create new library <10 min using EXCEL templates.

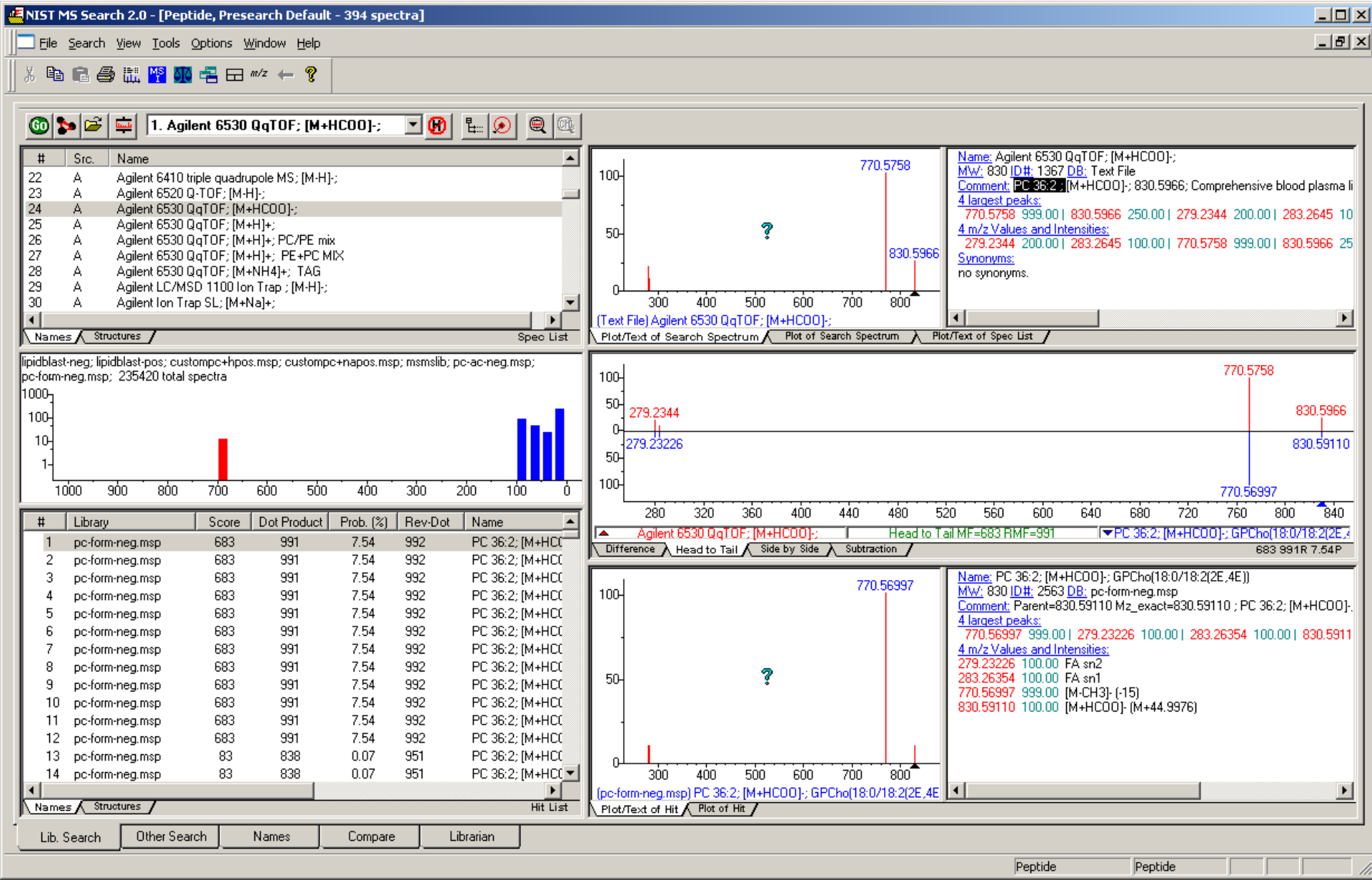
Q-TOF spectrum of PC 36:2 ; [M+HCOO]-; m/z 830.5966 is falsely identified as PE (with low hit score).
A custom library can be created to model specific m/z values (next slide).

Source MS/MS data Agilent 6530 QqTOF; [M+H]+;
Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry;
Sandra K, Pereira Ados S, Vanhoenacker G, David F, Sandra P.; Journal of Chromatography A, 1217 (2010) 4087-4099



Q-TOF spectrum of PC 36:2 ; [M+HCOO]-; m/z 830.5966 is correctly identified using the custom format pc-form-neg library.

Source MS/MS data Agilent 6530 QqTOF; [M+H]+;
Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry;
Sandra K, Pereira Ados S, Vanhoenacker G, David F, Sandra P.; Journal of Chromatography A, 1217 (2010) 4087-4099



LipidBlast - In silico created MS/MS libraries for lipid profiling

Supplement data mass spectral search
All raw files and software can be found under:

http://fiehnlab.ucdavis.edu/projects/LipidBlast

Tobias Kind, Kwang-Hyeon Liu, Do Yup Lee, Oliver Fiehn
FiehnLab – Metabolomics
UC Davis Genome Center, Davis, USA

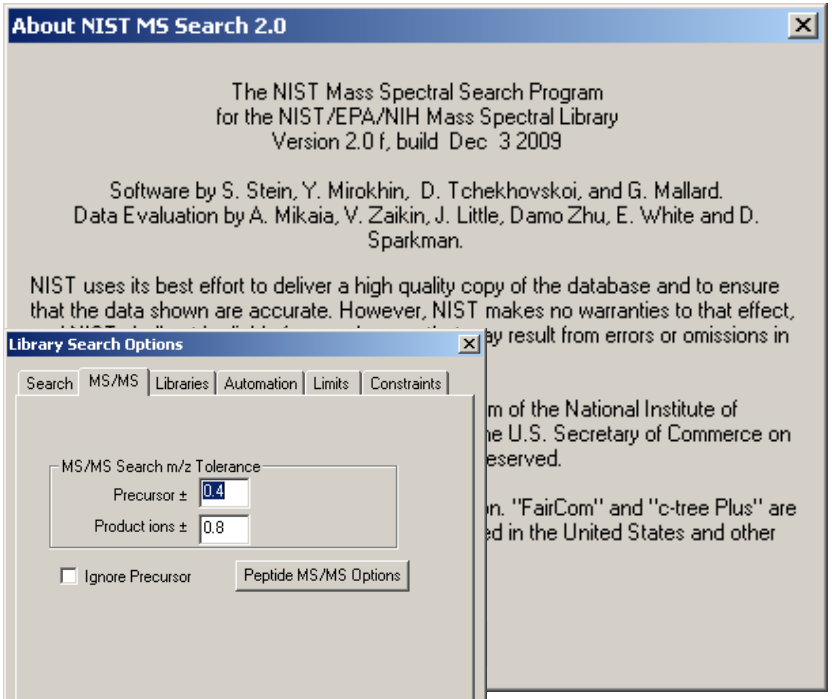
The MS/MS search results are shown here for peer review and proof of concept. The complete set of the electronic 134 spectra (*.MSP) is found in the supplement section.

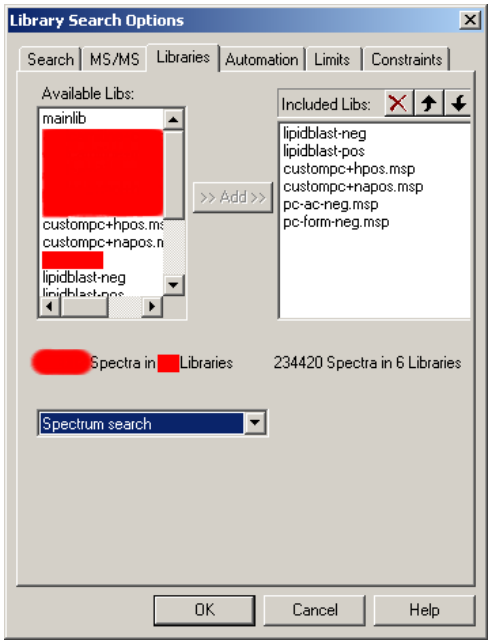
All machine readable spectra and all supplement data can be found at:
http://fiehnlab.ucdavis.edu/projects/LipidBlast

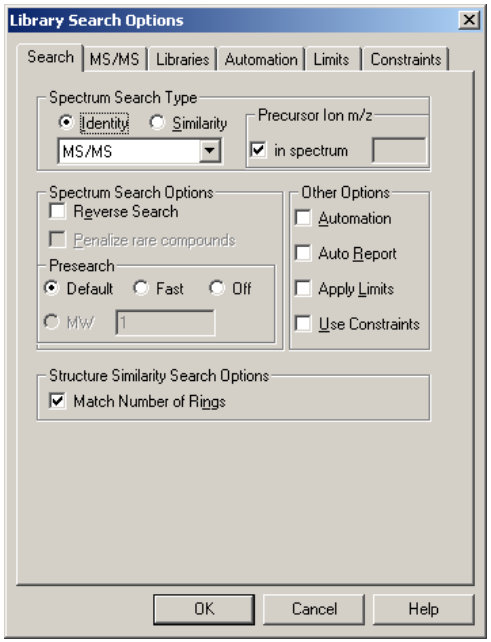
For questions please contact the curator: Dr. Tobias Kind
http://fiehnlab.ucdavis.edu/staff/kind/

NIST MS Search GUI – Search parameters

NIST MSPepSearch mass spectral library search program
Written by Dmitrii V. Tchekhovskoi and Stephen E. Stein
Mass Spectrometry Data Center
National Institute of Standards and Technology (NIST)
Visit http://peptide.nist.gov or http://chemdata.nist.gov for more information, software, or MS libraries.

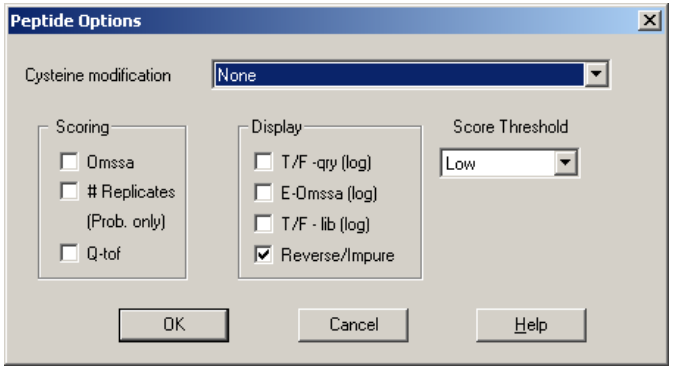




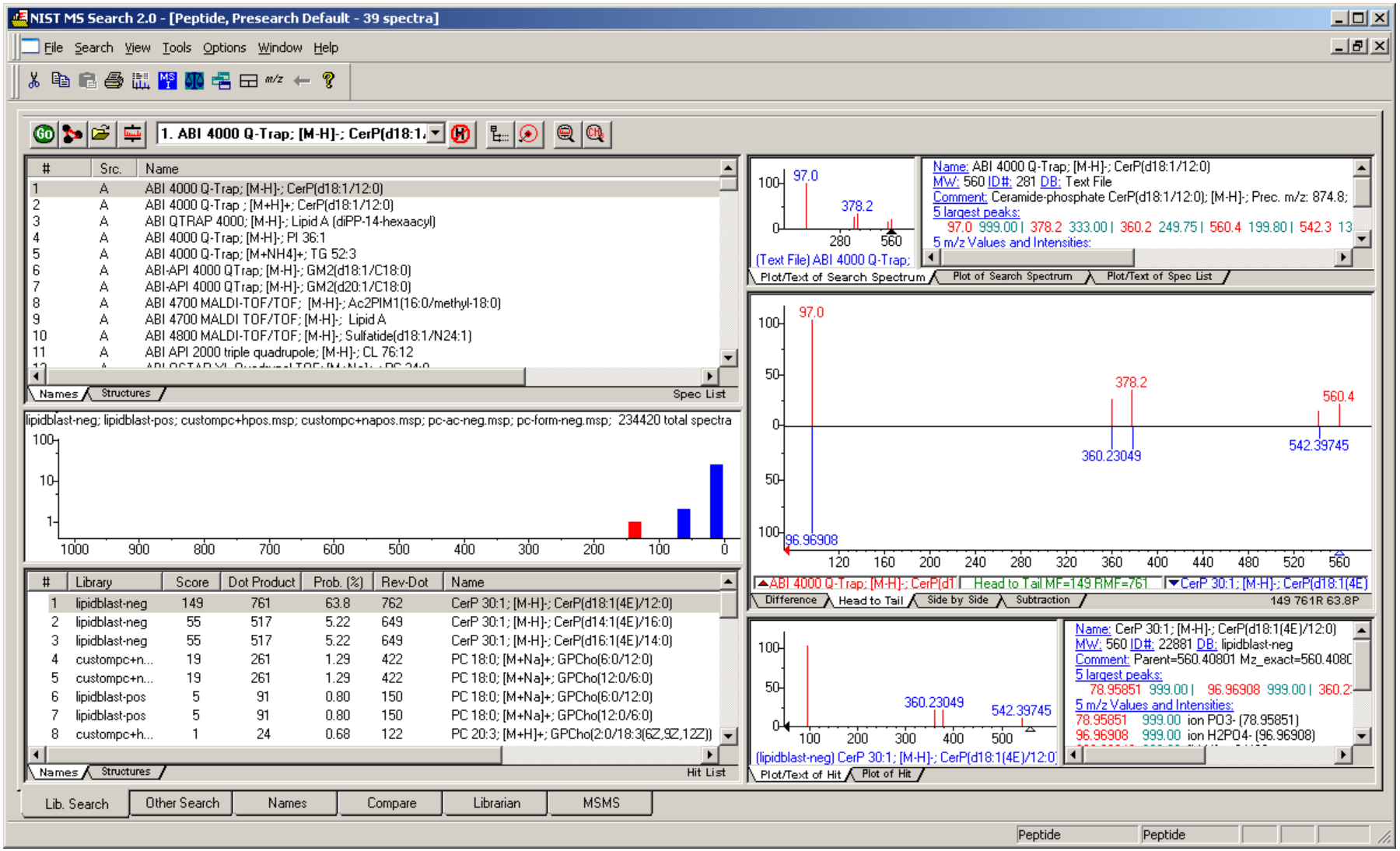


This is a special compiled version
NIST MS Search 2.0
The built date must be minimum May 2010
Version 2.0g 2011 produces slightly different hit scores.

The latest NIST.EXE is available from
http://peptide.nist.gov/
Search scores can change slightly with new versions.
NIST MS Search is an independent product from LipidBlast.

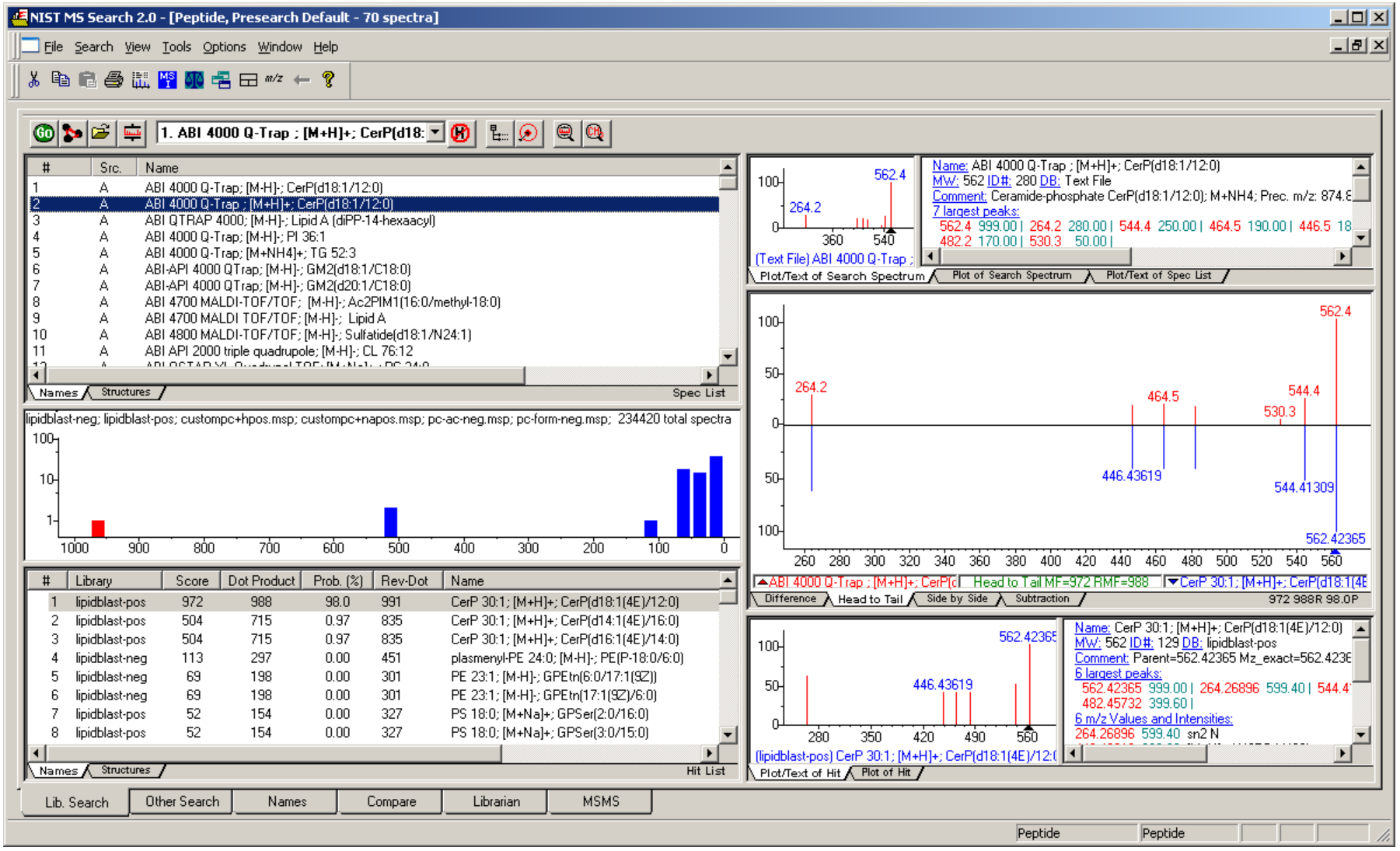


4000 Q-Trap mass spectrometer; [M-H]-
Ceramide-phosphate CerP(d18:1/12:0); [M-H]-; Prec. m/z: 874.8; LipidMaps http://www.lipidmaps.org/data/standards/standards.php?lipidclass=LMSP



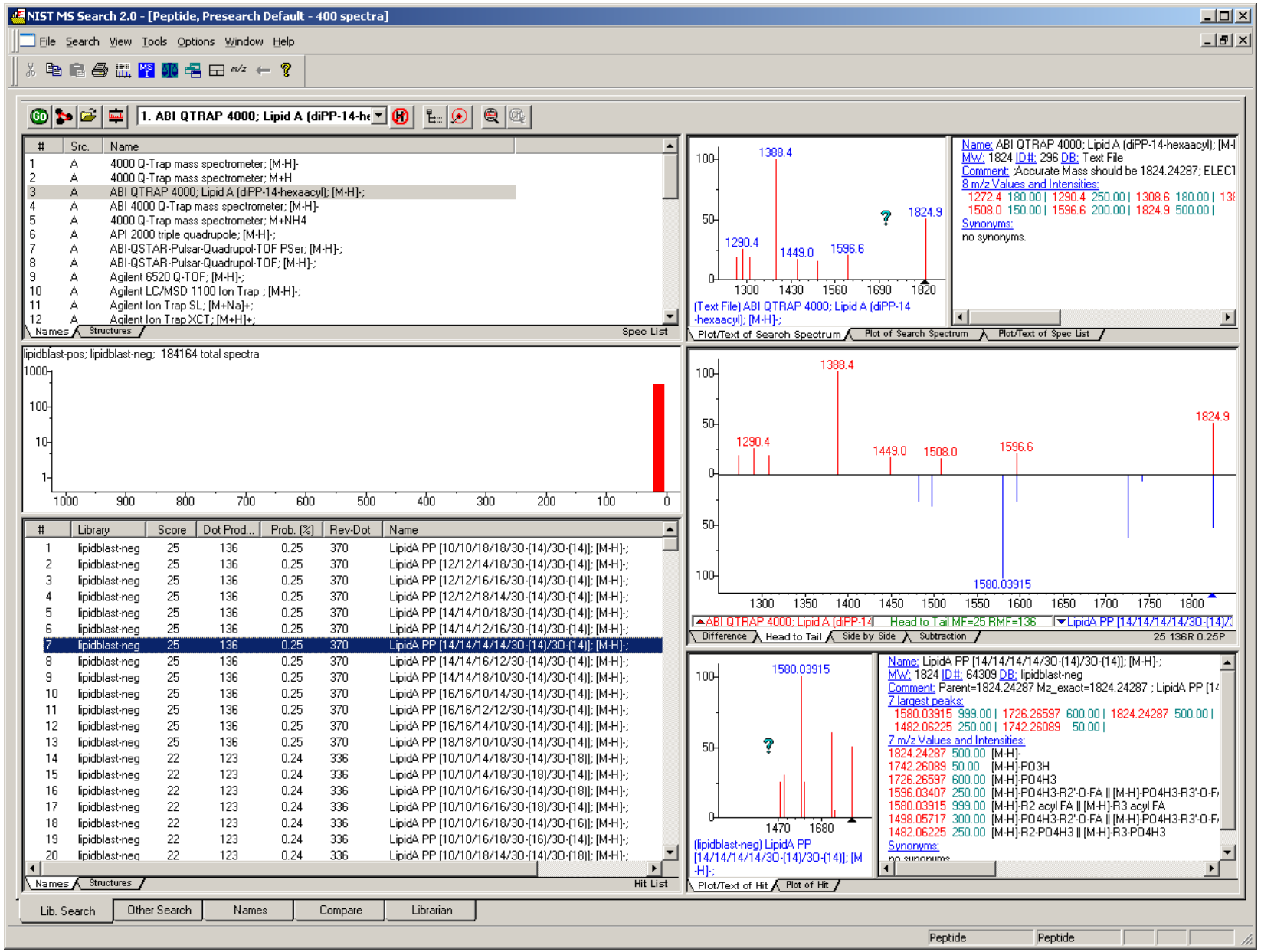
4000 Q-Trap mass spectrometer; M+H

Ceramide-phosphate CerP(d18:1/12:0); M+H; Prec. m/z: 874.8; LipidMaps http://www.lipidmaps.org/data/standards/standards.php?lipidclass=LMSP



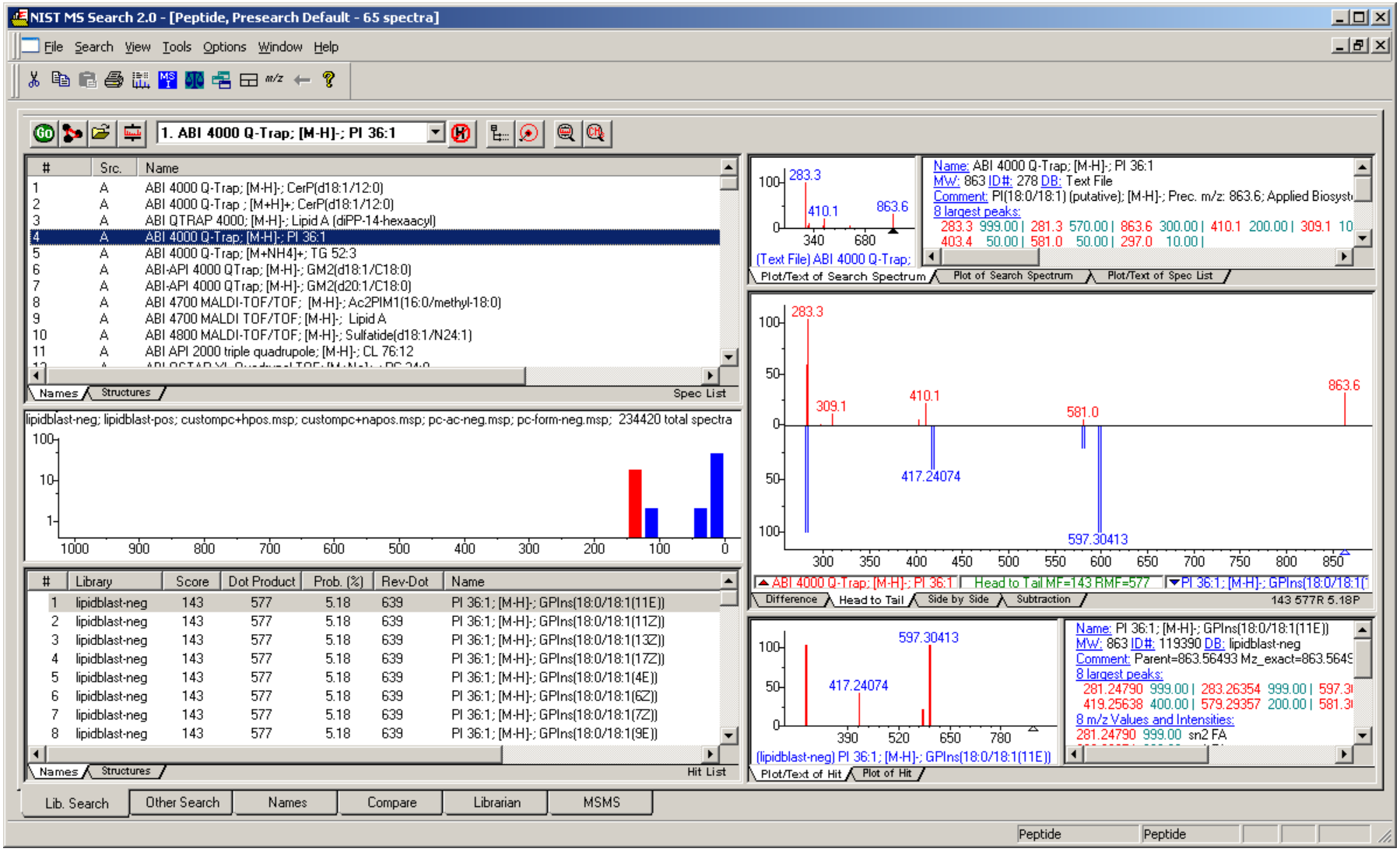
ABI QTRAP 4000; Lipid A (diPP-14-hexaacyl); [M-H]-;
Accurate Mass should be 1824.24287; ELECTROPHORESIS, Volume 29, Issue 10 (p 2171-2181) ;Characterization of intact lipopolysaccharides

0.8 precursor SET



Comment Curator: Precursor Search set to 0.8 Da (accurate mass not reported in publication)

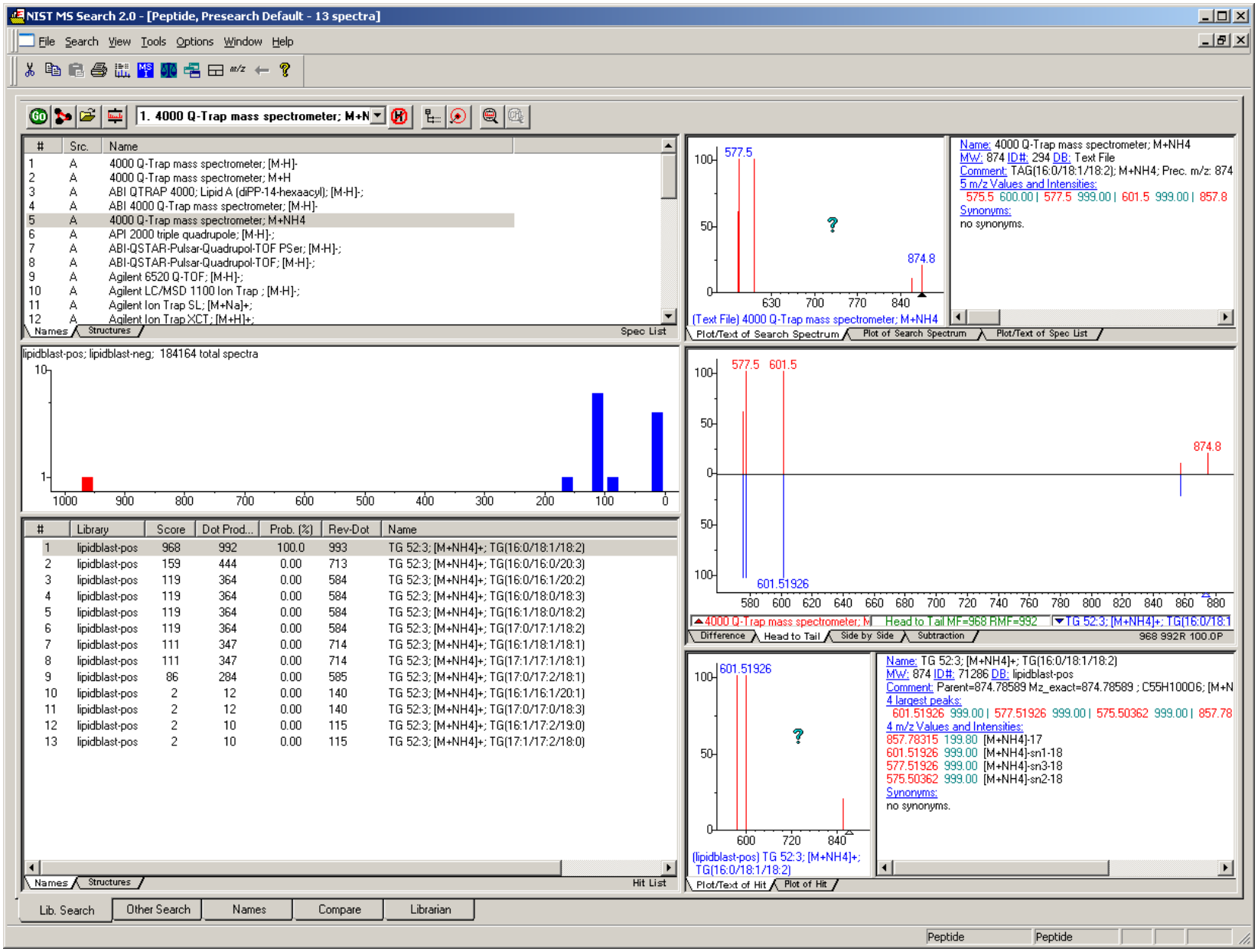
ABI 4000 Q-Trap mass spectrometer; [M-H]-
PI(18:0/18:1) (putative); [M-H]-; Prec. m/z: 863.6; Applied Biosystems/MDS Sciex;
Metabolomic identification of potential phospholipid biomarkers for chronic glomerulonephritis by using high performance liquid chromatography-mass spectrometry;
Lewen Jia, Chang Wang, Sumin Zhao, Xin Lu and Guowang Xu



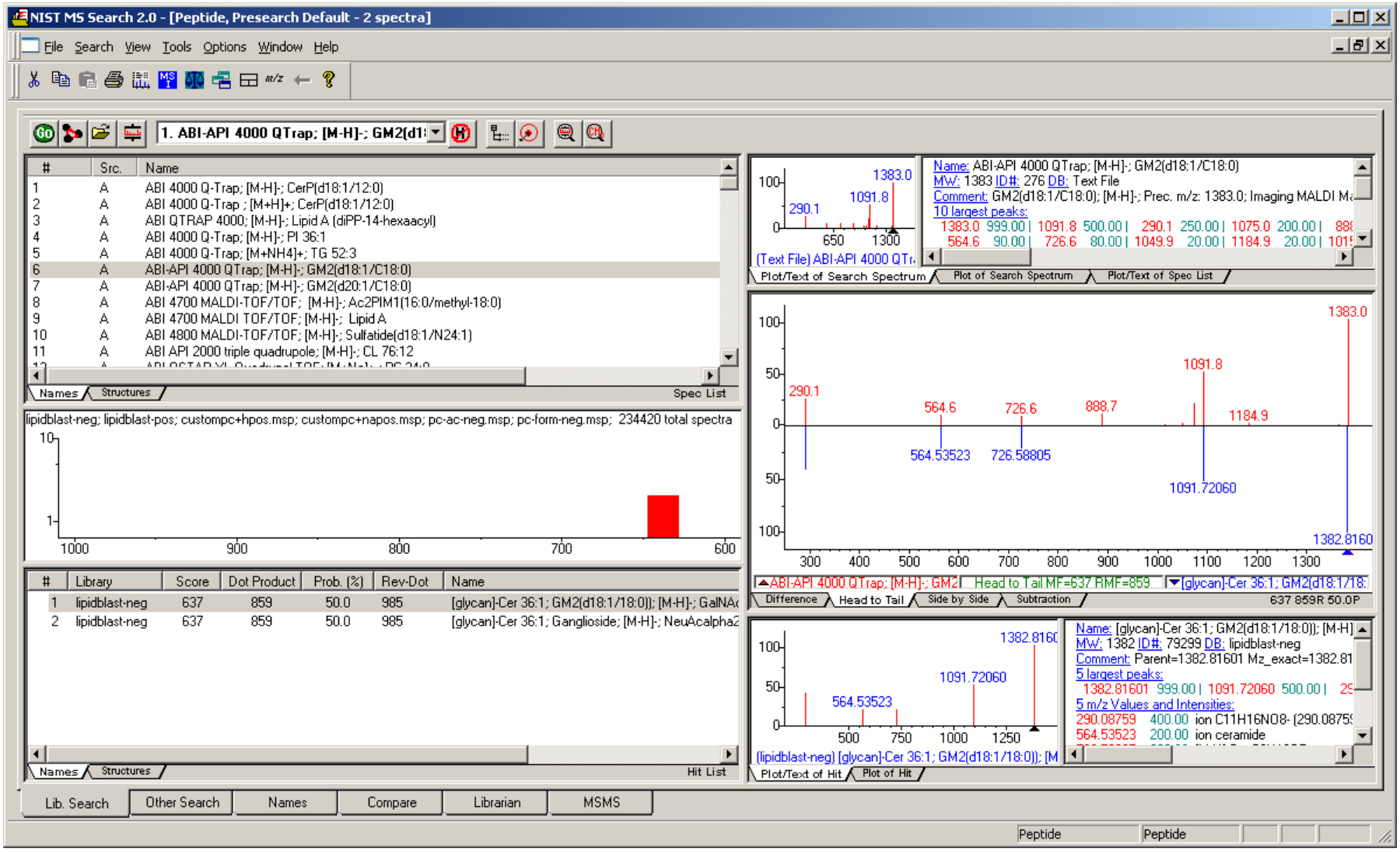
4000 Q-Trap mass spectrometer; M+NH4

TAG(16:0/18:1/18:2); M+NH4; Prec. m/z: 874.8; Detection of the abundance of diacylglycerolnext term and triacylglycerol molecular species in cells using neutral loss mass spectrometry; doi:10.1016/j.ab.2007.03.012; Robert C. Murphy, Corresponding Author Contact Information, E-mail

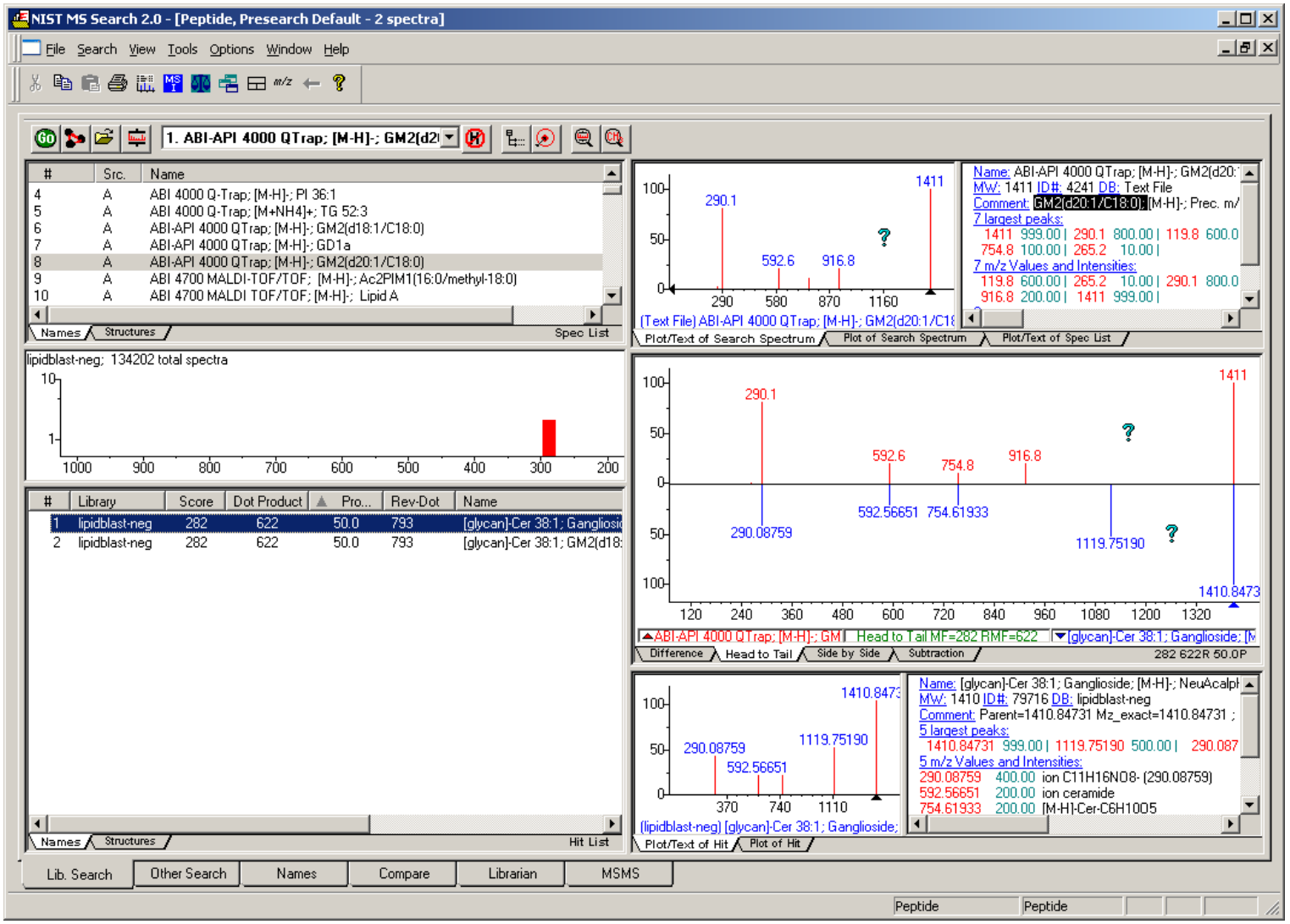
The Corresponding Author, Patrick F. James, Andrew M. McAnoy, Jessica Krank, Eva Duchoslav and Robert M. Barkley



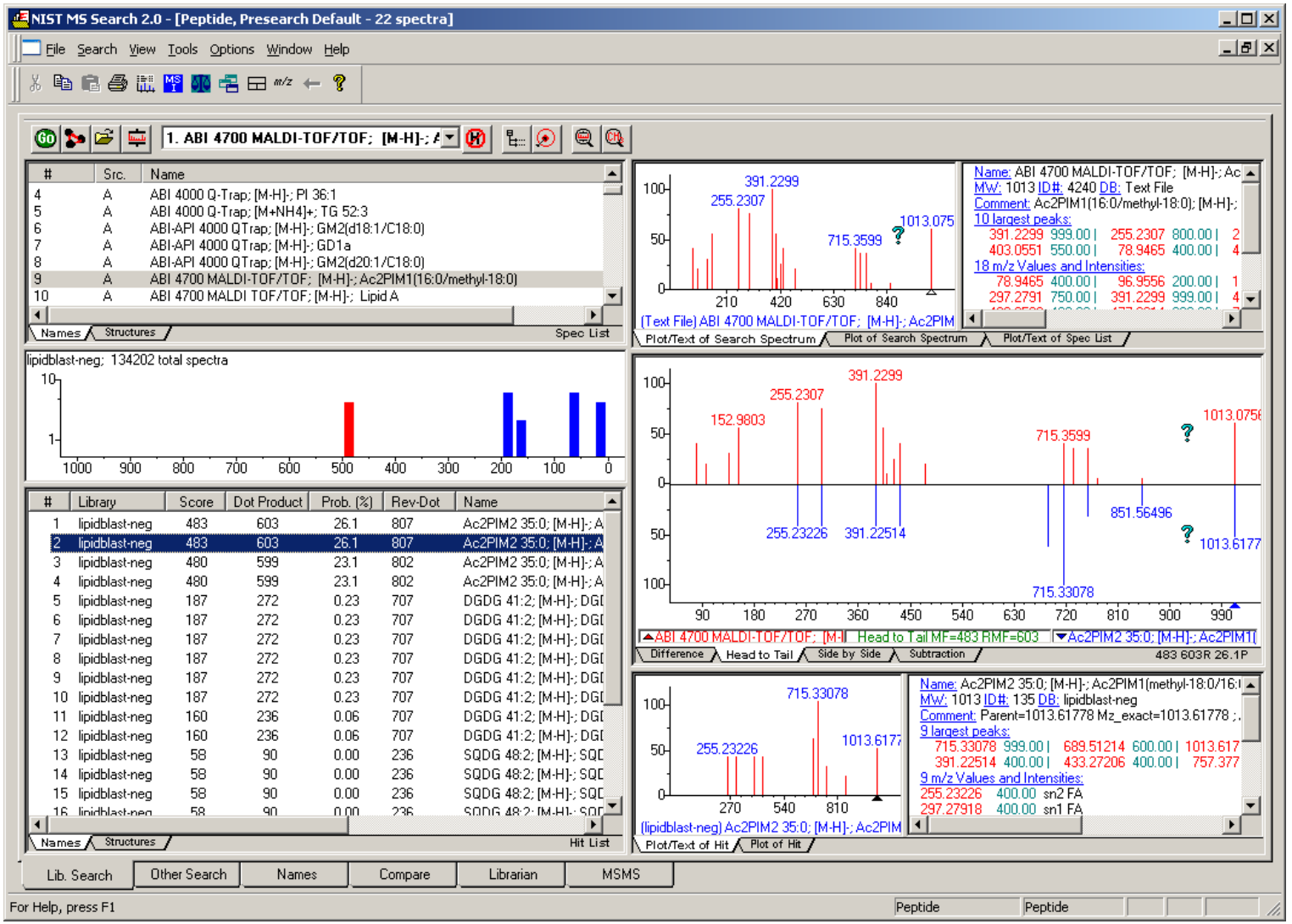
Name: ABI-API 4000 QTrap; [M-H]-; GM2(d18:1/C18:0)
MW: 1383 ID#: 276 DB: Text File
Comment: GM2(d18:1/C18:0); [M-H]-; Prec. m/z: 1383.0; Imaging MALDI Mass Spectrometry Using an Oscillating Capillary Nebulizer Matrix Coating System and Its Application to Analysis of Lipids in Brain from a Mouse Model of Tay-Sachs/Sandhoff Disease; Anal. Chem., 2008, 80 (8), pp 2780-2788; http://pubs.acs.org/doi/full/10.1021/ac702350g
10 largest peaks:



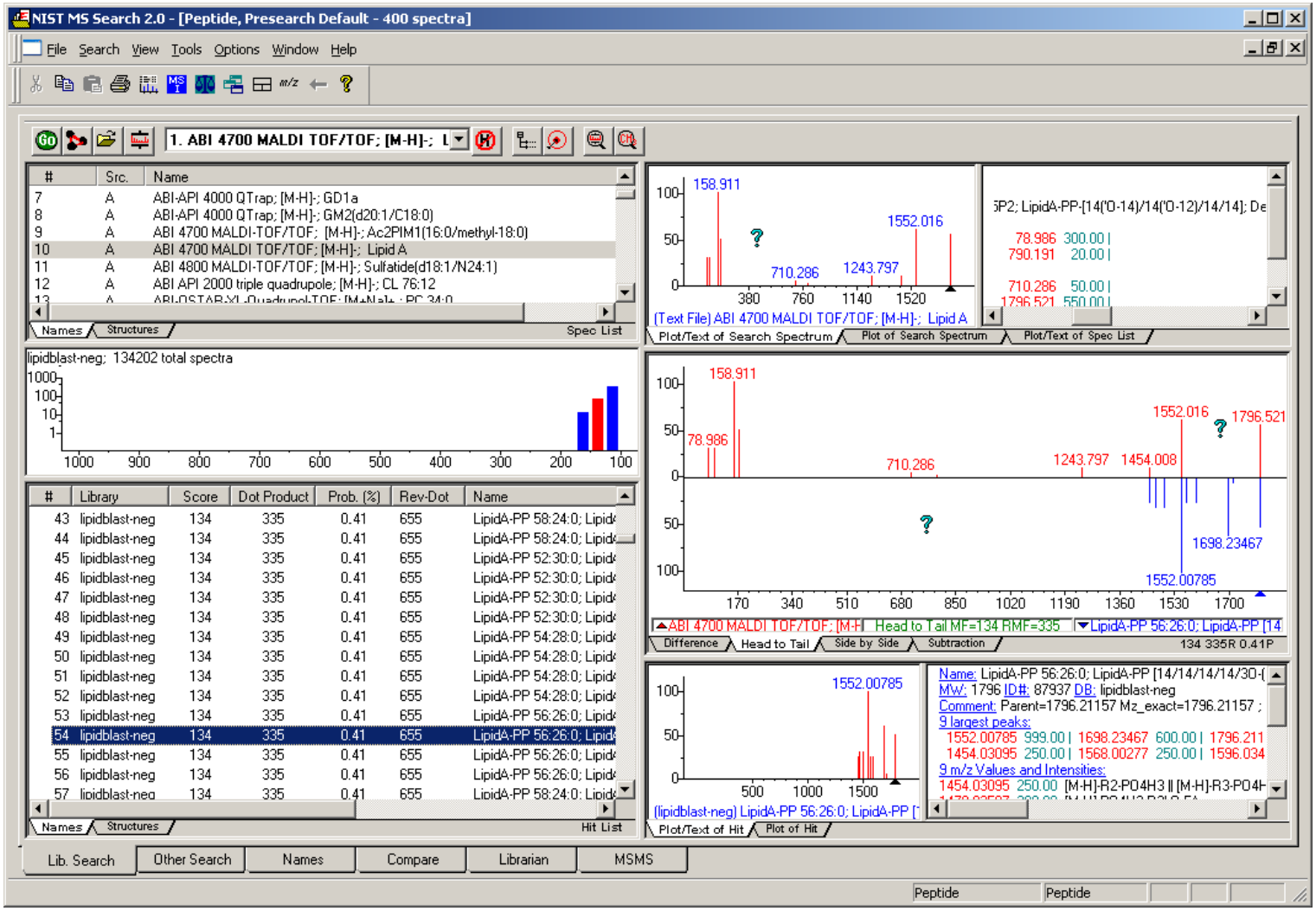
Name: ABI-API 4000 QTrap; [M-H]-; GM2(d20:1/C18:0)
MW: 1411 ID#: 4241 DB: Text File
Comment: GM2(d20:1/C18:0); [M-H]-; Prec. m/z: 1411; Imaging MALDI Mass Spectrometry of Sphingolipids Using an Oscillating Capillary Nebulizer Matrix Application System Series: Methods in Molecular Biology | Volume: 656 | Year: 2010 | Page ; 10.1007/978-1-60761-746-4_7



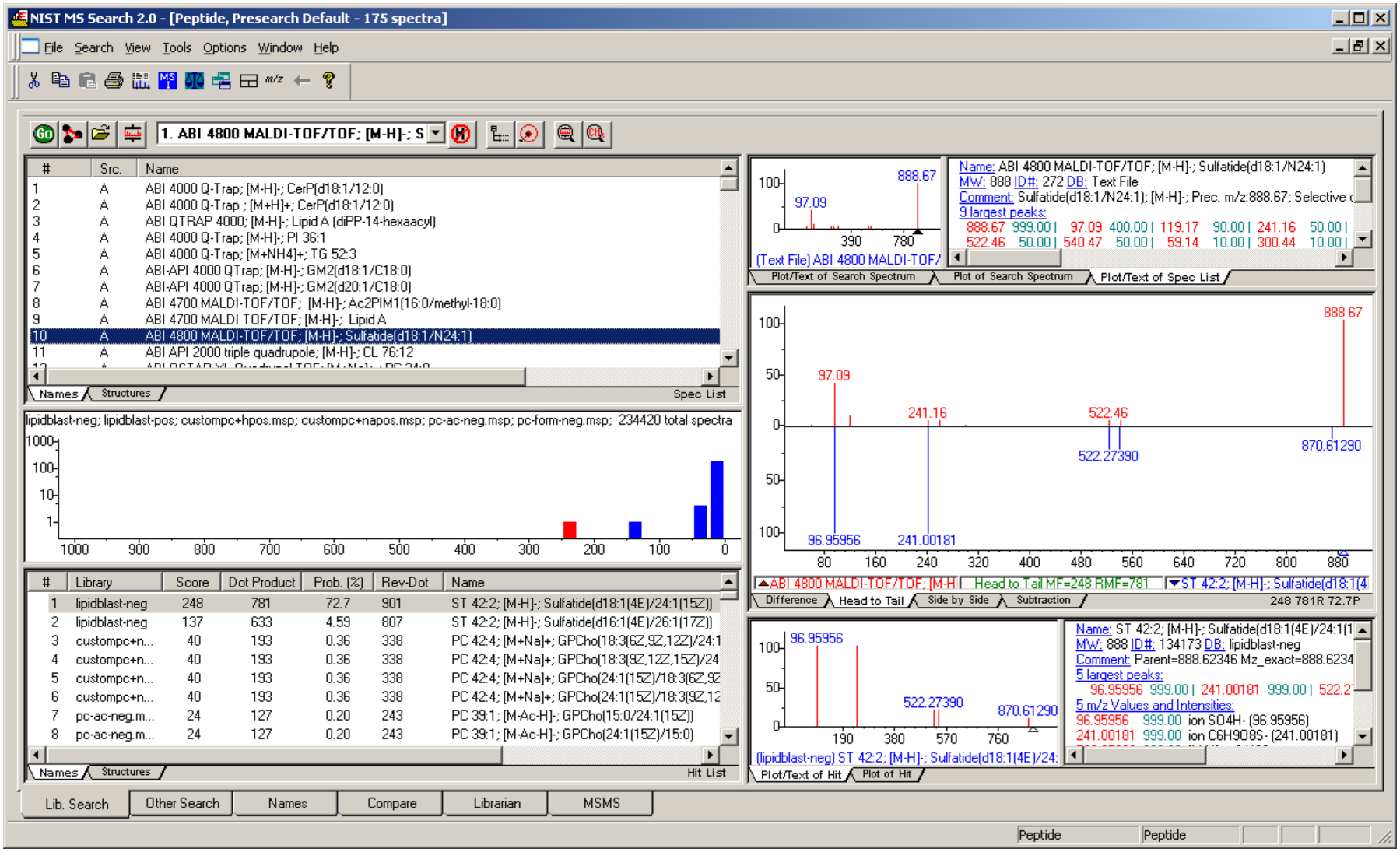
Name: ABI 4700 MALDI-TOF/TOF; [M-H]-; Ac2PIM1(16:0/methyl-18:0)
MW: 1013 ID#: 4240 DB: Text File
Comment: Ac2PIM1(16:0/methyl-18:0); [M-H]-; Prec. m/z:1013.63; Synthesis and Structure of Phosphatidylinositol Dimannoside; http://pubs.acs.org/doi/full/10.1021/jo0625599; Supplement



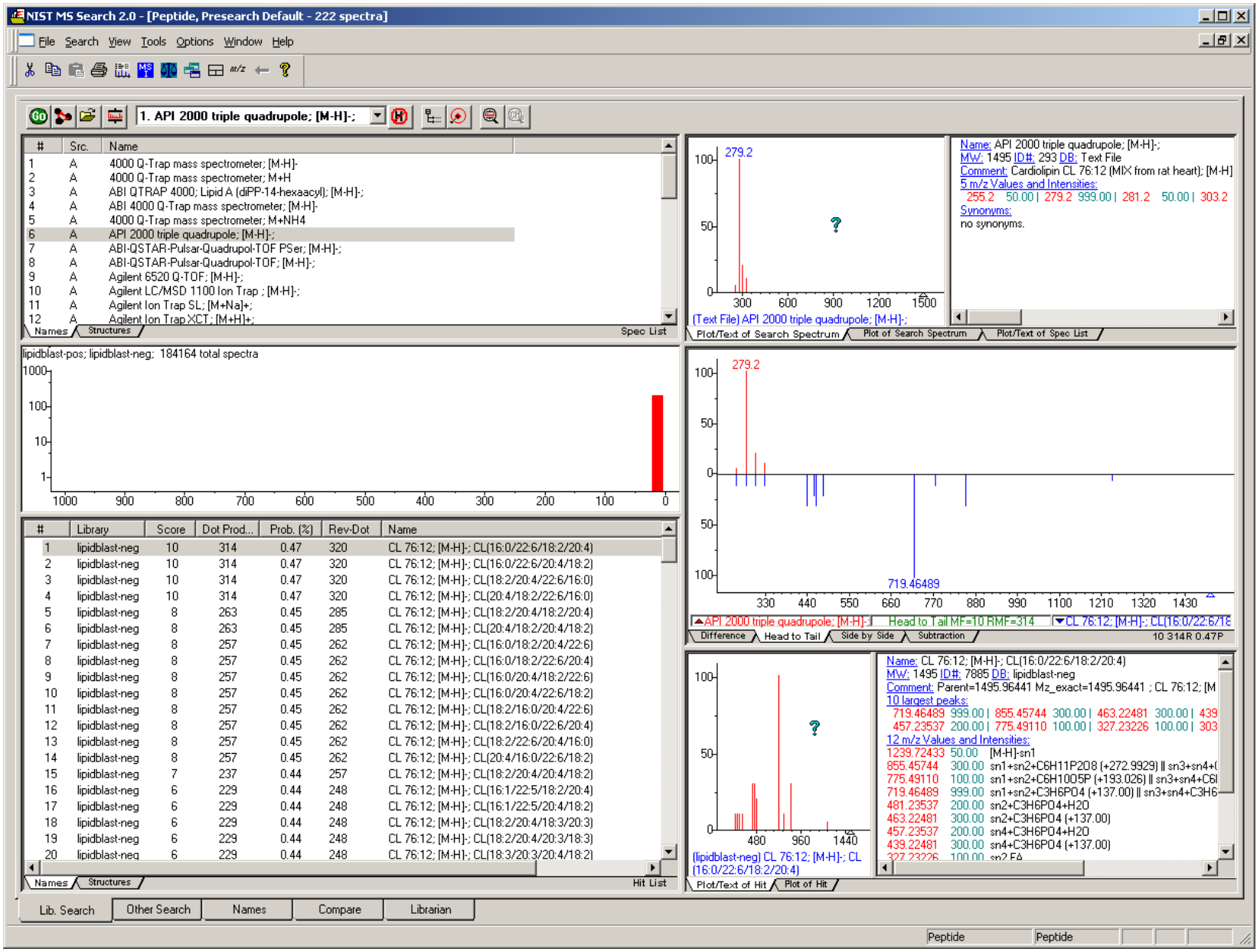
Name: ABI 4700 MALDI TOF/TOF; [M-H]-; Lipid A
MW: 1796 ID#: 4239 DB: Text File
Comment: Lipid A from E coli F583; [M-H]-; Prec. m/z: 1796.521; C94H178N2O25P2; LipidA-PP-[14('O-14)/14('O-12)/14/14]; Determination of pyrophosphorylated forms of lipid A in Gram-negative bacteria using a multivaried mass spectrometric approach; DOI: 10.1073/pnas.0800445105



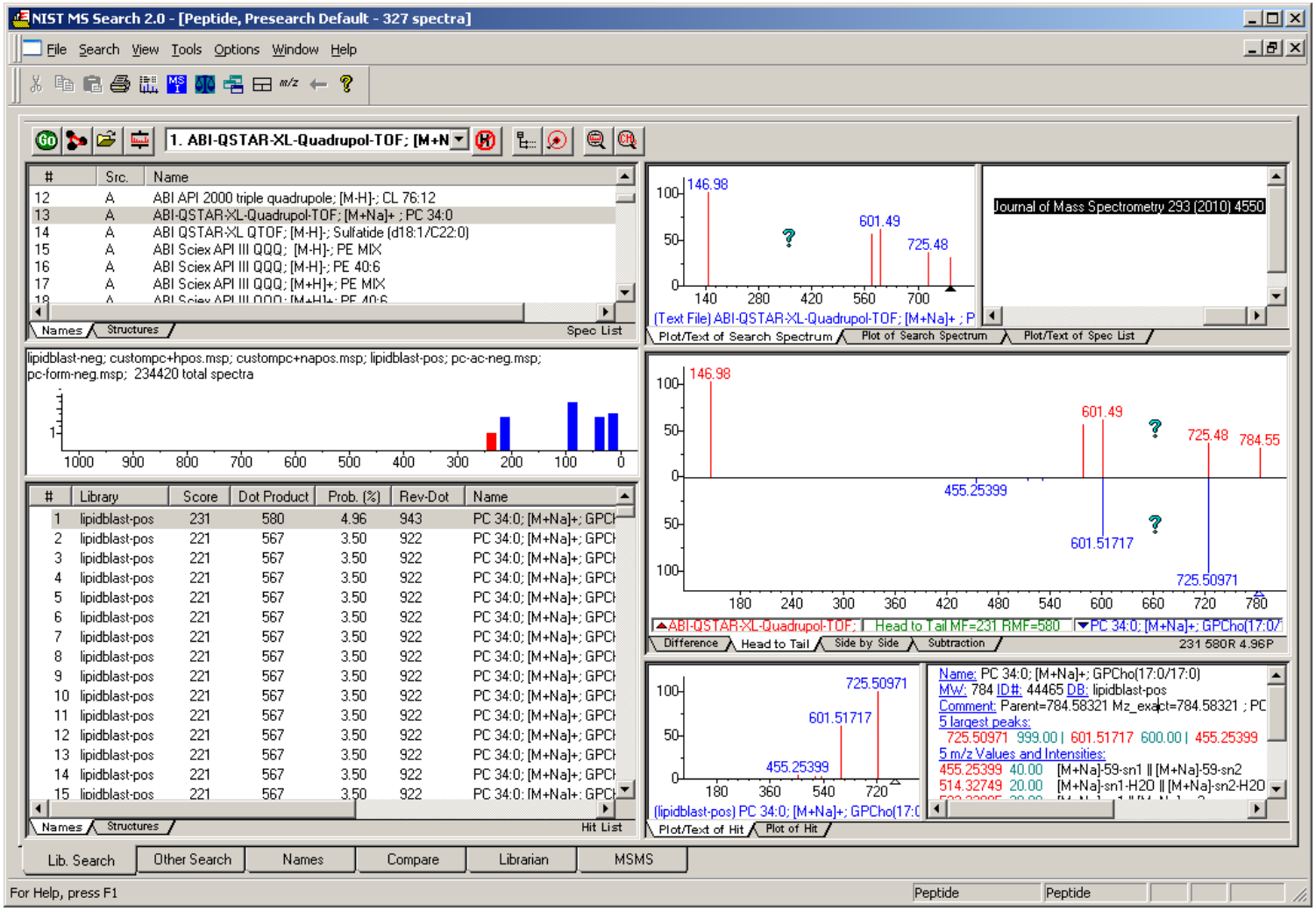
Name: ABI 4800 MALDI-TOF/TOF; [M-H]-; Sulfatide(d18:1/N24:1)
MW: 888 ID#: 272 DB: Text File
Comment: Sulfatide(d18:1/N24:1); [M-H]-; Prec. m/z:888.67; Selective desorption/ionization of sulfatides by MALDI-MS facilitated using 9- aminoacridine as matrix;Hua Cheng, Gang Sun, Kui Yang, Richard W. Gross, and Xianlin Han;Journal of Lipid Research, Vol. 51, 1599-1609, June 2010
9 largest peaks:



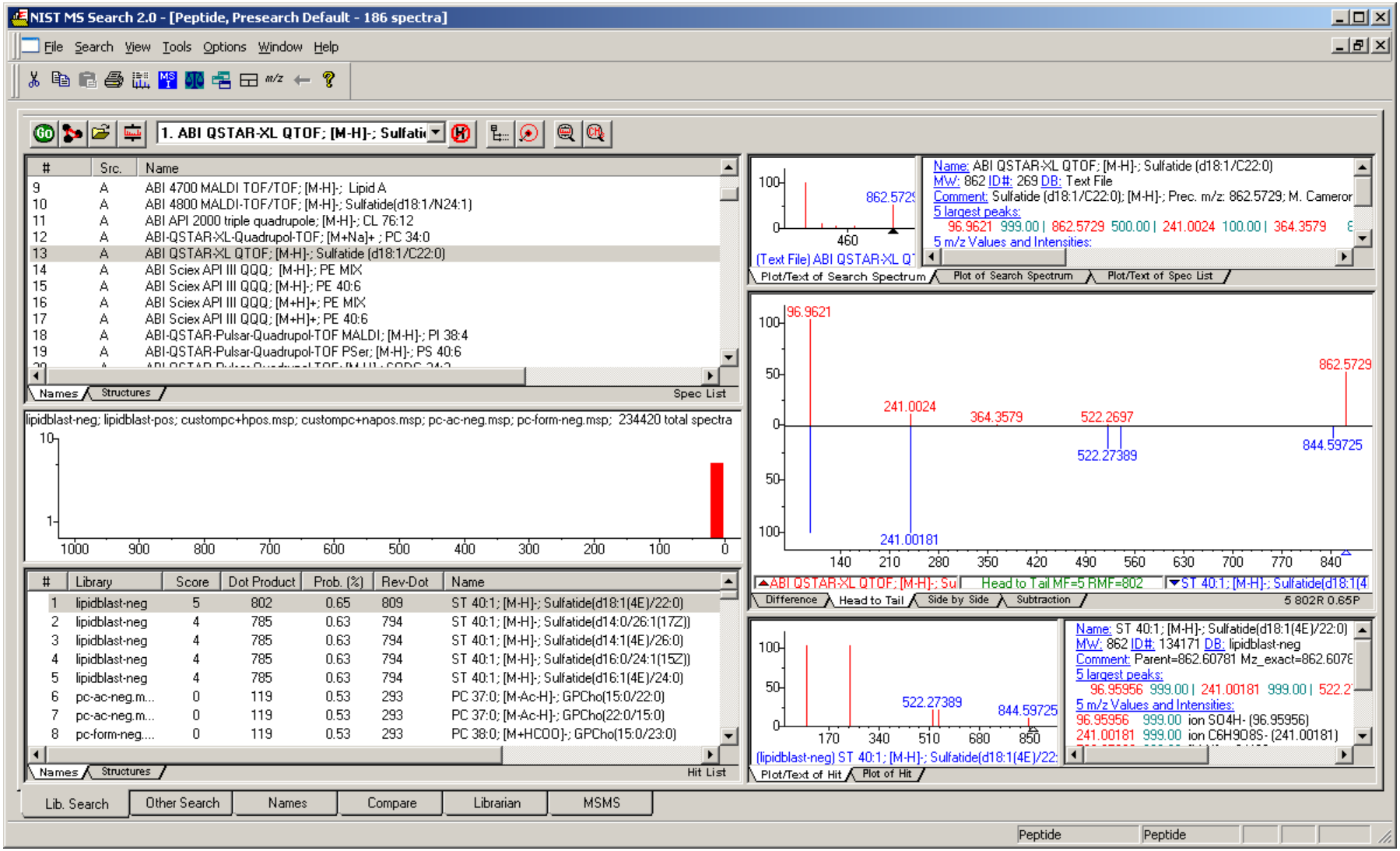
API 2000 triple quadrupole; [M-H]-;
Cardiolipin CL 76:12 (MIX from rat heart); [M-H]-; Prec. m/z: 1495.97;
Journal of Lipid ResearchVolume 46, 2005;
Quantitation of cardiolipin molecular species in spontaneously hypertensive heart failure rats using electrospray ionization mass spectrometry



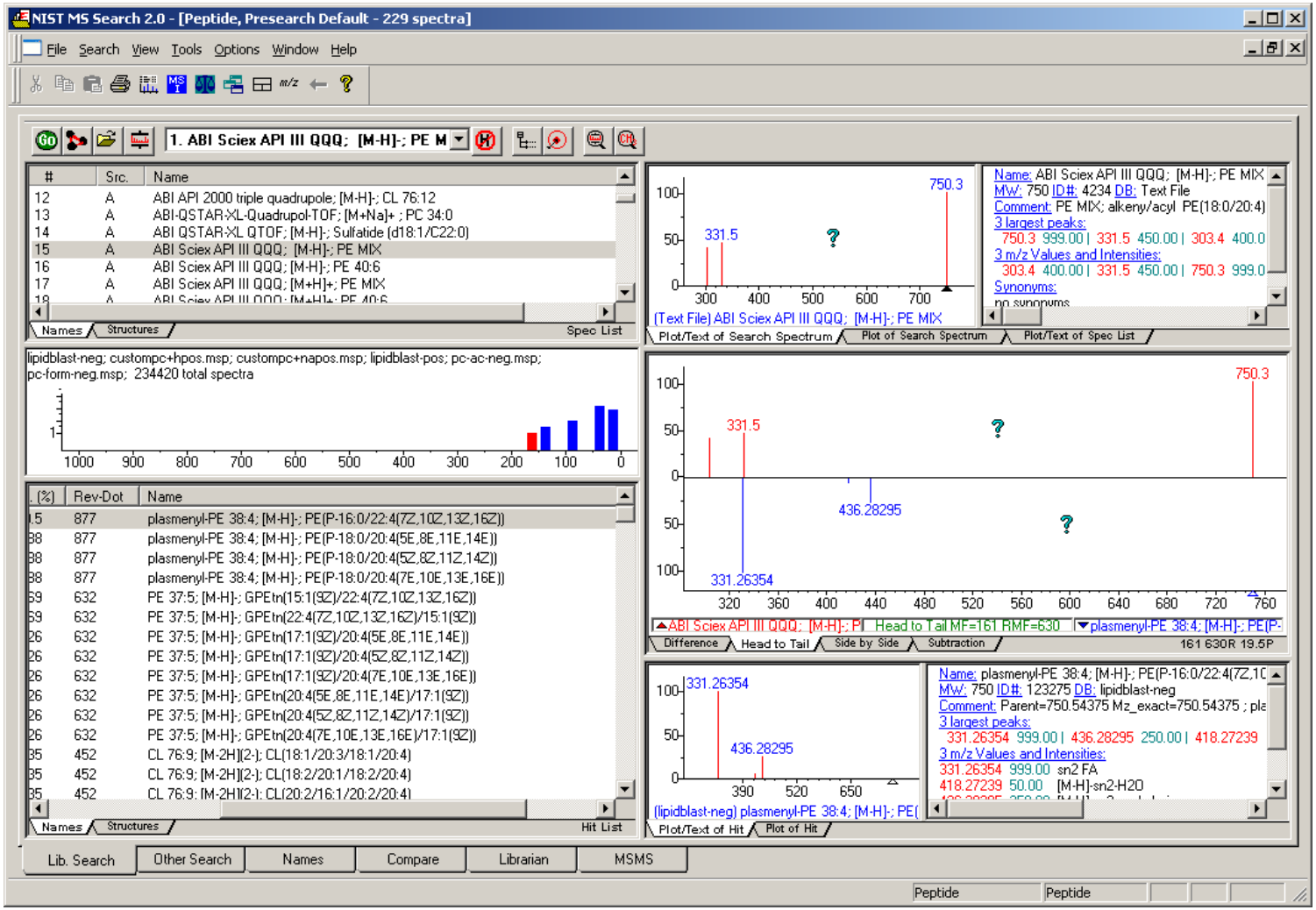
Name: ABI-QSTAR-XL-Quadrupol-TOF; [M+Na]+ ; PC 34:0
MW: N/A ID#: 4236 DB: Text File
Comment: PC 34:0; [M+Na]+ ; Prec. m/z: 784.55; Application of electrospray ionization mass spectrometry to characterize glycerophospholipids in Francisella tularensis subsp. novicida;X. Wang et al. / International Journal of Mass Spectrometry 293 (2010) 4550



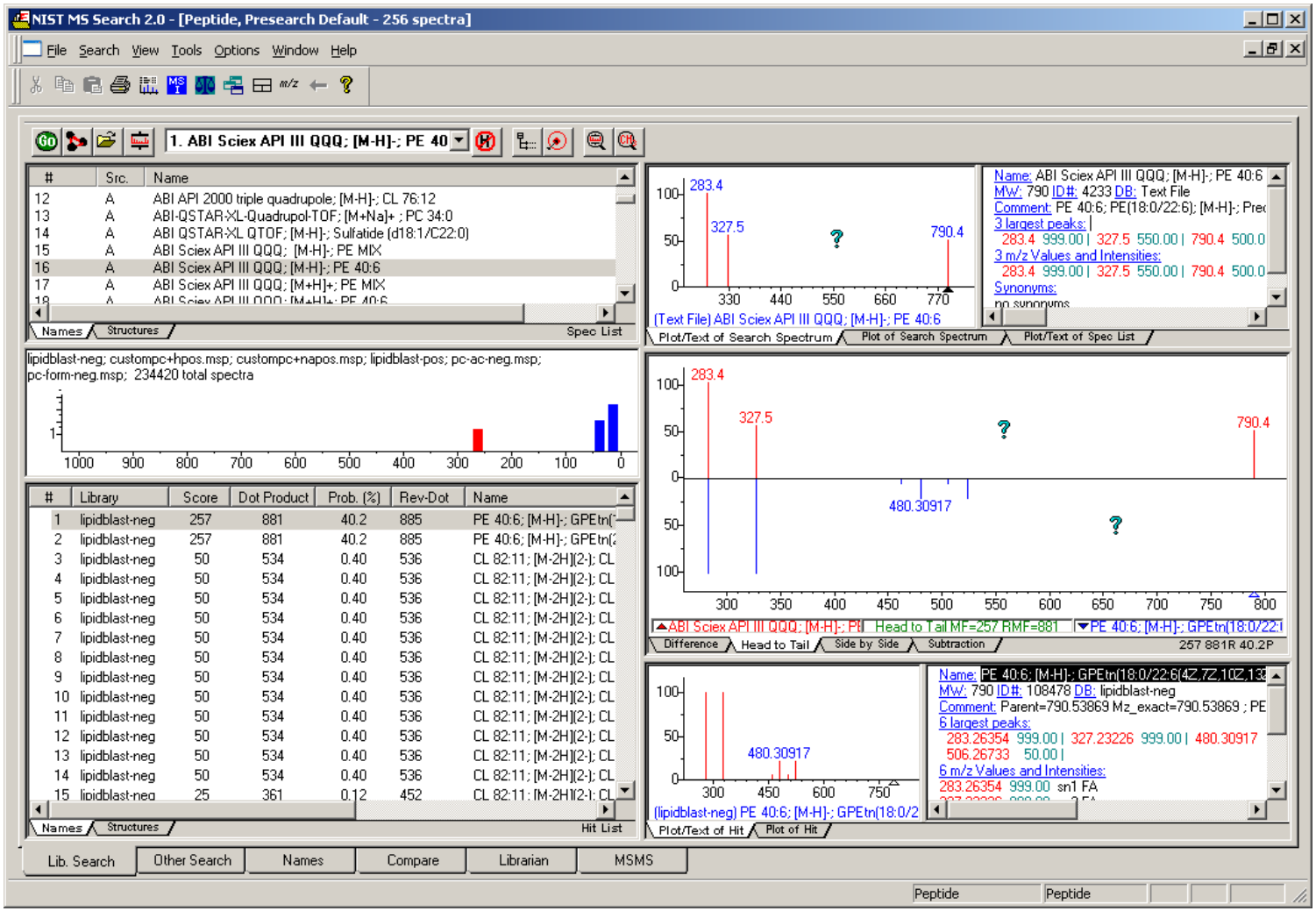
Name: ABI QSTAR-XL QTOF; [M-H]-; Sulfatide (d18:1/C22:0)
MW: 862 ID#: 269 DB: Text File
Comment: Sulfatide (d18:1/C22:0); [M-H]-; Prec. m/z: 862.5729; M. Cameron Sullards, Jeremy C. Allegood, and Alfred H. Merrill, Jr.; Identification and Structure Determination of Sulfatides using Chip-based NanoESI with Hybrid Q-TOF MS and MS/MS;
5 largest peaks:



Name: ABI Sciex API III QQQ; [M-H]-; PE MIX not found
MW: 750 ID#: 4234 DB: Text File
Comment: PE MIX; alkeny/acyl PE(18:0/20:4) and PE(16:0/22:4); [M-H]-; Prec. m/z:750.3; JL Kerwin, AR Tuininga, and LH Ericsson; Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry; J. Lipid Res., Jun 1994; 35: 1102 - 1114.

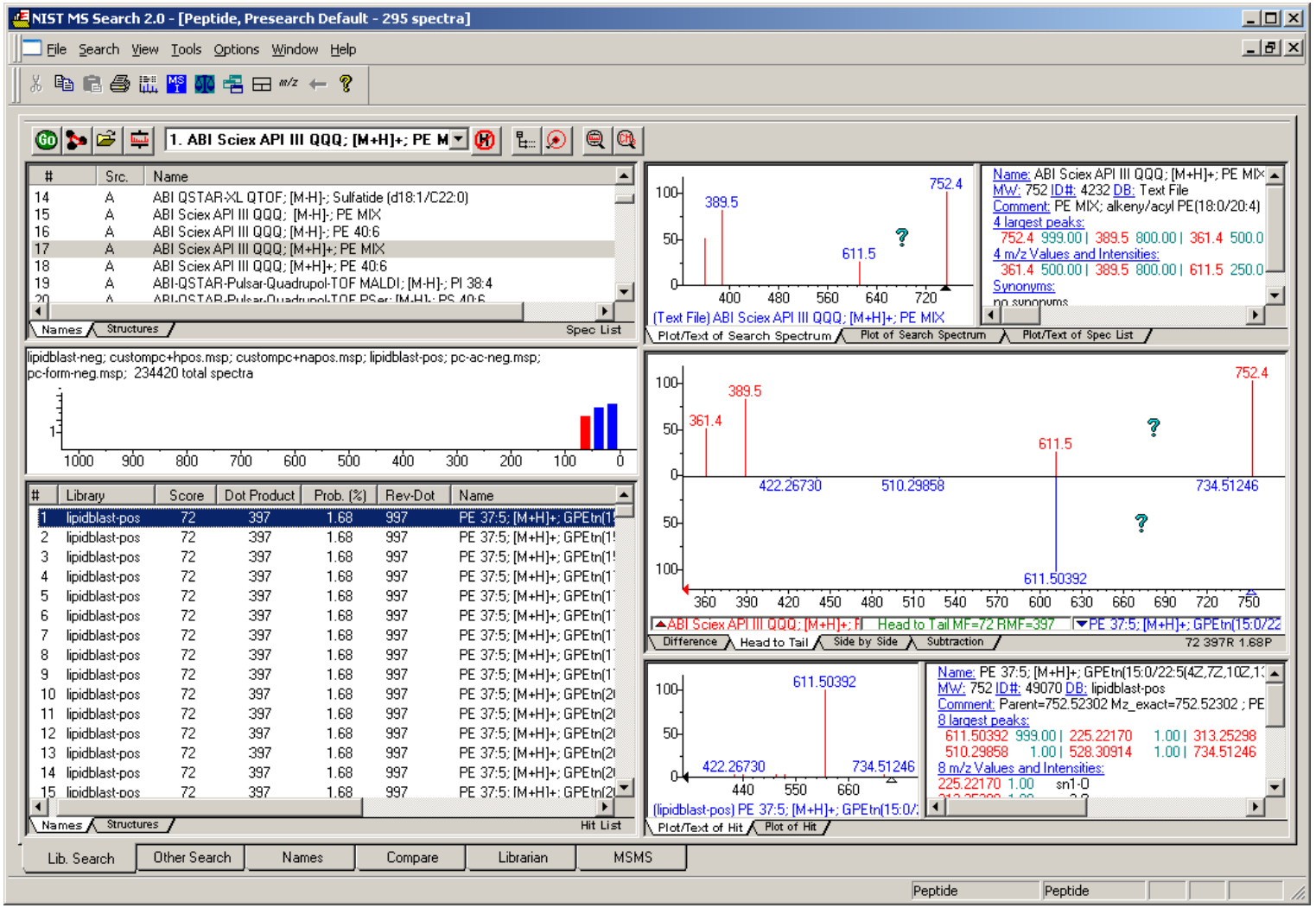


Name: ABI Sciex API III QQQ; [M-H]-; PE 40:6
MW: 790 ID#: 4233 DB: Text File
Comment: PE 40:6; PE(18:0/22:6); [M-H]-; Prec. m/z:790.4; JL Kerwin, AR Tuininga, and LH Ericsson; Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry; J. Lipid Res., Jun 1994; 35: 1102 - 1114.

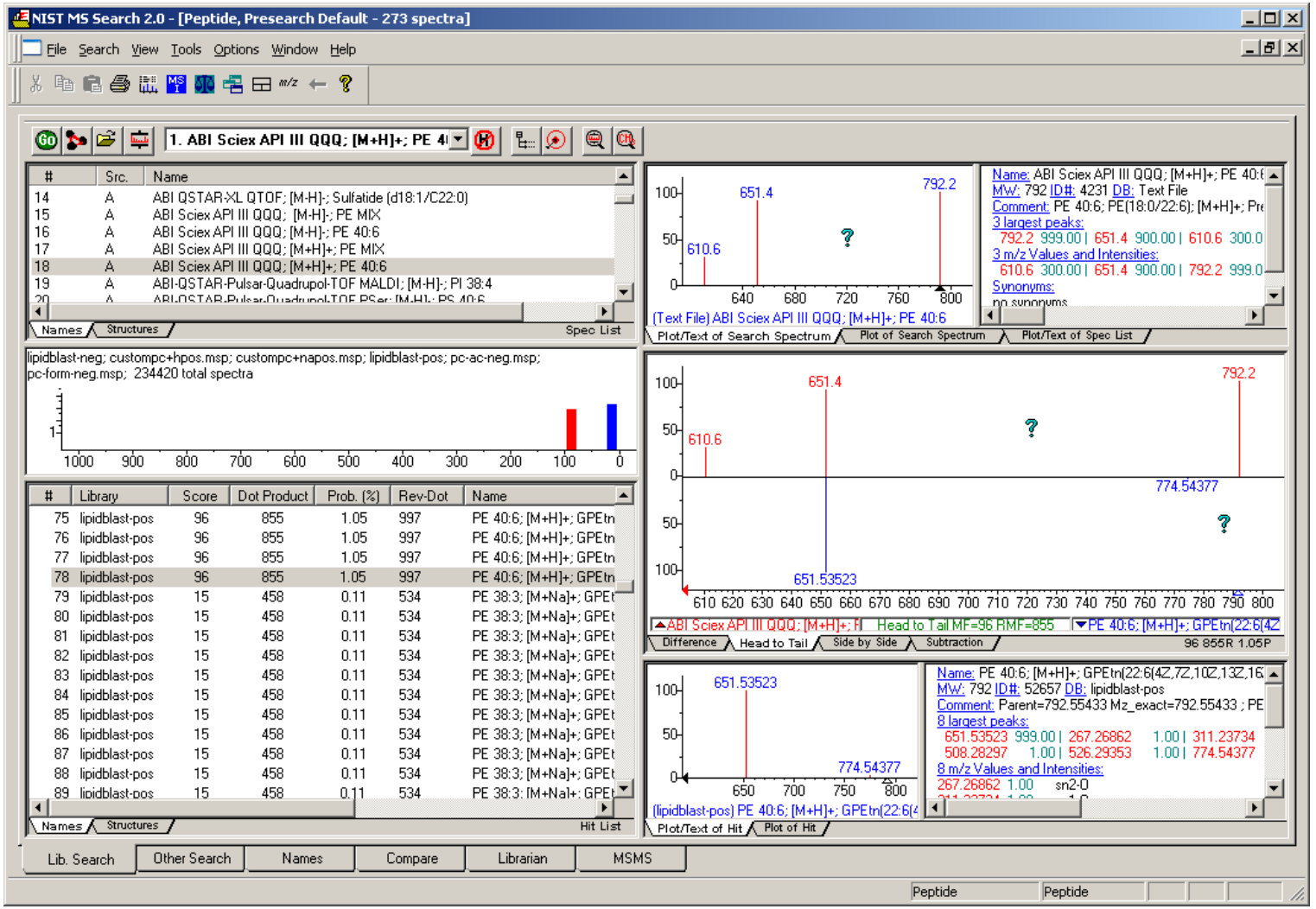


Name: ABI Sciex API III QQQ; [M+H]+; PE MIX
MW: 752 ID#: 4232 DB: Text File
Comment: PE MIX; alkeny/acyl PE(18:0/20:4) and PE(16:0/22:4) alkenyl-acyl PE; [M+H]+; Prec. m/z:752.4; JL Kerwin, AR Tuininga, and LH Ericsson; Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry; J. Lipid Res., Jun 1994; 35: 1102 - 1114.

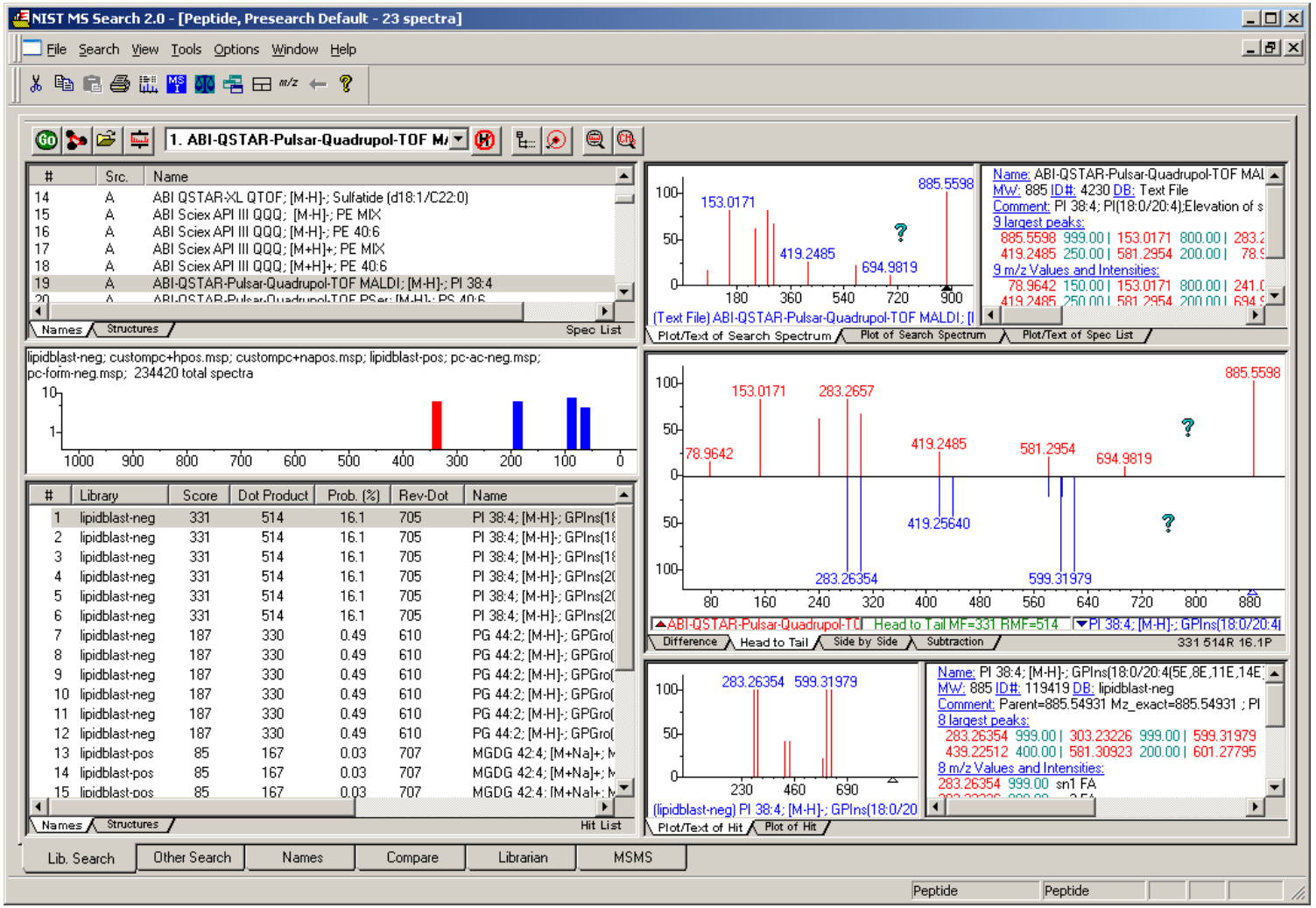
not found



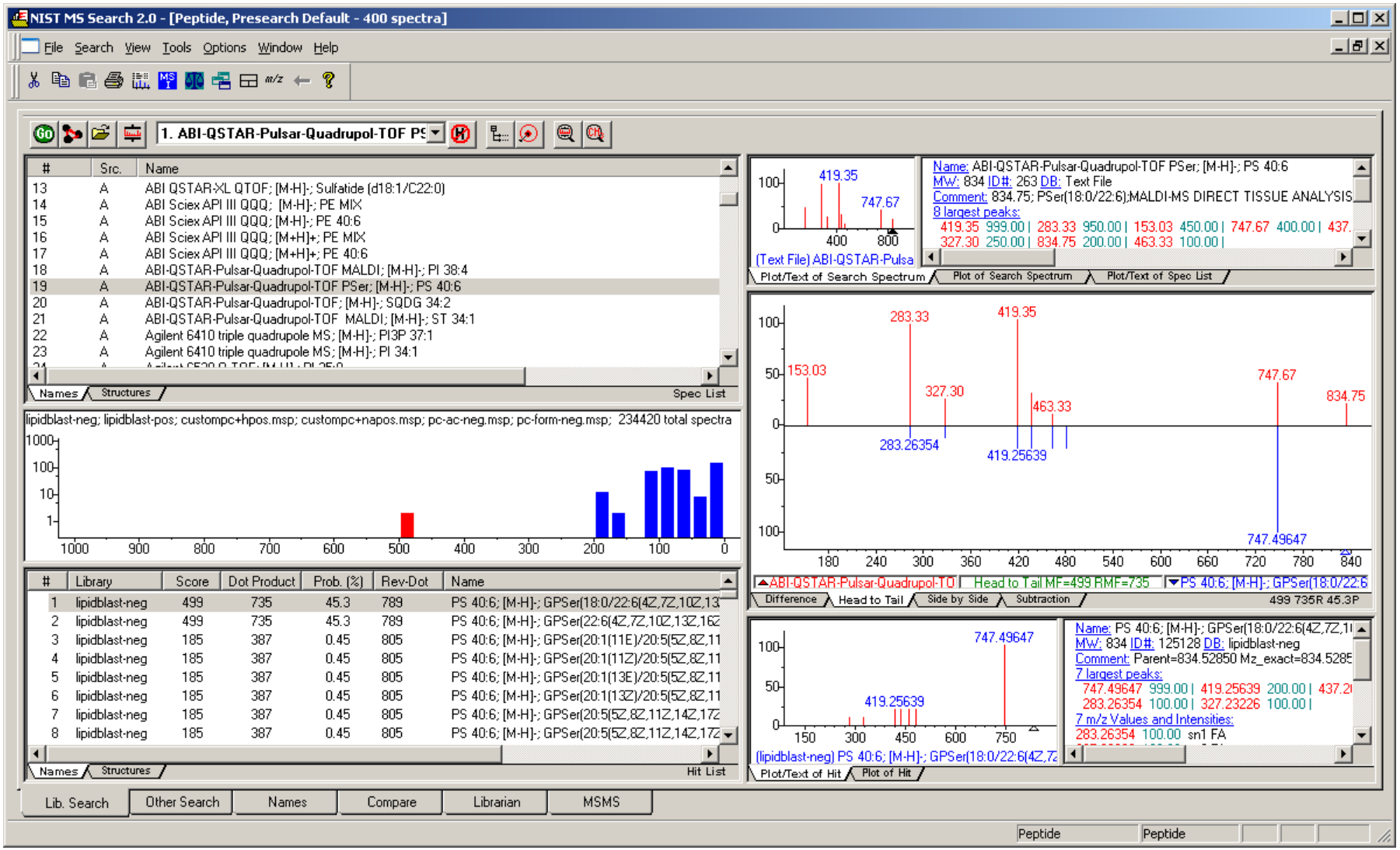
Name: ABI Sciex API III QQQ; [M+H]+; PE 40:6
MW: 792 ID#: 4231 DB: Text File
Comment: PE 40:6; PE(18:0/22:6); [M+H]+; Prec. m/z:792.2; JL Kerwin, AR Tuininga, and LH Ericsson; Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry; J. Lipid Res., Jun 1994; 35: 1102 - 1114.



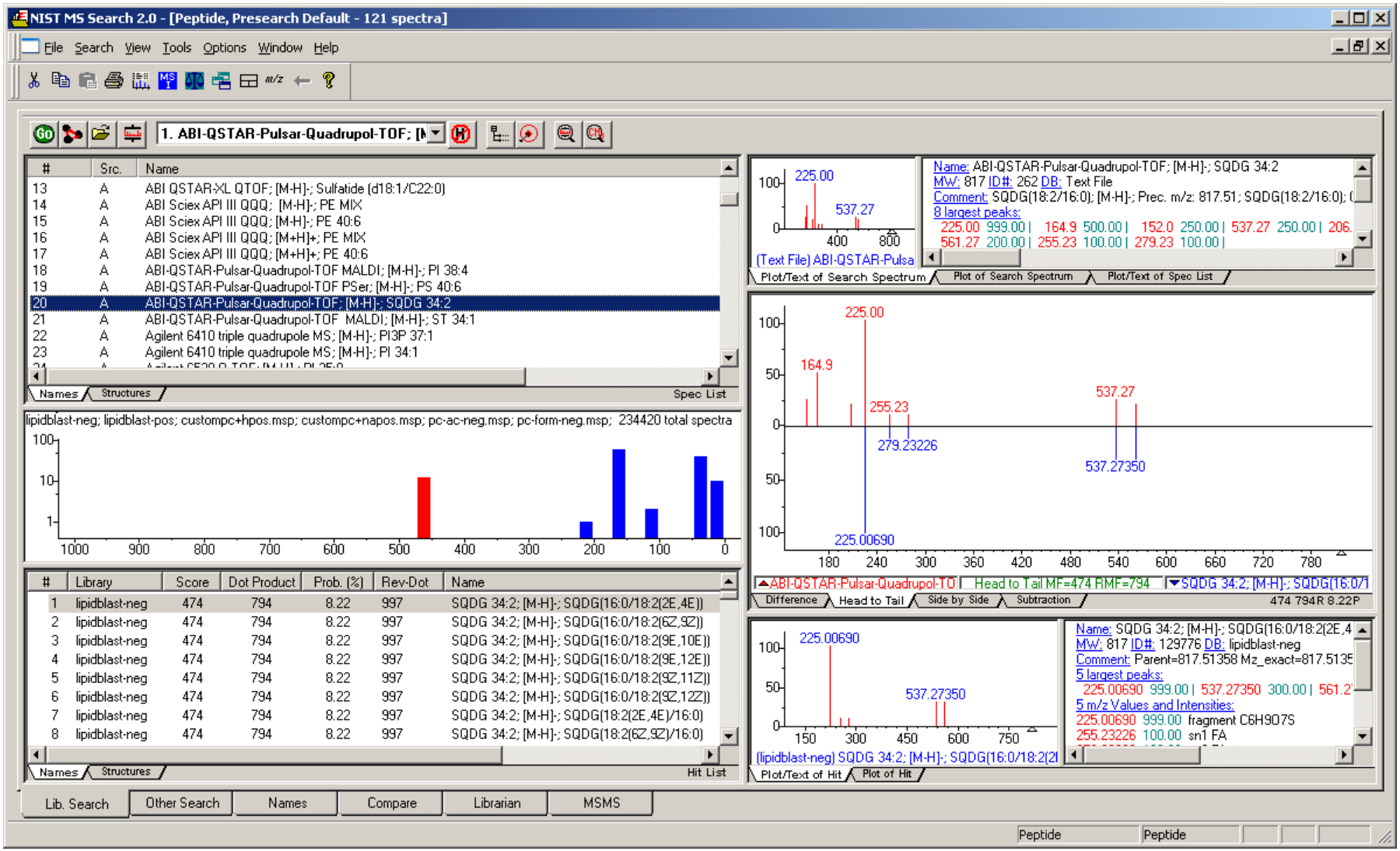
Name: ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H]-; PI 38:4
MW: 885 ID#: 4230 DB: Text File
Comment: PI 38:4; PI(18:0/20:4);Elevation of sulfatides in ovarian cancer: An integrated transcriptomic and lipidomic analysis including tissue-imaging mass spectrometry;;doi:10.1186/1476-4598-9-186



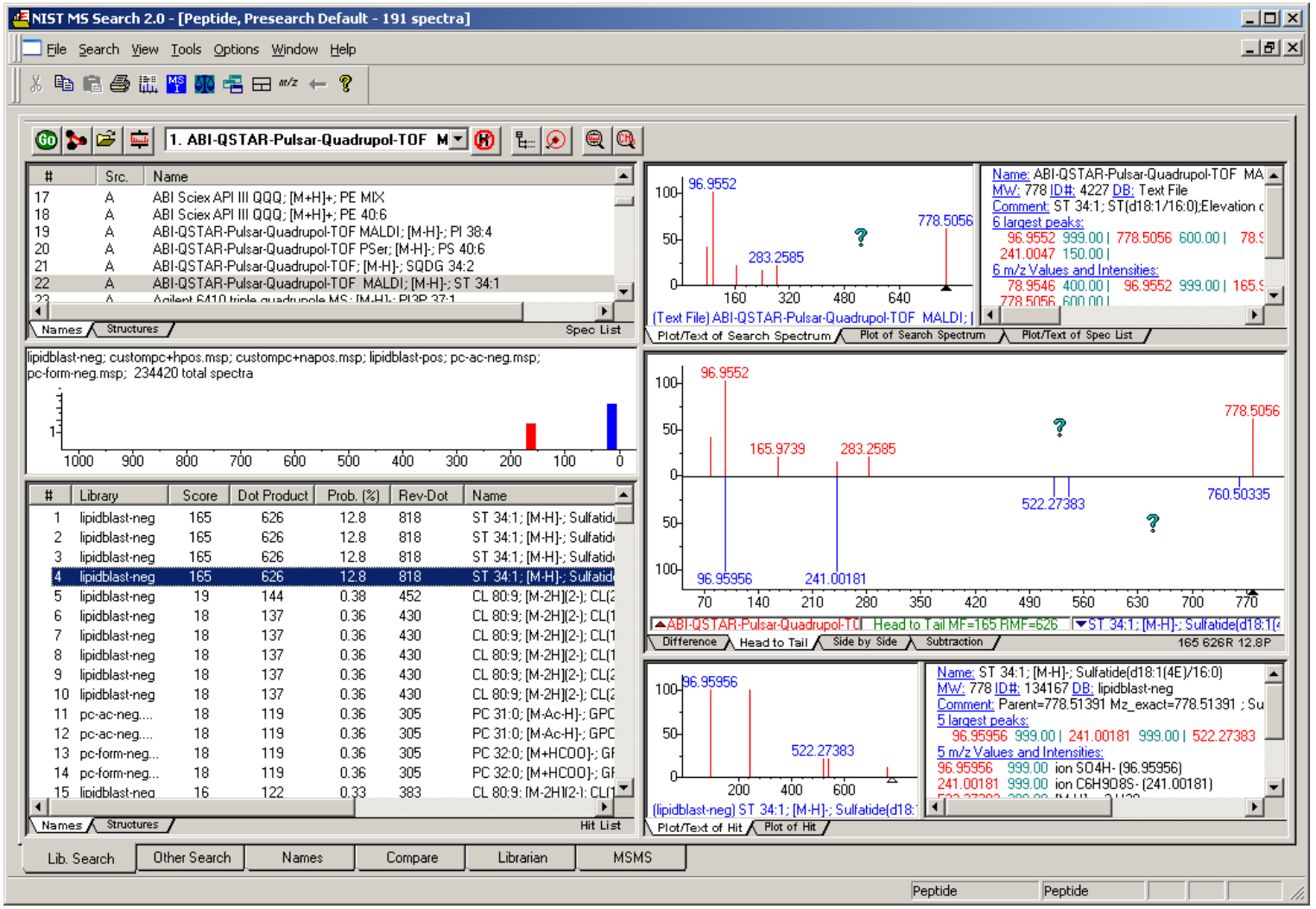
Name: ABI-QSTAR-Pulsar-Quadrupol-TOF PSer; [M-H]-; PS 40:6
MW: 834 ID#: 263 DB: Text File
Comment: 834.75; PSer(18:0/22:6);MALDI-MS DIRECT TISSUE ANALYSIS OF PROTEINS:IMPROVING SIGNAL SENSITIVITY USING ORGANIC TREATMENTS;R. Lemaire, M. Wisztorski, A. Desmons, J.C. Tabet, R. Day, M.Salzet, I. Fournier;DOI : 10.1021/ac060565z
8 largest peaks:



Name: ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H]-; SQDG 34:2
MW: 817 ID#: 262 DB: Text File
Comment: SQDG(18:2/16:0); [M-H]-; Prec. m/z: 817.51; SQDG(18:2/16:0); Characterization by high-performance liquid chromatography/electrospray ionization quadrupole time-of-flight mass spectrometry of the lipid fraction of Spirulina platensis pressurized ethanol extract; Rapid Commun. Mass Spectrom. 2007; 21: 1729-1738;Miguel Herrero, Maria J. Vicente, Alejandro Cifuentes and Elena Ibanez
8 largest peaks:

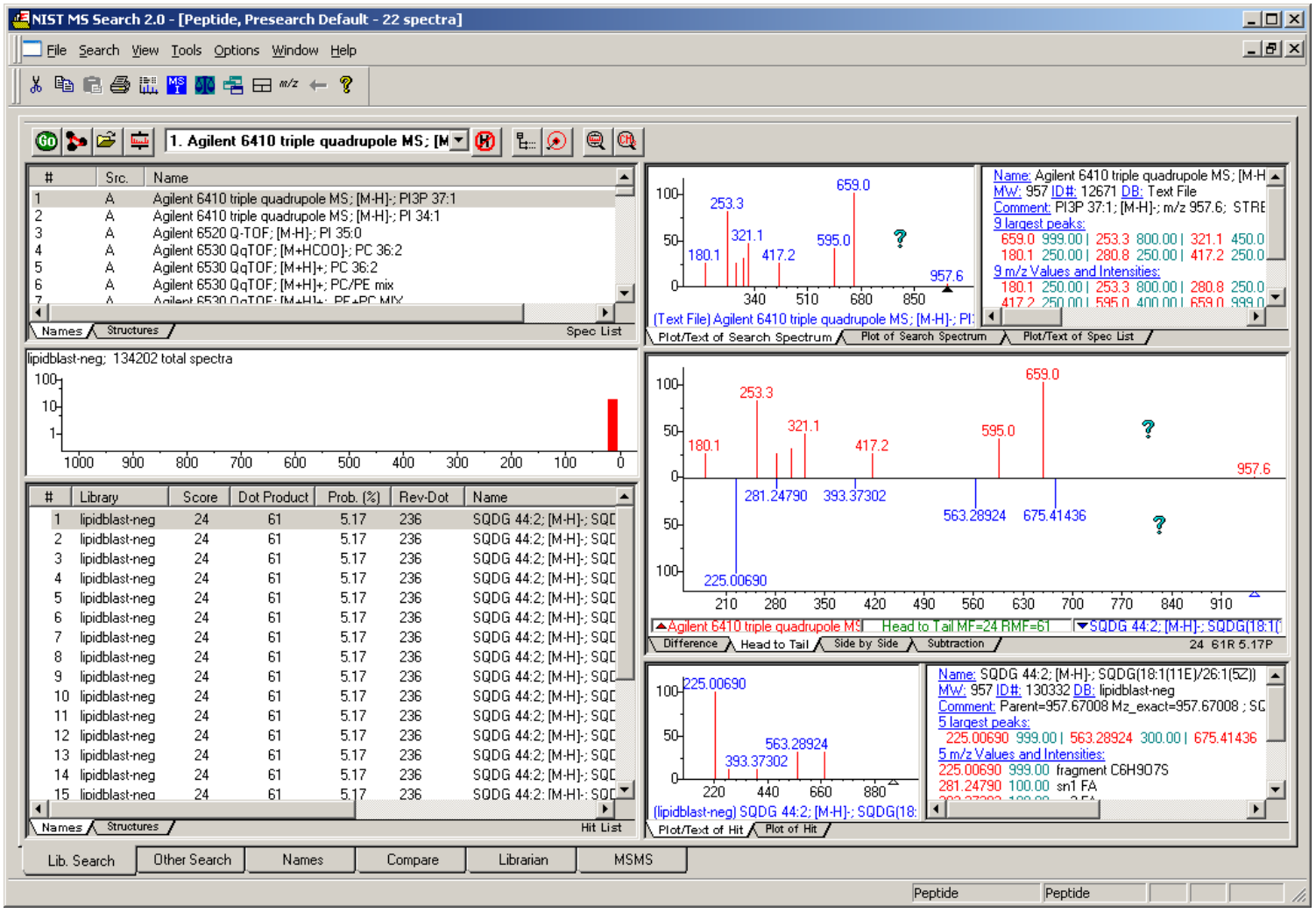


Name: ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H]-; ST 34:1
MW: 778 ID#: 4227 DB: Text File
Comment: ST 34:1; ST(d18:1/16:0);Elevation of sulfatides in ovarian cancer: An integrated transcriptomic and lipidomic analysis including tissue-imaging mass spectrometry;;doi:10.1186/1476-4598-9-186

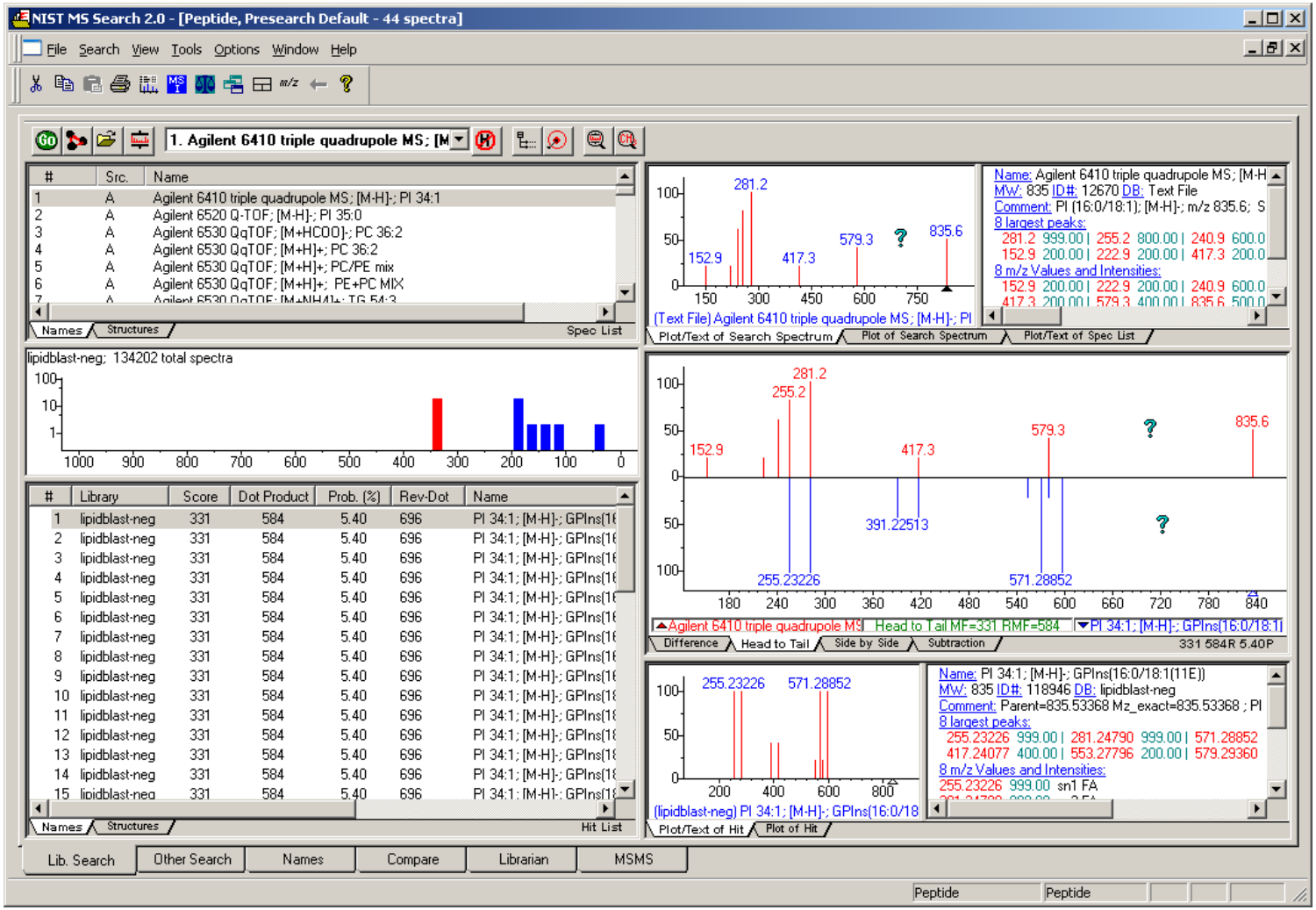


Name: Agilent 6410 triple quadrupole MS; [M-H]-; PI3P 37:1
MW: 957 ID#: 12671 DB: Text File
Comment: PI3P 37:1; [M-H]-; m/z 957.6; STRESS-INDUCED SYNTHESIS OF PHOSPHATIDYLINOSITOL 3-PHOSPHATE IN MYCOBACTERIA; http://www.jbc.org/cgi/doi/10.1074/jbc.M110.119263
9 largest peaks:

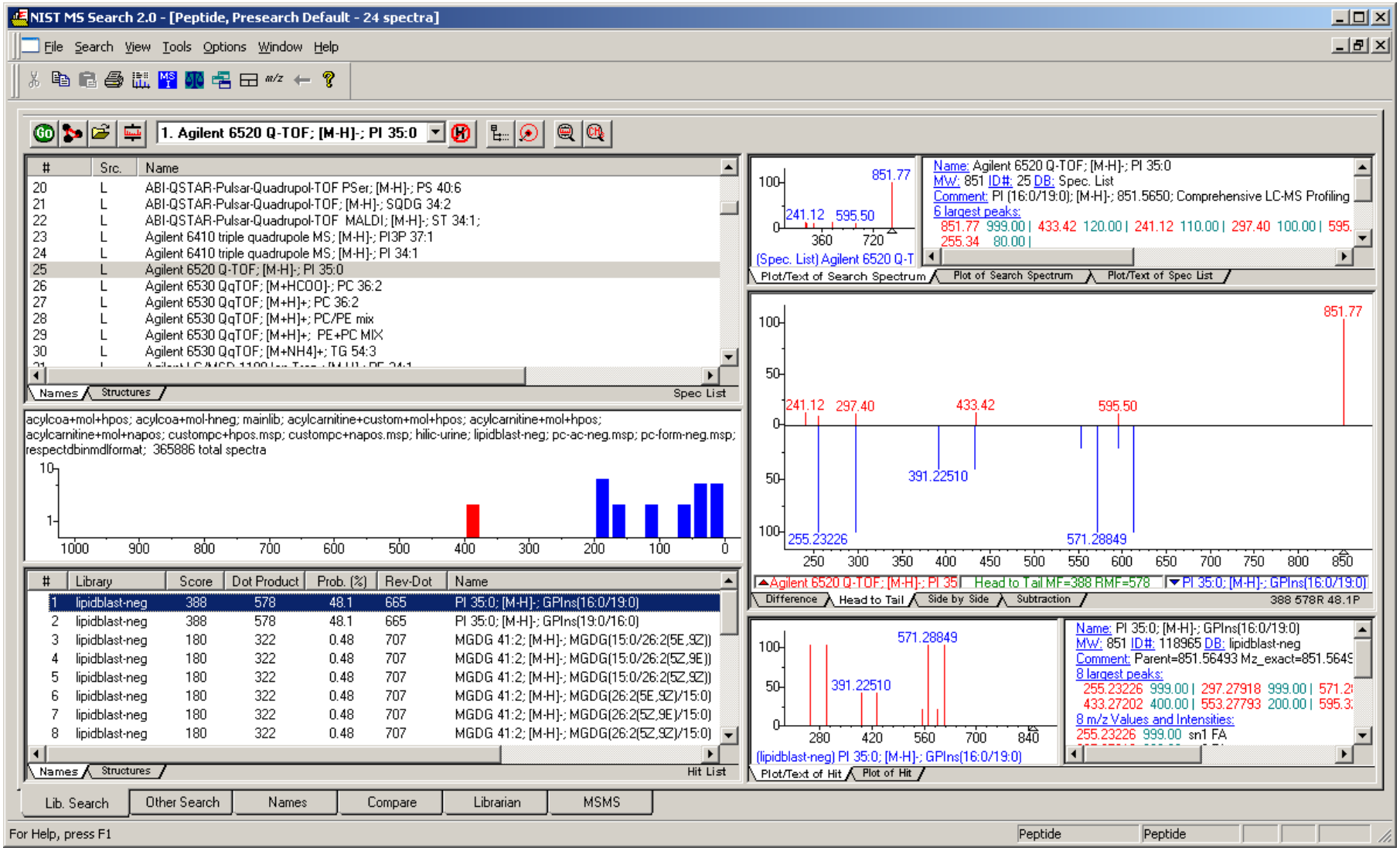
PI3P species (Phosphatidylinositol 3-Phosphates) not in LipidBlast – very low hit score (24) therefore false ID



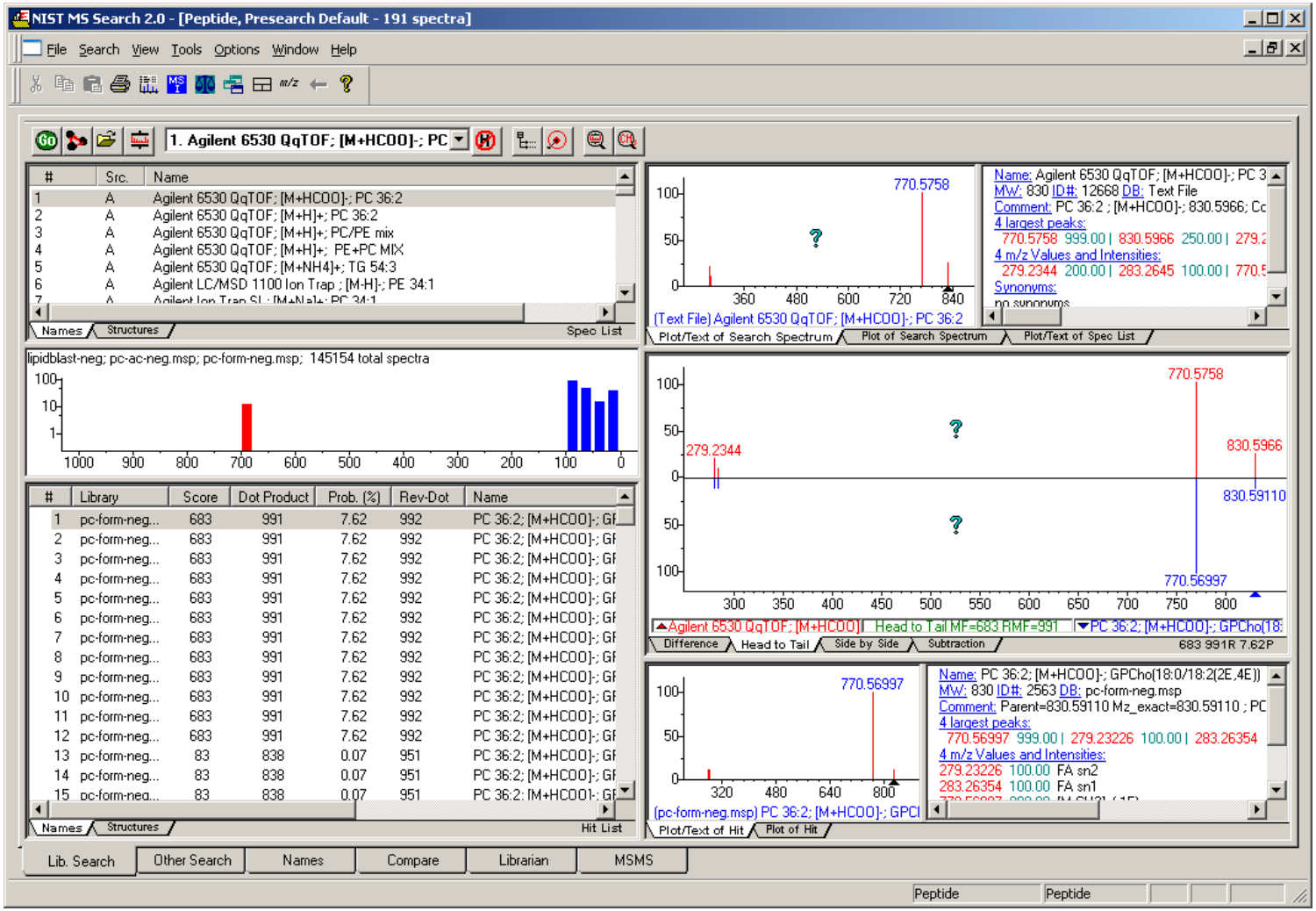
Name: Agilent 6410 triple quadrupole MS; [M-H]-; PI 34:1
MW: 835 ID#: 12670 DB: Text File
Comment: PI (16:0/18:1); [M-H]-; m/z 835.6; STRESS-INDUCED SYNTHESIS OF PHOSPHATIDYLINOSITOL 3-PHOSPHATE IN MYCOBACTERIA; http://www.jbc.org/cgi/doi/10.1074/jbc.M110.119263
8 largest peaks:



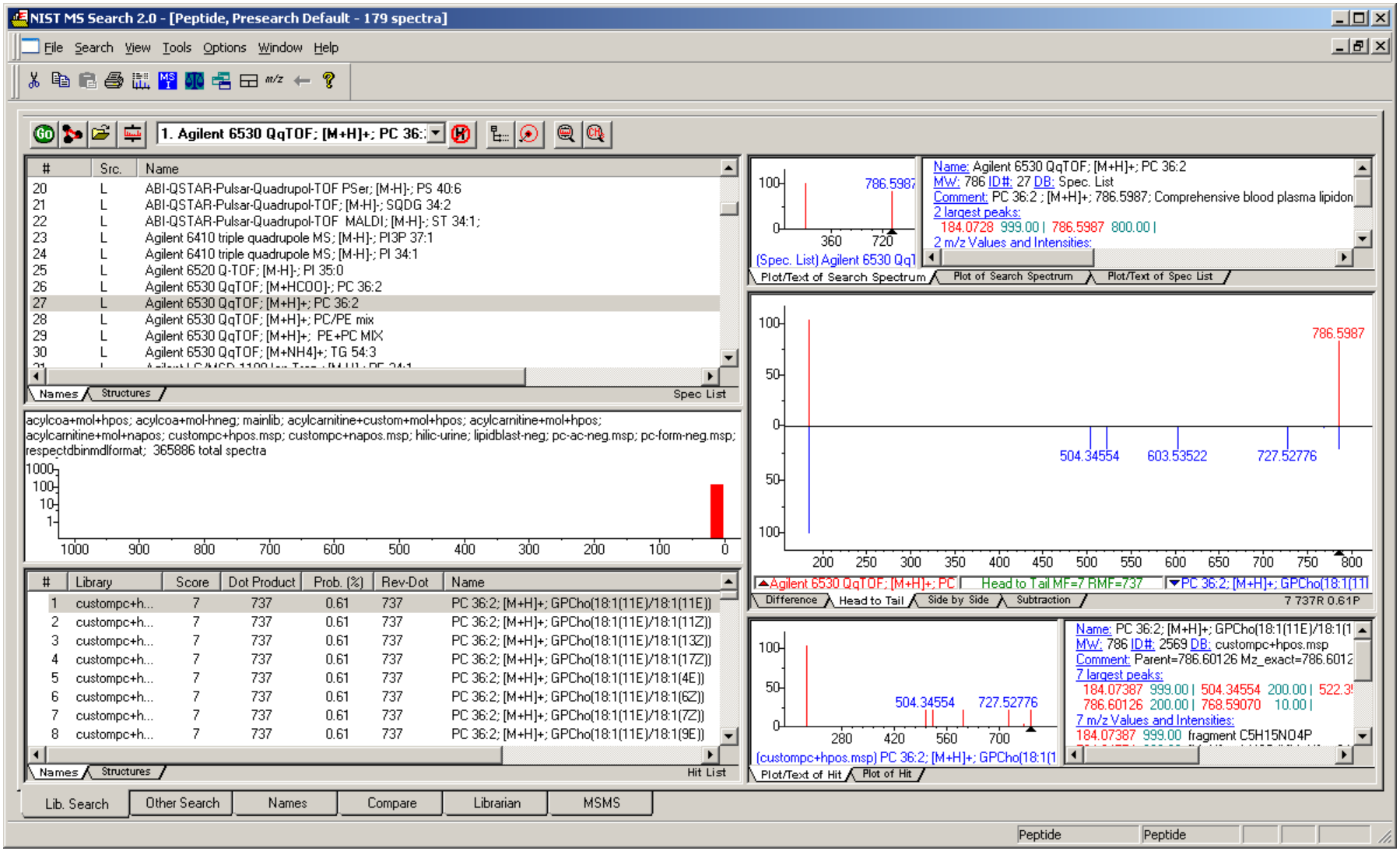
Name: Agilent 6520 Q-TOF; [M-H]-; PI 35:0
MW: 851 ID#: 25 DB: Spec. List
Comment: PI (16:0/19:0); [M-H]-; 851.5650; Comprehensive LC-MS Profiling of Mycobacterium tuberculosis Complex Lipids; Mark J. Sartain; COSMOS 2009
6 largest peaks:



Name: Agilent 6530 QqTOF; [M+HCOO]-; PC 36:2
MW: 830 ID#: 12668 DB: Text File
Comment: PC 36:2 ; [M+HCOO]-; 830.5966; Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry; Journal of Chromatography A, 1217 (2010) 4087-4099
4 largest peaks:

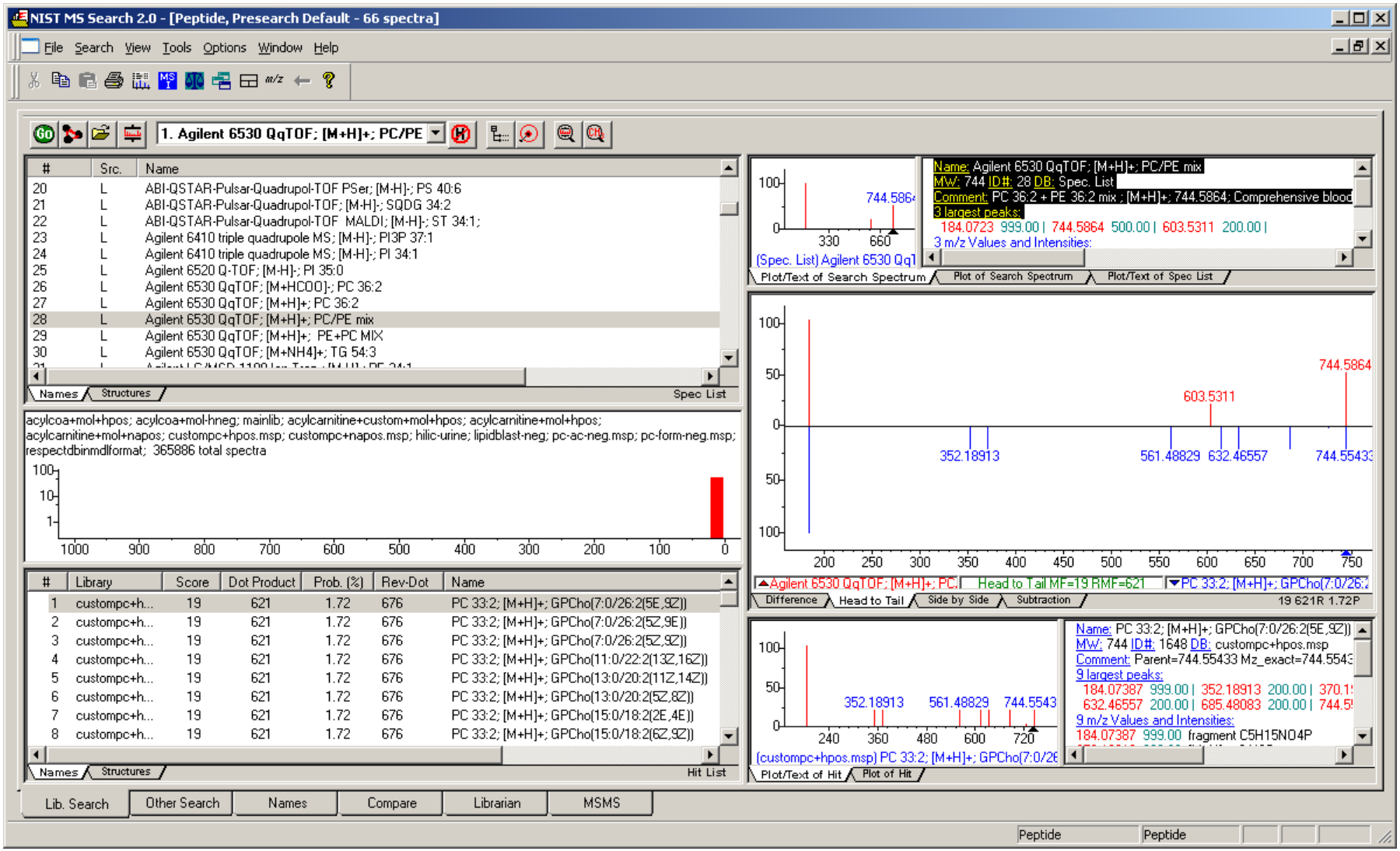


Name: Agilent 6530 QqTOF; [M+H]+; PC 36:2
MW: 786 ID#: 27 DB: Spec. List
Comment: PC 36:2 ; [M+H]+; 786.5987; Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry; Journal of Chromatography A, 1217 (2010) 4087-4099
2 largest peaks:

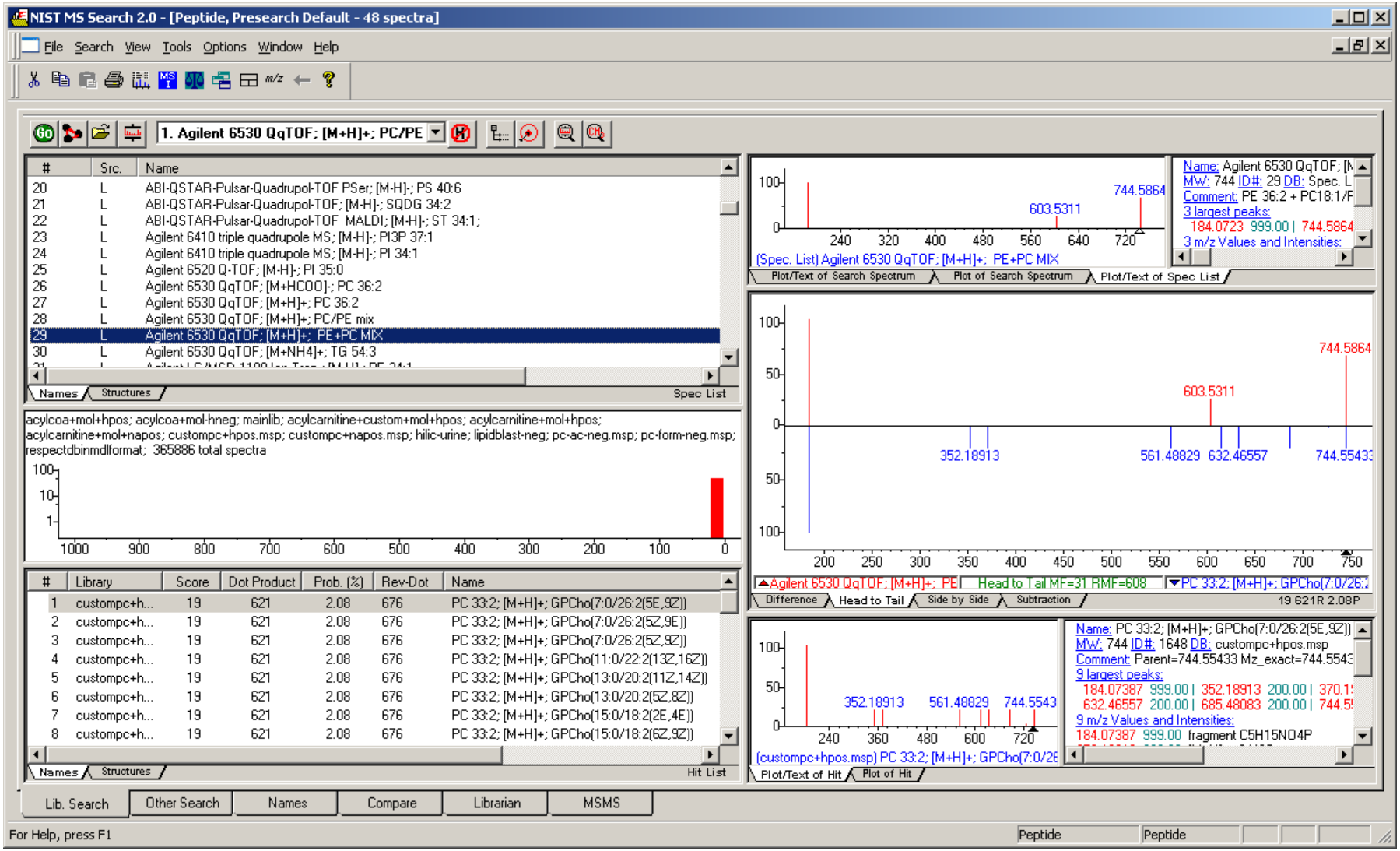


Name: Agilent 6530 QqTOF; [M+H]+; PC/PE mix
MW: 744 ID#: 28 DB: Spec. List
Comment: PC 36:2 + PE 36:2 mix ; [M+H]+; 744.5864; Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry; Journal of Chromatography A, 1217 (2010) 4087-4099
3 largest peaks:

MIX of different compounds (here annotated as PC36:2

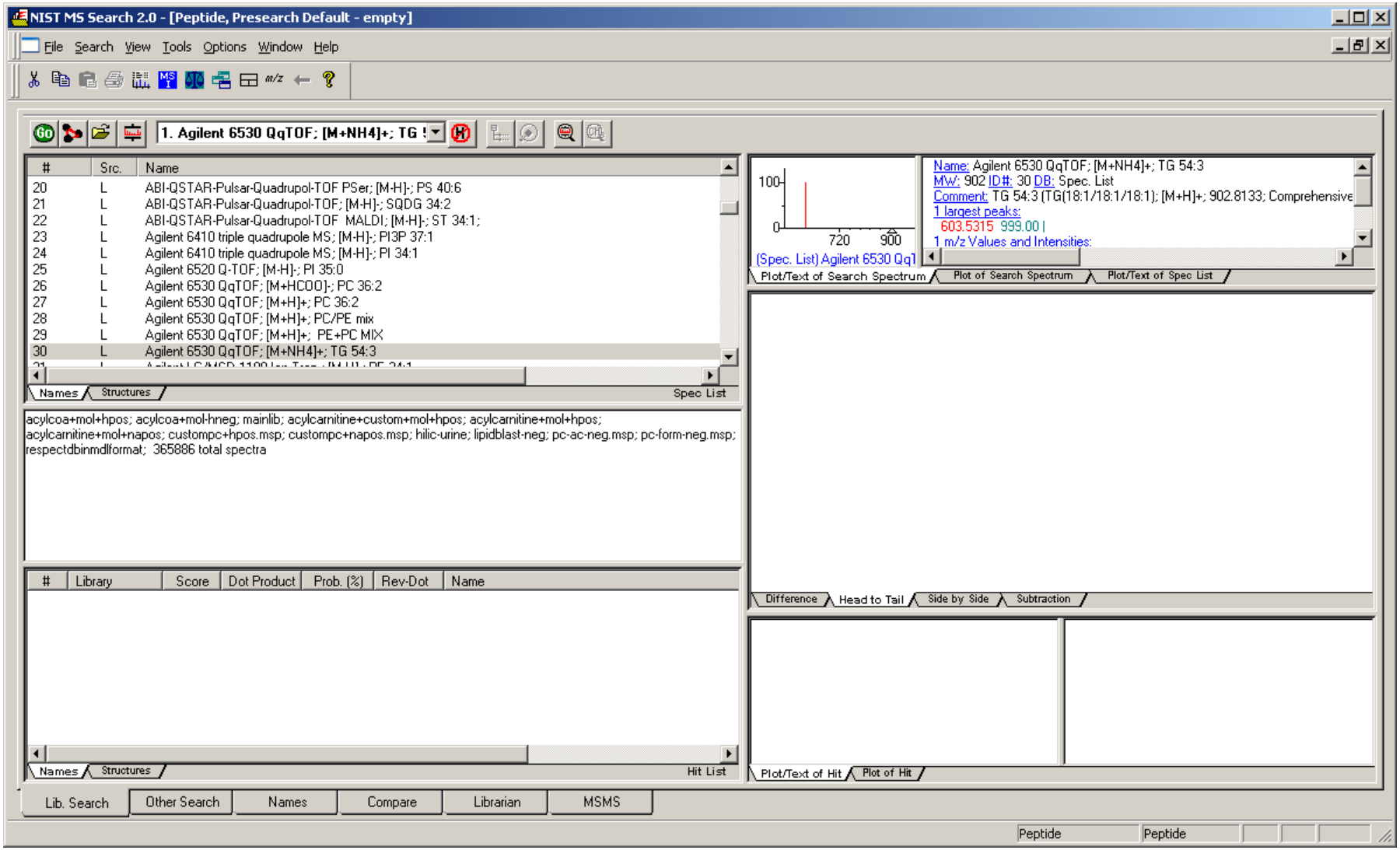


Name: Agilent 6530 QqTOF; [M+H]+; PE+PC MIX
MW: 744 ID#: 29 DB: Spec. List
Comment: PE 36:2 + PC18:1/P-16:0; [M+H]+; 744.5538; Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry; Journal of Chromatography A, 1217 (2010) 4087-4099
3 largest peaks:

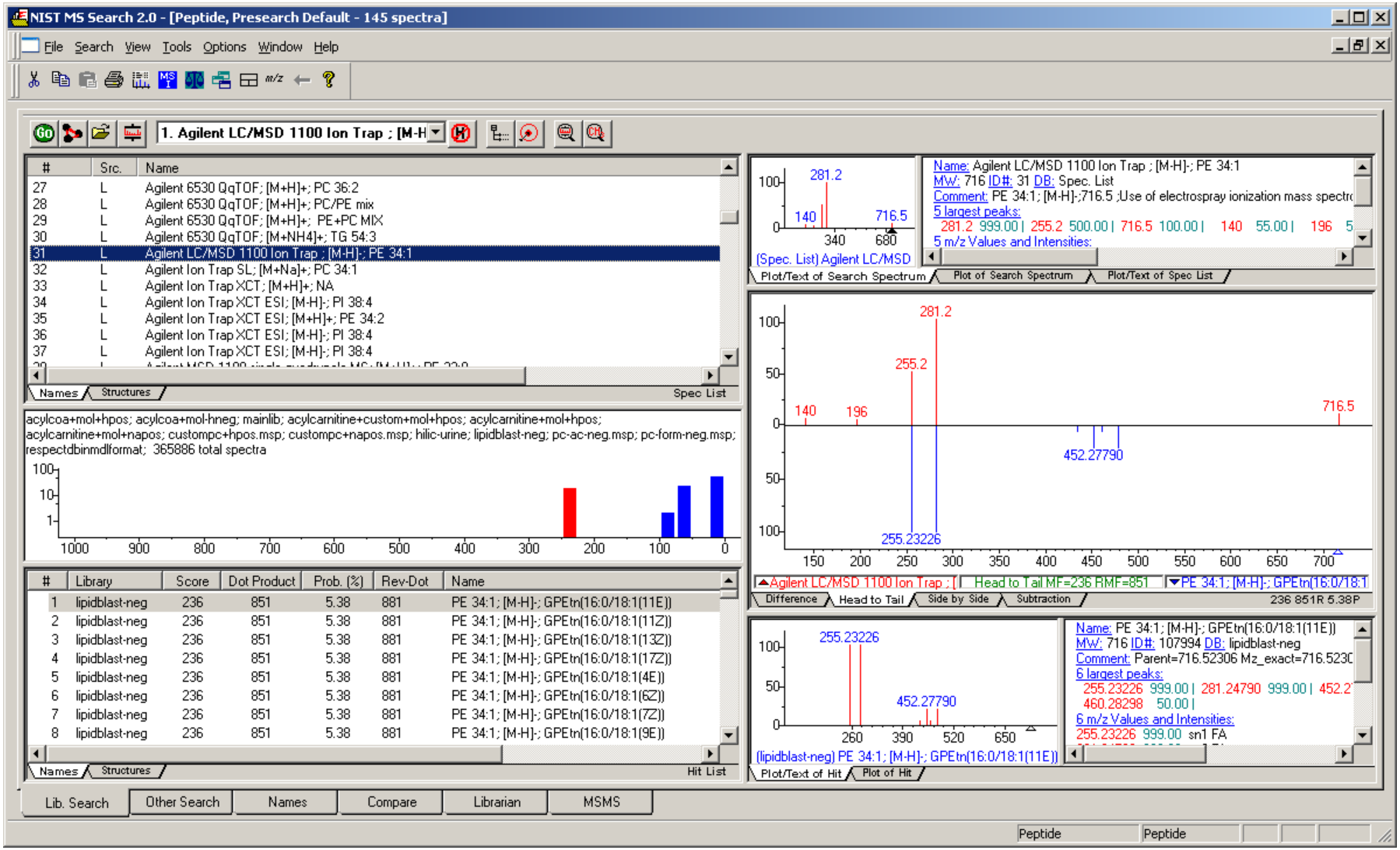


Name: Agilent 6530 QqTOF; [M+NH4]+; TG 54:3
MW: 902 ID#: 30 DB: Spec. List
Comment: TG 54:3 (TG(18:1/18:1/18:1); [M+H]+; 902.8133; Comprehensive blood plasma lipidomics by liquid chromatography/quadrupole time-of-flight mass spectrometry; Journal of Chromatography A, 1217 (2010) 4087-4099
1 largest peaks:

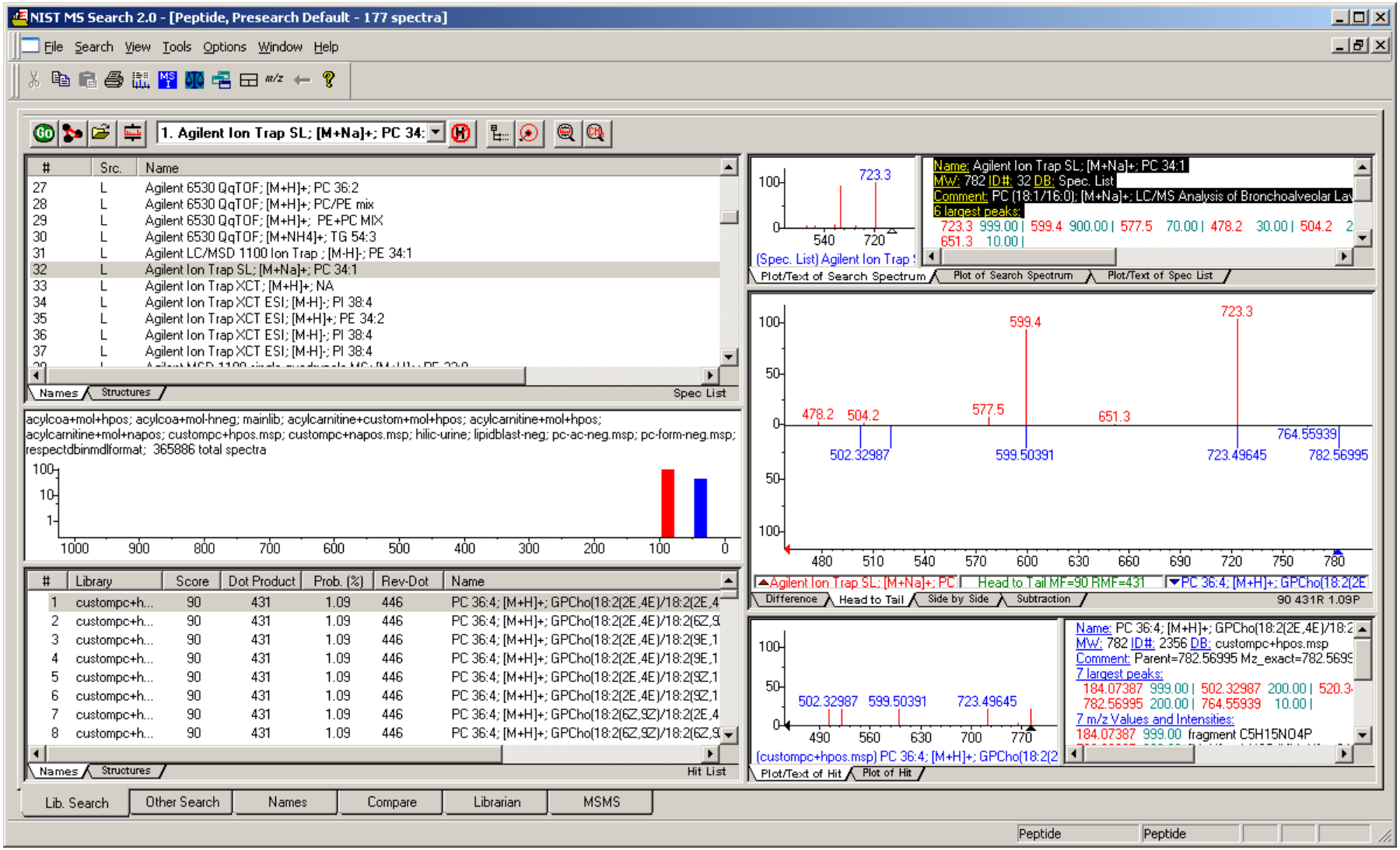
TAG M+H adduct not in library



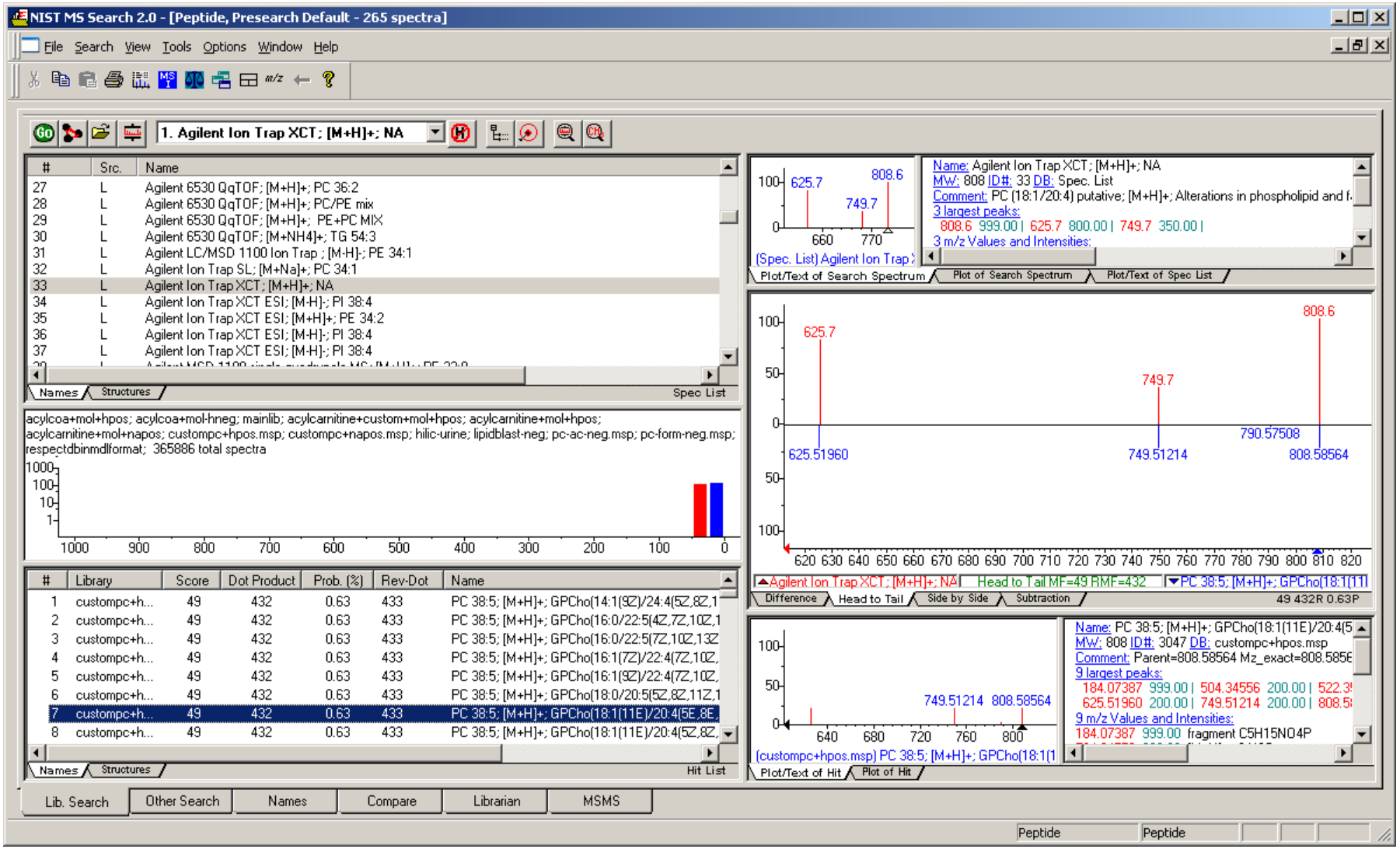
Name: Agilent LC/MSD 1100 Ion Trap ; [M-H]-; PE 34:1
MW: 716 ID#: 31 DB: Spec. List
Comment: PE 34:1; [M-H]-;716.5 ;Use of electrospray ionization mass spectrometry for profiling of crude oil effects on the phospholipid molecular species of two marine bacteria; DOI: 10.1002/rcm.2231
5 largest peaks:



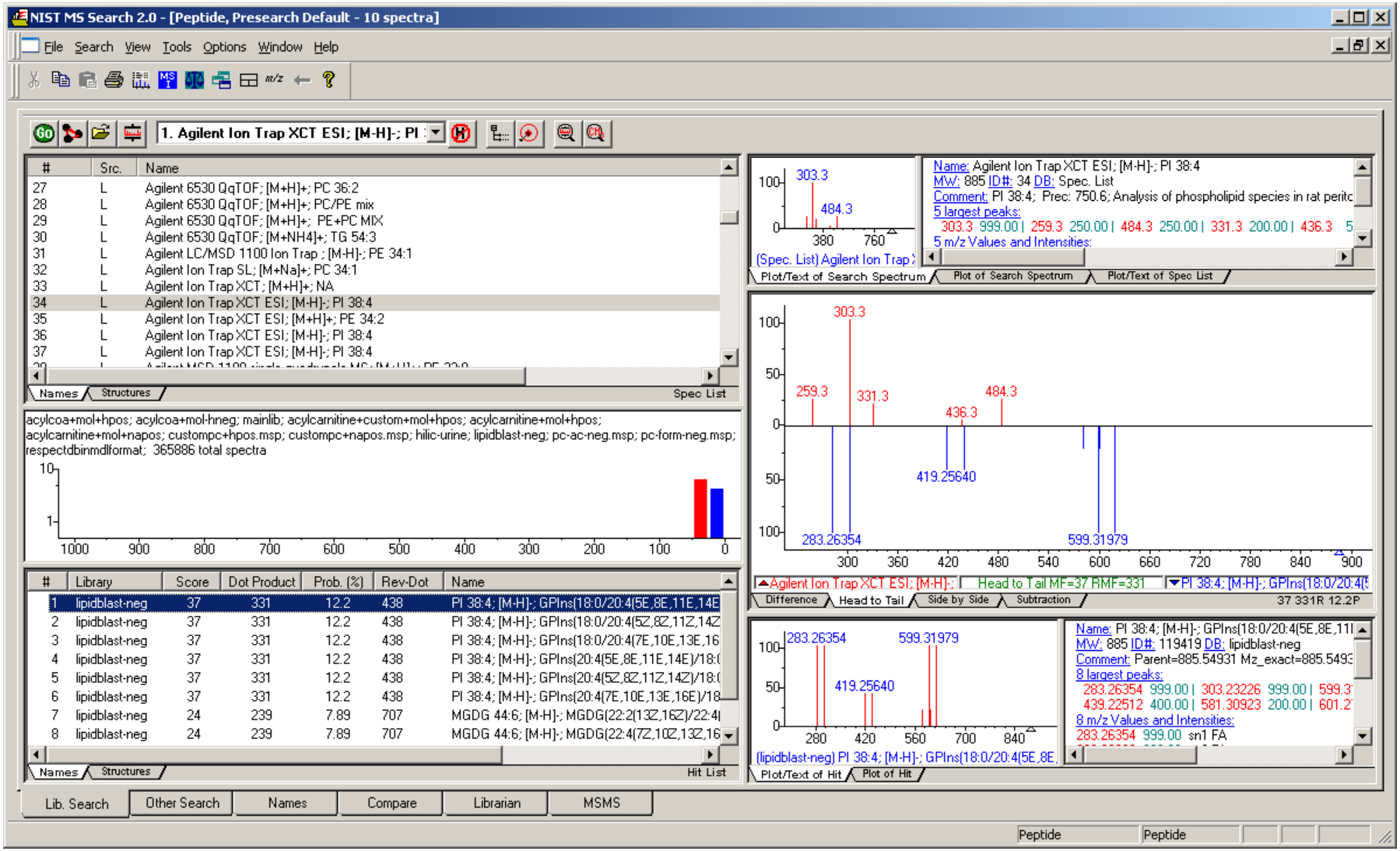
Name: Agilent Ion Trap SL; [M+Na]+; PC 34:1
MW: 782 ID#: 32 DB: Spec. List
Comment: PC (18:1/16:0); [M+Na]+; LC/MS Analysis of Bronchoalveolar Lavage Fluid Phospholipids as Biomarkers for Chronic Lung Inflammation; 5989-1491EN; Barroso, Bischoff
6 largest peaks:



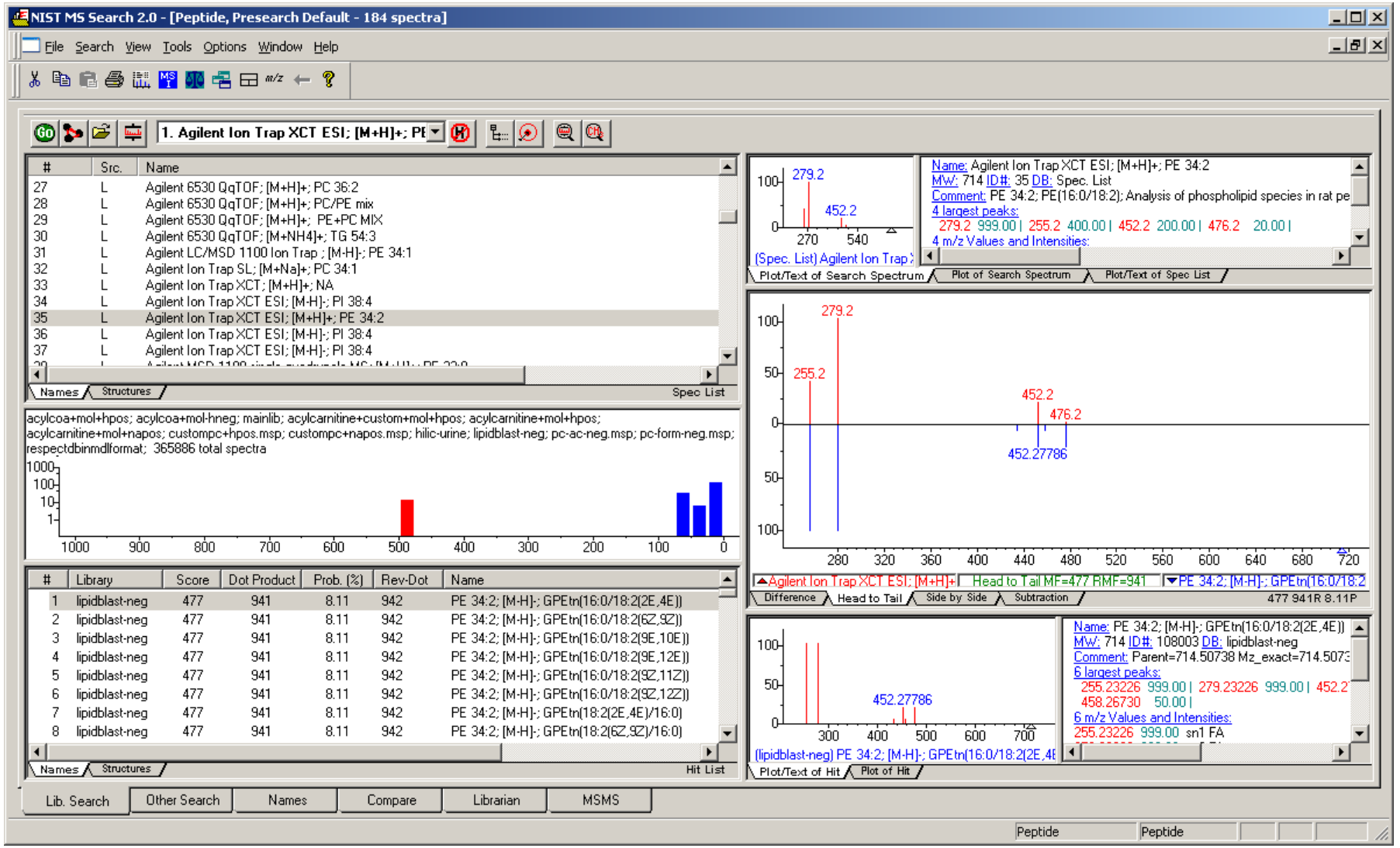
Name: Agilent Ion Trap XCT; [M+H]+; NA
MW: 808 ID#: 33 DB: Spec. List
Comment: PC (18:1/20:4) putative; [M+H]+; Alterations in phospholipid and fatty acid lipid profiles in primary neocortical cells during oxidant-induced cell injury; http://dx.doi.org/10.1016/j.cbi.2008.05.028
3 largest peaks:



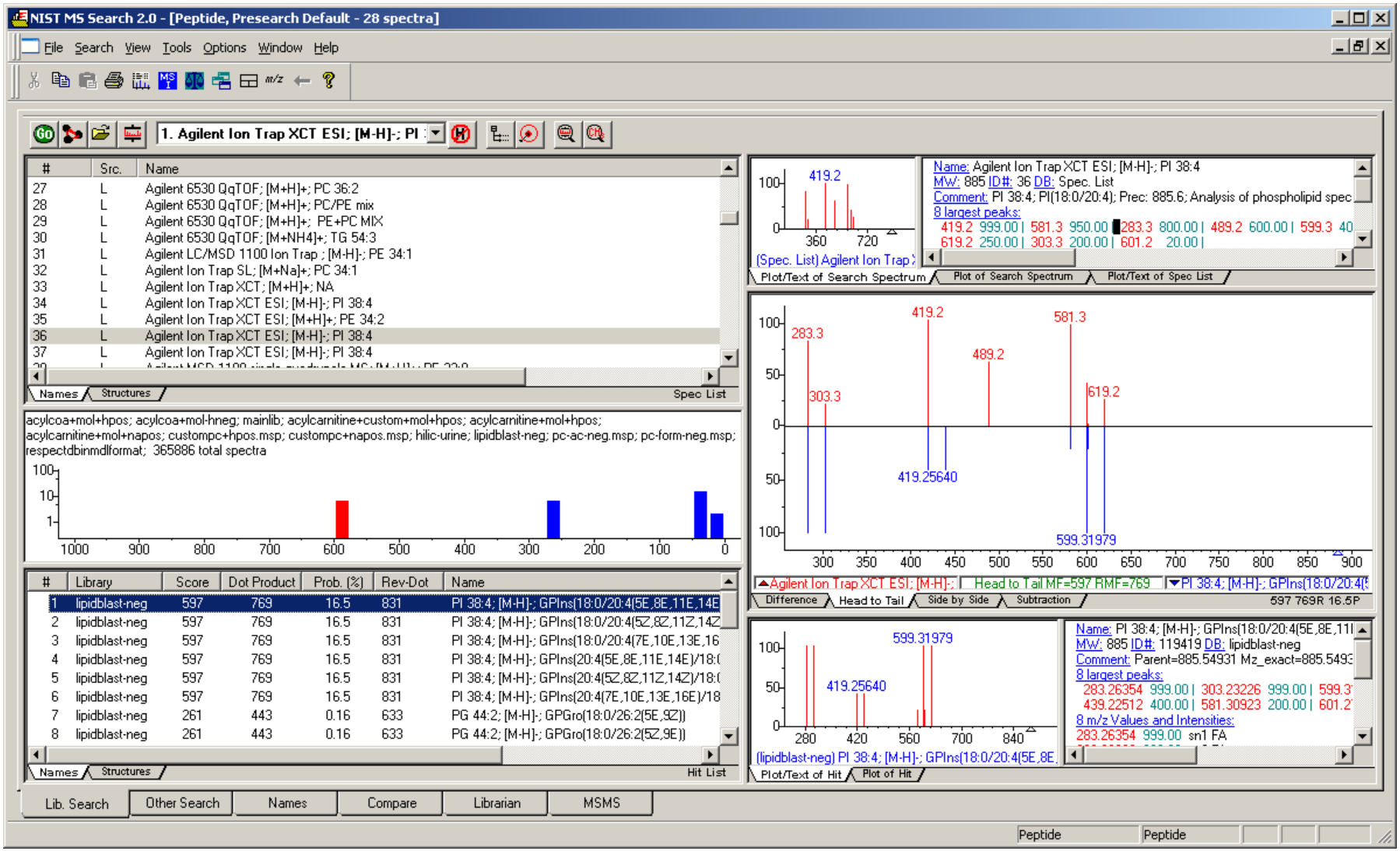
Name: Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
MW: 885 ID#: 34 DB: Spec. List
Comment: PI 38:4; Prec: 750.6; Analysis of phospholipid species in rat peritoneal surface layer by liquid chromatography/electrospray ionization ion-trap mass spectrometry ;http://dx.doi.org/10.1016/j.bbalip.2006.03.022
5 largest peaks:



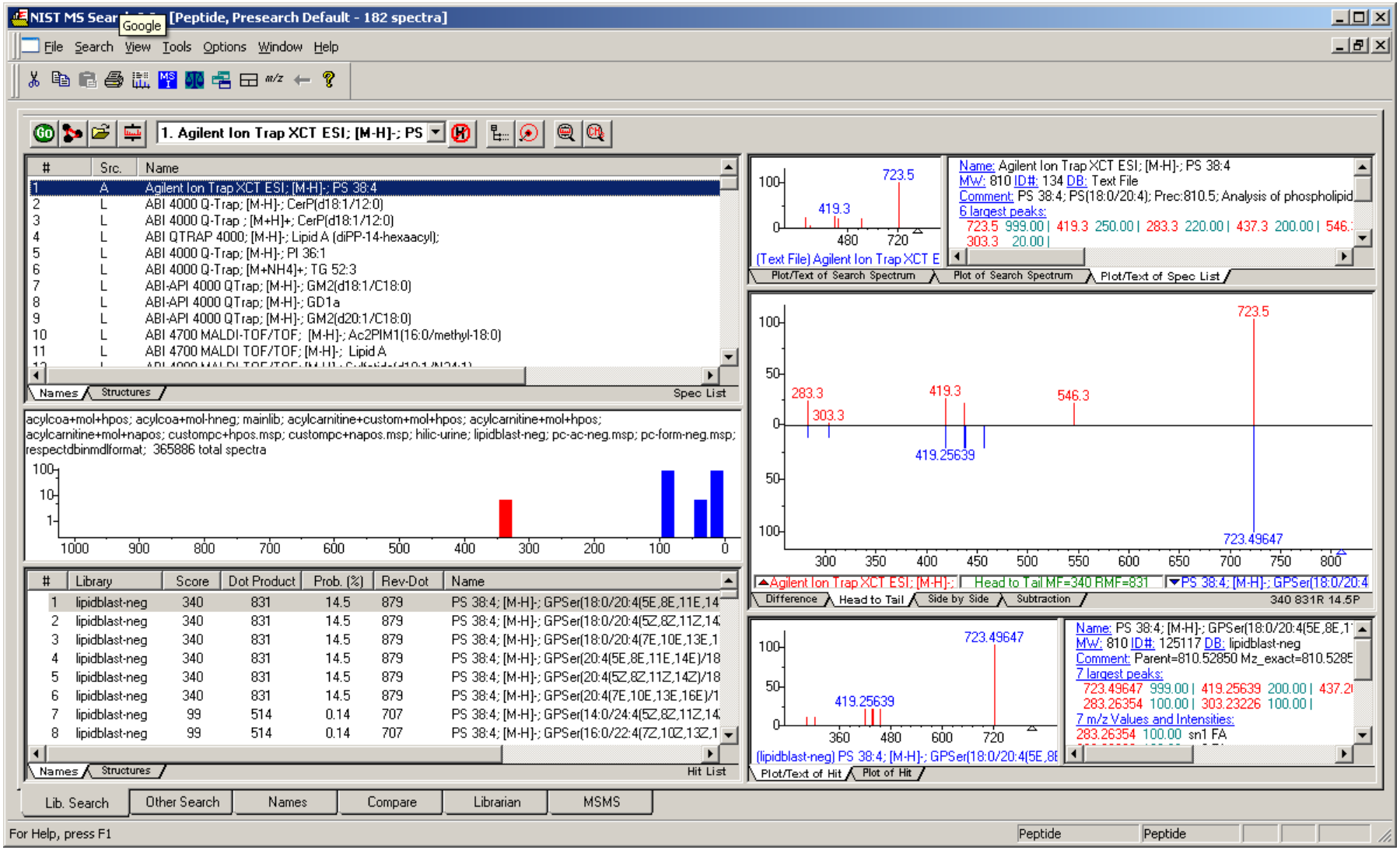
Name: Agilent Ion Trap XCT ESI; [M+H]+; PE 34:2
MW: 714 ID#: 35 DB: Spec. List
Comment: PE 34:2; PE(16:0/18:2); Analysis of phospholipid species in rat peritoneal surface layer by liquid chromatography/electrospray ionization ion-trap mass spectrometry ;http://dx.doi.org/10.1016/j.bbalip.2006.03.022
4 largest peaks:



Name: Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
MW: 885 ID#: 36 DB: Spec. List
Comment: PI 38:4; PI(18:0/20:4); Prec: 885.6; Analysis of phospholipid species in rat peritoneal surface layer by liquid chromatography/electrospray ionization ion-trap mass spectrometry ;http://dx.doi.org/10.1016/j.bbalip.2006.03.022
8 largest peaks:

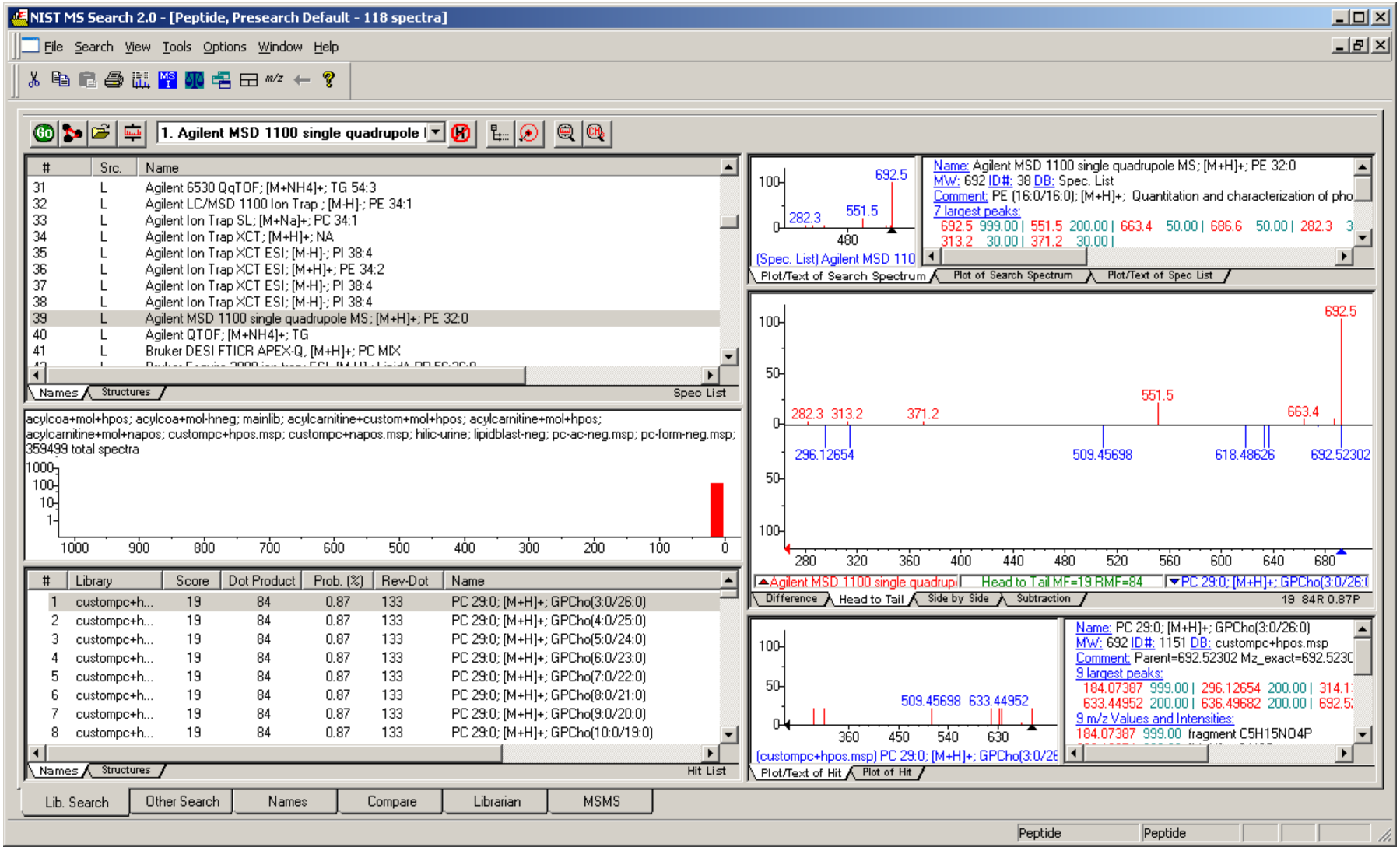


Name: Agilent Ion Trap XCT ESI; [M-H]-; PS 38:4
MW: 810 ID#: 134 DB: Text File
Comment: PS 38:4; PS(18:0/20:4); Prec:810.5; Analysis of phospholipid species in rat peritoneal surface layer by liquid chromatography/electrospray ionization ion-trap mass spectrometry ;http://dx.doi.org/10.1016/j.bbalip.2006.03.022
6 largest peaks:



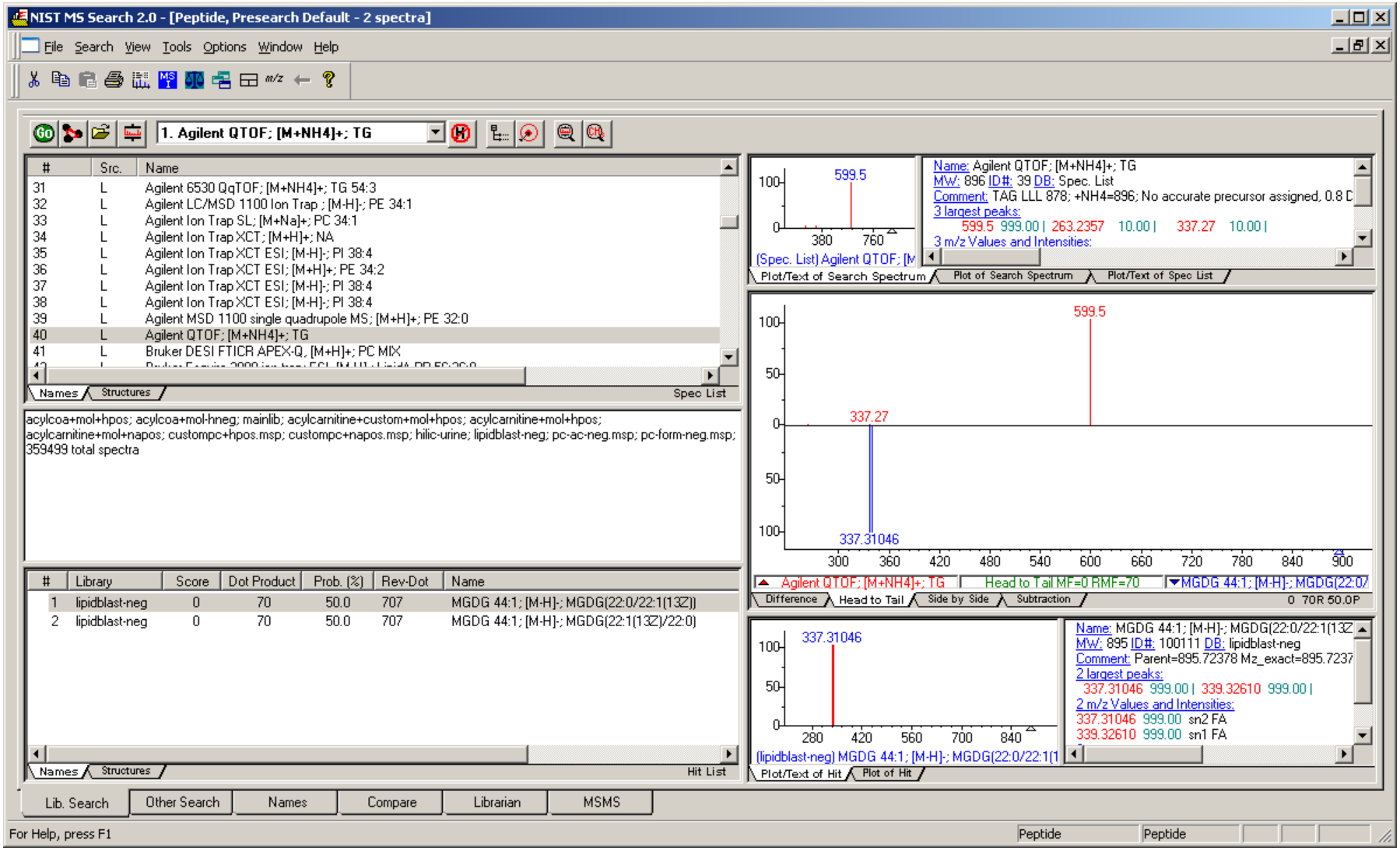
Name: Agilent MSD 1100 single quadrupole MS; [M+H]+; PE 32:0
MW: 692 ID#: 38 DB: Spec. List
Comment: PE (16:0/16:0); [M+H]+; Quantitation and characterization of phospholipids in pharmaceutical formulations by liquid chromatography-mass spectrometry; http://dx.doi.org/10.1016/S0021-9673(00)00148-5
7 largest peaks:

Hit score lower than 20, or 100 in dot product, non-hit, also obtained from single quad, no-MSMS



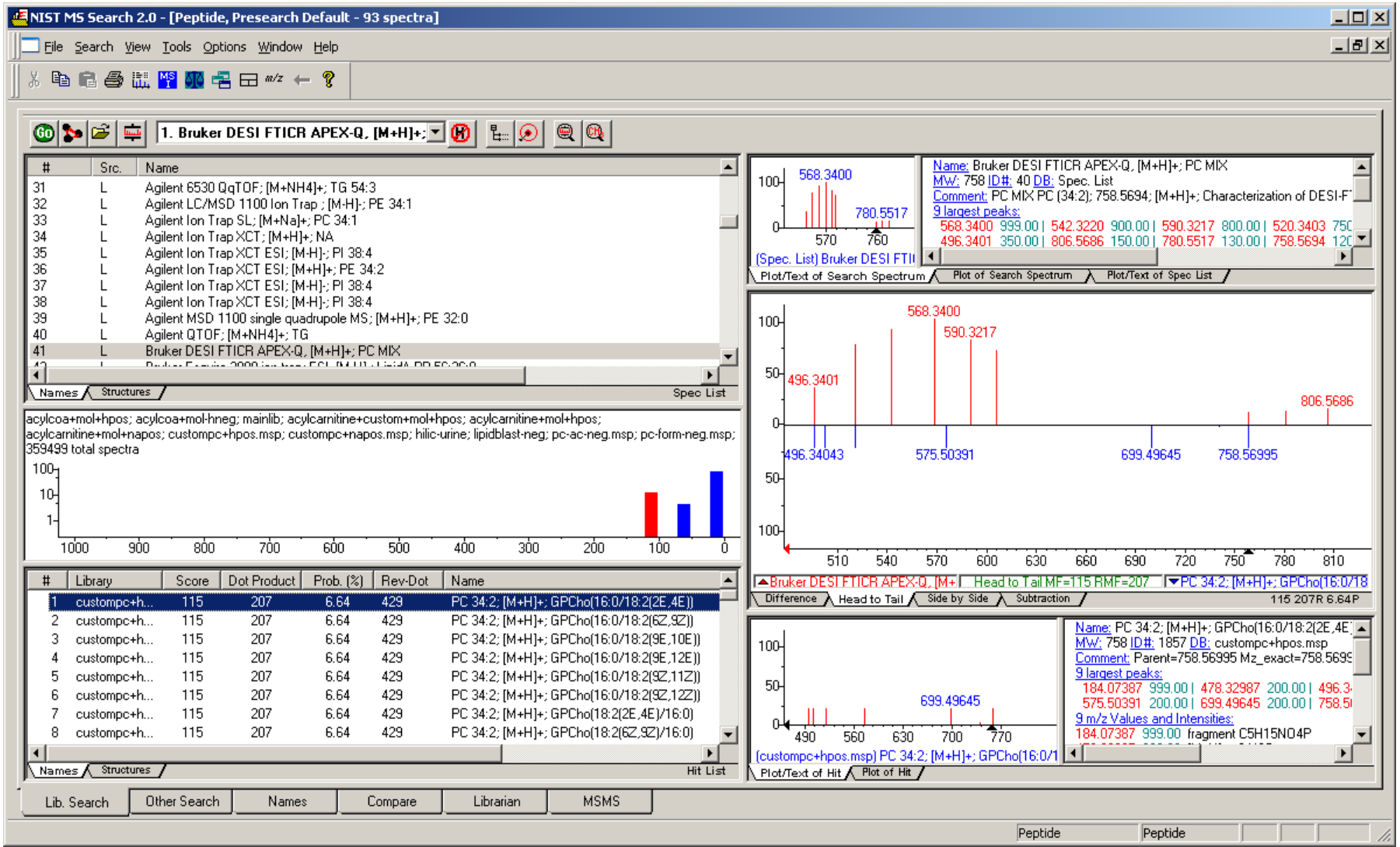
Name: Agilent QTOF; [M+NH4]+; TG
MW: 896 ID#: 39 DB: Spec. List
Comment: TAG LLL 878; +NH4=896; No accurate precursor assigned, 0.8 Da error;Maximizing Detection of Complex Hydrophobic Lipids: Optimization Efficiency and Nano-Chromatography; ASMS 2009 David A. Weil1, Michael Woodman and Carol Ball, Agilent Technologies Inc.,Schaumburg, IL1 and Raleigh, NC2
3 largest peaks:

no precursor assigned, hit score = 0

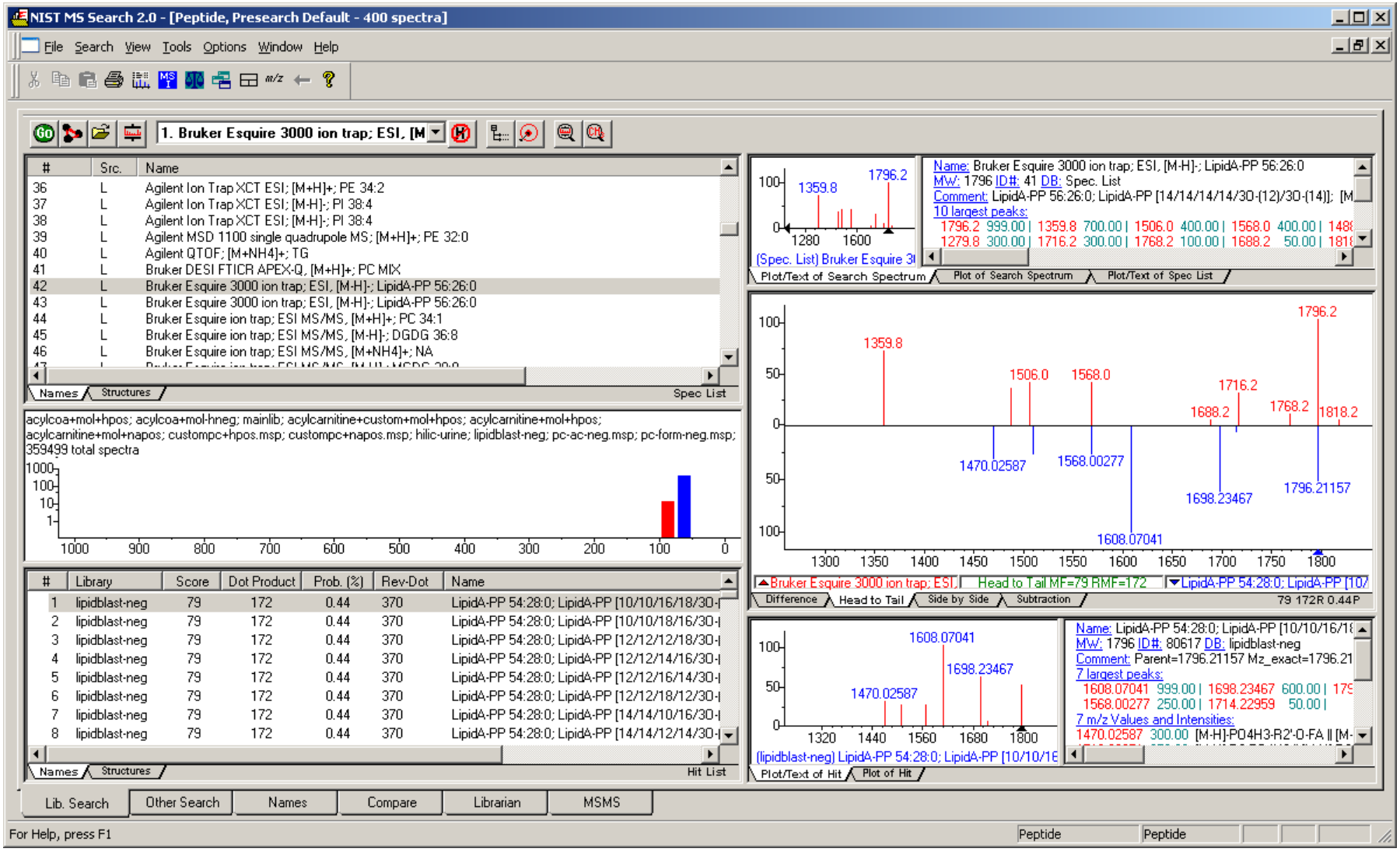


Name: Bruker DESI FTICR APEX-Q, [M+H]+; PC MIX
MW: 758 ID#: 40 DB: Spec. List
Comment: PC MIX PC (34:2); 758.5694; [M+H]+; Characterization of DESI-FTICR mass spectrometry from ECD to accurate mass tissue analysis
9 largest peaks:

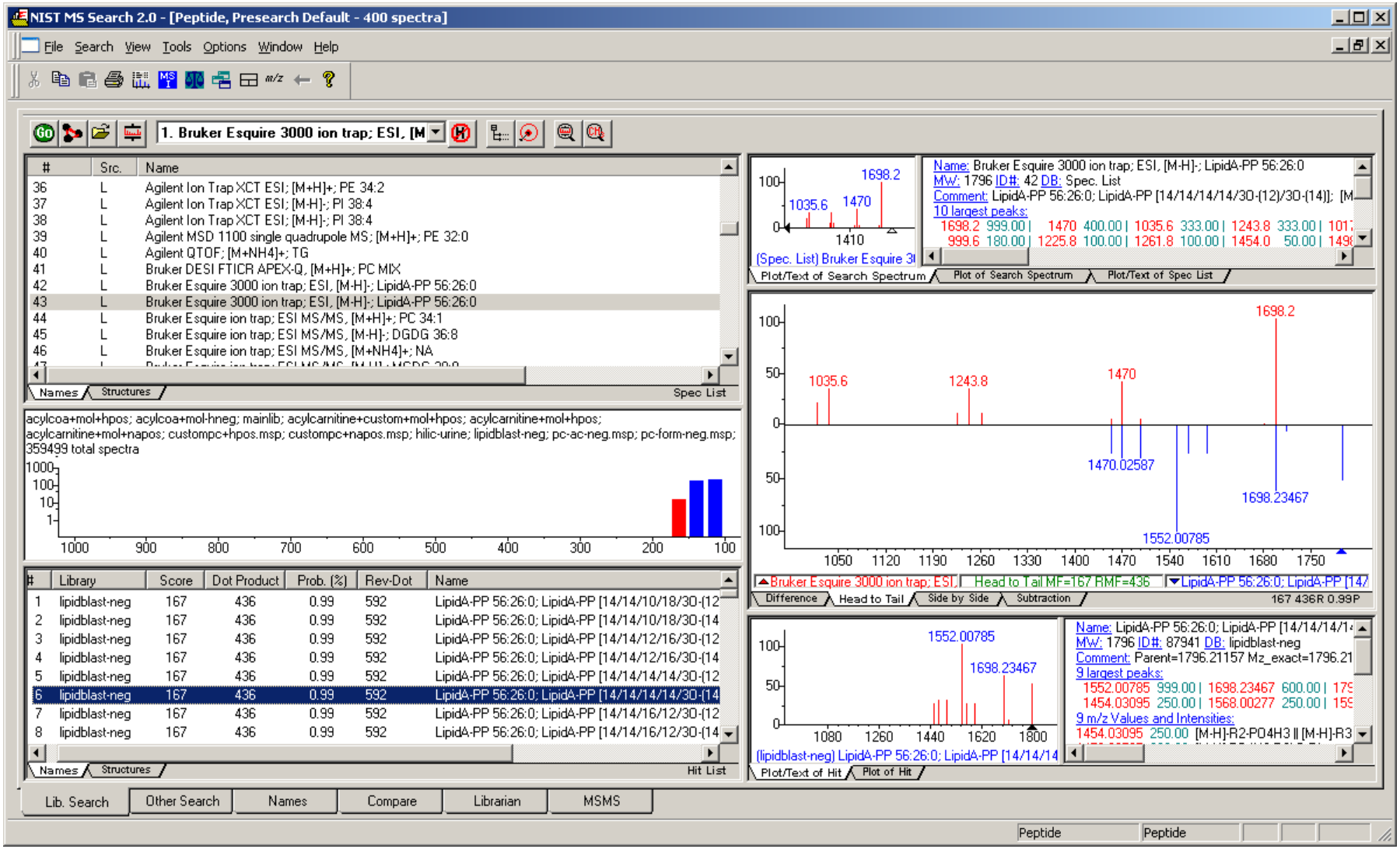
PC -MIX



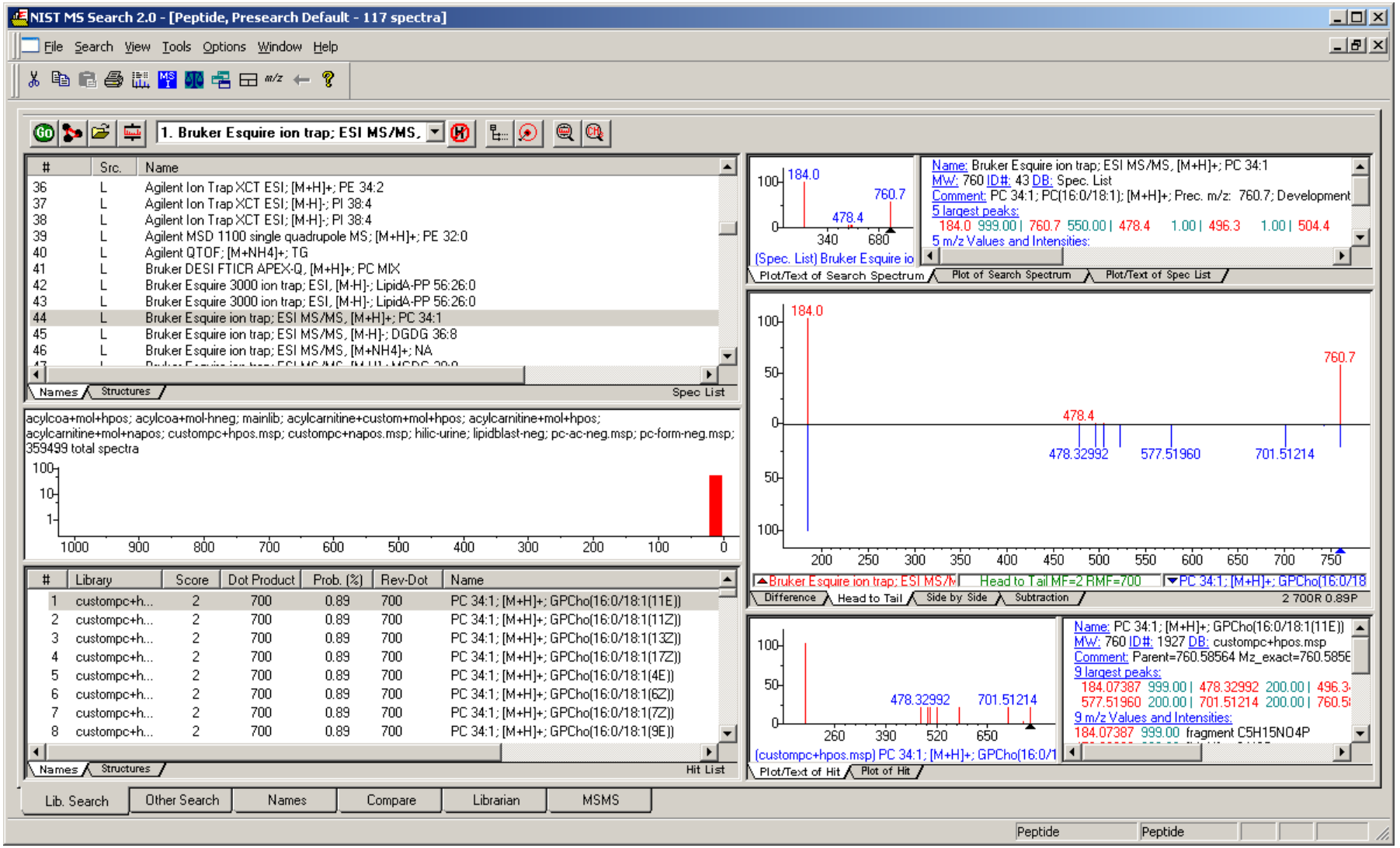
Name: Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
MW: 1796 ID#: 41 DB: Spec. List
Comment: LipidA-PP 56:26:0; LipidA-PP [14/14/14/14/3O-(12)/3O-(14)]; [M+H]+; Prec. m/z: 1796.2;Gram-negative bacterial lipid A analysis by negative electrospray Gram-negative bacterial lipid A analysis by negative electrospray Gram-negative bacterial lipid A analysis by negative electrospray; International Journal of Mass Spectrometry 249250 (2006) 7792
10 largest peaks:



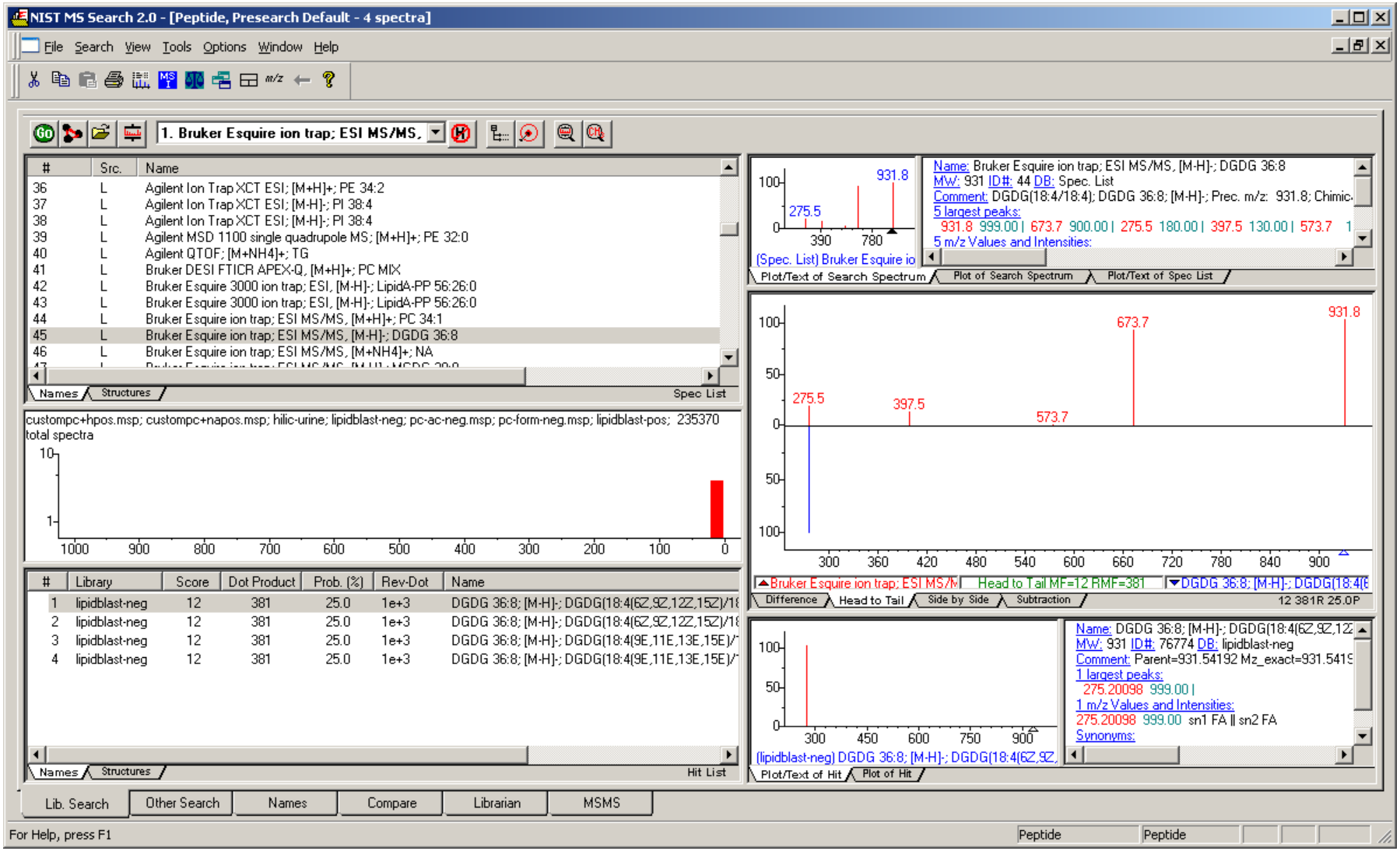
Name: Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
MW: 1796 ID#: 42 DB: Spec. List
Comment: LipidA-PP 56:26:0; LipidA-PP [14/14/14/14/3O-(12)/3O-(14)]; [M+H]+; Prec. m/z: 1796.2;Gram-negative bacterial lipid A analysis by negative electrospray Gram-negative bacterial lipid A analysis by negative electrospray Gram-negative bacterial lipid A analysis by negative electrospray; International Journal of Mass Spectrometry 249250 (2006) 7792
10 largest peaks:



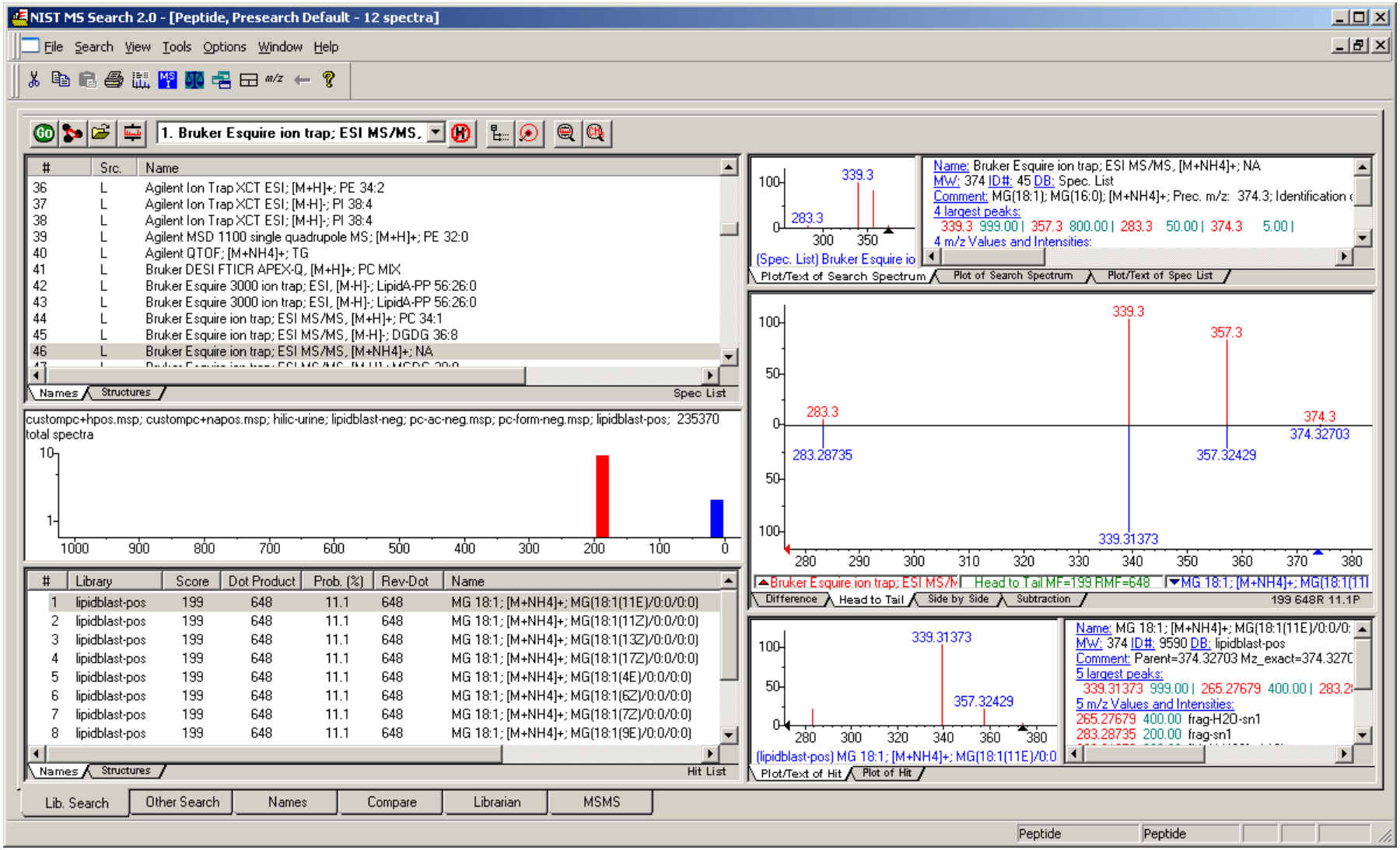
Name: Bruker Esquire ion trap; ESI MS/MS, [M+H]+; PC 34:1
MW: 760 ID#: 43 DB: Spec. List
Comment: PC 34:1; PC(16:0/18:1); [M+H]+; Prec. m/z: 760.7; Developmental profiling by mass spectrometry of phosphocholine containing phospholipids in the rat nervous system reveals temporo-spatial gradients; DOI: 10.1111/j.1471-4159.2010.06836.x
5 largest peaks:



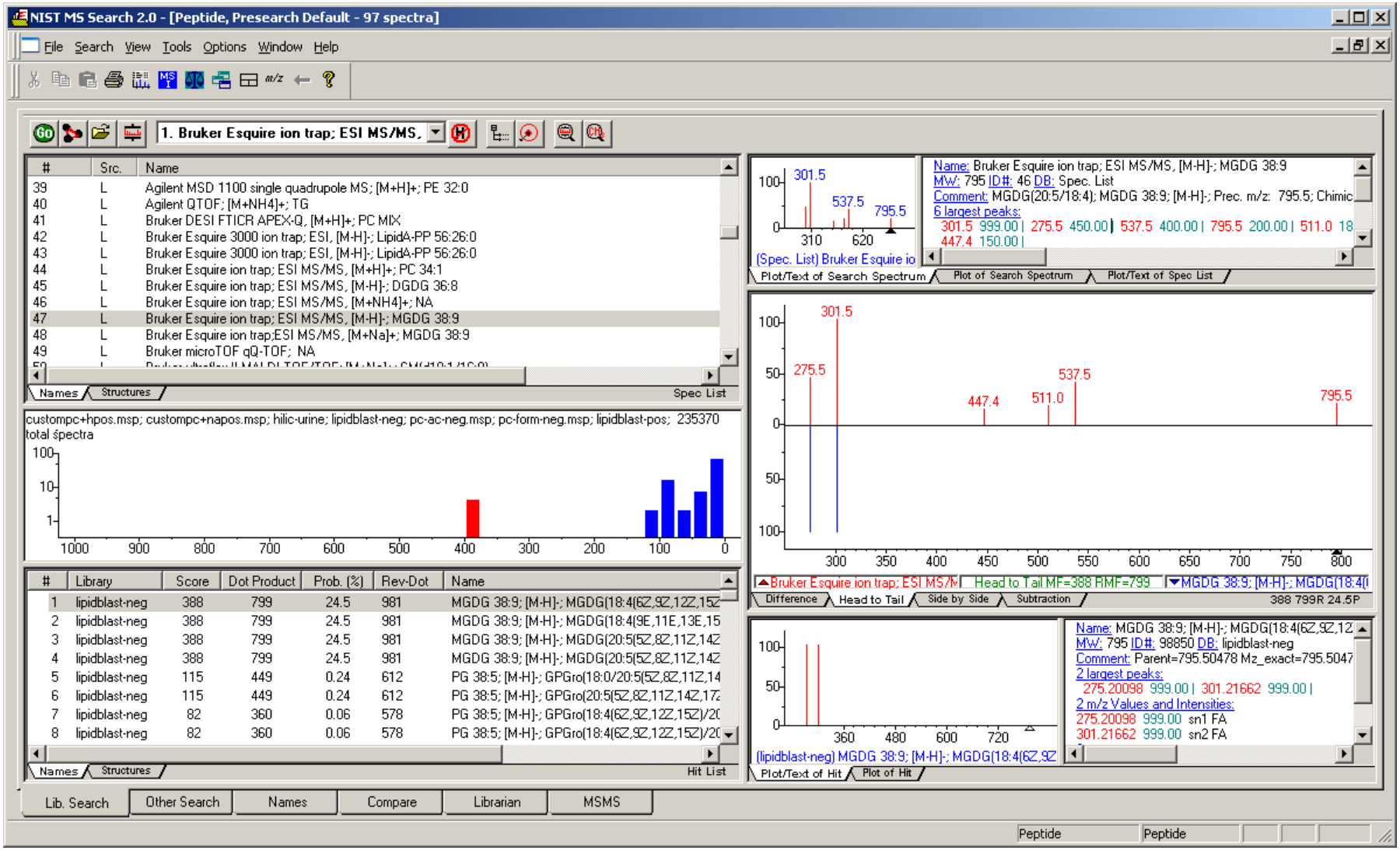
Name: Bruker Esquire ion trap; ESI MS/MS, [M-H]-; DGDG 36:8
MW: 931 ID#: 44 DB: Spec. List
Comment: DGDG(18:4/18:4); DGDG 36:8; [M-H]-; Prec. m/z: 931.8; Chimica e biologia a confronto: pigmenti e altri metaboliti secondari prodotti da dinoflagellati del Lago di Tovel; Studi Trent. Sci. Nat., Acta Biol., 81 (2004), Suppl. 2: 413-426;Rita FRASSANITO, Ines MANCINI & Graziano GUELLA
5 largest peaks:



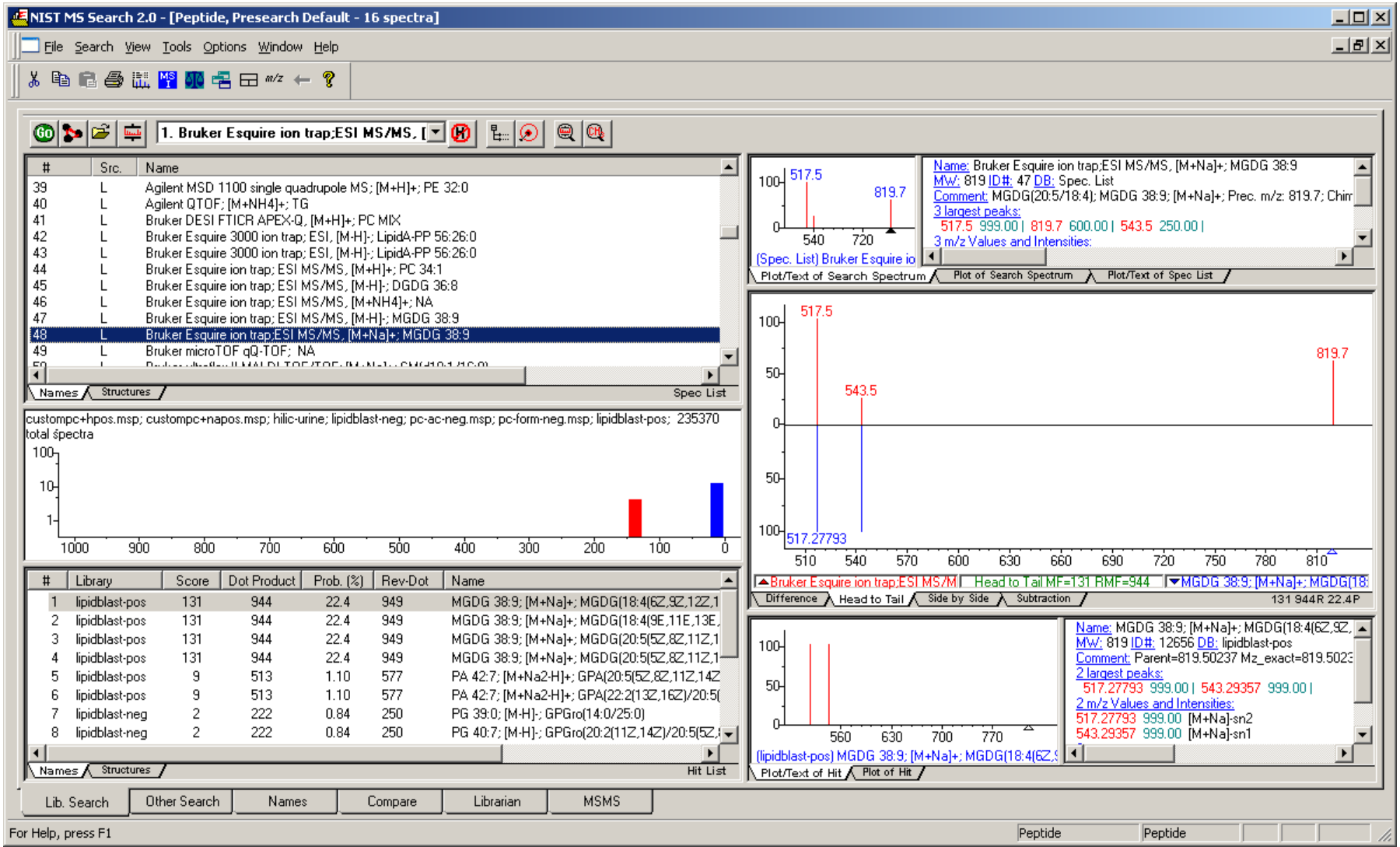
Name: Bruker Esquire ion trap; ESI MS/MS, [M+NH4]+; NA
MW: 374 ID#: 45 DB: Spec. List
Comment: MG(18:1); MG(16:0); [M+NH4]+; Prec. m/z: 374.3; Identification of molecular species of simple lipids by normal phase liquid chromatographypositive electrospray tandem mass spectrometry, and application of developed methods in comprehensive analysis of low erucic acid rapeseed oil lipids
4 largest peaks:



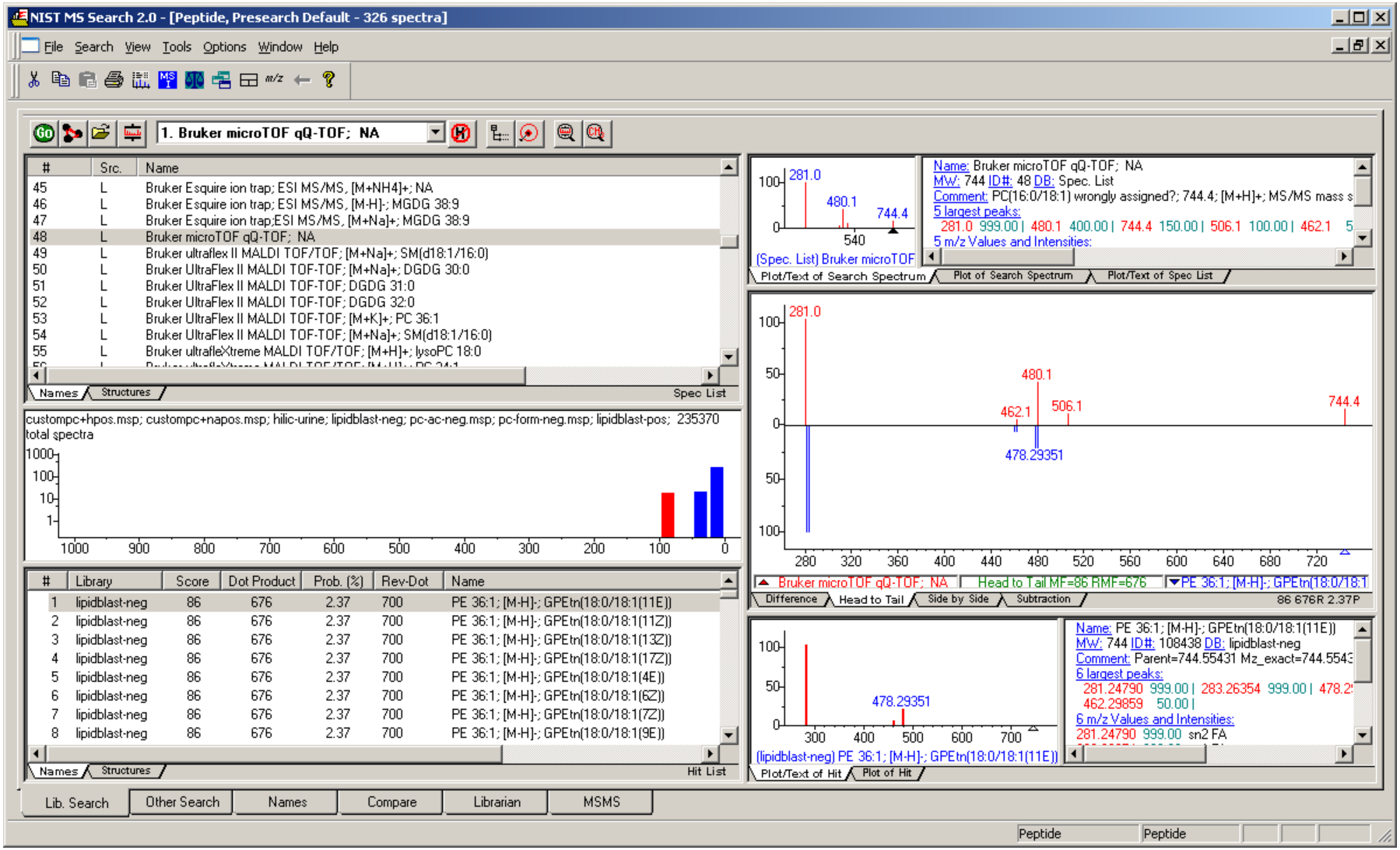
Name: Bruker Esquire ion trap; ESI MS/MS, [M-H]-; MGDG 38:9
MW: 795 ID#: 46 DB: Spec. List
Comment: MGDG(20:5/18:4); MGDG 38:9; [M-H]-; Prec. m/z: 795.5; Chimica e biologia a confronto: pigmenti e altri metaboliti secondari prodotti da dinoflagellati del Lago di Tovel; Studi Trent. Sci. Nat., Acta Biol., 81 (2004), Suppl. 2: 413-426;Rita FRASSANITO, Ines MANCINI & Graziano GUELLA
6 largest peaks:



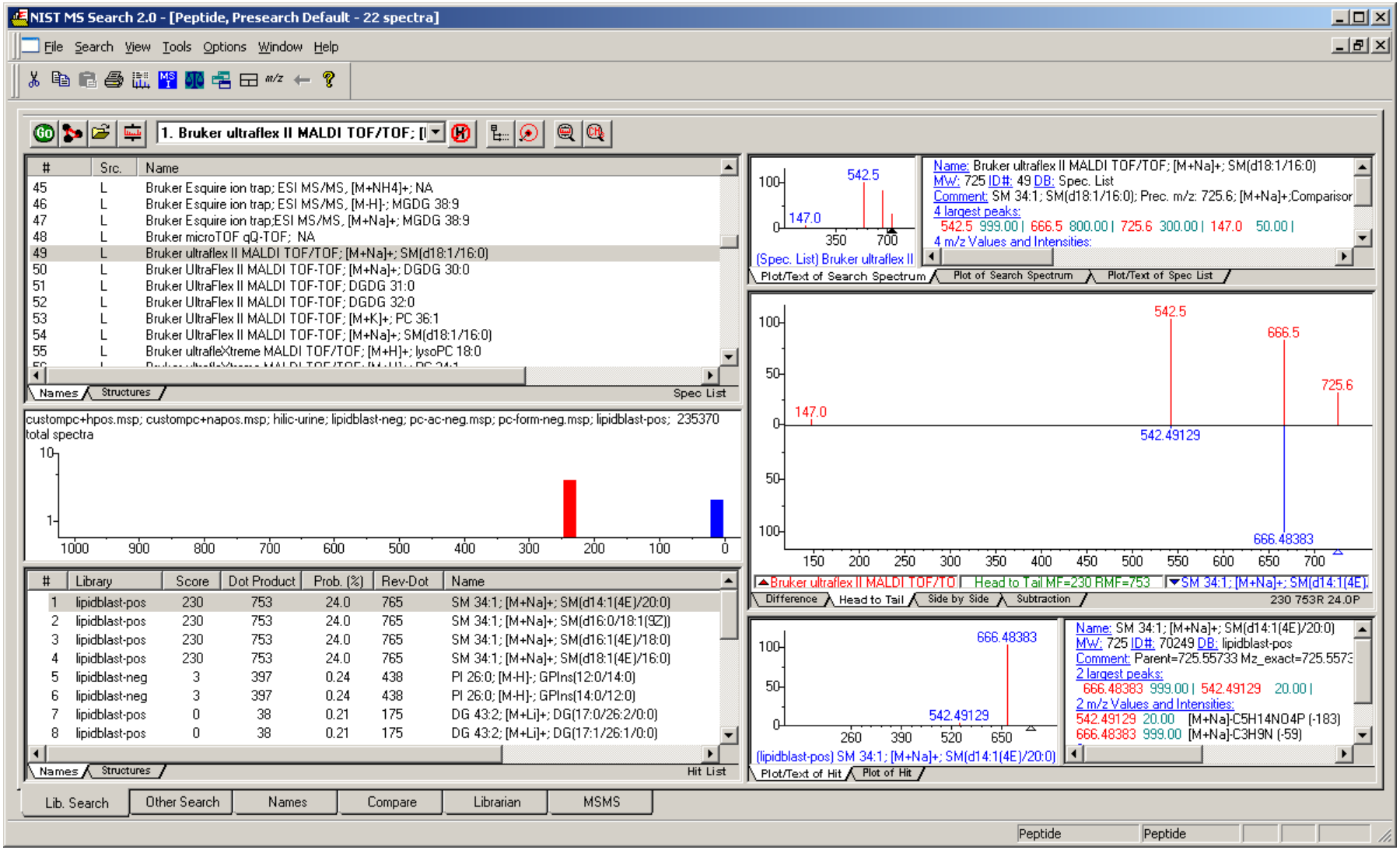
Name: Bruker Esquire ion trap;ESI MS/MS, [M+Na]+; MGDG 38:9
MW: 819 ID#: 47 DB: Spec. List
Comment: MGDG(20:5/18:4); MGDG 38:9; [M+Na]+; Prec. m/z: 819.7; Chimica e biologia a confronto: pigmenti e altri metaboliti secondari prodotti da dinoflagellati del Lago di Tovel; Studi Trent. Sci. Nat., Acta Biol., 81 (2004), Suppl. 2: 413-426;Rita FRASSANITO, Ines MANCINI & Graziano GUELLA
3 largest peaks:



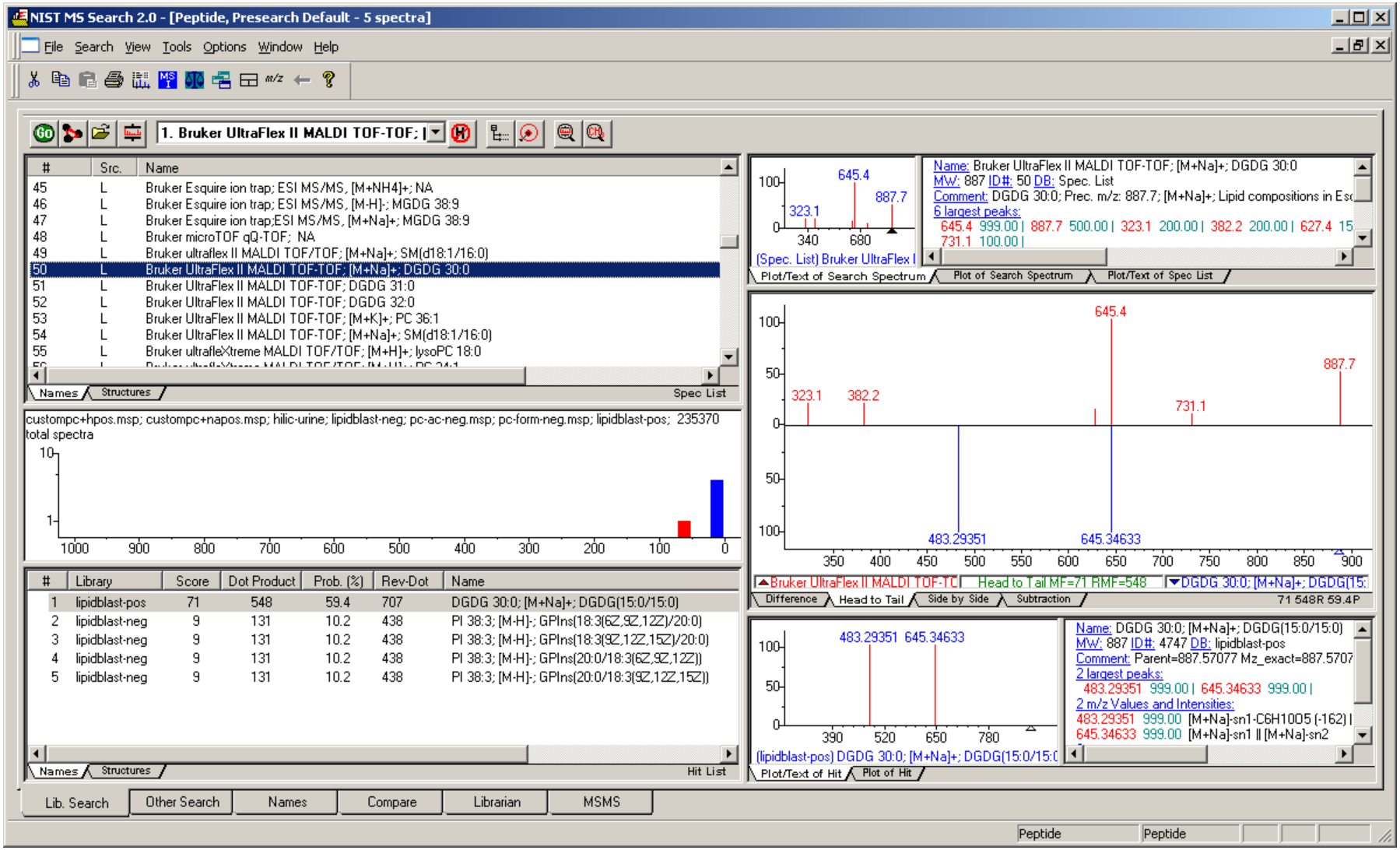
Name: Bruker microTOF qQ-TOF; NA
MW: 744 ID#: 48 DB: Spec. List
Comment: PC(16:0/18:1) wrongly assigned?; 744.4; [M+H]+; MS/MS mass spectra of 1-palmitoyl-, 2-oleyl-phosphatidycholine; Hyphenated Tools for Lipidomics;Jan Willmann1,Herbert Thiele2, Dieter Leibfritz1;HUPO 2007, Poster M-195
5 largest peaks:



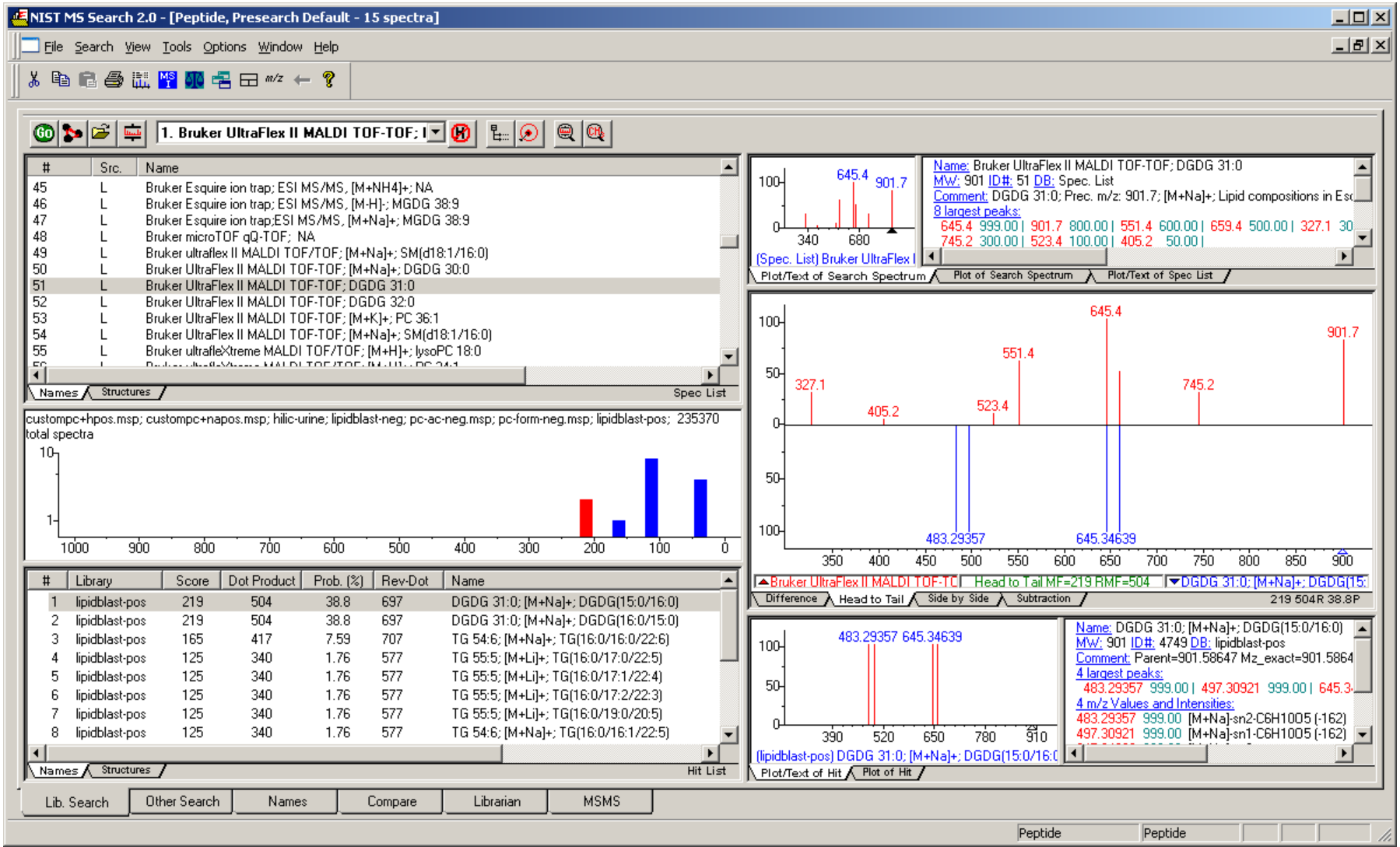
Name: Bruker ultraflex II MALDI TOF/TOF; [M+Na]+; SM(d18:1/16:0)
MW: 725 ID#: 49 DB: Spec. List
Comment: SM 34:1; SM(d18:1/16:0); Prec. m/z: 725.6; [M+Na]+;Comparison of Phospholipid Molecular Species between Terminal and Stem Villi of Human Term Placenta by Imaging Mass Spectrometry;Placenta 31 (2010) 245248; http://dx.doi.org/10.1016/j.placenta.2009.12.026
4 largest peaks:



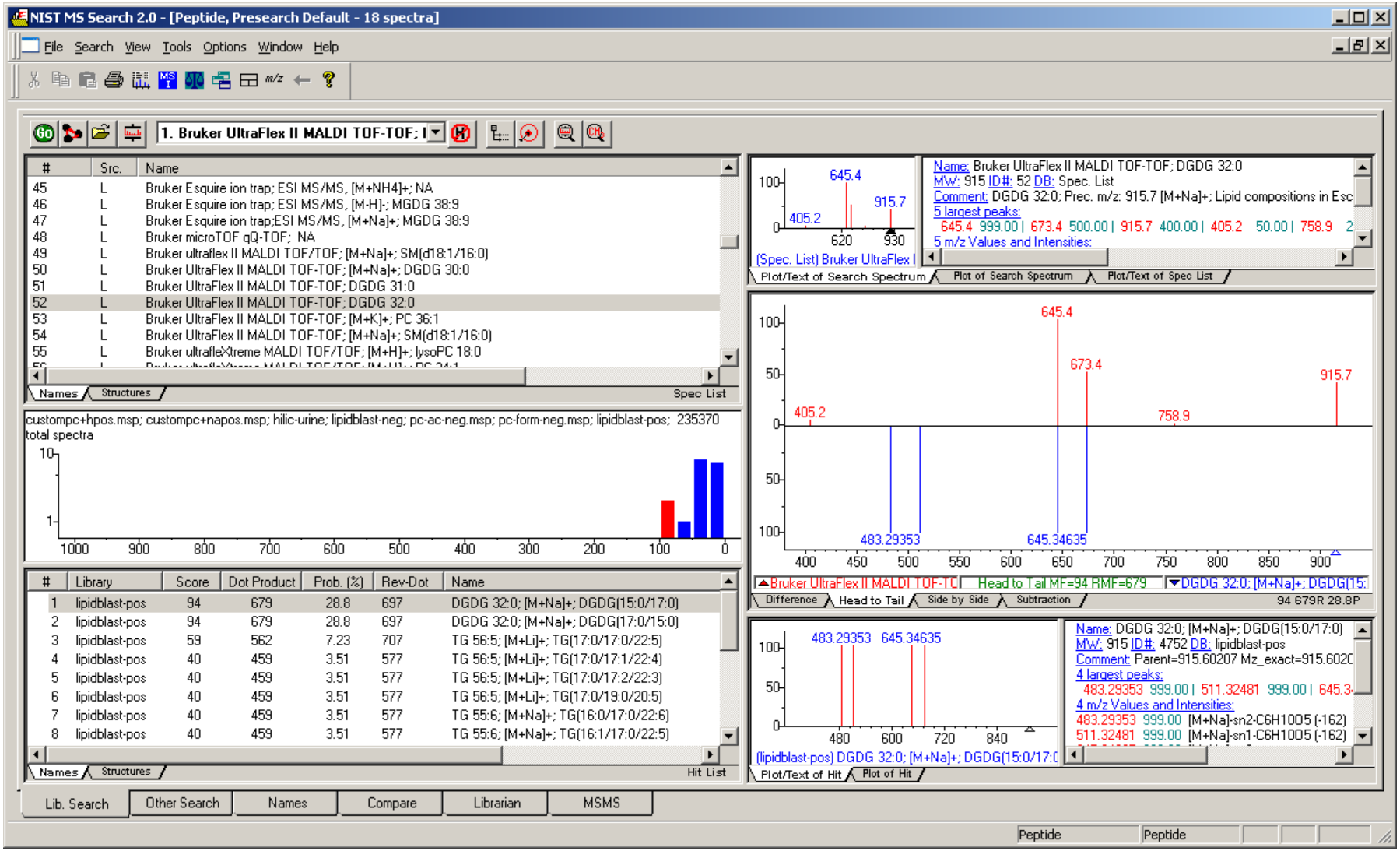
Name: Bruker UltraFlex II MALDI TOF-TOF; [M+Na]+; DGDG 30:0
MW: 887 ID#: 50 DB: Spec. List
Comment: DGDG 30:0; Prec. m/z: 887.7; [M+Na]+; Lipid compositions in Escherichia coli and Bacillus subtilis during growth as determined by MALDI-TOF and TOF/TOF mass spectrometry;
6 largest peaks:



Name: Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
MW: 901 ID#: 51 DB: Spec. List
Comment: DGDG 31:0; Prec. m/z: 901.7; [M+Na]+; Lipid compositions in Escherichia coli and Bacillus subtilis during growth as determined by MALDI-TOF and TOF/TOF mass spectrometry;
8 largest peaks:

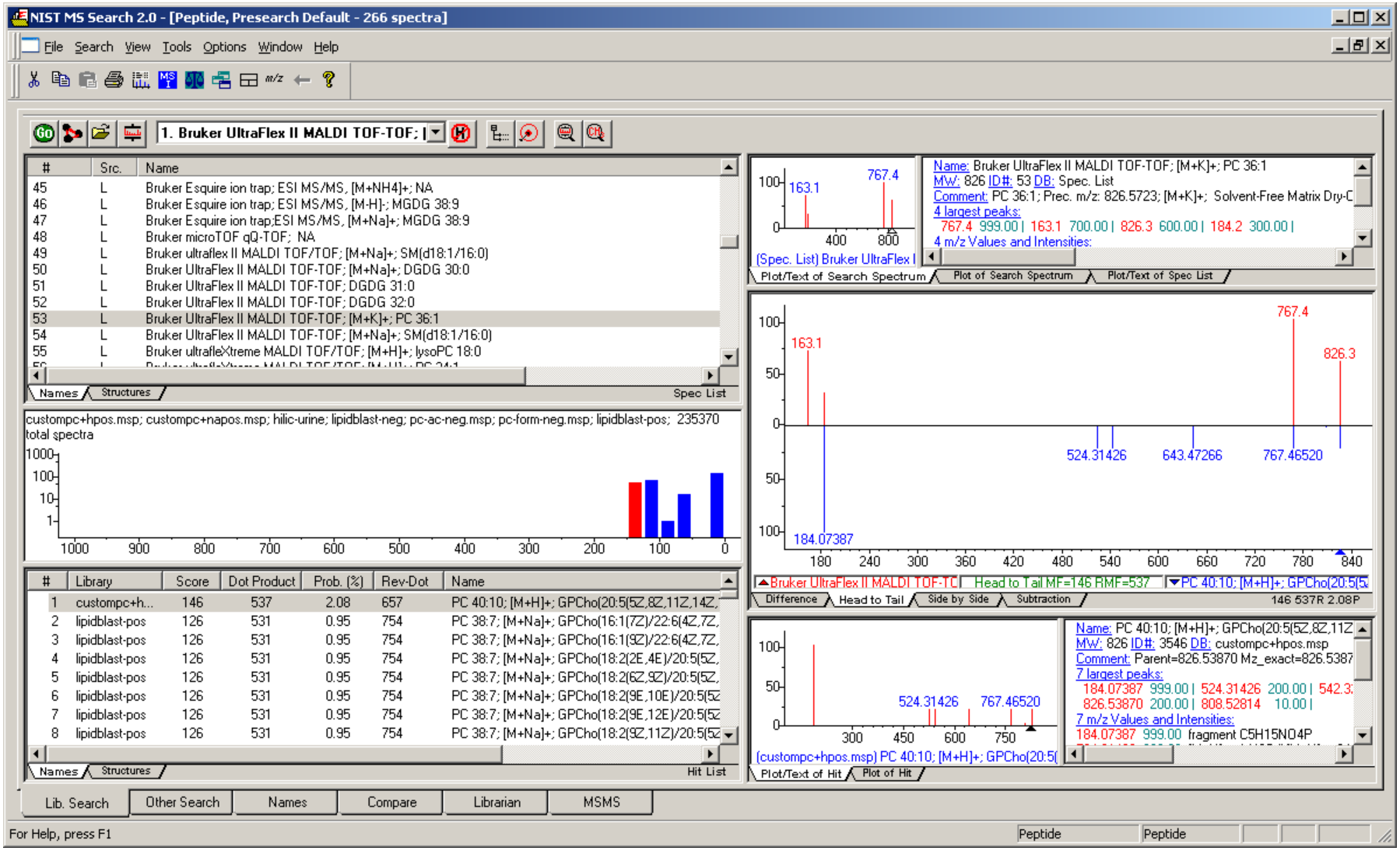


Name: Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
MW: 915 ID#: 52 DB: Spec. List
Comment: DGDG 32:0; Prec. m/z: 915.7 [M+Na]+; Lipid compositions in Escherichia coli and Bacillus subtilis during growth as determined by MALDI-TOF and TOF/TOF mass spectrometry;
5 largest peaks:

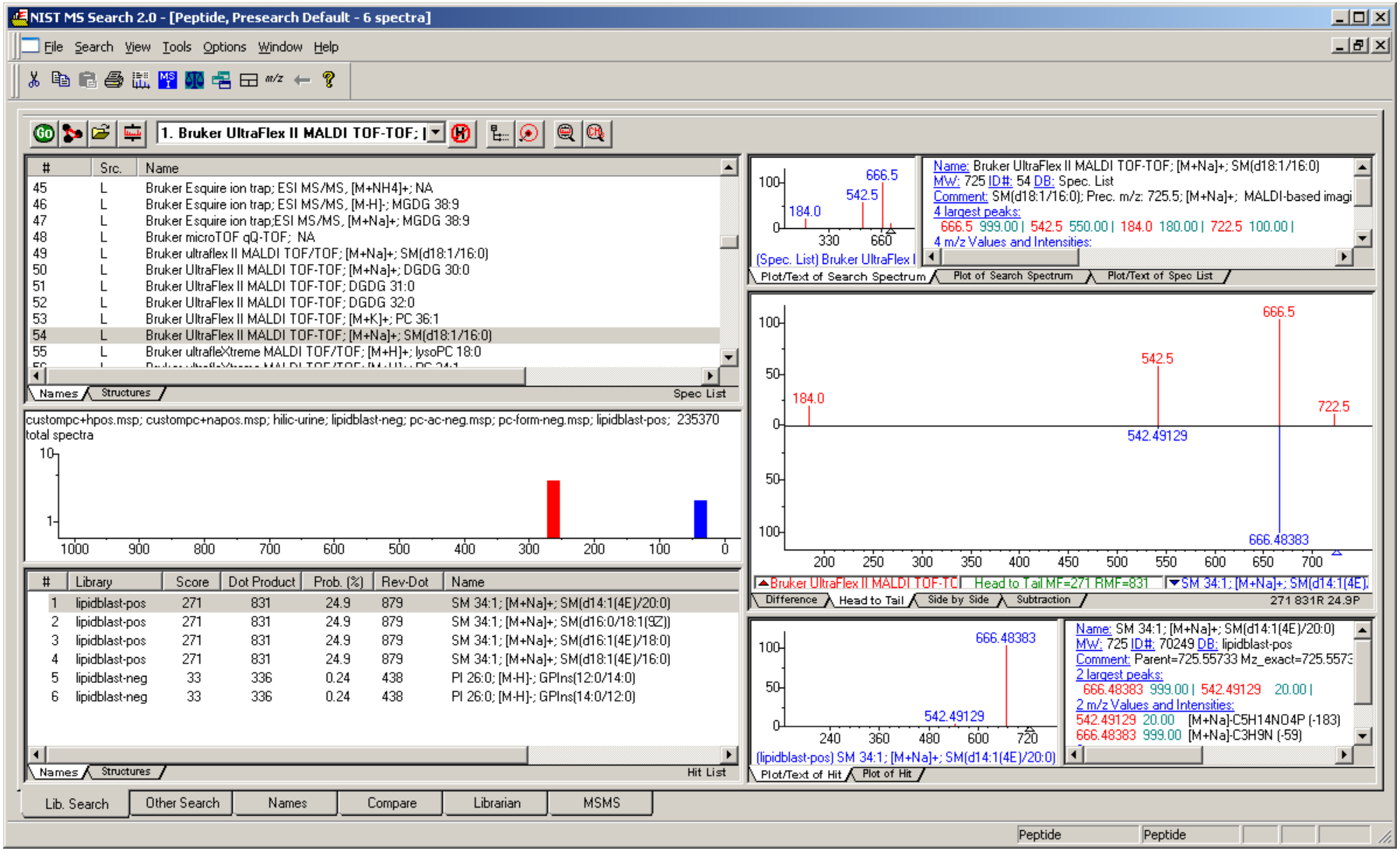


Name: Bruker UltraFlex II MALDI TOF-TOF; [M+K]+; PC 36:1
MW: 826 ID#: 53 DB: Spec. List
Comment: PC 36:1; Prec. m/z: 826.5723; [M+K]+; Solvent-Free Matrix Dry-Coating for MALDI Imaging of Phospholipids ;Satu M. Puolitaival, Kristin E. Burnum, D. Shannon Cornett, Richard M. Caprioli; doi:10.1016/j.jasms.2008.02.013
4 largest peaks:

FALSE Positive ID
M+K not in LipidBlast

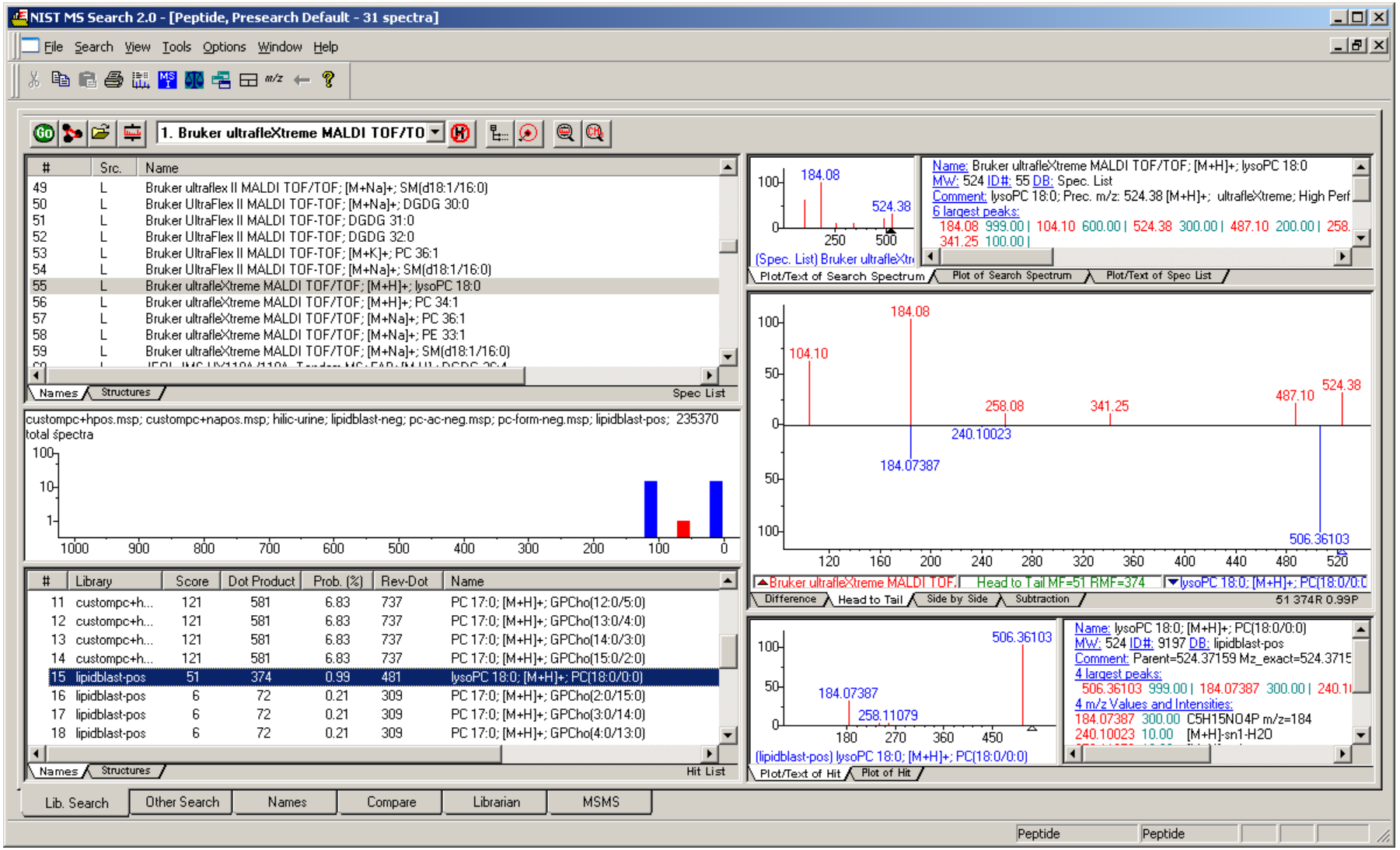


Name: Bruker UltraFlex II MALDI TOF-TOF; [M+Na]+; SM(d18:1/16:0)
MW: 725 ID#: 54 DB: Spec. List
Comment: SM(d18:1/16:0); Prec. m/z: 725.5; [M+Na]+; MALDI-based imaging mass spectrometry revealed abnormal distribution of phospholipids in colon cancer liver metastasis; http://dx.doi.org/10.1016/j.jchromb.2007.02.037
4 largest peaks:

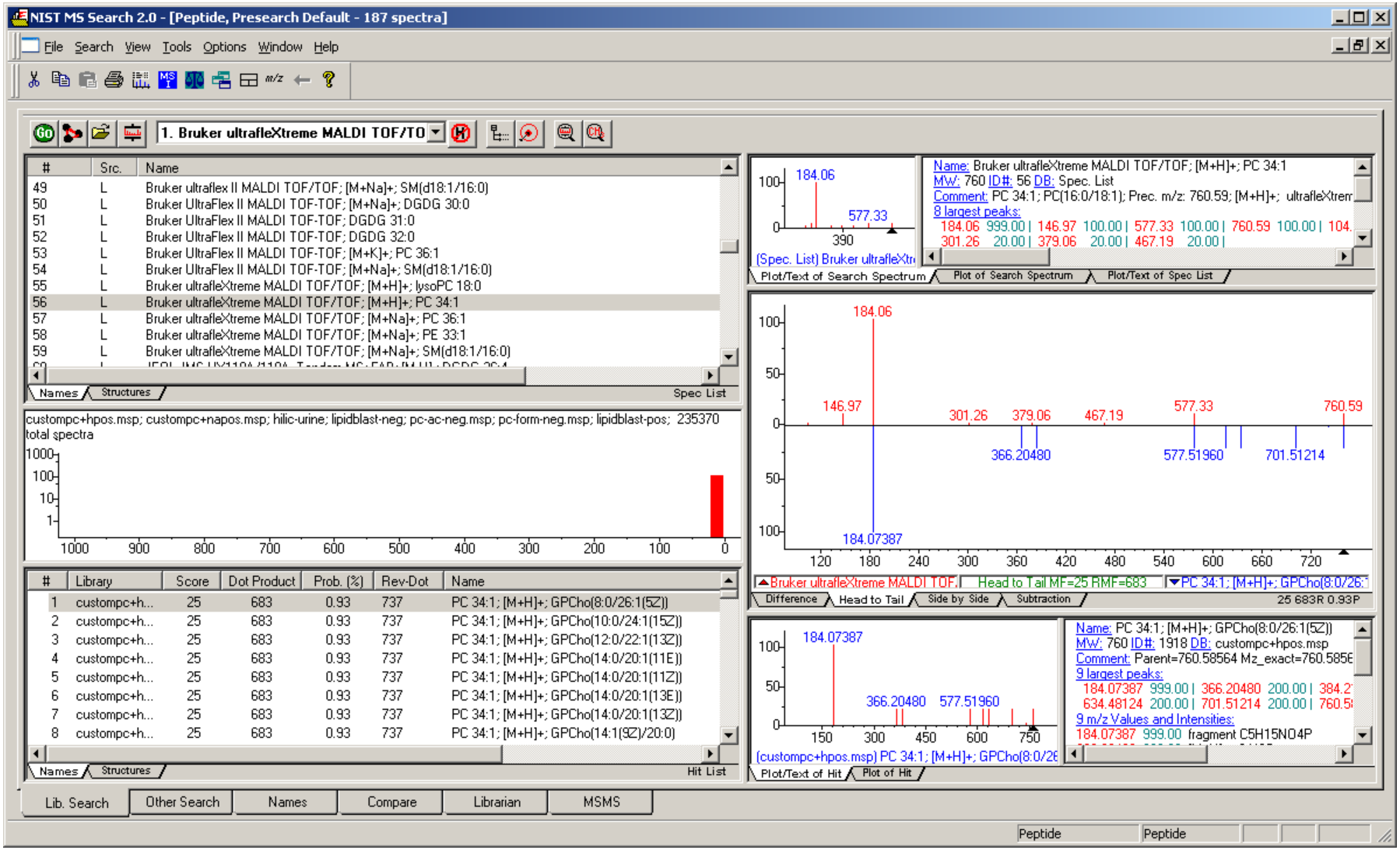


2nd probability group

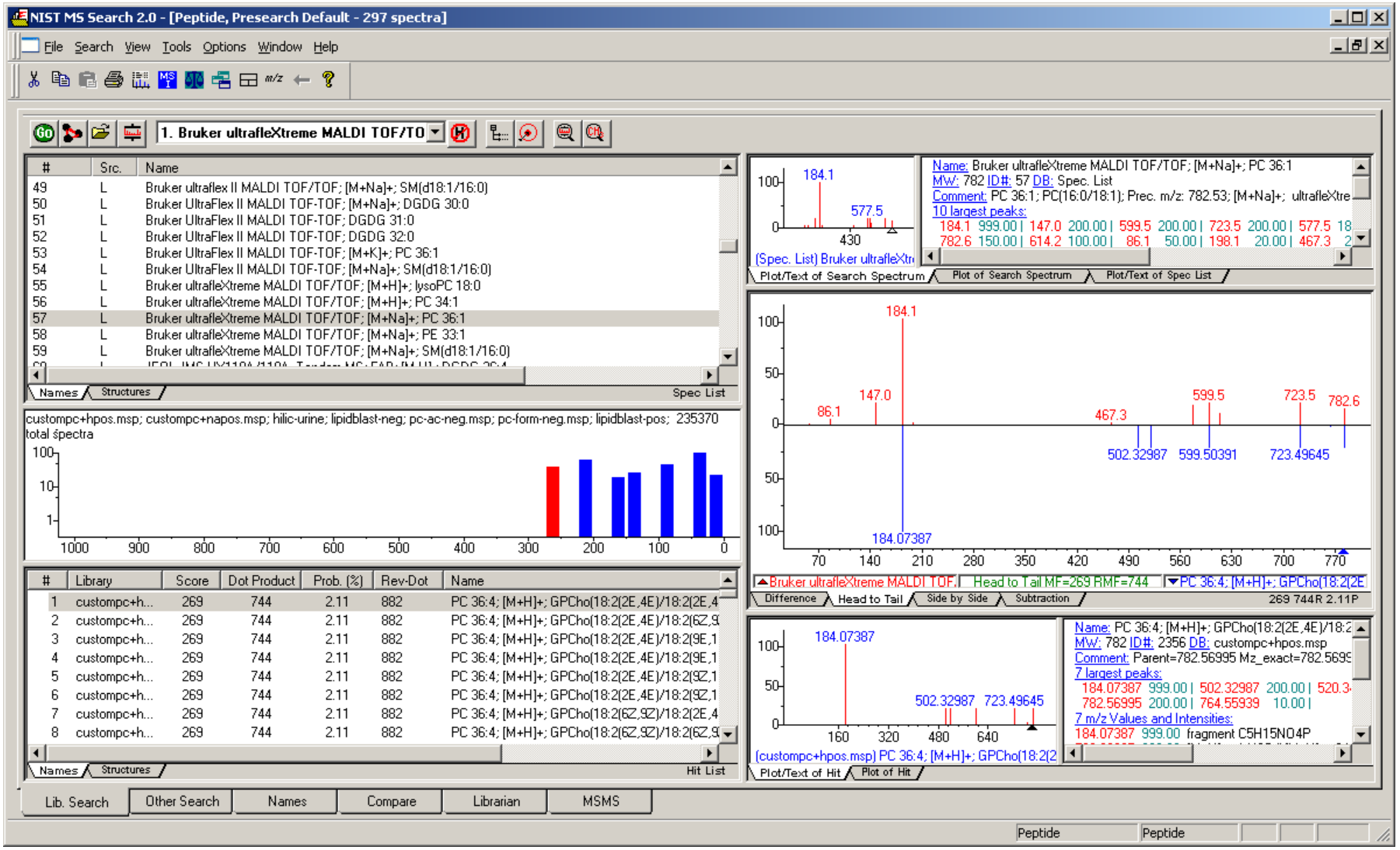
Name: Bruker ultrafleXtreme MALDI TOF/TOF; [M+H]+; lysoPC 18:0
MW: 524 ID#: 55 DB: Spec. List
Comment: lysoPC 18:0; Prec. m/z: 524.38 [M+H]+; ultrafleXtreme; High Performance TLC-MALDI; Martin Schürenberg, Beate Fuchs, Annabell Bischoff, Rosemarie Sü, Detlev Suckau, Jürgen Schiller, Gerda Morlock and Ulrike Anders; DGMS2010_185_Poster_TLC-MALDI.pd
6 largest peaks:



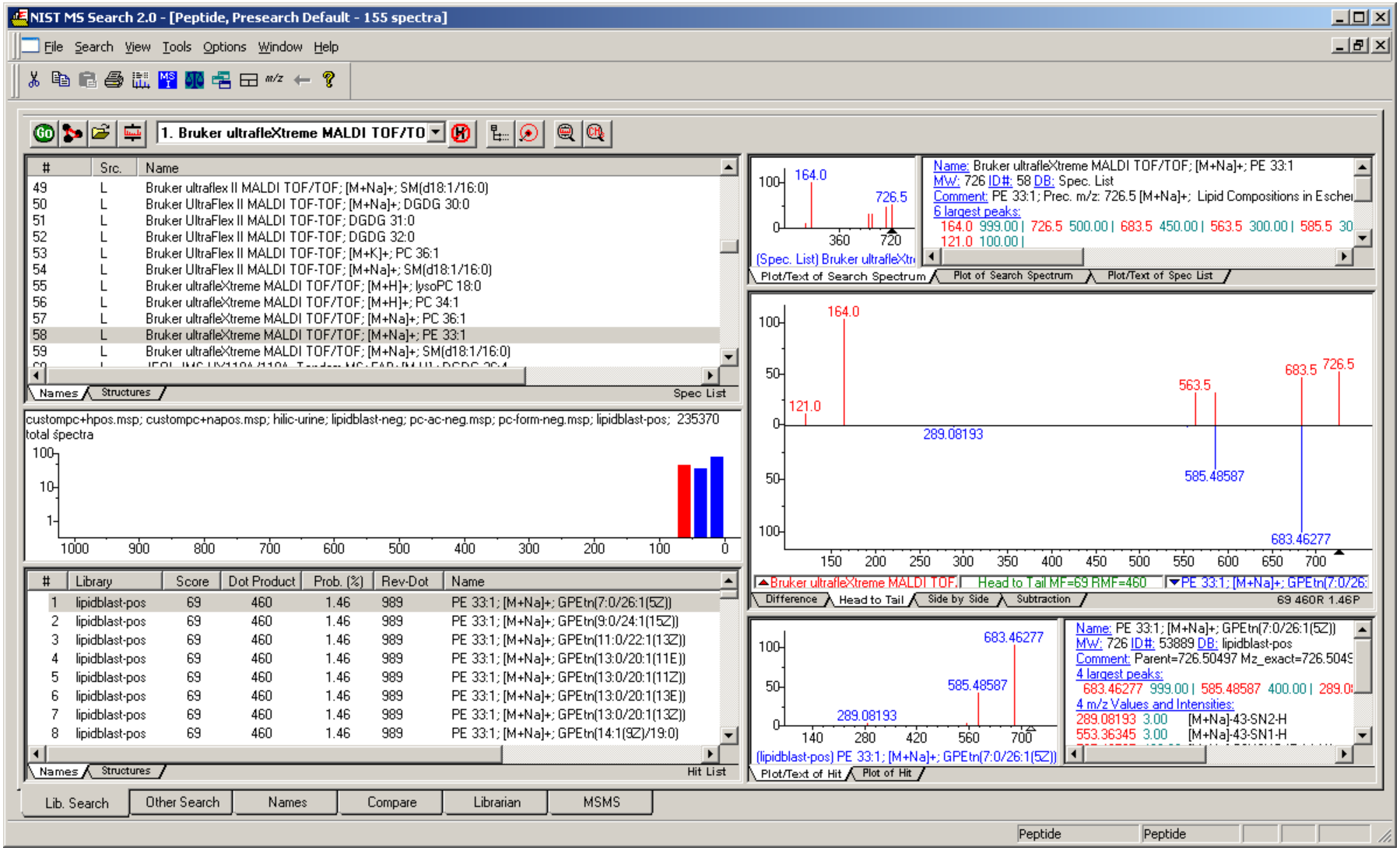
Name: Bruker ultrafleXtreme MALDI TOF/TOF; [M+H]+; PC 34:1
MW: 760 ID#: 56 DB: Spec. List
Comment: PC 34:1; PC(16:0/18:1); Prec. m/z: 760.59; [M+H]+; ultrafleXtreme; High Performance TLC-MALDI; Martin Schürenberg, Beate Fuchs, Annabell Bischoff, Rosemarie Sü, Detlev Suckau, Jürgen Schiller, Gerda Morlock and Ulrike Anders; DGMS2010_185_Poster_TLC-MALDI.pd
8 largest peaks:



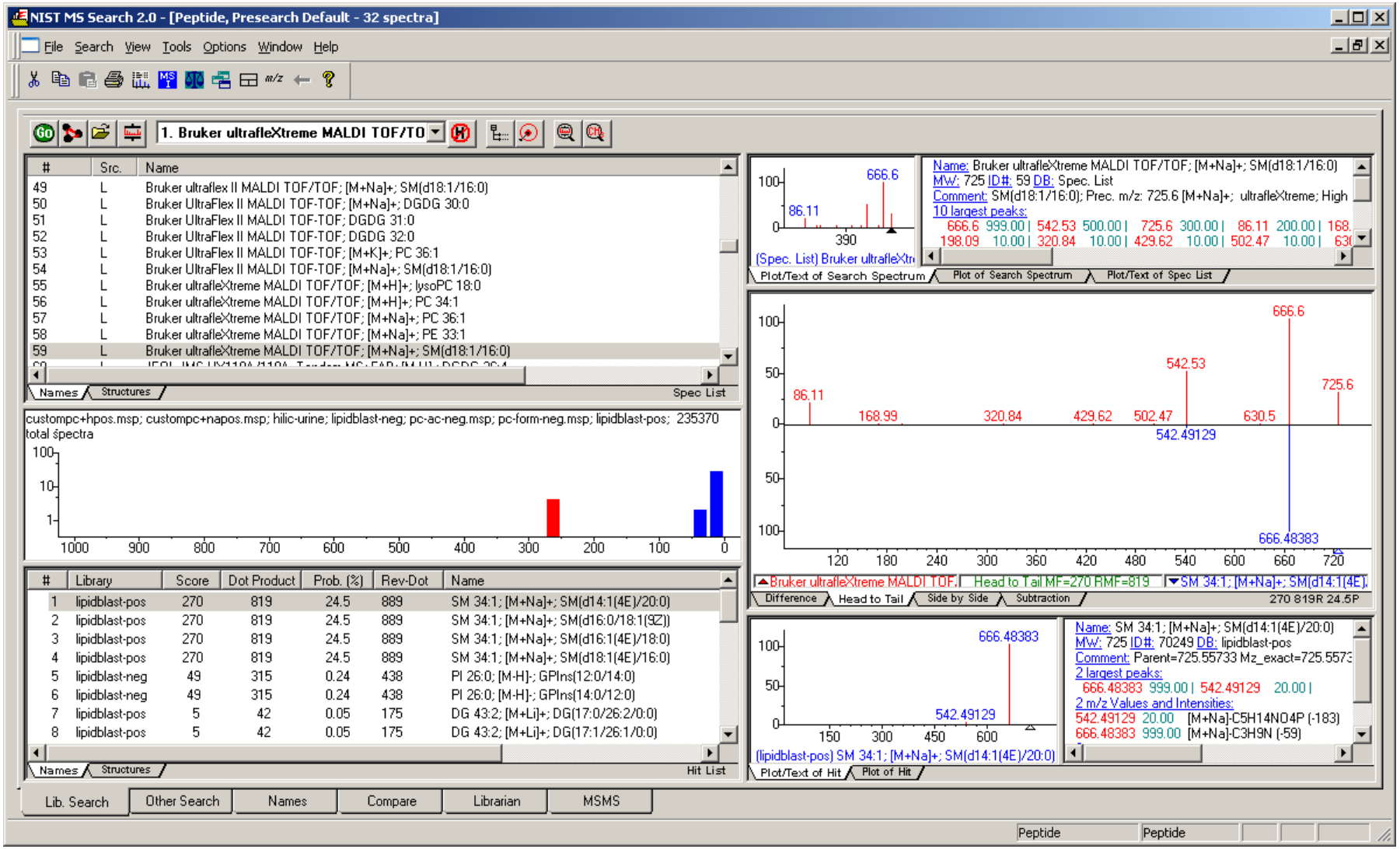
Name: Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na]+; PC 36:1
MW: 782 ID#: 57 DB: Spec. List
Comment: PC 36:1; PC(16:0/18:1); Prec. m/z: 782.53; [M+Na]+; ultrafleXtreme; BDAL; http://www.bdal.de/uploads/media/ultrafleXtreme-eBook.pdf
10 largest peaks:



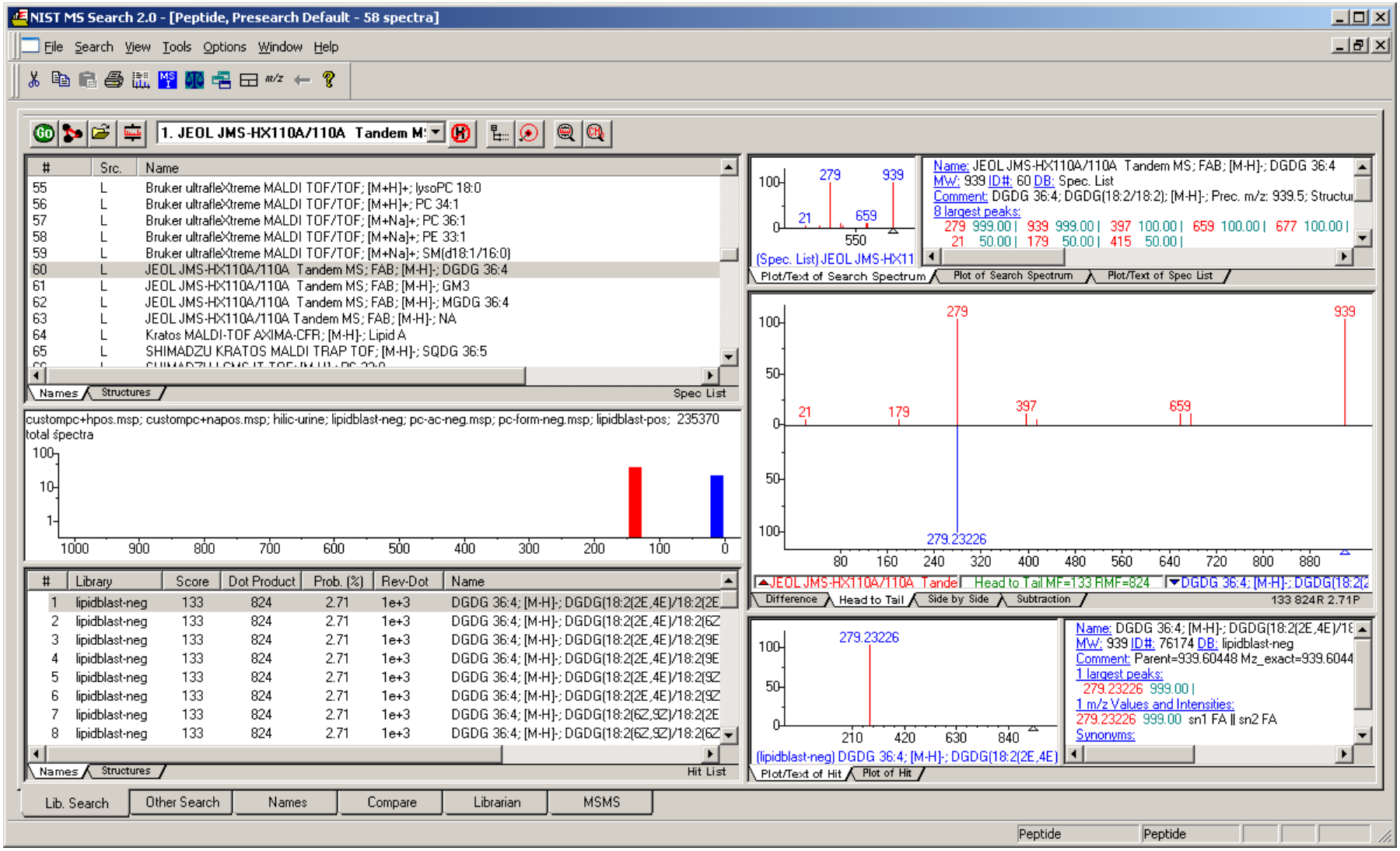
Name: Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na]+; PE 33:1
MW: 726 ID#: 58 DB: Spec. List
Comment: PE 33:1; Prec. m/z: 726.5 [M+Na]+; Lipid Compositions in Escherichia coli and Bacillus subtilis During Growth as Determined by MALDI-TOF and TOF/TOF Mass Spectrometry; doi:10.1016/j.ijms.2009.03.005.
6 largest peaks:



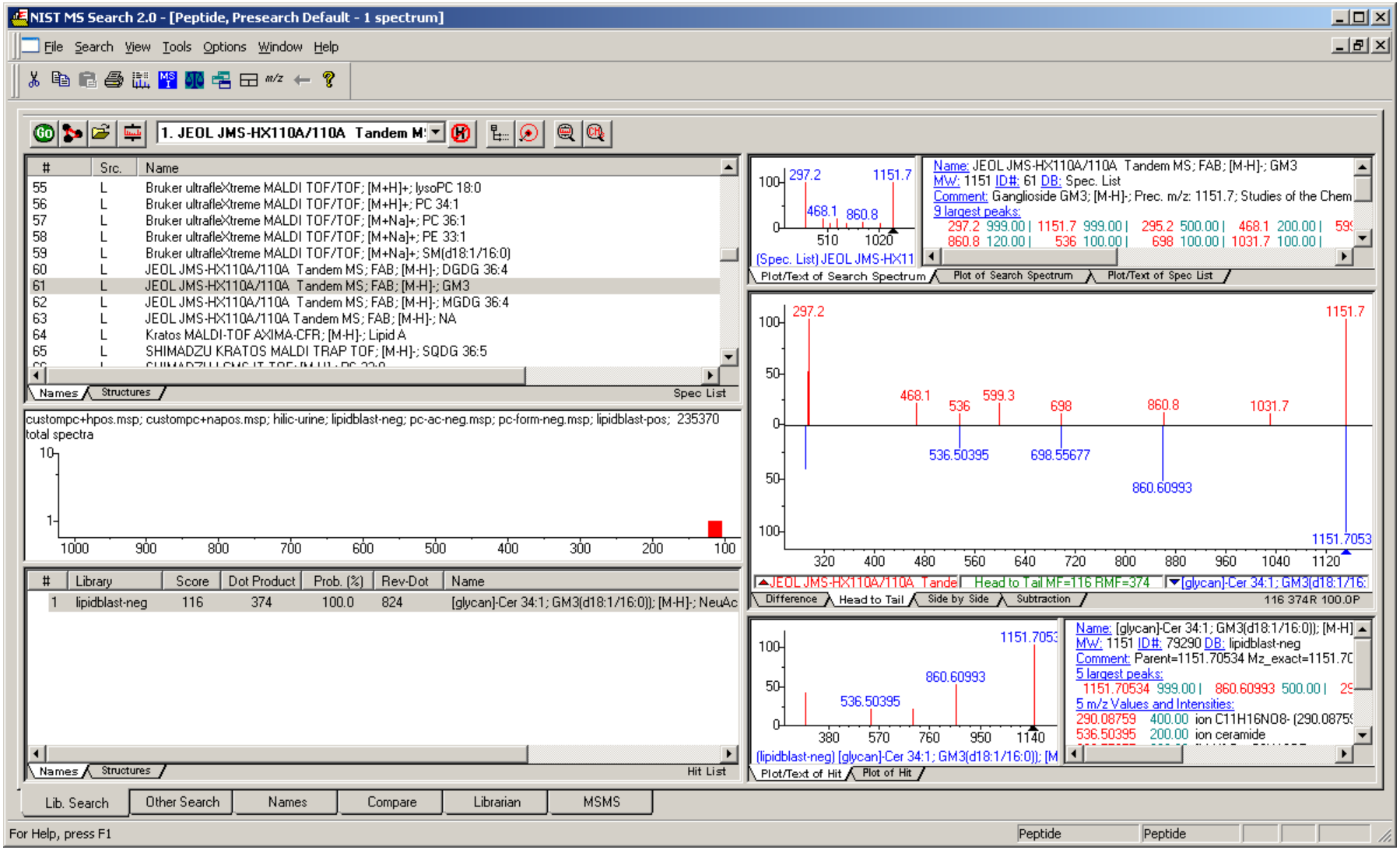
Name: Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na]+; SM(d18:1/16:0)
MW: 725 ID#: 59 DB: Spec. List
Comment: SM(d18:1/16:0); Prec. m/z: 725.6 [M+Na]+; ultrafleXtreme; High Performance TLC-MALDI; Martin Schürenberg, Beate Fuchs, Annabell Bischoff, Rosemarie Sü, Detlev Suckau, Jürgen Schiller, Gerda Morlock and Ulrike Anders; DGMS2010_185_Poster_TLC-MALDI.pd
10 largest peaks:



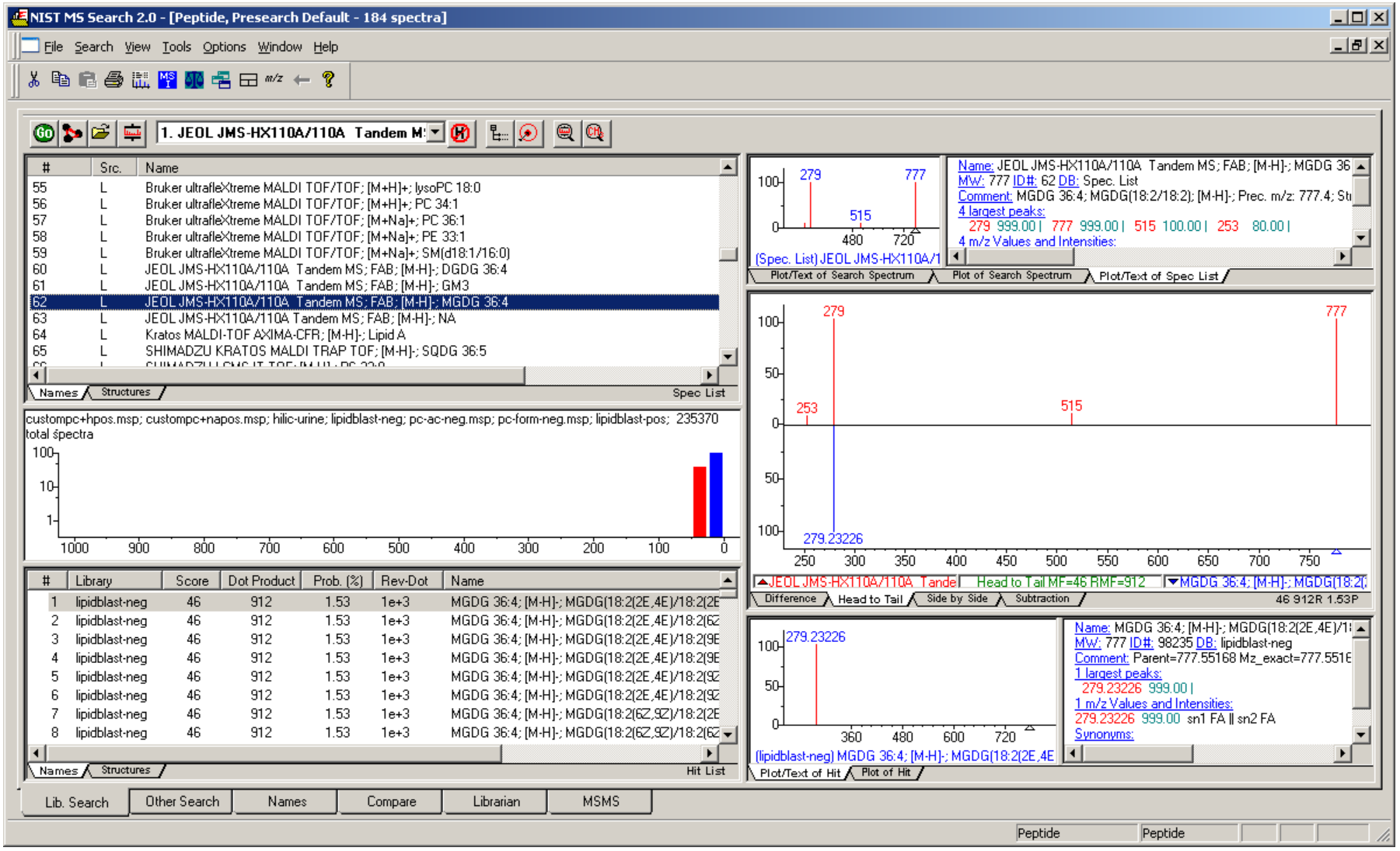
Name: JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]-; DGDG 36:4
MW: 939 ID#: 60 DB: Spec. List
Comment: DGDG 36:4; DGDG(18:2/18:2); [M-H]-; Prec. m/z: 939.5; Structural Characterization of Sulfoquinovosyl, Monogalactosyl and Digalactosyl Diacylglycerols by FAB-CID-MS/MS; JOURNAL OF MASS SPECTROMETRY, VOL. 32, 968-977 (1997)
8 largest peaks:



Name: JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]-; GM3
MW: 1151 ID#: 61 DB: Spec. List
Comment: Ganglioside GM3; [M-H]-; Prec. m/z: 1151.7; Studies of the Chemical Structure of Gangliosides in Deer Antler, Cervus nippon; Chem. Pharm. Bull. 47(1) 123-127 (1999)
9 largest peaks:

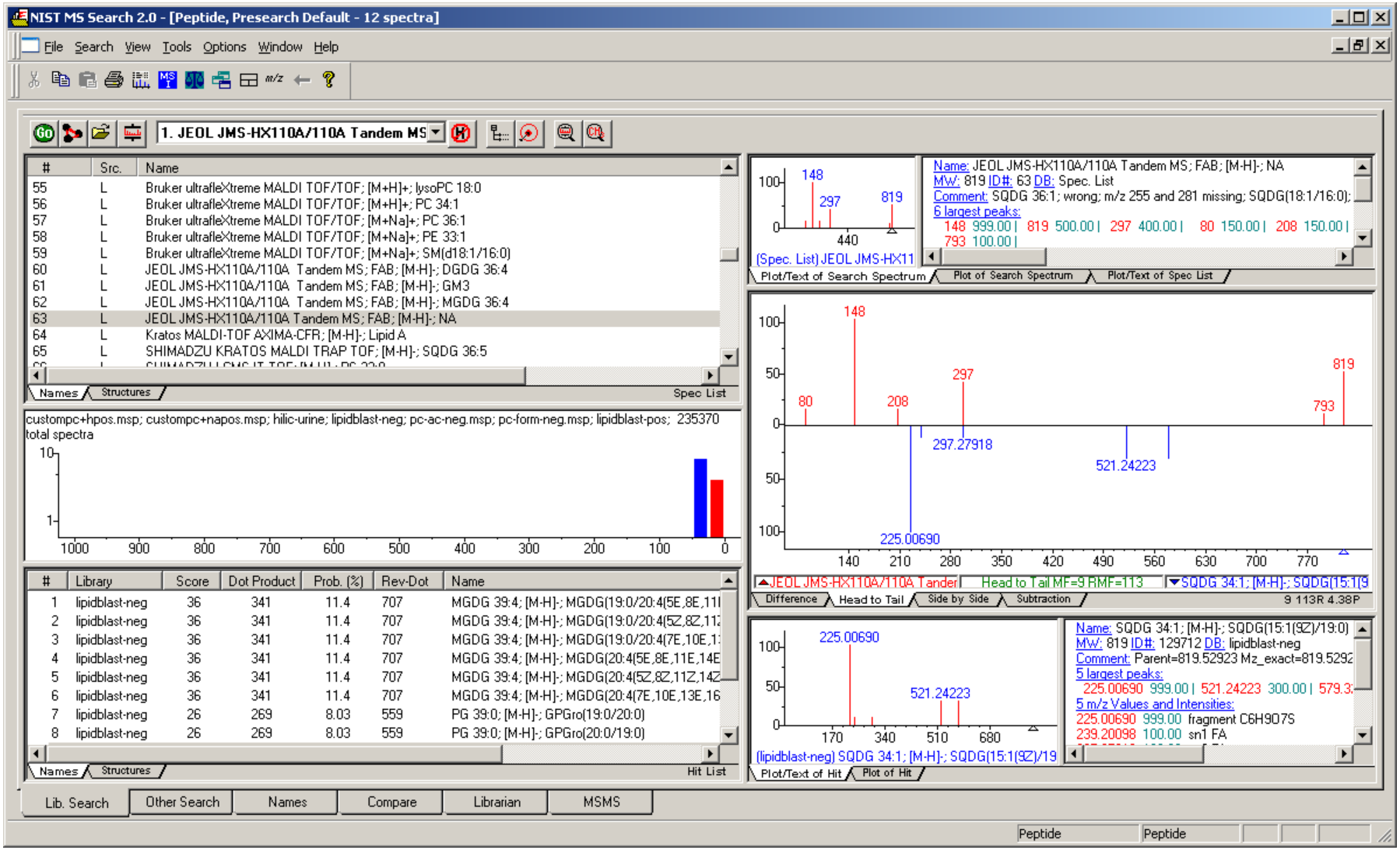


Name: JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]-; MGDG 36:4
MW: 777 ID#: 62 DB: Spec. List
Comment: MGDG 36:4; MGDG(18:2/18:2); [M-H]-; Prec. m/z: 777.4; Structural Characterization of Sulfoquinovosyl, Monogalactosyl and Digalactosyl Diacylglycerols by FAB-CID-MS/MS; JOURNAL OF MASS SPECTROMETRY, VOL. 32, 968-977 (1997)
4 largest peaks:

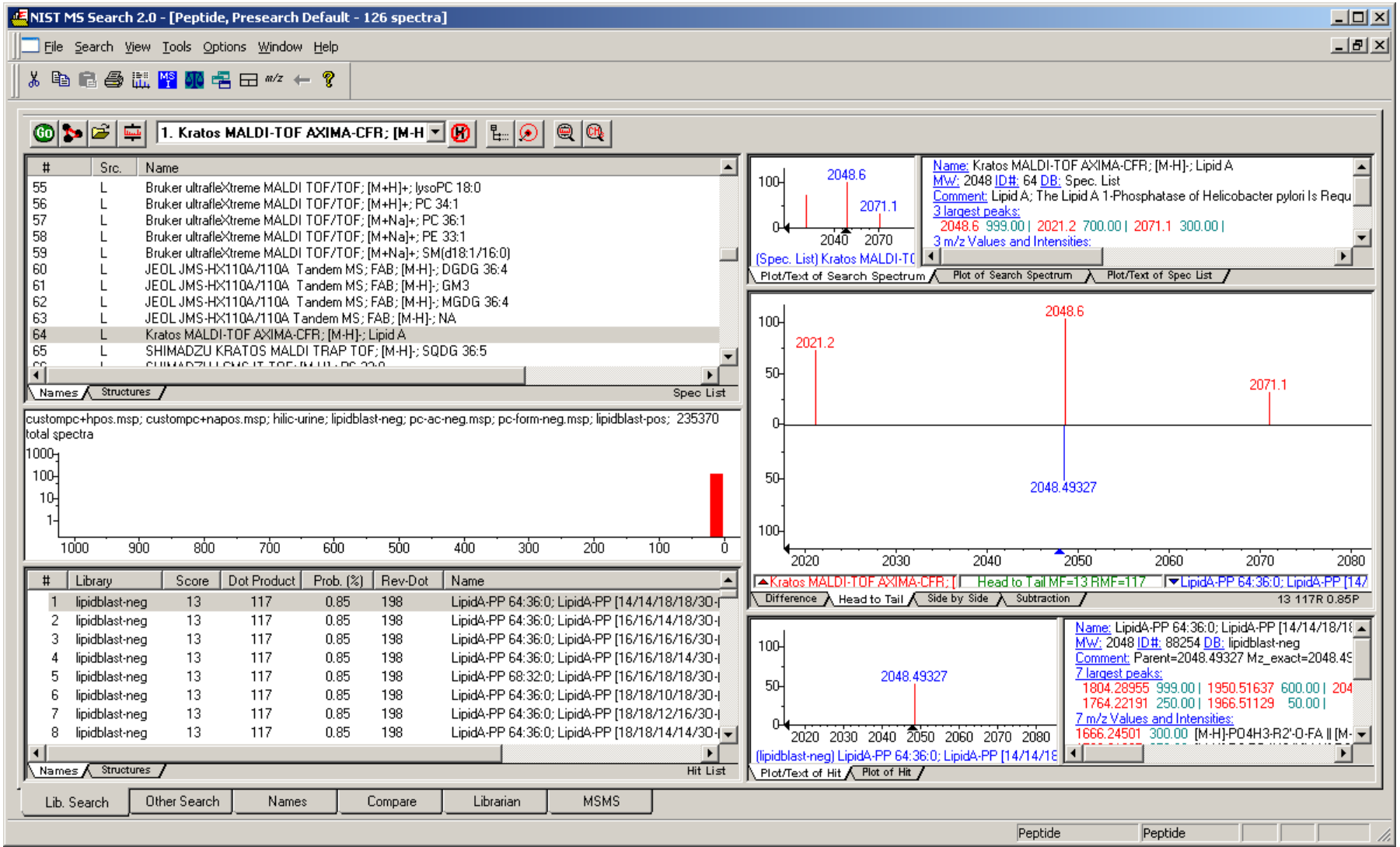


Name: JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]-; NA
MW: 819 ID#: 63 DB: Spec. List
Comment: SQDG 36:1; wrong; m/z 255 and 281 missing; SQDG(18:1/16:0); [M-H]-; Prec. m/z: 819.6; Structural Characterization of Sulfoquinovosyl, Monogalactosyl and Digalactosyl Diacylglycerols by FAB-CID-MS/MS; JOURNAL OF MASS SPECTROMETRY, VOL. 32, 968-977 (1997)
6 largest peaks:

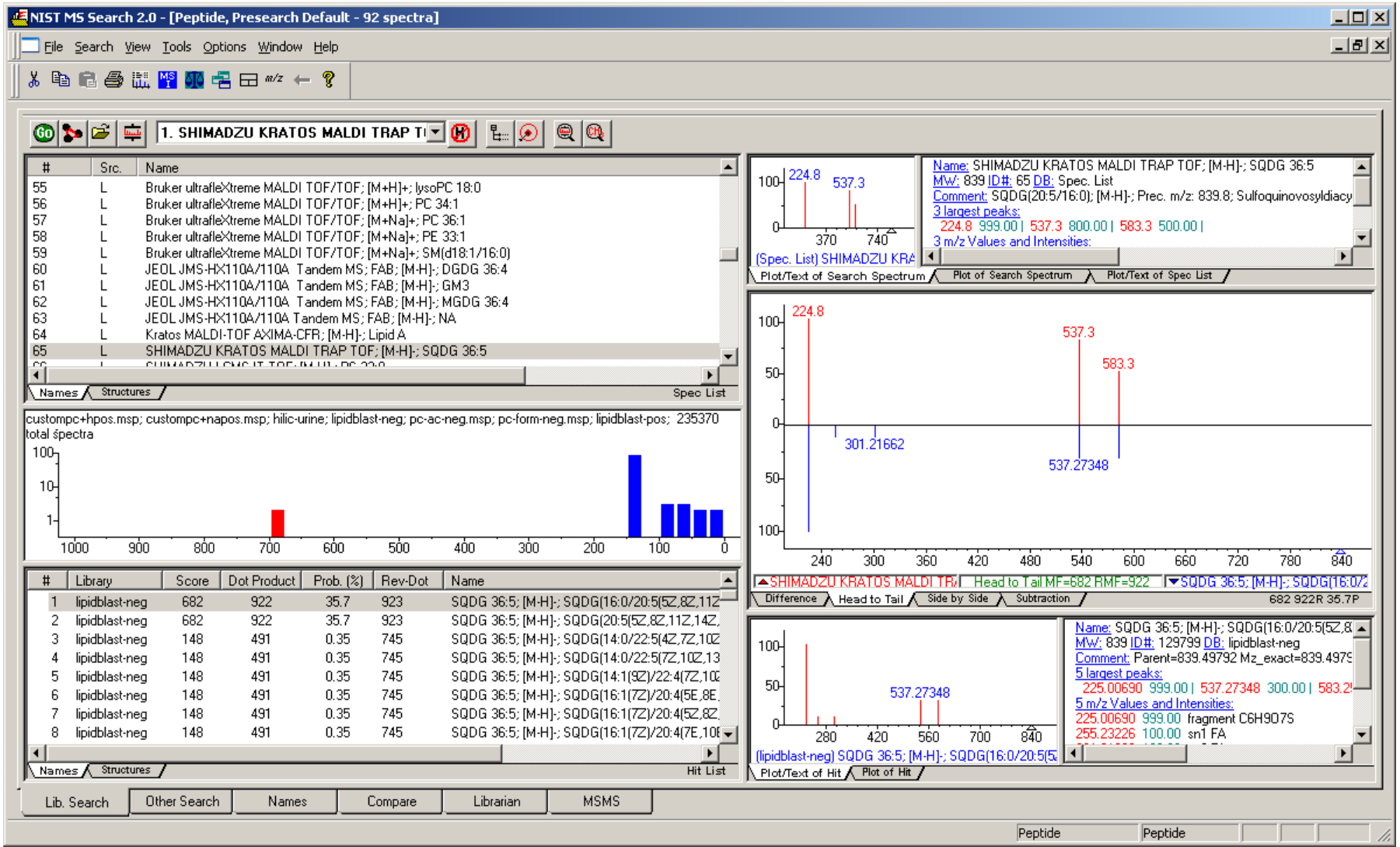
Wrong assignment:
SQDG 36:1; wrong; m/z 255 and 281 missing; SQDG(18:1/16:0); [M-H]-; Prec. m/z:



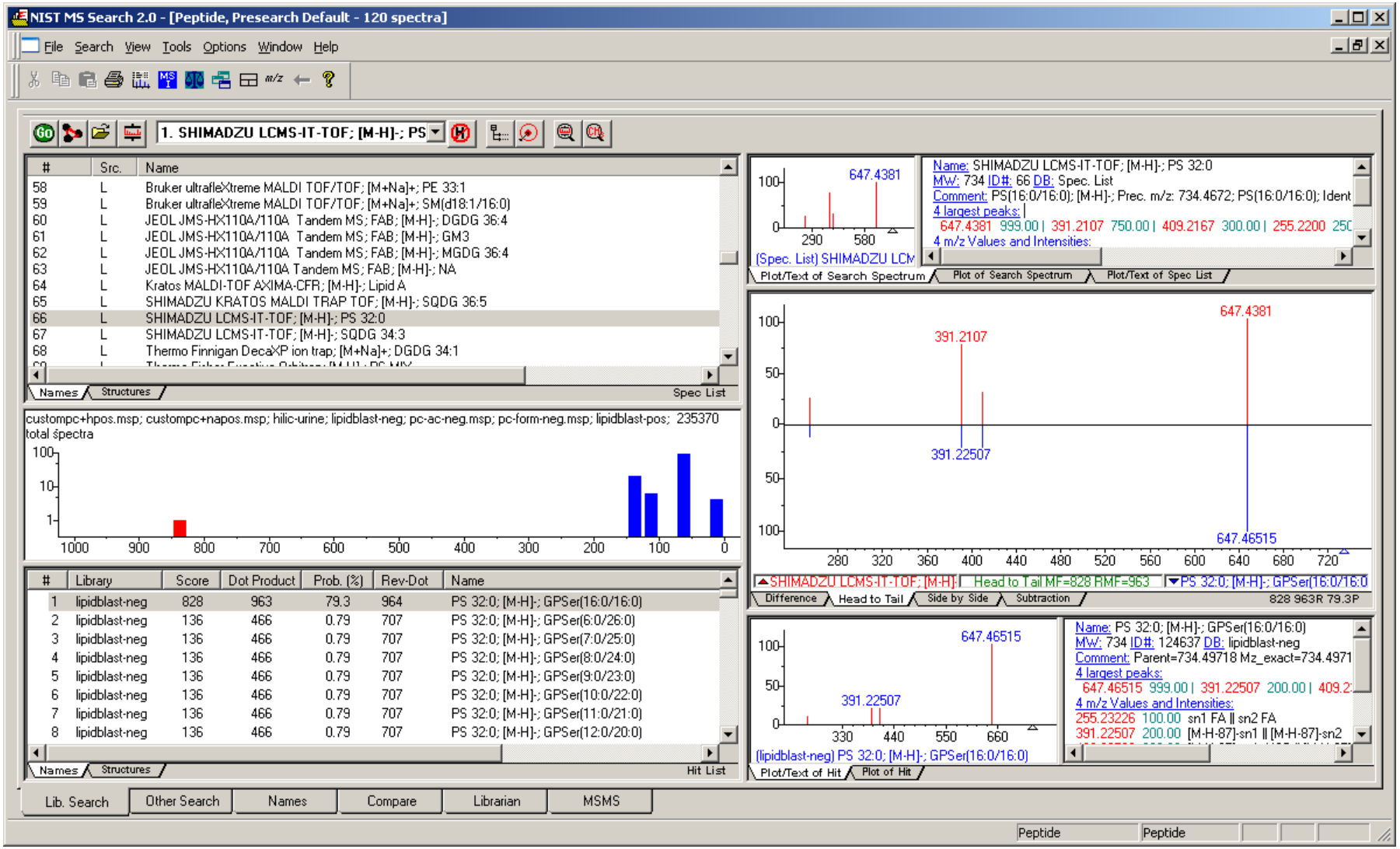
Name: Kratos MALDI-TOF AXIMA-CFR; [M-H]-; Lipid A
MW: 2048 ID#: 64 DB: Spec. List
Comment: Lipid A; The Lipid A 1-Phosphatase of Helicobacter pylori Is Required for Resistance to the Antimicrobial Peptide Polymyxin;JOURNAL OF BACTERIOLOGY, June 2006, p. 45314541
3 largest peaks:



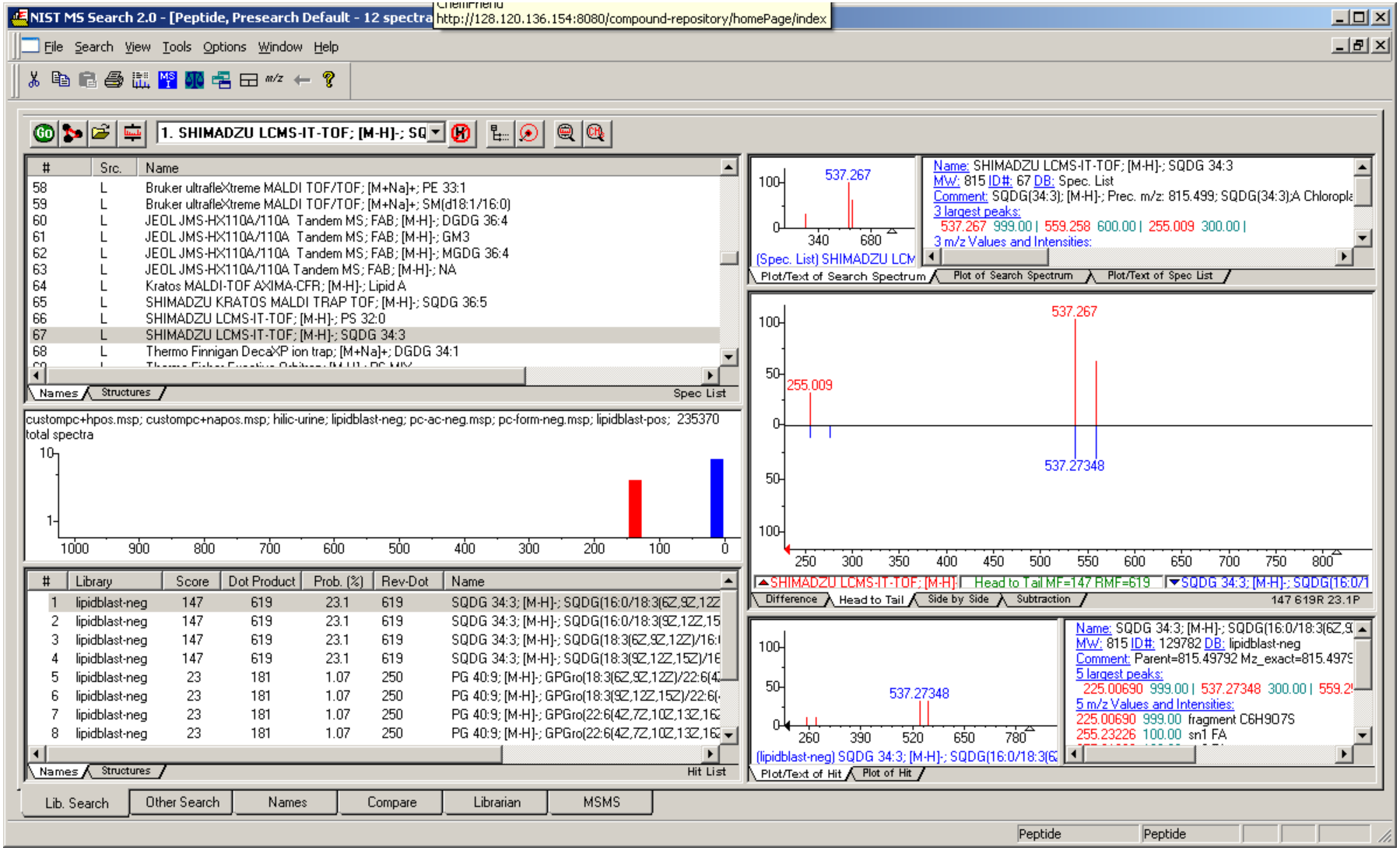
Name: SHIMADZU KRATOS MALDI TRAP TOF; [M-H]-; SQDG 36:5
MW: 839 ID#: 65 DB: Spec. List
Comment: SQDG(20:5/16:0); [M-H]-; Prec. m/z: 839.8; Sulfoquinovosyldiacylglyceride - antiviral aktive Substanzen; Diss Universitt Erlangen-Nürnberg; 2009; Ivonne Naumann
3 largest peaks:



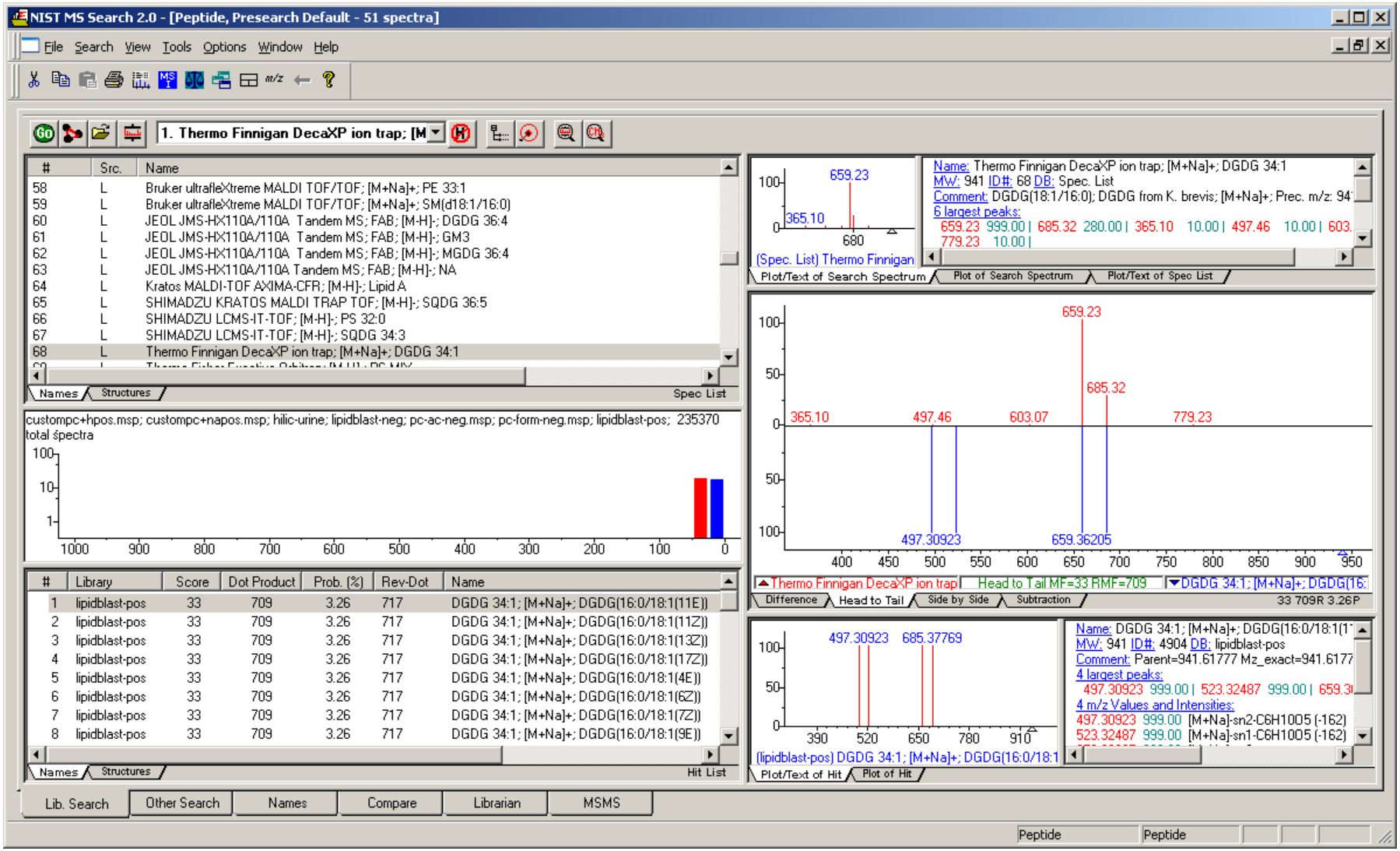
Name: SHIMADZU LCMS-IT-TOF; [M-H]-; PS 32:0
MW: 734 ID#: 66 DB: Spec. List
Comment: PS(16:0/16:0); [M-H]-; Prec. m/z: 734.4672; PS(16:0/16:0); Identification of Phospholipid Molecular Species Using Neutral Loss Survey and MS3 Analysis; Shimadzu Technical Report
4 largest peaks:



Name: SHIMADZU LCMS-IT-TOF; [M-H]-; SQDG 34:3
MW: 815 ID#: 67 DB: Spec. List
Comment: SQDG(34:3); [M-H]-; Prec. m/z: 815.499; SQDG(34:3);A Chloroplastic UDP-Glucose Pyrophosphorylase from Arabidopsis Is the Committed Enzyme for the First Step of Sulfolipid Biosynthesis;Plant Cell Okazaki et al. 21: 892 ;
http://www.plantcell.org/cgi/data/tpc.108.063925/DC1/1;
3 largest peaks:

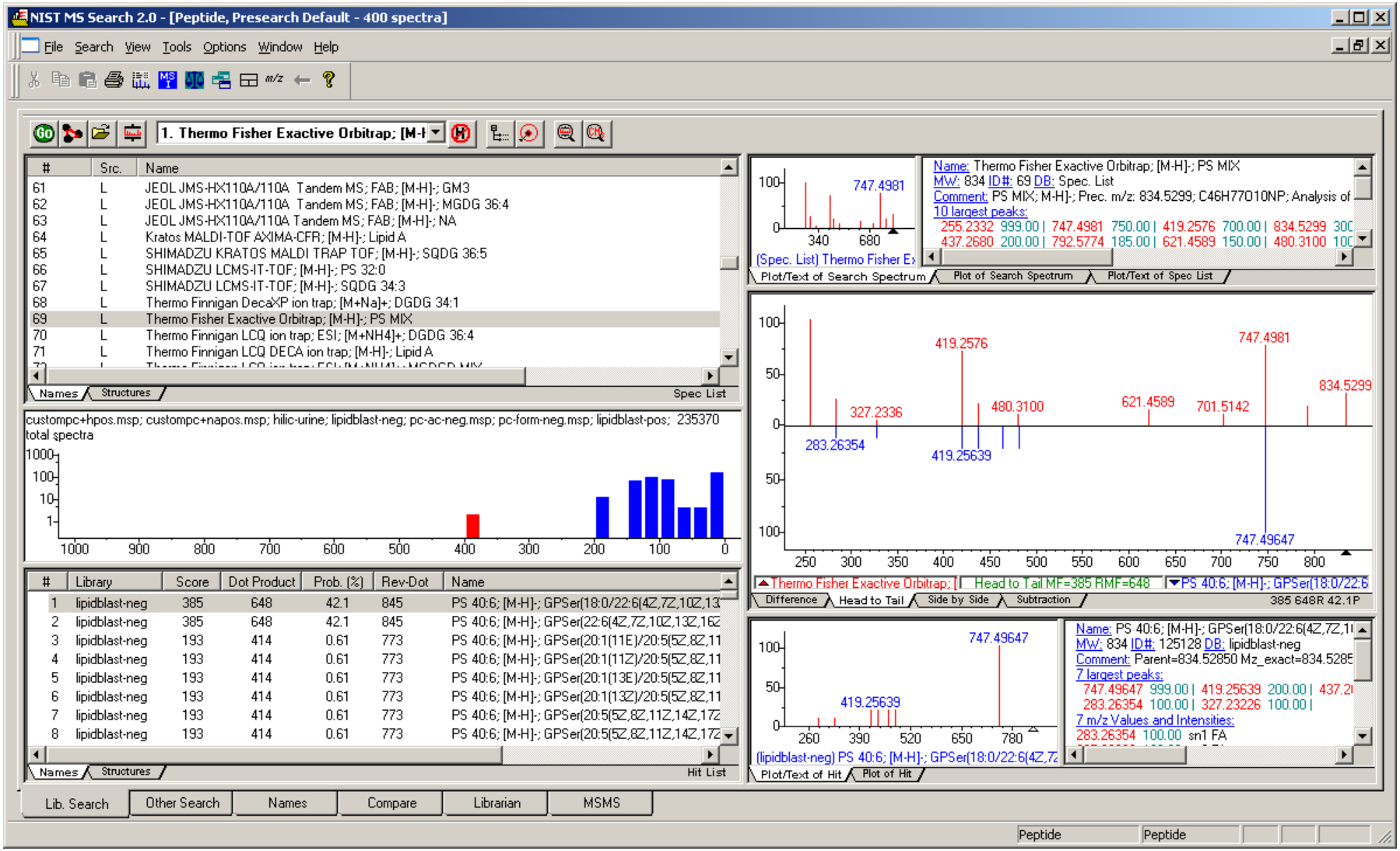


Name: Thermo Finnigan DecaXP ion trap; [M+Na]+; DGDG 34:1
MW: 941 ID#: 68 DB: Spec. List
Comment: DGDG(18:1/16:0); DGDG from K. brevis; [M+Na]+; Prec. m/z: 941.41;
6 largest peaks:



Name: Thermo Fisher Exactive Orbitrap; [M-H]-; PS MIX
MW: 834 ID#: 69 DB: Spec. List
Comment: PS MIX; M-H]-; Prec. m/z: 834.5299; C46H77O10NP; Analysis of whole lipid extracts using on-line high resolution LC-MS; Catharina Crone, Eric Genin and Helmut Muenster
10 largest peaks:

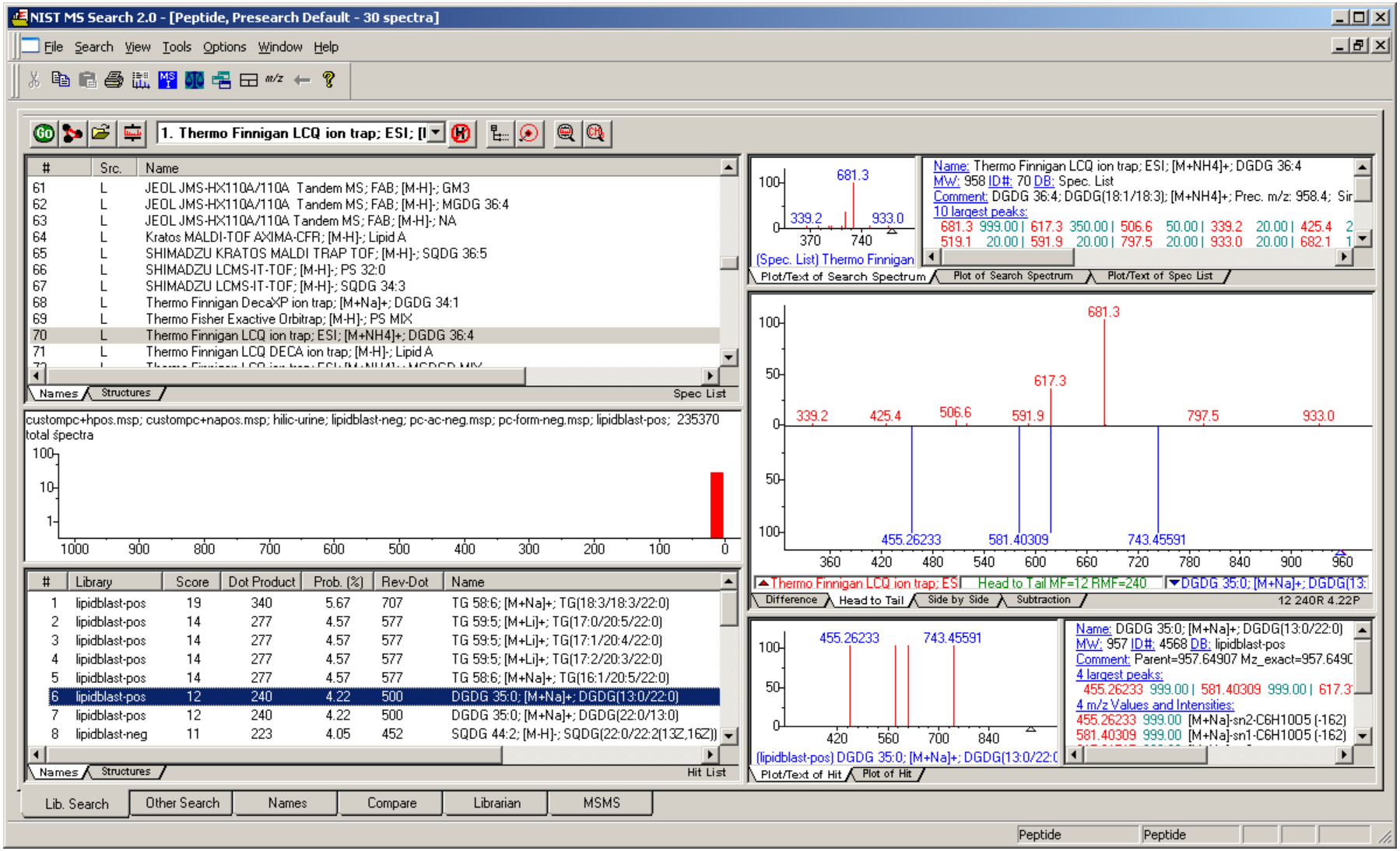
PS-MIX



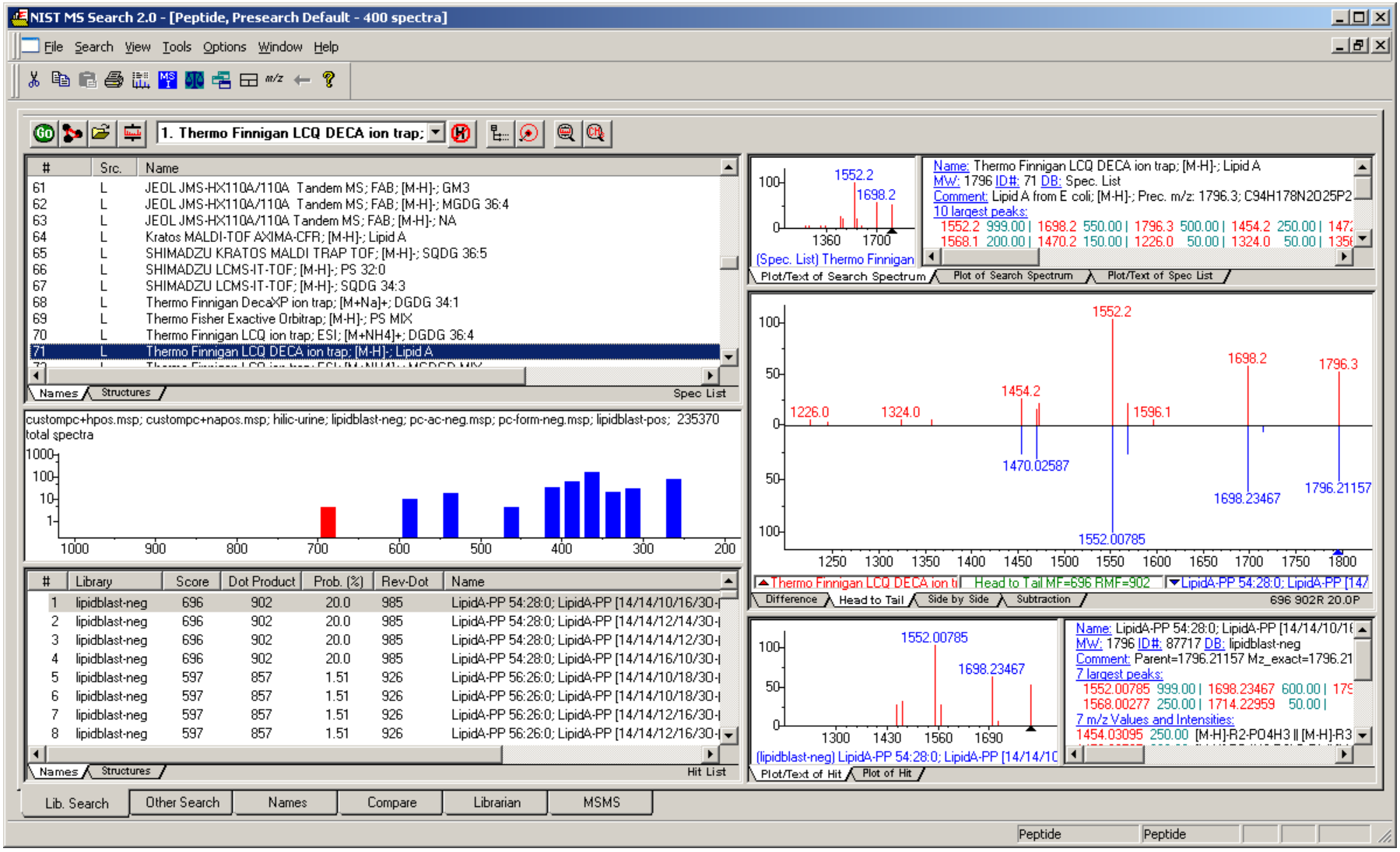
Name: Thermo Finnigan LCQ ion trap; ESI; [M+NH4]+; DGDG 36:4
MW: 958 ID#: 70 DB: Spec. List
Comment: DGDG 36:4; DGDG(18:1/18:3); [M+NH4]+; Prec. m/z: 958.4; Simultaneous analysis of glycolipids and phospholids molecular species in avocado (Persea americana Mill) fruit; http://dx.doi.org/10.1016/j.chroma.2006.10.022
10 largest peaks:

3rd probability group

(exclude M+Li)

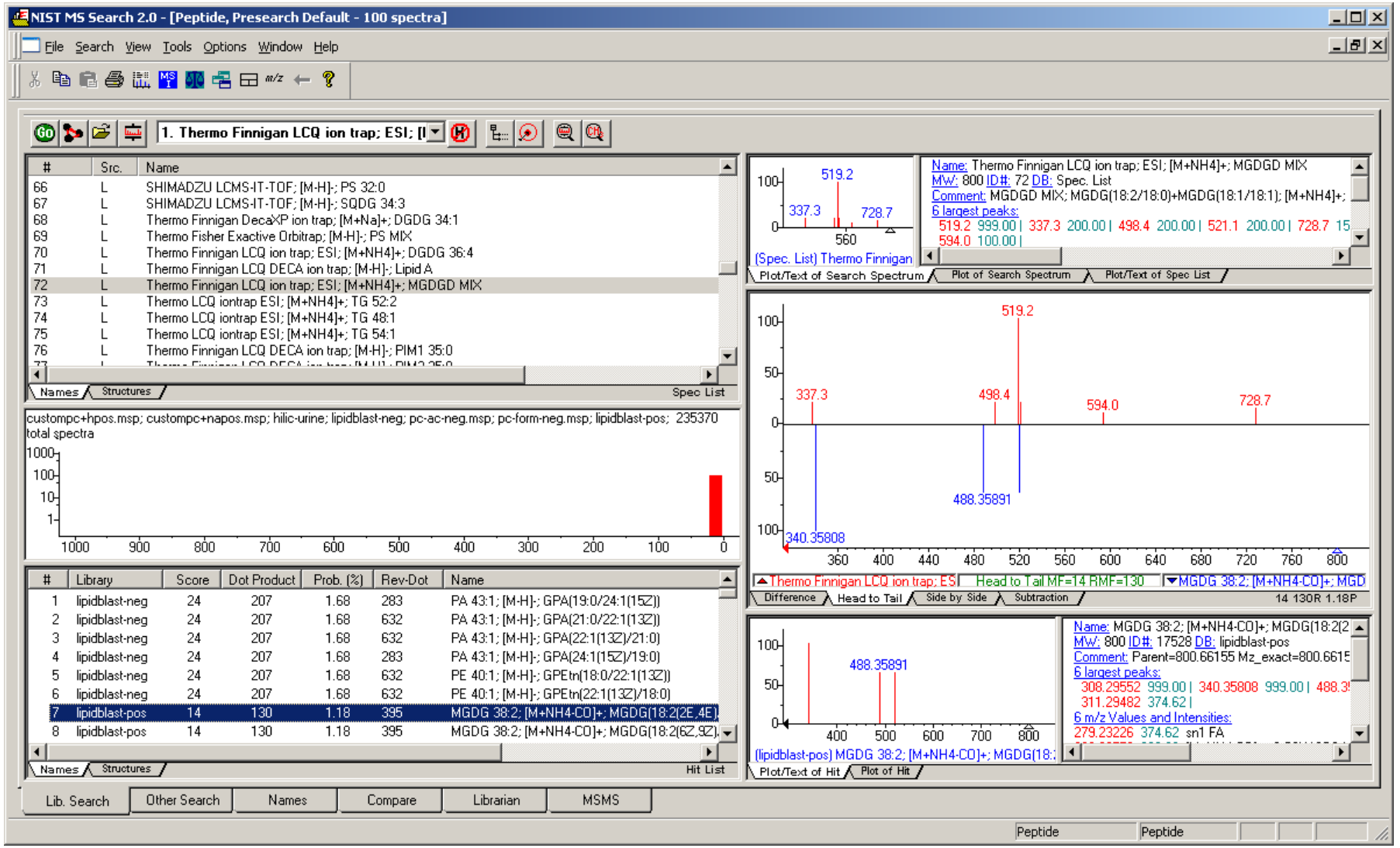


Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; Lipid A
MW: 1796 ID#: 71 DB: Spec. List
Comment: Lipid A from E coli; [M-H]-; Prec. m/z: 1796.3; C94H178N2O25P2; LipidA-PP-[R2(14:0)(3-OH)/R3(14:0)(3-OH)/R2'(14:0)/R3('14:0)/R2'-3-O-(12:0)/R3'-3O-(14:0)]; DOI: 10.1002/jms.614; Structural analysis of lipid A from Escherichia coli O157:H7:K- using thin-layer chromatography and ion-trap mass spectrometry
10 largest peaks:

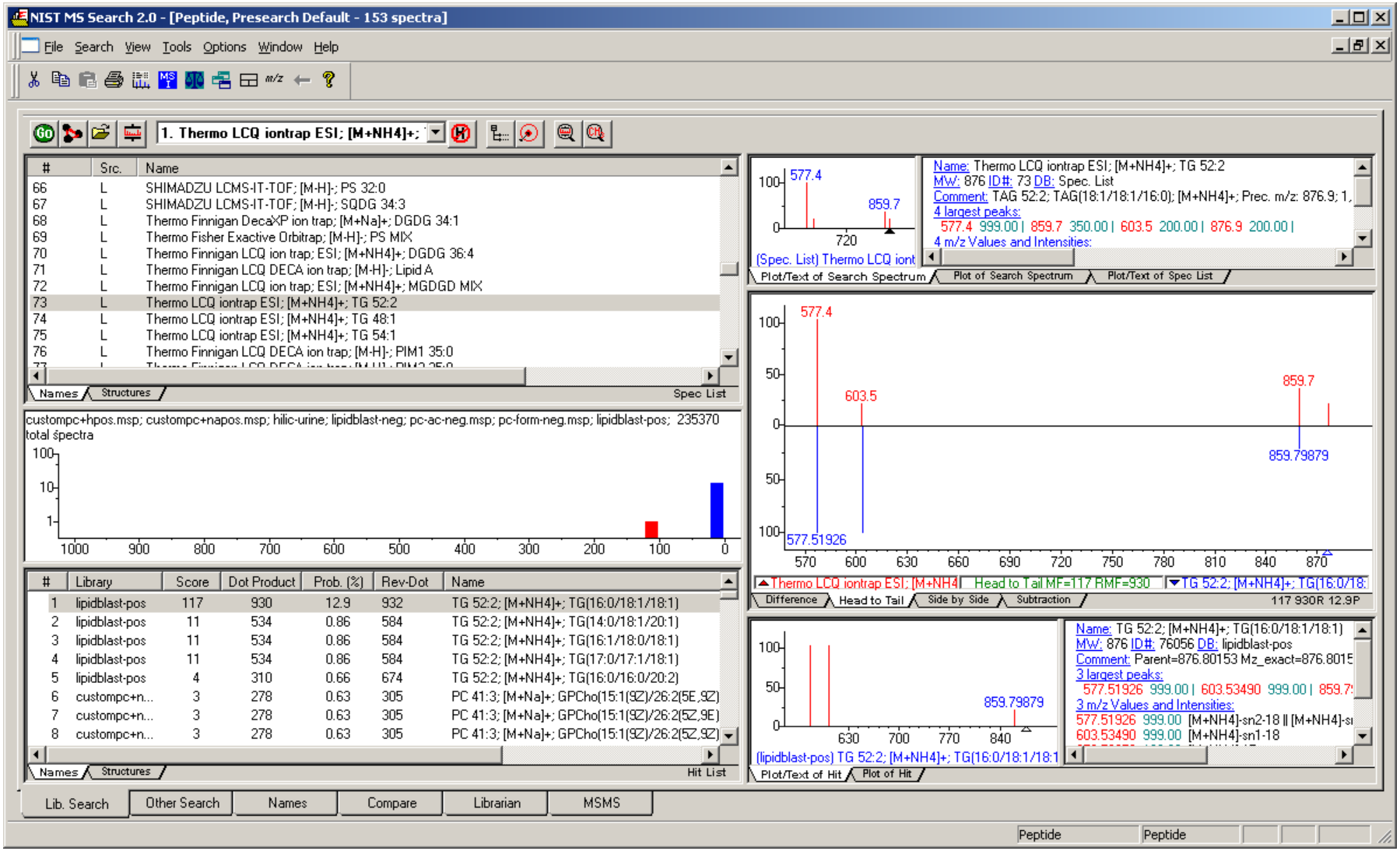


Name: Thermo Finnigan LCQ ion trap; ESI; [M+NH4]+; MGDGD MIX
MW: 800 ID#: 72 DB: Spec. List
Comment: MGDGD MIX; MGDG(18:2/18:0)+MGDG(18:1/18:1); [M+NH4]+; Prec. m/z: 800.4; Simultaneous analysis of glycolipids and phospholids molecular species in avocado (Persea americana Mill) fruit; http://dx.doi.org/10.1016/j.chroma.2006.10.022
6 largest peaks:

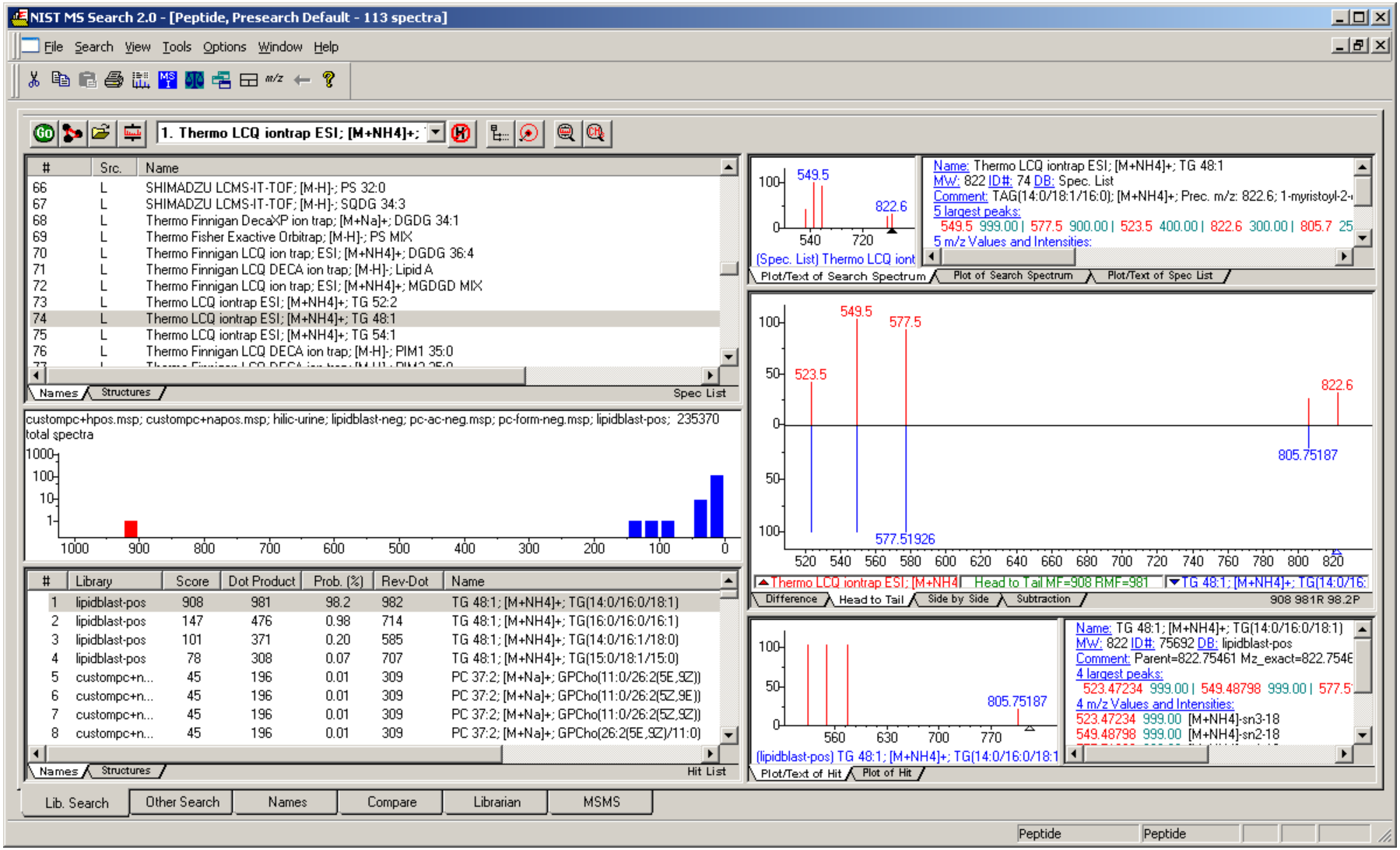
MGDG MIX



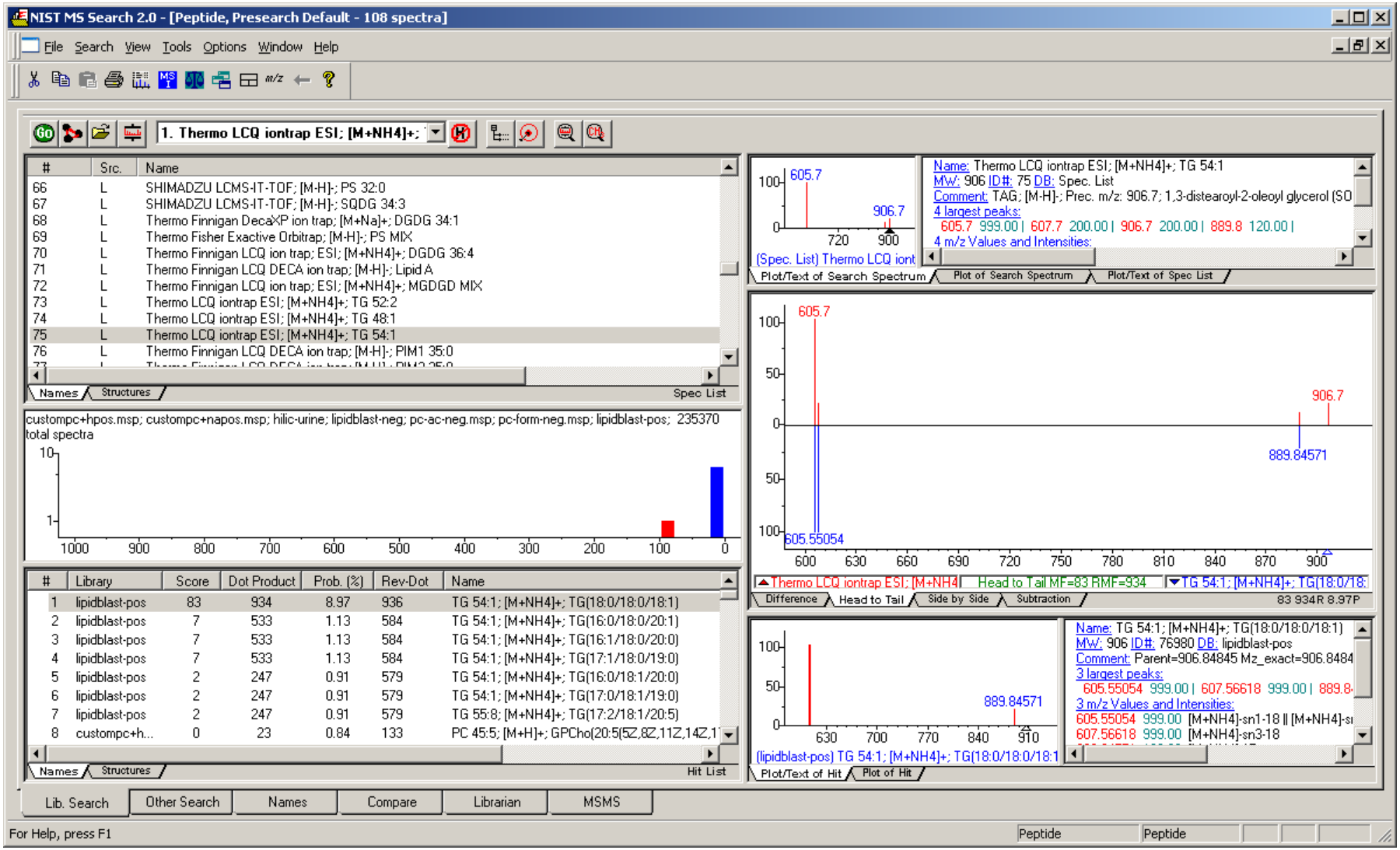
Name: Thermo LCQ iontrap ESI; [M+NH4]+; TG 52:2
MW: 876 ID#: 73 DB: Spec. List
Comment: TAG 52:2; TAG(18:1/18:1/16:0); [M+NH4]+; Prec. m/z: 876.9; 1,3-dioleoyl-2-palmitoyl-glycerol (OPO); Structural Characterization of Triacylglycerols Using Electrospray Ionization-MSn Ion-Trap MS; 10.1007/s11746-003-0676-2
4 largest peaks:



Name: Thermo LCQ iontrap ESI; [M+NH4]+; TG 48:1
MW: 822 ID#: 74 DB: Spec. List
Comment: TAG(14:0/18:1/16:0); [M+NH4]+; Prec. m/z: 822.6; 1-myristoyl-2-oleoyl-3-palmitoyl glycerol (MOP); Structural Characterization of Triacylglycerols Using Electrospray Ionization-MSn Ion-Trap MS; 10.1007/s11746-003-0676-2
5 largest peaks:

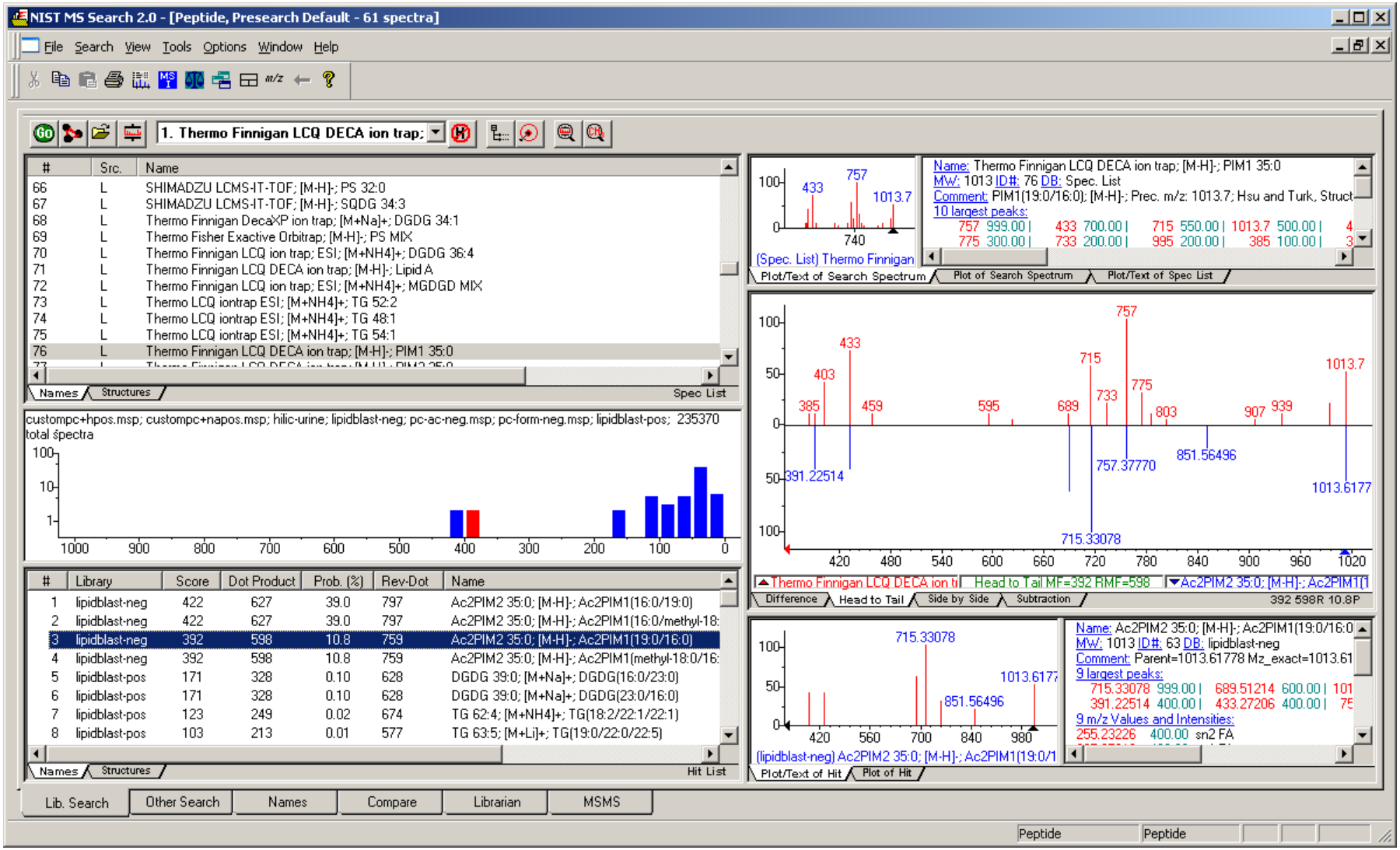


Name: Thermo LCQ iontrap ESI; [M+NH4]+; TG 54:1
MW: 906 ID#: 75 DB: Spec. List
Comment: TAG; [M-H]-; Prec. m/z: 906.7; 1,3-distearoyl-2-oleoyl glycerol (SOS); Structural Characterization of Triacylglycerols Using Electrospray Ionization-MSn Ion-Trap MS; 10.1007/s11746-003-0676-2
4 largest peaks:

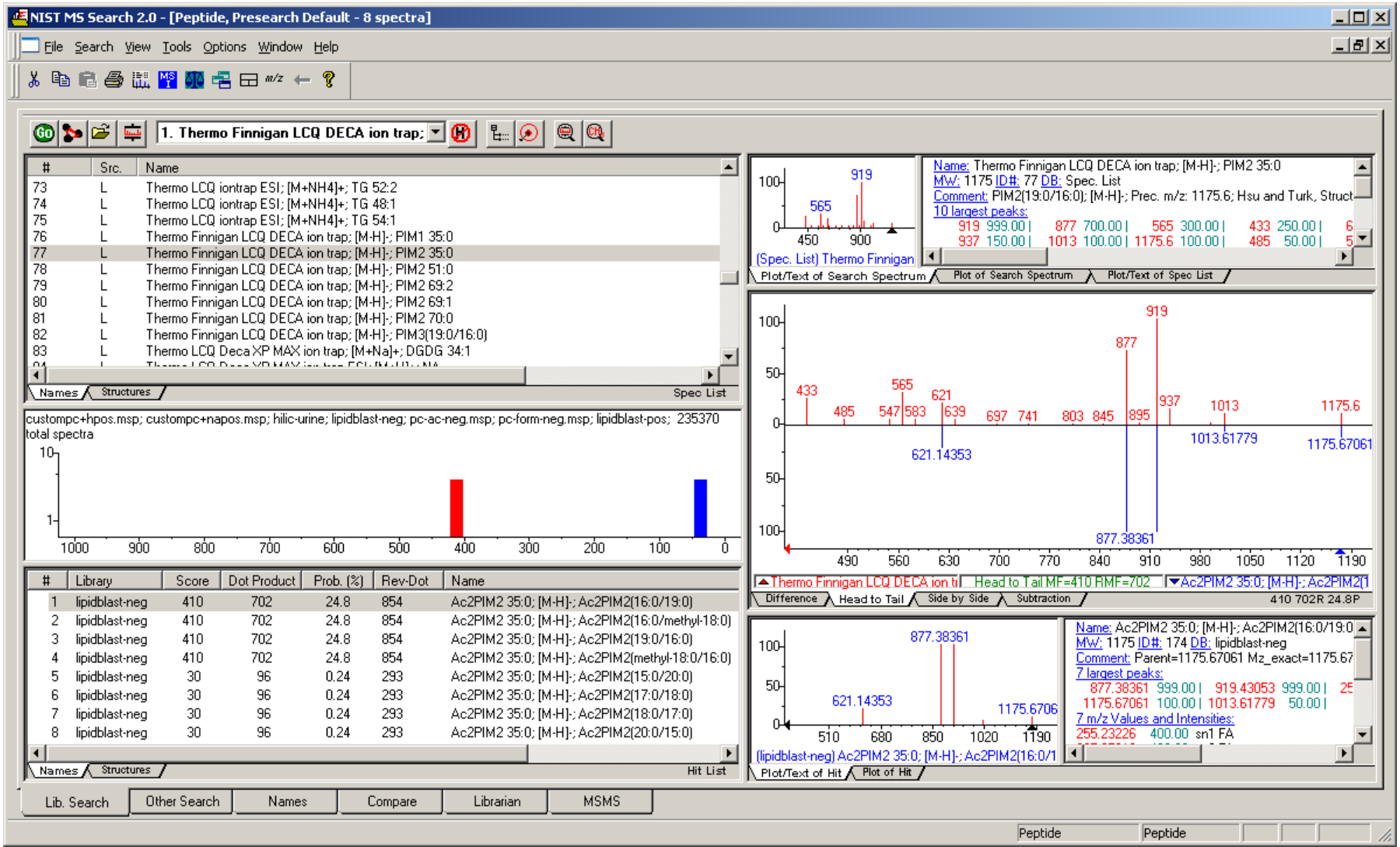


Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM1 35:0
MW: 1013 ID#: 76 DB: Spec. List
Comment: PIM1(19:0/16:0); [M-H]-; Prec. m/z: 1013.7; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. I. PIMs and lyso-PIMs.
10 largest peaks:

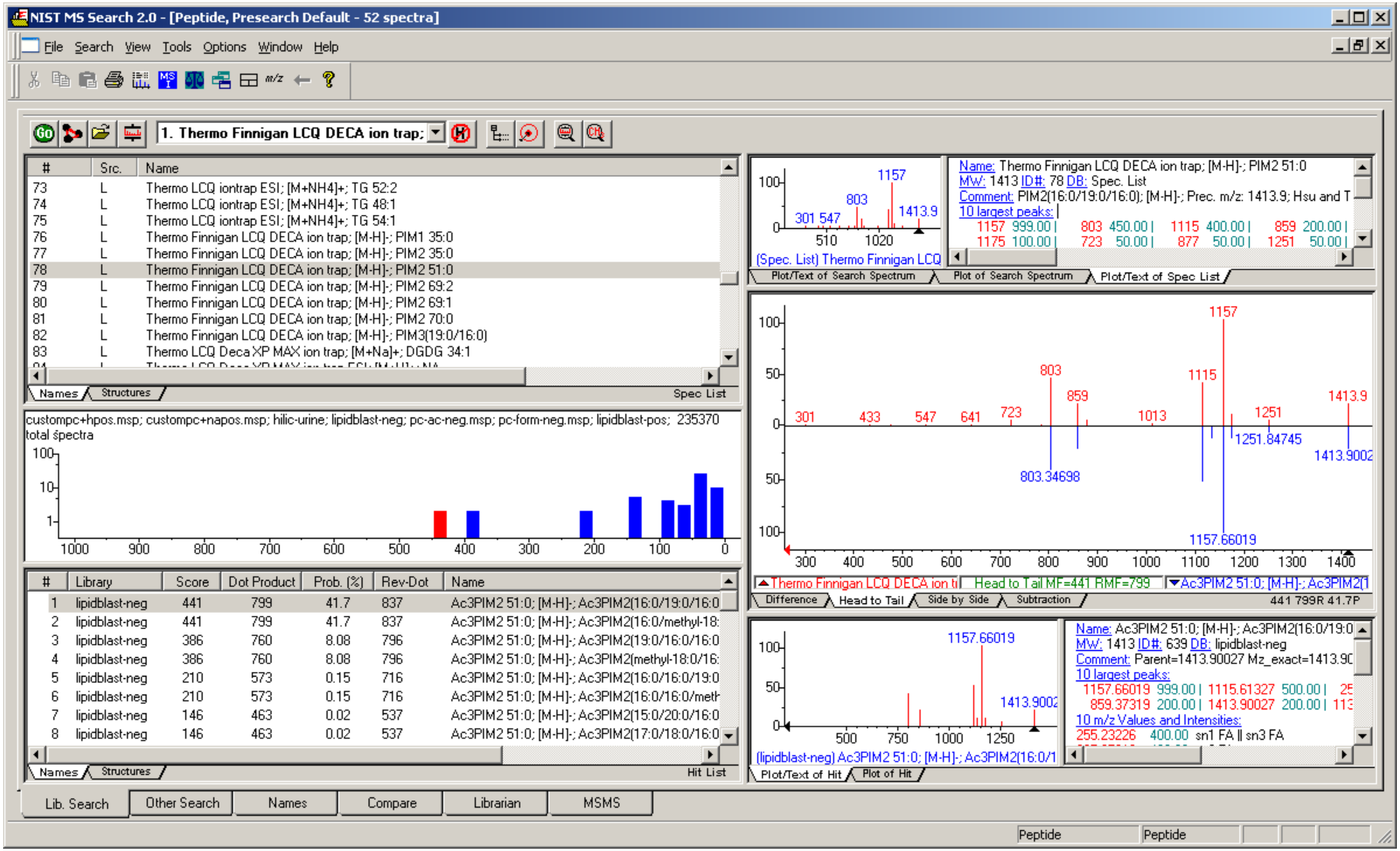
757	999.00 |



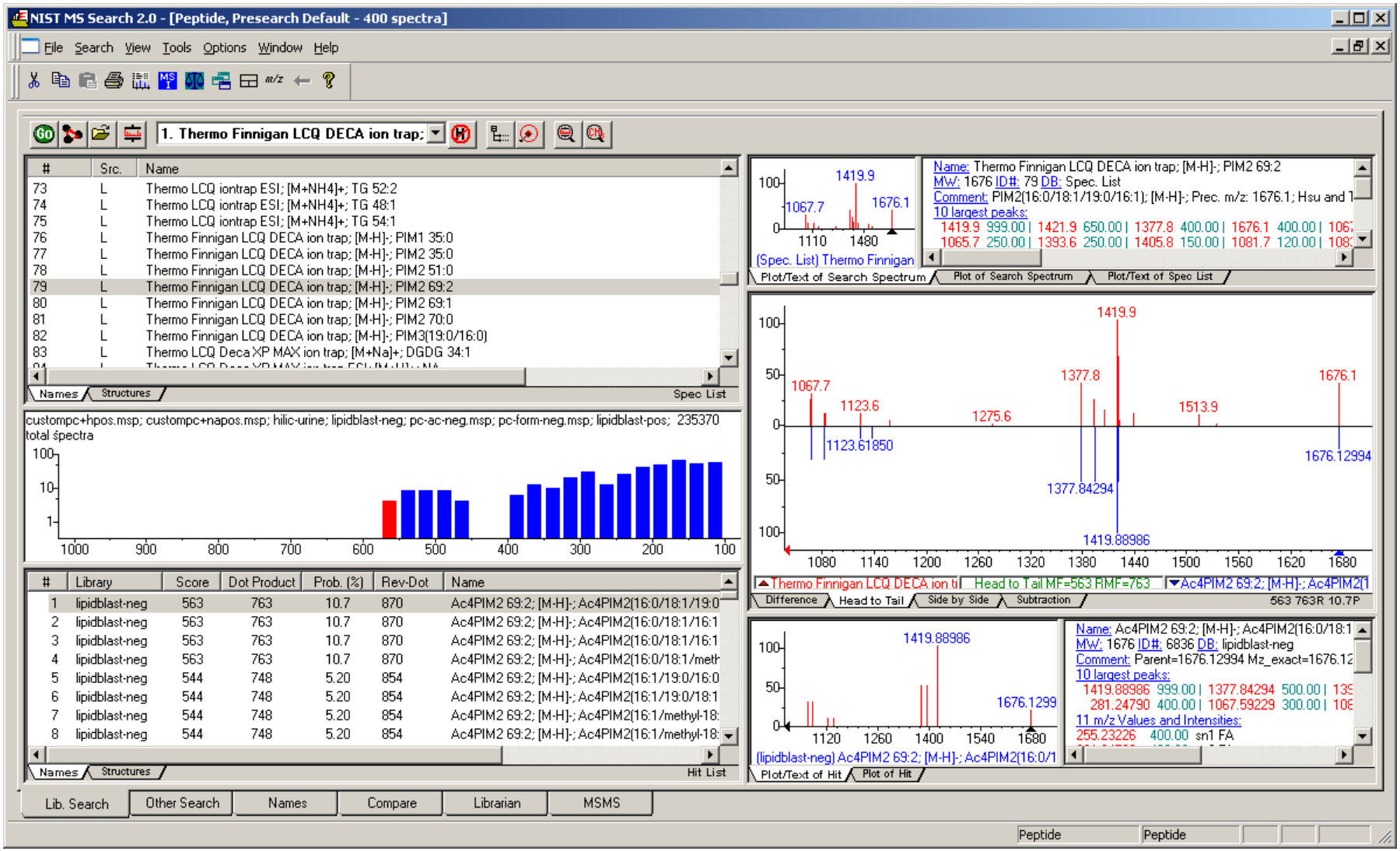
Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM2 35:0
MW: 1175 ID#: 77 DB: Spec. List
Comment: PIM2(19:0/16:0); [M-H]-; Prec. m/z: 1175.6; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. I. PIMs and lyso-PIMs.
10 largest peaks:



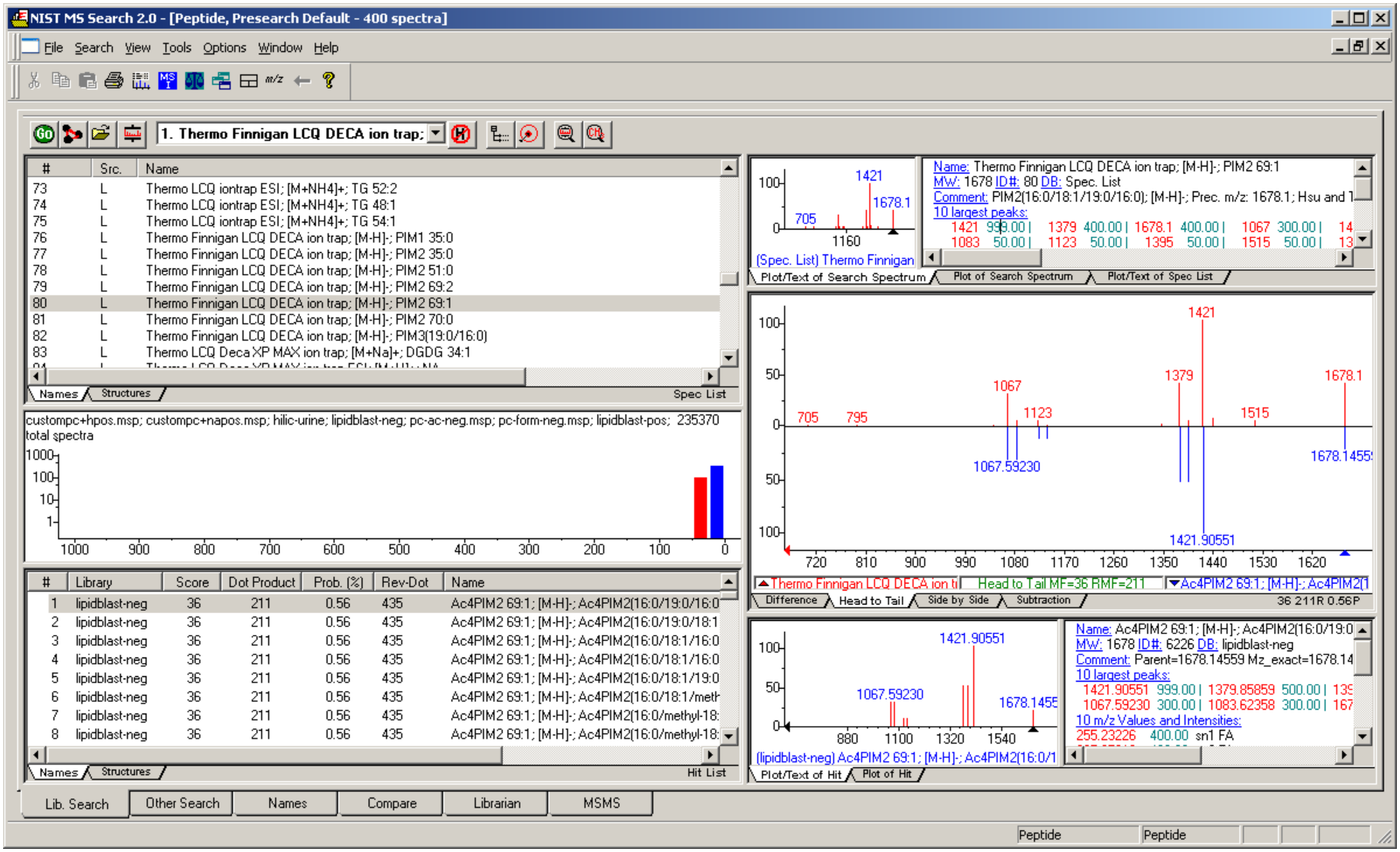
Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM2 51:0
MW: 1413 ID#: 78 DB: Spec. List
Comment: PIM2(16:0/19:0/16:0); [M-H]-; Prec. m/z: 1413.9; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. II. Monoacyl- and Diacyl-PIMs
10 largest peaks:



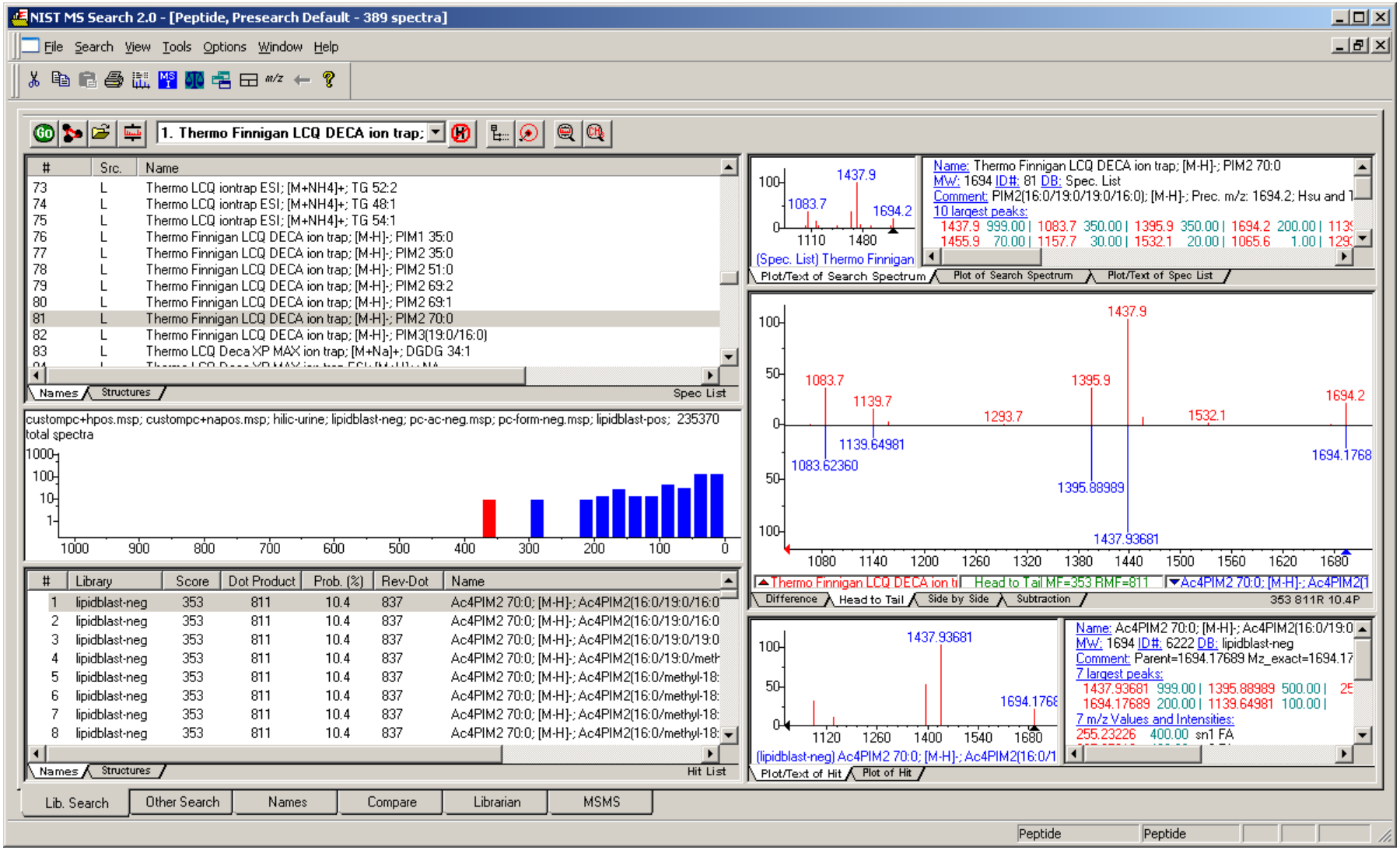
Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM2 69:2
MW: 1676 ID#: 79 DB: Spec. List
Comment: PIM2(16:0/18:1/19:0/16:1); [M-H]-; Prec. m/z: 1676.1; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. II. Monoacyl- and Diacyl-PIMs
10 largest peaks:



Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM2 69:1
MW: 1678 ID#: 80 DB: Spec. List
Comment: PIM2(16:0/18:1/19:0/16:0); [M-H]-; Prec. m/z: 1678.1; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. II. Monoacyl- and Diacyl-PIMs
10 largest peaks:

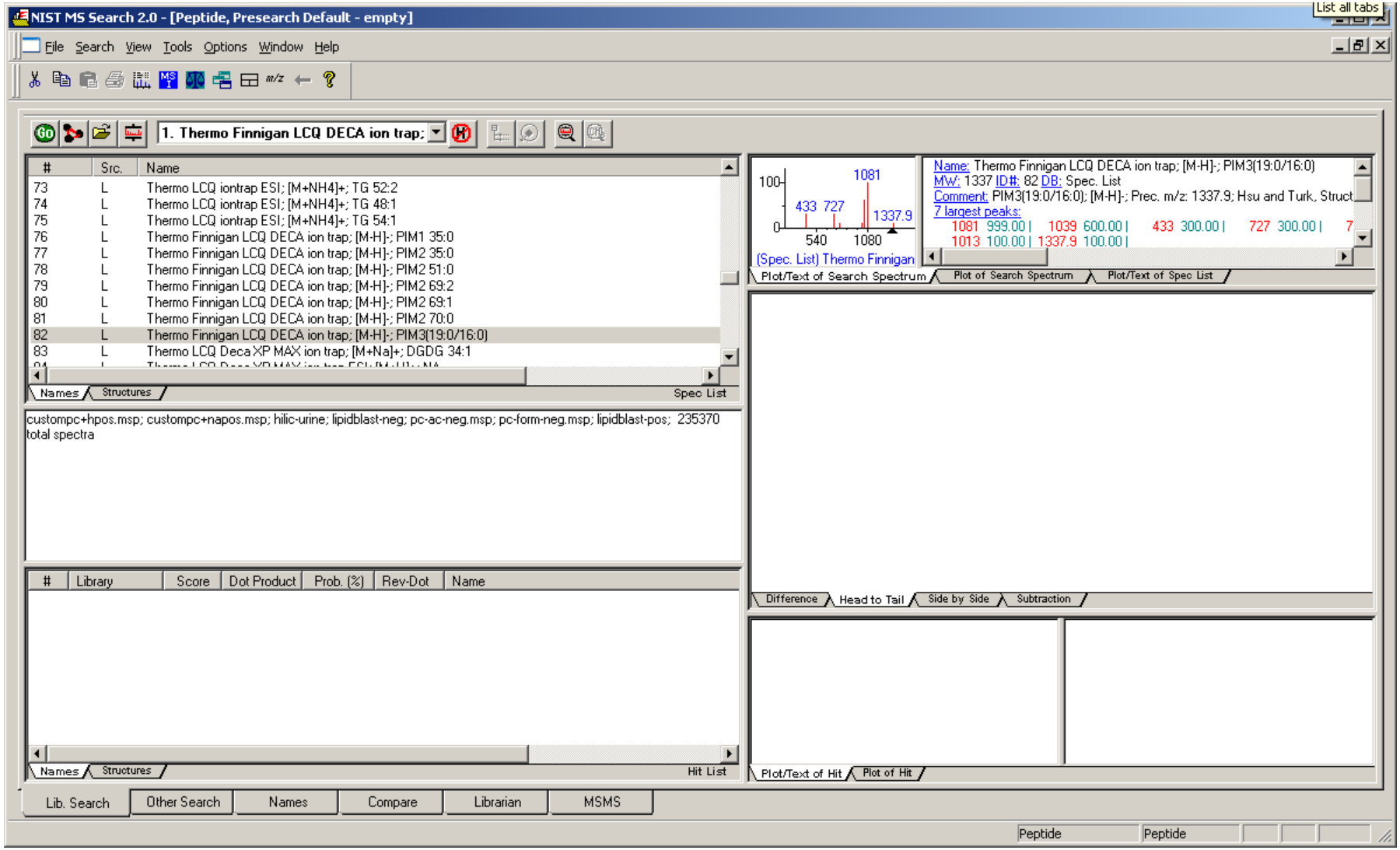


Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM2 70:0
MW: 1694 ID#: 81 DB: Spec. List
Comment: PIM2(16:0/19:0/19:0/16:0); [M-H]-; Prec. m/z: 1694.2; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. II. Monoacyl- and Diacyl-PIMs
10 largest peaks:

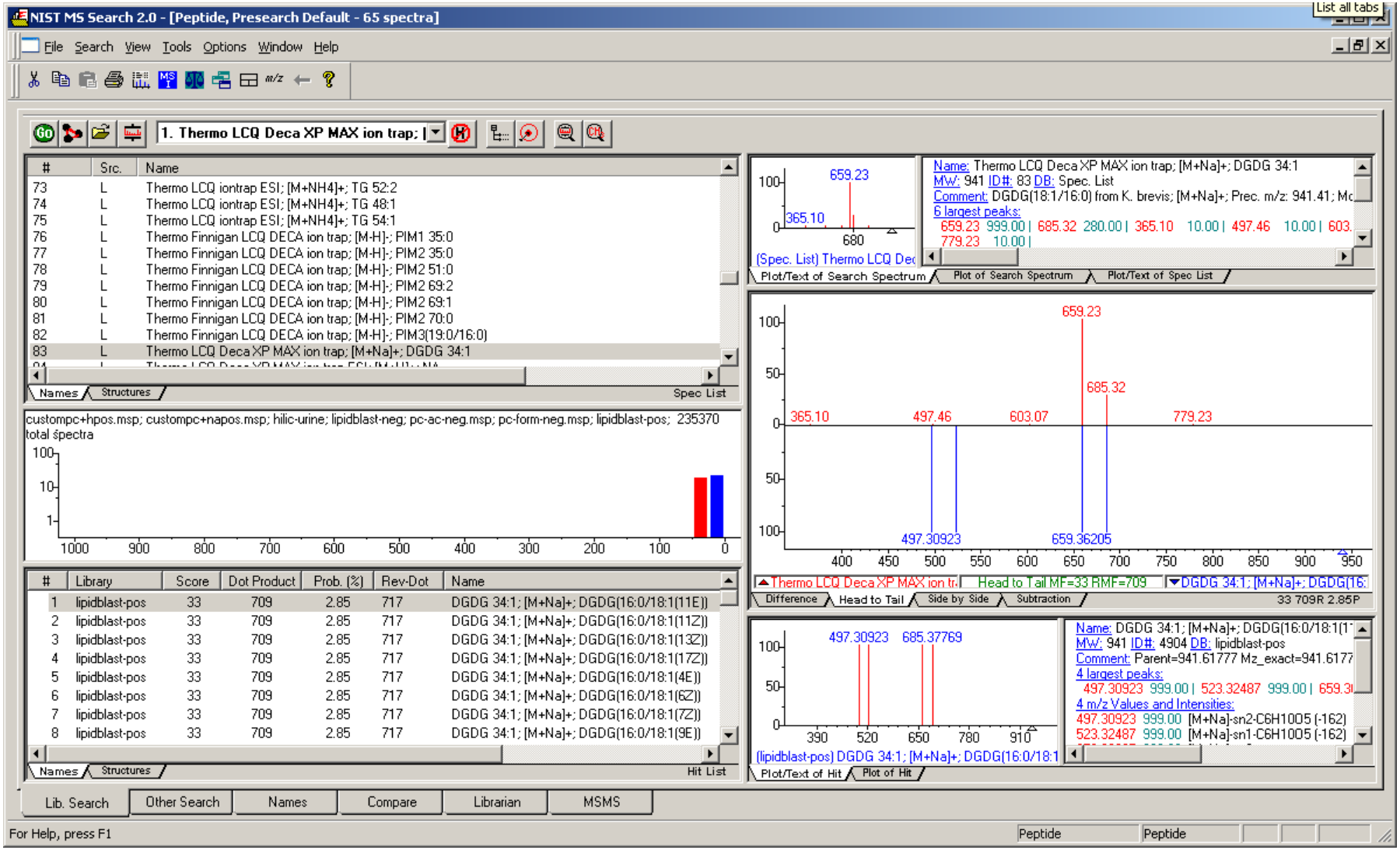


Name: Thermo Finnigan LCQ DECA ion trap; [M-H]-; PIM3(19:0/16:0)
MW: 1337 ID#: 82 DB: Spec. List
Comment: PIM3(19:0/16:0); [M-H]-; Prec. m/z: 1337.9; Hsu and Turk, Structural characterization of phosphatidyl-myo-inositol mannosides from Mycobacterium bovis Bacillus Calmette Gurin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. I. PIMs and lyso-PIMs.
7 largest peaks:

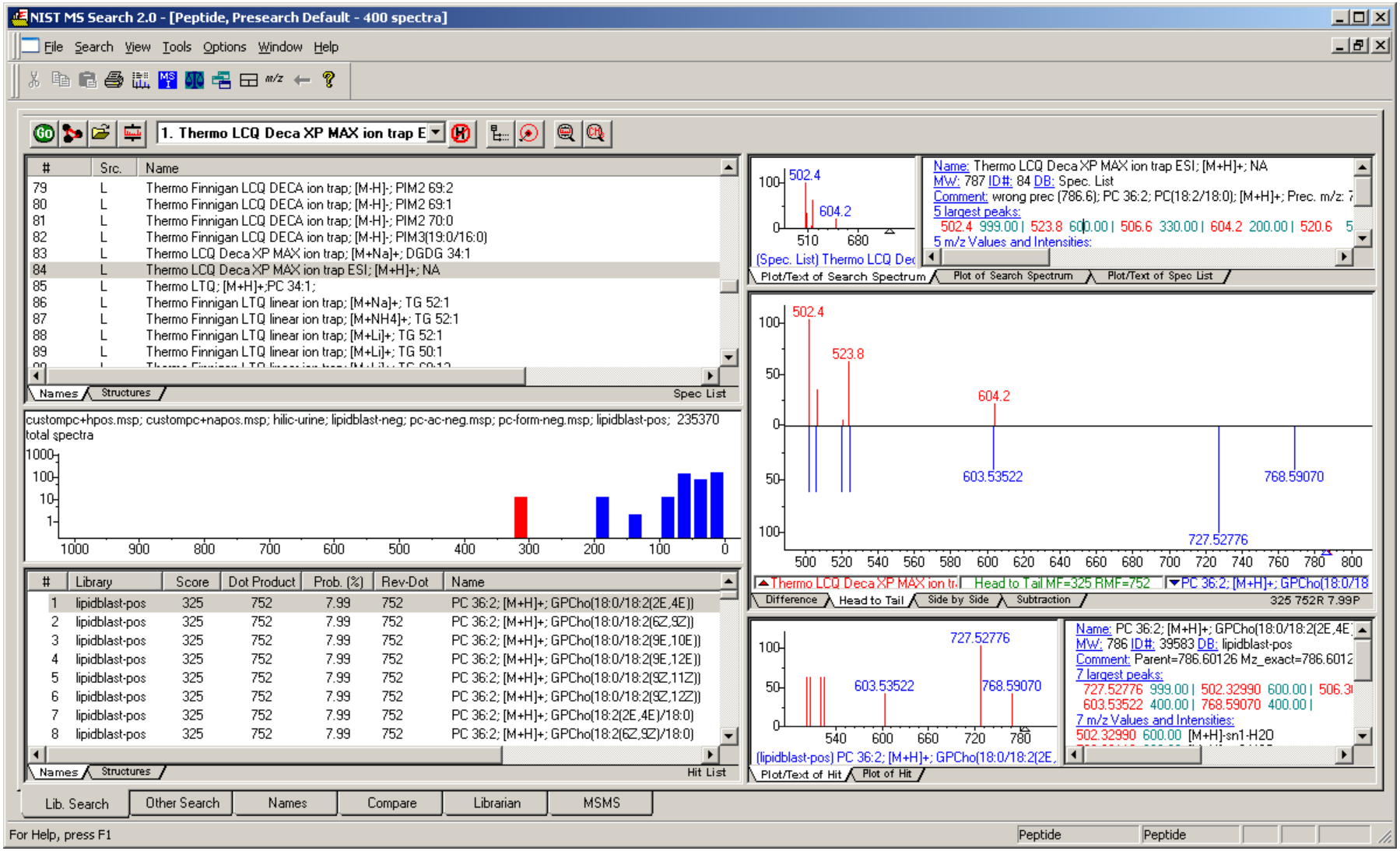
Compounds not in LipidBlast



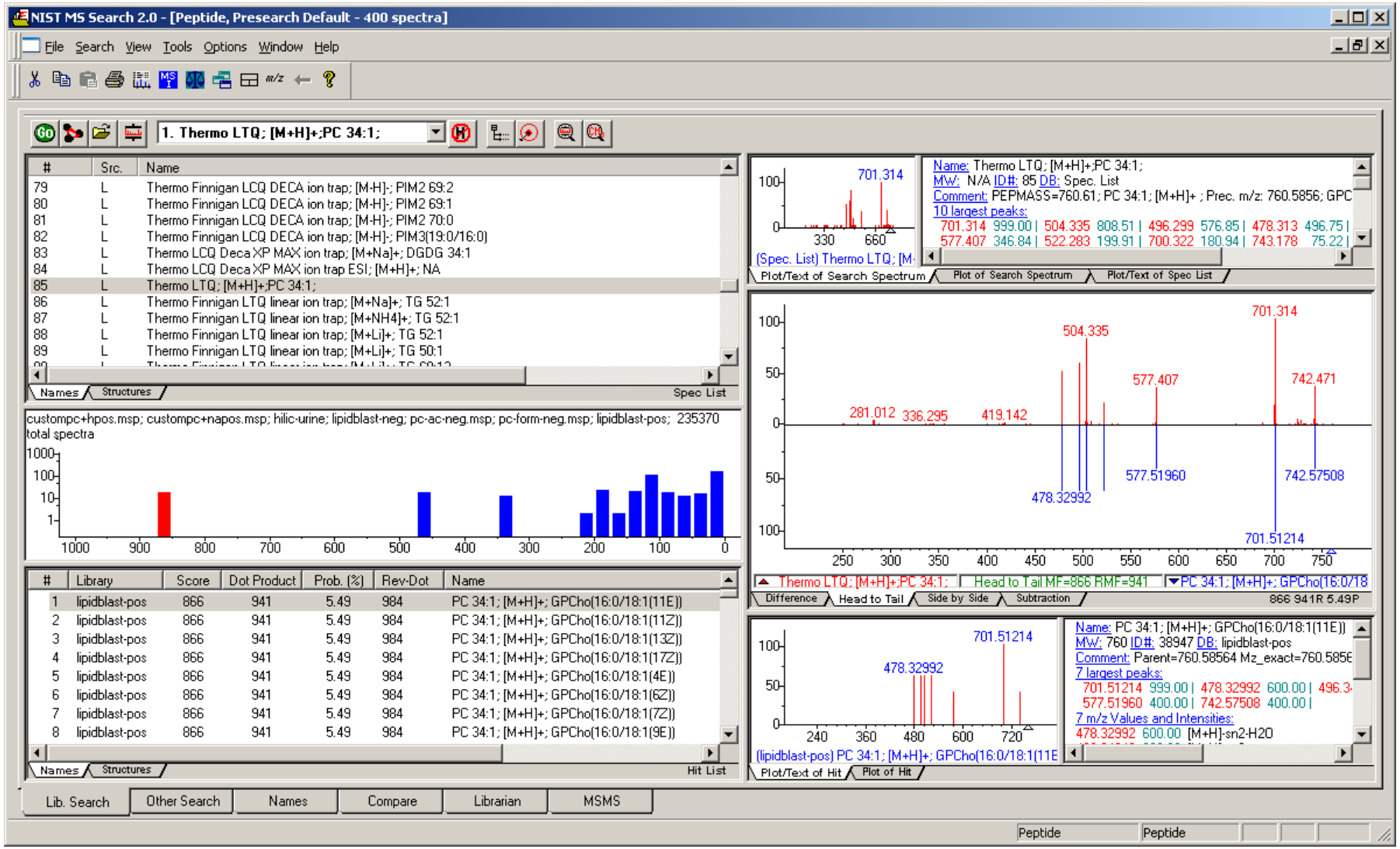
Name: Thermo LCQ Deca XP MAX ion trap; [M+Na]+; DGDG 34:1
MW: 941 ID#: 83 DB: Spec. List
Comment: DGDG(18:1/16:0) from K. brevis; [M+Na]+; Prec. m/z: 941.41; Mono- and digalactosyldiacylglycerol composition of dinoflagellates. II. Lepidodinium chlorophorum, Karenia brevis, and Kryptoperidinium foliaceum, three dinoflagellates with aberrant plastids Jeffrey D. Leblond ; Andrew D. Lasiter;European Journal of Phycology, 1469-4433, Volume 44, Issue 2, First published 2009, Pages 199 - 205
6 largest peaks:



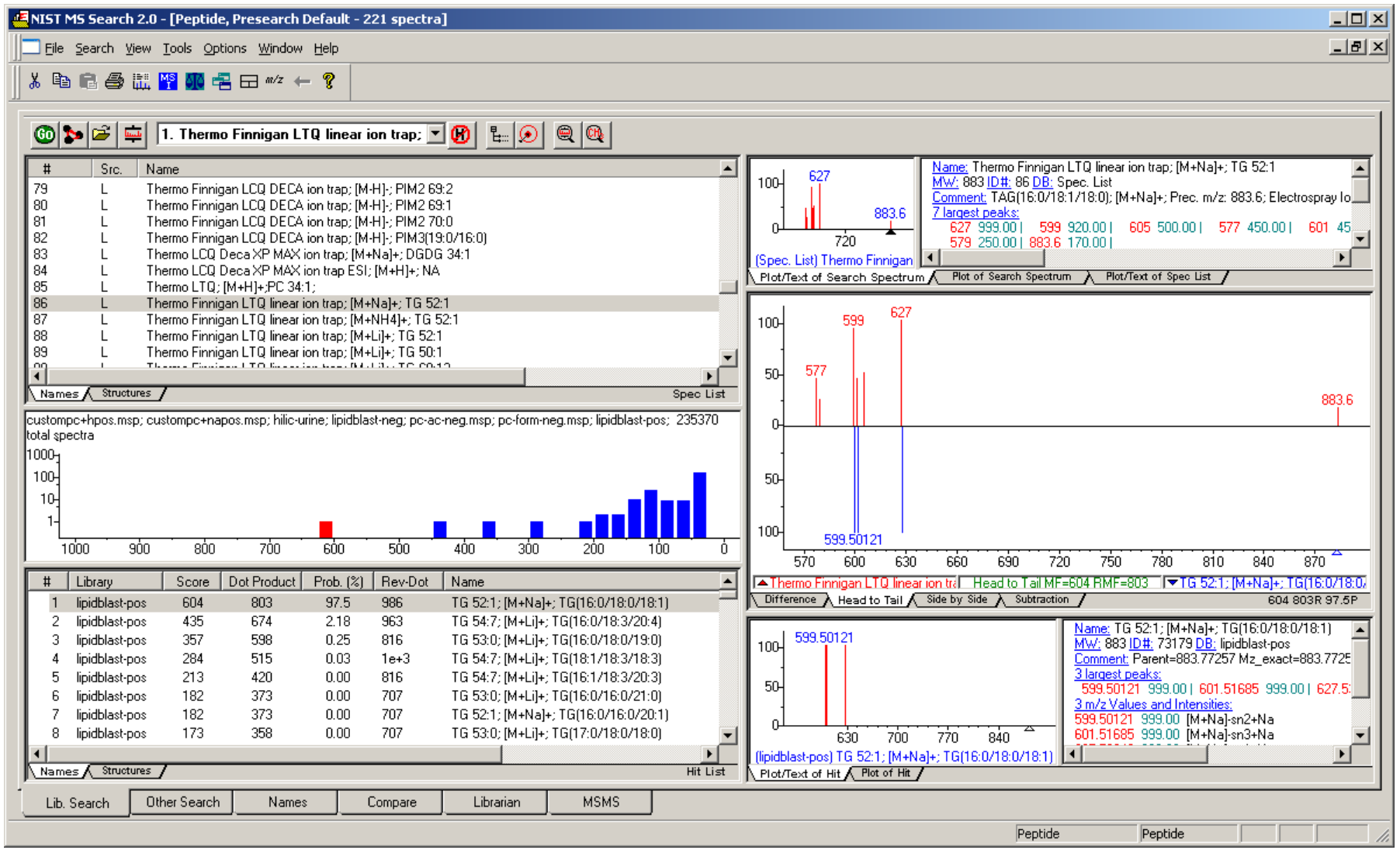
Name: Thermo LCQ Deca XP MAX ion trap ESI; [M+H]+; NA
MW: 787 ID#: 84 DB: Spec. List
Comment: wrong prec (786.6); PC 36:2; PC(18:2/18:0); [M+H]+; Prec. m/z: 787.3; Profiling of phospholipids in lipoproteins by multiplexed hollow fiber flow field-flow fractionation and nanoflow liquid chromatographytandem mass spectrometry ;http://dx.doi.org/10.1016/j.chroma.2010.01.006
5 largest peaks:



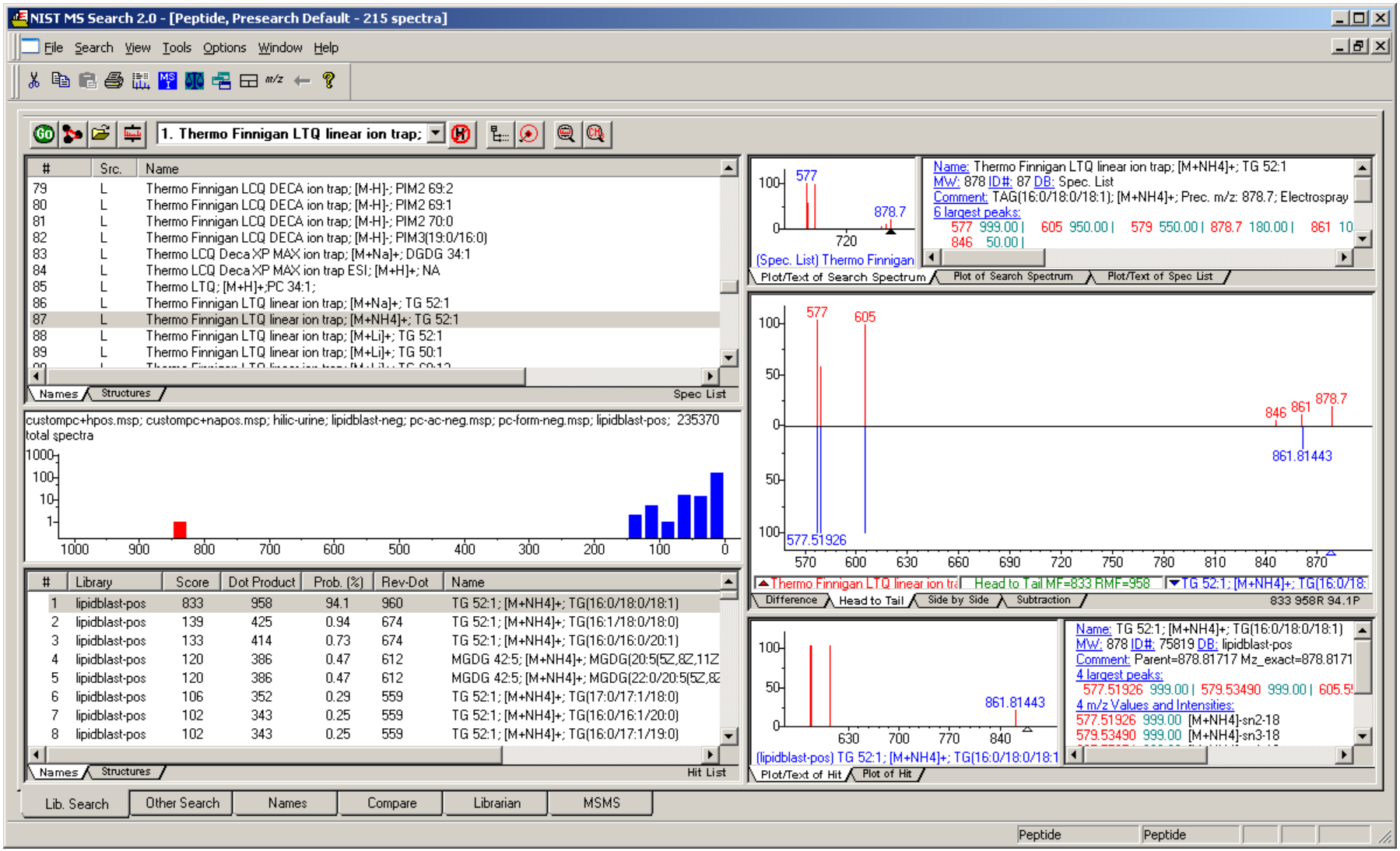
Name: Thermo LTQ; [M+H]+;PC 34:1;
MW: N/A ID#: 85 DB: Spec. List
Comment: PEPMASS=760.61; PC 34:1; [M+H]+ ; Prec. m/z: 760.5856; GPCho(16:0/18:1(11E));
C42H82NO8P
10 largest peaks:



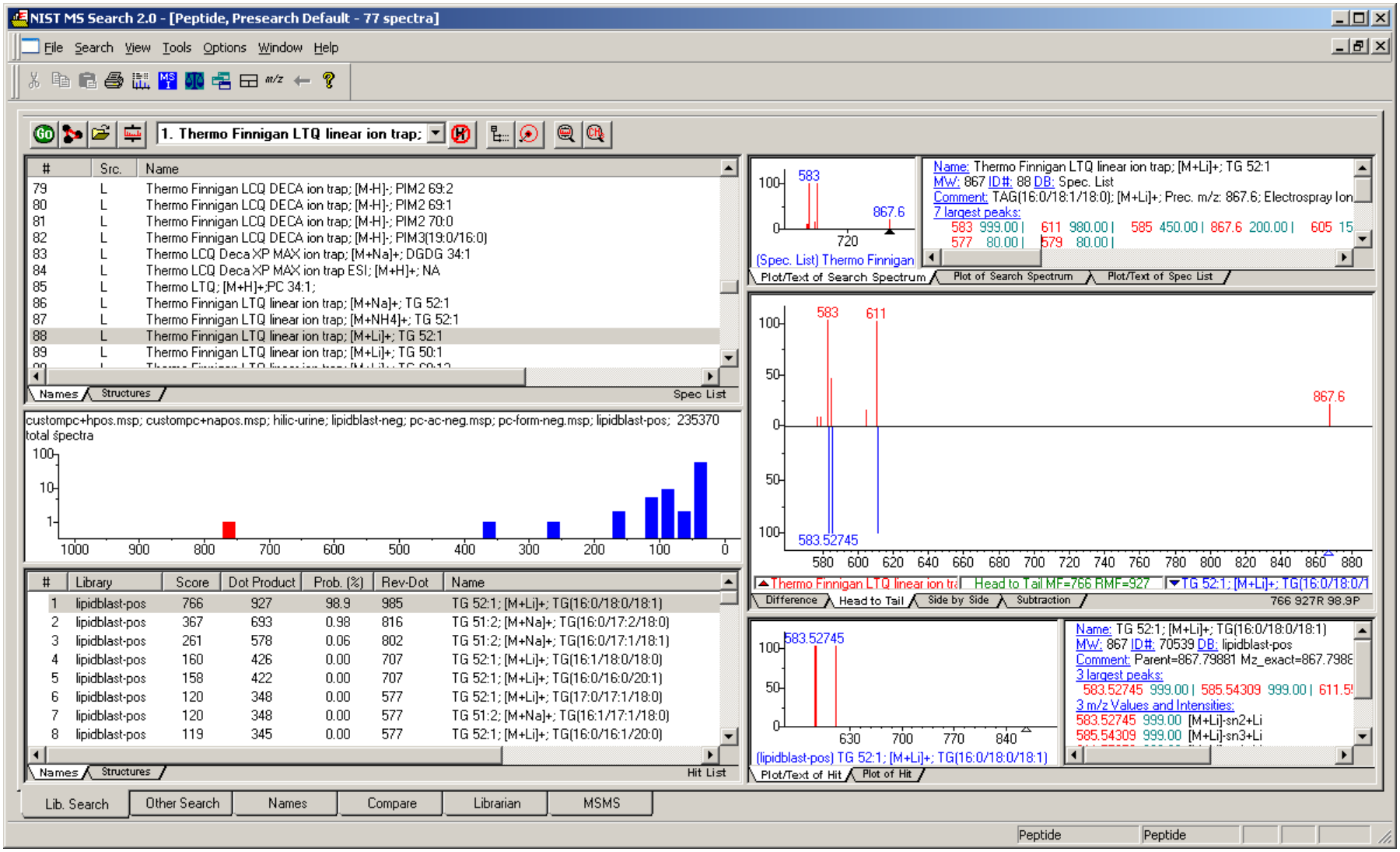
Name: Thermo Finnigan LTQ linear ion trap; [M+Na]+; TG 52:1
MW: 883 ID#: 196 DB: Text File
Comment: TAG(16:0/18:1/18:0); [M+Na]+; Prec. m/z: 883.6; Electrospray Ionization Multiple-Stage Linear Ion-trap Mass Spectrometry for Structural Elucidation of Triacylglycerols: Assignment of Fatty Acyl Groups on the Glycerol Backbone and Location of Double Bonds; Fong-Fu Hsu and John Turk
7 largest peaks:



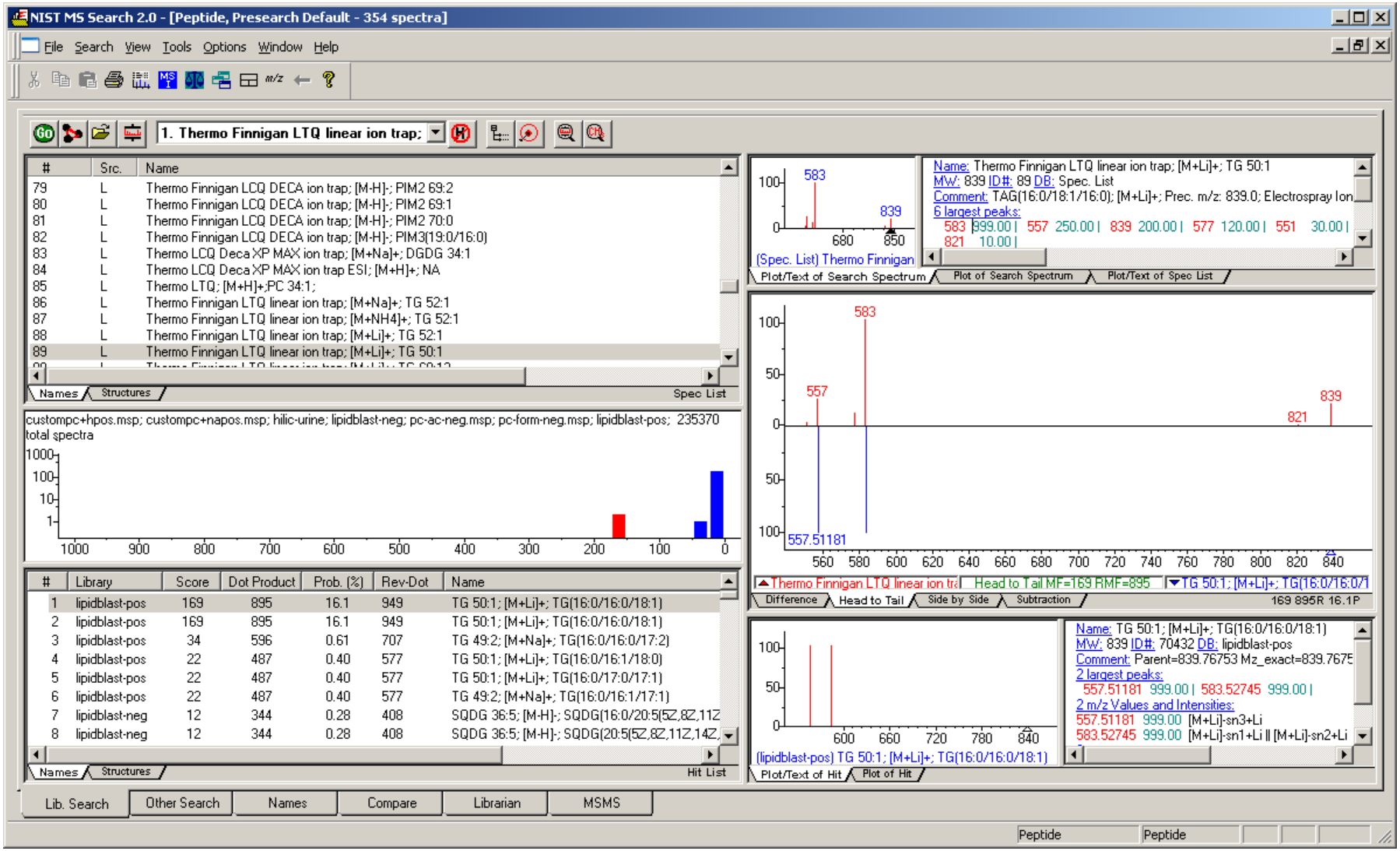
Name: Thermo Finnigan LTQ linear ion trap; [M+NH4]+; TG 52:1
MW: 878 ID#: 87 DB: Spec. List
Comment: TAG(16:0/18:0/18:1); [M+NH4]+; Prec. m/z: 878.7; Electrospray Ionization Multiple-Stage Linear Ion-trap Mass Spectrometry for Structural Elucidation of Triacylglycerols: Assignment of Fatty Acyl Groups on the Glycerol Backbone and Location of Double Bonds; Fong-Fu Hsu and John Turk
6 largest peaks:



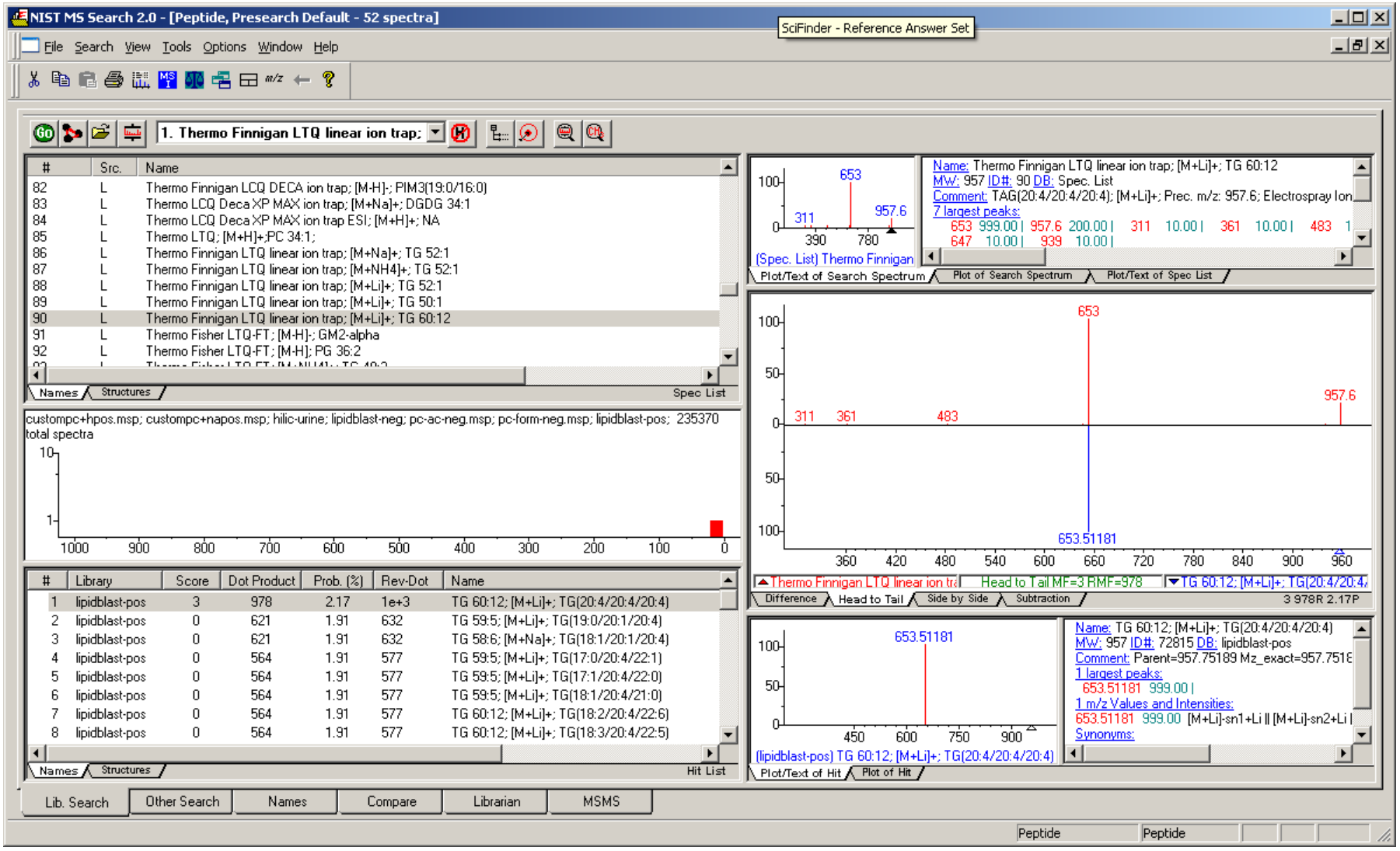
Name: Thermo Finnigan LTQ linear ion trap; [M+Li]+; TG 52:1
MW: 867 ID#: 88 DB: Spec. List
Comment: TAG(16:0/18:1/18:0); [M+Li]+; Prec. m/z: 867.6; Electrospray Ionization Multiple-Stage Linear Ion-trap Mass Spectrometry for Structural Elucidation of Triacylglycerols: Assignment of Fatty Acyl Groups on the Glycerol Backbone and Location of Double Bonds; Fong-Fu Hsu and John Turk
7 largest peaks:



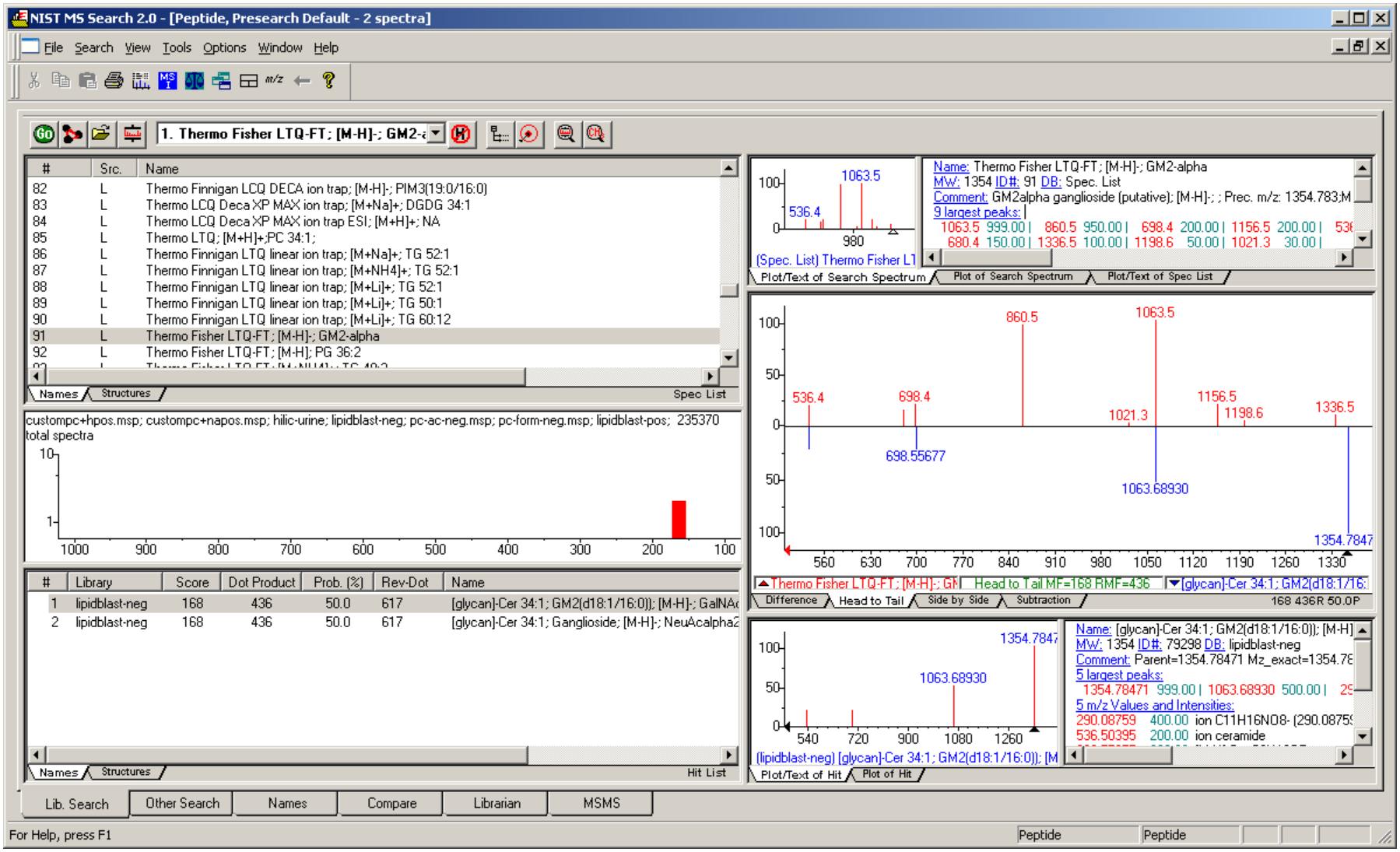
Name: Thermo Finnigan LTQ linear ion trap; [M+Li]+; TG 50:1
MW: 839 ID#: 89 DB: Spec. List
Comment: TAG(16:0/18:1/16:0); [M+Li]+; Prec. m/z: 839.0; Electrospray Ionization Multiple-Stage Linear Ion-trap Mass Spectrometry for Structural Elucidation of Triacylglycerols: Assignment of Fatty Acyl Groups on the Glycerol Backbone and Location of Double Bonds; Fong-Fu Hsu and John Turk
6 largest peaks:



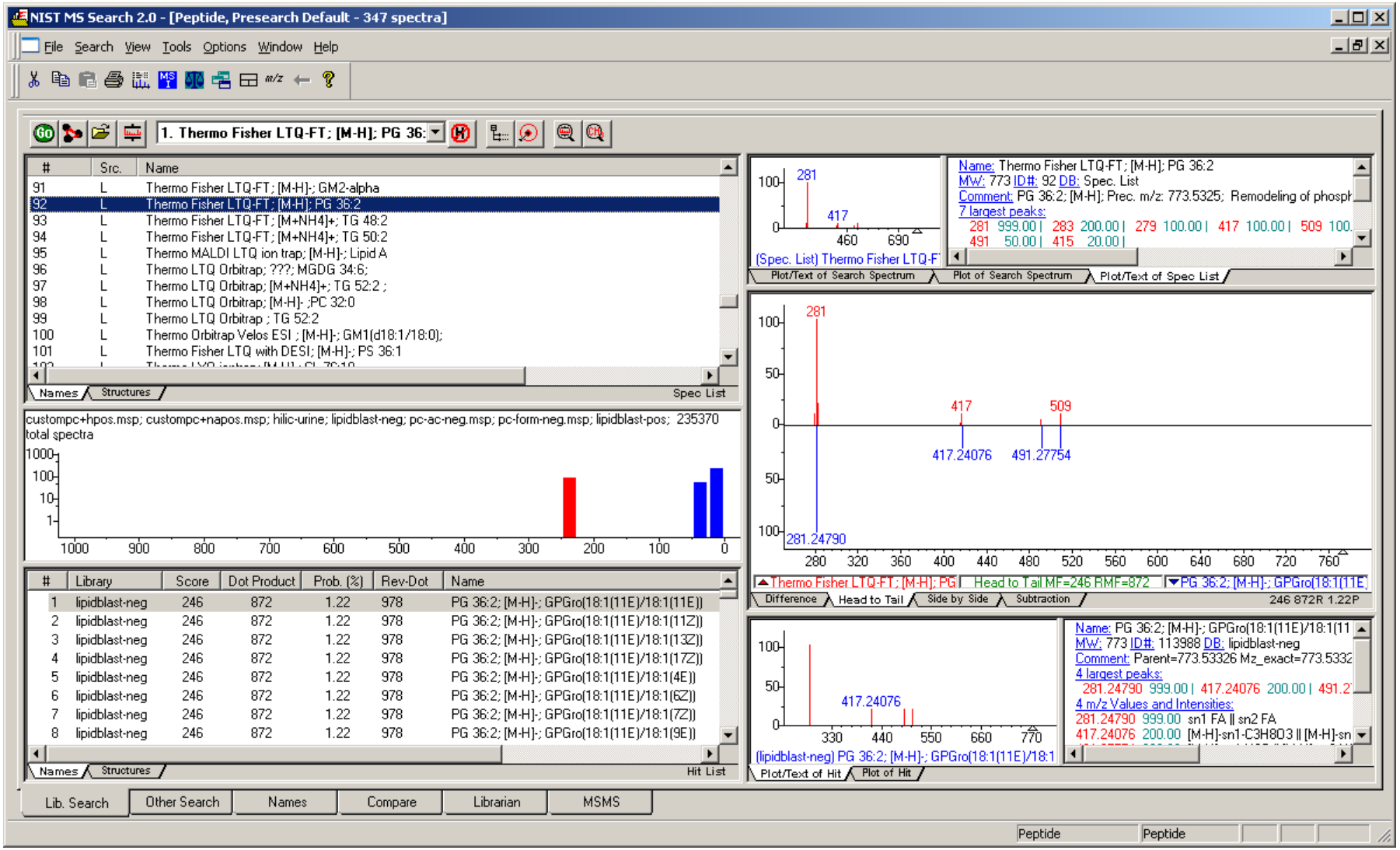
Name: Thermo Finnigan LTQ linear ion trap; [M+Li]+; TG 60:12
MW: 957 ID#: 90 DB: Spec. List
Comment: TAG(20:4/20:4/20:4); [M+Li]+; Prec. m/z: 957.6; Electrospray Ionization Multiple-Stage Linear Ion-trap Mass Spectrometry for Structural Elucidation of Triacylglycerols: Assignment of Fatty Acyl Groups on the Glycerol Backbone and Location of Double Bonds; Fong-Fu Hsu and John Turk
7 largest peaks:



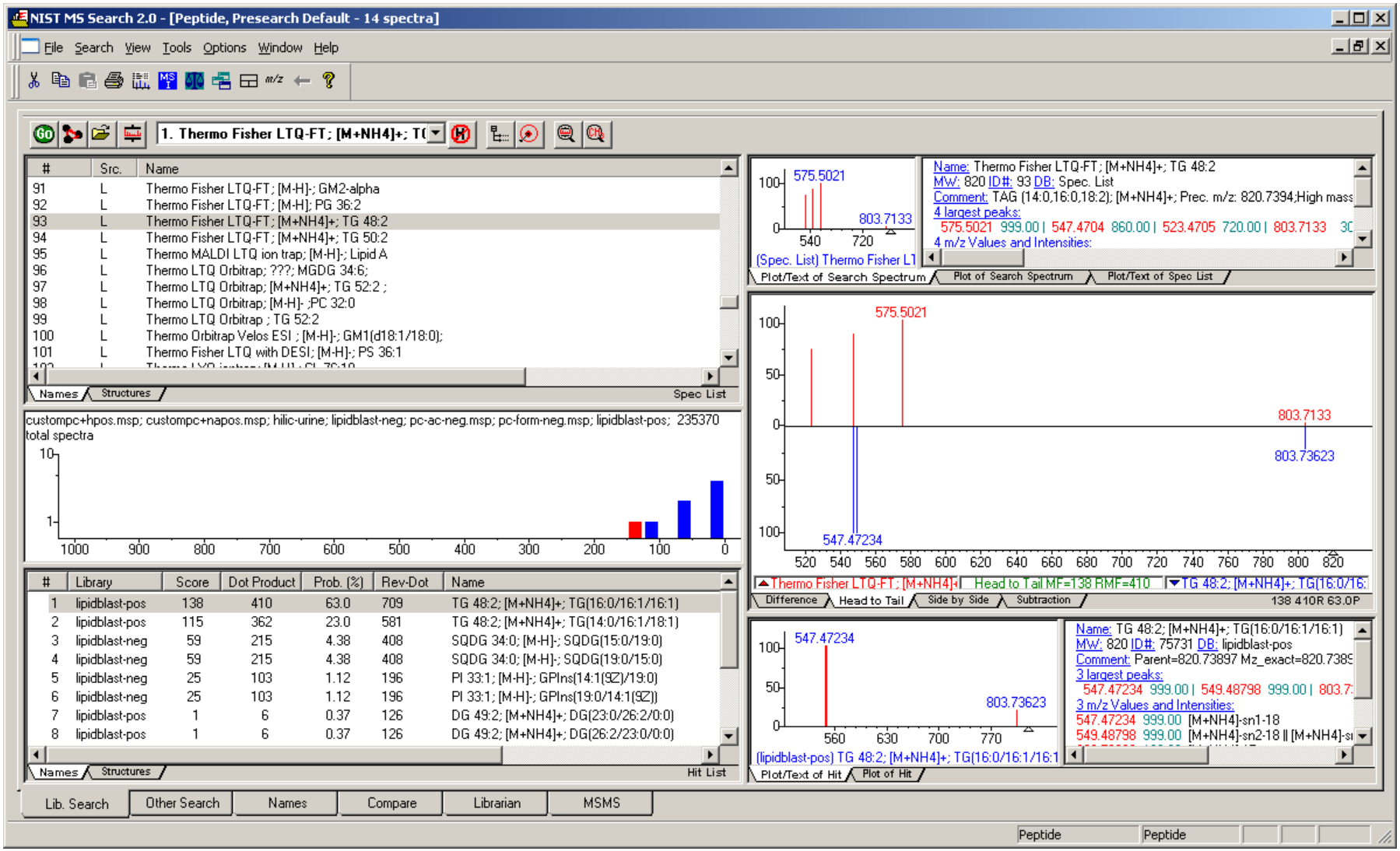
Name: Thermo Fisher LTQ-FT; [M-H]-; GM2-alpha
MW: 1354 ID#: 91 DB: Spec. List
Comment: GM2alpha ganglioside (putative); [M-H]-; ; Prec. m/z: 1354.783;Method for Lipidomic Analysis: p53 Expression Modulation of Sulfatide, Ganglioside, and Phospholipid Composition of U87 MG Glioblastoma Cells; Anal. Chem., 2007, 79 (22), pp 84238430; 10.1021/ac071413m
9 largest peaks:



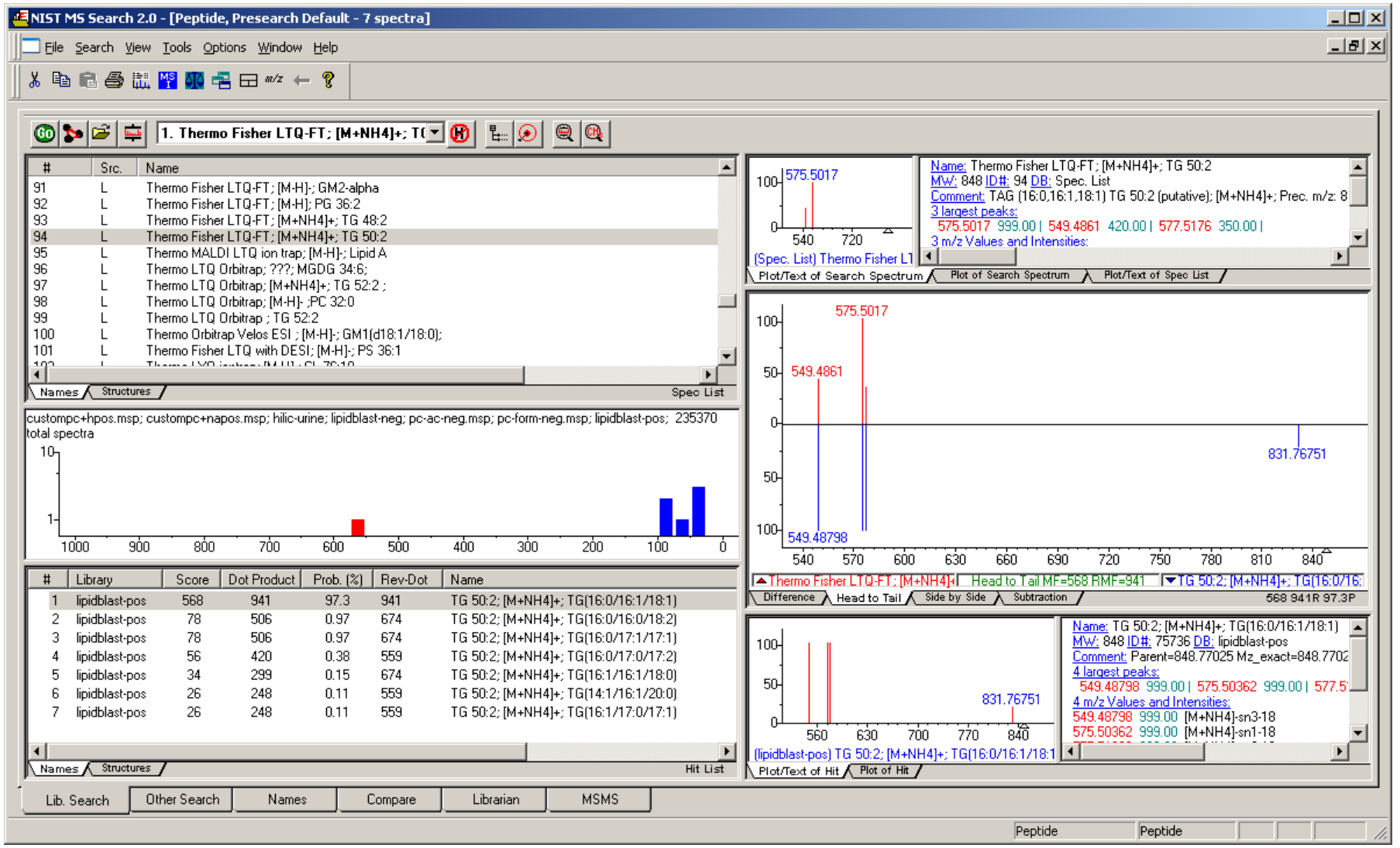
Name: Thermo Fisher LTQ-FT; [M-H]; PG 36:2
MW: 773 ID#: 92 DB: Spec. List
Comment: PG 36:2; [M-H]; Prec. m/z: 773.5325; Remodeling of phosphatidylglycerol in Synechocystis PCC6803 ;http://dx.doi.org/10.1016/j.bbalip.2009.10.009
7 largest peaks:



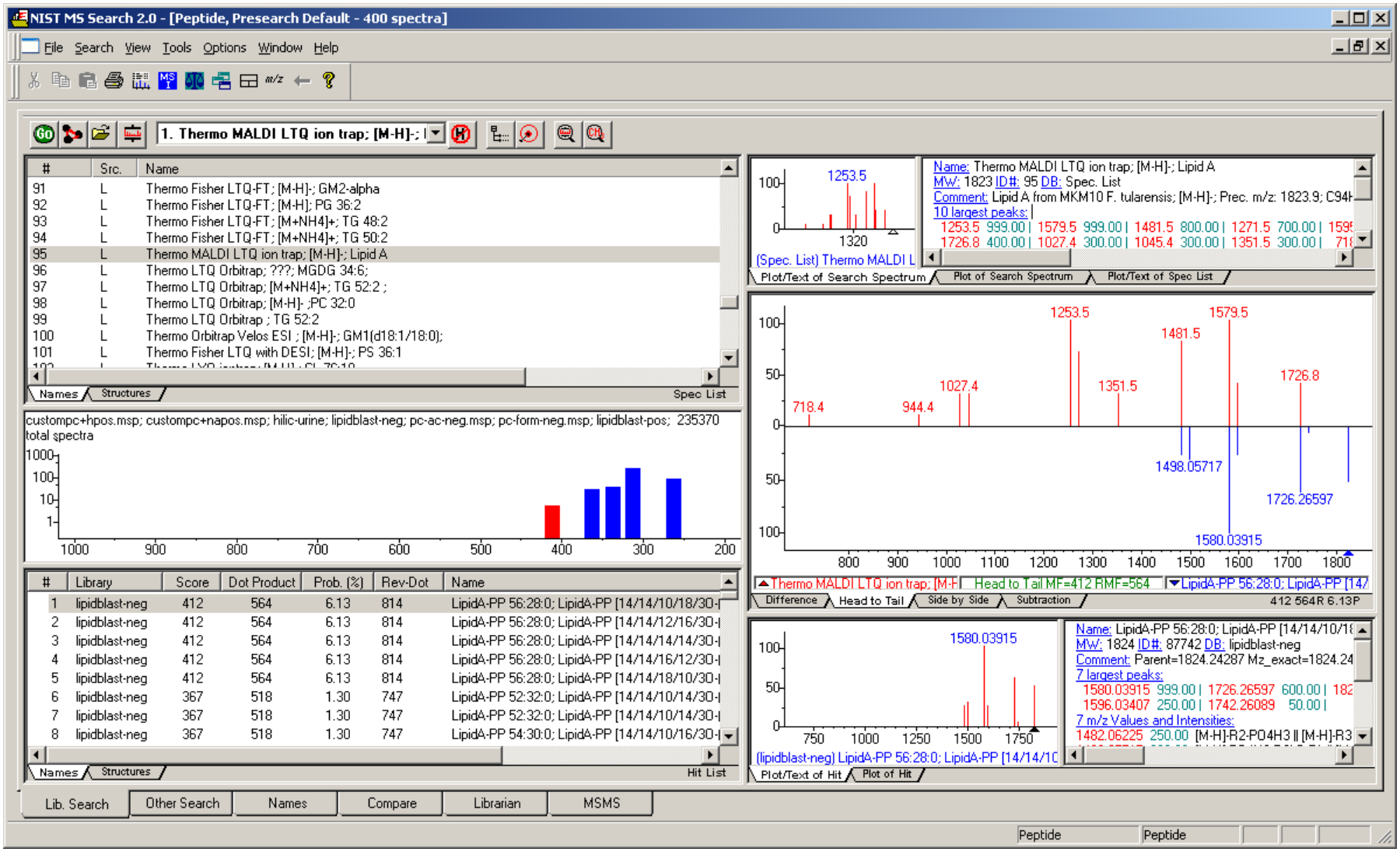
Name: Thermo Fisher LTQ-FT; [M+NH4]+; TG 48:2
MW: 820 ID#: 93 DB: Spec. List
Comment: TAG (14:0,16:0,18:2); [M+NH4]+; Prec. m/z: 820.7394;High mass measurement accuracy MS/MS utilizing LTQ-FT; Application of the accurate mass and time tag approach in studies of the human blood lipidome;Jie Ding, Christina M. Sorensen, Navdeep Jaitly, Hongliang Jiang, Daniel J. Orton, Matthew E. Monroe, Ronald J. Moore, Richard D. Smith, Thomas O. Metz;
4 largest peaks:



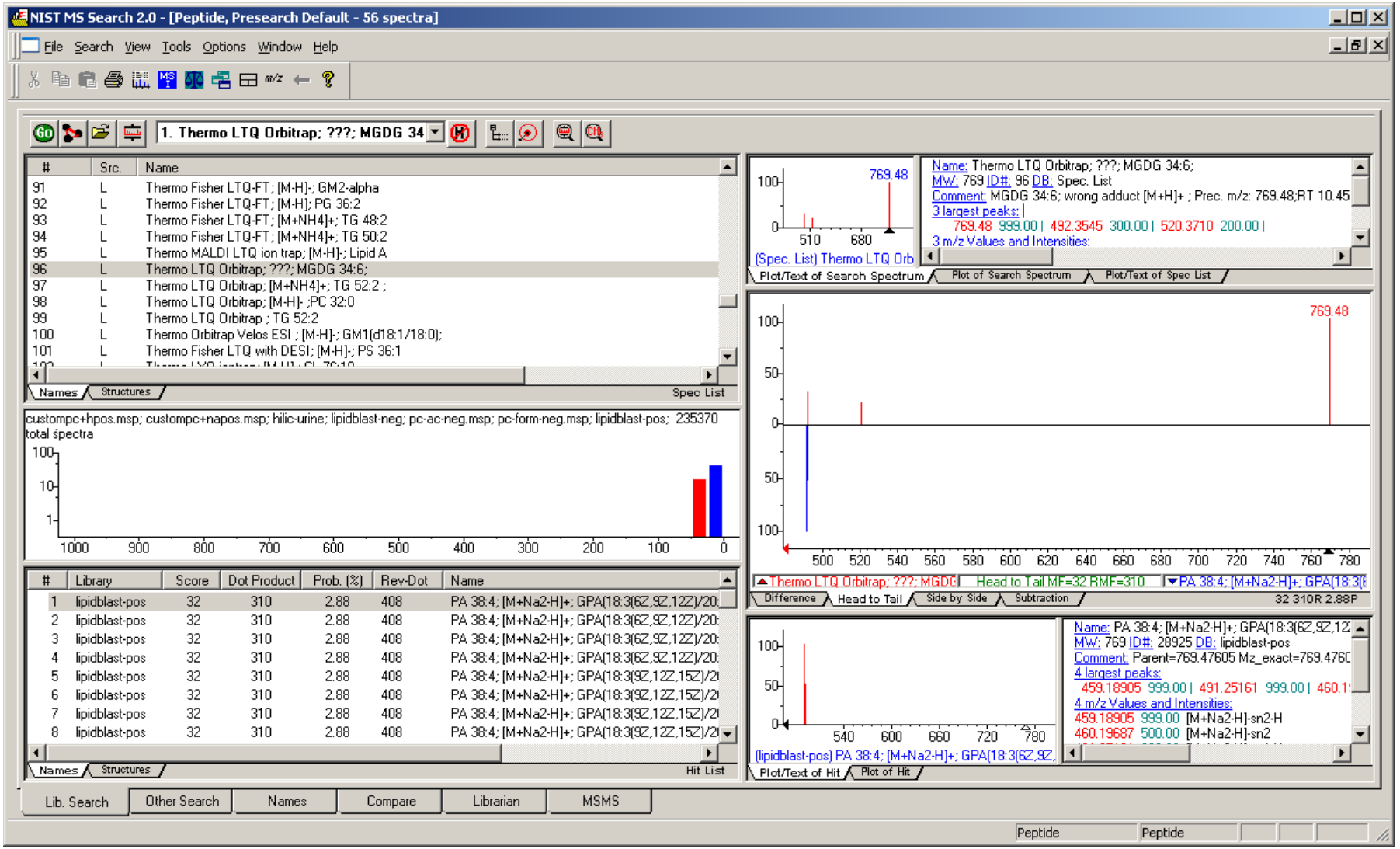
Name: Thermo Fisher LTQ-FT; [M+NH4]+; TG 50:2
MW: 848 ID#: 94 DB: Spec. List
Comment: TAG (16:0,16:1,18:1) TG 50:2 (putative); [M+NH4]+; Prec. m/z: 848.7707; High mass measurement accuracy MS/MS utilizing LTQ-FT; Application of the accurate mass and time tag approach in studies of the human blood lipidome;Jie Ding, Christina M. Sorensen, Navdeep Jaitly, Hongliang Jiang, Daniel J. Orton, Matthew E. Monroe, Ronald J. Moore, Richard D. Smith, Thomas O. Metz;
3 largest peaks:



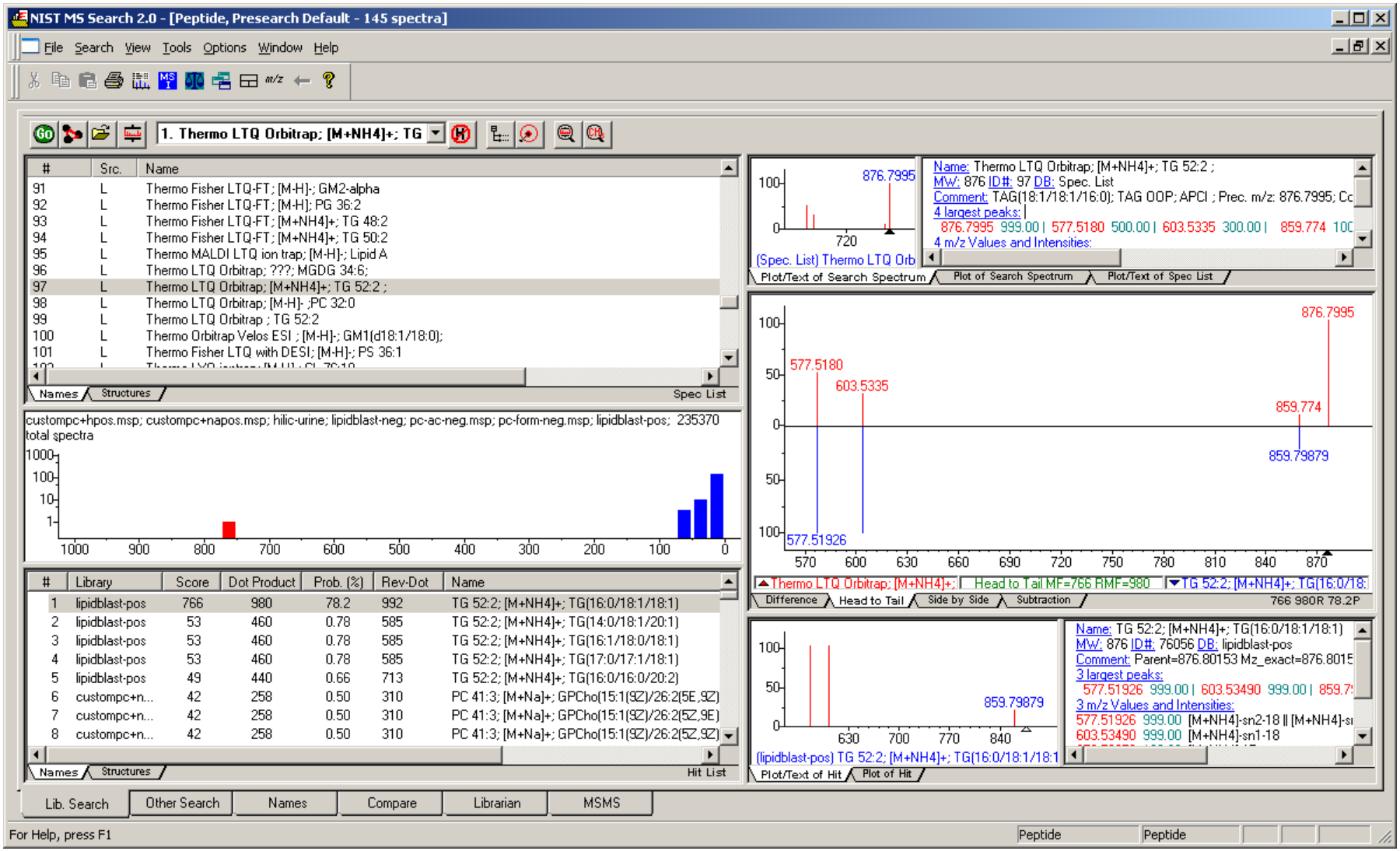
Name: Thermo MALDI LTQ ion trap; [M-H]-; Lipid A
MW: 1823 ID#: 95 DB: Spec. List
Comment: Lipid A from MKM10 F. tularensis; [M-H]-; Prec. m/z: 1823.9; C94H178N2O25P2; LipidA-PP-[14/14/14/14/14/14]; DOI: 10.1002/jms.614; Identification of LpxL, a Late Acyltransferase of Francisella tularensis; 10.1128/IAI.01288-06
10 largest peaks:



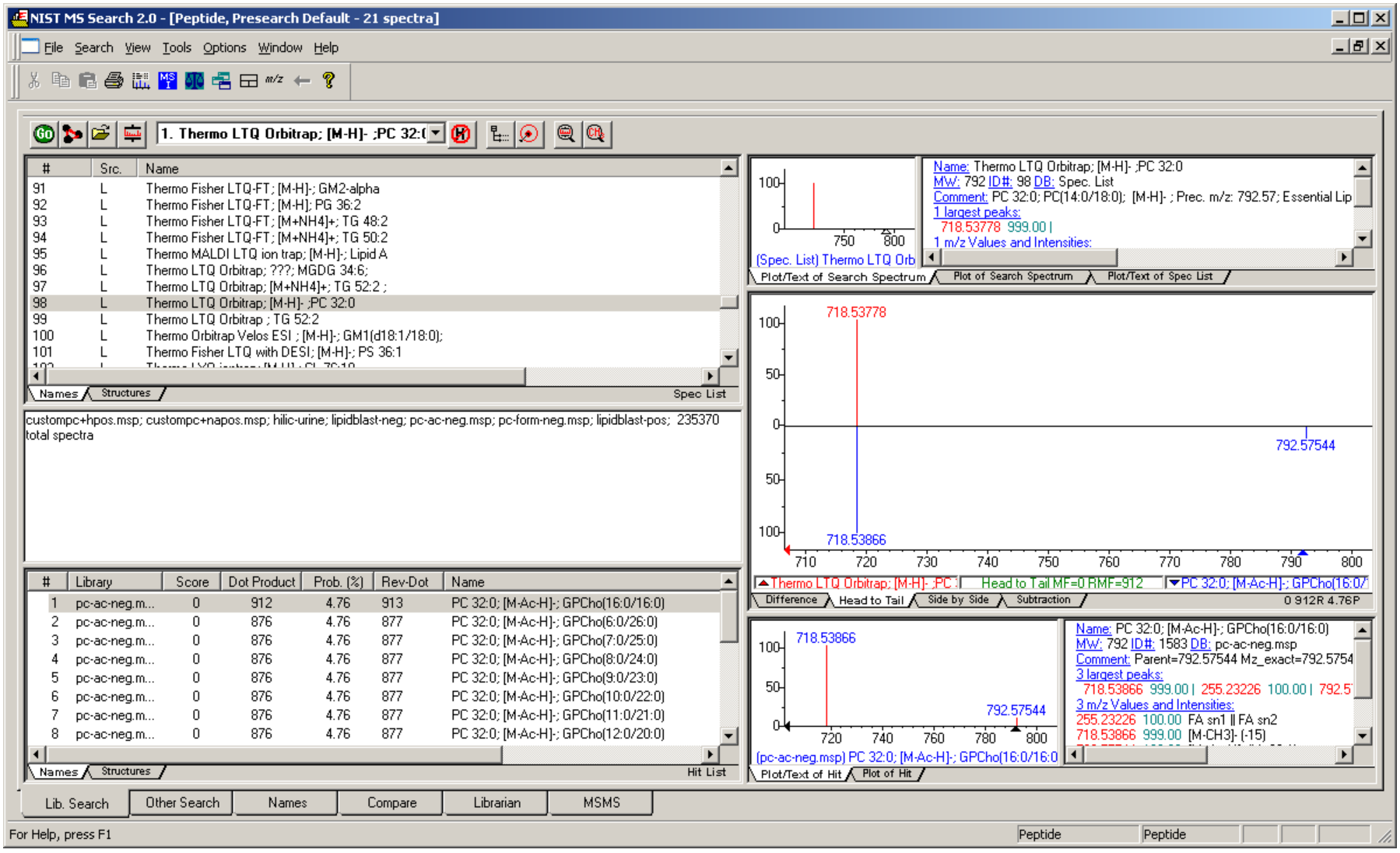
Name: Thermo LTQ Orbitrap; ???; MGDG 34:6;
MW: 769 ID#: 96 DB: Spec. List
Comment: MGDG 34:6; wrong adduct [M+H]+ ; Prec. m/z: 769.48;RT 10.45 min ; Advanced Mass Spectrometry Methods for Analysis of Lipids from Photosynthetic Organisms; Bettina Seiwert, Patrick Giavalisco, and Lothar Willmitzer; dx.doi.org/10.1007/978-90-481-2863-1_20
3 largest peaks:



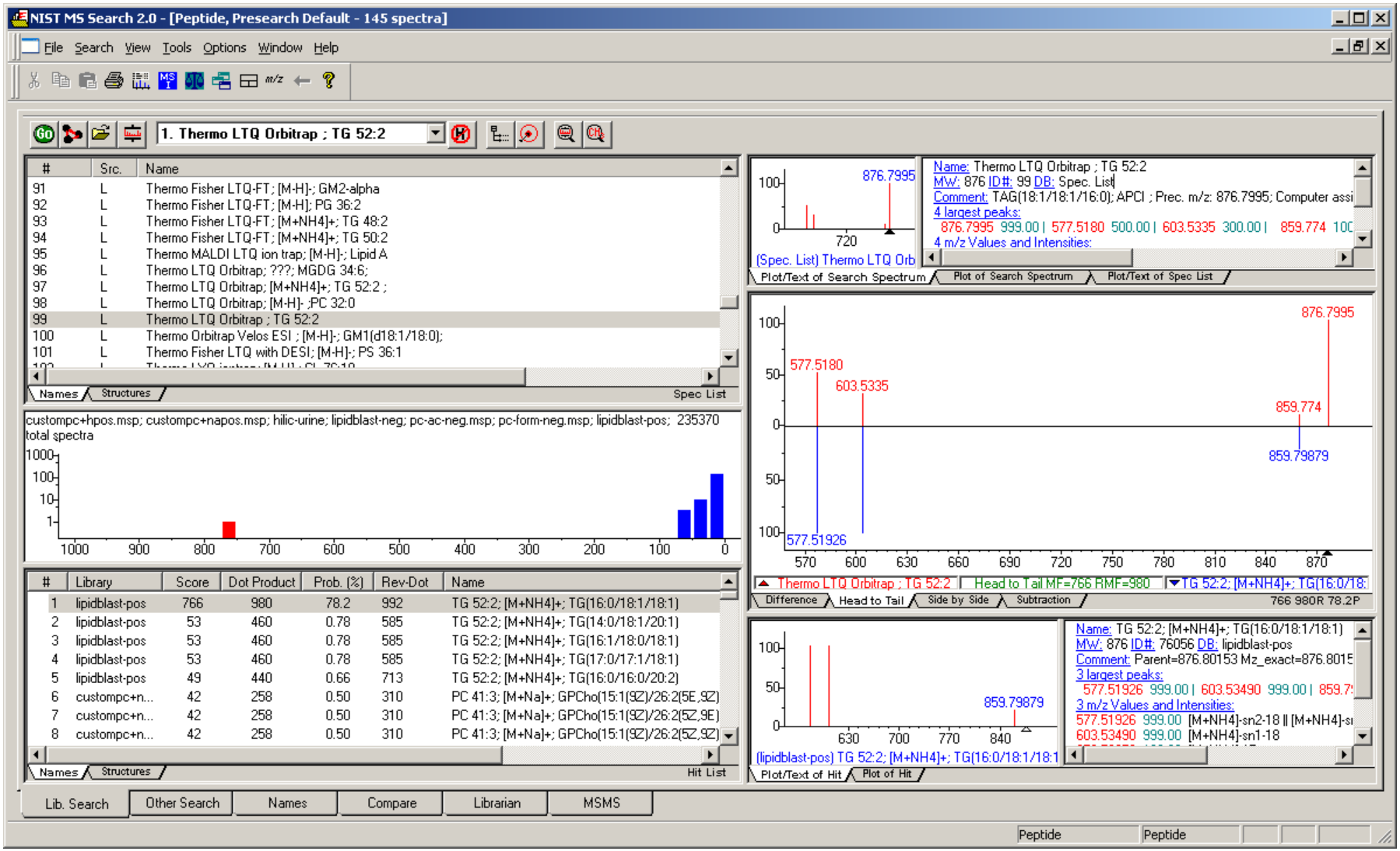
Name: Thermo LTQ Orbitrap; [M+NH4]+; TG 52:2 ;
MW: 876 ID#: 97 DB: Spec. List
Comment: TAG(18:1/18:1/16:0); TAG OOP; APCI ; Prec. m/z: 876.7995; Computer assisted Interpretation of Triacylglycerols Mass Spectra;Josef Cvacka and Edita Kofronová
4 largest peaks:



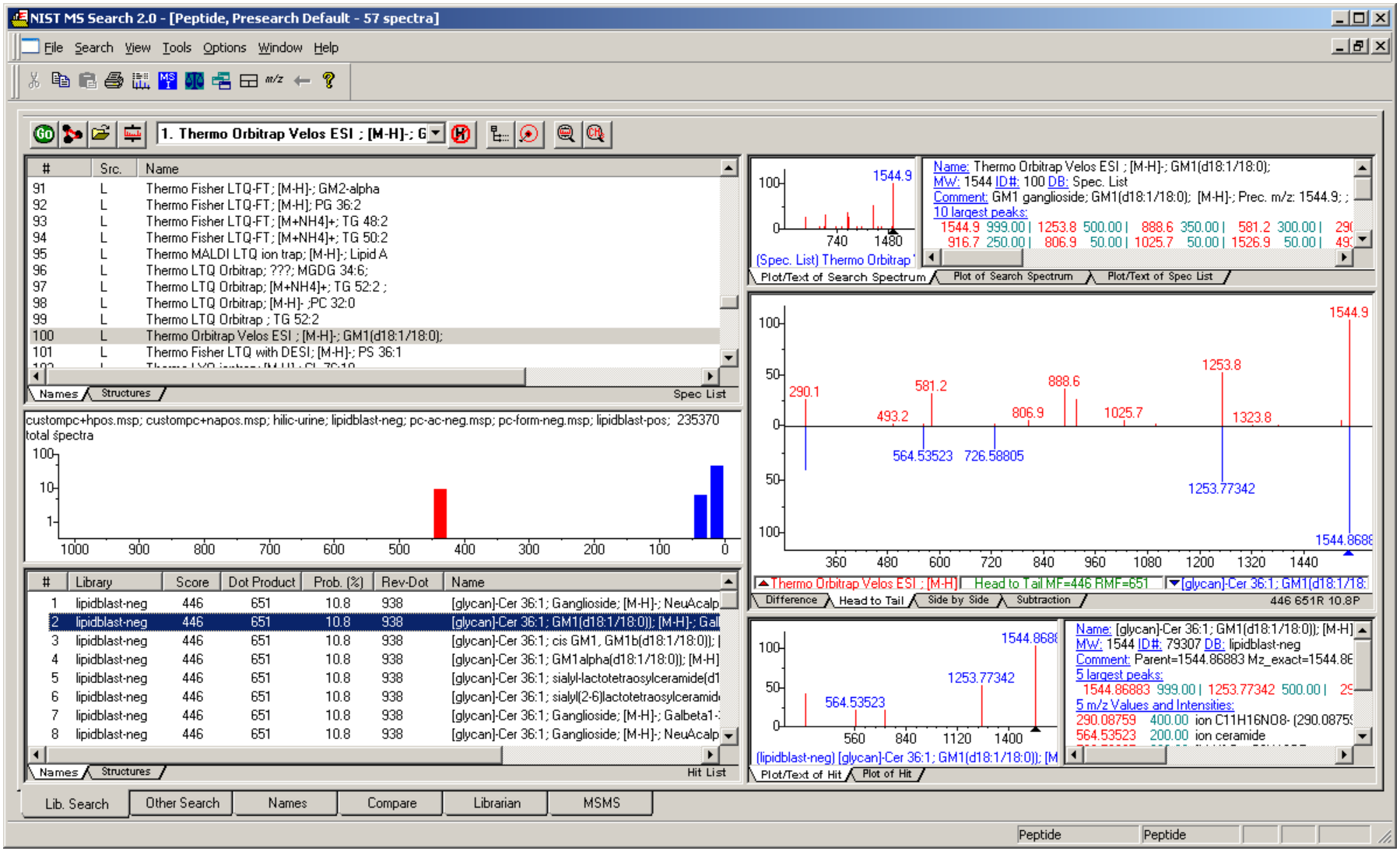
Name: Thermo LTQ Orbitrap; [M-H]- ;PC 32:0
MW: 792 ID#: 98 DB: Spec. List
Comment: PC 32:0; PC(14:0/18:0); [M-H]- ; Prec. m/z: 792.57; Essential Lipidomics Experiments Using the LTQ Orbitrap Hybrid Mass Spectrometer; Thermo Application Note 367
1 largest peaks:



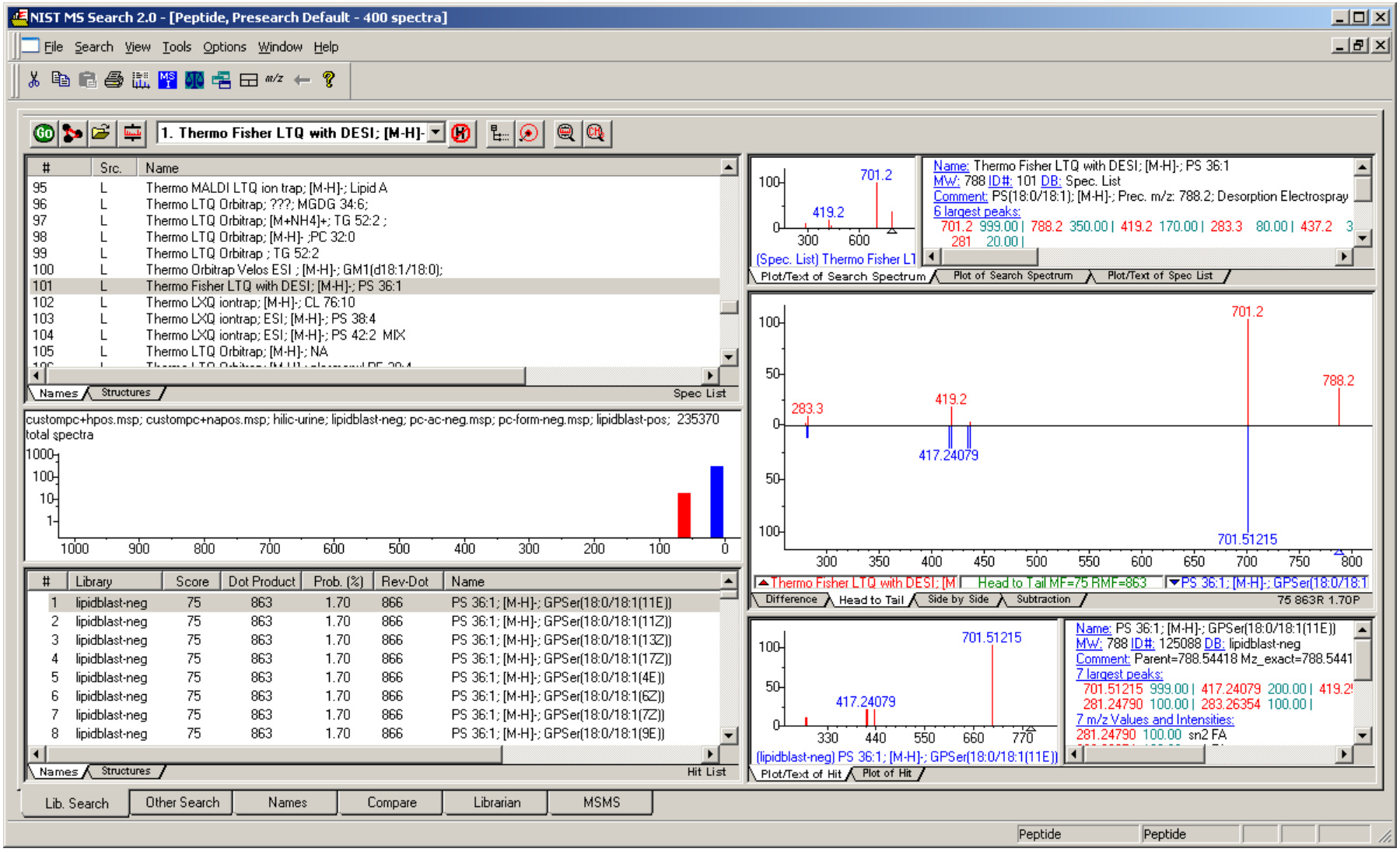
Name: Thermo LTQ Orbitrap ; TG 52:2
MW: 876 ID#: 99 DB: Spec. List
Comment: TAG(18:1/18:1/16:0); APCI ; Prec. m/z: 876.7995; Computer assisted Interpretation of Triacylglycerols Mass Spectra;Josef Cvacka and Edita Kofronová
4 largest peaks:



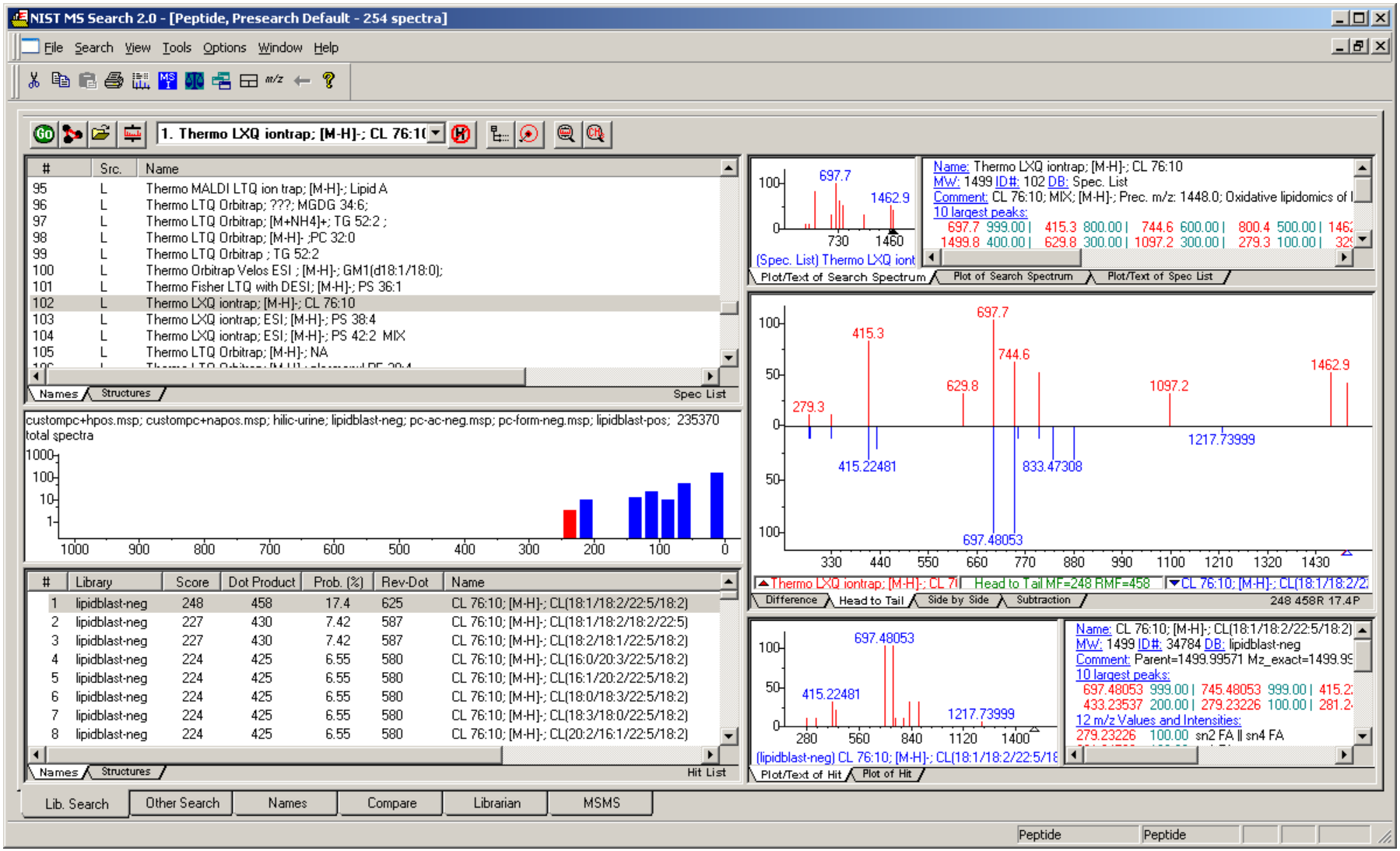
Name: Thermo Orbitrap Velos ESI ; [M-H]-; GM1(d18:1/18:0);
MW: 1544 ID#: 100 DB: Spec. List
Comment: GM1 ganglioside; GM1(d18:1/18:0); [M-H]-; Prec. m/z: 1544.9; ; Localization, Imaging and Structural Analysis of Sialylated Glycosphingolipids in Brain Tissue Sections by Mass Spectrometry.; Benoit Colsch1, Shelley N. Jackson1, Sucharita M. Dutta2, Alice M. Delvolv1, Amina S. Woods1.; ASMS2010;
http://www.asms.org/asms10pdf/ASMS201020798.0375VER.4.pdf
10 largest peaks:



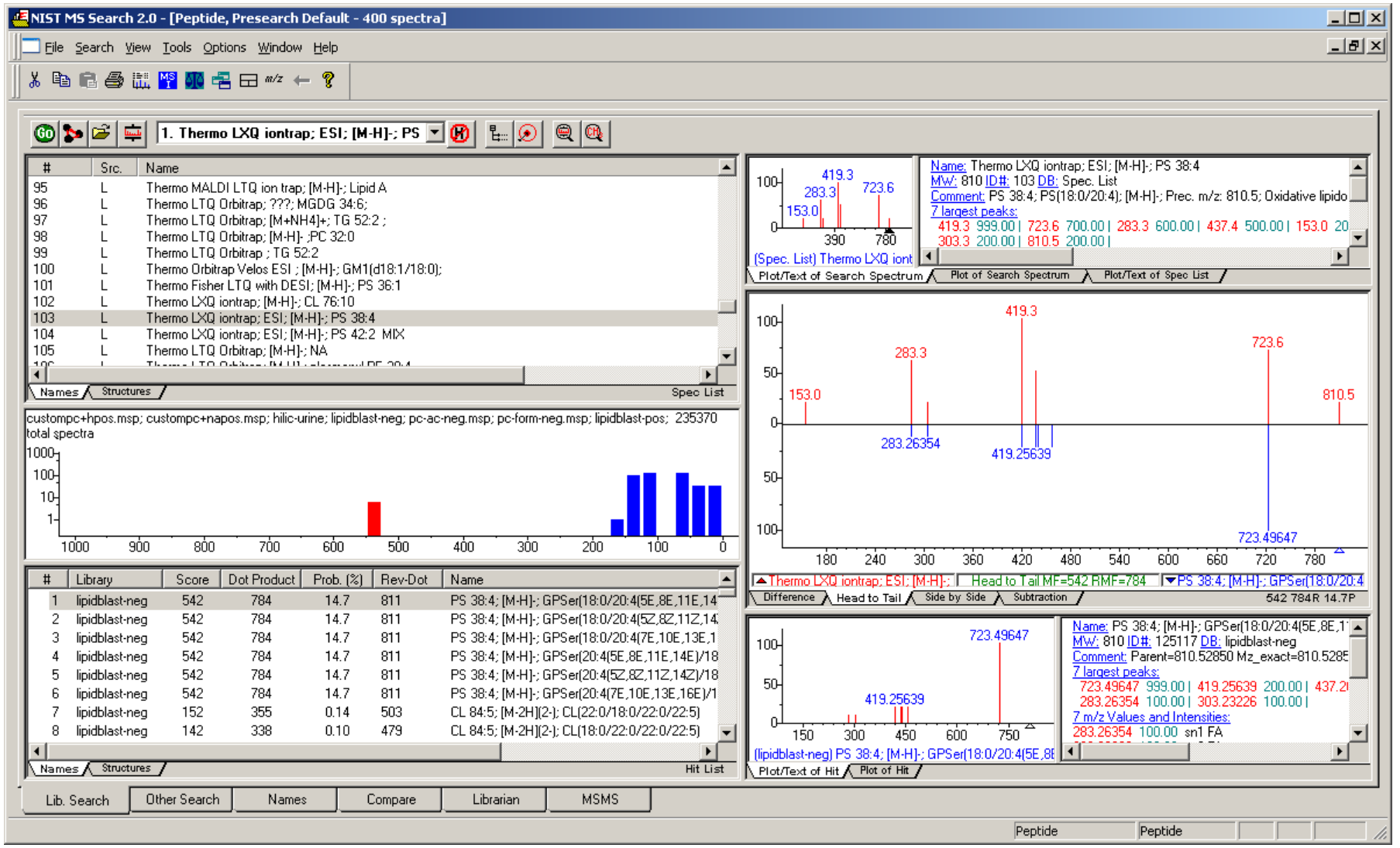
Name: Thermo Fisher LTQ with DESI; [M-H]-; PS 36:1
MW: 788 ID#: 101 DB: Spec. List
Comment: PS(18:0/18:1); [M-H]-; Prec. m/z: 788.2; Desorption Electrospray Ionization (DESI) Mass Spectrometry and Tandem Mass Spectrometry (MS/MS) of Phospholipids and Sphingolipids: Ionization, Adduct Formation, and Fragmentation; Nicholas E. Manicke, Justin M. Wiseman, Demian R. Ifa and R. Graham Cooks;
6 largest peaks:



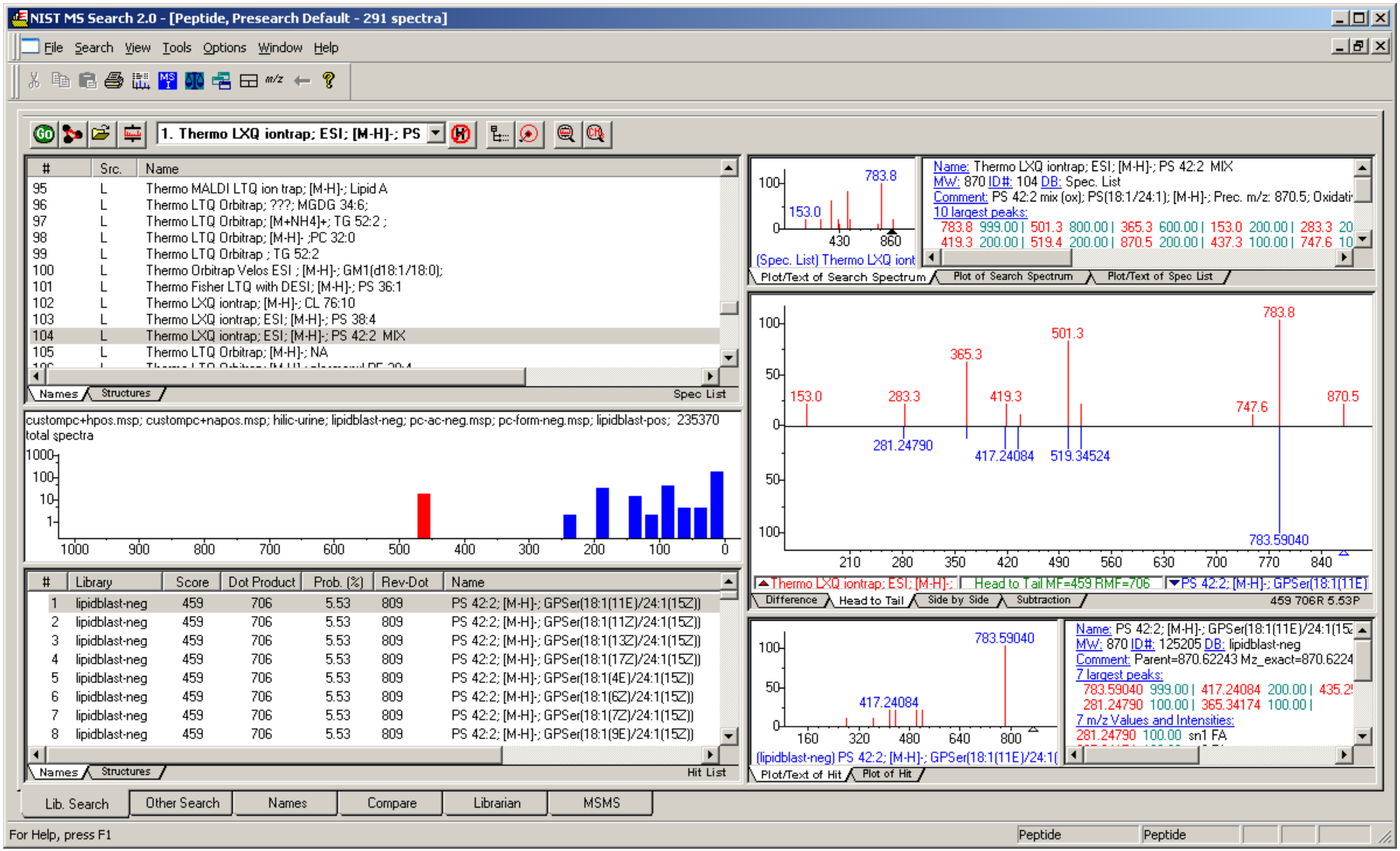
Name: Thermo LXQ iontrap; [M-H]-; CL 76:10
MW: 1499 ID#: 102 DB: Spec. List
Comment: CL 76:10; MIX; [M-H]-; Prec. m/z: 1448.0; Oxidative lipidomics of hyperoxic acute lung injury: mass spectrometric characterization of cardiolipin and phosphatidylserine peroxidation; doi:10.1152/ajplung.00035.2010
10 largest peaks:



Name: Thermo LXQ iontrap; ESI; [M-H]-; PS 38:4
MW: 810 ID#: 103 DB: Spec. List
Comment: PS 38:4; PS(18:0/20:4); [M-H]-; Prec. m/z: 810.5; Oxidative lipidomics of hyperoxic acute lung injury: mass spectrometric characterization of cardiolipin and phosphatidylserine peroxidation; doi:10.1152/ajplung.00035.2010
7 largest peaks:

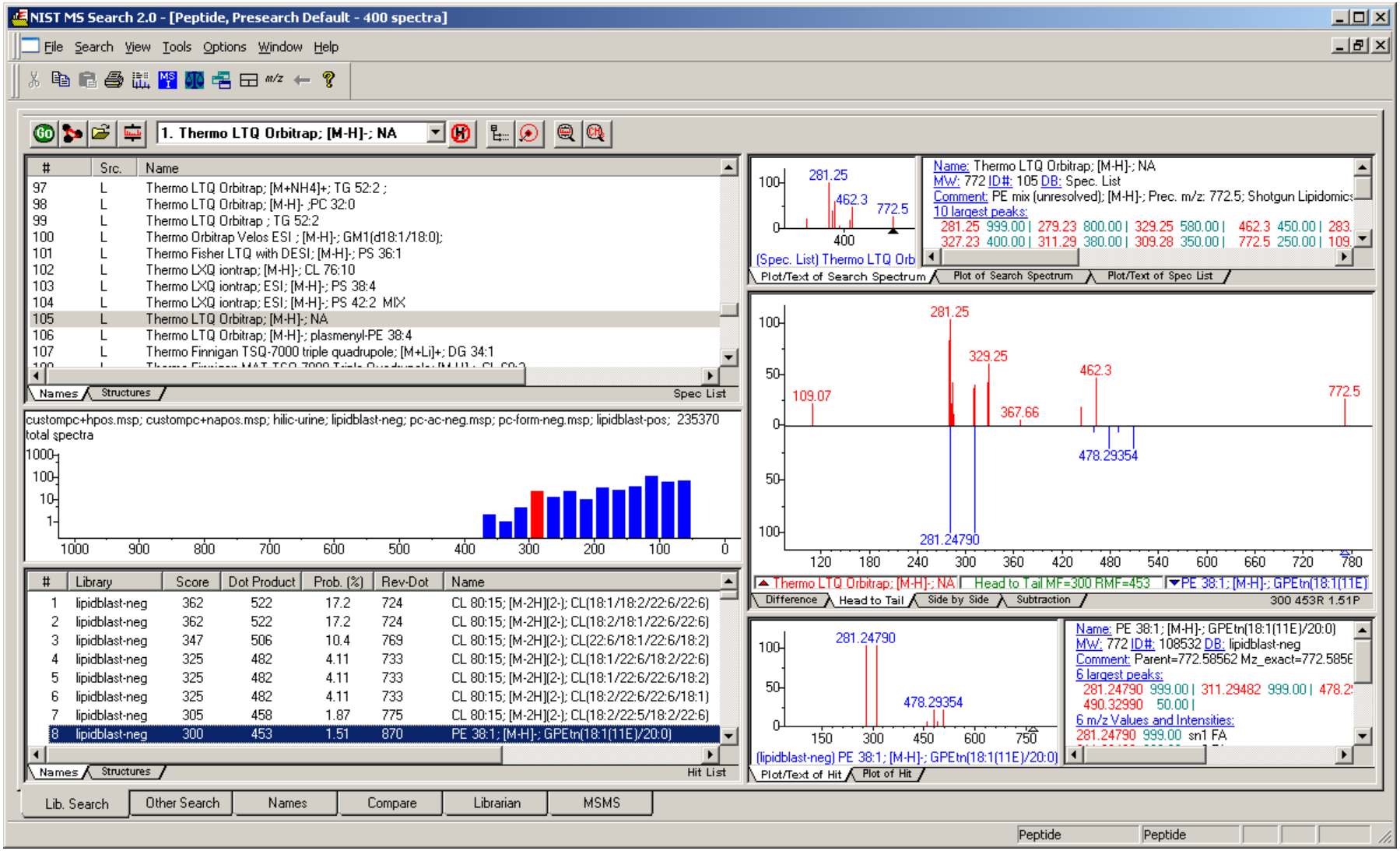


Name: Thermo LXQ iontrap; ESI; [M-H]-; PS 42:2 MIX
MW: 870 ID#: 104 DB: Spec. List
Comment: PS 42:2 mix (ox); PS(18:1/24:1); [M-H]-; Prec. m/z: 870.5; Oxidative lipidomics of hyperoxic acute lung injury: mass spectrometric characterization of cardiolipin and phosphatidylserine peroxidation; doi:10.1152/ajplung.00035.2010
10 largest peaks:

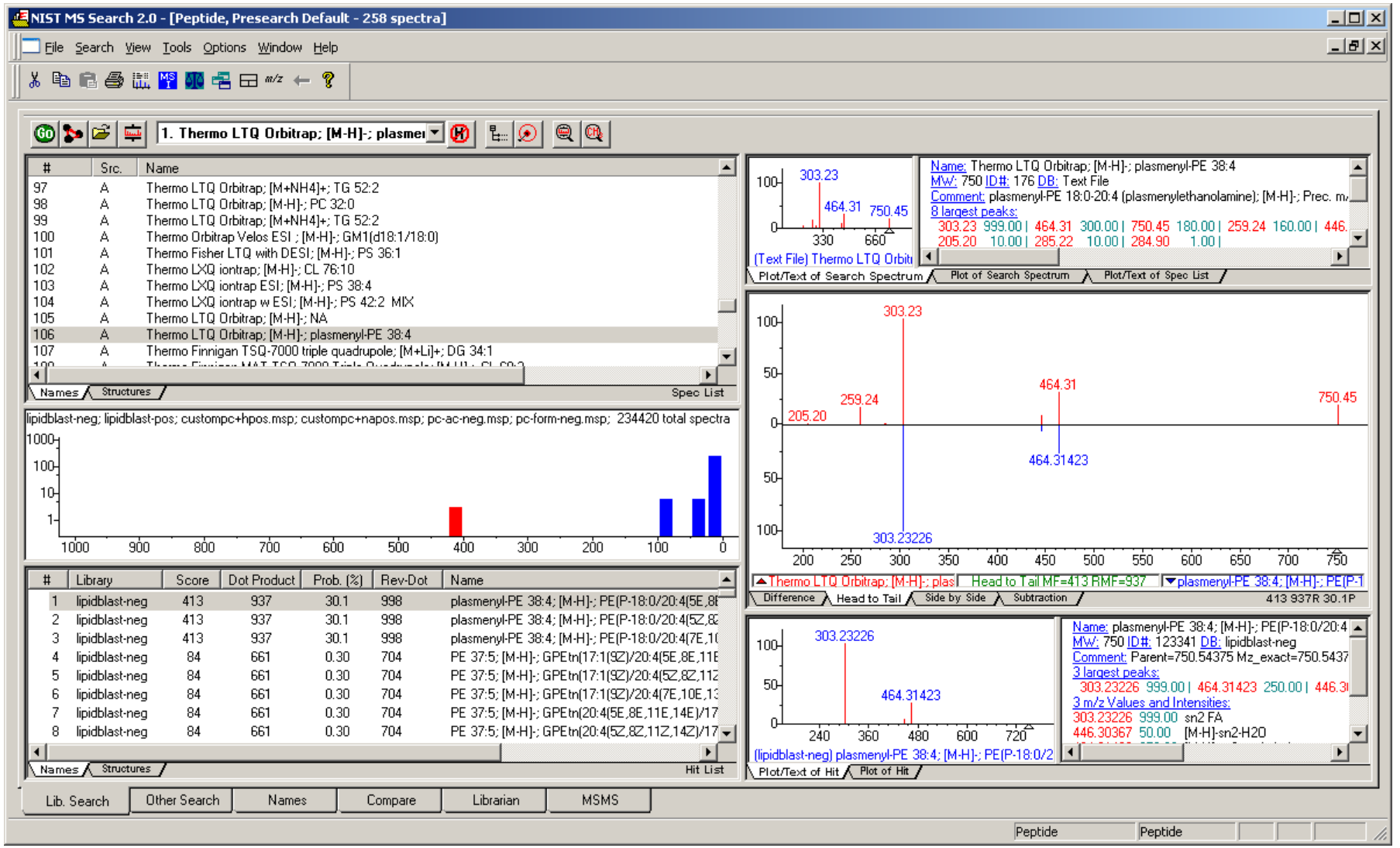


Name: Thermo LTQ Orbitrap; [M-H]-; NA
MW: 772 ID#: 105 DB: Spec. List
Comment: PE mix (unresolved); [M-H]-; Prec. m/z: 772.5; Shotgun Lipidomics Identifies a Paired Rule for the Presence of Isomeric Ether Phospholipid Molecular Species; Kui Yang, Zhongdan Zhao, Richard W. Gross, Xianlin Han
10 largest peaks:

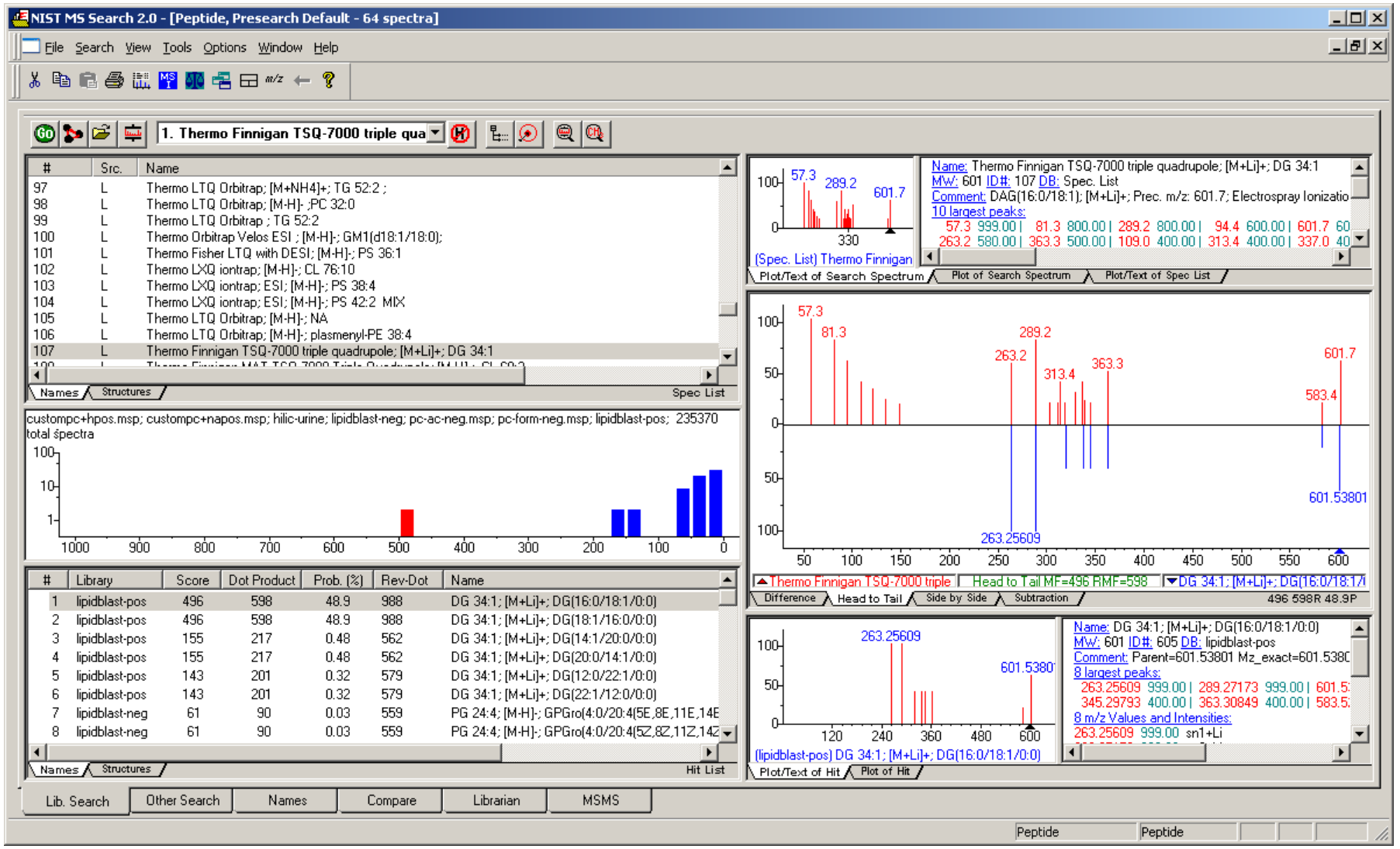
PE MIX (unresolved)



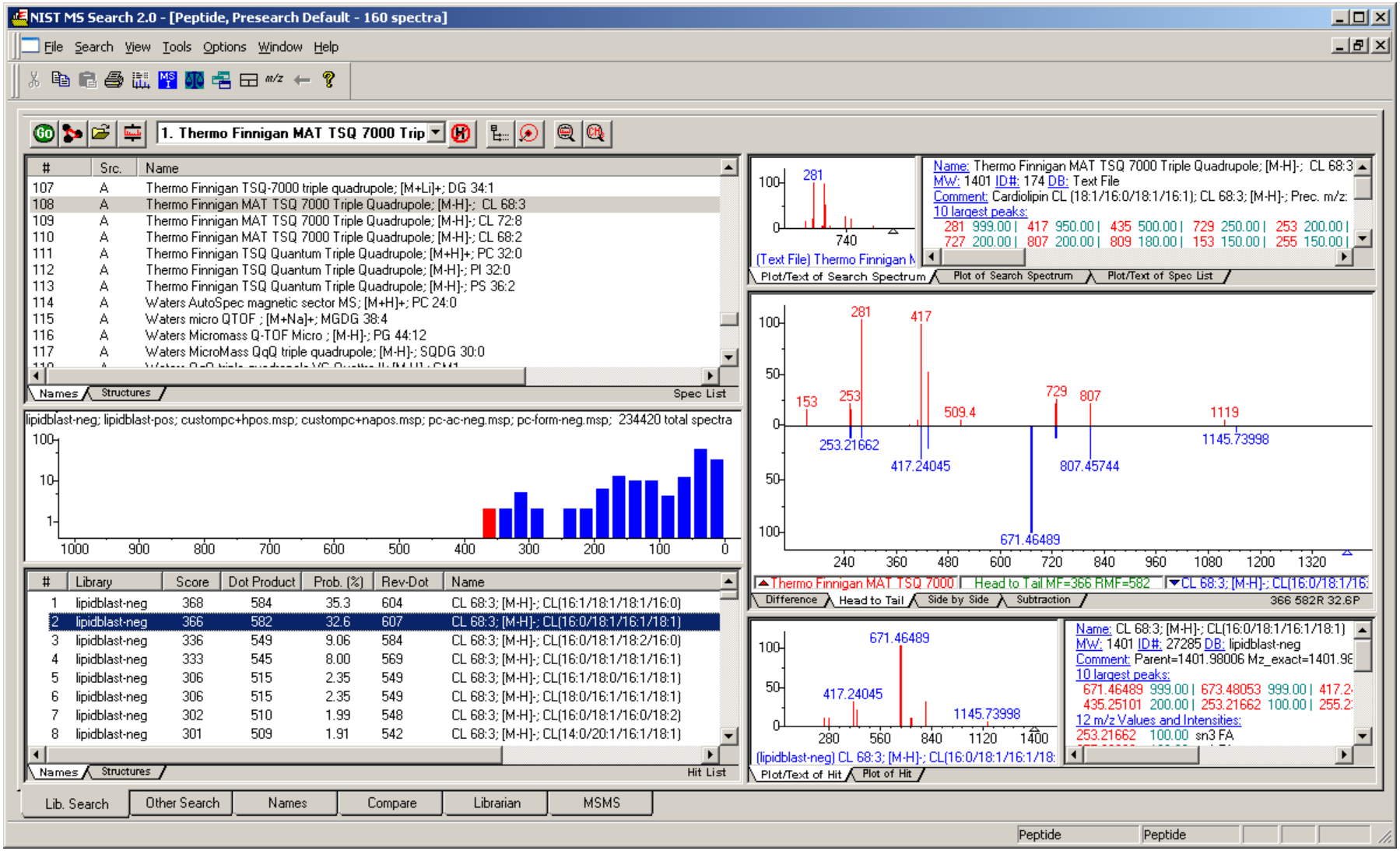
Name: Thermo LTQ Orbitrap; [M-H]-; plasmenyl-PE 38:4
MW: 750 ID#: 176 DB: Text File
Comment: plasmenyl-PE 18:0-20:4 (plasmenylethanolamine); [M-H]-; Prec. m/z: 750.54; Shotgun Lipidomics Identifies a Paired Rule for the Presence of Isomeric Ether Phospholipid Molecular Species; Kui Yang, Zhongdan Zhao, Richard W. Gross, Xianlin Han
8 largest peaks:



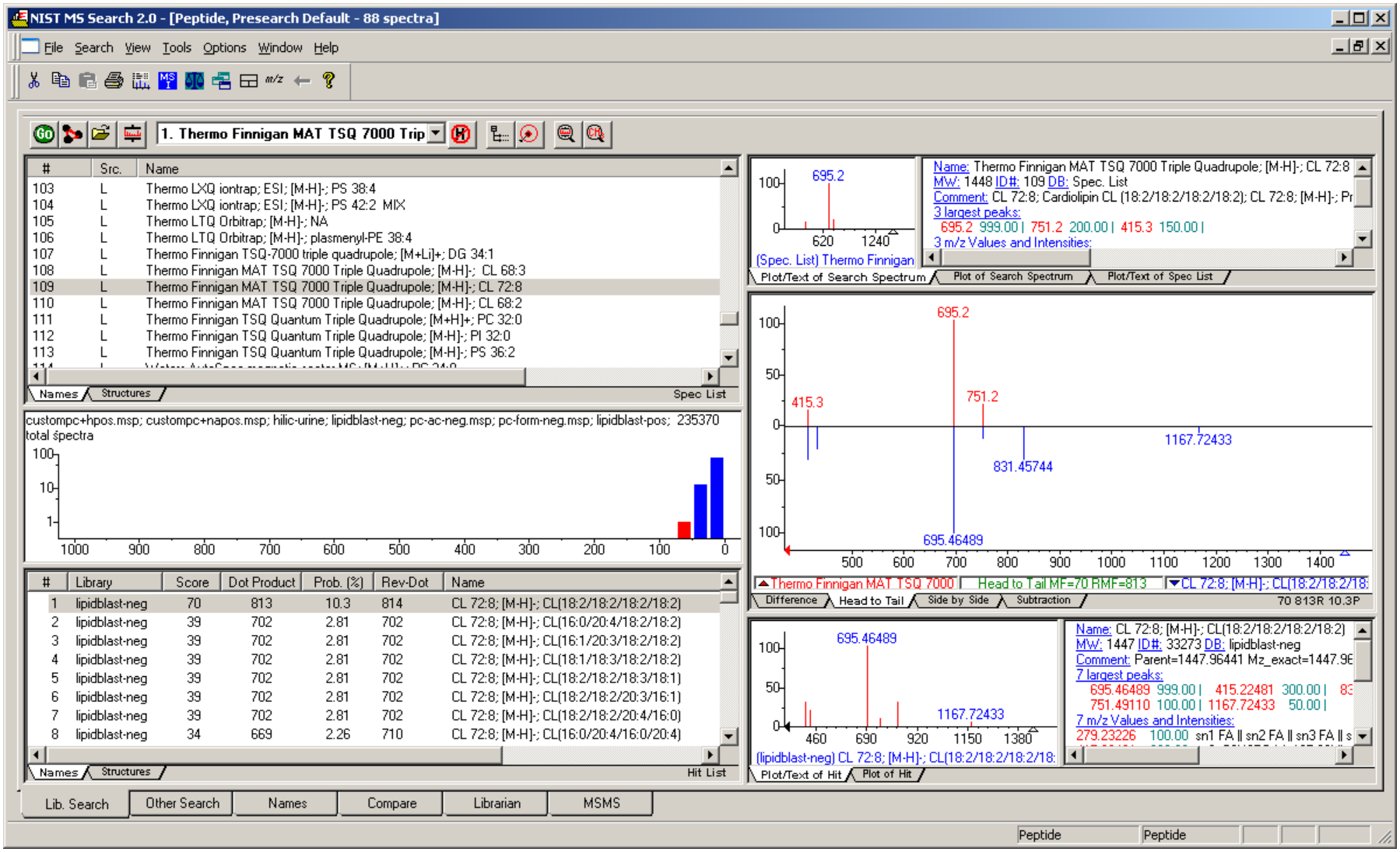
Name: Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li]+; DG 34:1
MW: 601 ID#: 107 DB: Spec. List
Comment: DAG(16:0/18:1); [M+Li]+; Prec. m/z: 601.7; Electrospray Ionization/Mass Spectrometric Analyses of Human Promonocytic U937 Cell Glycerolipids and Evidence That Differentiation Is Associated with Membrane Lipid Composition Changes That Facilitate Phospholipase A2 Activation; DOI 10.1074/jbc.M908342199
10 largest peaks:



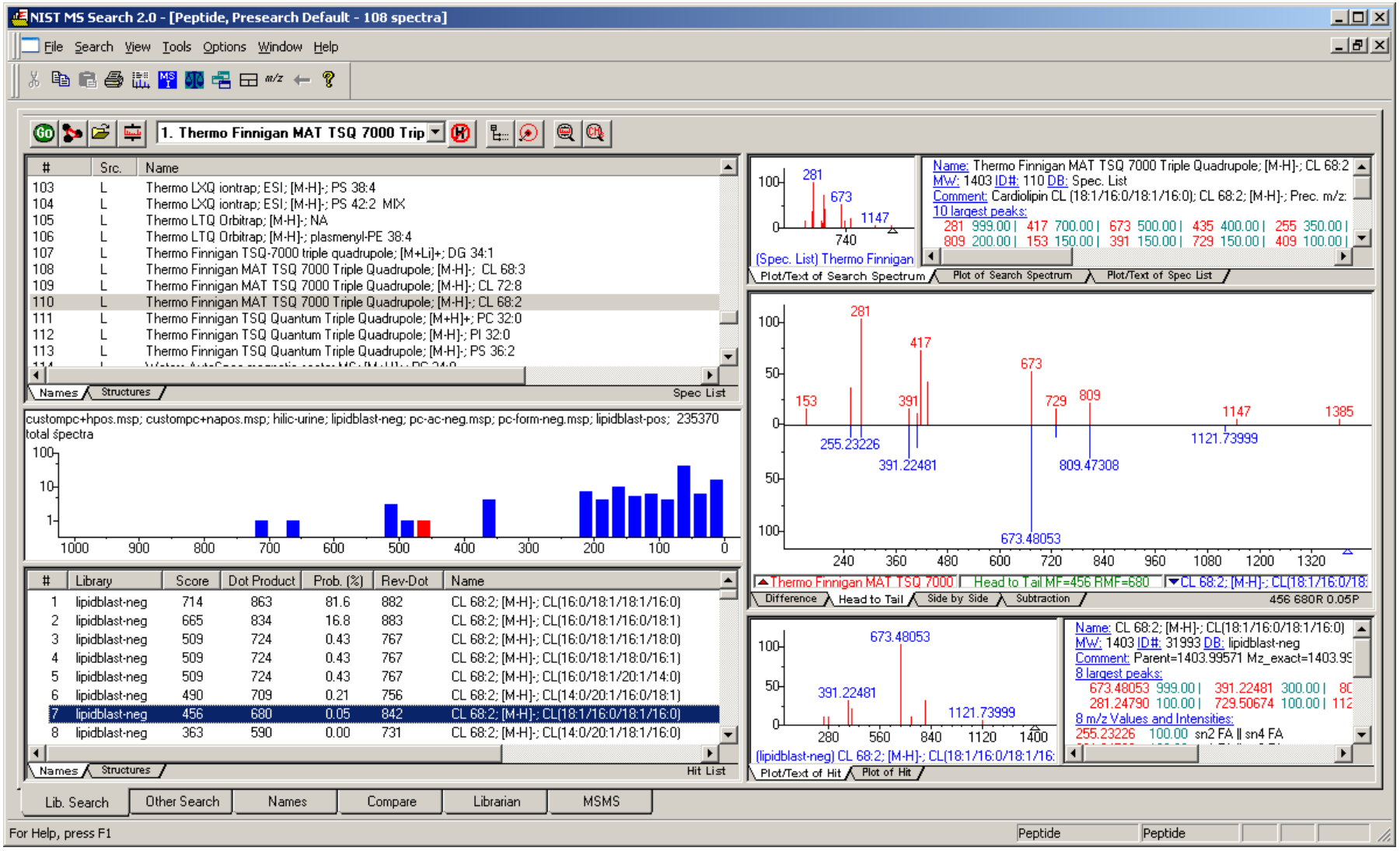
Name: Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H]-; CL 68:3
MW: 1401 ID#: 174 DB: Text File
Comment: Cardiolipin CL (18:1/16:0/18:1/16:1); CL 68:3; [M-H]-; Prec. m/z: 1401.9; Structural Characterization of Cardiolipin by Tandem Quadrupole and Multiple-Stage Quadrupole Ion-Trap Mass Spectrometry with Electrospray Ionization;John Turk, Elizabeth R. Rhoades, David G. Russell, Yixin Shi and Eduardo A. Groisman;http://dx.doi.org/10.1016/j.jasms.2004.12.015
10 largest peaks:



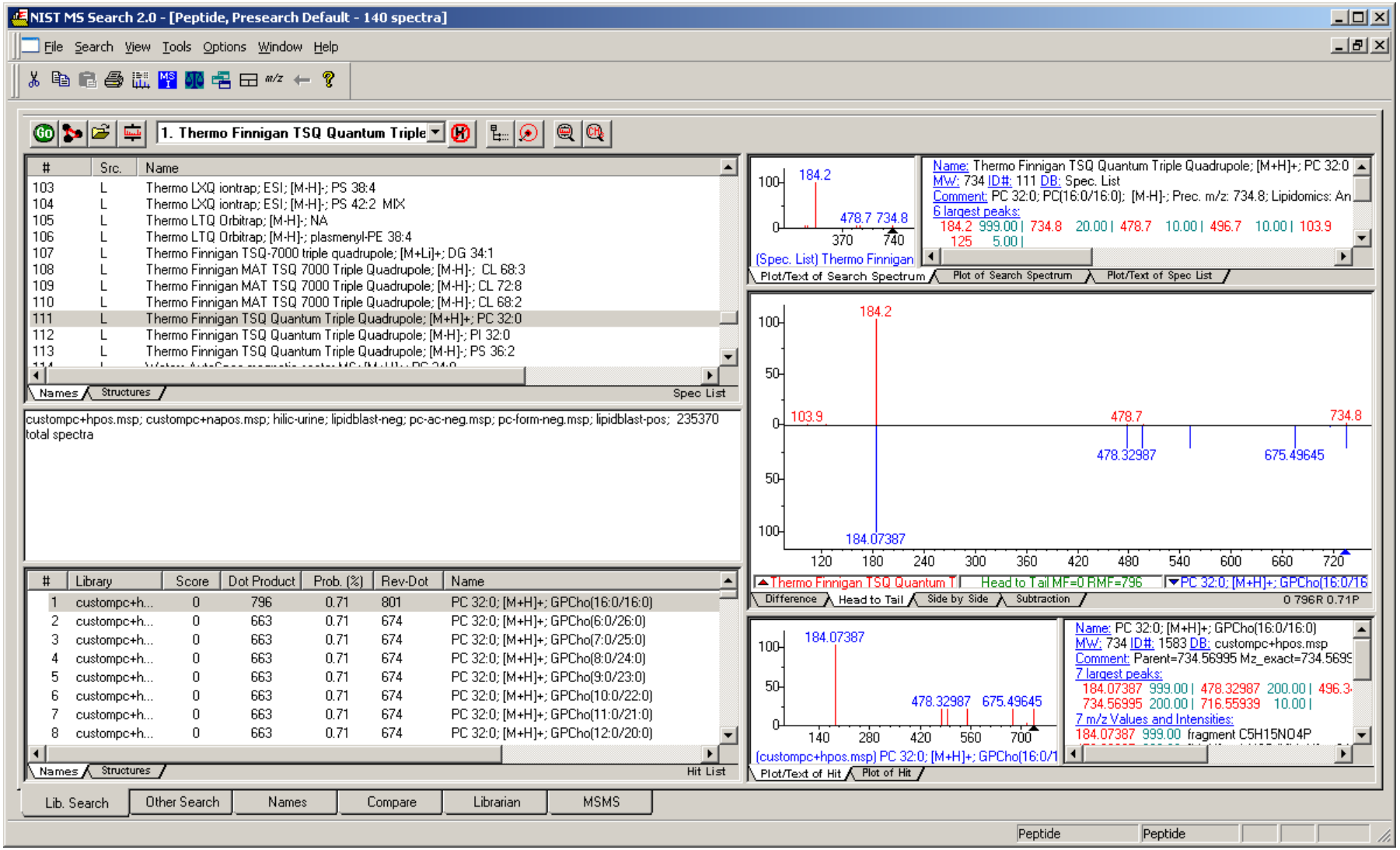
Name: Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H]-; CL 72:8
MW: 1448 ID#: 109 DB: Spec. List
Comment: CL 72:8; Cardiolipin CL (18:2/18:2/18:2/18:2); CL 72:8; [M-H]-; Prec. m/z: 1448.0; CARDIOLIPIN LOSS DURING MYOCARDIAL ISCHEMIA; Am J Physiol Heart Circ Physiol 280: H2770-H2778, 2001
3 largest peaks:



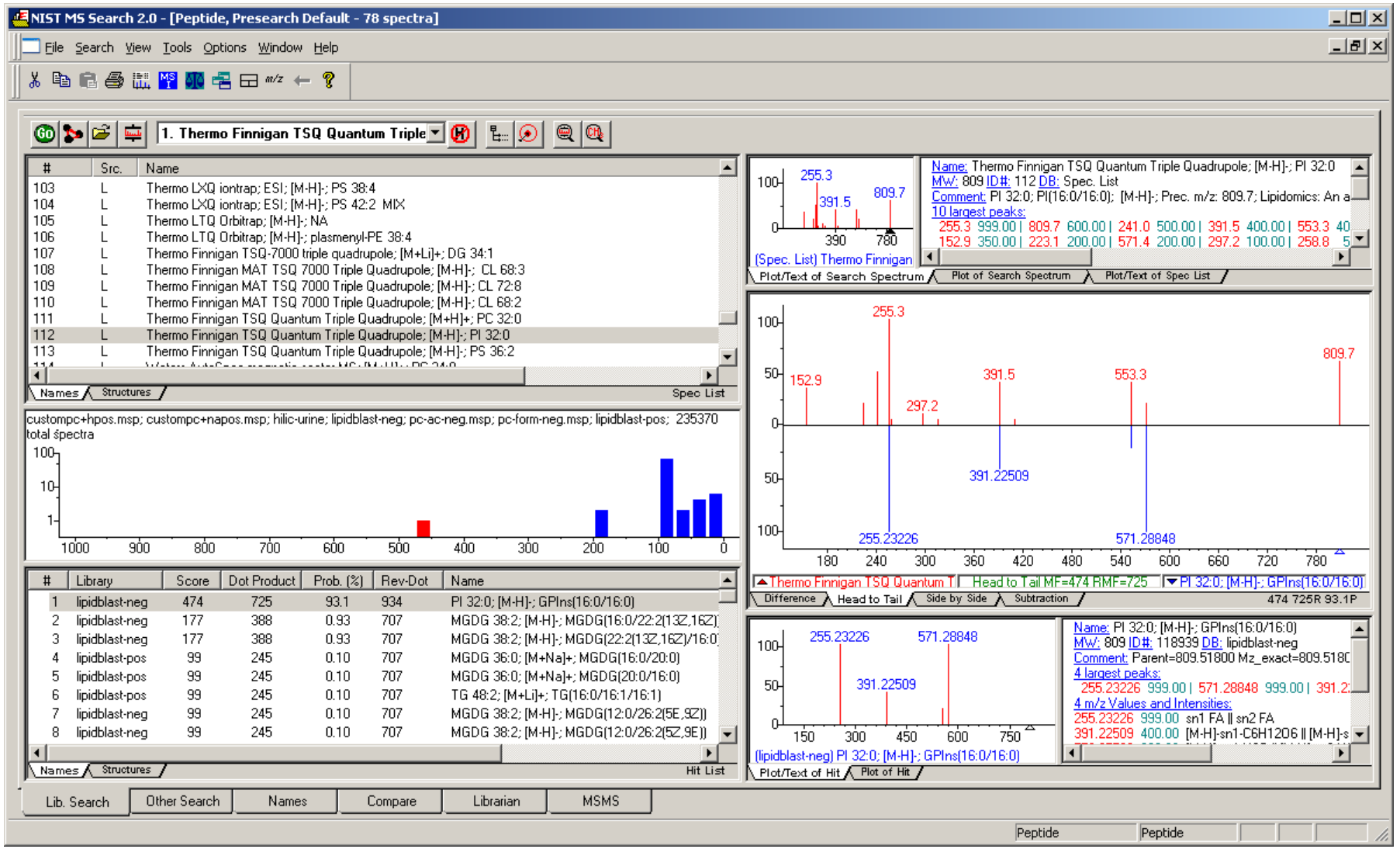
Name: Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H]-; CL 68:2
MW: 1403 ID#: 110 DB: Spec. List
Comment: Cardiolipin CL (18:1/16:0/18:1/16:0); CL 68:2; [M-H]-; Prec. m/z: 1403.9; Structural Characterization of Cardiolipin by Tandem Quadrupole and Multiple-Stage Quadrupole Ion-Trap Mass Spectrometry with Electrospray Ionization
10 largest peaks:



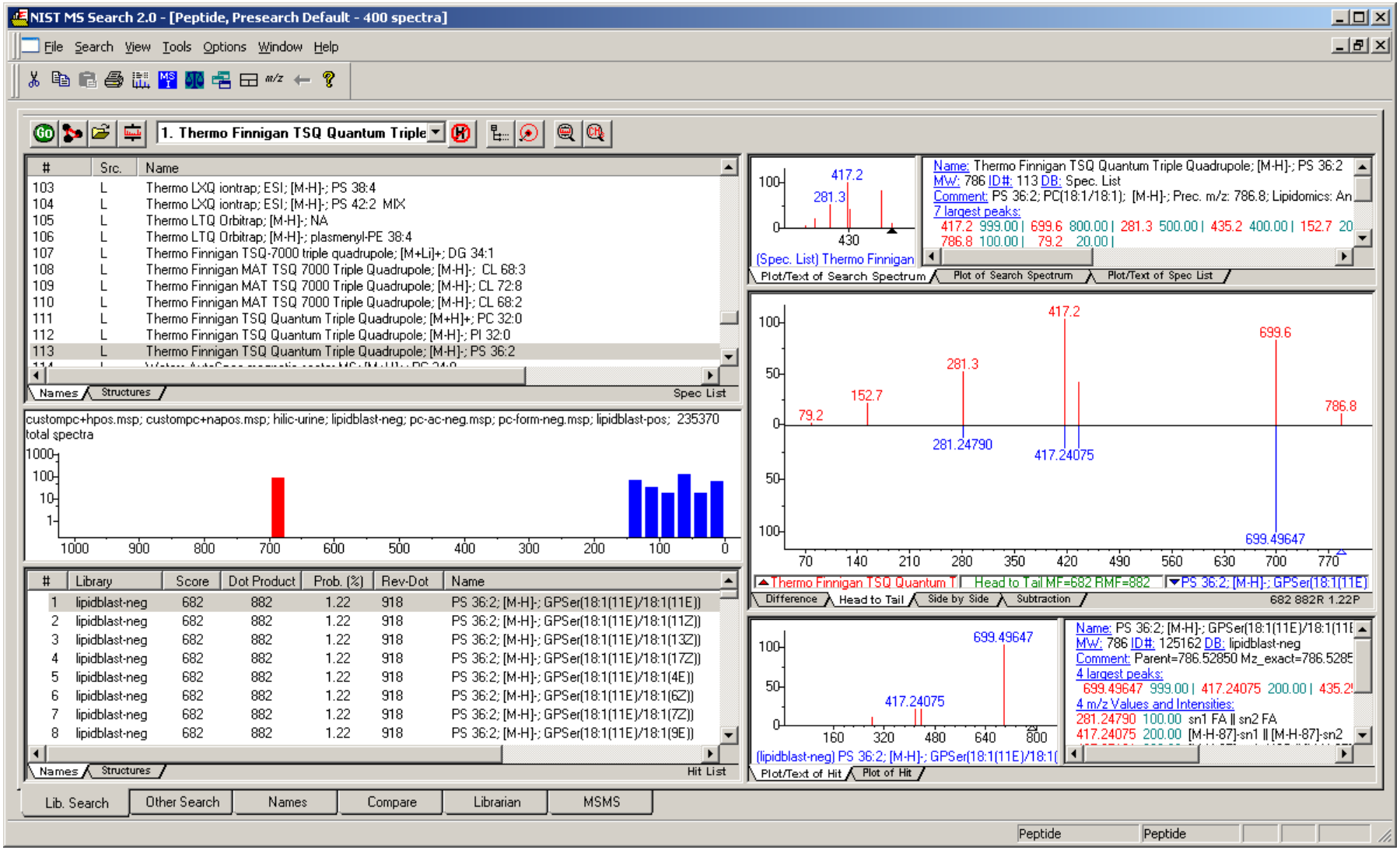
Name: Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H]+; PC 32:0
MW: 734 ID#: 111 DB: Spec. List
Comment: PC 32:0; PC(16:0/16:0); [M-H]-; Prec. m/z: 734.8; Lipidomics: An analysis of cellular lipids by ESI-MS; Stephen Milne, Pavlina Ivanova, JeVrey Forrester, H. Alex Brown; Methods 39 (2006) 92-103
6 largest peaks:



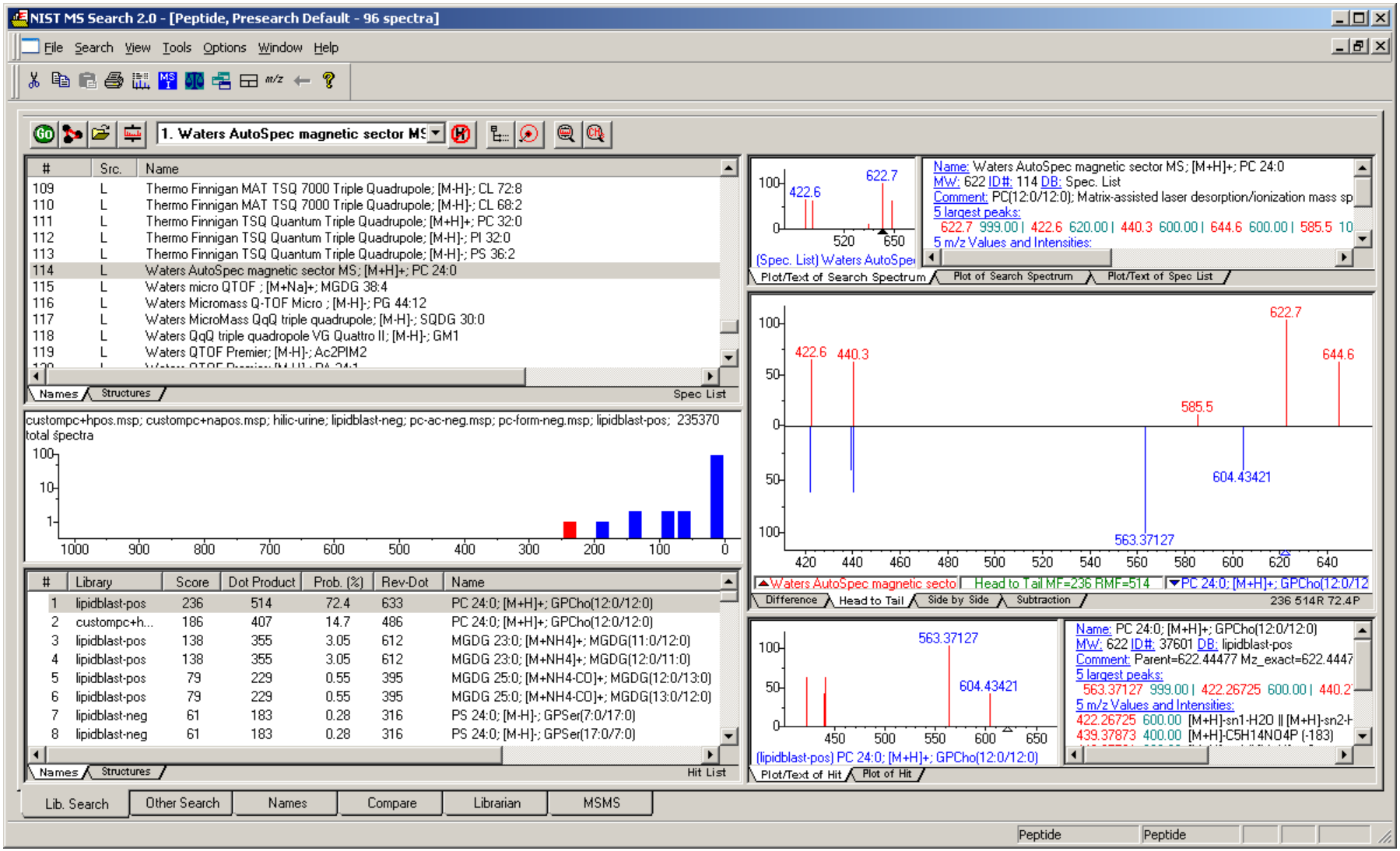
Name: Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H]-; PI 32:0
MW: 809 ID#: 112 DB: Spec. List
Comment: PI 32:0; PI(16:0/16:0); [M-H]-; Prec. m/z: 809.7; Lipidomics: An analysis of cellular lipids by ESI-MS; Stephen Milne, Pavlina Ivanova, JeVrey Forrester, H. Alex Brown; Methods 39 (2006) 92-103
10 largest peaks



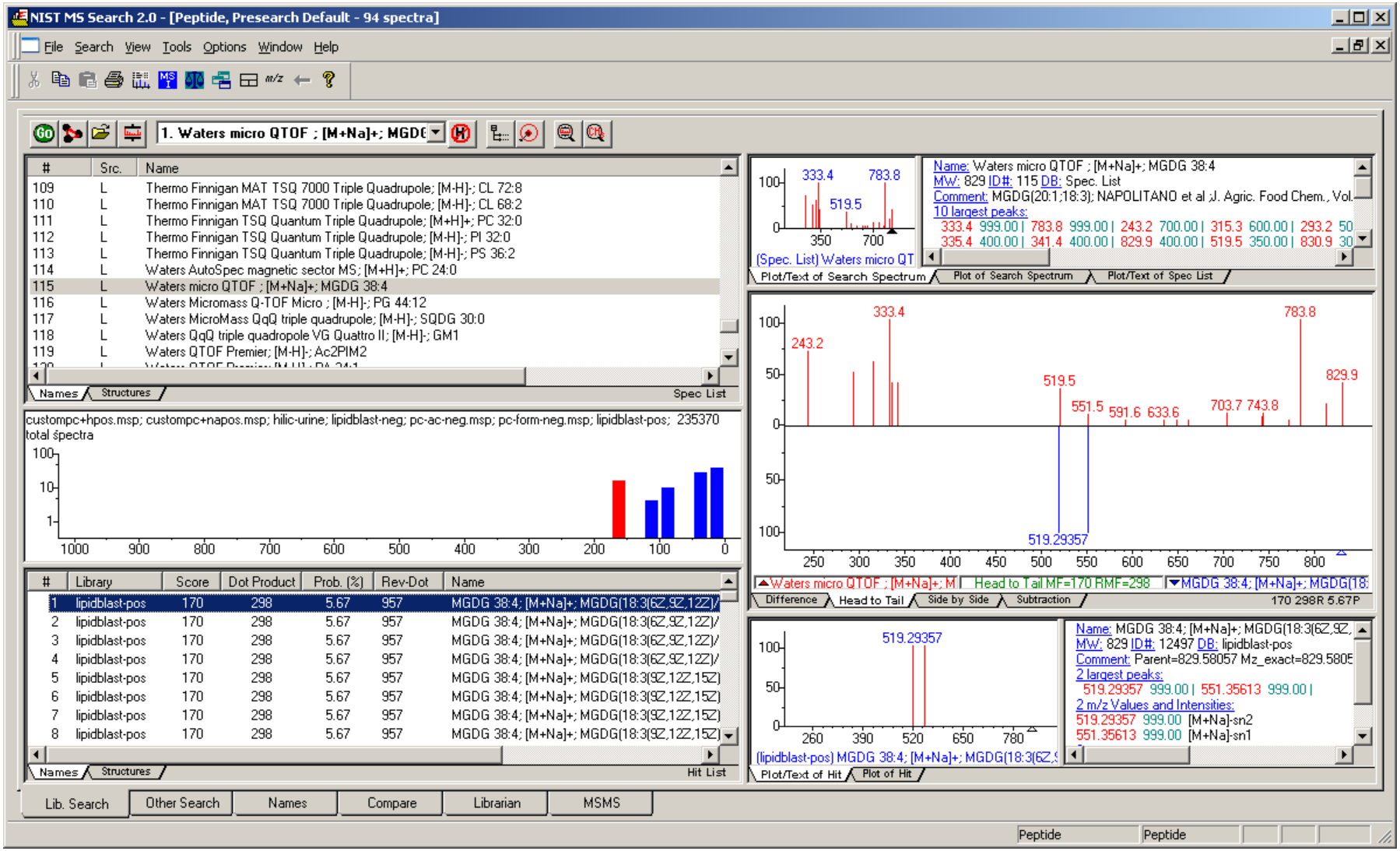
Name: Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H]-; PS 36:2
MW: 786 ID#: 113 DB: Spec. List
Comment: PS 36:2; PC(18:1/18:1); [M-H]-; Prec. m/z: 786.8; Lipidomics: An analysis of cellular lipids by ESI-MS; Stephen Milne, Pavlina Ivanova, JeVrey Forrester, H. Alex Brown; Methods 39 (2006) 92-103
7 largest peaks:



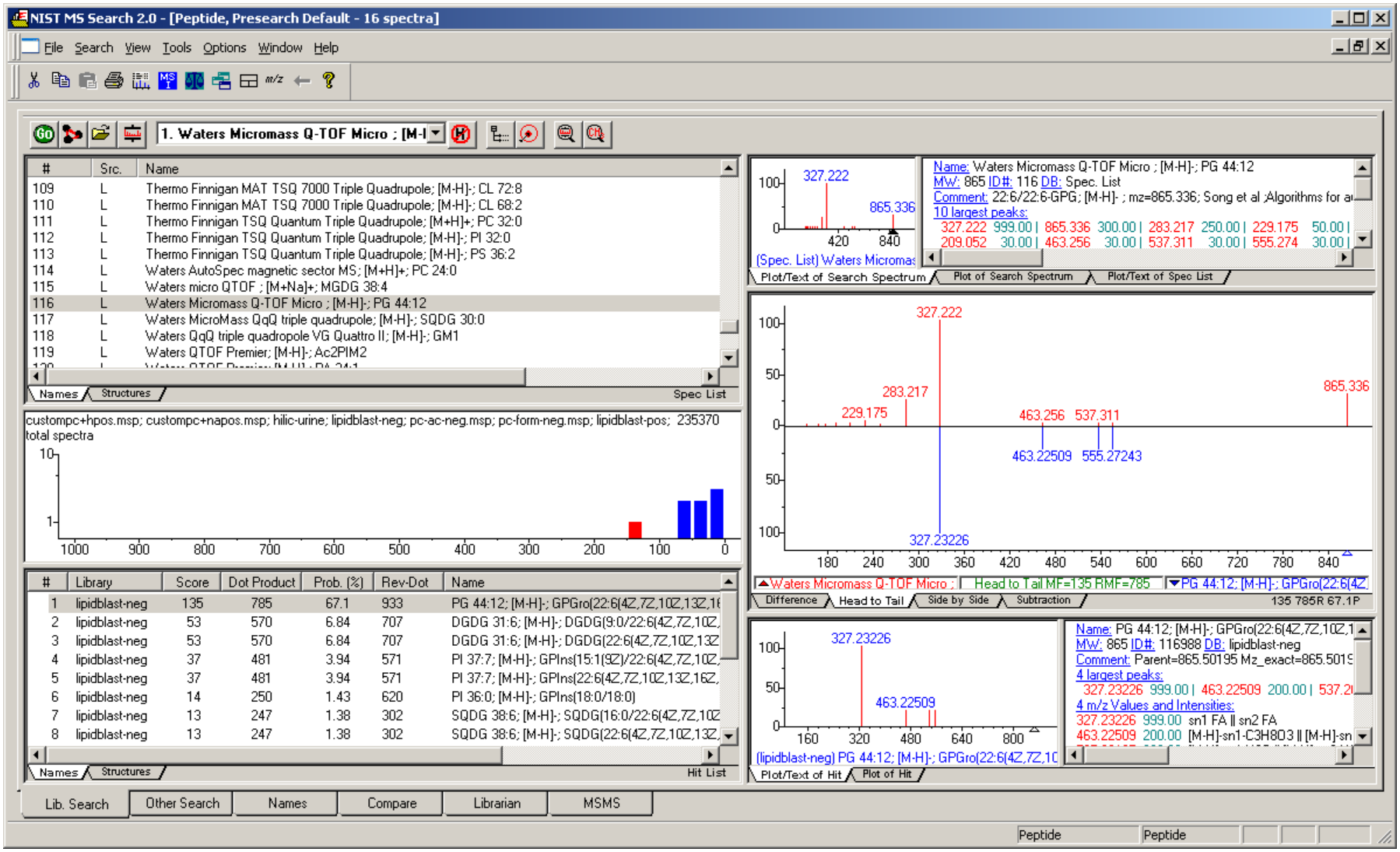
Name: Waters AutoSpec magnetic sector MS; [M+H]+; PC 24:0
MW: 622 ID#: 114 DB: Spec. List
Comment: PC(12:0/12:0); Matrix-assisted laser desorption/ionization mass spectrometry of phospholipids; D. J. Harvey; Journal of Mass Spectrometry, Volume 30, Issue 9 (p 1333-1346)
5 largest peaks:



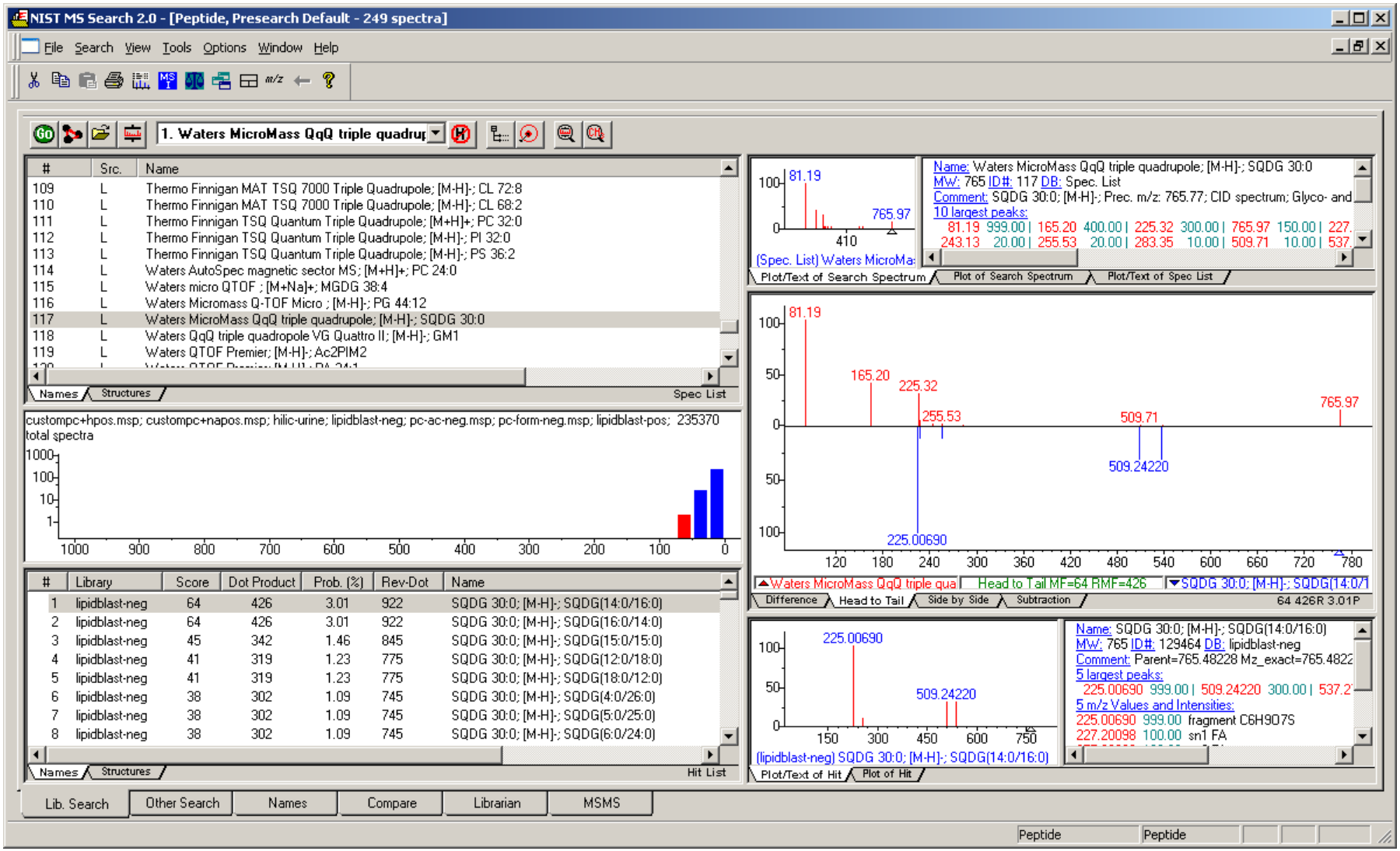
Name: Waters micro QTOF ; [M+Na]+; MGDG 38:4
MW: 829 ID#: 115 DB: Spec. List
Comment: MGDG(20:1;18:3); NAPOLITANO et al ;J. Agric. Food Chem., Vol. 55, No. 25, 2007; Novel Galactolipids from the Leaves of Ipomoea batatas L.: Characterization by Liquid Chromatography Coupled with Electrospray IonizationQuadrupole Time-of-Flight Tandem Mass Spectrometry
10 largest peaks:



Name: Waters Micromass Q-TOF Micro ; [M-H]-; PG 44:12
MW: 865 ID#: 116 DB: Spec. List
Comment: 22:6/22:6-GPG; [M-H]- ; mz=865.336; Song et al ;Algorithms for automatic processing of data from mass spectrometric analyses of lipids; Journal of chromatography. B, Analytical technologies in the biomedical and life sciences [1570-0232] Song (2009) volume: 877 issue: 26 page: 2847-2854
10 largest peaks:



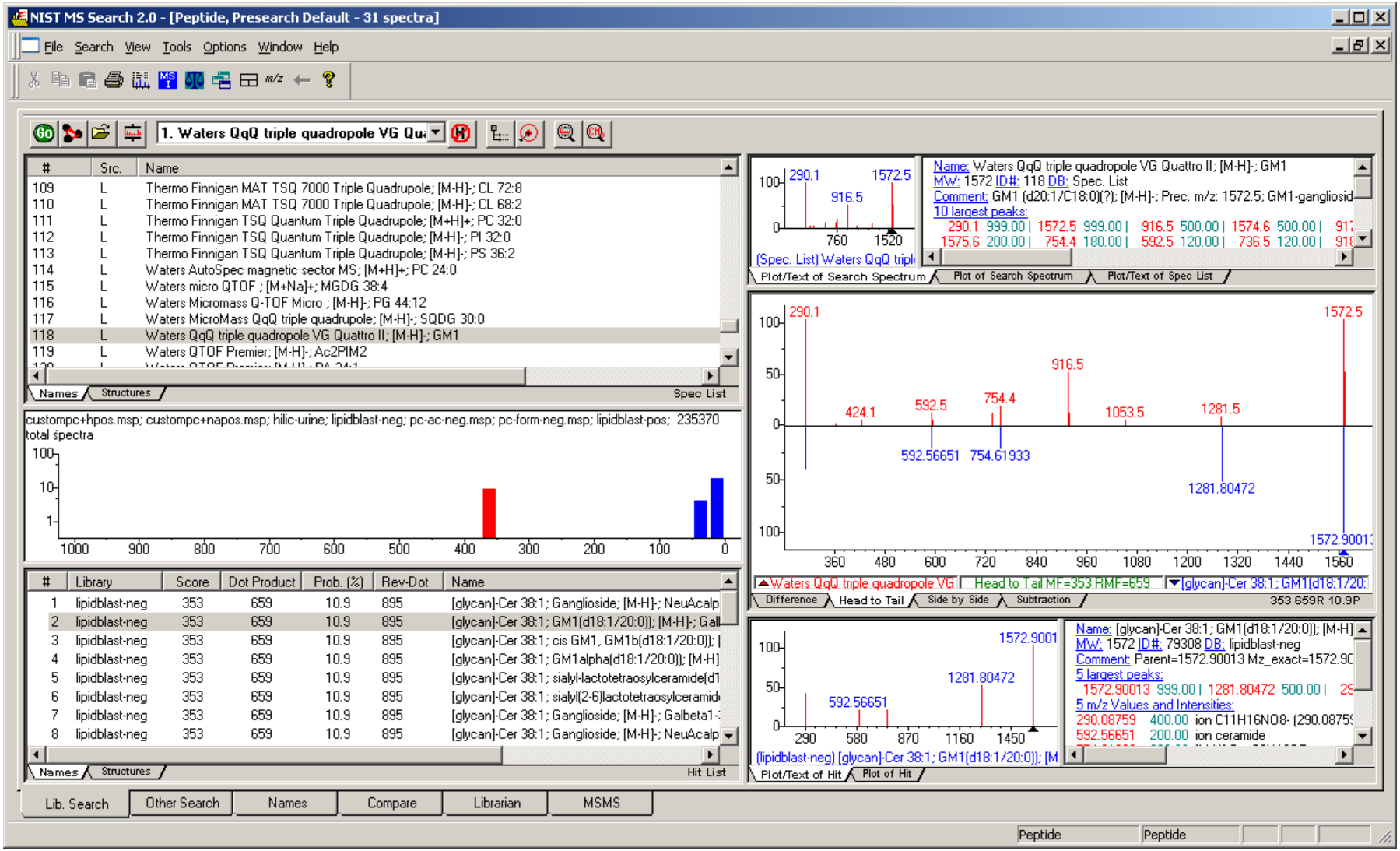
Name: Waters MicroMass QqQ triple quadrupole; [M-H]-; SQDG 30:0
MW: 765 ID#: 117 DB: Spec. List
Comment: SQDG 30:0; [M-H]-; Prec. m/z: 765.77; CID spectrum; Glyco- and sphingophosphonolipids from the medusa Phyllorhiza punctata: NMR and ESI-MS/MS fingerprints; http://dx.doi.org/10.1016/j.chemphyslip.2006.11.001
10 largest peaks:



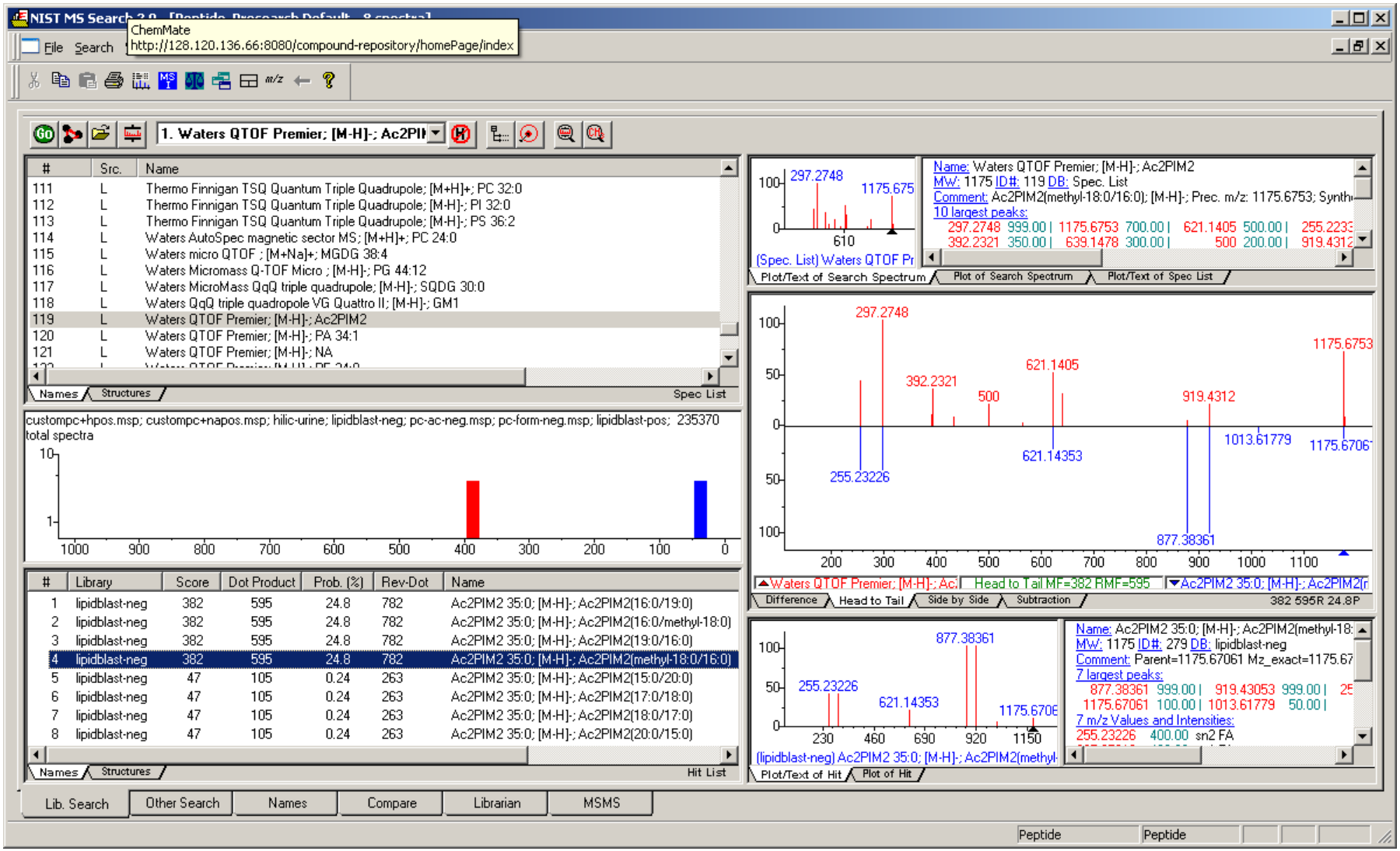
Name: Waters QqQ triple quadropole VG Quattro II; [M-H]-; GM1
MW: 1572 ID#: 118 DB: Spec. List
Comment: GM1 (d20:1/C18:0)(?); [M-H]-; Prec. m/z: 1572.5; GM1-gangliosidosis in a cross-bred dog confirmed by detection of GM1-ganglioside using electrospray ionisation-tandem mass spectrometry;DOI 10.1007/s004010000187
10 largest peaks:

Comment from Publication:
Purified bovine brain monosialoganglioside-GM1 consisting of GM1(d18:1–C18:0) and GM1 (d20:1–C18:0) was obtained from Sigma (Poole, UK).

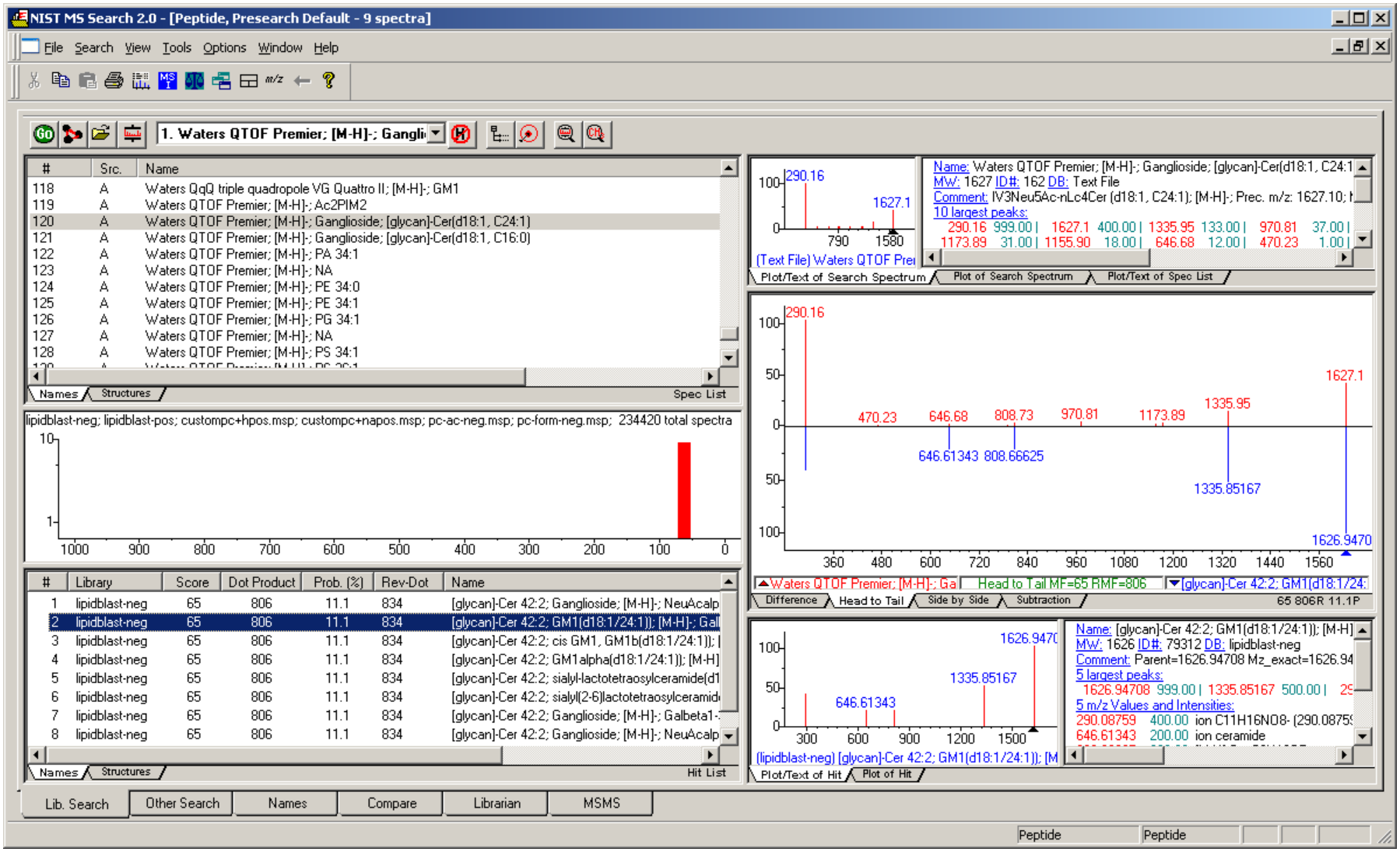
Also magnification (OCR) error possible



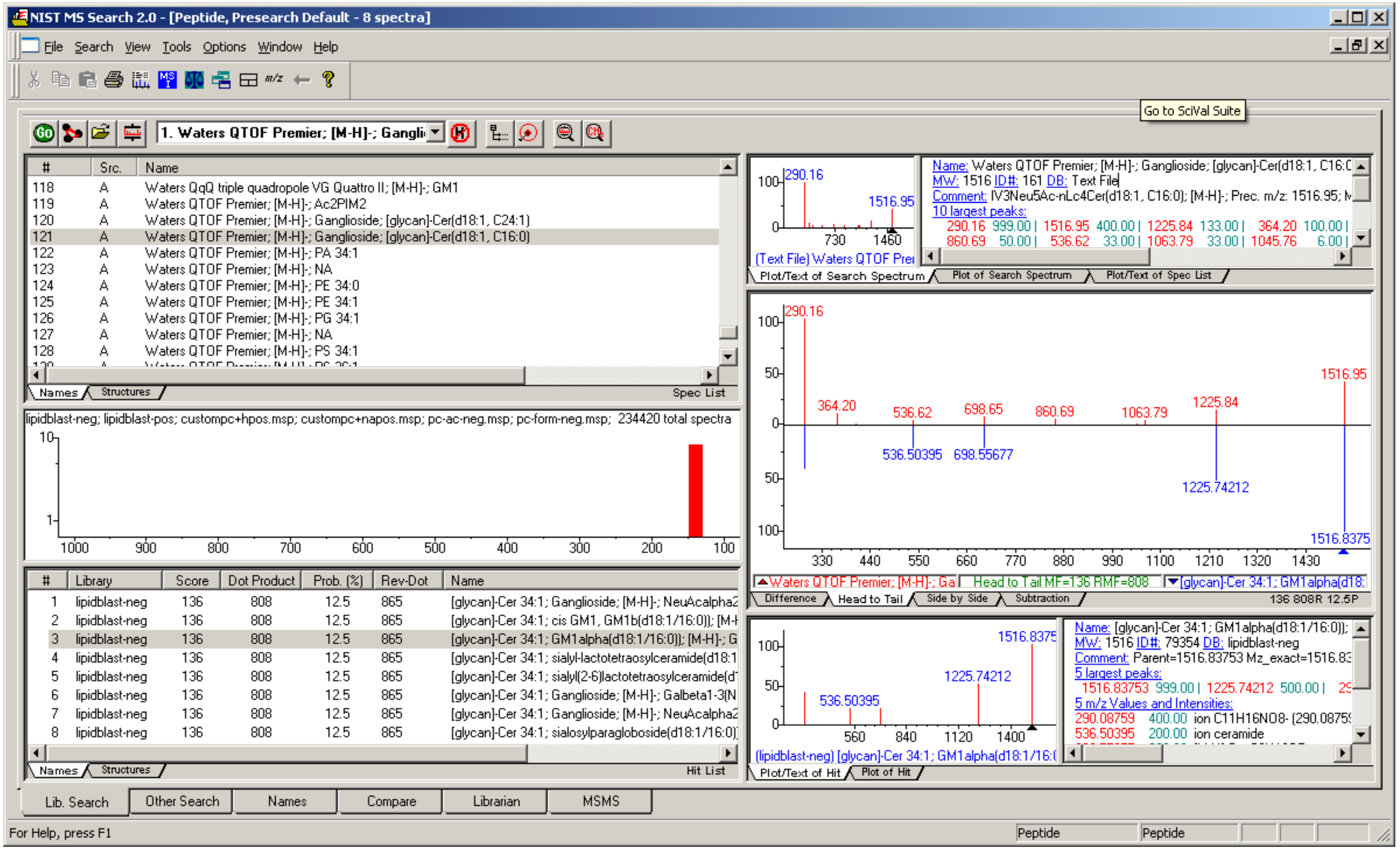
Name: Waters QTOF Premier; [M-H]-; Ac2PIM2
MW: 1175 ID#: 119 DB: Spec. List
Comment: Ac2PIM2(methyl-18:0/16:0); [M-H]-; Prec. m/z: 1175.6753; Synthesis and Structure of Phosphatidylinositol Dimannoside;J. Org. Chem., 2007, 72 (9), pp 3282-3288; 10.1021/jo0625599
10 largest peaks:



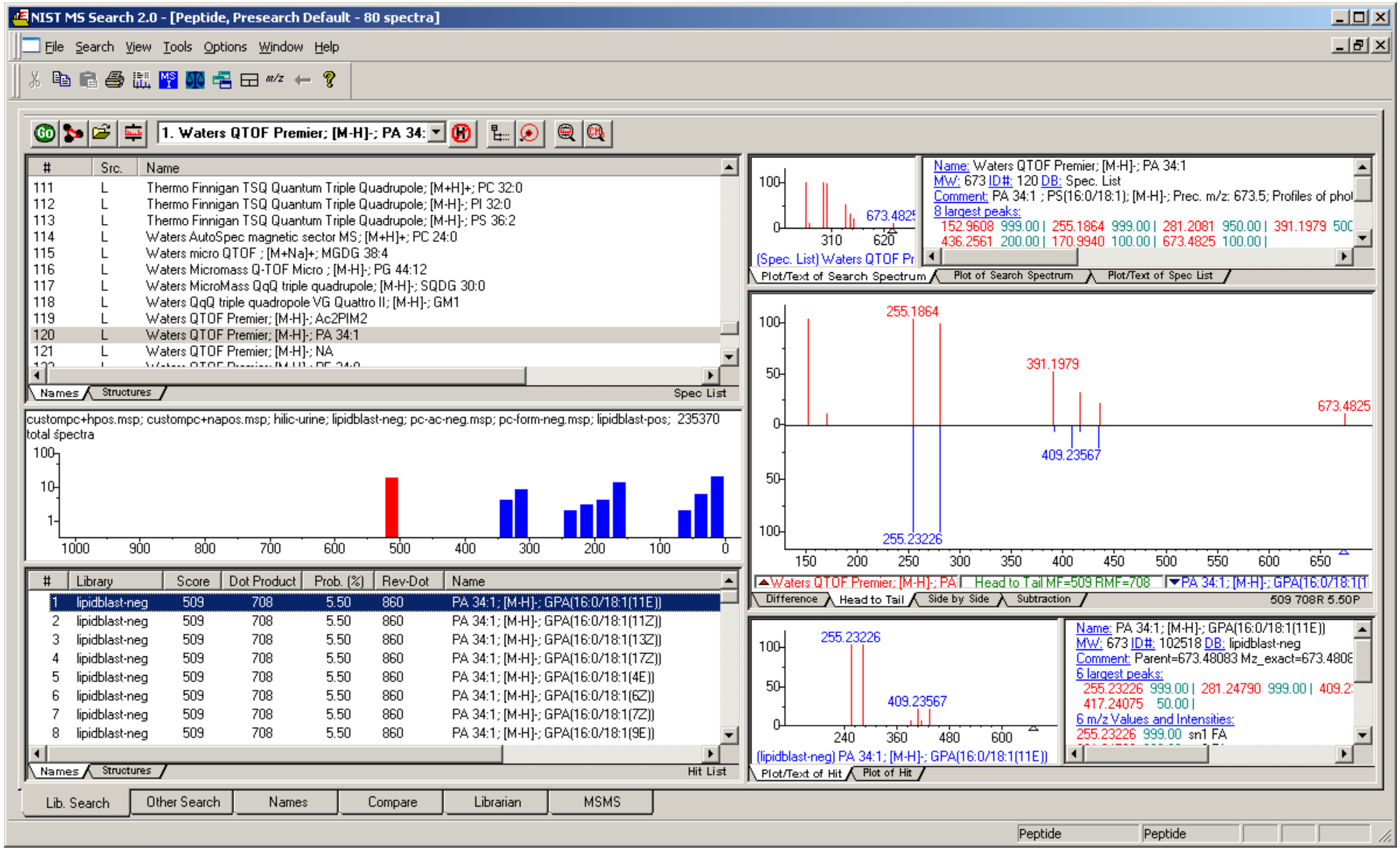
Name: Waters QTOF Premier; [M-H]-; Ganglioside; [glycan]-Cer(d18:1, C24:1)
MW: 1627 ID#: 162 DB: Text File
Comment: IV3Neu5Ac-nLc4Cer (d18:1, C24:1); [M-H]-; Prec. m/z: 1627.10; Mass Spectrometry ReviewsVolume 29, Issue 3, DOI:10.1002/mas.20253
10 largest peaks:



Name: Waters QTOF Premier; [M-H]-; Ganglioside; [glycan]-Cer(d18:1, C16:0)
MW: 1516 ID#: 161 DB: Text File
Comment: IV3Neu5Ac-nLc4Cer(d18:1, C16:0); [M-H]-; Prec. m/z: 1516.95; Mass Spectrometry ReviewsVolume 29, Issue 3, DOI:10.1002/mas.20253
10 largest peaks:

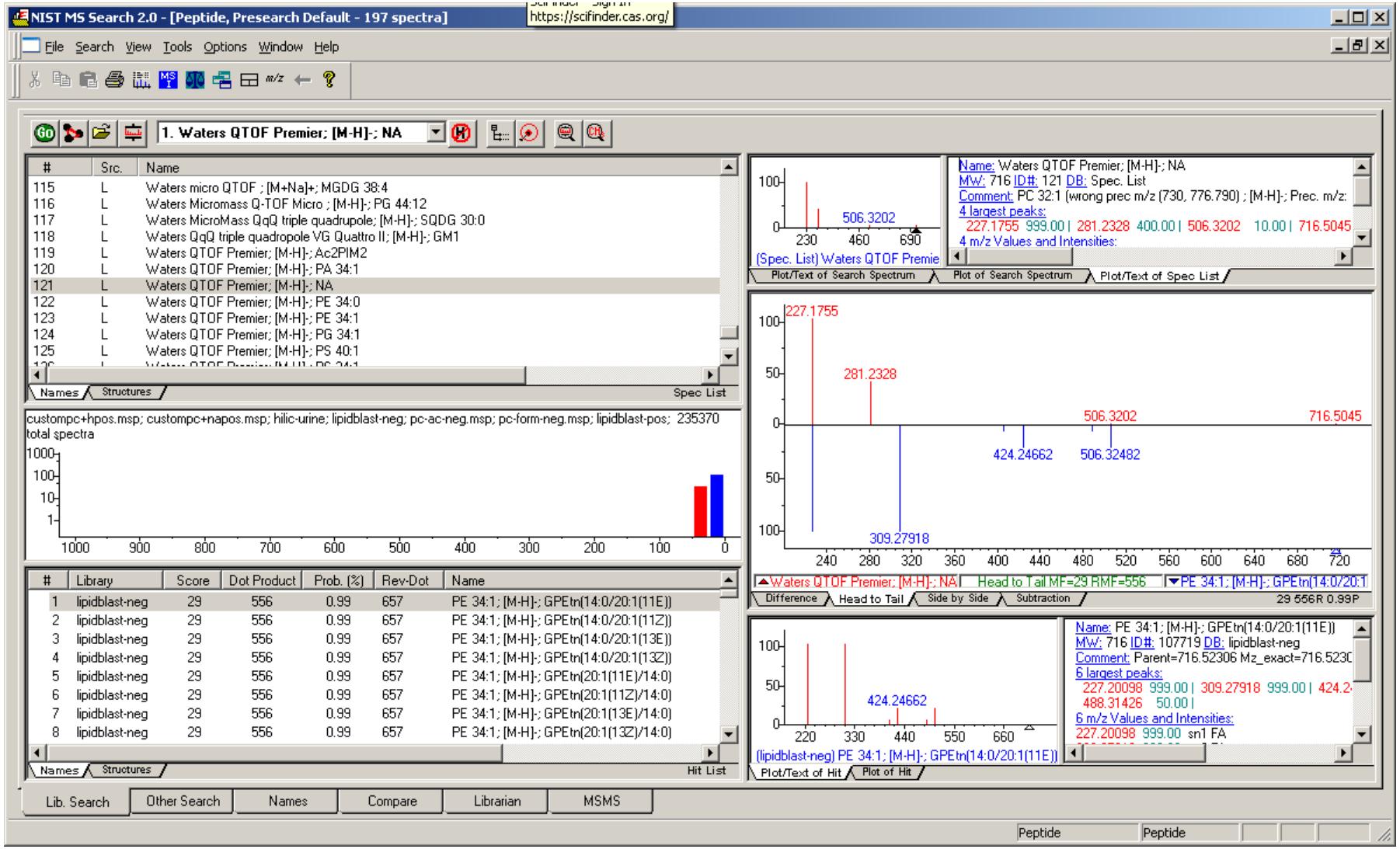


Name: Waters QTOF Premier; [M-H]-; PA 34:1
MW: 673 ID#: 120 DB: Spec. List
Comment: PA 34:1 ; PS(16:0/18:1); [M-H]-; Prec. m/z: 673.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
8 largest peaks:

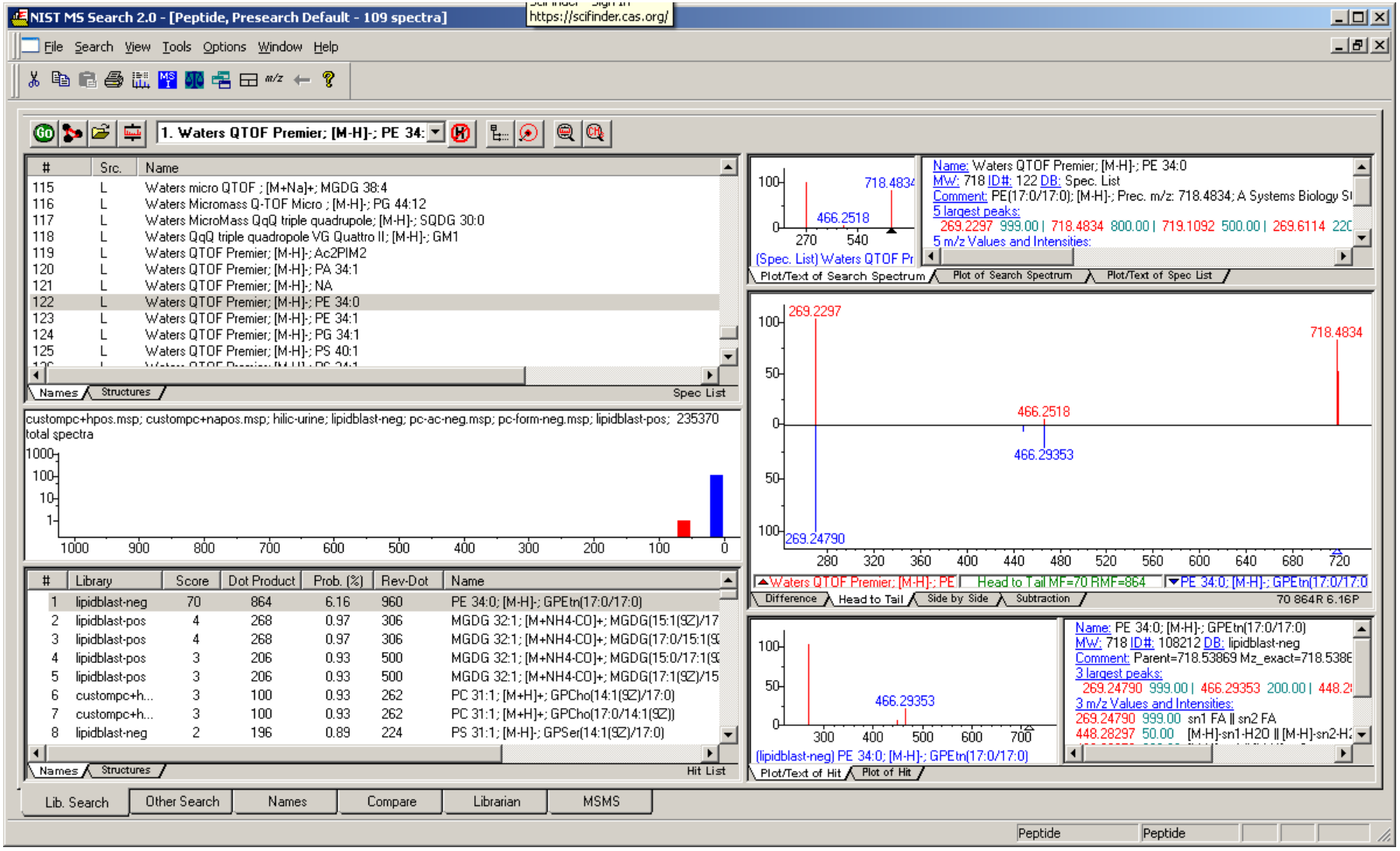


Name: Waters QTOF Premier; [M-H]-; NA
MW: 716 ID#: 121 DB: Spec. List
Comment: PC 32:1 (wrong prec m/z (730, 776.790) ; [M-H]-; Prec. m/z: 716.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
4 largest peaks:

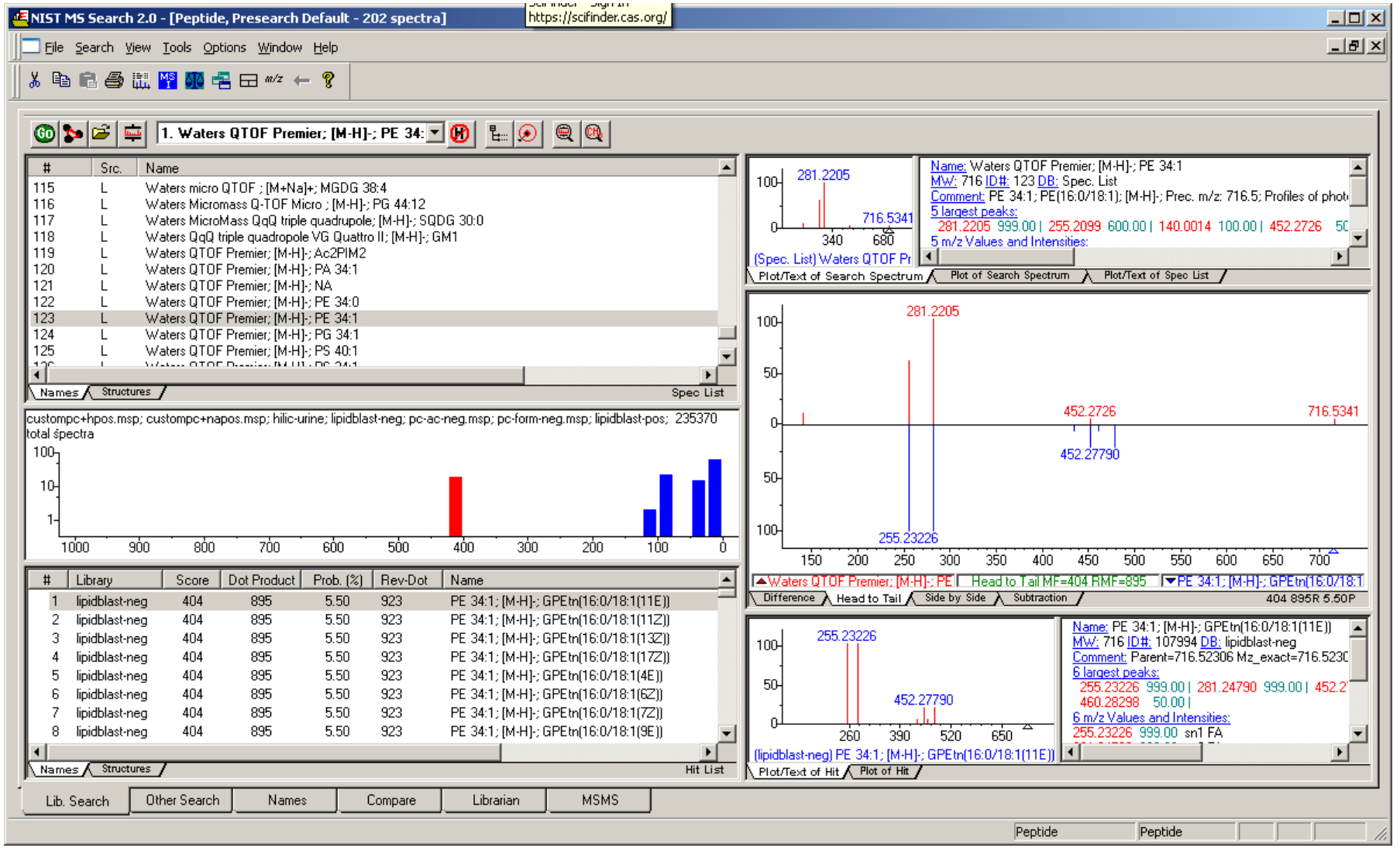
Wrong precursor, wrong ID, probably mixed spectrum



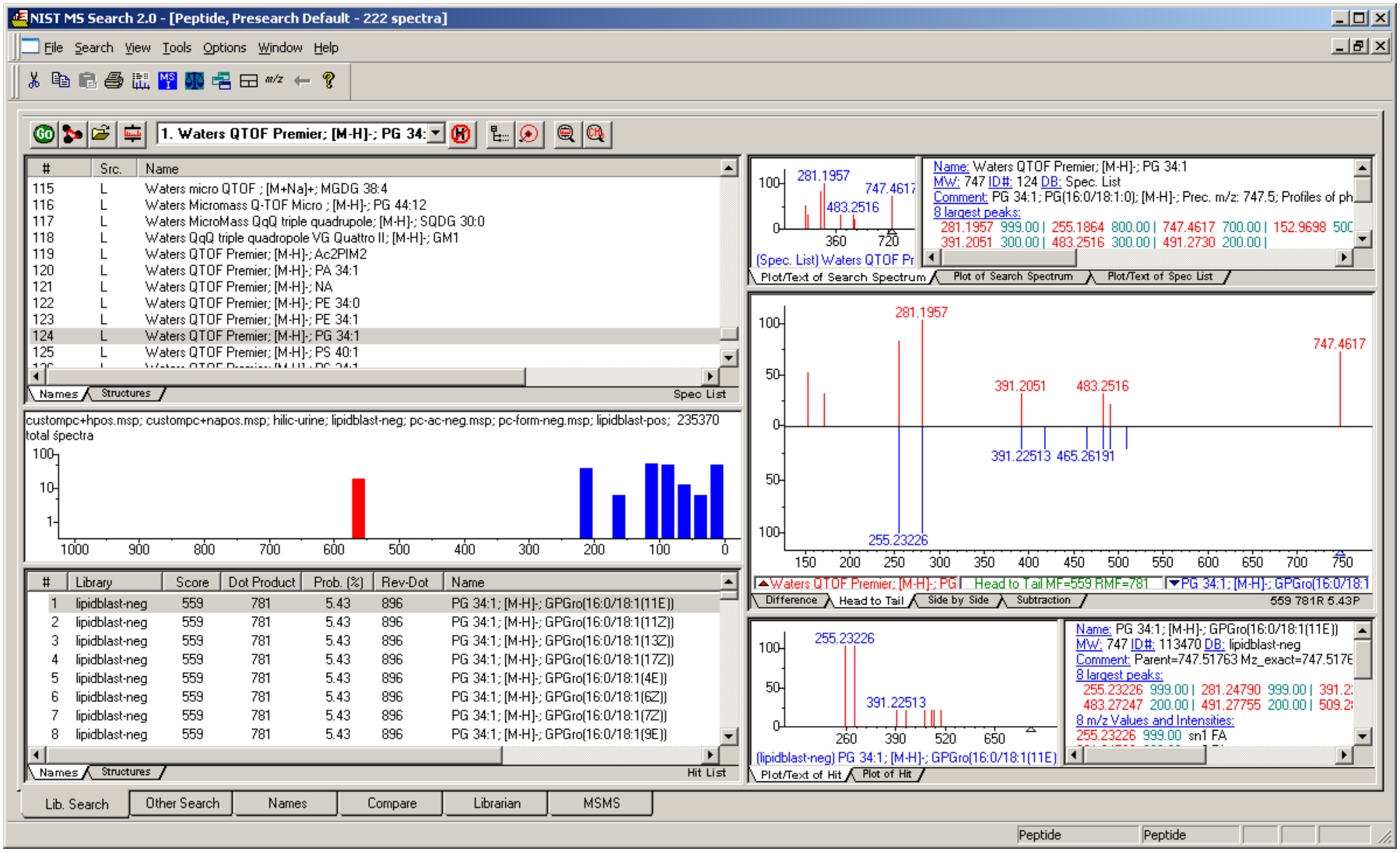
Name: Waters QTOF Premier; [M-H]-; PE 34:0
MW: 718 ID#: 122 DB: Spec. List
Comment: PE(17:0/17:0); [M-H]-; Prec. m/z: 718.4834; A Systems Biology Strategy Reveals Biological Pathways and Plasma Biomarker Candidates for Potentially Toxic Statin-Induced Changes in Muscle; 10.1371/journal.pone.0000097
5 largest peaks:



Name: Waters QTOF Premier; [M-H]-; PE 34:1
MW: 716 ID#: 123 DB: Spec. List
Comment: PE 34:1; PE(16:0/18:1); [M-H]-; Prec. m/z: 716.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
5 largest peaks:

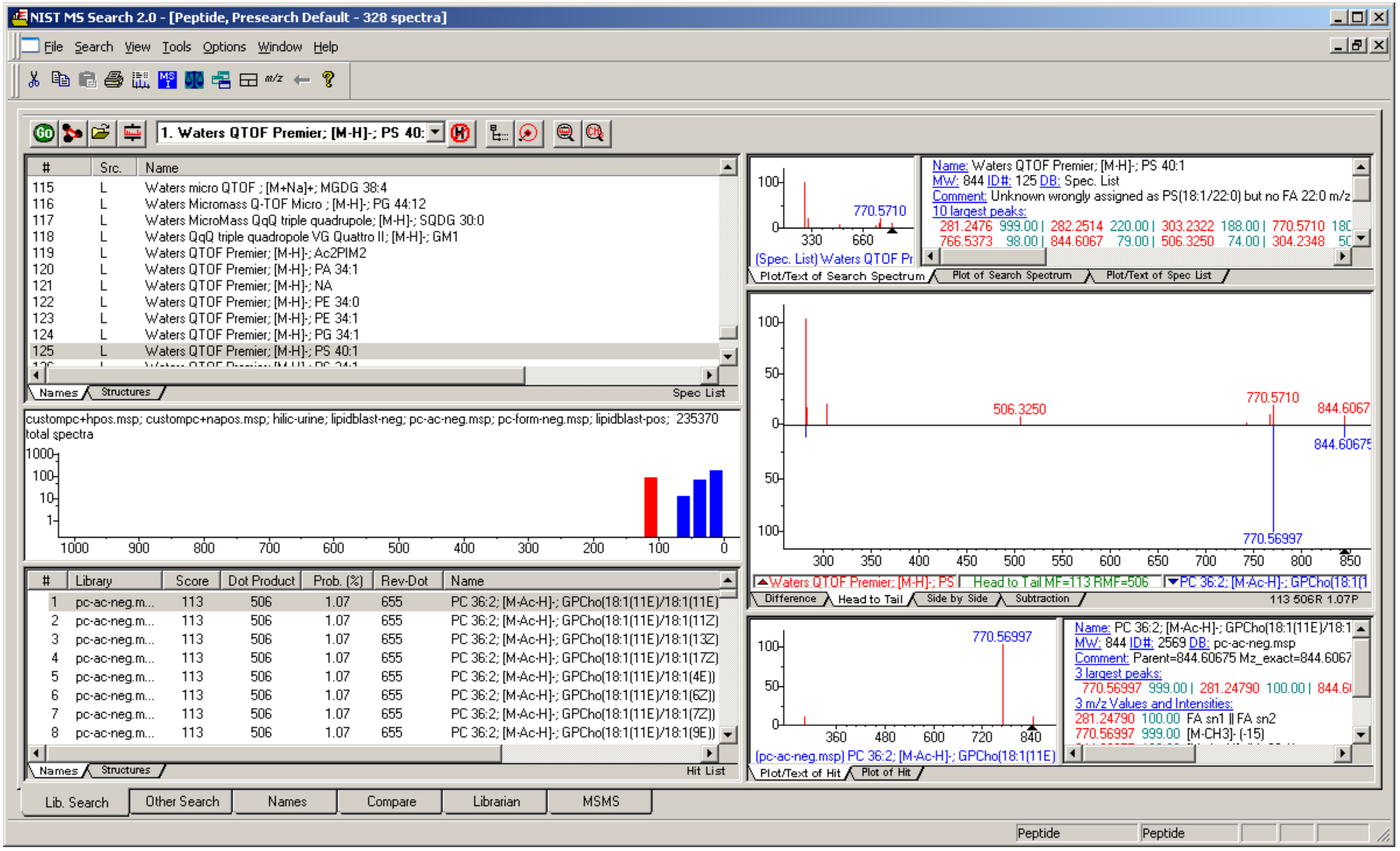


Name: Waters QTOF Premier; [M-H]-; PG 34:1
MW: 747 ID#: 124 DB: Spec. List
Comment: PG 34:1; PG(16:0/18:1:0); [M-H]-; Prec. m/z: 747.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
8 largest peaks:

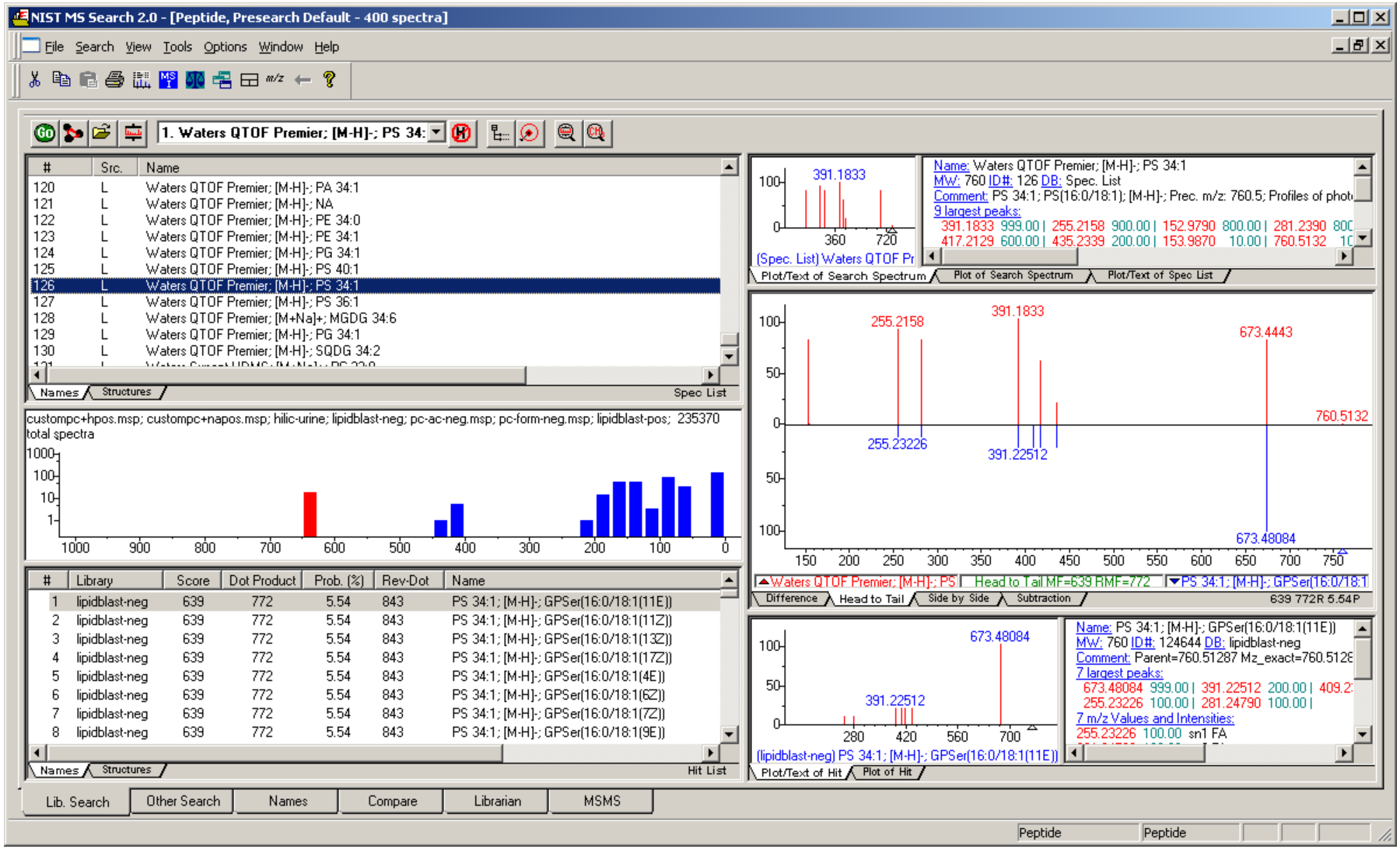


Name: Waters QTOF Premier; [M-H]-; PS 40:1
MW: 844 ID#: 125 DB: Spec. List
Comment: Unknown wrongly assigned as PS(18:1/22:0) but no FA 22:0 m/z 339.3; [M-H]-; Prec. m/z: 844.6063; RT: 9.71 min; Lipidomics: Study of Total Phospholipids in Immortalized Liver Cells Exposed to Different Fatty Acid Substrates: Pagliasotti,Prenni,Ryan,Rainville,Baker; 720001756EN;
10 largest peaks:

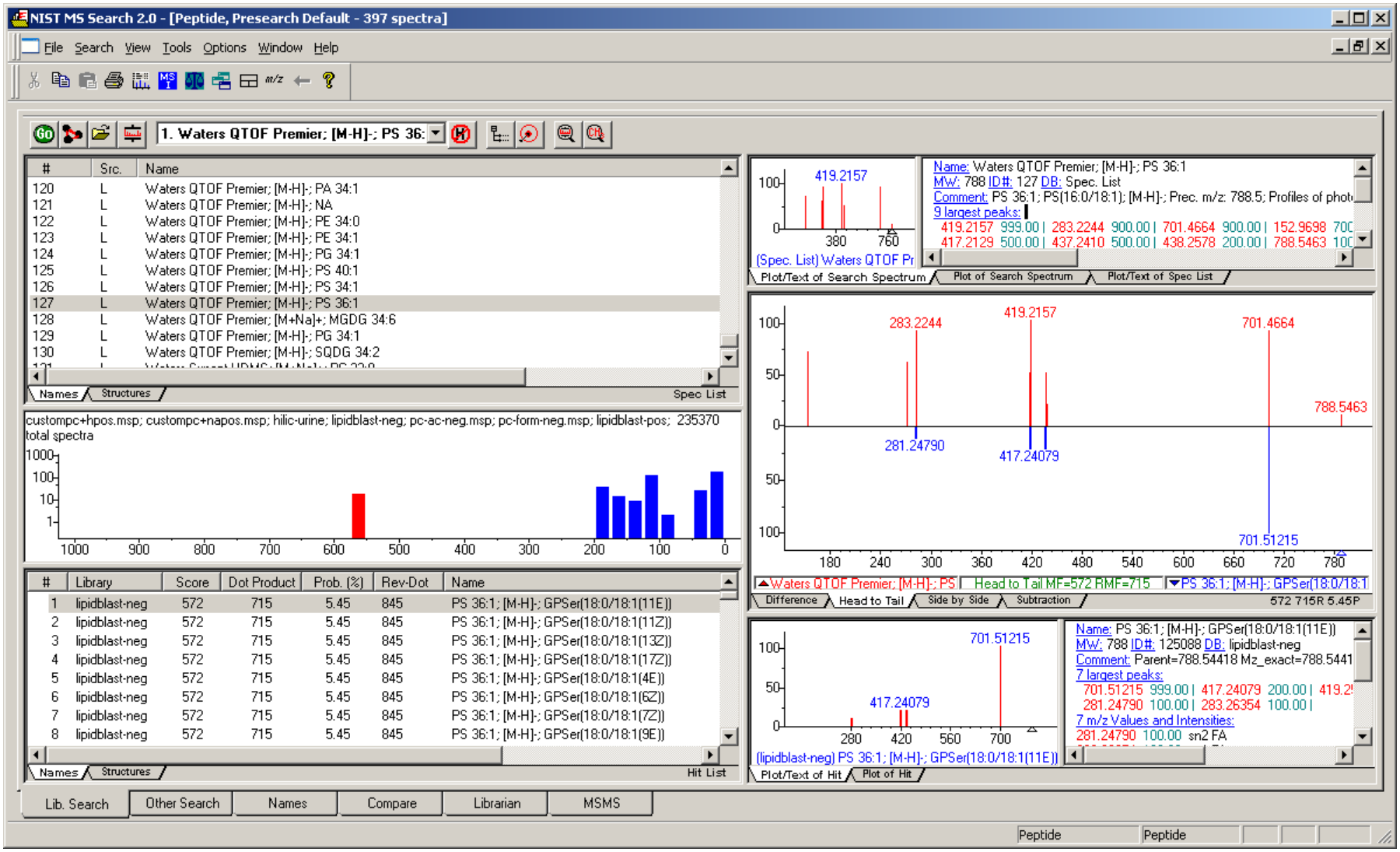
Unknown wrongly assigned FA missing



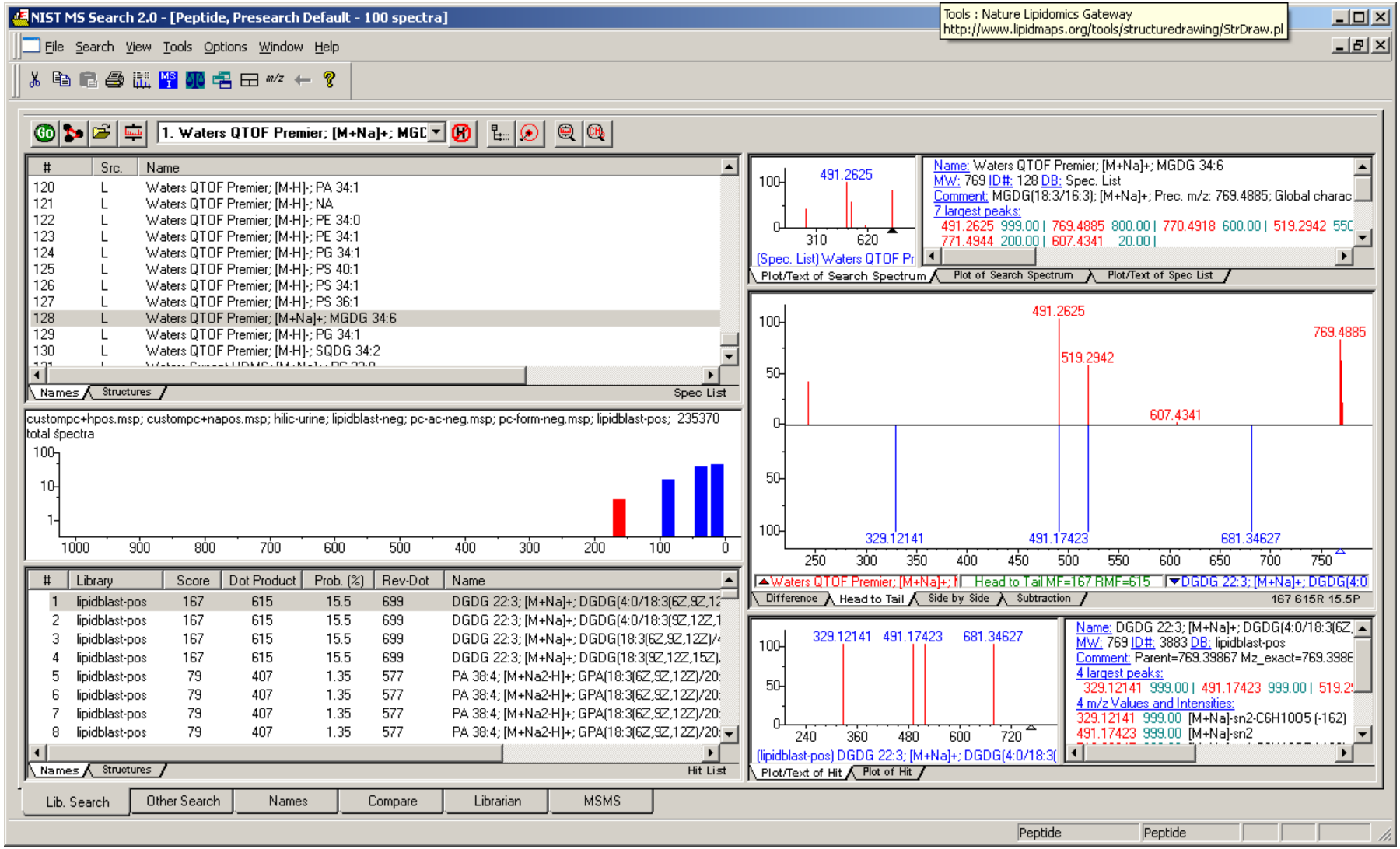
Name: Waters QTOF Premier; [M-H]-; PS 34:1
MW: 760 ID#: 126 DB: Spec. List
Comment: PS 34:1; PS(16:0/18:1); [M-H]-; Prec. m/z: 760.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
9 largest peaks:



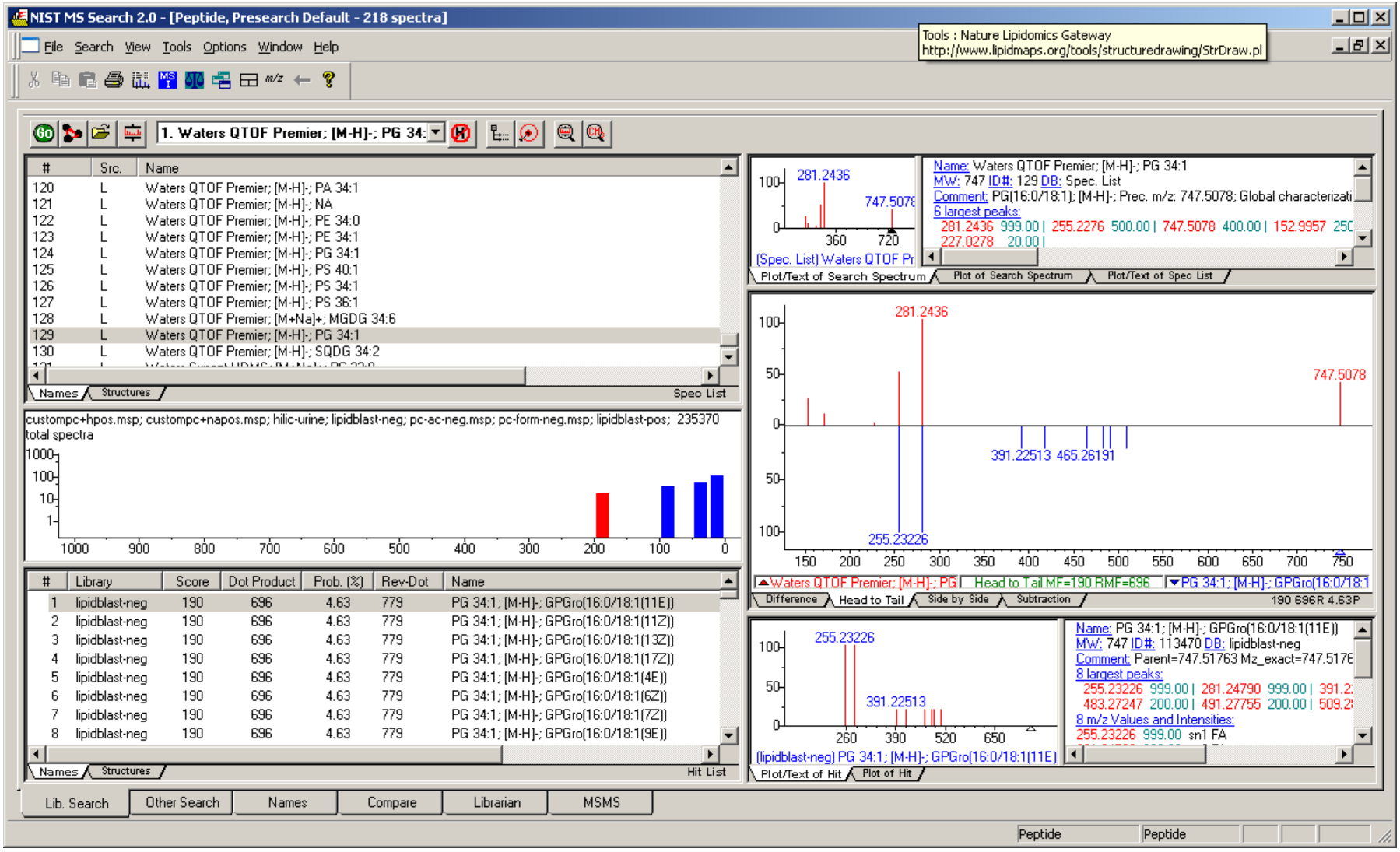
Name: Waters QTOF Premier; [M-H]-; PS 36:1
MW: 788 ID#: 127 DB: Spec. List
Comment: PS 36:1; PS(16:0/18:1); [M-H]-; Prec. m/z: 788.5; Profiles of photosynthetic glycerolipids in three strains of Skeletonema determined by UPLC-Q-TOF-MS; Journal of Applied Phycology; DOI: 10.1007/s10811-010-9553-3
9 largest peaks:



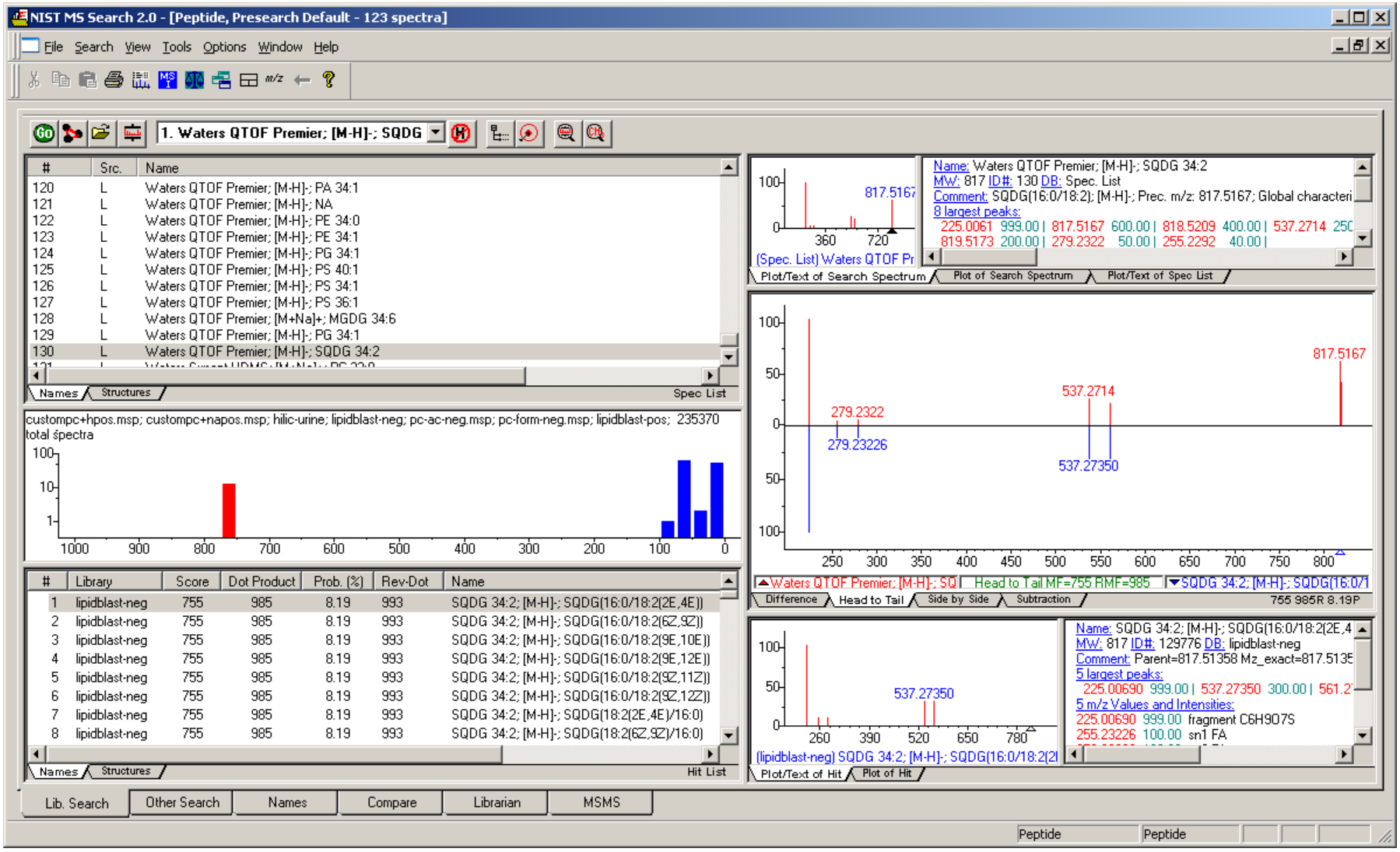
Name: Waters QTOF Premier; [M+Na]+; MGDG 34:6
MW: 769 ID#: 128 DB: Spec. List
Comment: MGDG(18:3/16:3); [M+Na]+; Prec. m/z: 769.4885; Global characterization of the photosynthetic glycerolipids from a marine diatom Stephanodiscus sp. by ultra performance liquid chromatography coupled with electrospray ionization-quadrupole-time of flight mass spectrometry ;http://dx.doi.org/10.1016/j.aca.2010.01.026
7 largest peaks:



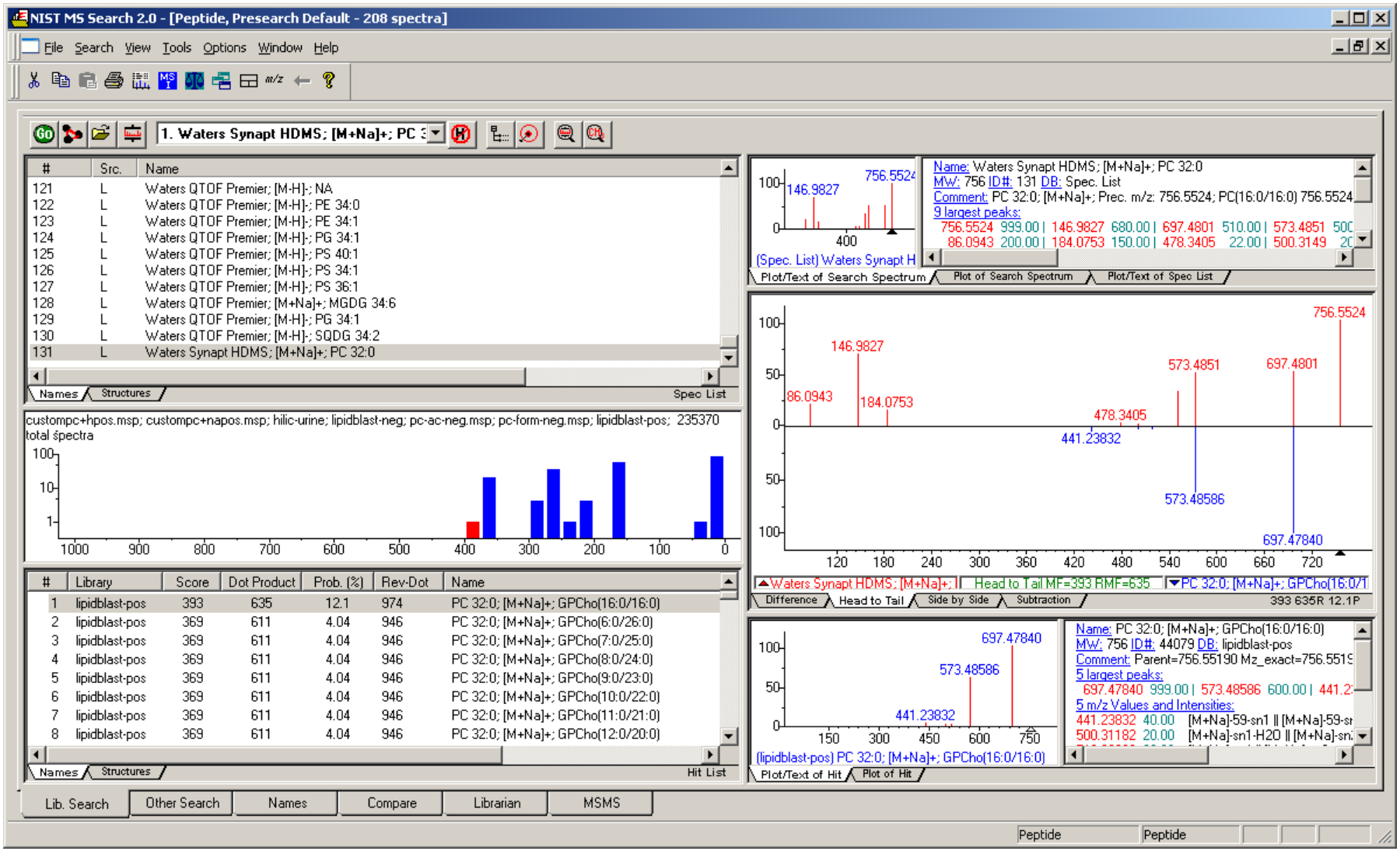
Name: Waters QTOF Premier; [M-H]-; PG 34:1
MW: 747 ID#: 129 DB: Spec. List
Comment: PG(16:0/18:1); [M-H]-; Prec. m/z: 747.5078; Global characterization of the photosynthetic glycerolipids from a marine diatom Stephanodiscus sp. by ultra performance liquid chromatography coupled with electrospray ionization-quadrupole-time of flight mass spectrometry ;http://dx.doi.org/10.1016/j.aca.2010.01.026
6 largest peaks:



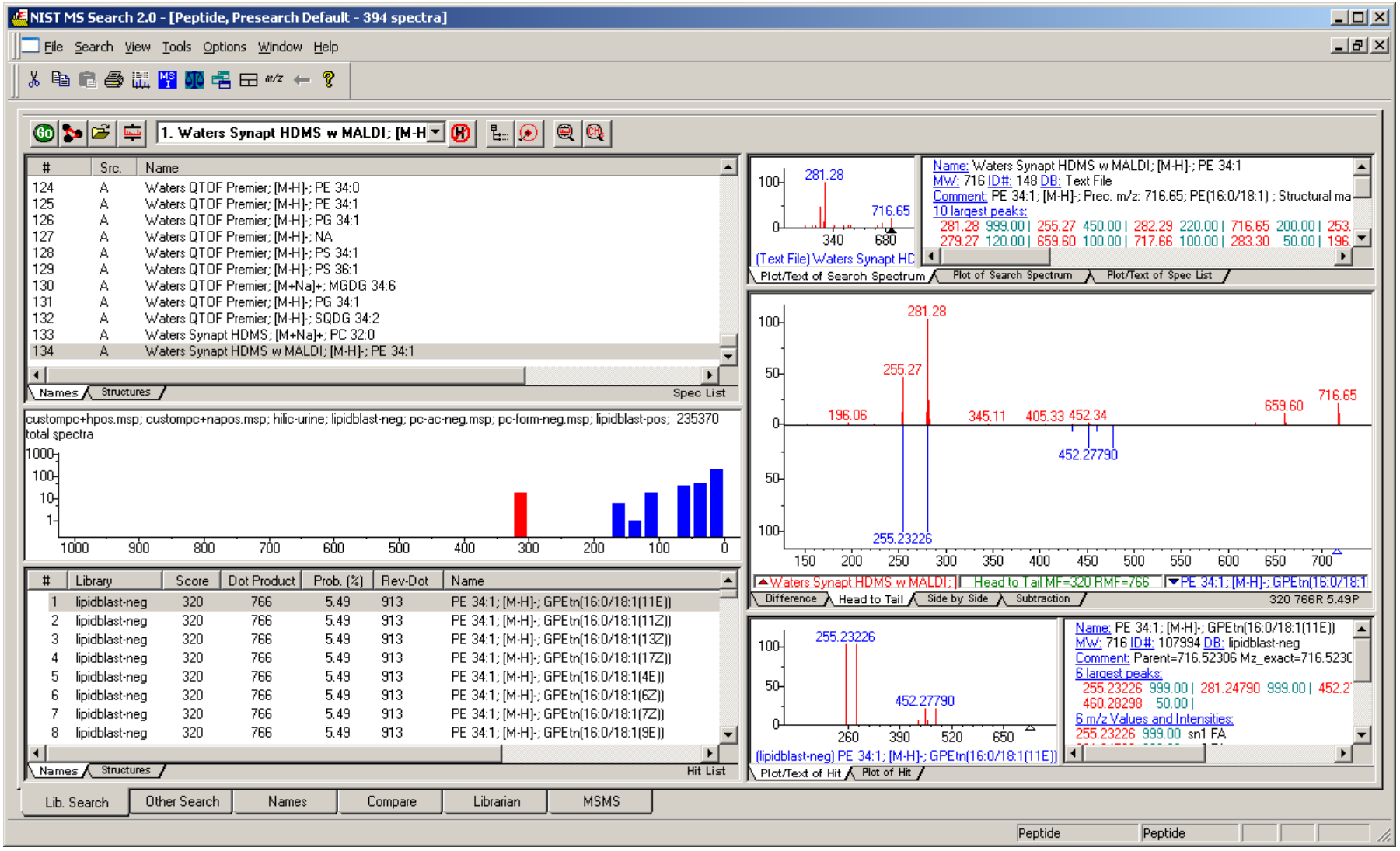
Name: Waters QTOF Premier; [M-H]-; SQDG 34:2
MW: 817 ID#: 130 DB: Spec. List
Comment: SQDG(16:0/18:2); [M-H]-; Prec. m/z: 817.5167; Global characterization of the photosynthetic glycerolipids from a marine diatom Stephanodiscus sp. by ultra performance liquid chromatography coupled with electrospray ionization-quadrupole-time of flight mass spectrometry ;http://dx.doi.org/10.1016/j.aca.2010.01.026
8 largest peaks



Name: Waters Synapt HDMS; [M+Na]+; PC 32:0
MW: 756 ID#: 131 DB: Spec. List
Comment: PC 32:0; [M+Na]+; Prec. m/z: 756.5524; PC(16:0/16:0) 756.5524; Direct Tissue Imaging and Characterization of Phospholipids Using MALDI SYNAPT HDMS System; Emmanuelle Claude, Marten Snel, Therese McKenna, James Langridge; APNT10011751
9 largest peaks:



Name: Waters Synapt HDMS w MALDI; [M-H]-; PE 34:1
MW: 716 ID#: 148 DB: Text File
Comment: PE 34:1; [M-H]-; Prec. m/z: 716.65; PE(16:0/18:1) ; Structural mass spectrometry analysis of lipid changes in a Drosophila epilepsy model brain ; Michal Kliman, Niranjana Vijayakrishnan, Lily Wang, John T. Tapp, Kendal Broadie and John A. McLean;
DOI:10.1039/B927494D
10 largest peaks:



LipidBlast evaluation using Agilent 6530 QTOF-MS/MS spectra

Curator: Tobias Kind
Spectra: John K. Meissen and Brian DeFelice
PI: Oliver Fiehn
Date: Sept 2011

Spectra: LipidBlast
Molecule Images: Avanti Polar Lipids or Sigma

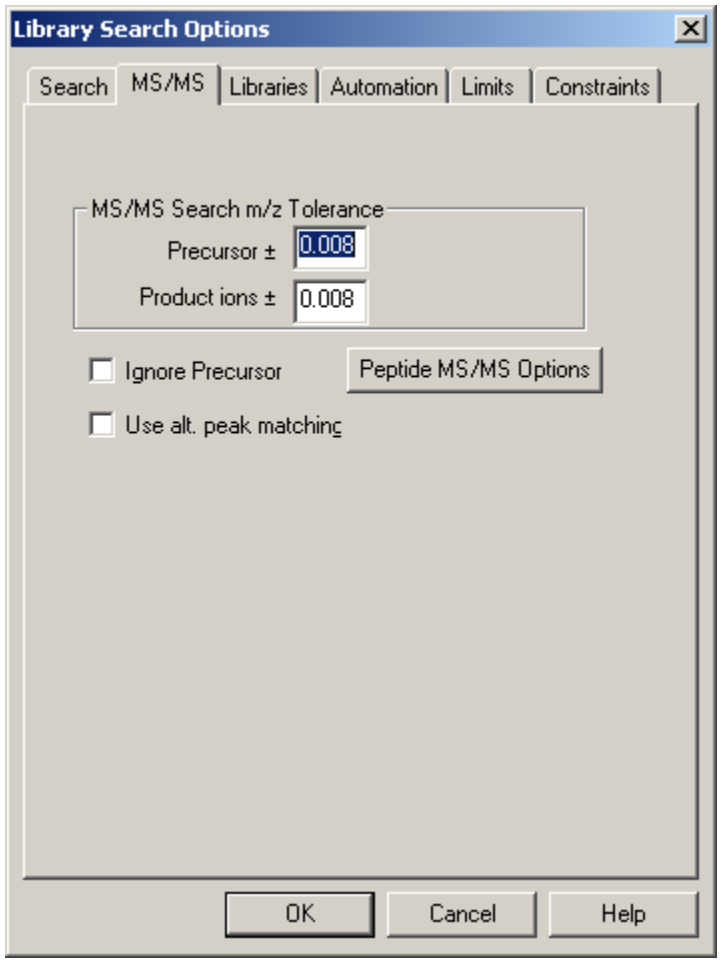
RAW MGF or MSP MS/MS spectra can be found under
http://fiehnlab.ucdavis.edu/projects/LipidBlast

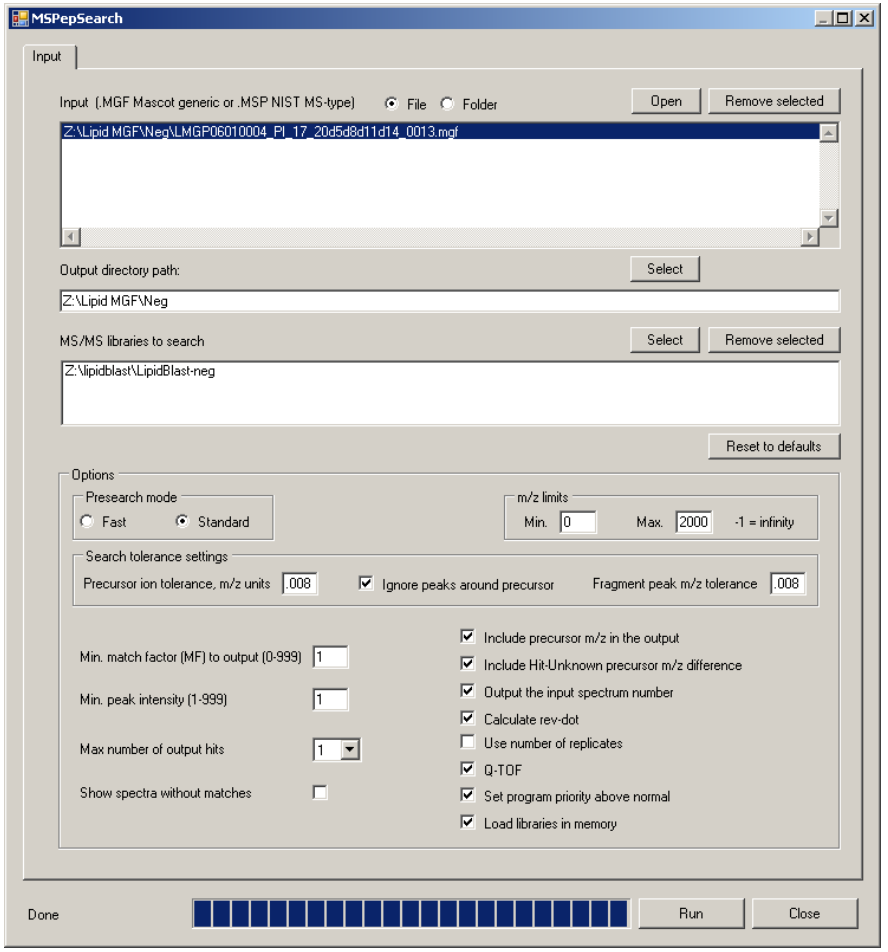
NIST MSPepSearch

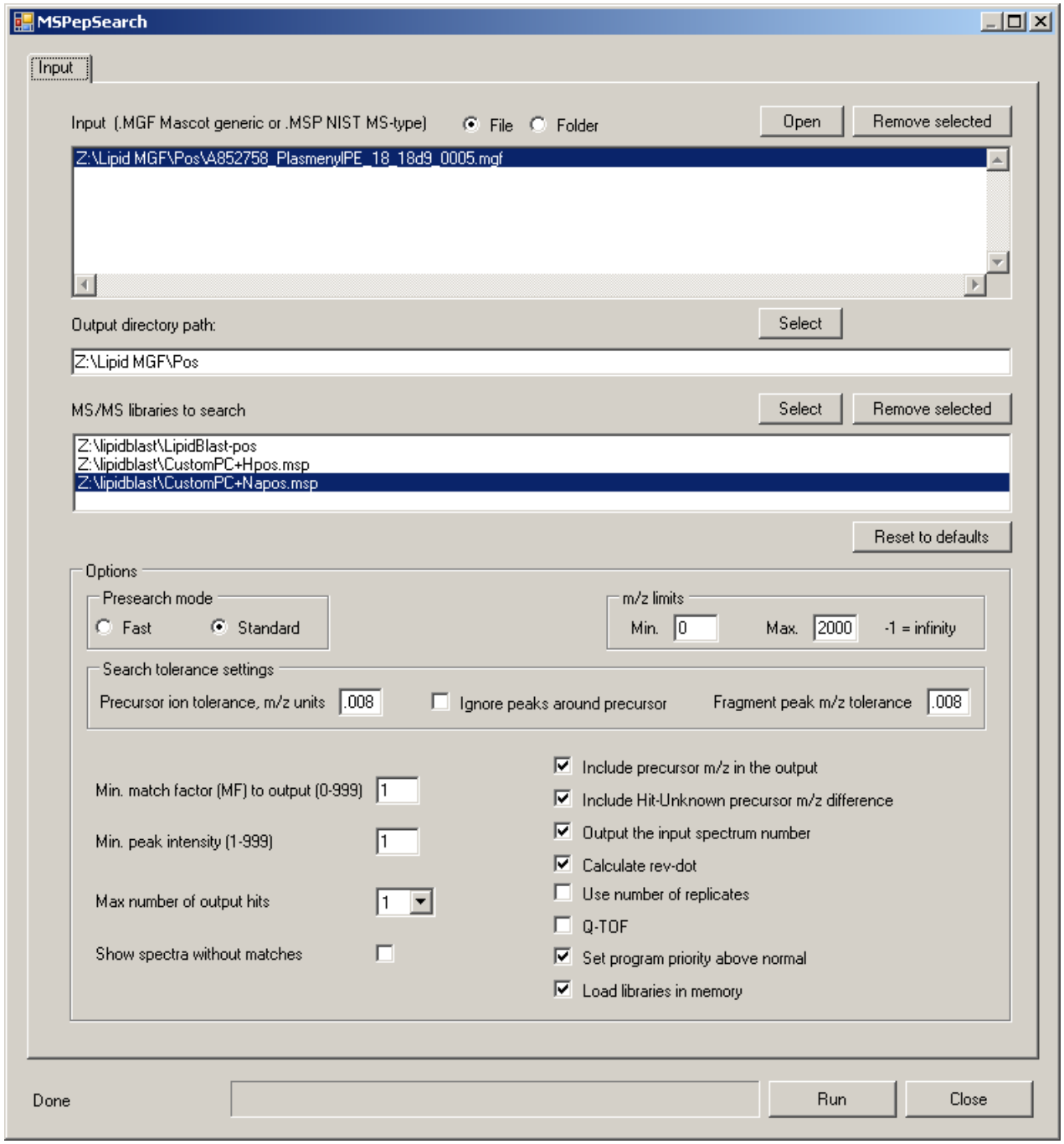
Software for batch interpretation of tandem mass spectra

Independent from LipidBlast. Can be freely obtained from http://peptide.nist.gov/

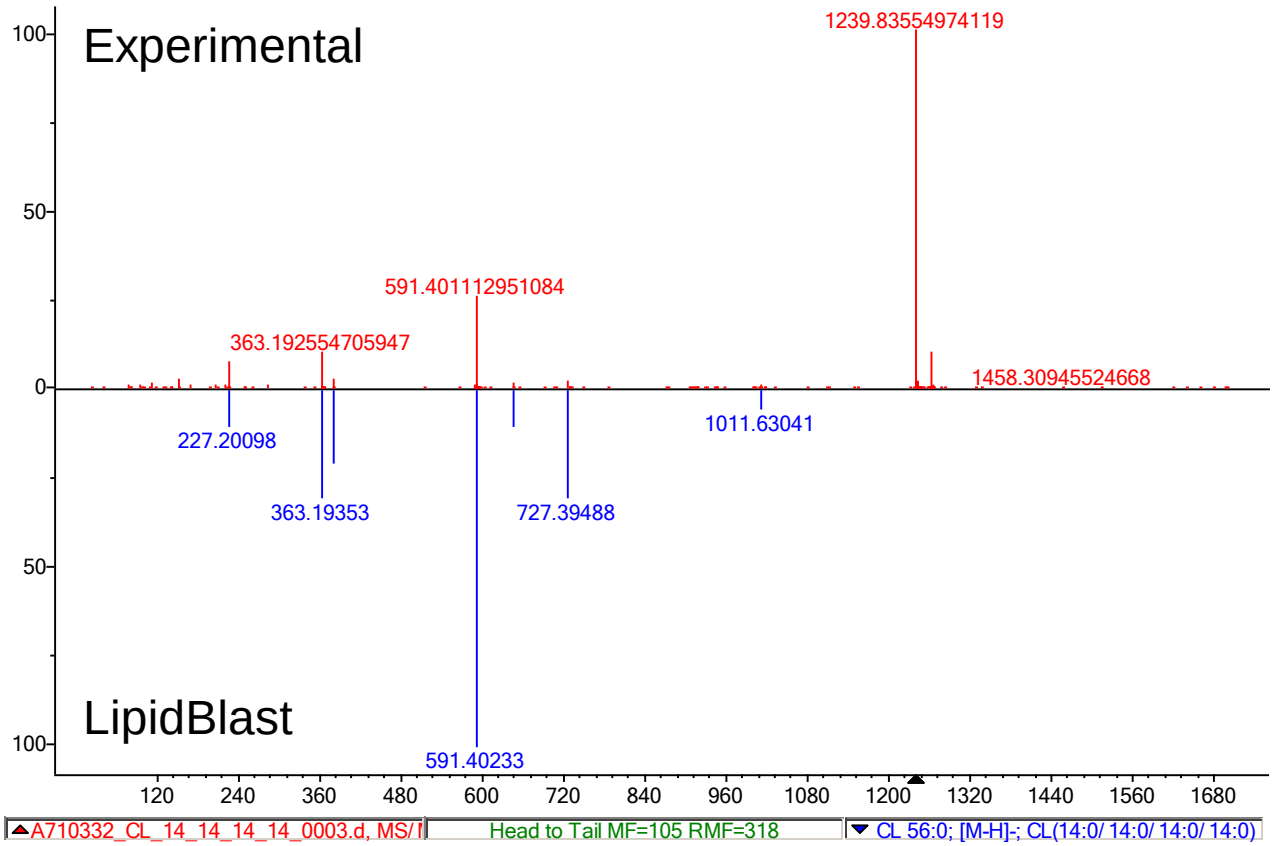
Library search settings for accurate mass spectrometry: Precursor accuracy +/-0.008 Da; product ion accuracy +/-0.008 Da;






MSPepSearch
Input
Input (.MGF Mascot generic or .MSP NIST MS-type)
File
Folder
Open
Remove selected
Z:\Lipid MGF\Pos\A852758_PlasmenylPE_18_18d9_0005.mgf
Output directory path:
Select
Z:\Lipid MGF\Pos
MS/MS libraries to search
Select
Remove selected
Z:\lipidblast\LipidBlast-pos
Z:\lipidblast\CustomPC+Hpos.msp
Z:\lipidblast\CustomPC+Napos.msp
Reset to defaults
Options
Presearch mode
Fast
Standard
m/z limits
Min.
0
Max.
2000
-1 = infinity
Search tolerance settings
Precursor ion tolerance, m/z units
.008
Ignore peaks around precursor
Fragment peak m/z tolerance
.008
Min. match factor (MF) to output (0-999)
1
Min. peak intensity (1-999)
1
Max number of output hits
1
Show spectra without matches
Include precursor m/z in the output
Include Hit-Unknown precursor m/z difference
Output the input spectrum number
Calculate rev-dot
Use number of replicates
Q-TOF
Set program priority above normal
Load libraries in memory
Done
Run
Close

1) Standard Cardiolipin - ESI(-)
CL(1'-[14:0/14:0],3'-[14:0/14:0]); C65H132N2O17P2



ID in LipidBlast – single hit OK

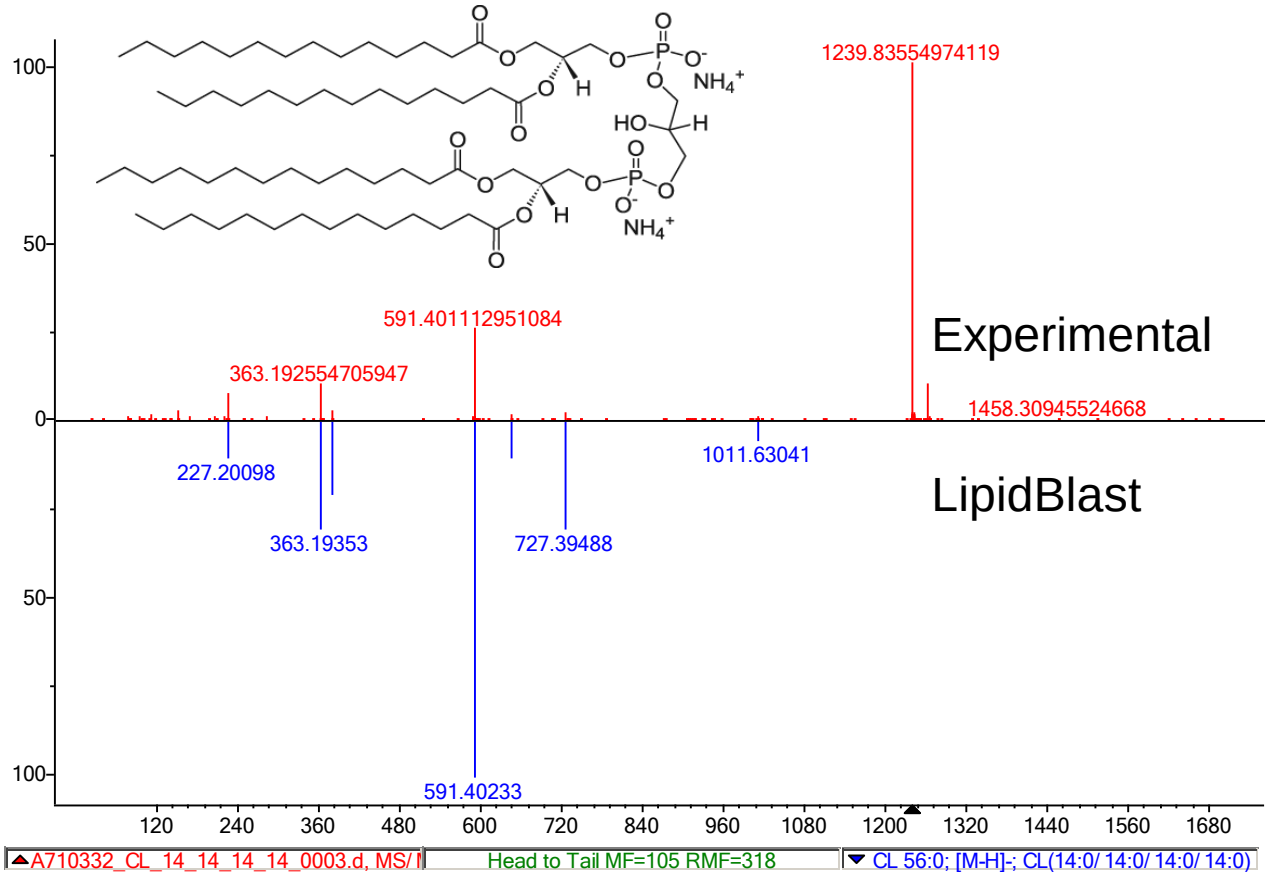
Name: CL 56:0; [M-H]-; CL(14:0/14:0/14:0/14:0)

MW: 1239 ID#: 22921 DB: lipidblast-neg

Comment: Parent=1239.83921 Mz_exact=1239.83921 ; CL 56:0; [M-H]-; CL(14:0/14:0/14:0/14:0); C65H126O17P2

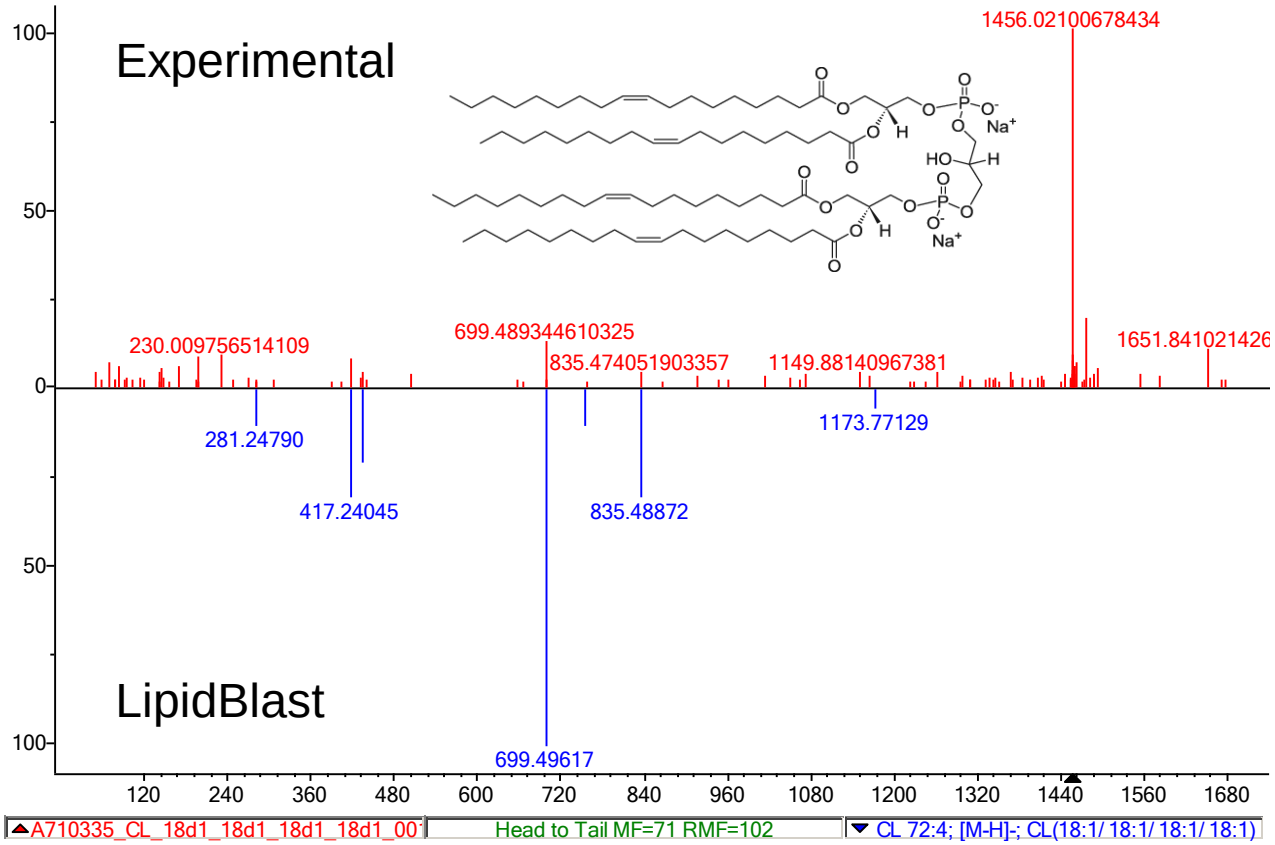
Source: A710332_CL_14_14_14_14_0003.d, MS/MS of 1239.839965820 1+ at 1.4901

Automatic LipidBlast explanation of fragments: Cardiolipin CL(1'-[14:0/14:0],3'-[14:0/14:0]); C65H132N2O17P2



227.20098	100.00	sn1 FA || sn2 FA || sn3 FA || sn4 FA
363.19353	300.00	sn2+C3H6PO4 (+137.00) || sn4+C3H6PO4 (+137.00)
381.20409	200.00	sn2+C3H6PO4+H2O || sn4+C3H6PO4+H2O
591.40233	999.00	sn1+sn2+C3H6PO4 (+137.00) || sn3+sn4+C3H6PO4 (+137.00)
647.42854	100.00	sn1+sn2+C6H10O5P (+193.026) || sn3+sn4+C6H10O5P (+193.026)
727.39488	300.00	sn1+sn2+C6H11P2O8 (+272.9929) || sn3+sn4+C6H11P2O8 (+272.9929)
1011.63041	50.00	[M-H]-sn1

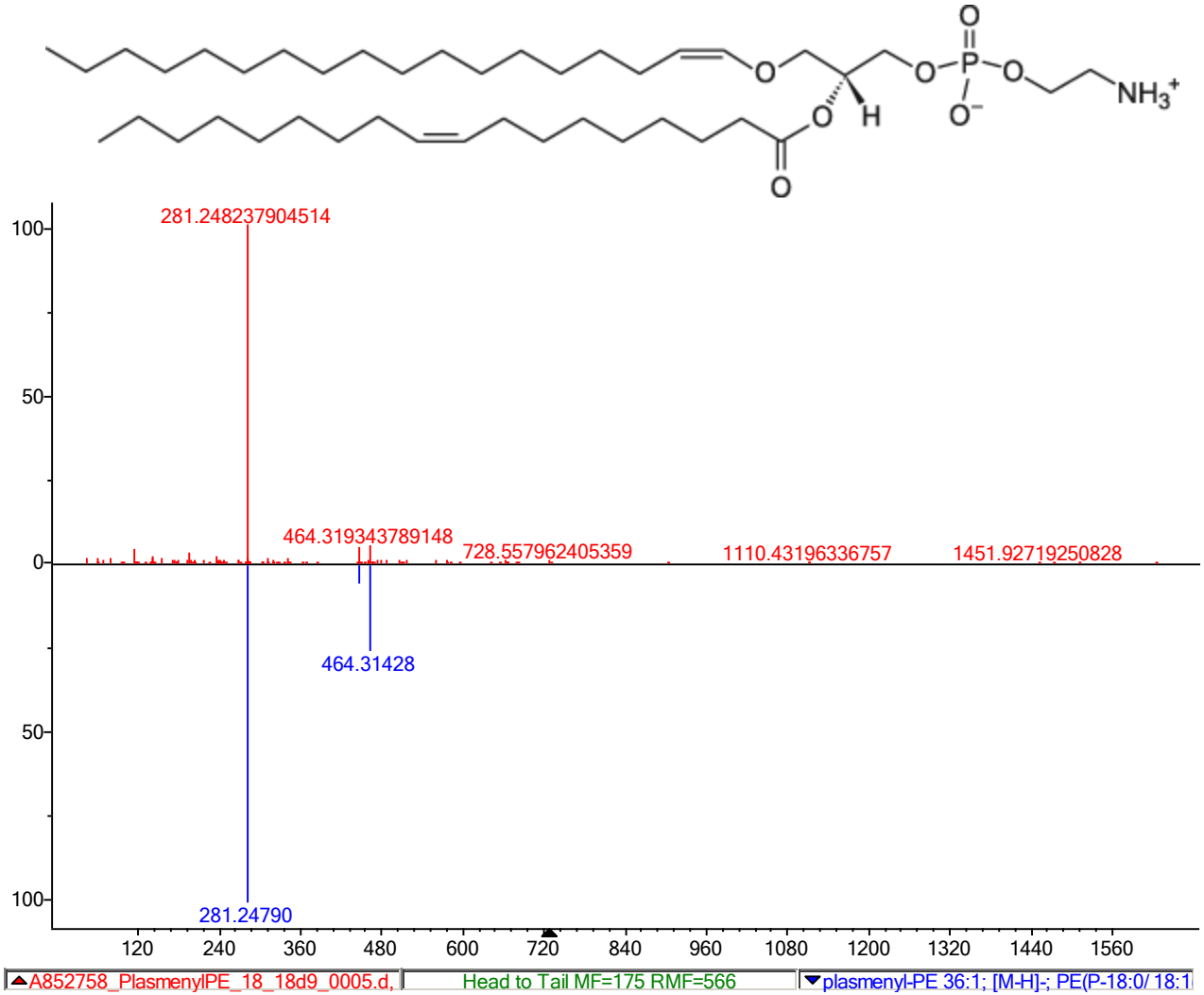
2) Standard Cardiolipin ESI(-)
CL(1'-[18:1/18:1(9Z)],3'-[18:1/18:1(9Z)])



ID in LipidBlast – First HIT

Name: CL 72:4; [M-H]-; CL(18:1/18:1/18:1/18:1)
MW: 1456 ID#: 33228 DB: lipidblast-neg
Comment: Parent=1456.02701 Mz_exact=1456.02701 ; CL 72:4; [M-H]-; CL(18:1/18:1/18:1/18:1); C81H150O17P2
7 largest peaks:

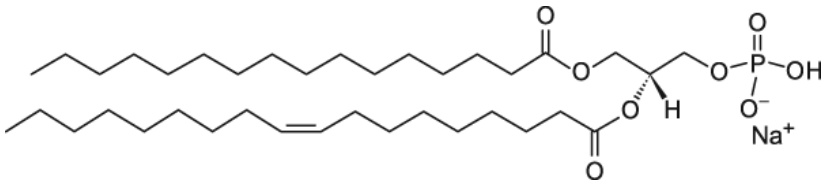
3) Standard Plasmenyl-PE; GPEtn(18:0p/18:1(9Z)) - ESI(-)

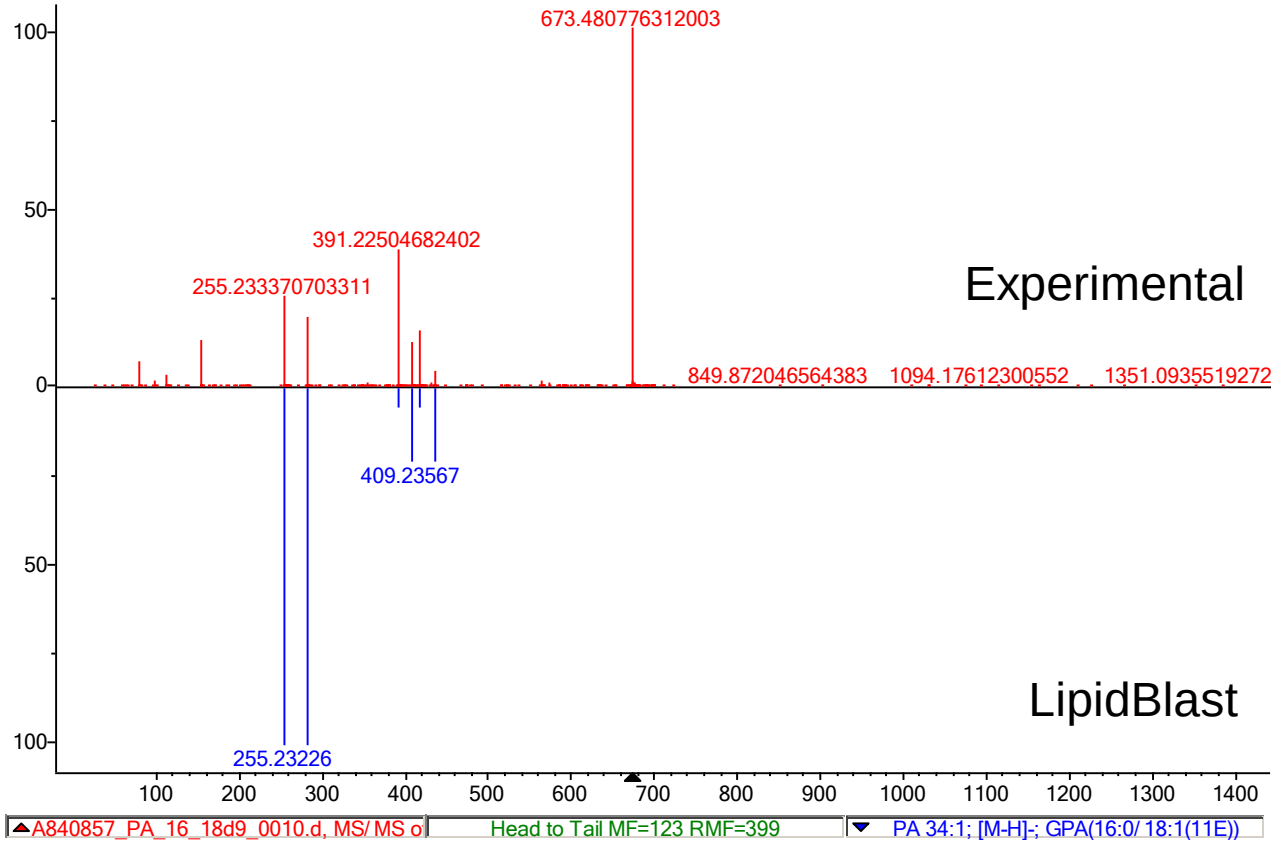


ID in LipidBlast – First HIT

Name: plasmenyl-PE 36:1; [M-H]-; PE(P-18:0/18:1(11E))
MW: 728 ID#: 123312 DB: lipidblast-neg
Comment: Parent=728.55944 Mz_exact=728.55944 ; plasmenyl-PE 36:1; [M-H]-; PE(P-18:0/18:1(11E)); C41H80NO7P

4) Standard Phosphatidic Acid: PA(16:0/18:1(9Z)) - ESI(-)

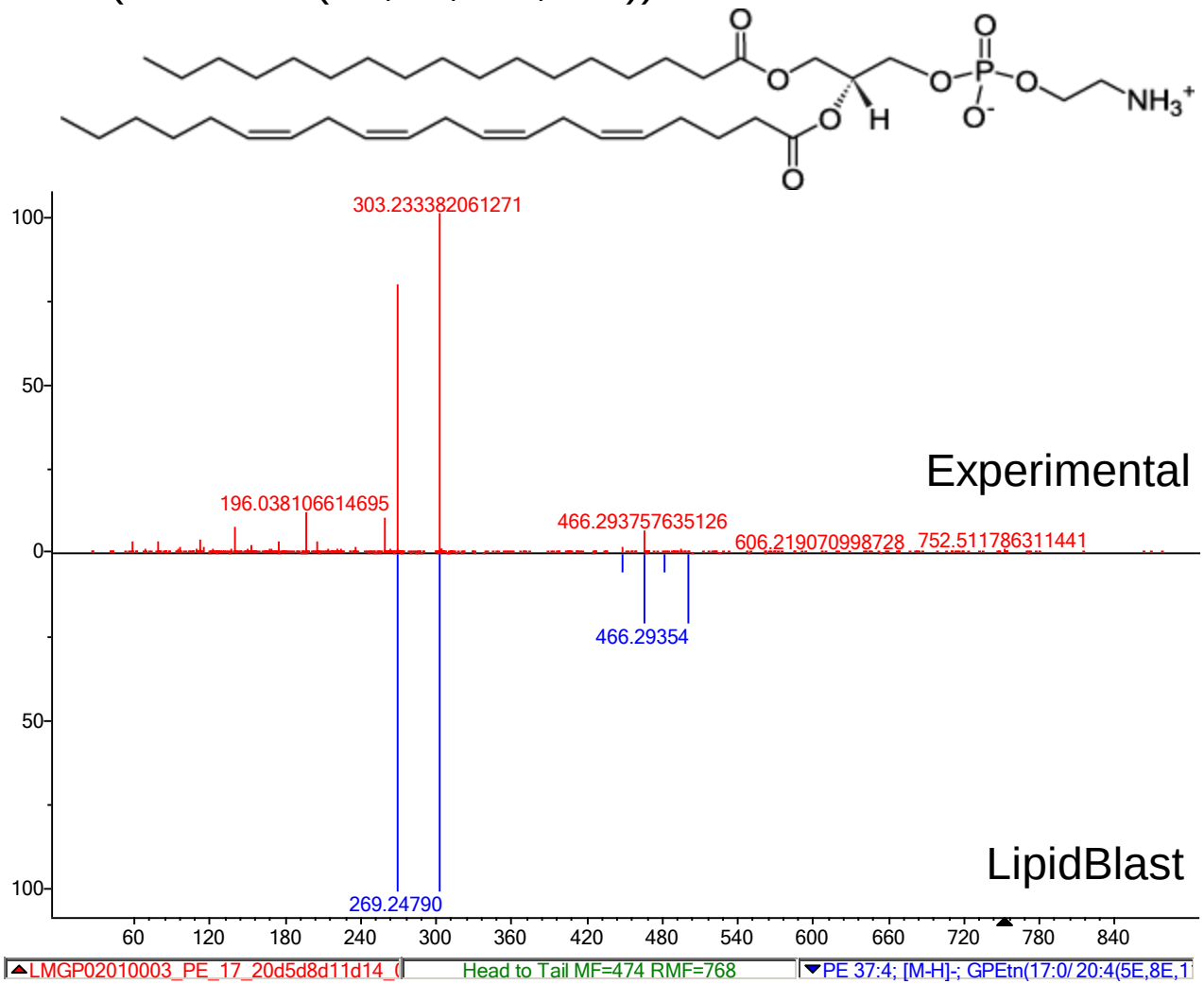




ID in LipidBlast – First HIT

Name: PA 34:1; [M-H]-; GPA(16:0/18:1(11E)) – equivalent with GPA(16:0/18:1(9Z))
MW: 673 ID#: 102518 DB: lipidblast-neg
Comment: Parent=673.48083 Mz_exact=673.48083 ; PA 34:1; [M-H]-; GPA(16:0/18:1(11E)); C37H71O8P

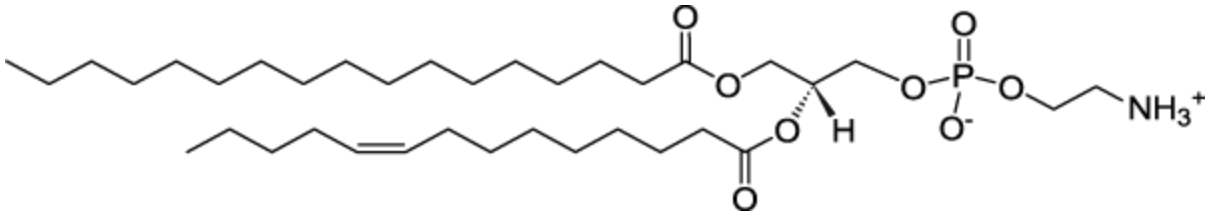
5) Standard phosphatidylethanolamine – ESI (-)
PE(17:0/20:4(5Z,8Z,11Z,14Z))

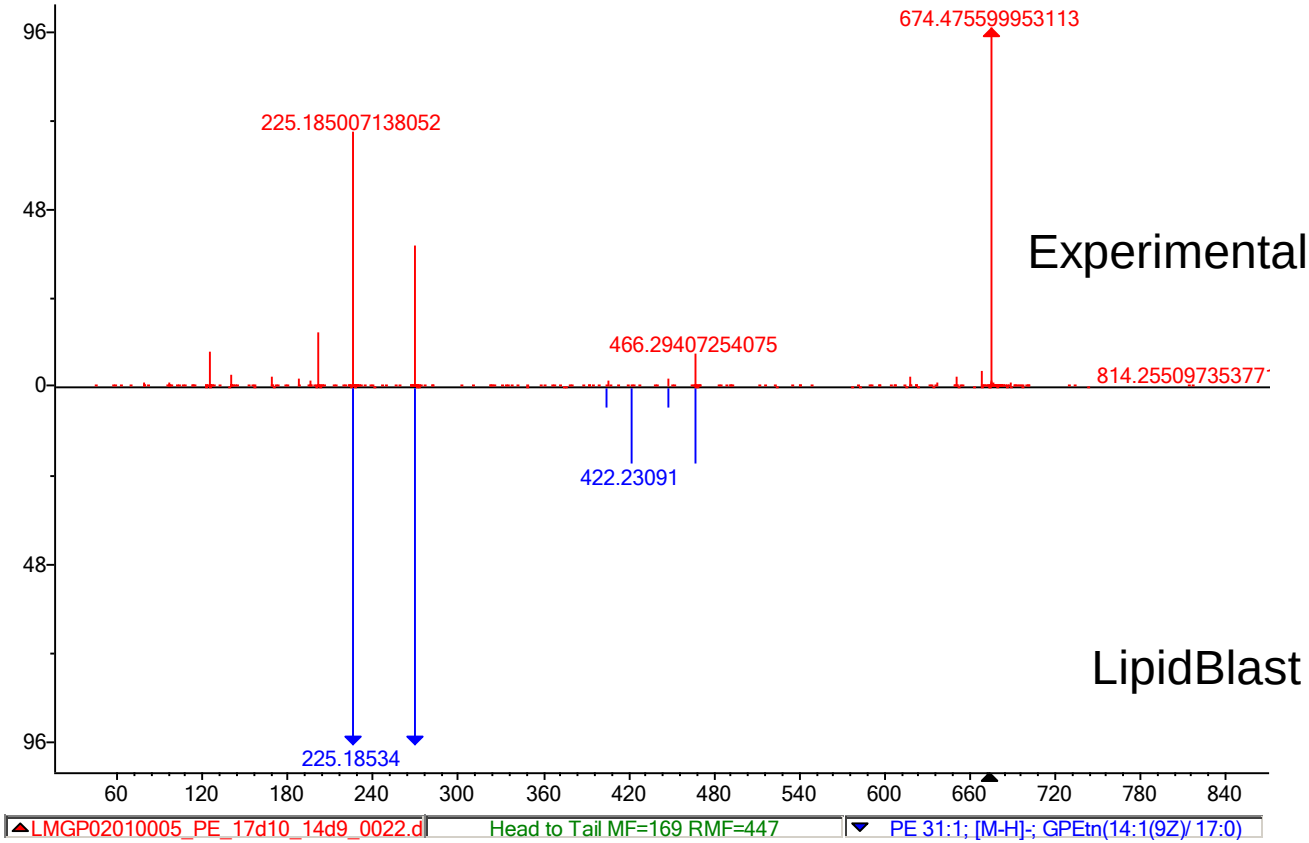


ID in LipidBlast – First HIT

Name: PE 37:4; [M-H]-; GPEtn(17:0/20:4(5E,8E,11E,14E)) - equivalent with GPEtn(17:0/20:4(5Z,8Z,11Z,14Z))
MW: 752 ID#: 108245 DB: lipidblast-neg
Comment: Parent=752.52306 Mz_exact=752.52306 ; PE 37:4; [M-H]-; GPEtn(17:0/20:4(5E,8E,11E,14E)); C42H76NO8P

6) Standard phosphatidylethanolamine – ESI(-)
PE(17:1/14:1(9Z))



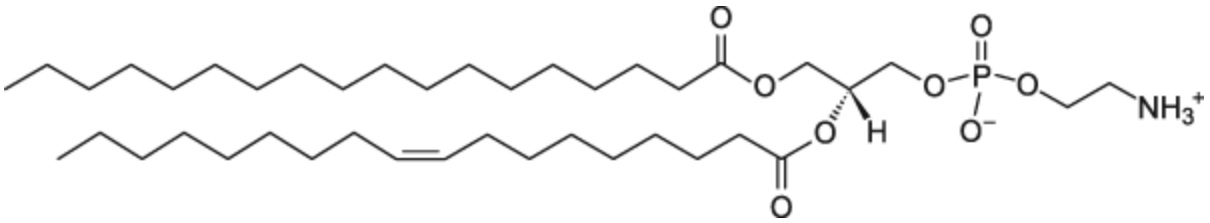


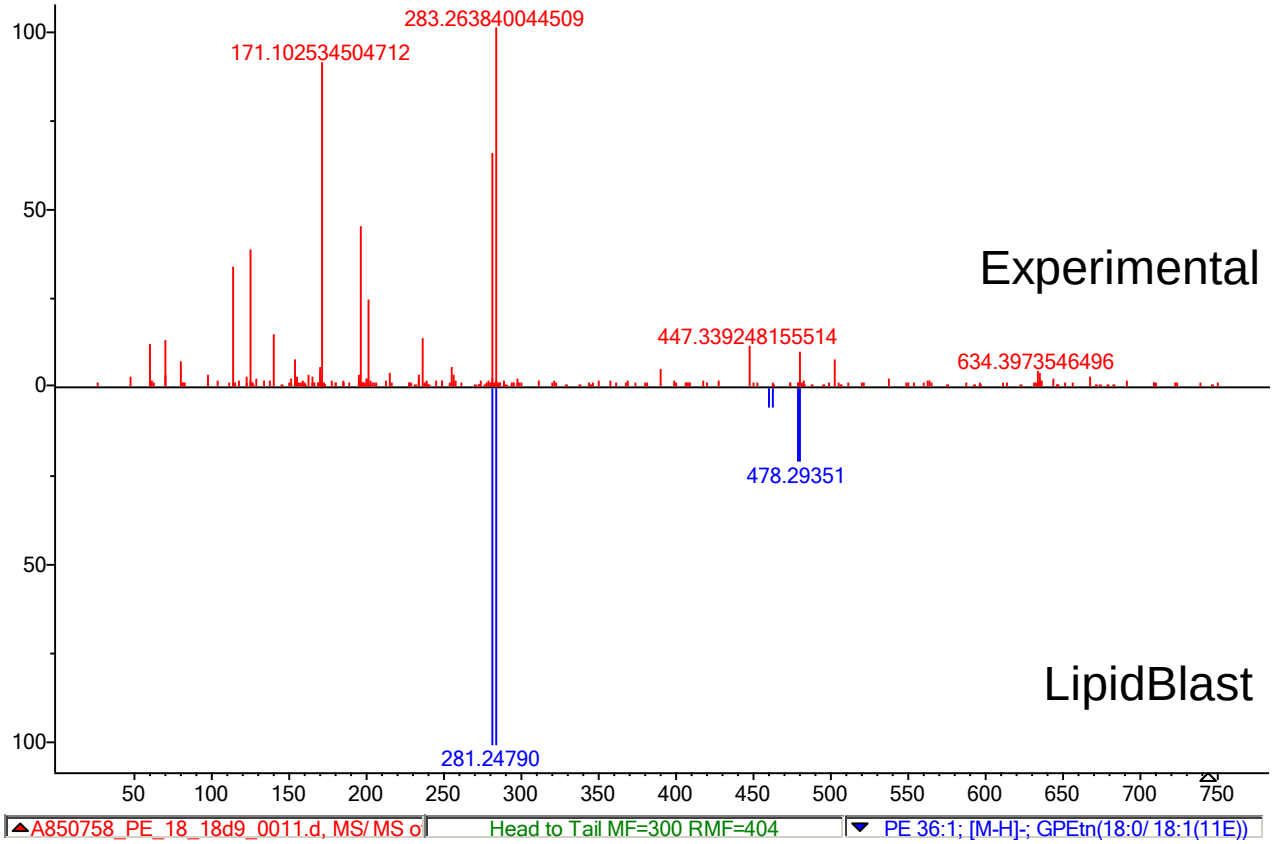
Experimental

LipidBlast

ID in LipidBlast – First HIT
Name: PE 31:1; [M-H]-; GPEtn(14:1(9Z)/17:0)
MW: 674 ID#: 107768 DB: lipidblast-neg
Comment: Parent=674.47607 Mz_exact=674.47607 ; PE 31:1; [M-H]-; GPEtn(14:1(9Z)/17:0); C36H70NO8P

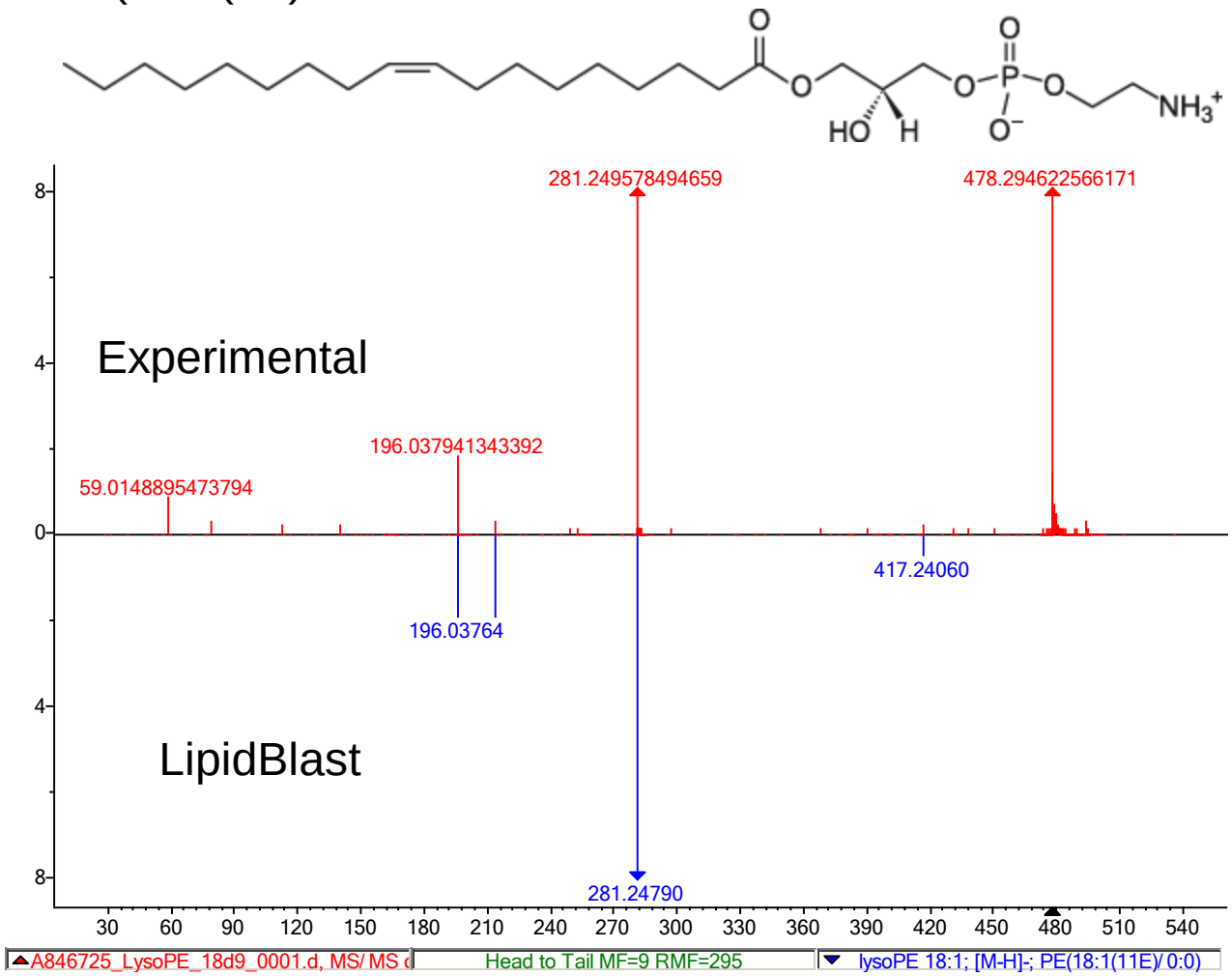
7) Standard phosphatidylethanolamine – ESI(-)
PE(18:0/18:1(9Z))





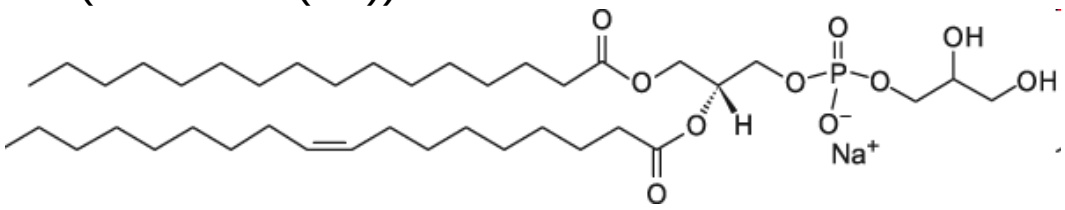
ID in LipidBlast – First HIT
Name: PE 36:1; [M-H]-; GPEtn(18:0/18:1(11E))
MW: 744 ID#: 108438 DB: lipidblast-neg
Comment: Parent=744.55431 Mz_exact=744.55431 ; PE 36:1; [M-H]-; GPEtn(18:0/18:1(11E)); C41H80NO8P

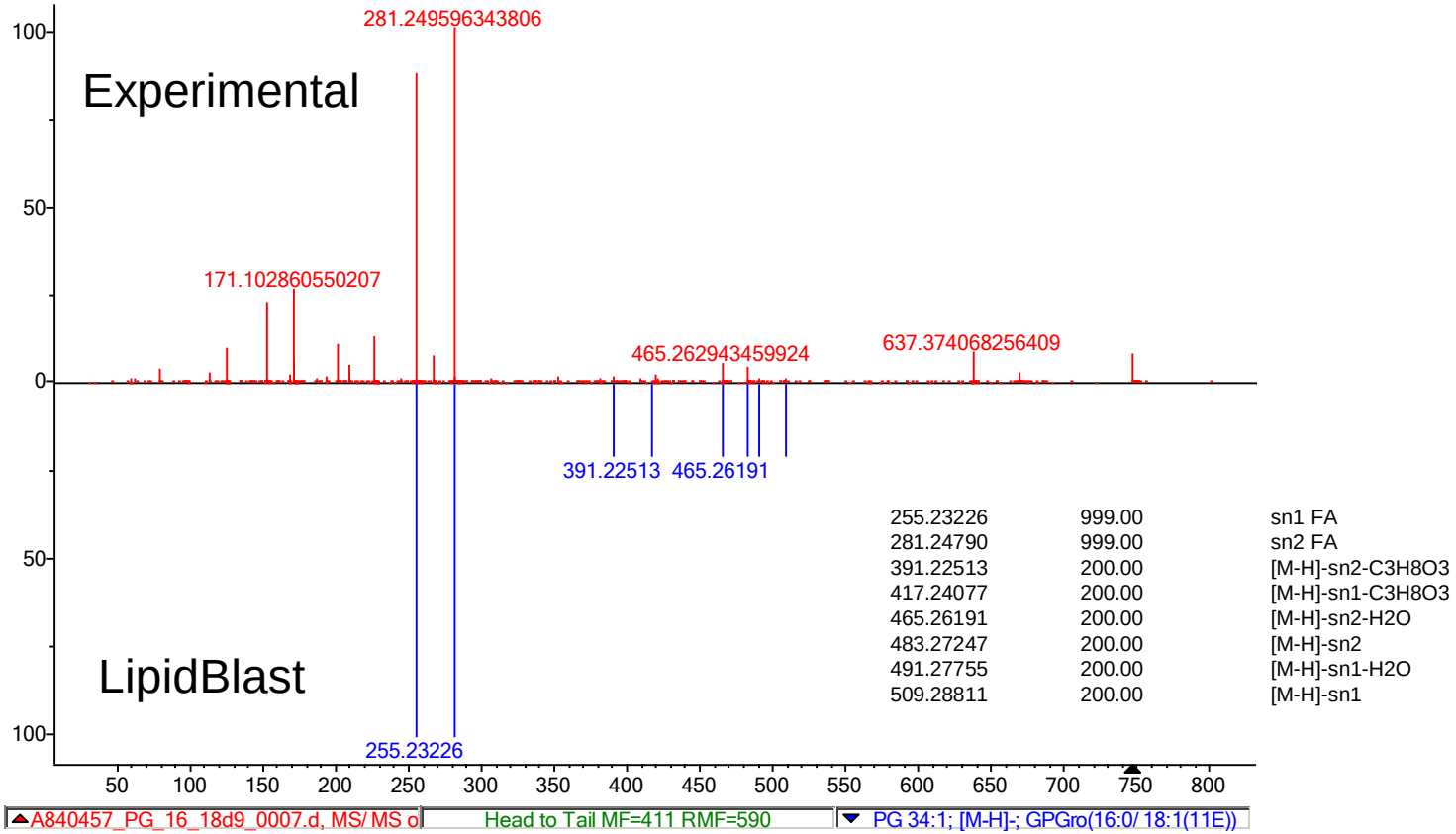
8) Standard Lyso-phosphatidylethanolamine – ESI(-)
PE(18:1(9Z)/0:0



ID in LipidBlast – First HIT
Name: lysoPE 18:1; [M-H]-; PE(18:1(11E)/0:0)
MW: 478 ID#: 95782 DB: lipidblast-neg
Comment: Parent=478.29336 Mz_exact=478.29336 ; lysoPE 18:1; [M-H]-; PE(18:1(11E)/0:0); C23H46NO7P

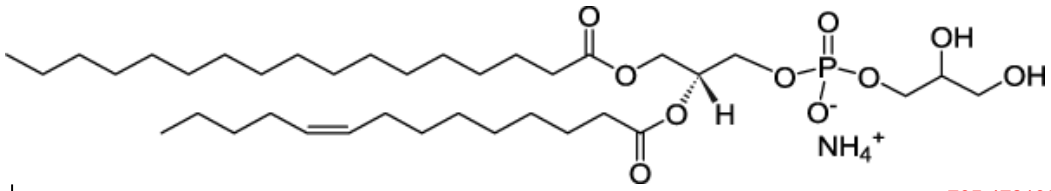
9) Standard phosphatidylglycerol – ESI(-)
PG(17:0/14:1(9Z))

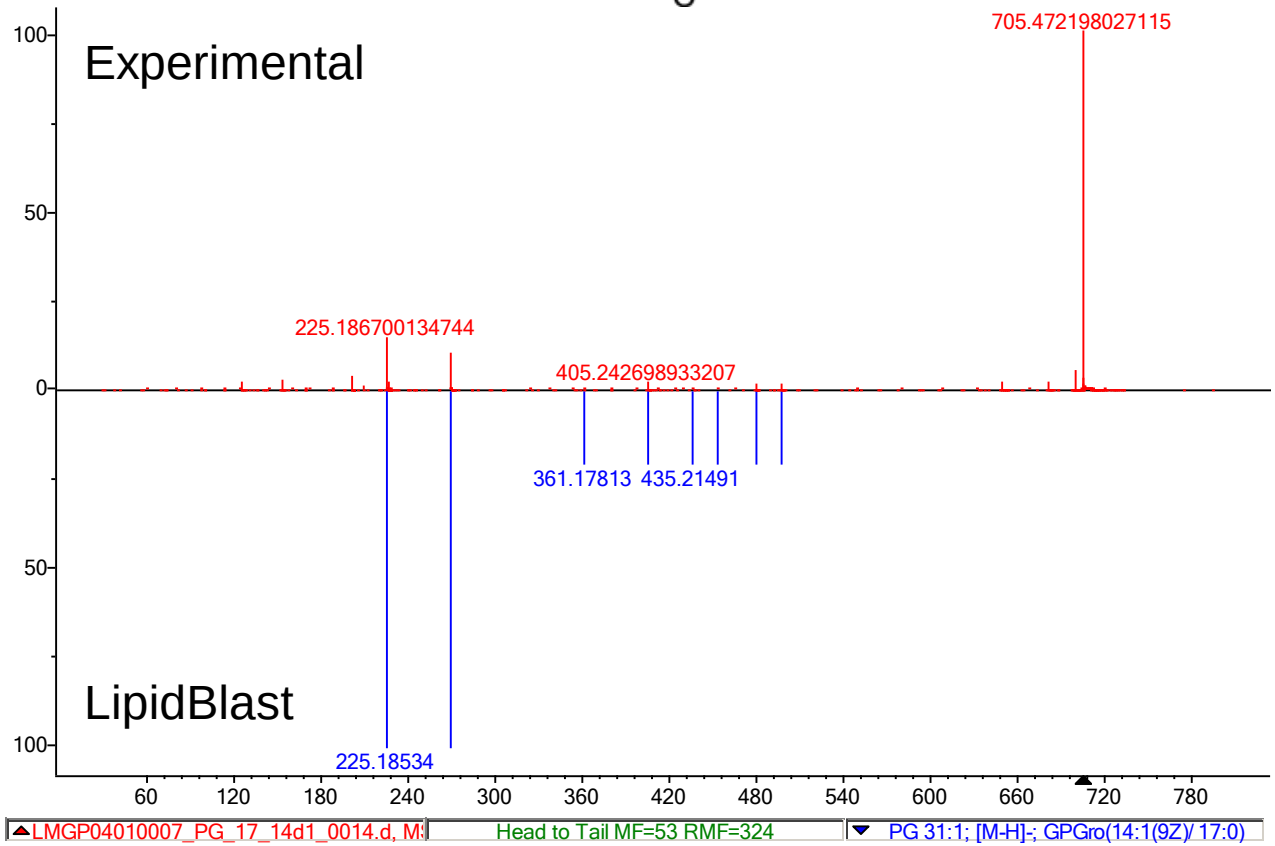




255.23226	999.00	sn1 FA
281.24790	999.00	sn2 FA
391.22513	200.00	[M-H]-sn2-C3H8O3
417.24077	200.00	[M-H]-sn1-C3H8O3
465.26191	200.00	[M-H]-sn2-H2O
483.27247	200.00	[M-H]-sn2
491.27755	200.00	[M-H]-sn1-H2O
509.28811	200.00	[M-H]-sn1

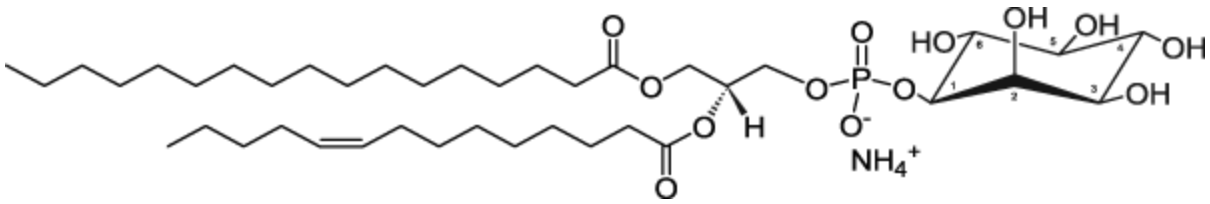
10) Standard phosphatidylglycerol – ESI(-)
PG(17:0/14:1(9Z))

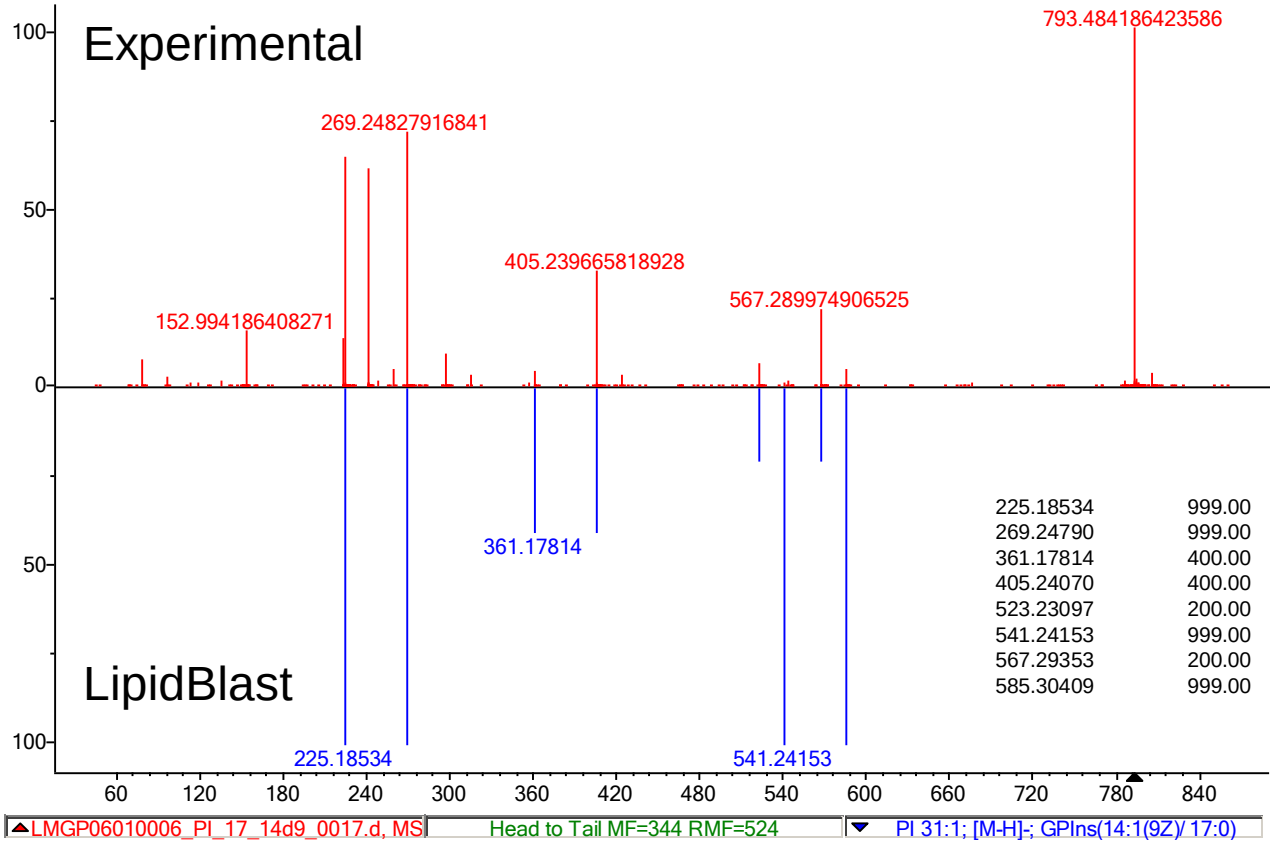




ID in LipidBlast – First HIT
Name: PG 31:1; [M-H]-; GPGro(14:1(9Z)/17:0)
MW: 705 ID#: 113244 DB: lipidblast-neg
Comment: Parent=705.47063 Mz_exact=705.47063 ; PG 31:1; [M-H]-; GPGro(14:1(9Z)/17:0); C37H71O10P

11) Standard phosphatidylinositol – ESI(-)
PI(17:0/14:1(9Z))



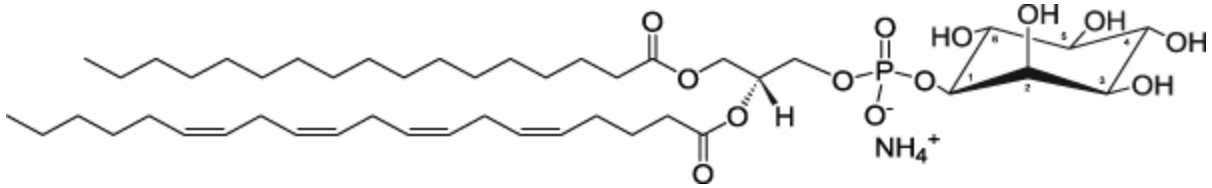


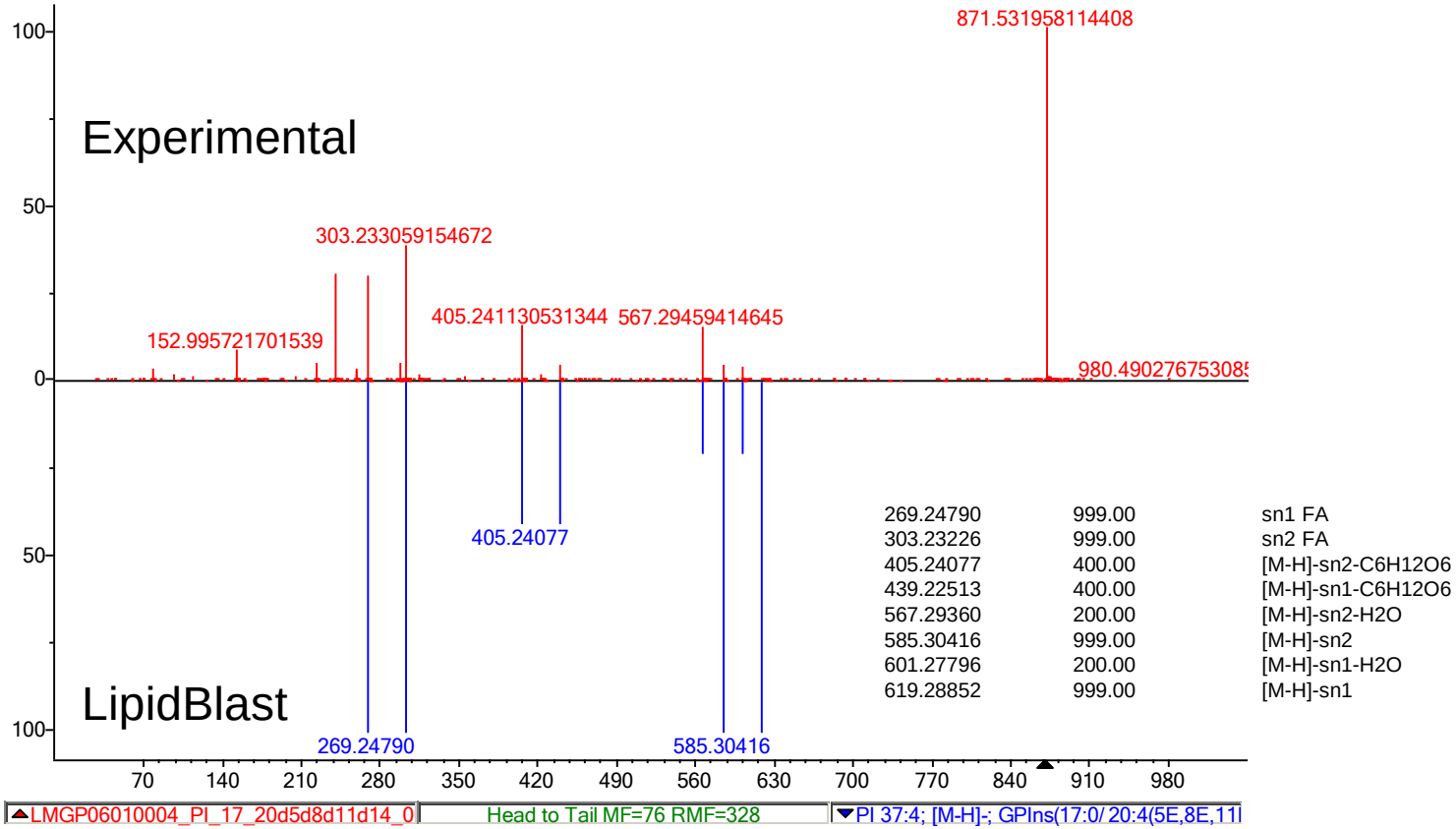
225.18534	999.00	sn1 FA
269.24790	999.00	sn2 FA
361.17814	400.00	[M-H]-sn2-C6H12O6
405.24070	400.00	[M-H]-sn1-C6H12O6
523.23097	200.00	[M-H]-sn2-H2O
541.24153	999.00	[M-H]-sn2
567.29353	200.00	[M-H]-sn1-H2O
585.30409	999.00	[M-H]-sn1

ID in LipidBlast – First HIT

Name: PI 31:1; [M-H]-; GPIns(14:1(9Z)/17:0)
MW: 793 ID#: 118720 DB: lipidblast-neg
Comment: Parent=793.48669 Mz_exact=793.48669 ; PI 31:1; [M-H]-; GPIns(14:1(9Z)/17:0); C40H75O13P

12) Standard phosphatidylinositol – ESI(-)
PI(17:0/20:4(5Z,8Z,11Z,14Z))



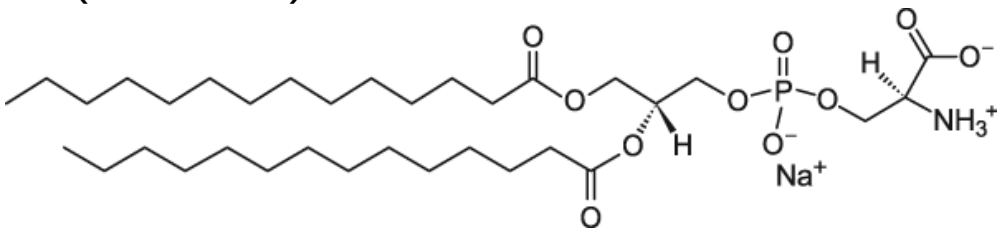


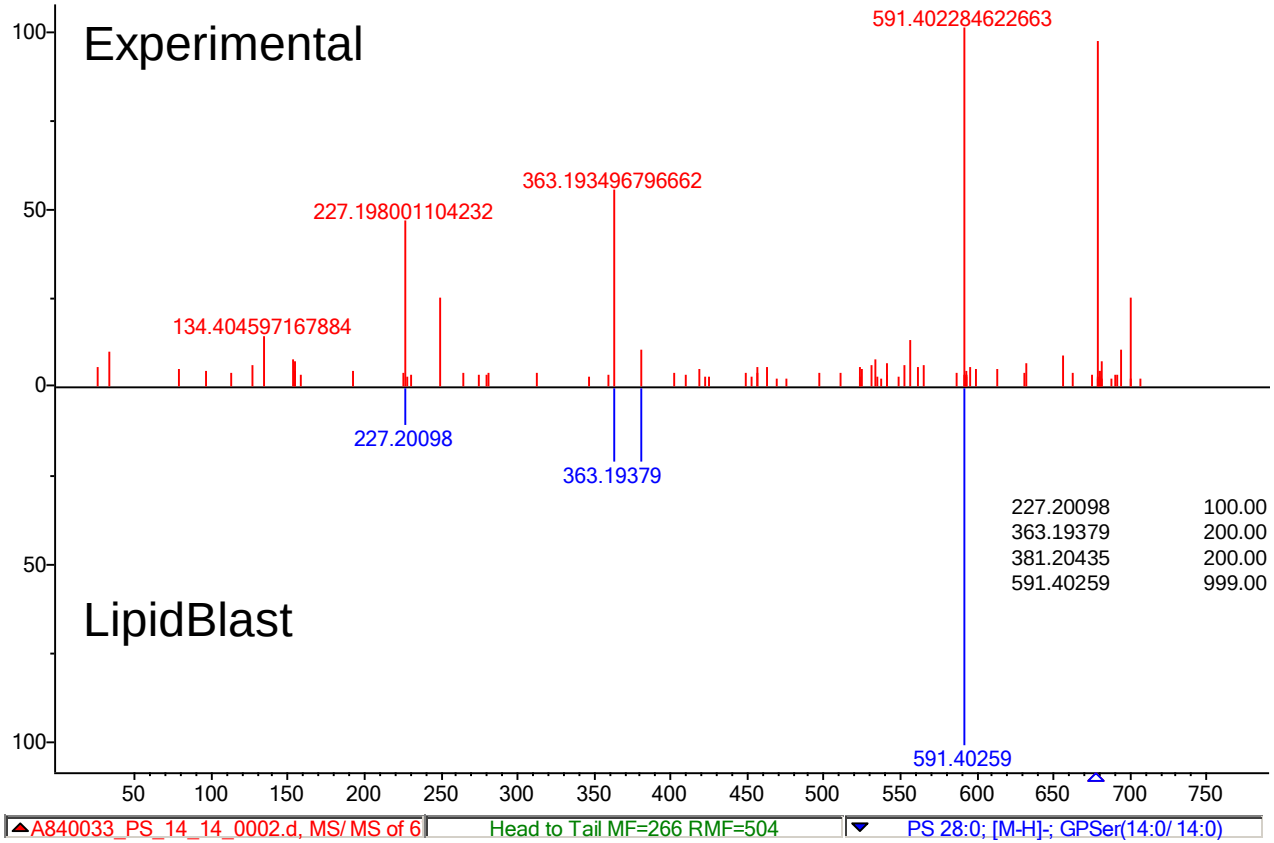
269.24790	999.00	sn1 FA
303.23226	999.00	sn2 FA
405.24077	400.00	[M-H]-sn2-C6H12O6
439.22513	400.00	[M-H]-sn1-C6H12O6
567.29360	200.00	[M-H]-sn2-H2O
585.30416	999.00	[M-H]-sn2
601.27796	200.00	[M-H]-sn1-H2O
619.28852	999.00	[M-H]-sn1

ID in LipidBlast – First HIT

Name: PI 37:4; [M-H]-; GPIns(17:0/20:4(5E,8E,11E,14E))
MW: 871 ID#: 119197 DB: lipidblast-neg
Comment: Parent=871.53368 Mz_exact=871.53368 ; PI 37:4; [M-H]-; GPIns(17:0/20:4(5E,8E,11E,14E)); C46H81O13P

13) Standard phosphatidylserine – ESI(-)
PS(14:0/14:0)



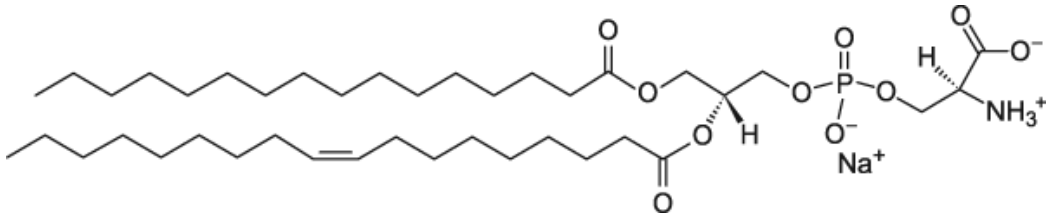


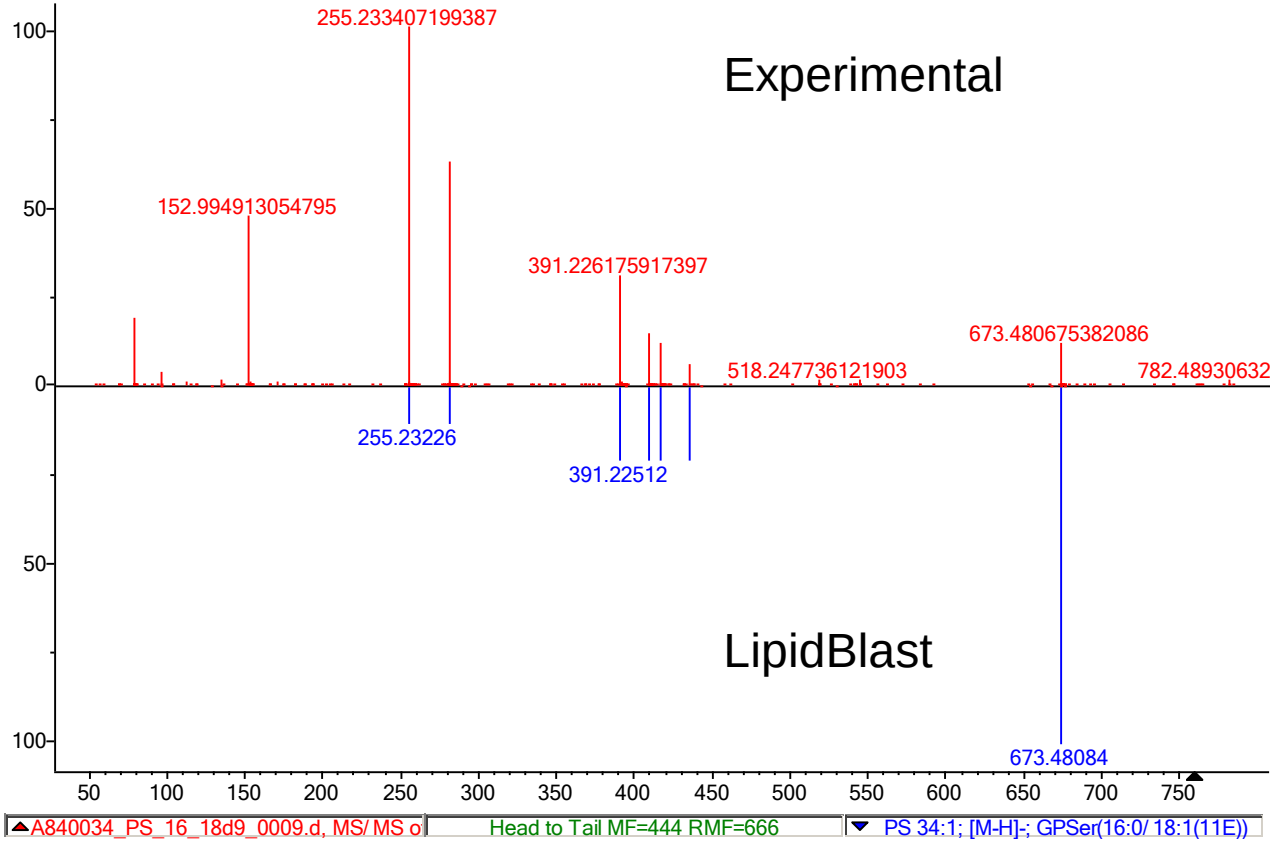
227.20098	100.00	sn1 FA || sn2 FA
363.19379	200.00	[M-H-87]-sn1 || [M-H-87]-sn2
381.20435	200.00	[M-H-87]-sn1+H2O || [M-H-87]-sn2+H2O
591.40259	999.00	[M-H]-C3H5NO2 (-87)

ID in LipidBlast – First HIT

Name: PS 28:0; [M-H]-; GPSer(14:0/14:0)
MW: 678 ID#: 124337 DB: lipidblast-neg
Comment: Parent=678.43462 Mz_exact=678.43462 ; PS 28:0; [M-H]-; GPSer(14:0/14:0);
C34H66NO10P

14) Standard phosphatidylserine – ESI(-)
PS(16:0/18:1(9Z))

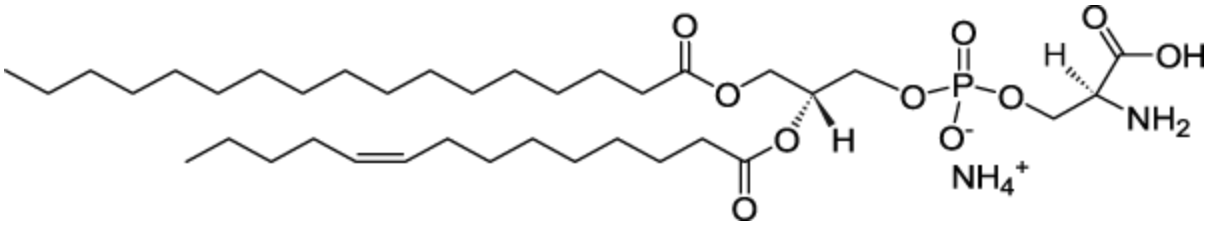


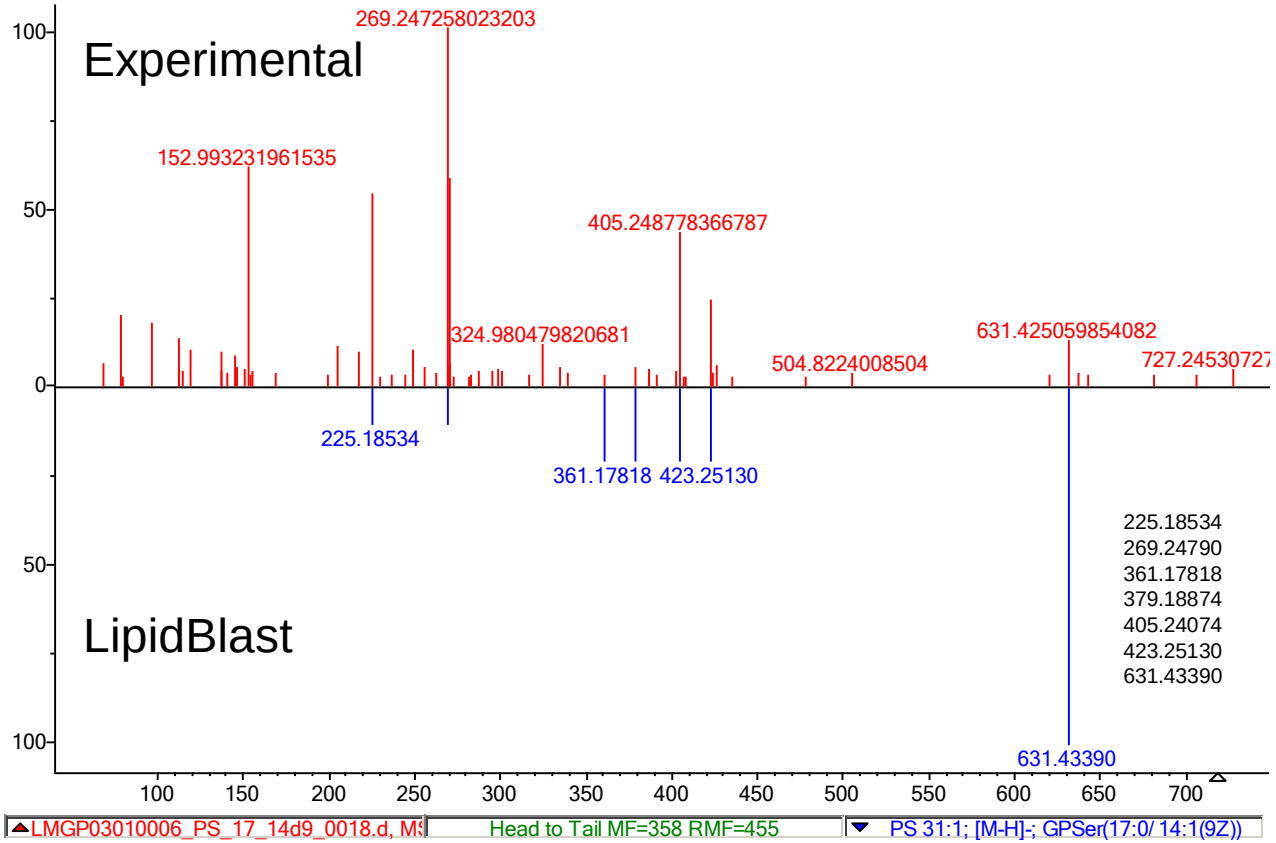


ID in LipidBlast – First HIT

Name: PS 34:1; [M-H]-; GPSer(16:0/18:1(11E)) equivalent with GPSer(16:0/18:1(9Z))
MW: 760 ID#: 124644 DB: lipidblast-neg
Comment: Parent=760.51287 Mz_exact=760.51287 ; PS 34:1; [M-H]-; GPSer(16:0/18:1(11E)); C40H76NO10P

15) Standard phosphatidylserine – ESI(-)
PS(17:0/14:1(9Z))

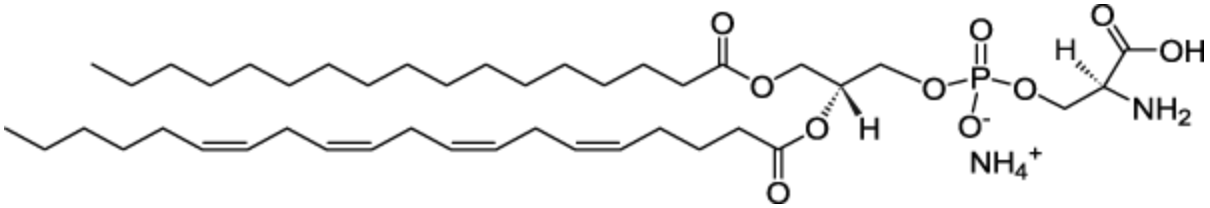


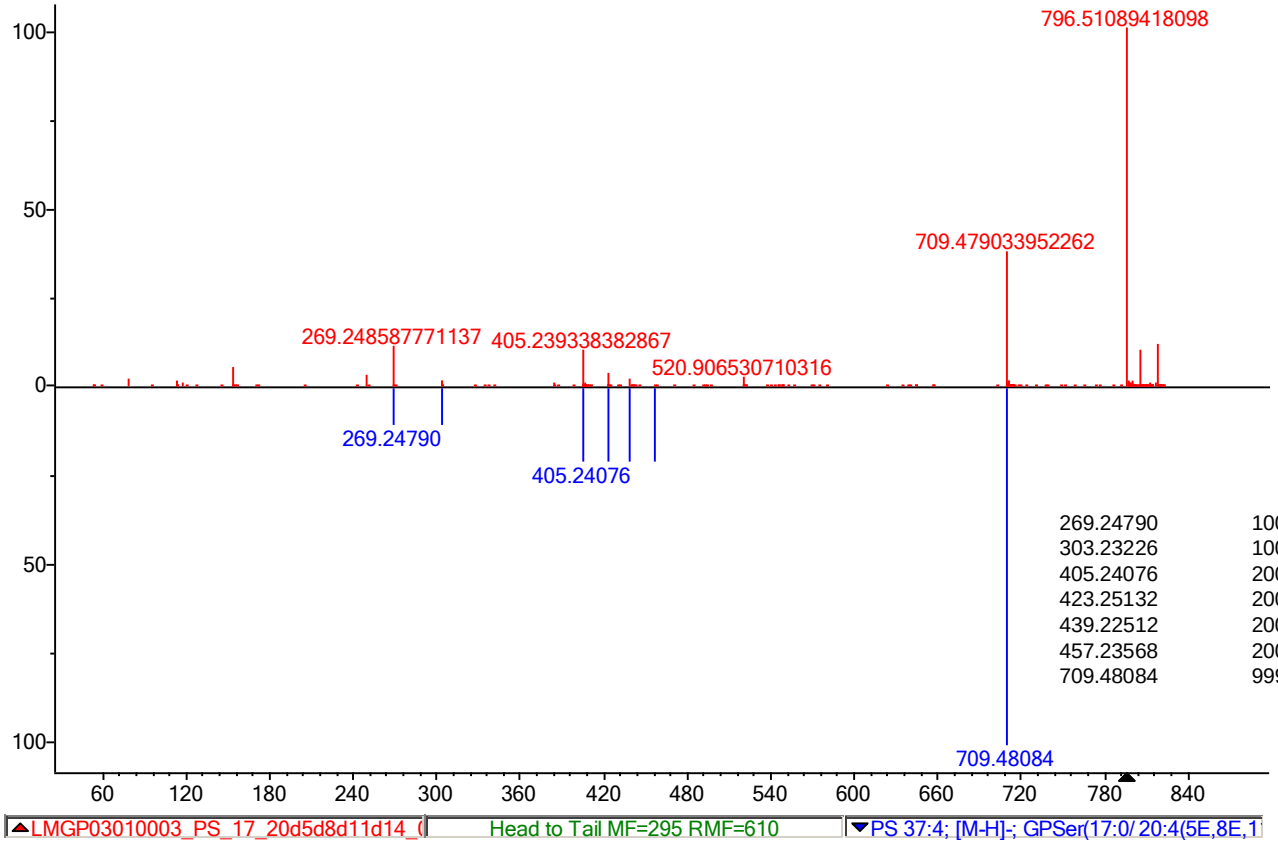


225.18534	100.00	sn2 FA
269.24790	100.00	sn1 FA
361.17818	200.00	[M-H-87]-sn1
379.18874	200.00	[M-H-87]-sn1+H2O
405.24074	200.00	[M-H-87]-sn2
423.25130	200.00	[M-H-87]-sn2+H2O
631.43390	999.00	[M-H]-C3H5NO2 (-87)

ID in LipidBlast – First HIT
Name: PS 31:1; [M-H]-; GPSer(17:0/14:1(9Z))
MW: 718 ID#: 124856 DB: lipidblast-neg
Comment: Parent=718.46593 Mz_exact=718.46593 ; PS 31:1; [M-H]-; GPSer(17:0/14:1(9Z)); C37H70NO10P

16) Standard phosphatidylserine – ESI(-)
PS(17:0/20:4(5Z,8Z,11Z,14Z))



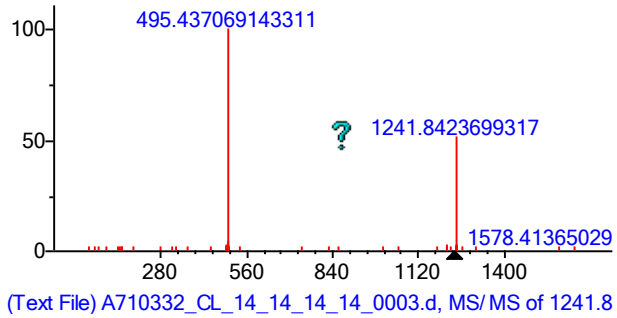


269.24790	100.00	sn1 FA
303.23226	100.00	sn2 FA
405.24076	200.00	[M-H-87]-sn2
423.25132	200.00	[M-H-87]-sn2+H2O
439.22512	200.00	[M-H-87]-sn1
457.23568	200.00	[M-H-87]-sn1+H2O
709.48084	999.00	[M-H]-C3H5NO2 (-87)

ID in LipidBlast – First HIT

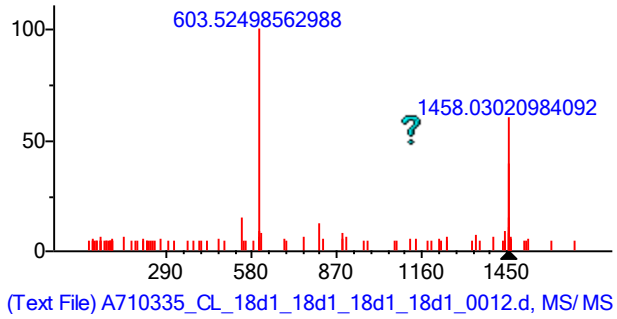
Name: PS 37:4; [M-H]-; GPSer(17:0/20:4(5E,8E,11E,14E)) equivalent to GPSer(17:0/20:4(5Z,8Z,11Z,14Z))
MW: 796 ID#: 124895 DB: lipidblast-neg
Comment: Parent=796.51287 Mz_exact=796.51287 ; PS 37:4; [M-H]-; GPSer(17:0/20:4(5E,8E,11E,14E)); C43H76NO10P

17) Standards – ESI(+)



Cardiolipin
CL(1'-[14:0/14:0],3'-[14:0/14:0]); C65H132N2O17P2

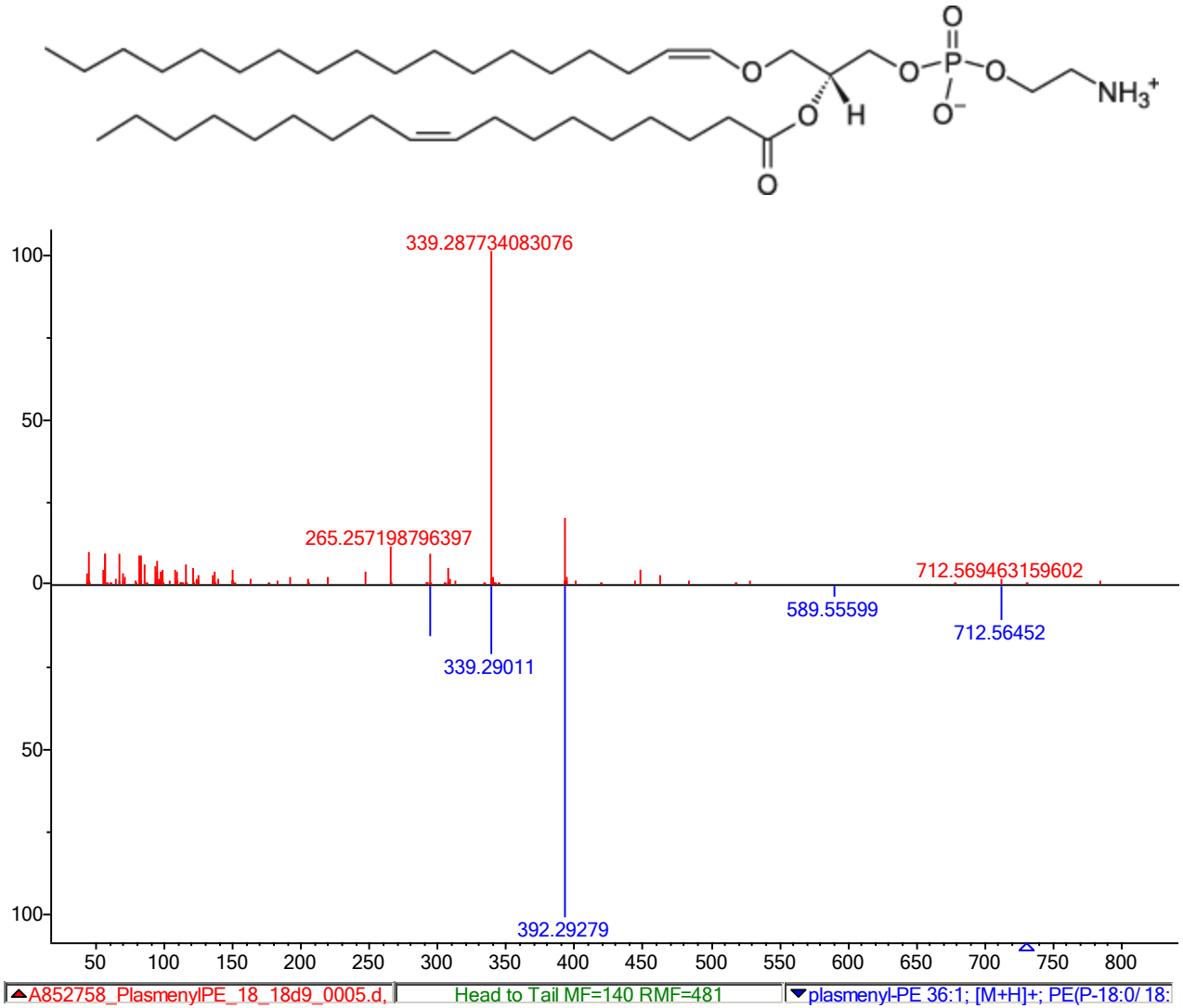
double negative charge, usually measured in negative mode.



Cardiolipin ESI(-)
CL(1'-[18:1/18:1(9Z)],3'-[18:1/18:1(9Z)])

double negative charge, usually measured in negative mode.

18) Standards ESI(+) plasmenylphosphatidylethanolamine; GPEtn(18:0p/18:1(9Z))



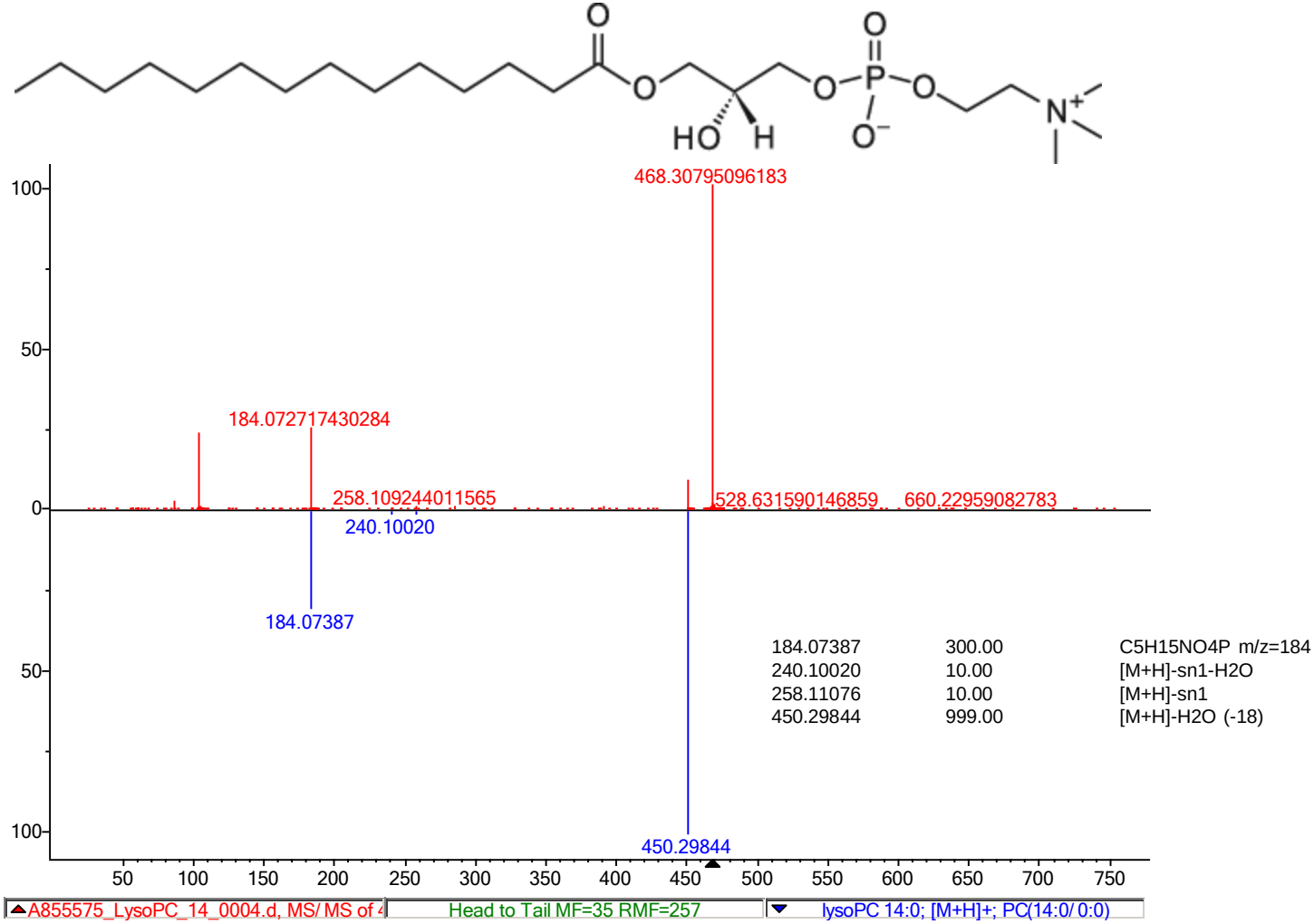
ID in LipidBlast – First HIT – issue with batch version

Name: plasmenyl-PE 36:1; [M+H]+; PE(P-18:0/18:1(11E)) equivalent to PE(P-18:0/18:1(11Z))

MW: 730 ID#: 59466 DB: lipidblast-pos

Comment: Parent=730.57508 Mz_exact=730.57508 ; plasmenyl-PE 36:1; [M+H]+; PE(P-18:0/18:1(11E)); C41H80NO7P

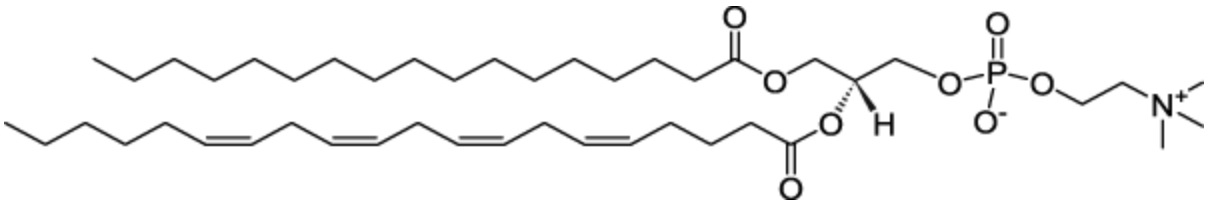
19) Standards ESI(+) lyso-PC; PC(14:0/0:0)

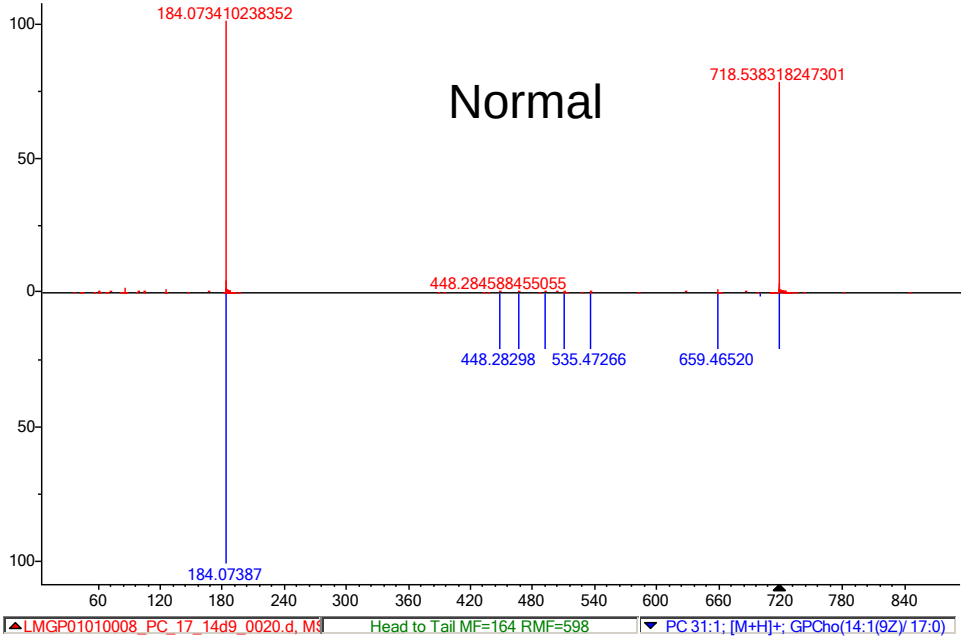


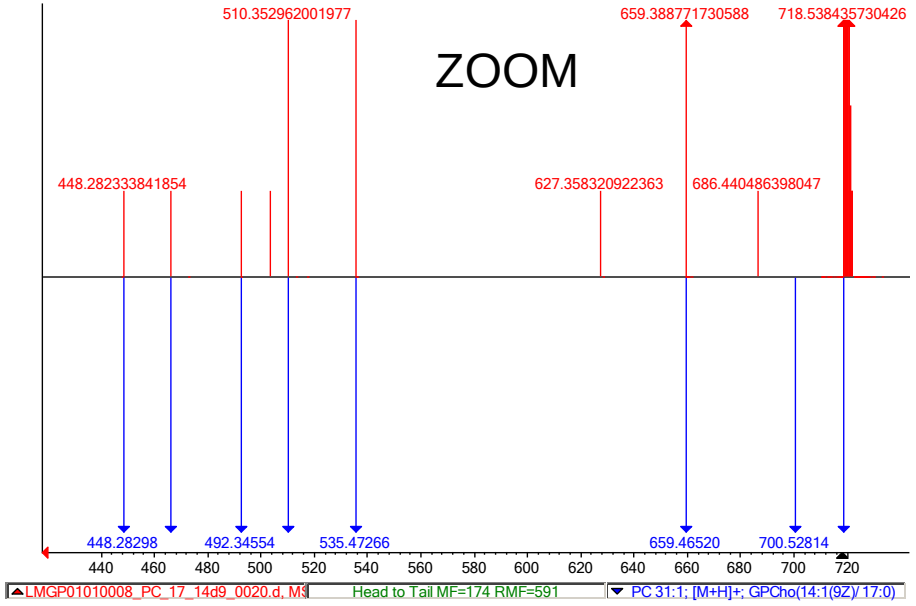
ID in LipidBlast – First HIT

Name: lysoPC 14:0; [M+H]+; PC(14:0/0:0)
MW: 468 ID#: 9185 DB: lipidblast-pos
Comment: Parent=468.30900 Mz_exact=468.30900 ; lysoPC 14:0; [M+H]+; PC(14:0/0:0); C22H46NO7P
4 largest peaks:

20) Standards ESI(+) ; Phosphatidylcholine; PC(17:0/14:1(9Z))

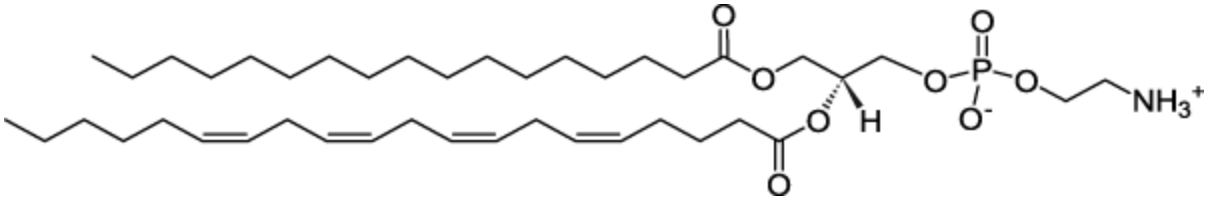


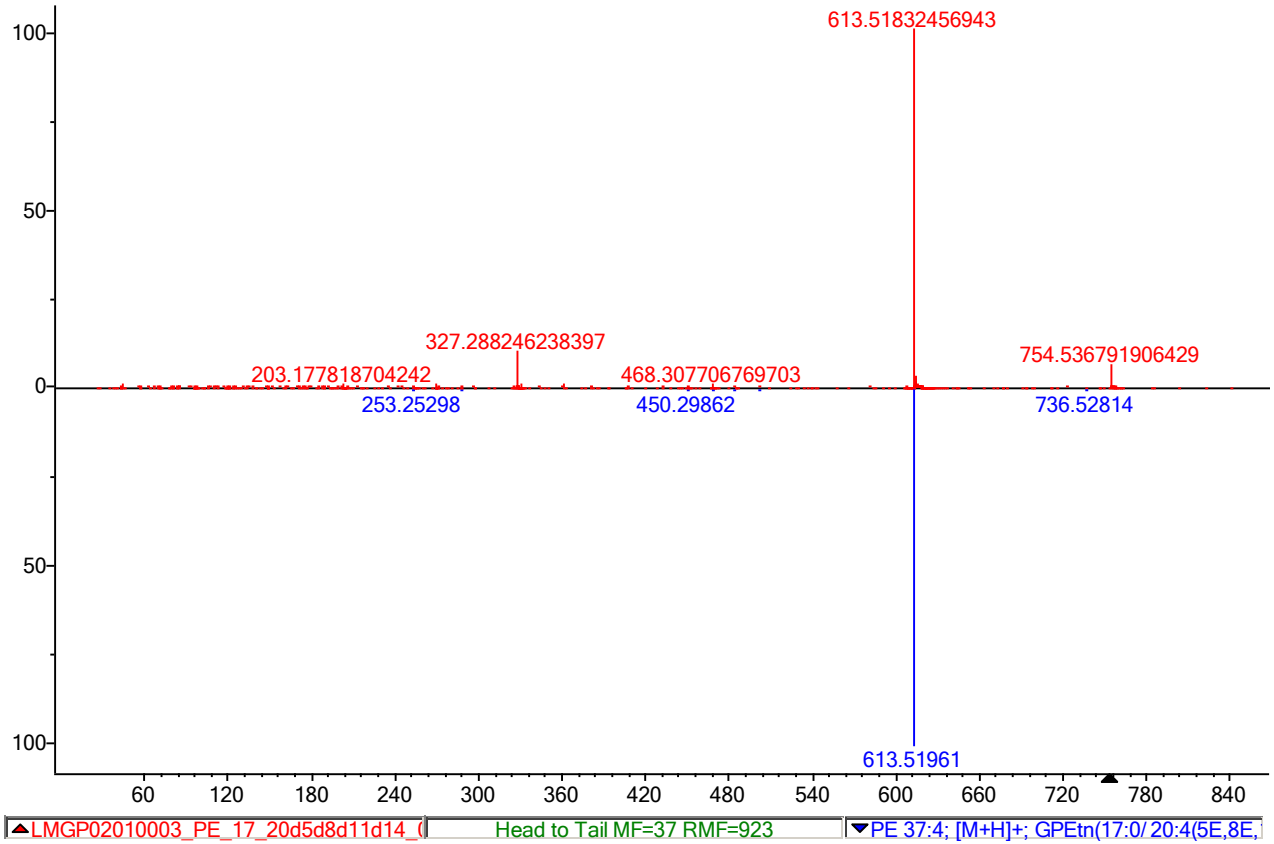




ID in LipidBlast – First HIT
Name: PC 31:1; [M+H]+; GPCho(14:1(9Z)/17:0)
MW: 718 ID#: 1382 DB: custompc+hpos.msp
Comment: Parent=718.53870 Mz_exact=718.53870 ; PC 31:1; [M+H]+; GPCho(14:1(9Z)/17:0); C39H76NO8P

21) Standards ESI(+) ; phosphatidylethanolamine; PE(17:0/20:4(5Z,8Z,11Z,14Z))

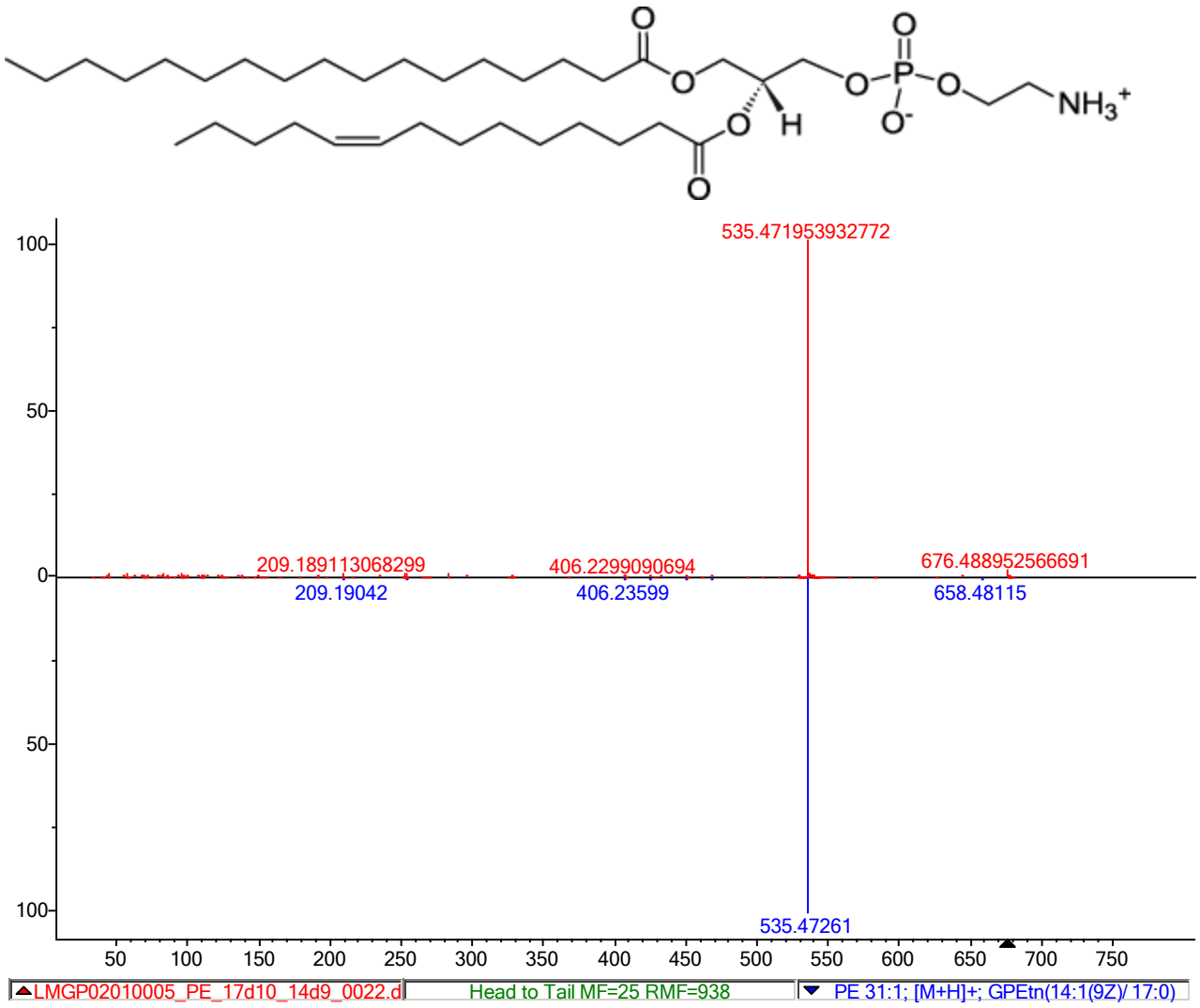




ID in LipidBlast – First HIT

Name: PE 37:4; [M+H]+; GPEtn(17:0/20:4(5E,8E,11E,14E))
MW: 754 ID#: 49431 DB: lipidblast-pos
Comment: Parent=754.53870 Mz_exact=754.53870 ; PE 37:4; [M+H]+; GPEtn(17:0/20:4(5E,8E,11E,14E)); C42H76NO8P

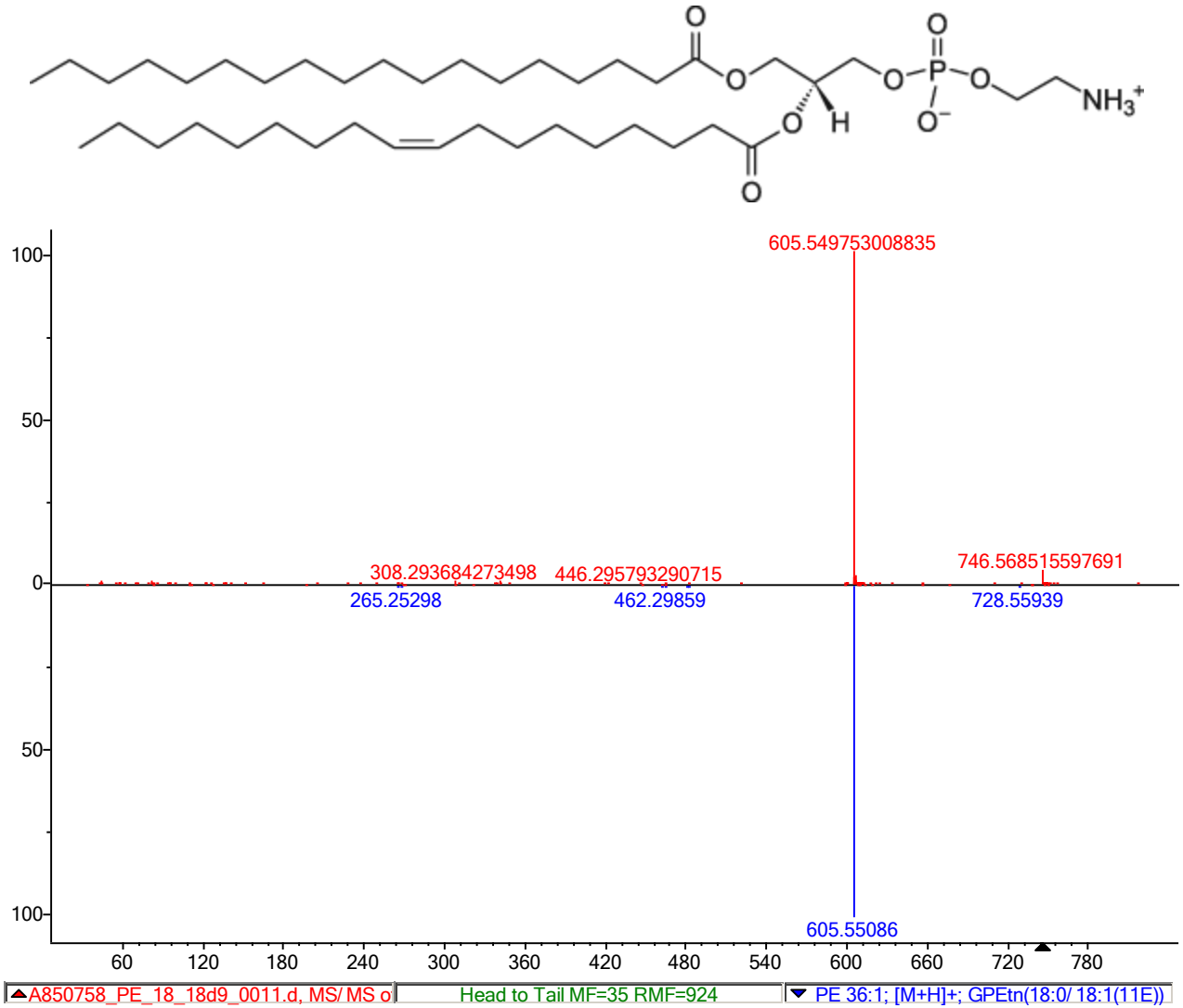
22) Standards ESI(+) ; phosphatidylethanolamine; PE(17:0/14:1(9Z))



Correct ID in LipidBlast – not first HIT – multiple probabilities (few fragments in pos mode)

Name: PE 31:1; [M+H]+; GPEtn(14:1(9Z)/17:0)
MW: 676 ID#: 48954 DB: lipidblast-pos
Comment: Parent=676.49171 Mz_exact=676.49171 ; PE 31:1; [M+H]+; GPEtn(14:1(9Z)/17:0); C36H70NO8P
8 largest peaks:

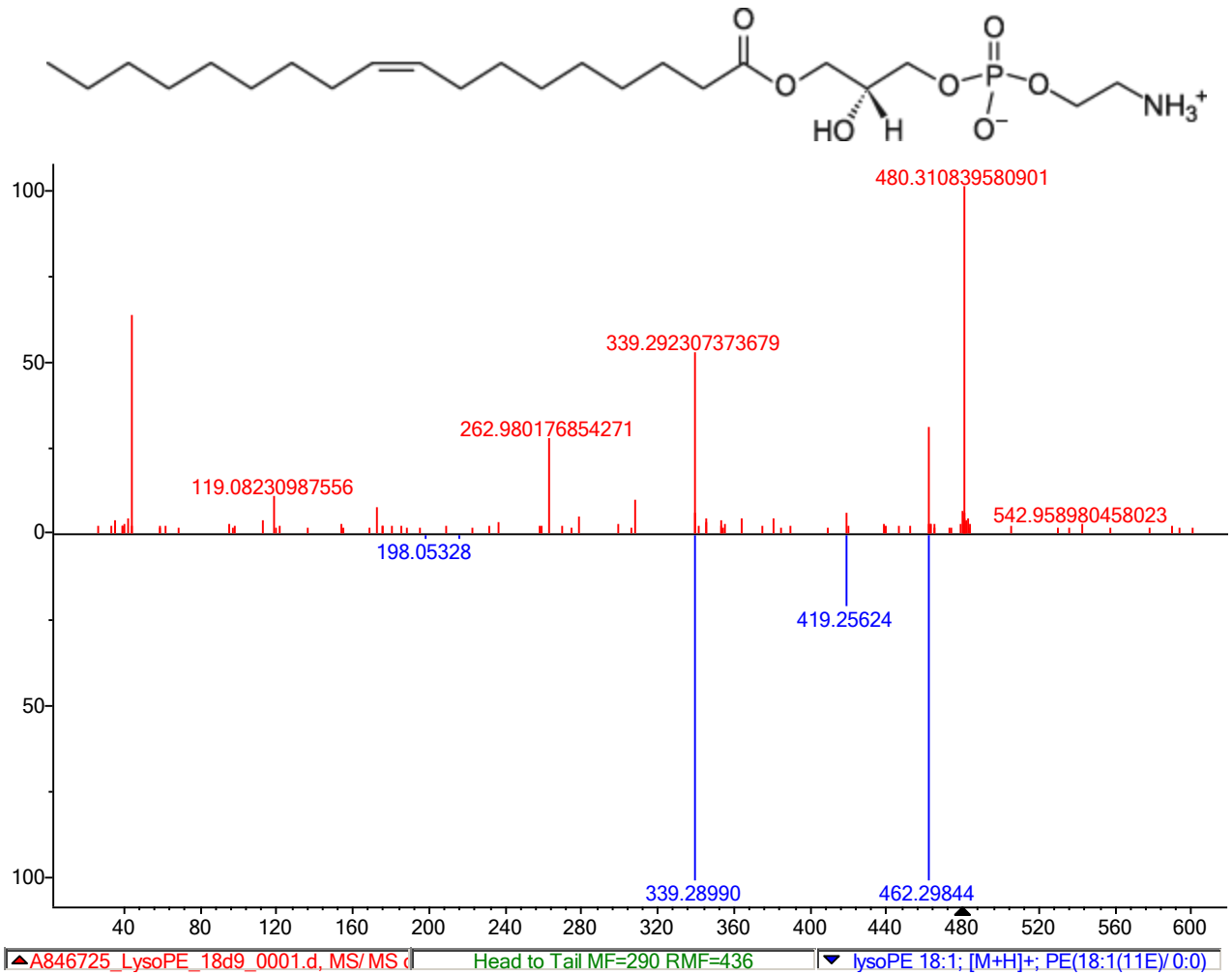
23) Standards ESI(+) ; phosphatidylethanolamine; PE(18:0/18:1(9Z))



ID in LipidBlast – First HIT

Name: PE 36:1; [M+H]+; GPEtn(18:0/18:1(11E))
MW: 746 ID#: 49624 DB: lipidblast-pos
Comment: Parent=746.56995 Mz_exact=746.56995 ; PE 36:1; [M+H]+; GPEtn(18:0/18:1(11E)); C41H80NO8P

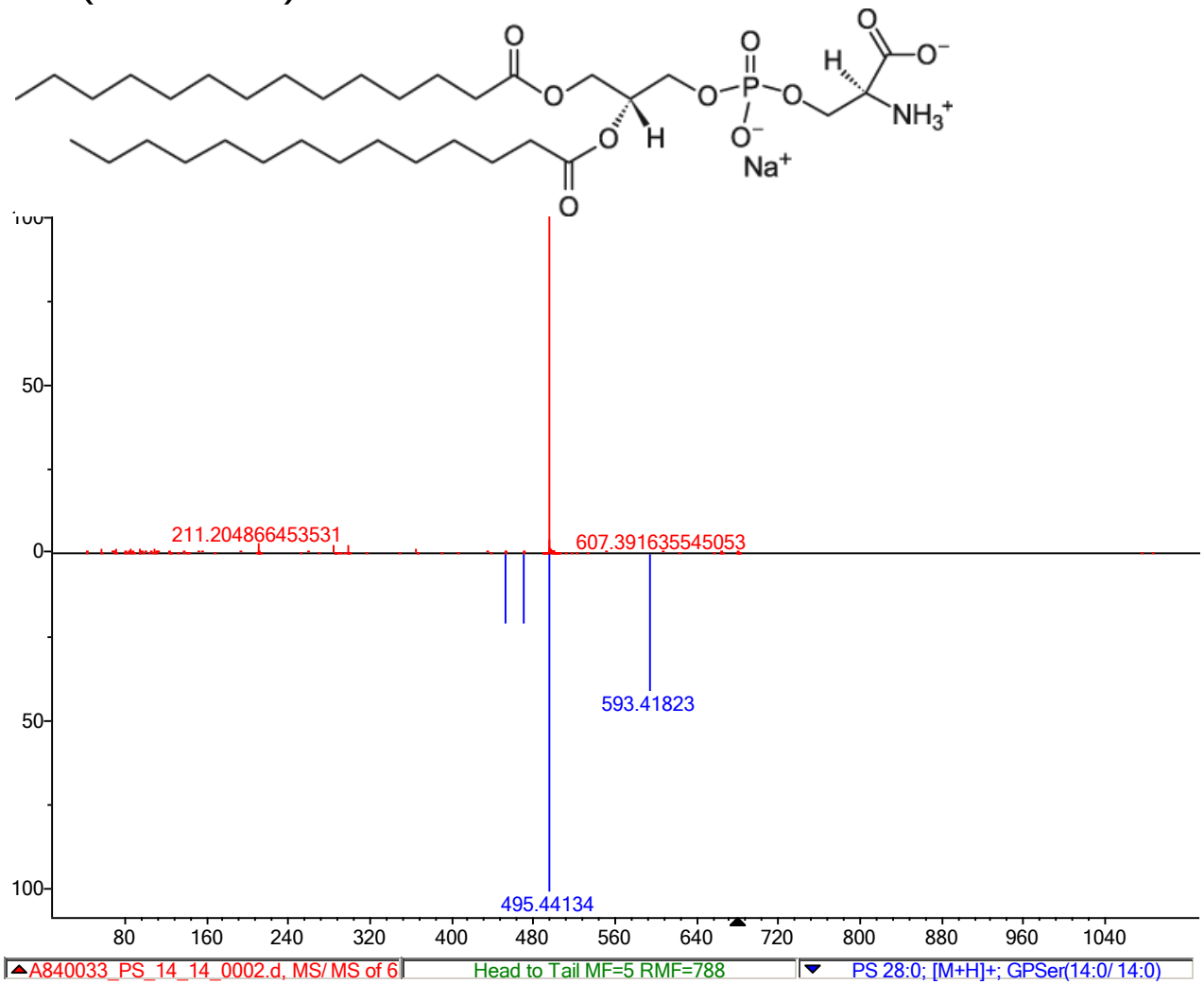
24) Standard Lyso-phosphatidylethanolamine – ESI(+)
PE(18:1(9Z)/0:0



ID in LipidBlast – First HIT

Name: lysoPE 18:1; [M+H]+; PE(18:1(11E)/0:0)
MW: 480 ID#: 9360 DB: lipidblast-pos
Comment: Parent=480.30900 Mz_exact=480.30900 ; lysoPE 18:1; [M+H]+; PE(18:1(11E)/0:0); C23H46NO7P
5 largest peaks:

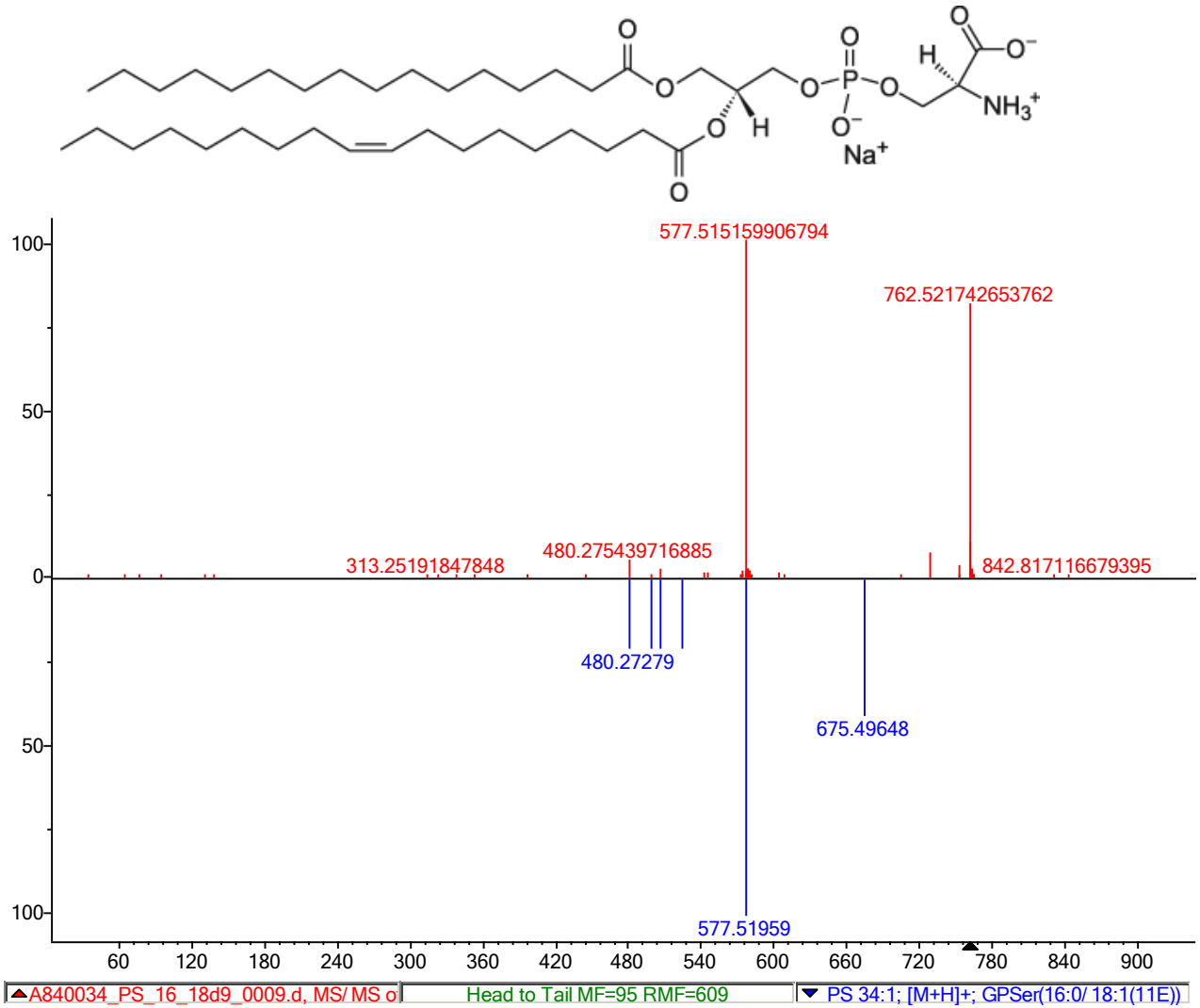
25) Standard phosphatidylserine – ESI(+)
PS(14:0/14:0)



ID in LipidBlast – First HIT

Name: PS 28:0; [M+H]+; GPSer(14:0/14:0)
MW: 680 ID#: 60713 DB: lipidblast-pos
Comment: Parent=680.45026 Mz_exact=680.45026 ; PS 28:0; [M+H]+; GPSer(14:0/14:0); C34H66NO10P
4 largest peaks:

26) Standard phosphatidylserine – ESI(+)
PS(16:0/18:1(9Z))

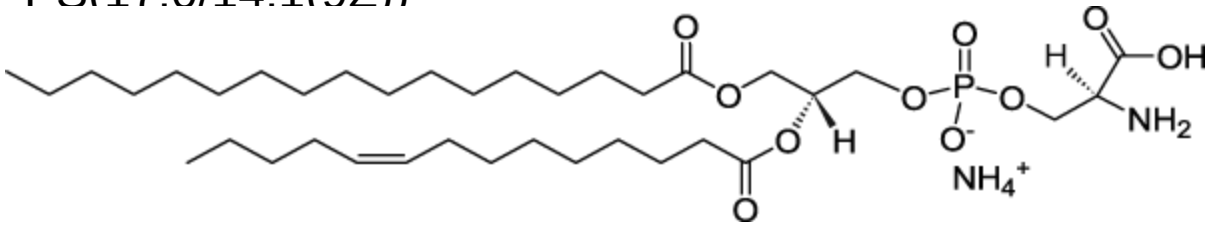


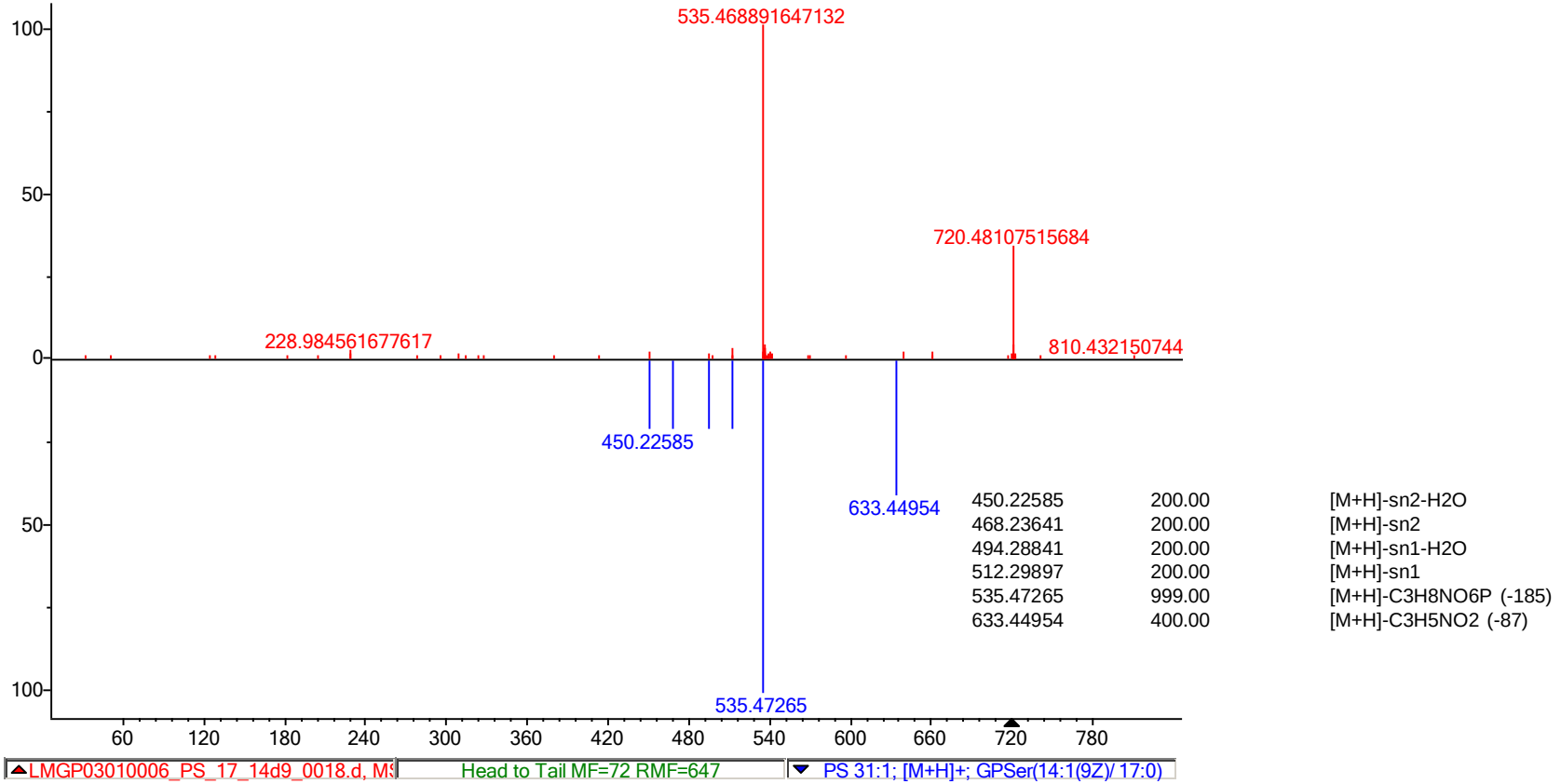
ID in LipidBlast – First HIT

Name: PS 34:1; [M+H]+; GPSer(16:0/18:1(11E))
MW: 762 ID#: 61020 DB: lipidblast-pos
Comment: Parent=762.52851 Mz_exact=762.52851 ; PS 34:1; [M+H]+; GPSer(16:0/18:1(11E)); C40H76NO10P

27) Standard phosphatidylserine – ESI(+)

PS(17:0/14:1(9Z))



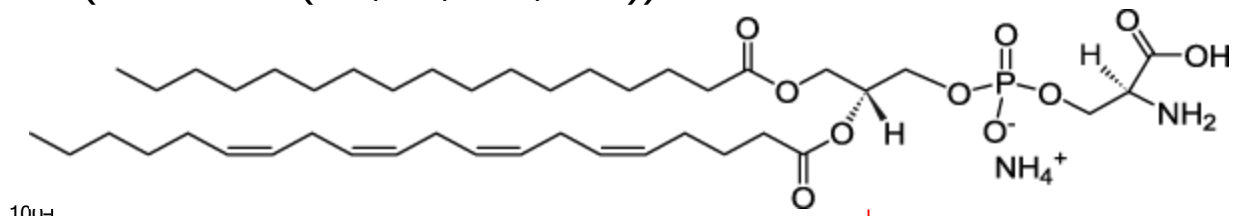


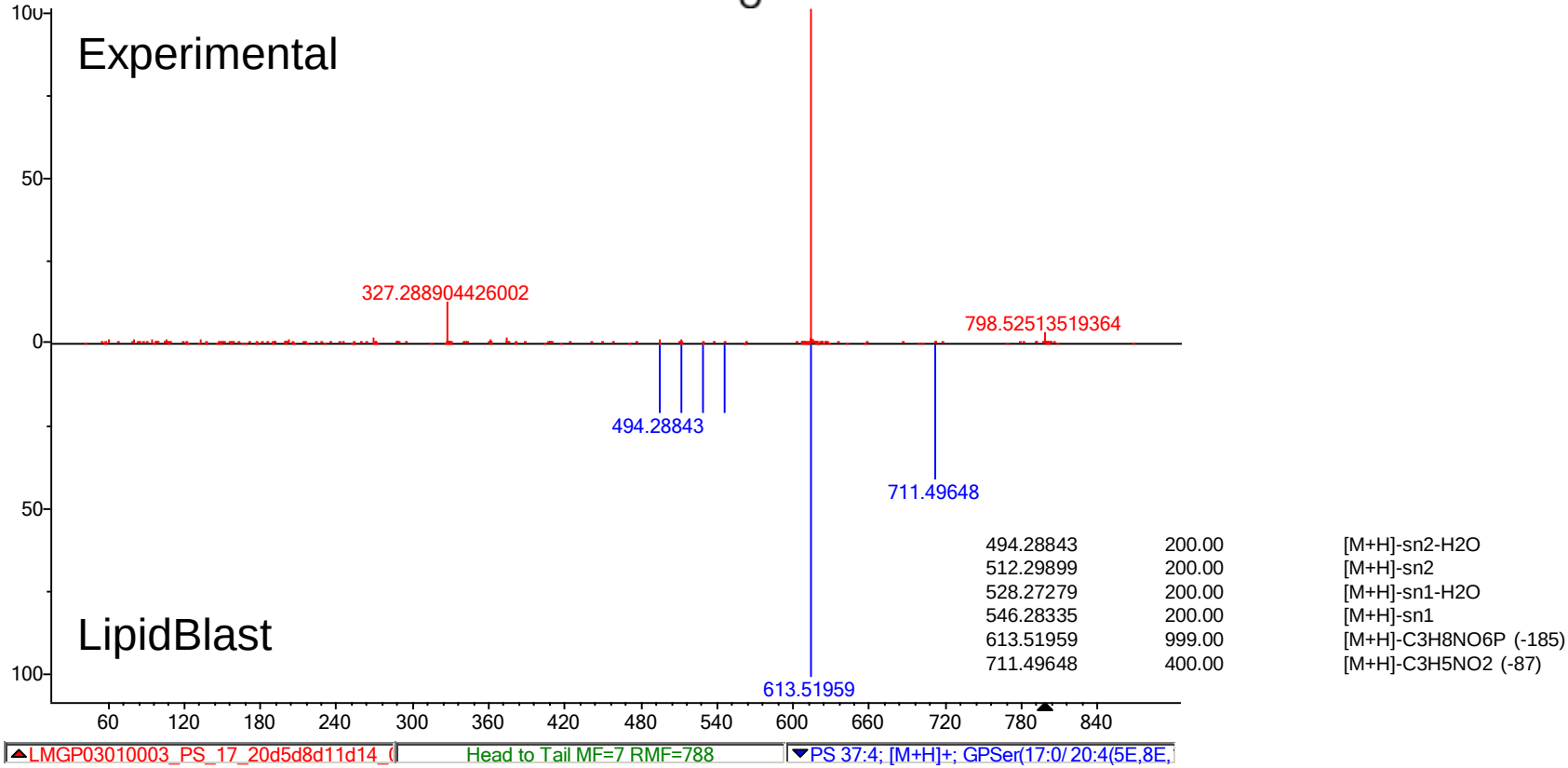
450.22585	200.00	[M+H]-sn2-H2O
468.23641	200.00	[M+H]-sn2
494.28841	200.00	[M+H]-sn1-H2O
512.29897	200.00	[M+H]-sn1
535.47265	999.00	[M+H]-C3H8NO6P (-185)
633.44954	400.00	[M+H]-C3H5NO2 (-87)

ID in LipidBlast – First HIT

Name: PS 31:1; [M+H]+; GPSer(14:1(9Z)/17:0)
MW: 720 ID#: 60794 DB: lipidblast-pos
Comment: Parent=720.48157 Mz_exact=720.48157 ; PS 31:1; [M+H]+; GPSer(14:1(9Z)/17:0); C37H70NO10P

28) Standard phosphatidylserine – ESI(+)
PS(17:0/20:4(5Z,8Z,11Z,14Z))

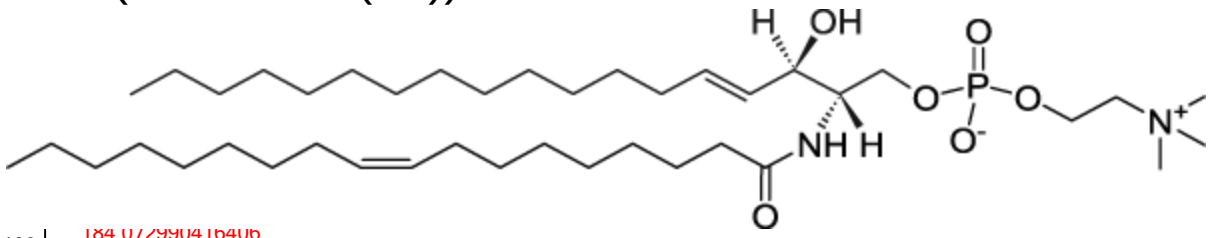


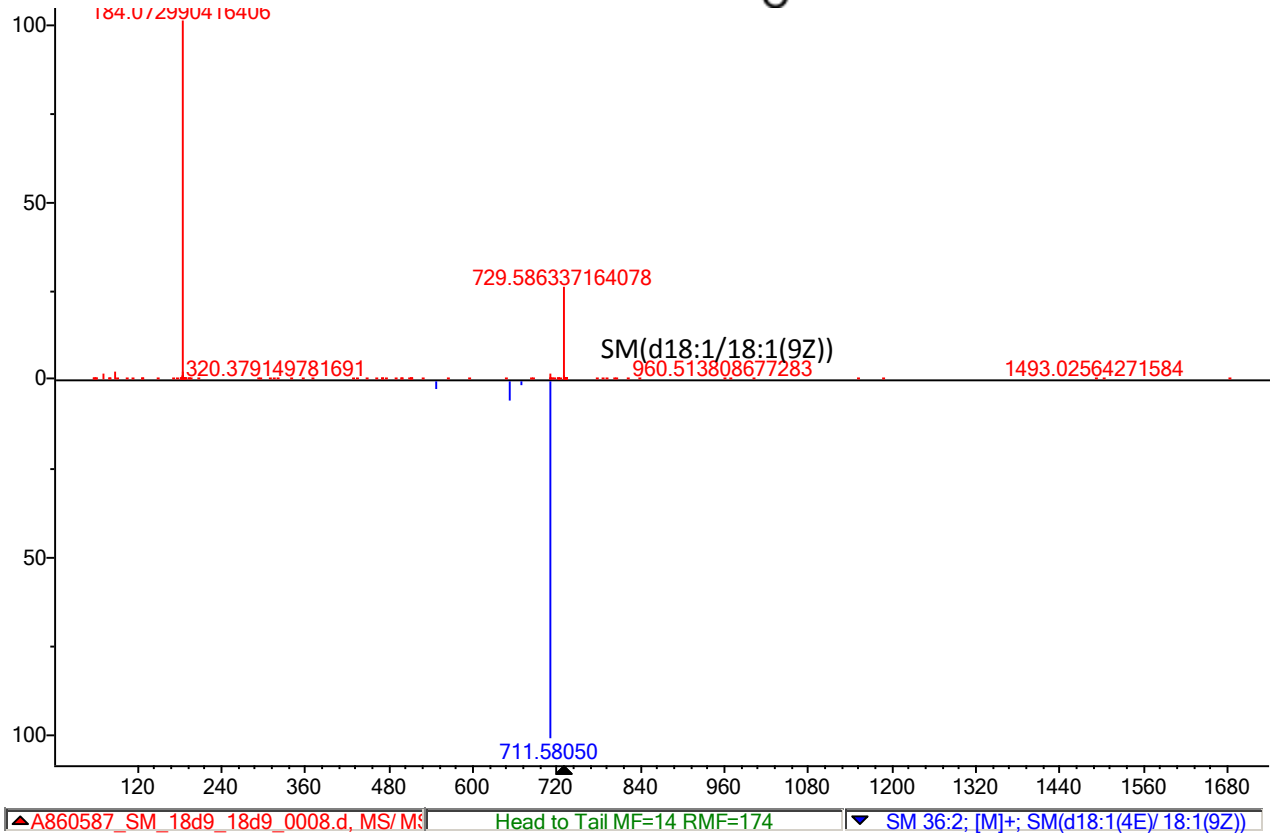


ID in LipidBlast – First HIT

Name: PS 37:4; [M+H]+; GPSer(17:0/20:4(5E,8E,11E,14E))
MW: 798 ID#: 61271 DB: lipidblast-pos
Comment: Parent=798.52851 Mz_exact=798.52851 ; PS 37:4; [M+H]+; GPSer(17:0/20:4(5E,8E,11E,14E)); C43H76NO10P
6 largest peaks:

29) Standard sphingomyleine – ESI+)
SM(d18:1/18:1(9Z))





ID in LipidBlast – First HIT

Name: SM 36:2; [M]+; SM(d18:1(4E)/18:1(9Z))
MW: 729 ID#: 70192 DB: lipidblast-pos
Comment: Parent=729.59106 Mz_exact=729.59106 ; SM 36:2; [M]+; SM(d18:1(4E)/18:1(9Z)); C41H82N2O6P
4 largest peaks:

Supplement Literature Collection for LipidBlast MS/MS library;
http://fiehnlab.ucdavis.edu/projects/LipidBlast

For questions please contact the curator: Dr. Tobias Kind (Date: May 2010)
http://fiehnlab.ucdavis.edu/staff/kind/

The development of the MS/MS LipidBlast libraries is based on own experimental data and more than ~300 external literature references. Not all references can be included into the publication due to publishing limits and therefore are given here. References from the paper itself may not be referenced here.

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End of supplement