

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

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

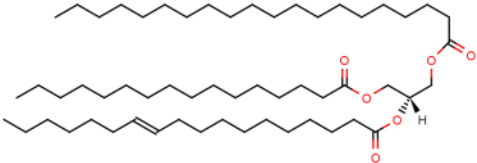
The structure drawing files (*.mrv) MarvinSketch
can be found under:

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

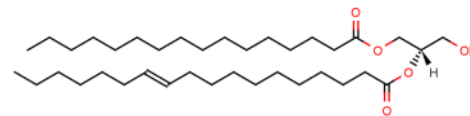
**Tobias Kind, Oliver Fiehn
FiehnLab – Metabolomics
UC Davis Genome Center, Davis, USA**

Covered structures and MS/MS spectra in LipidBlast

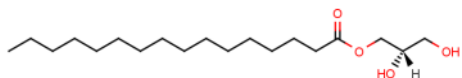
Num	Lipid class	PIC	Short Name	Number compounds	Number MS/MS spectra	Number MS/MS libraries
1	Phosphatidylcholines	ok	PC	5,476	10,952	2
2	Lysophosphatidylcholines	ok	lysoPC	80	160	2
3	Plasmenylphosphatidylcholines	ok	plasmenyl-PC	222	444	2
4	Phosphatidylethanolamines	ok	PE	5,476	16,428	3
5	Lysophosphatidylethanolamines	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



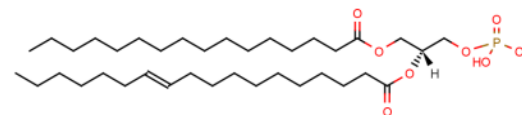
Abbreviation TG(16:0/18:1(11E)/20:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-3-eicosanoyl-sn-glycerol
Formula C57H108O6
Mass 888.81



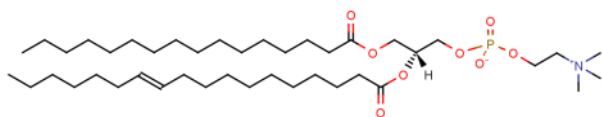
Abbreviation DG(16:0/18:1(11E)/0:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycerol
Formula C37H70O5
Mass 594.52



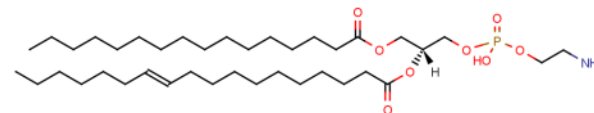
Abbreviation MG(16:0/0:0/0:0)
Systematic Name 1-hexadecanoyl-sn-glycerol
Formula C19H38O4
Mass 330.28



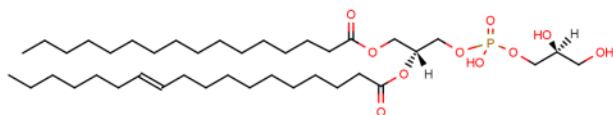
Abbreviation PA(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphate
Formula C37H71O8P
Mass 674.49



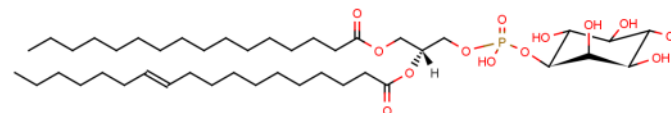
Abbreviation PC(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphocholine
Formula C42H82NO8P
Mass 759.58



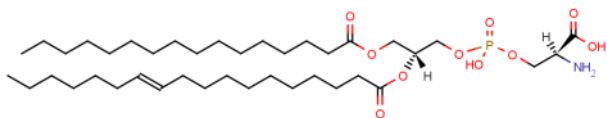
Abbreviation PE(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoethanolamine
Formula C39H76NO8P
Mass 717.53



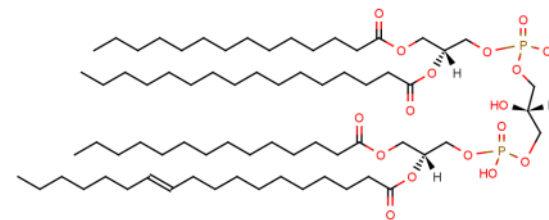
Abbreviation PG(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-sn-glycerol)
Formula C40H77O10P
Mass 748.53



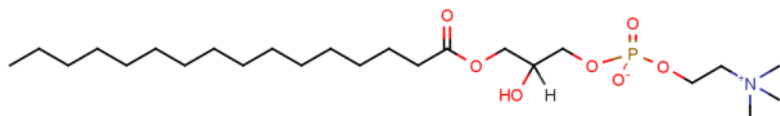
Abbreviation PI(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-myo-inositol)
Formula C43H81O13P
Mass 836.54



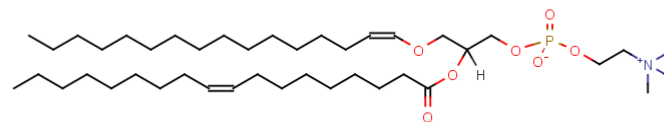
Abbreviation PS(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoserine
Formula C40H76NO10P
Mass 761.52



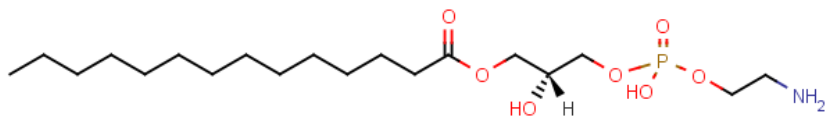
Abbreviation CL(1'-[14:0/16:0],3'-[14:0/18:1(11E)])
Systematic Name 1'-[1-tetradecanoyl-2-hexadecanoyl-sn-glycero-3-phospho],3'-[1-tetradecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho]-sn-glycerol
Formula C71H136O17P2
Mass 1322.93



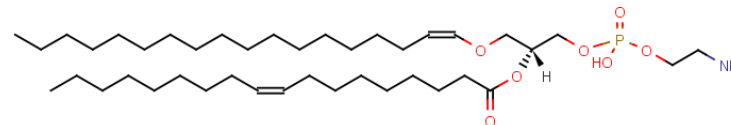
Common Name PC(16:0/0:0)[U] (lysoPC)
Systematic Name 1-hexadecanoyl-sn-glycero-3-phosphocholine
Exact Mass 495.33
Formula C24H50NO7P



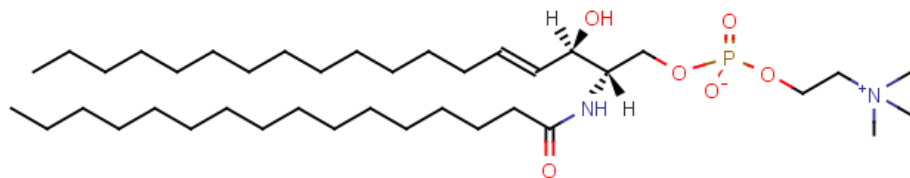
LM ID LMGP01030007 (plasmeyl-PC)
Common Name PC(P-16:0/18:1(9Z))[U]
Exact Mass 743.58
Formula C42H82NO7P



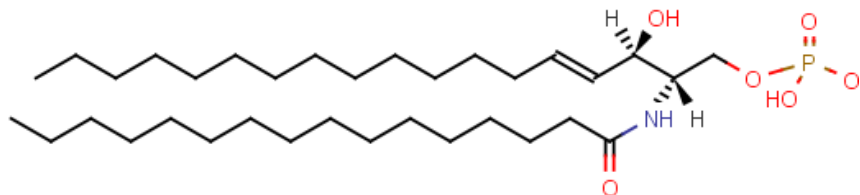
LM ID LMGP02050003 (lysoPE)
Common Name PE(14:0/0:0)
Exact Mass 425.25
Formula C19H40NO7P



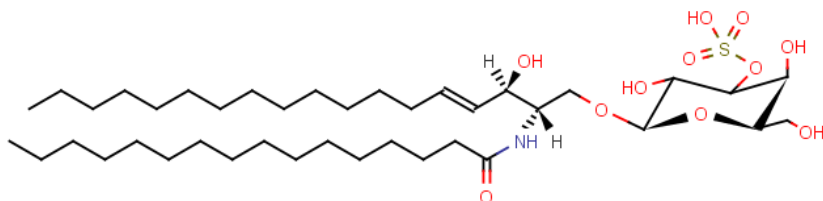
LM ID LMGP02030004 (plasmeyl-PE)
Common Name PE(P-18:0/18:1(9Z))
Exact Mass 729.57
Formula C41H80NO7P



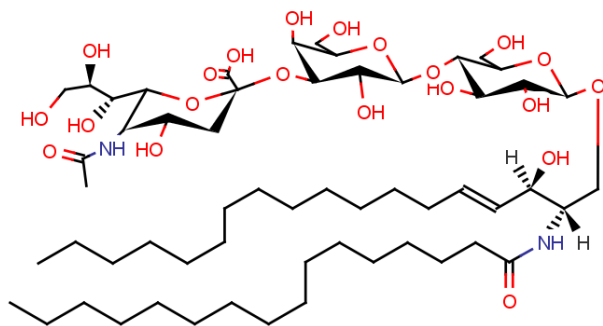
LM ID LMSP03010003
Common Name SM(d18:1/16:0)
Systematic Name N-(hexadecanoyl)-sphing-4-enine-1-phosphocholine
Synonyms C16 Sphingomyelin
Exact Mass 702.57
Formula C39H79N2O6P



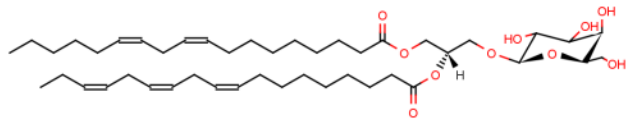
LM ID LMSP02050002 (Ceramide-phosphate)
Common Name CerP(d18:1/16:0)
Systematic Name N-(hexadecanoyl)-sphing-4-enine-1-phosphate
Synonyms C16 CerP
Exact Mass 617.48
Formula C34H68NO6P



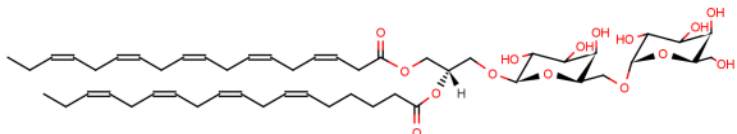
LM ID LMSP06020002
Common Name C16 Sulfatide
Systematic Name (3'-sulfo)Galβ-Cer(d18:1/16:0)
Synonyms C16 Sulfatide
Exact Mass 779.52
Formula C40H77NO11S



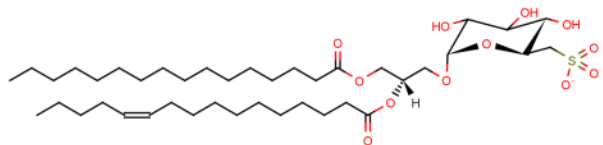
LM ID LMSP0601AJ01 (GM3 ganglioside)
Common Name -
Systematic Name NeuAca2-3Galβ1-4Glcβ-Cer(d18:1/16:0)
Synonyms -
Exact Mass 1152.71
Formula C57H104N2O21



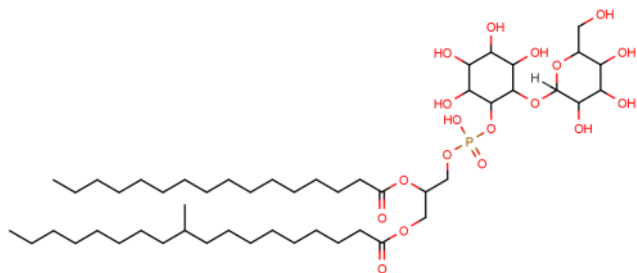
LM ID LMGL05010024
Common Name MGDG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Systematic Name 1-(9Z,12Z-octadecadienoyl)-2-(9Z,12Z,15Z-octadecatrienoyl)-3-O-β-D-galactosyl-sn-glycerol
Synonyms Monogalactosyldiacylglycerol(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Exact Mass 776.54
Formula C45H76O10



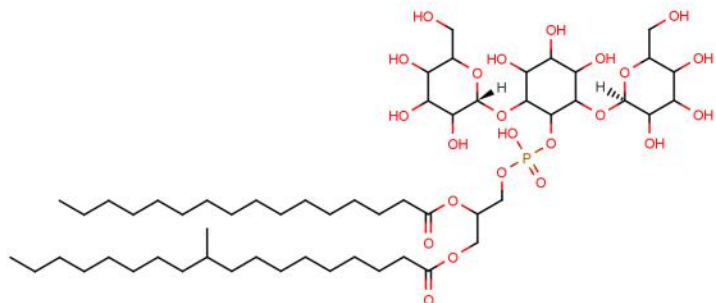
LM ID LMGL05010010
Common Name DGDG(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))
Systematic Name 1-(3Z,6Z,9Z,12Z,15Z-octadecapentaenoyl)-2-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-3-O-(6'-O-α-D-galactosyl-β-D-galactosyl)-sn-glycerol
Synonyms Digalactosyldiacylglycerol(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))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



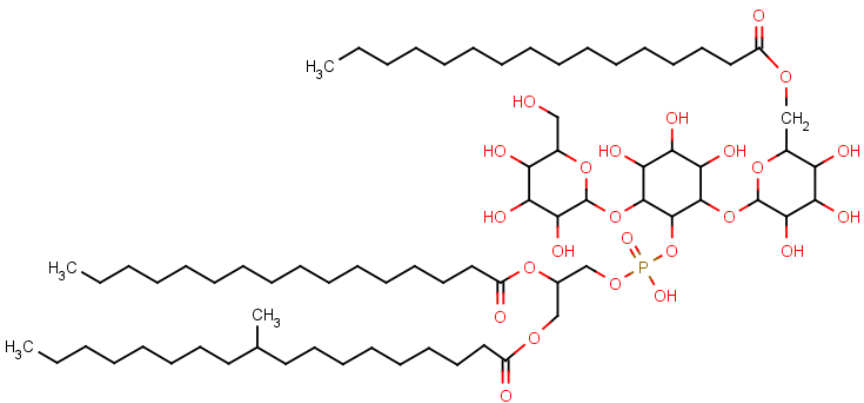
LM ID LMGL05010007
Common Name SQDG(16:0/16:1(11Z))
Systematic Name 1-hexadecanoyl-2-(11Z-hexadecenoyl)-3-(6'-sulfo-α-D-quinovosyl)-sn-glycerol
Synonyms sulfoquinovosyldiacylglycerols; SQDG(16:0/16:1)
Exact Mass 791.50
Formula C41H75O12S



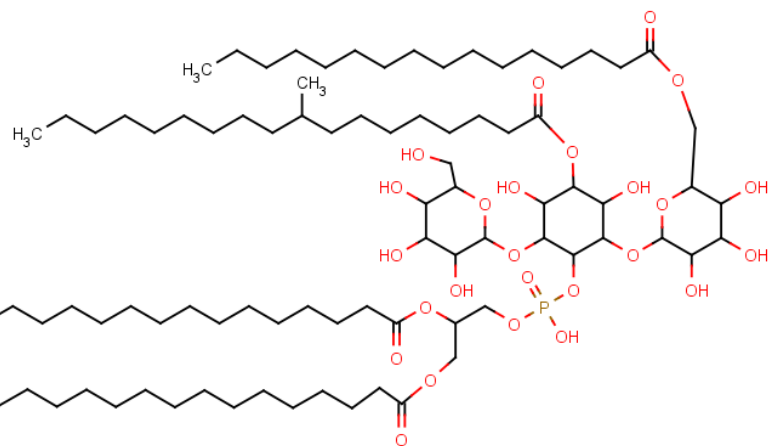
Diacylated phosphatidylinositol monomannoside Ac2PIM1
Ac2PIM1(16:0/methyl-18:0)
C50H95O18P
1014.625603



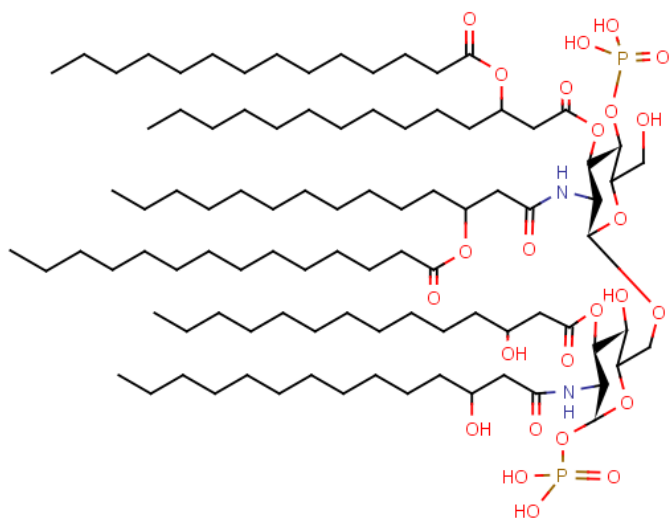
Diacylated phosphatidylinositol dimannoside Ac2PIM2
Ac2PIM2(16:0/methyl-18:0)
C56H105O23P
Mass: 1176.678426



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>

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

FiehnLab – Metabolomics

UC Davis Genome Center, Davis, USA

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 ⁺

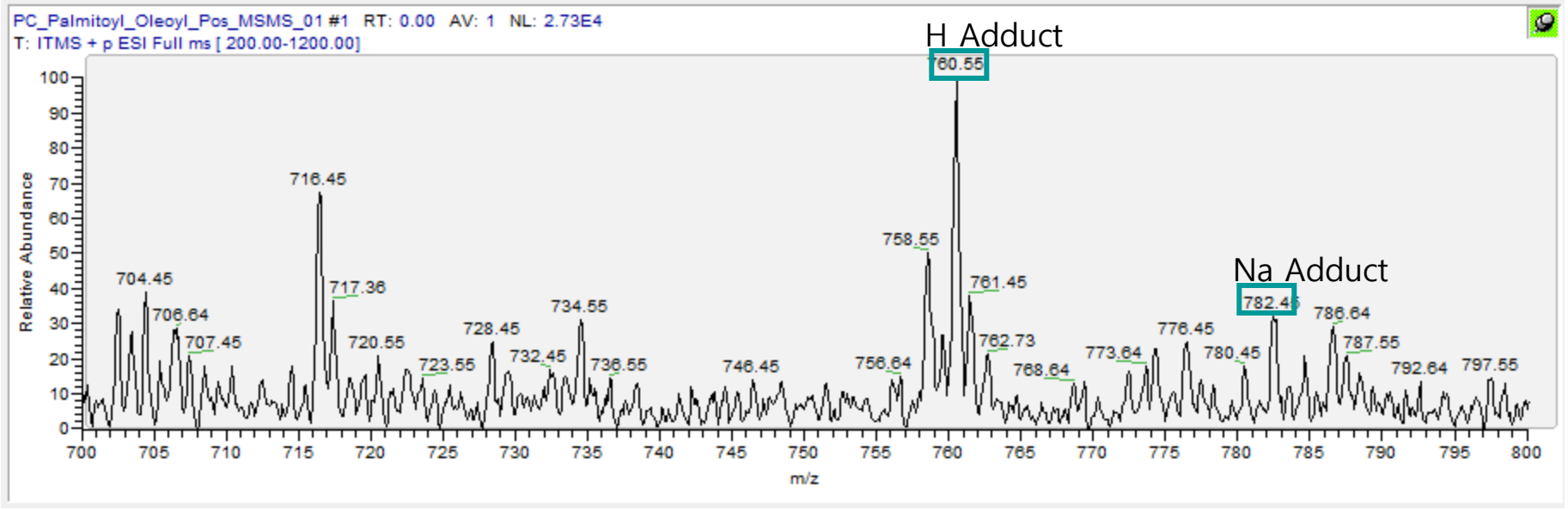
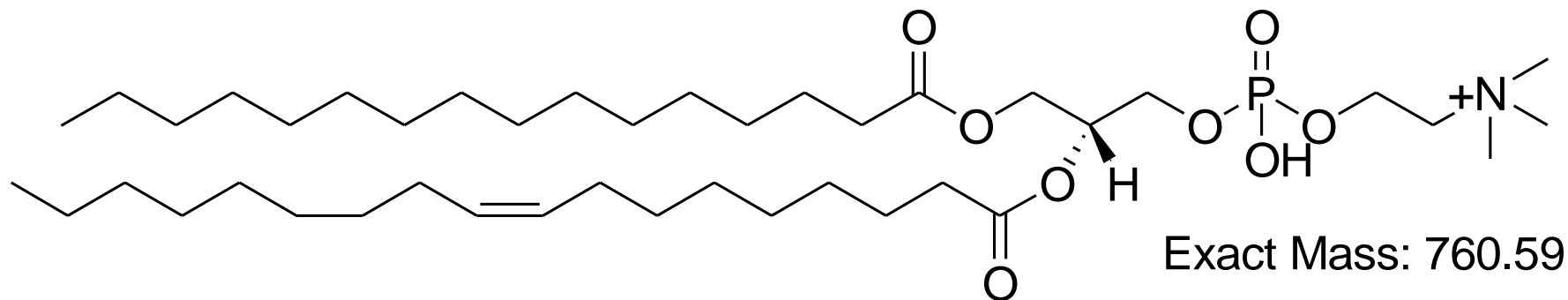
(Na⁺), (H⁺), (Ac⁻): Adduct Ion,
* Characteristic Fragment Ion

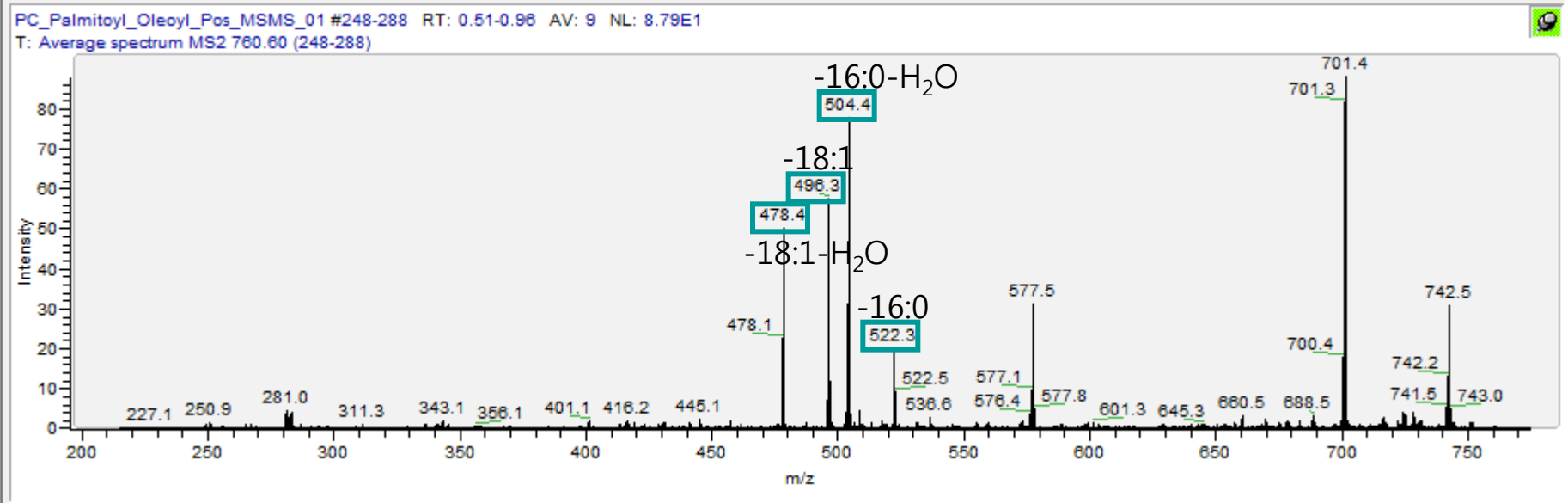
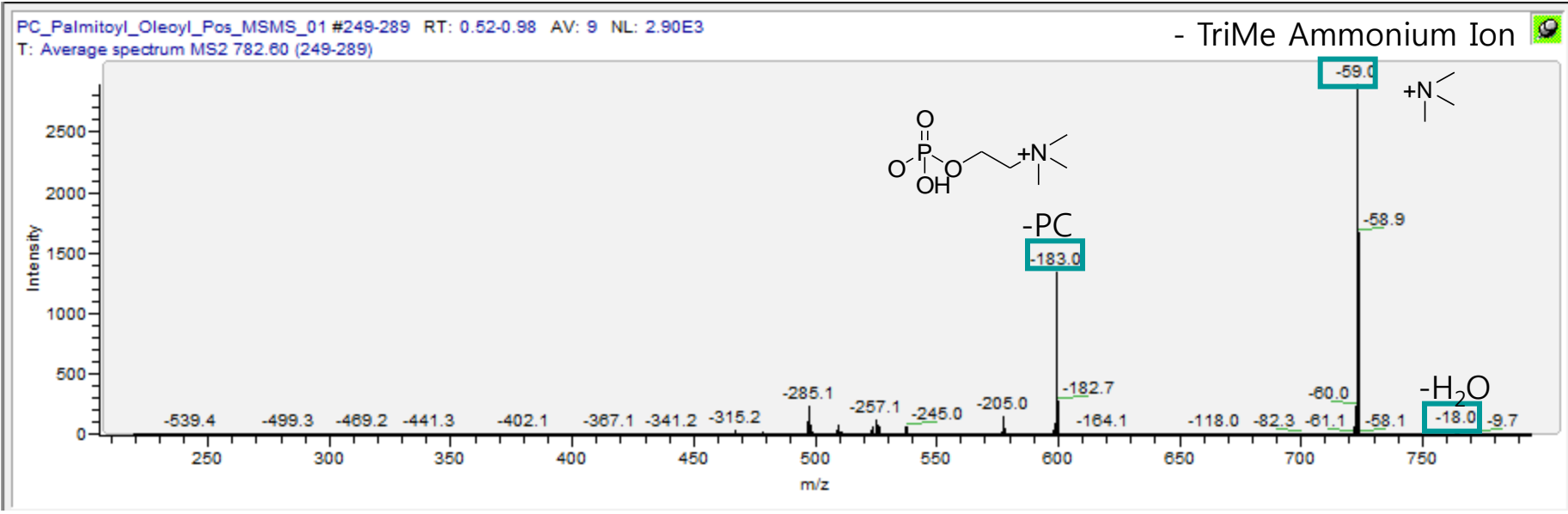
Both: (Na⁺) or (H⁺)

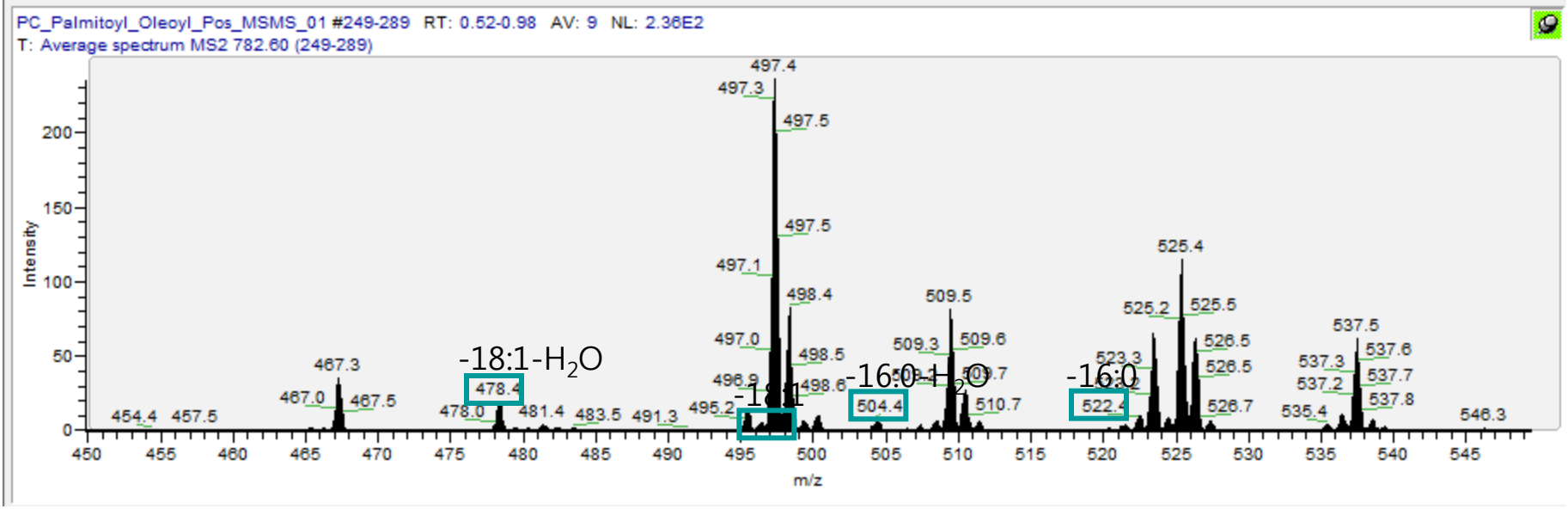
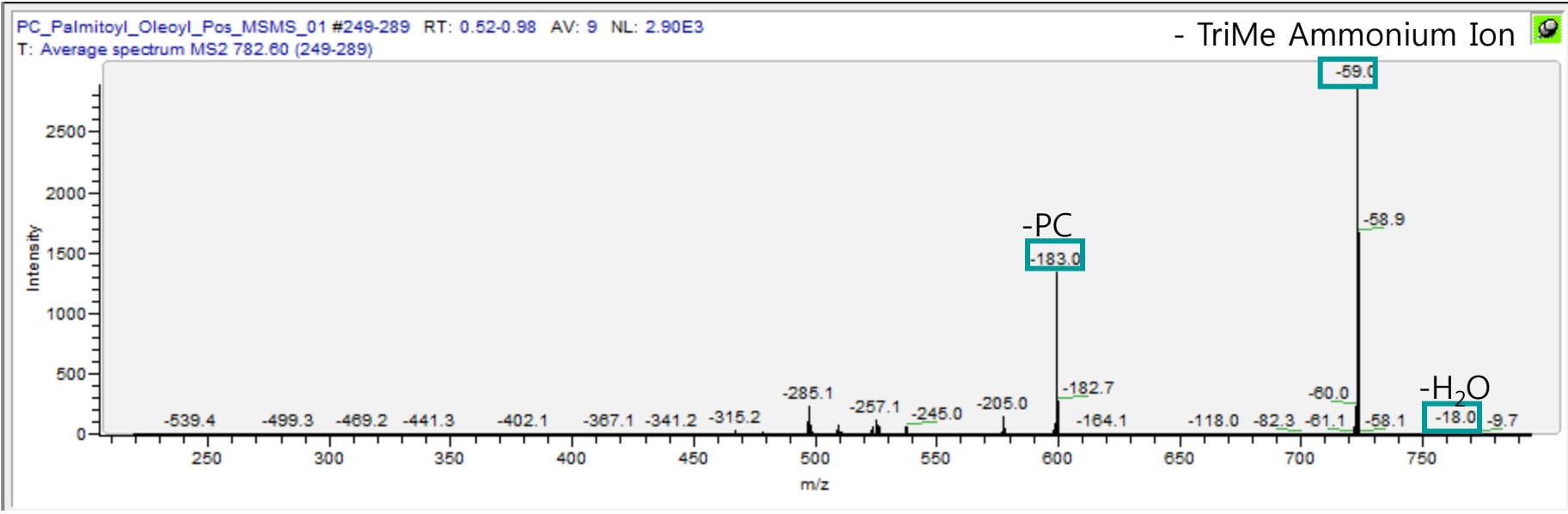
Phosphatidylcholine ID

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

Pos. Mode

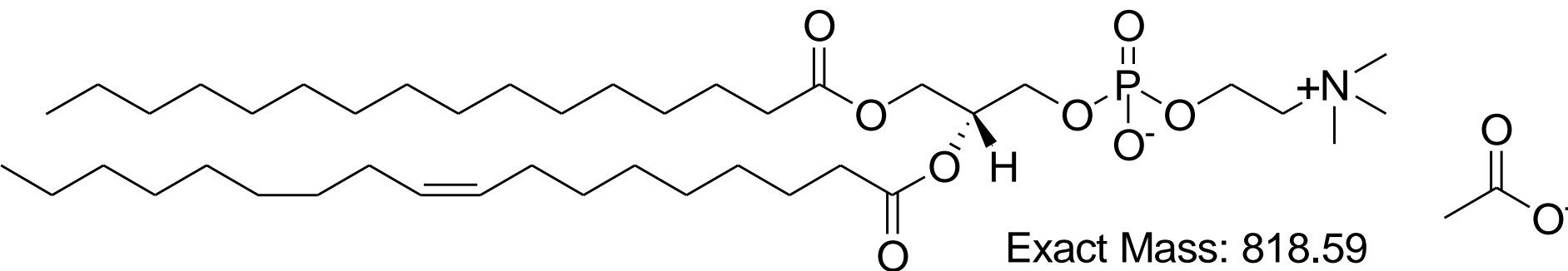




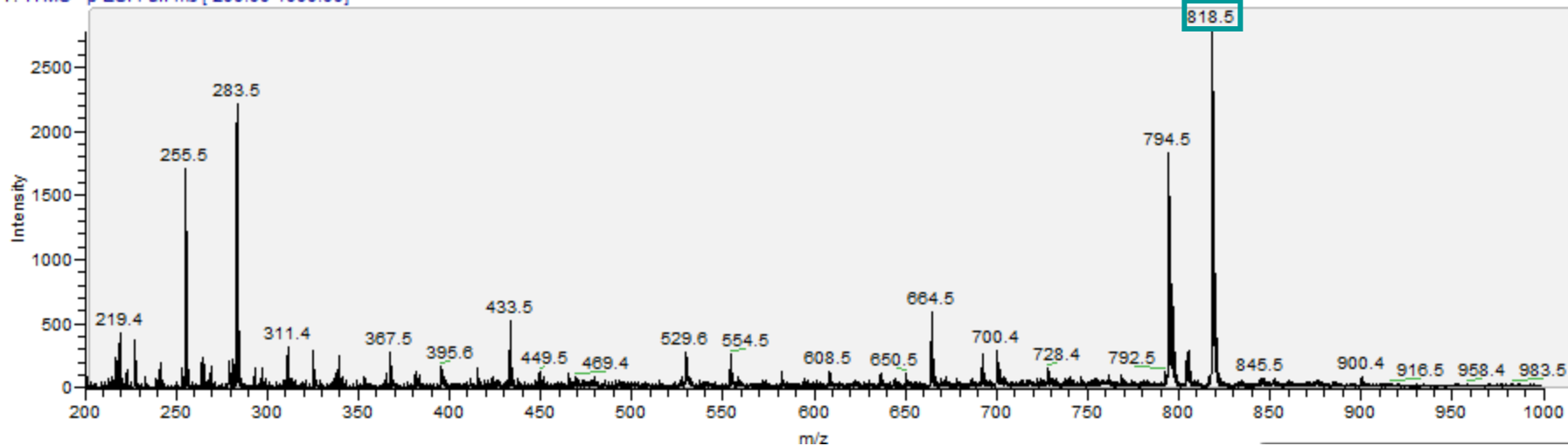


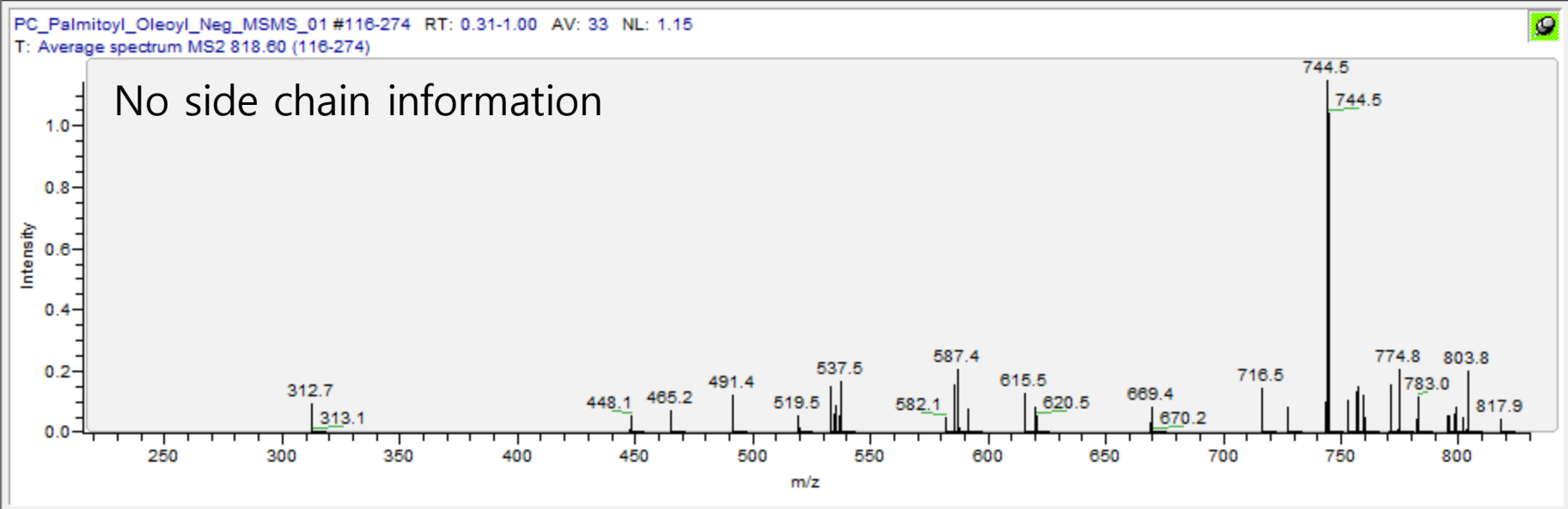
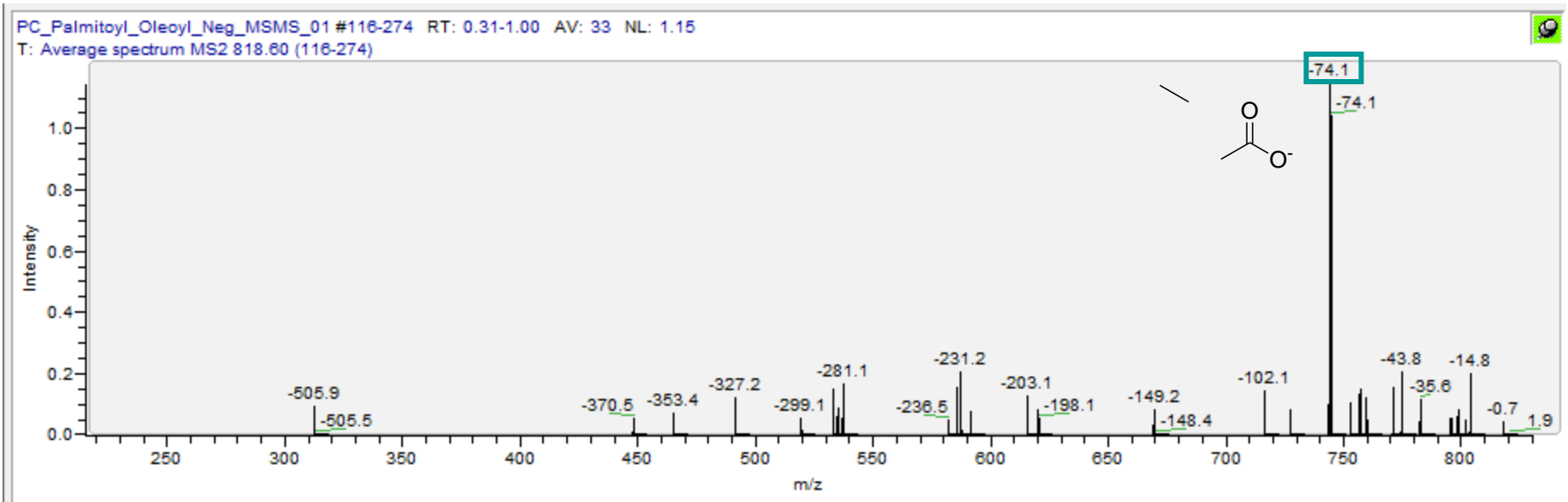
m/z 818.6 (PC 34:1, Acetate Adduct (16:0, 18:1))

Neg. Mode



PC_Palmitoyl_Oleoyl_Neg_MSMS_01 #18-113 RT: 0.05-0.30 AV: 96 NL: 2.78E3
T: ITMS - p ESI Full ms [200.00-1000.00]





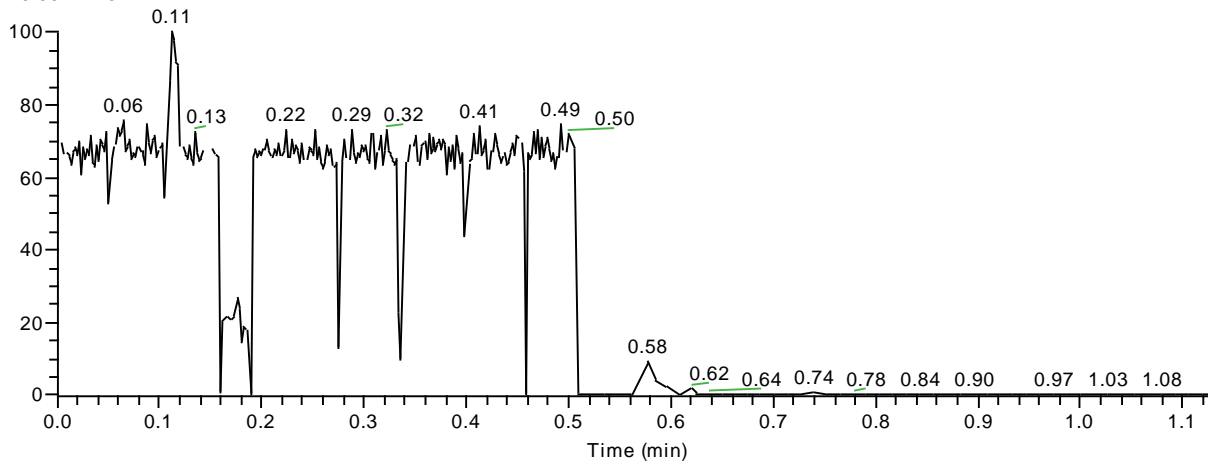
PC – Bovine brain

090325_PCs_Pos_CE25_MSMS_01

3/25/2009 10:44:40 AM

PL Standard

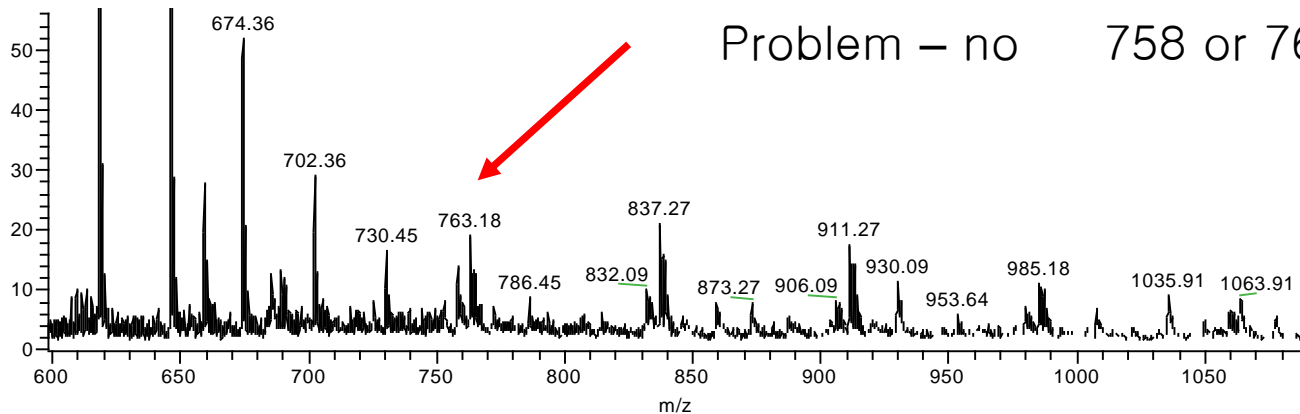
RT: 0.00 - 1.13



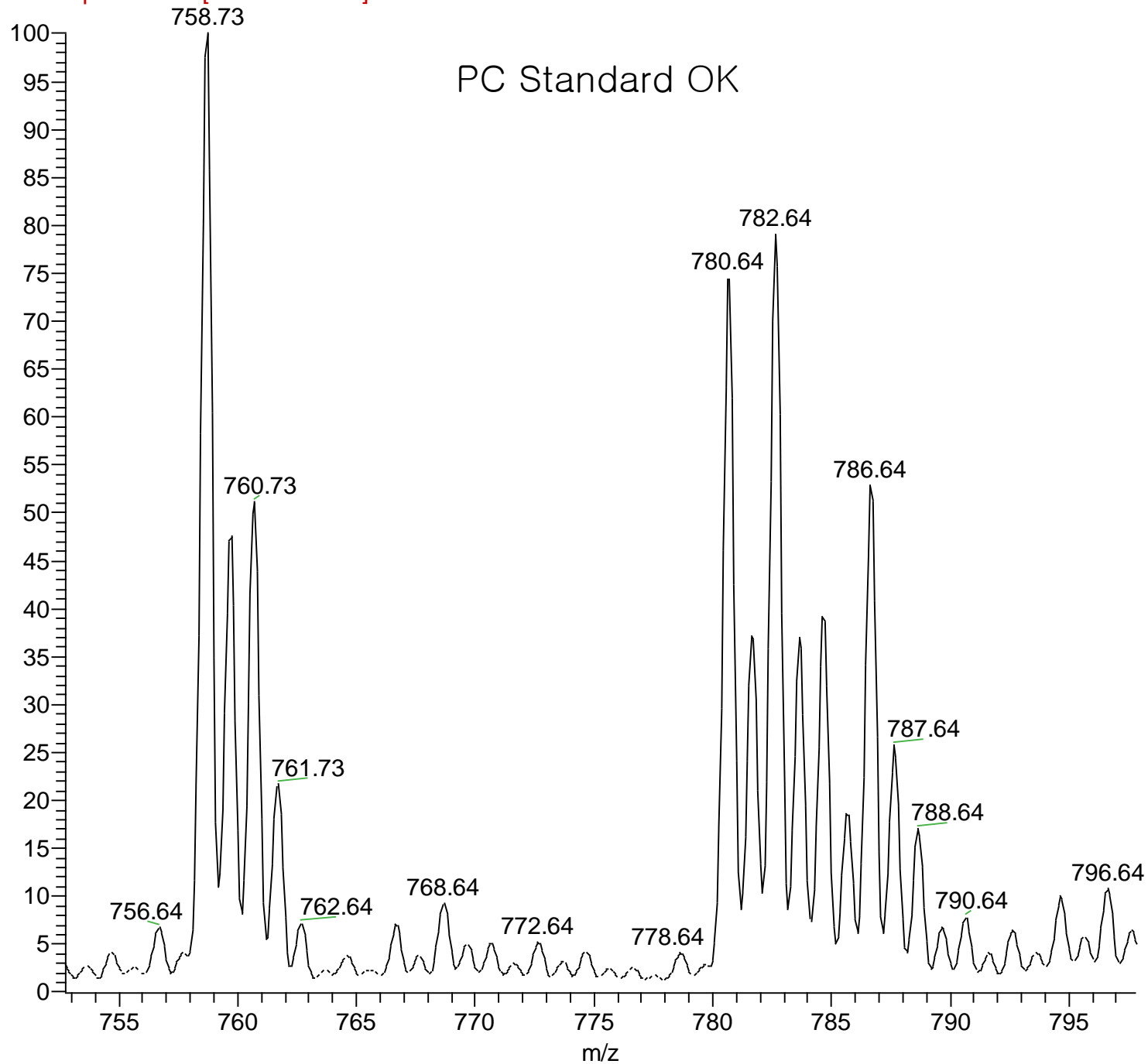
NL:
4.35E6
TIC MS
090325_PC
s_Pos_CE2
5_MSMS_0
1

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]



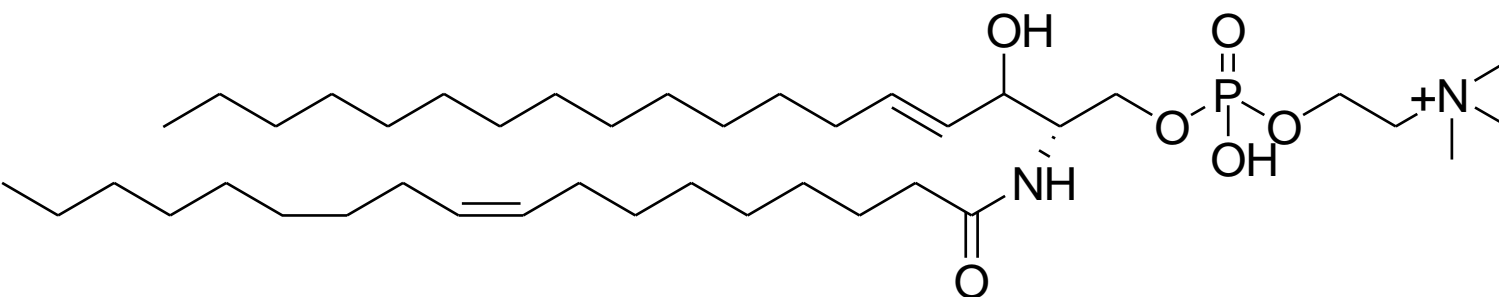
Problem – no 758 or 760



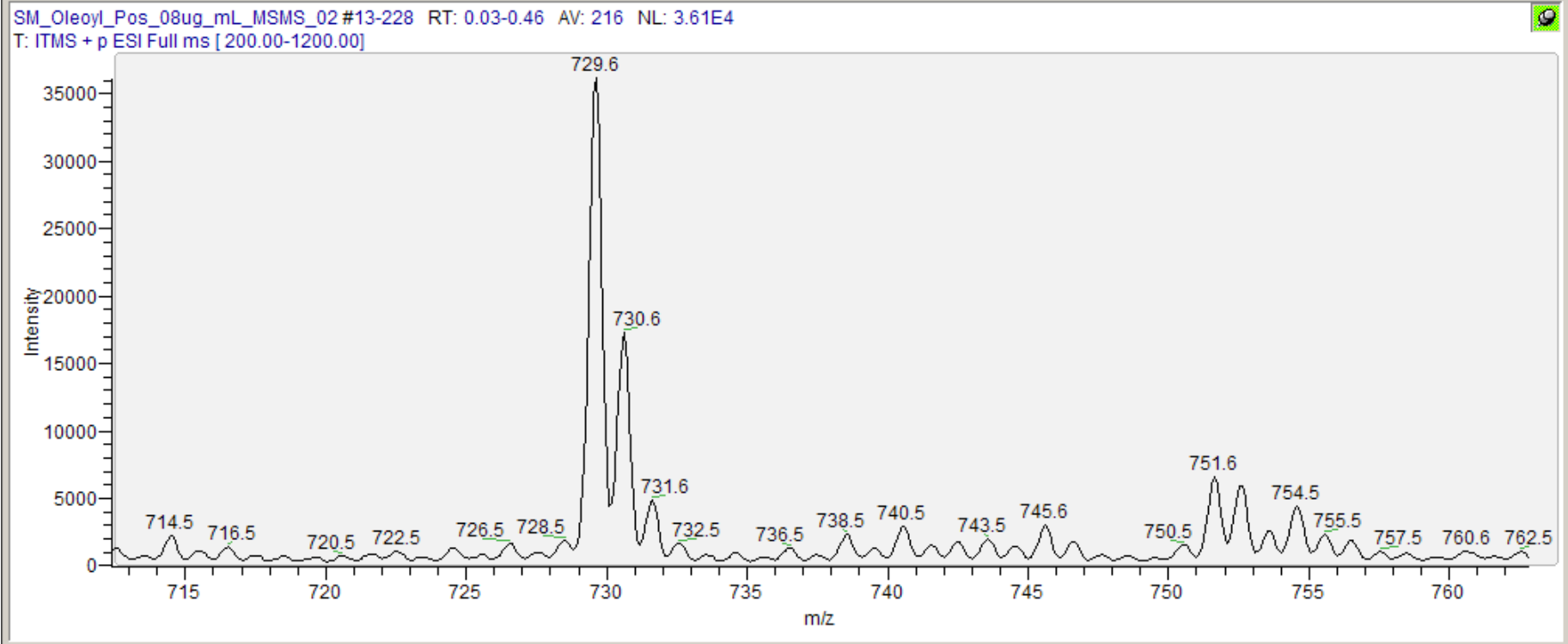
Sphingomyelin ID

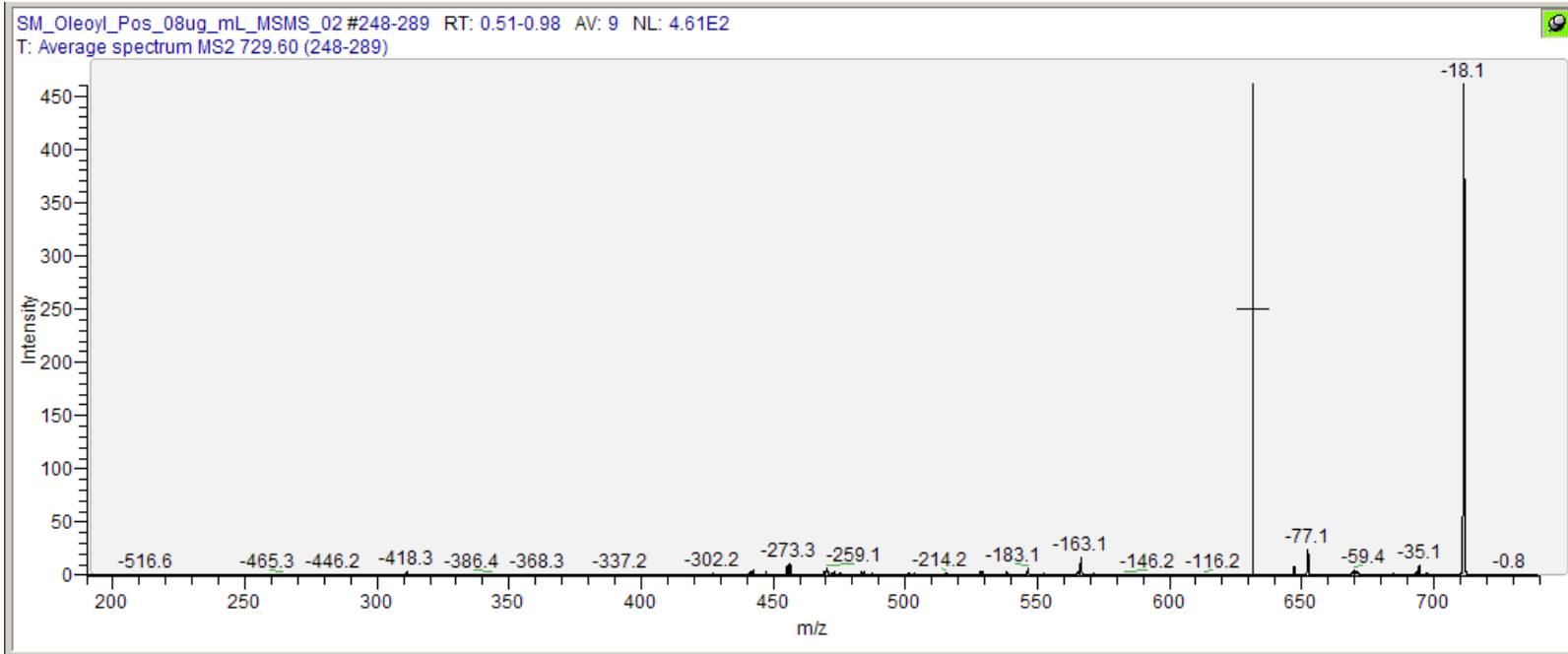
m/z 729.6 (SM 36:1 (18:1))

Pos. Mode



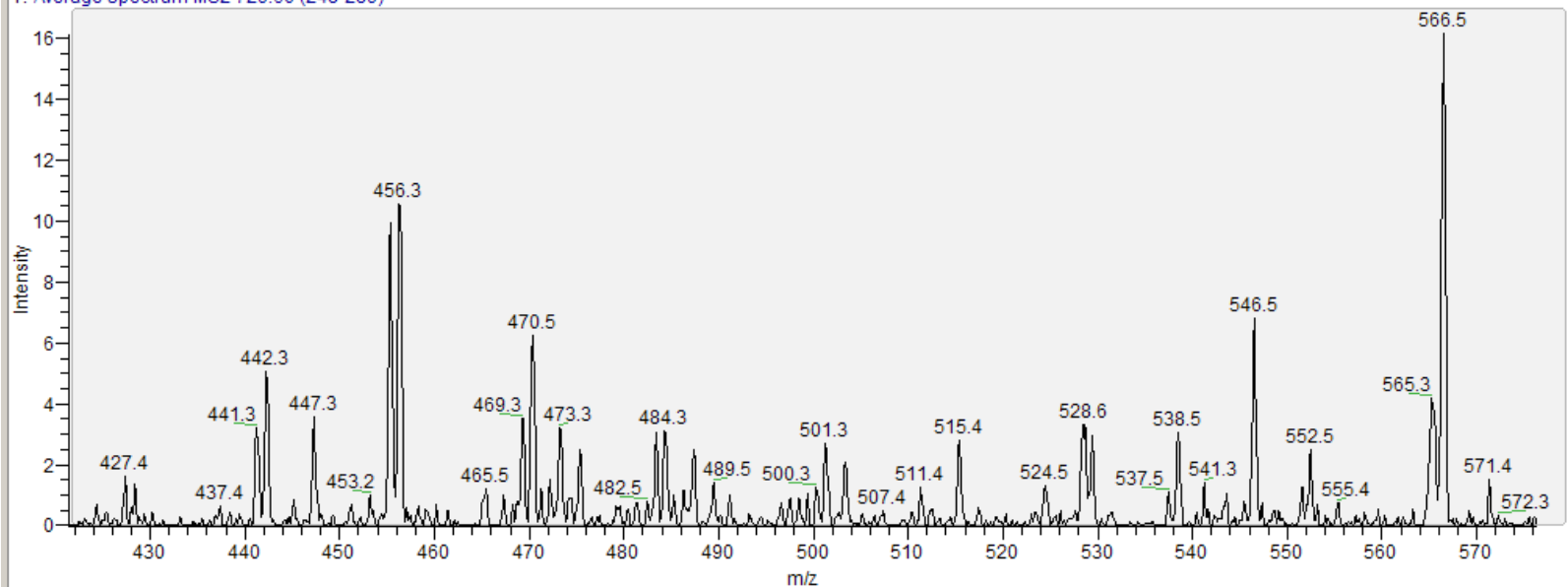
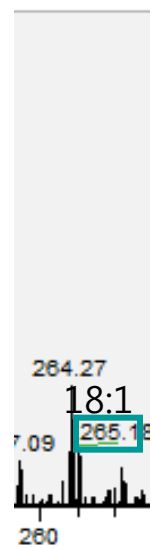
Exact Mass: 729.59





F: 0.51-0.98

SM_Oleoyl_Pos_08ug_mL_MSMS_02 #248-289 RT: 0.51-0.98 AV: 9 NL: 1.61E1
T: Average spectrum MS2 729.60 (248-289)



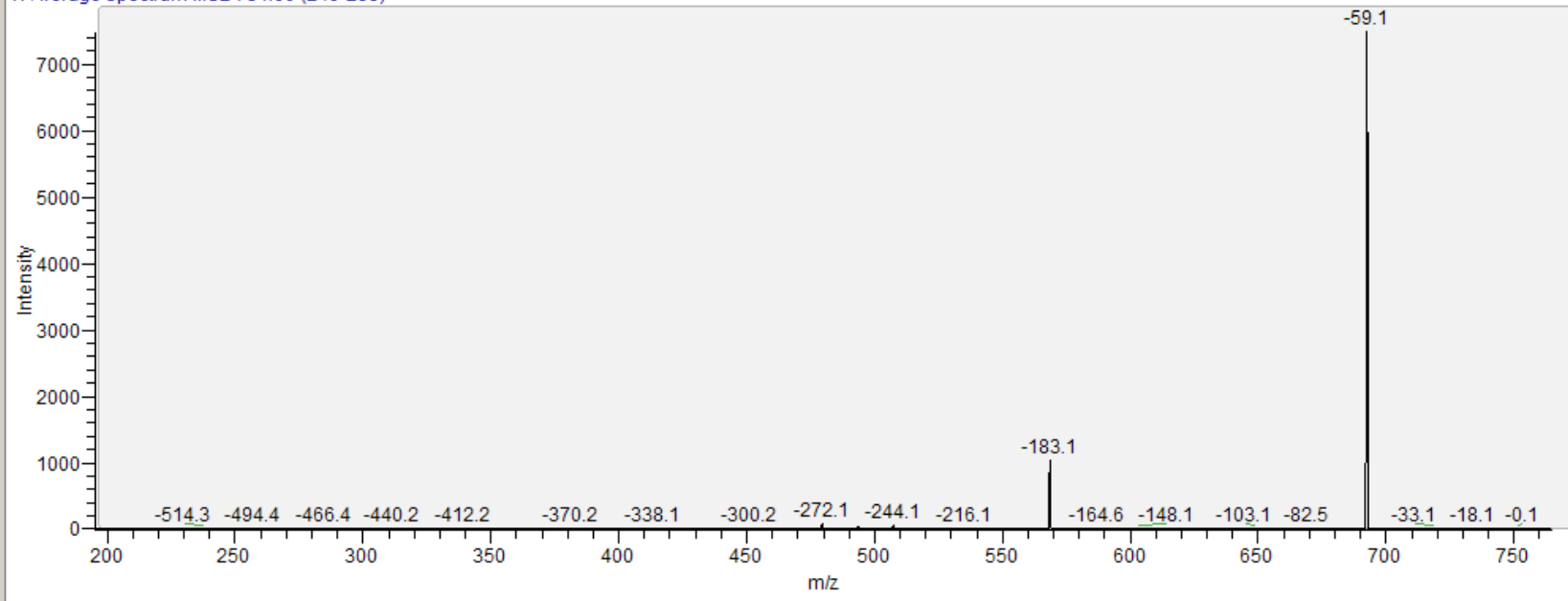
m/z 751.6 (SM 36:1, Sodium Adduct (18:1))

Pos. Mode

SM_Oleoyl_Pos_08ug_mL_MSMS_02#249-288 RT: 0.52-0.96 AV: 9 NL: 7.48E3

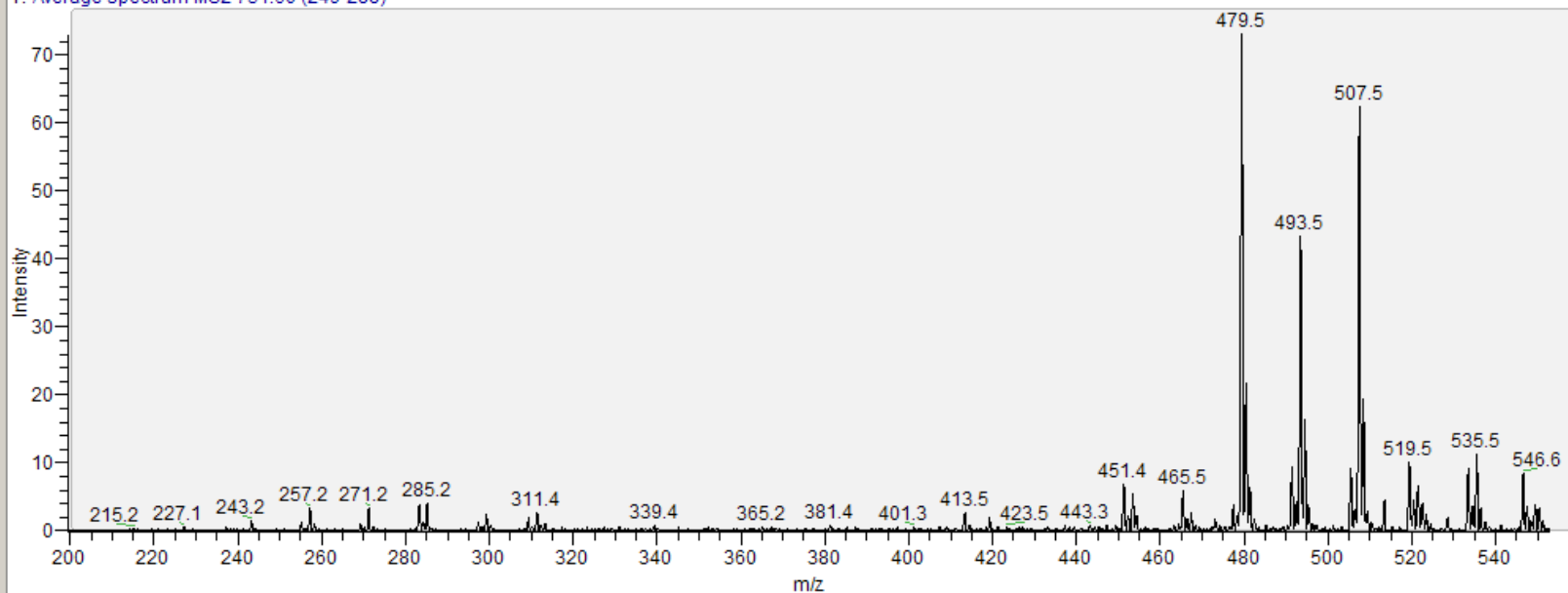
um Ion

T: Average spectrum MS2 751.60 (249-288)



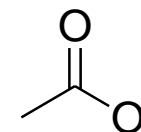
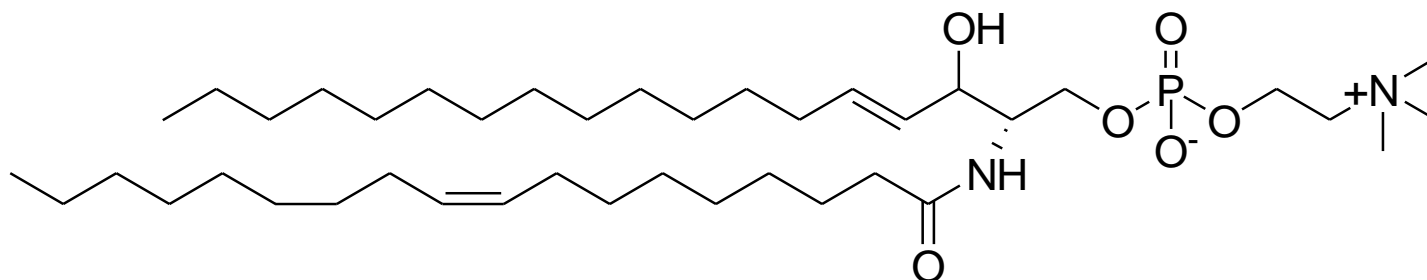
SM_Oleoyl_Pos_08ug_mL_MSMS_02#249-288 RT: 0.52-0.96 AV: 9 NL: 7.30E1

T: Average spectrum MS2 751.60 (249-288)



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

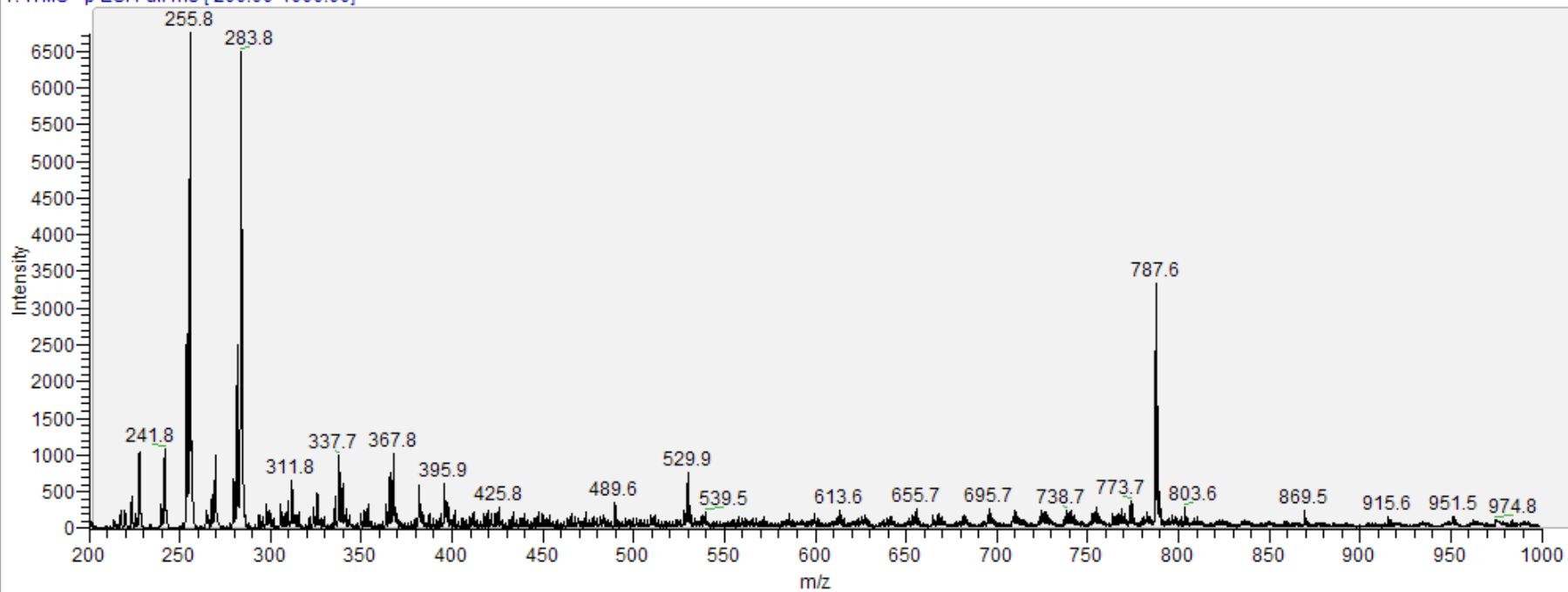
Neg. Mode

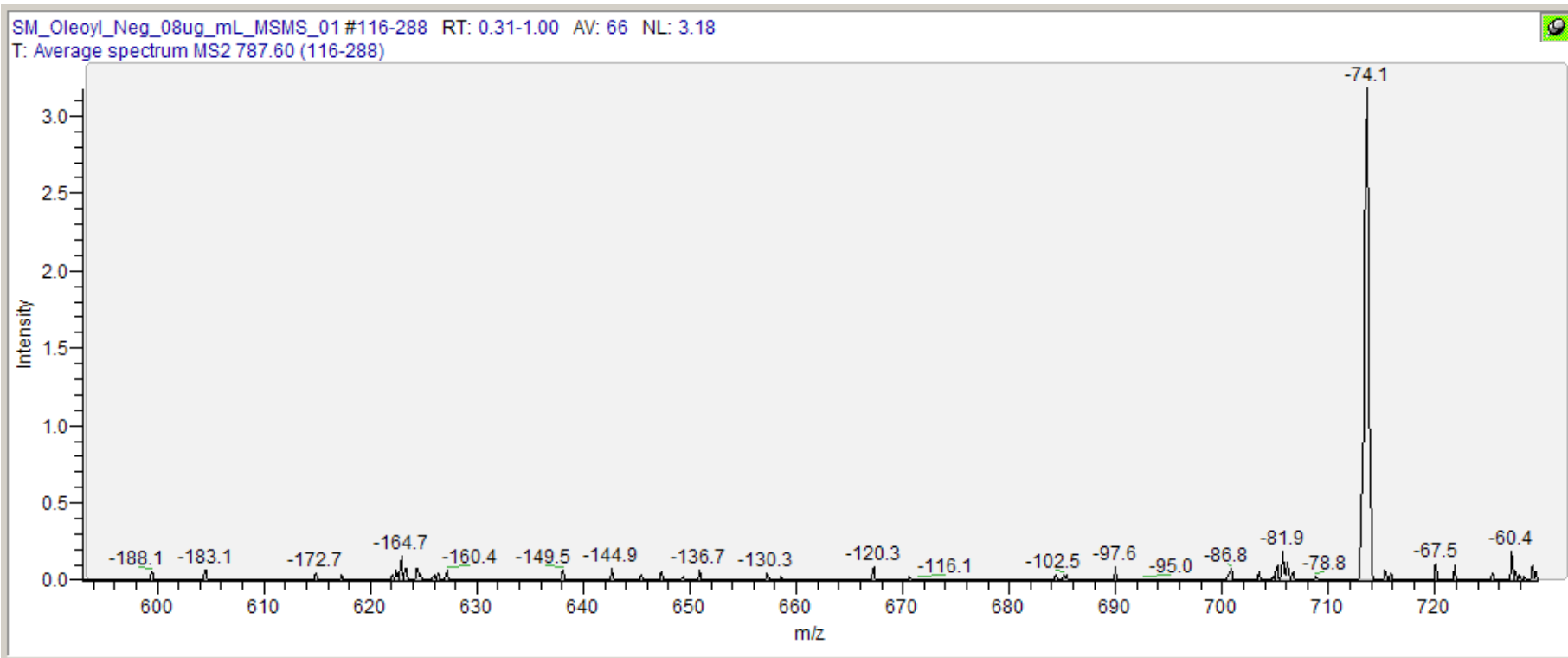


Exact Mass: 787.60

SM_Oleoyl_Neg_08ug_mL_MSMS_01 #6-97 RT: 0.02-0.25 AV: 92 NL: 6.74E3

T: ITMS - p ESI Full ms [200.00-1000.00]

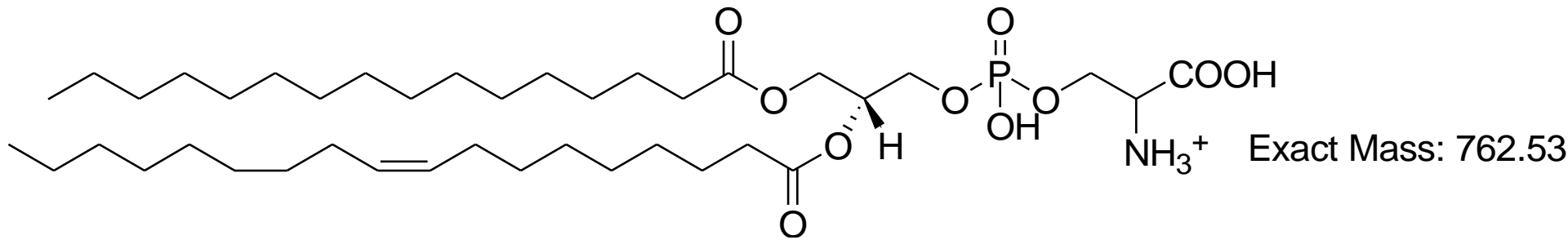




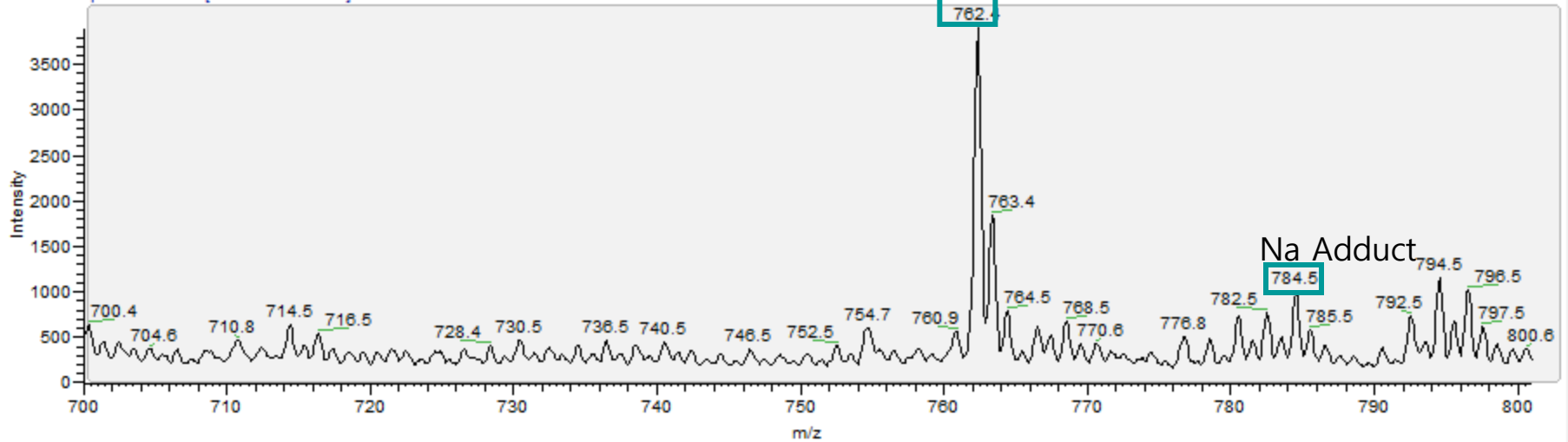
Phosphatidylserine ID

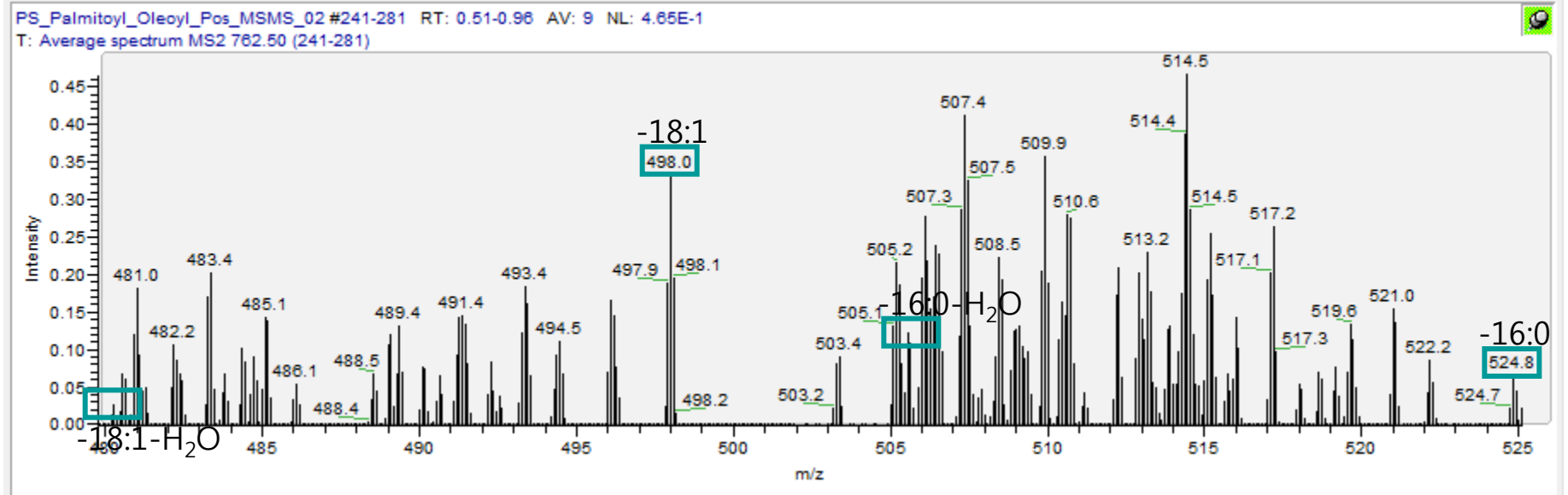
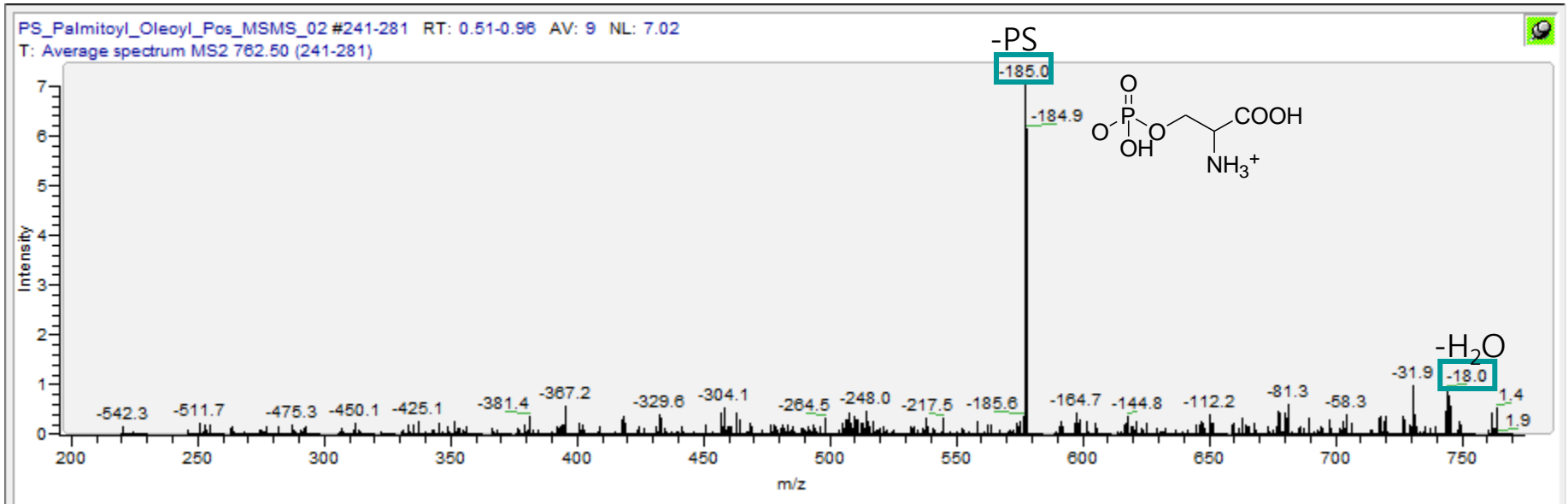
m/z 762.6 (PS 34:1 (16:0, 18:1))

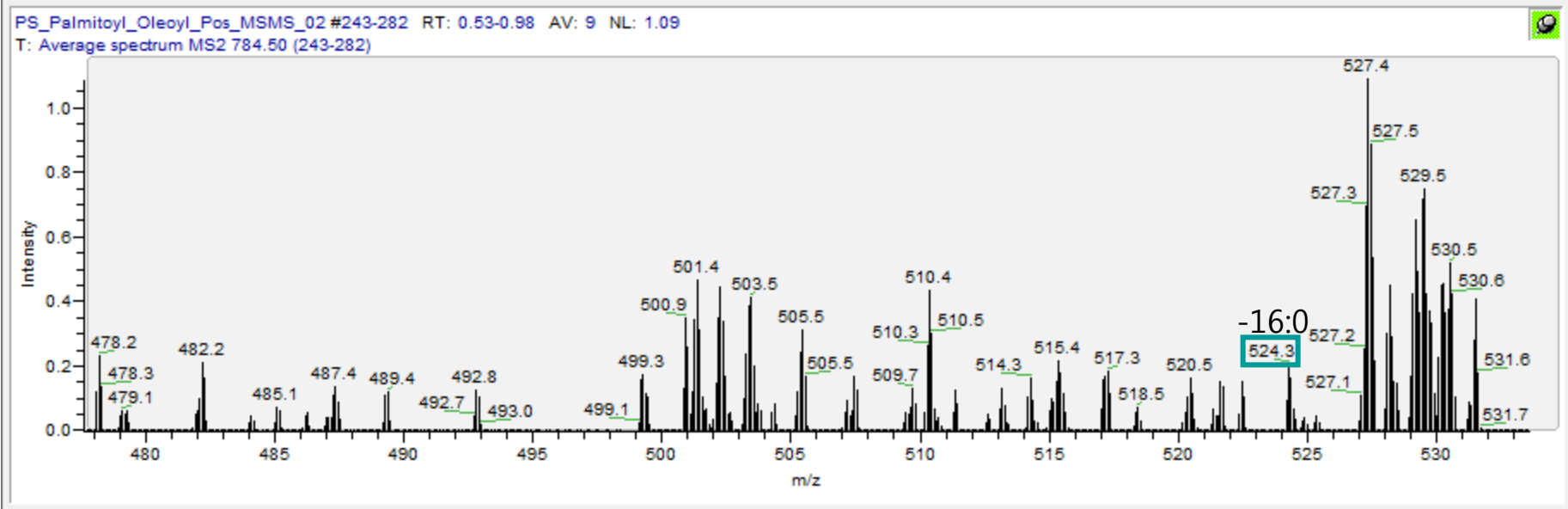
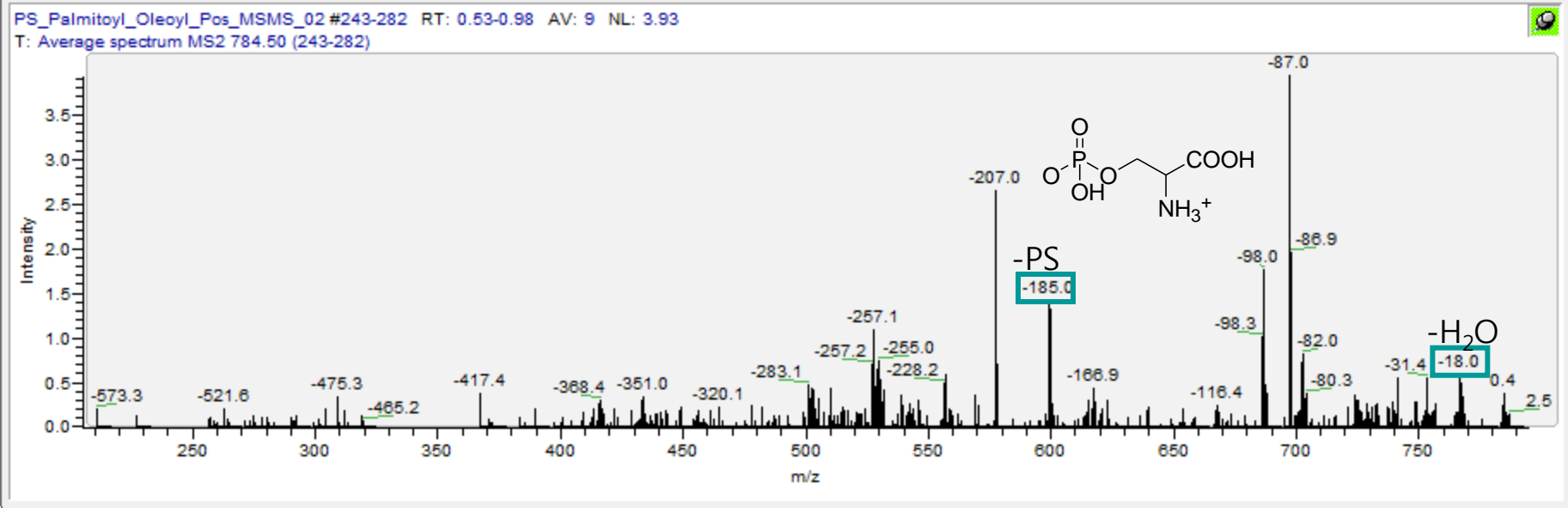
Pos. Mode



PS_Palmitoyl_Oleoyl_Pos_MSMS_02 #63-232 RT: 0.13-0.48 AV: 170 NL: 3.90E3
T: ITMS + p ESI Full ms [200.00-1200.00]

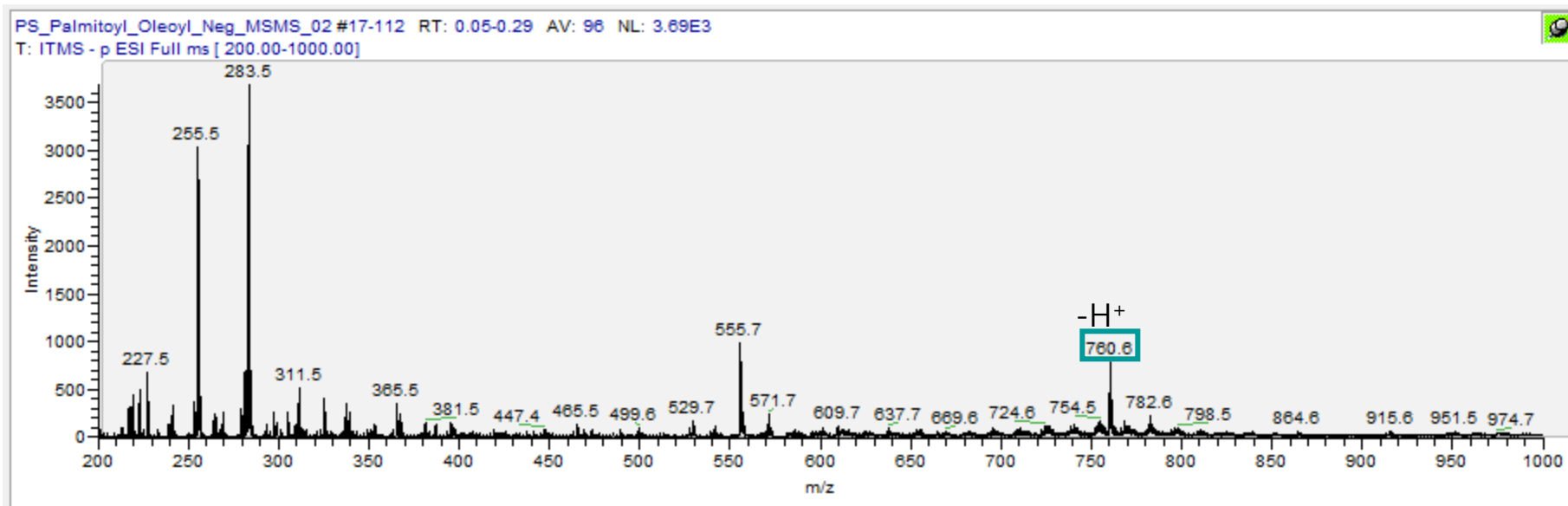
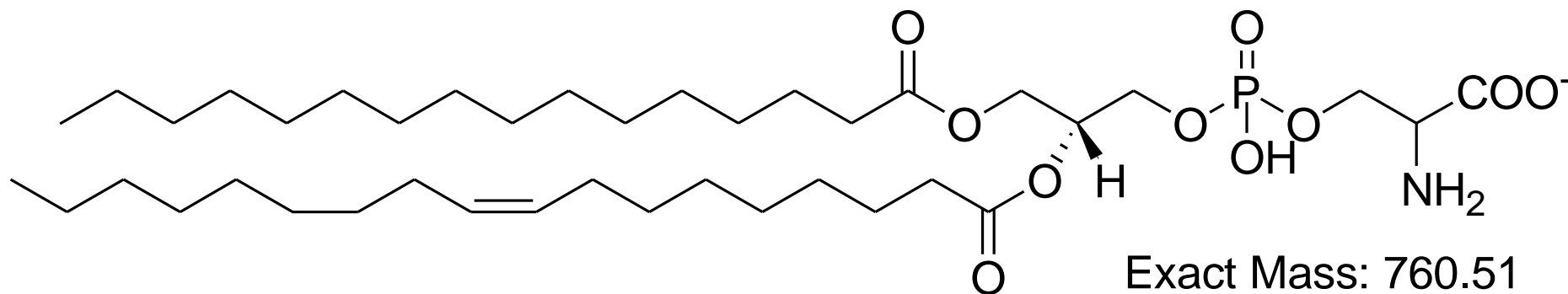


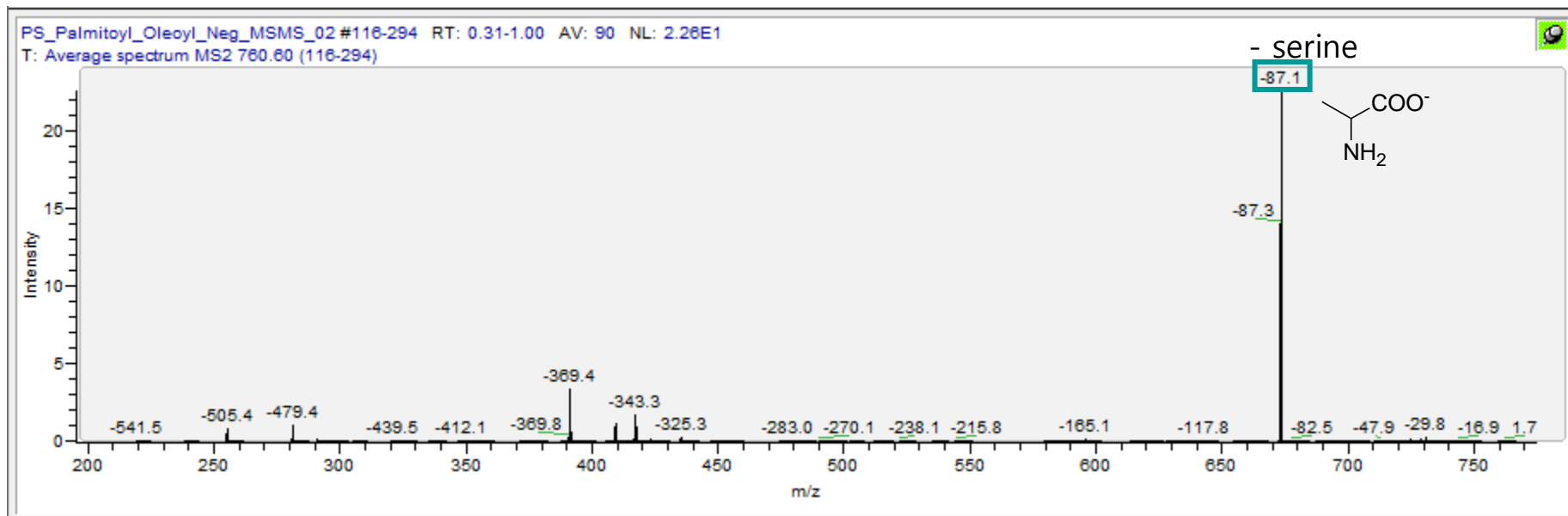




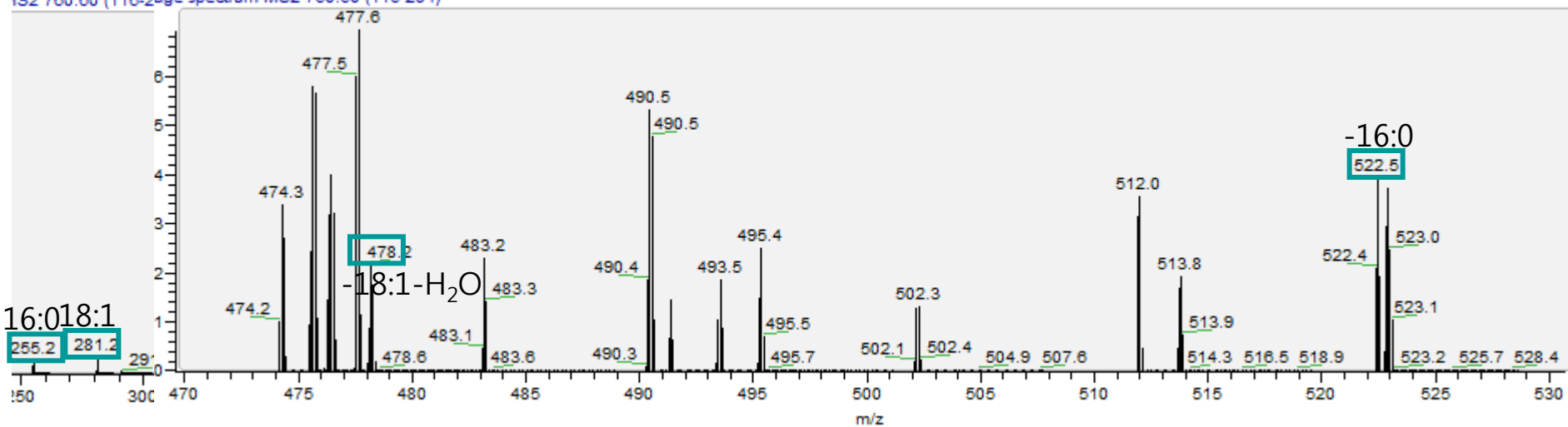
m/z 760.6 (PS 34:1 (16:0, 18:1))

Neg. Mode



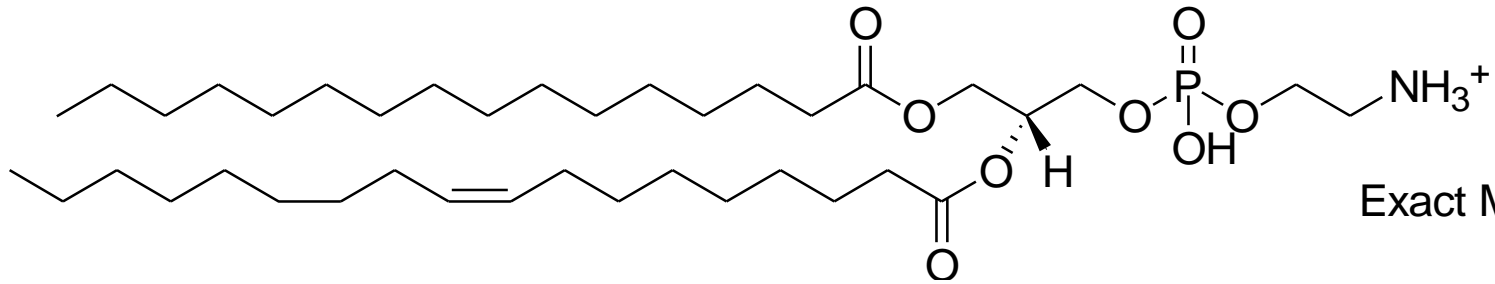


Neg_MSMS_02 #mitoyl_Oleoyl_Neg_MSMS_02 #116-294 RT: 0.31-1.00 AV: 90 NL: 6.93E-2
IS2 760.60 (116-2)age spectrum MS2 760.60 (116-294)



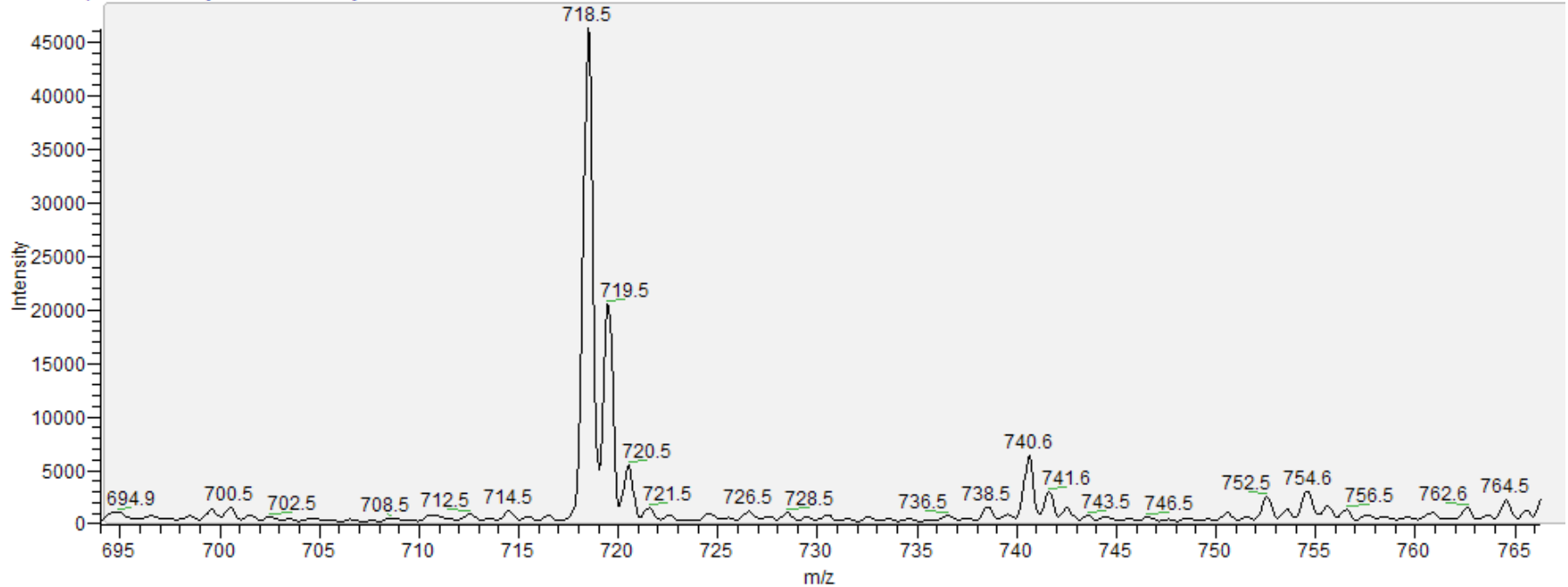
Phosphatidylethanolamine
ID

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



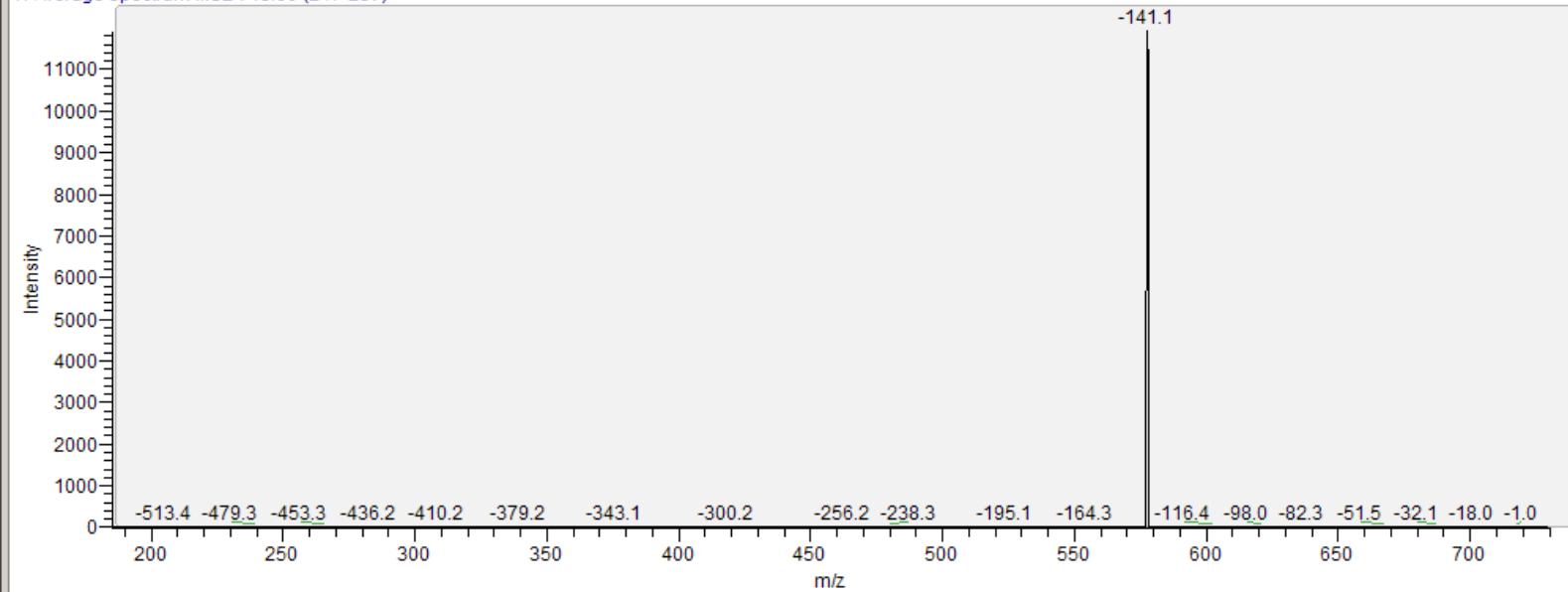
Exact Mass: 718.54

PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02 #8-241 RT: 0.02-0.49 AV: 234 NL: 4.63E4
T: ITMS + p ESI Full ms [200.00-1200.00]

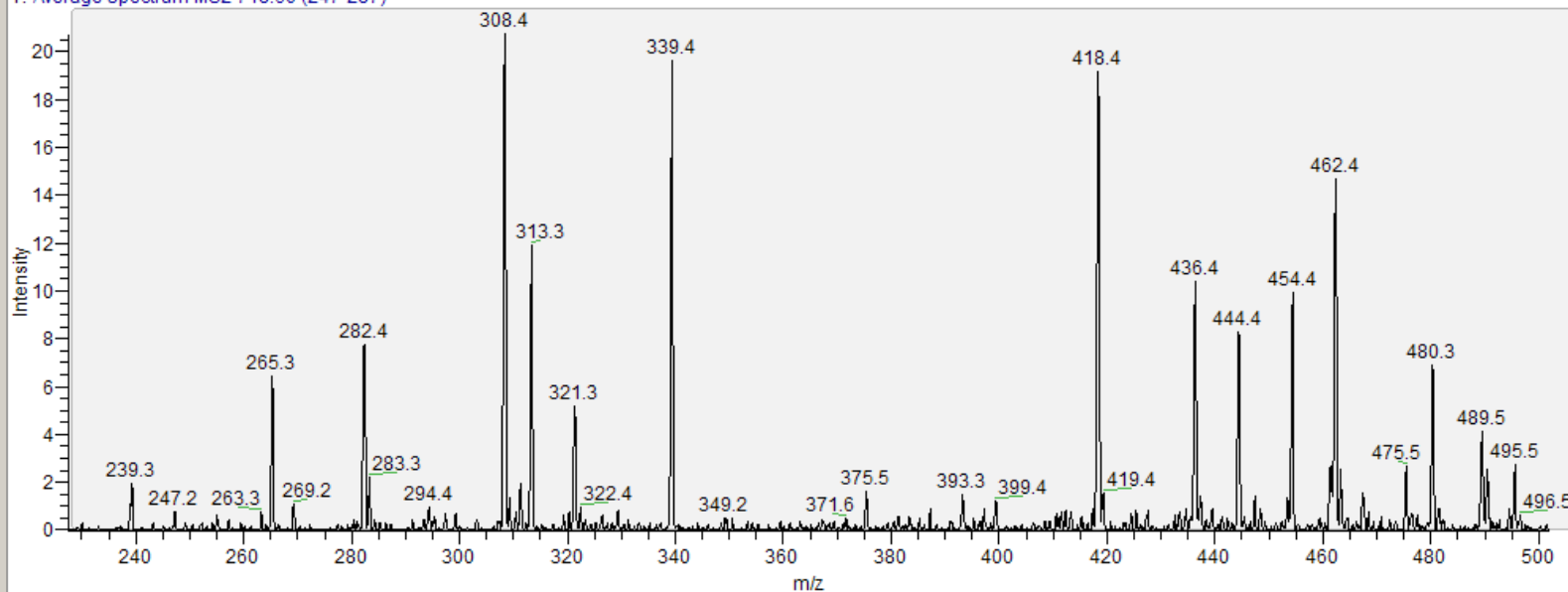


m/z 718.6 (PE 34:1 (16:0, 18:1))

PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02 #247-287 RT: 0.51-0.96 AV: 9 NL: 1.19E4
T: Average spectrum MS2 718.60 (247-287)

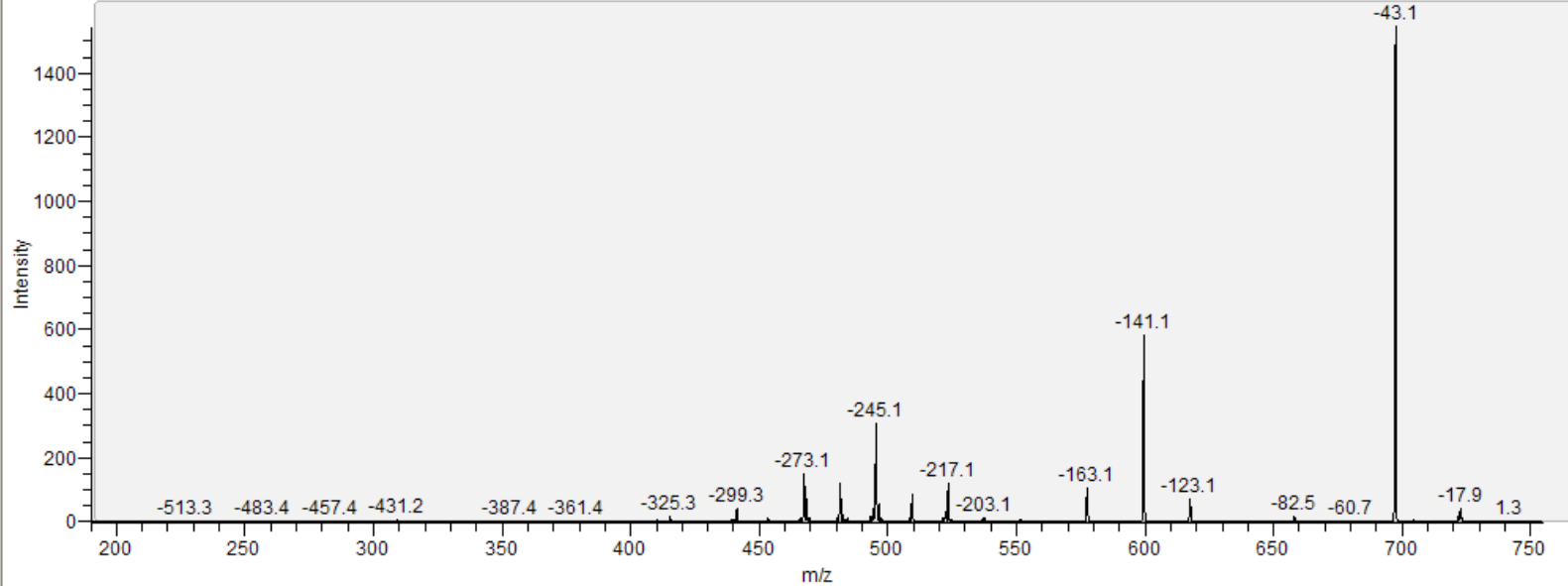


PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02 #247-287 RT: 0.51-0.96 AV: 9 NL: 2.07E1
T: Average spectrum MS2 718.60 (247-287)

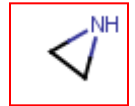
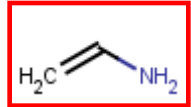
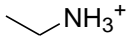


m/z 740.6 (PE 34:1, sodium adduct (16:0, 18:1))

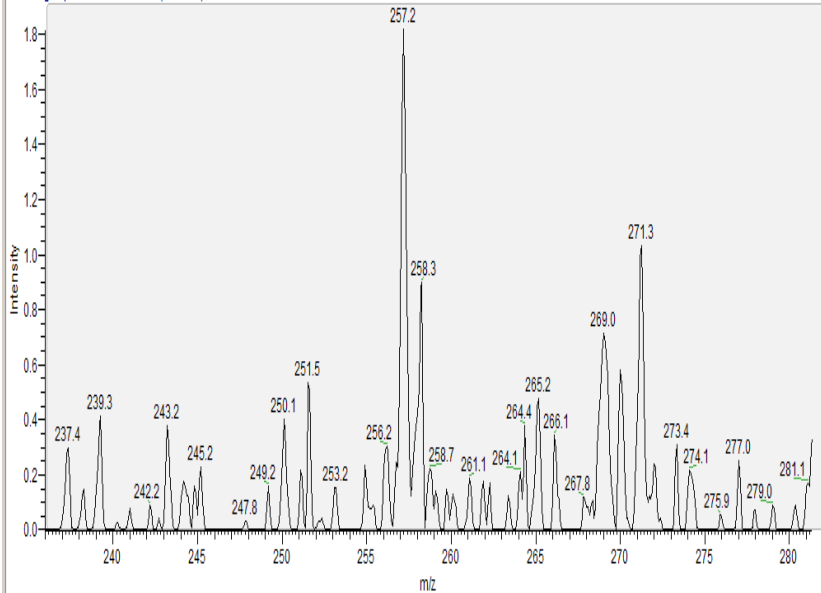
PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02#248-288 RT: 0.52-0.97 AV: 9 NL: 1.54E3
T: Average spectrum MS2 740.60 (248-288)



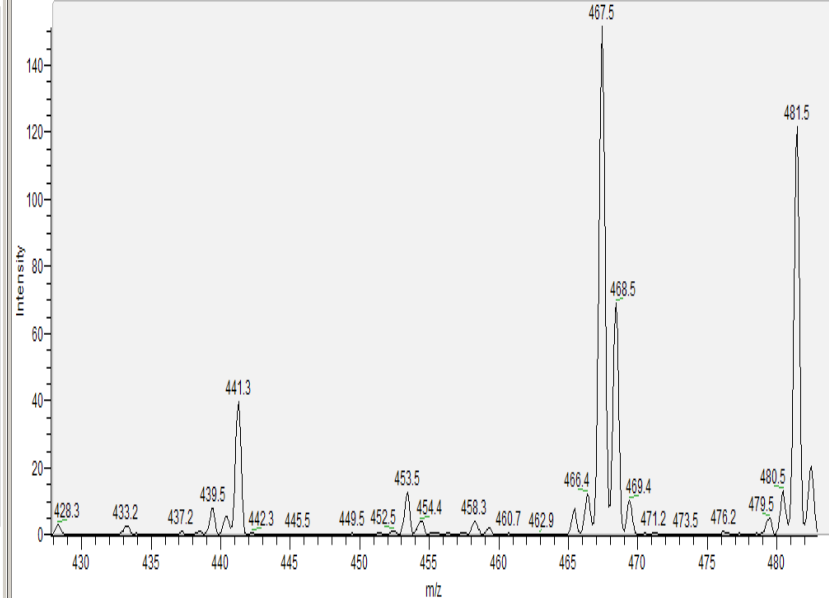
onium ion



PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02#248-288 RT: 0.52-0.97 AV: 9 NL: 1.82
T: Average spectrum MS2 740.60 (248-288)

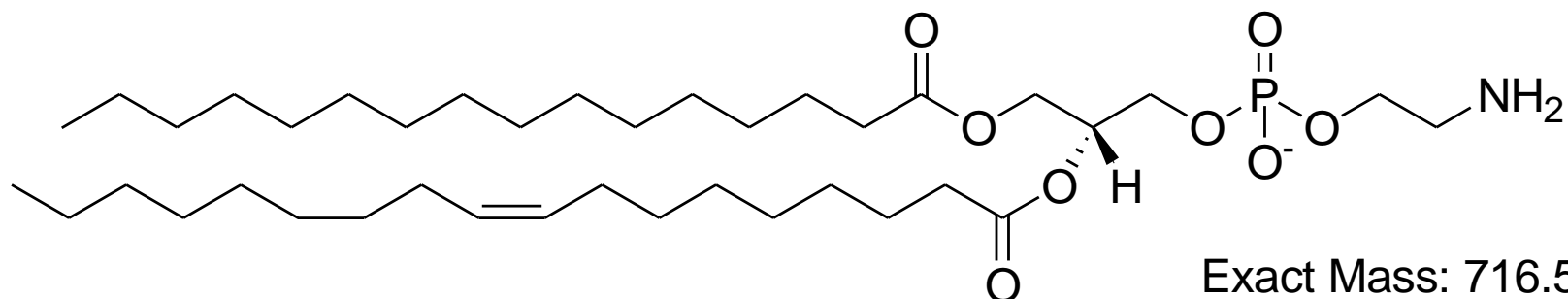


PE_Palmitoyl_Oleoyl_Pos_08ug_mL_MSMS_02#248-288 RT: 0.52-0.97 AV: 9 NL: 1.51E2
T: Average spectrum MS2 740.60 (248-288)



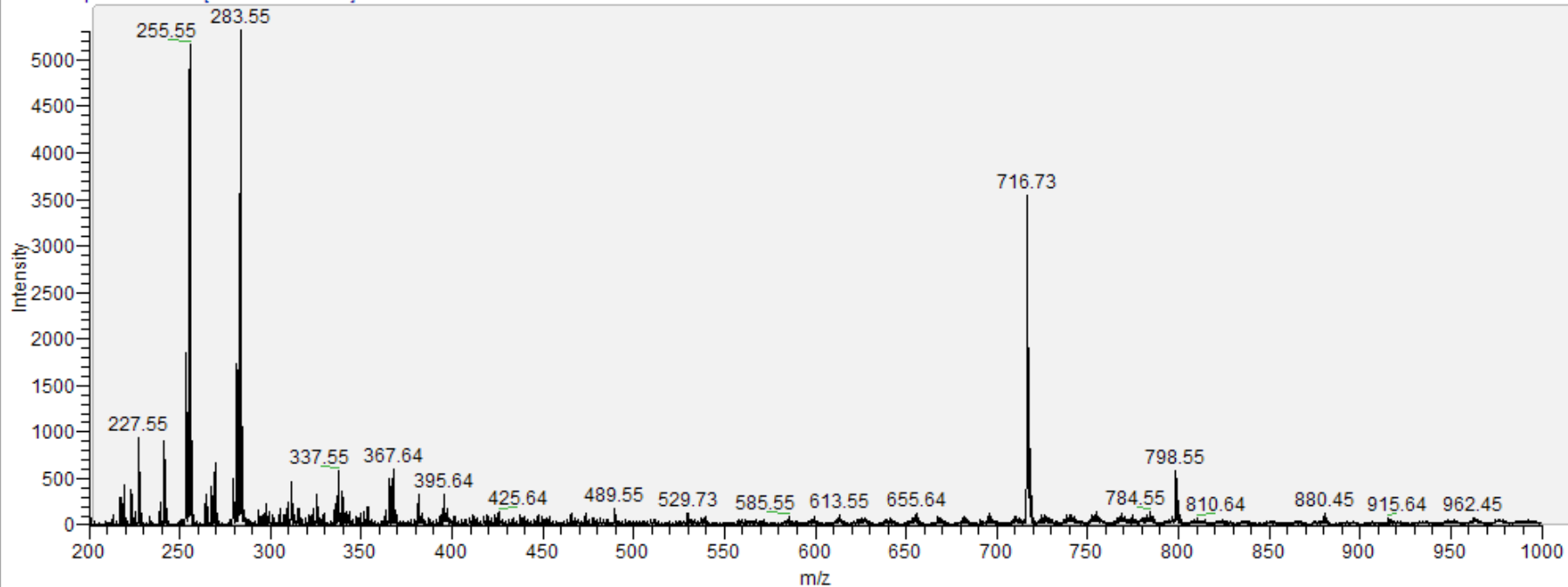
m/z 716.7 (PE 34:1 (16:0, 18:1))

Neg. Mode



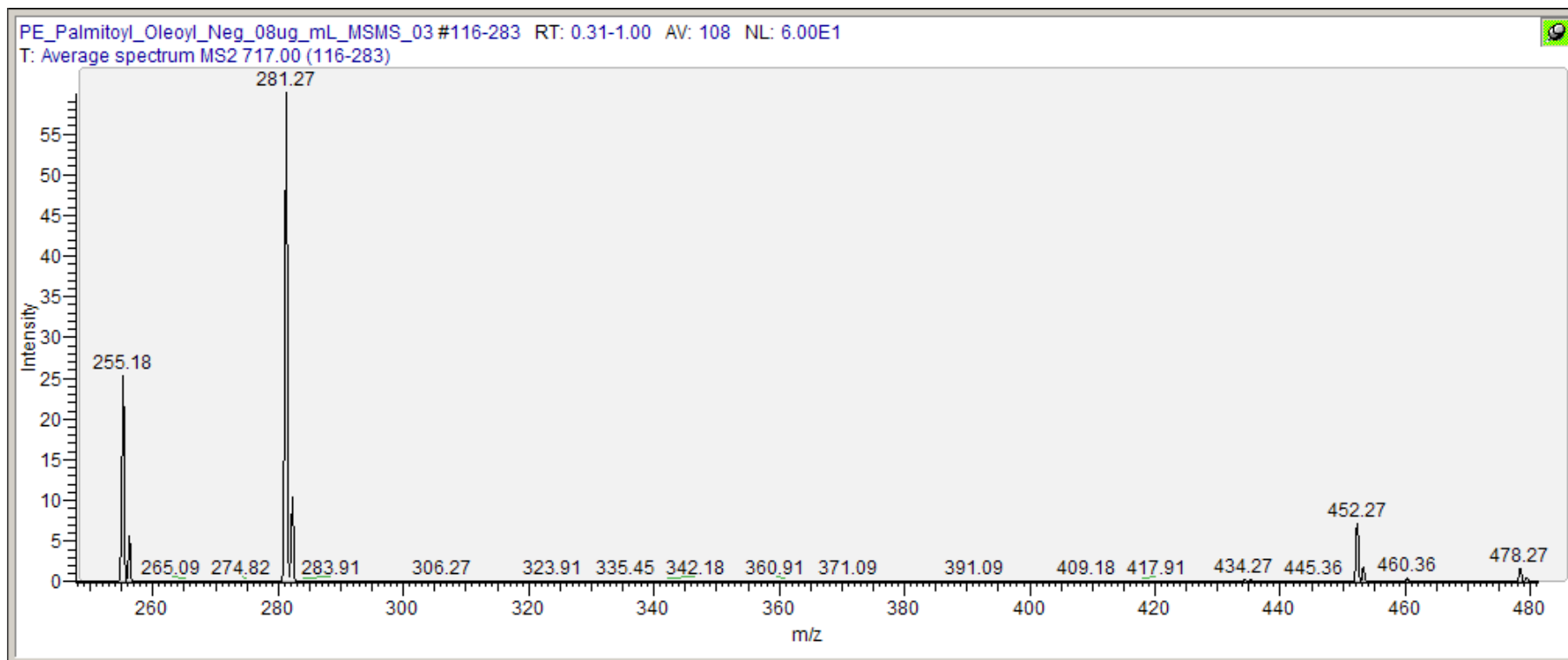
PE_Palmitoyl_Oleoyl_Neg_08ug_mL_MSMS_03#2-115 RT: 0.01-0.30 AV: 113 NL: 5.31E3

T: ITMS - p ESI Full ms [200.00-1000.00]



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

Neg. Mode

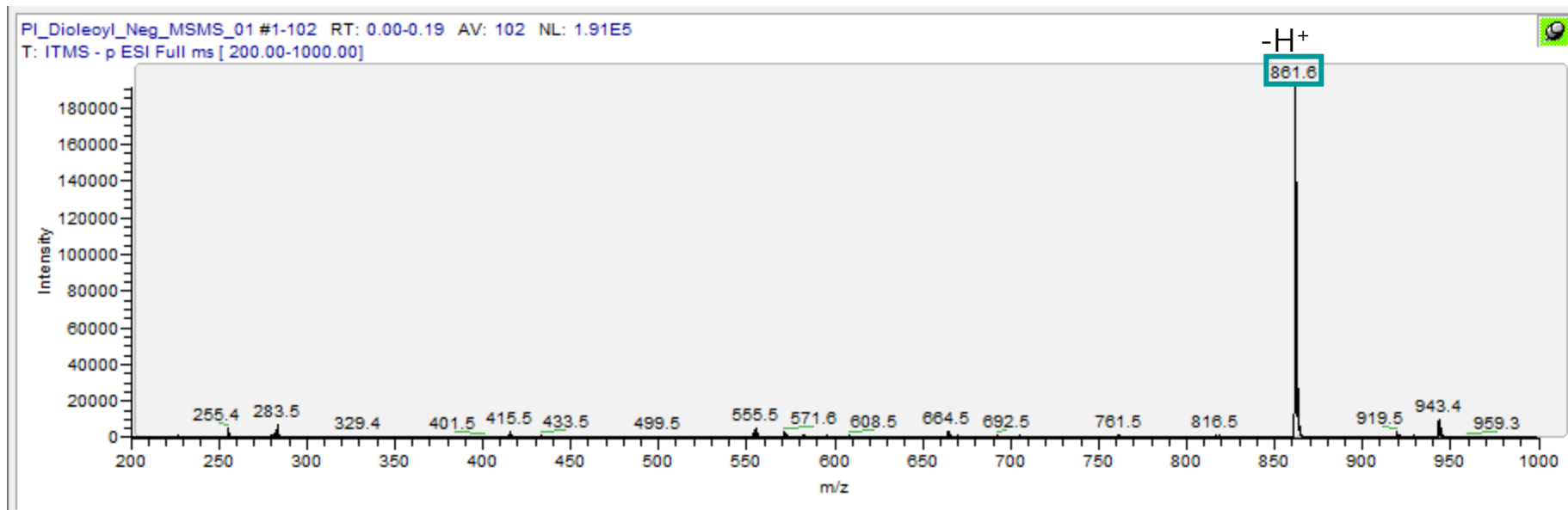
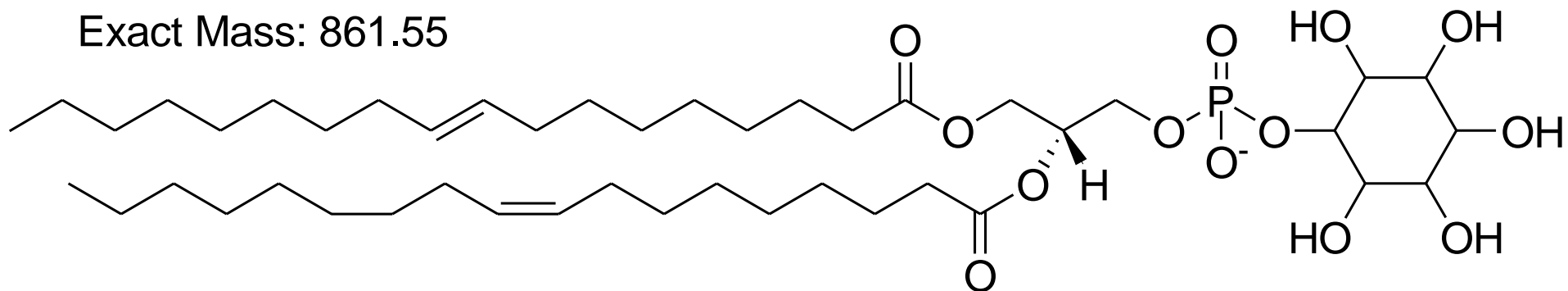


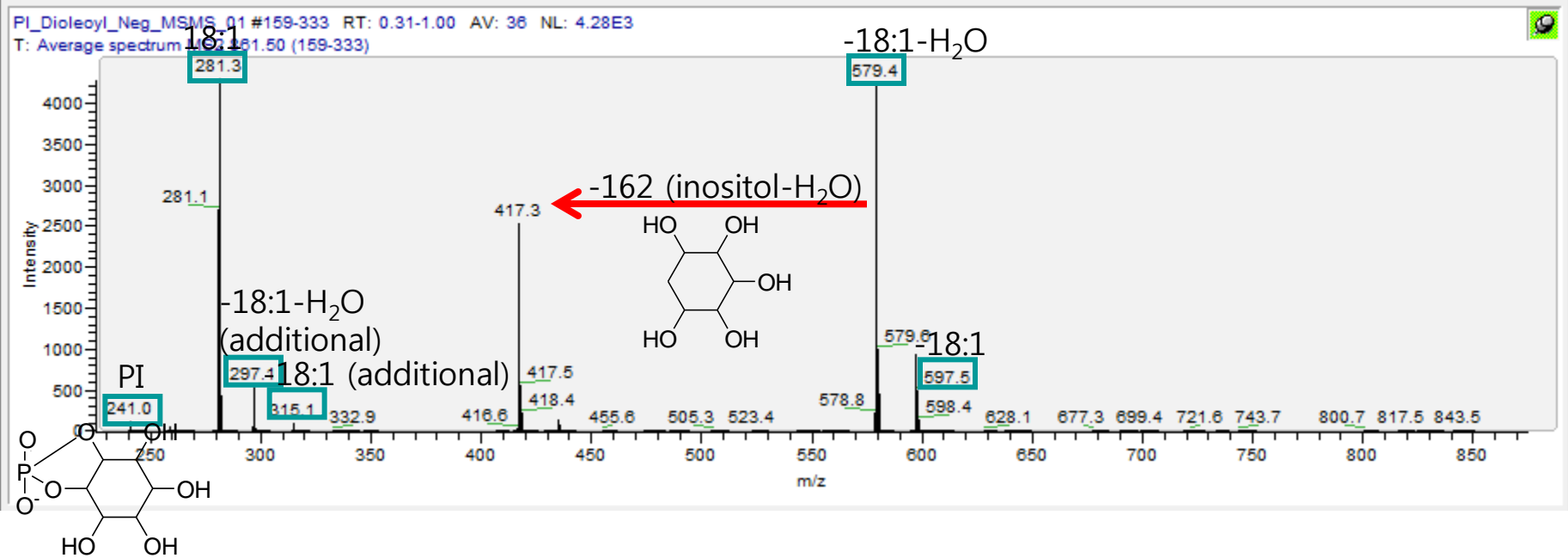
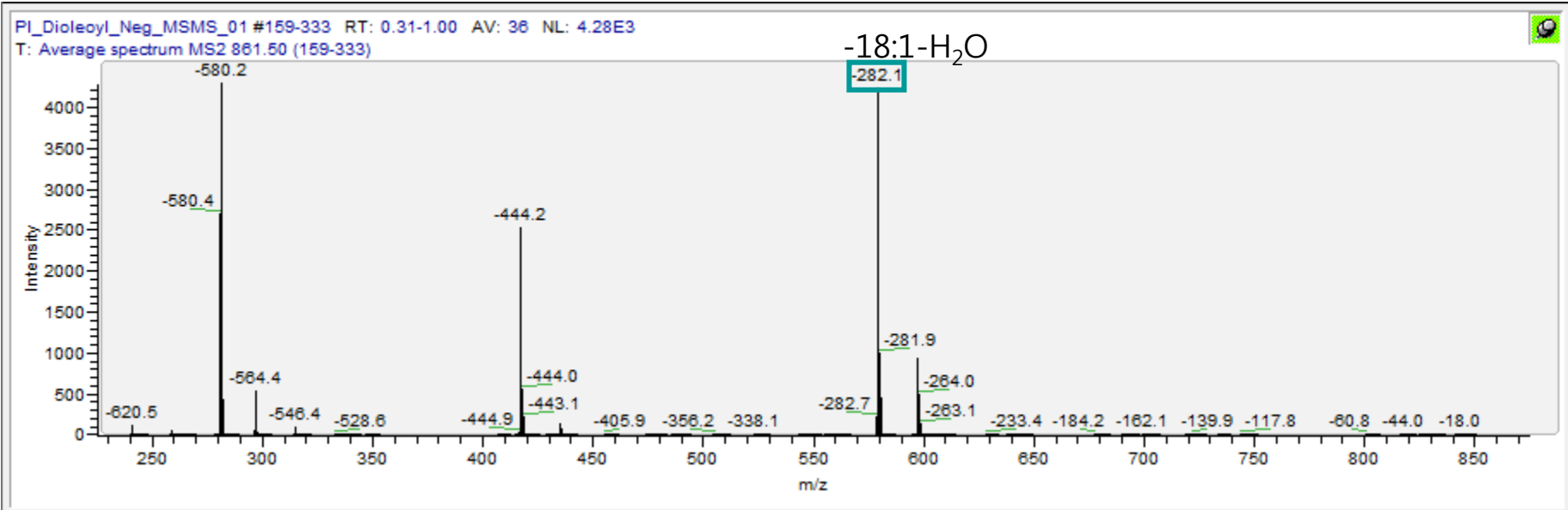
Phosphatidylinositol ID

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

Neg. Mode

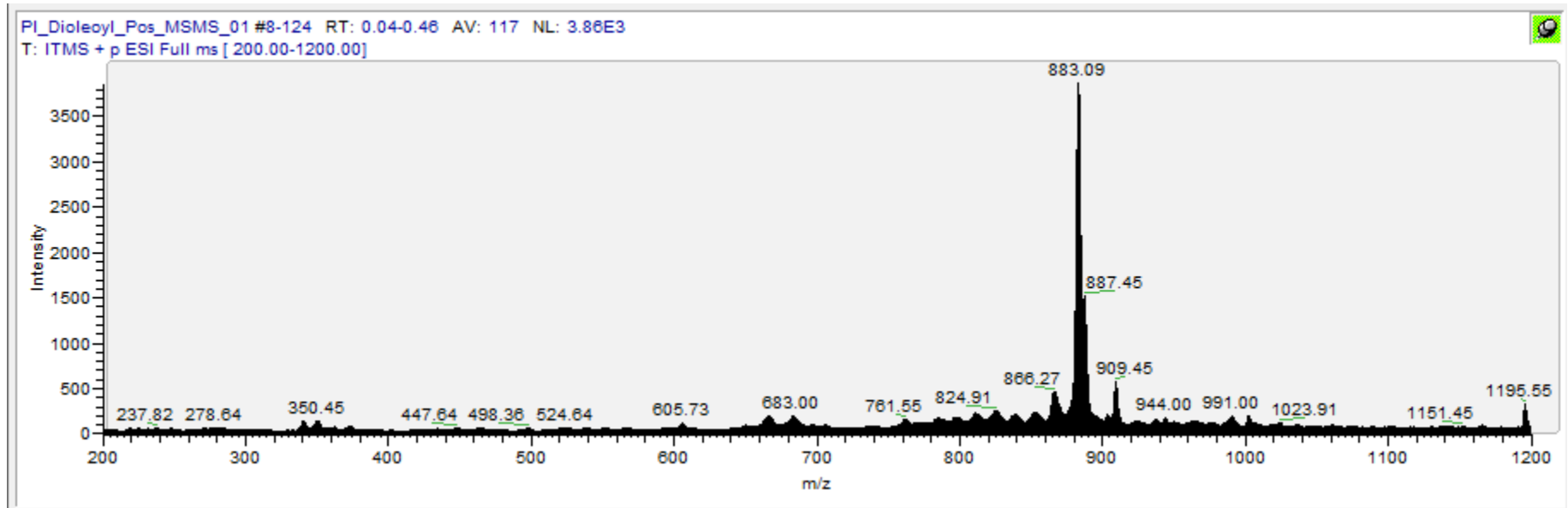
Exact Mass: 861.55





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

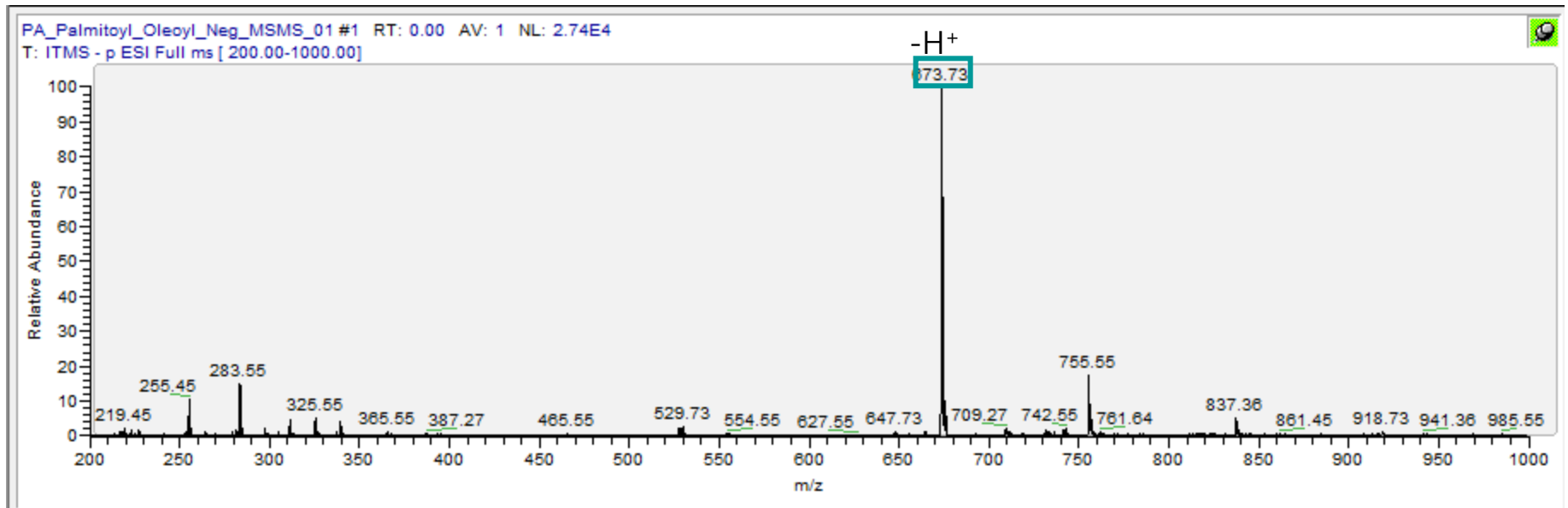
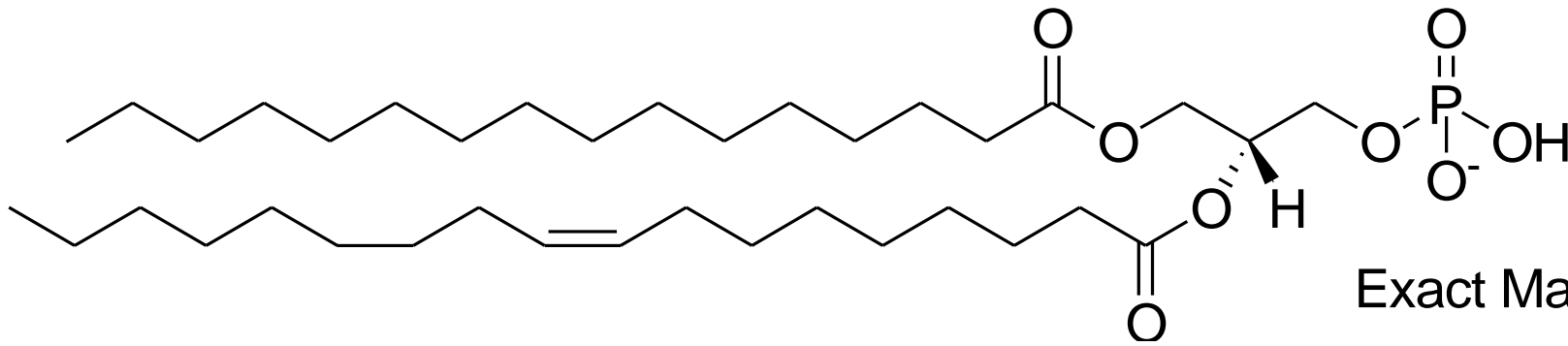
Pos. Mode

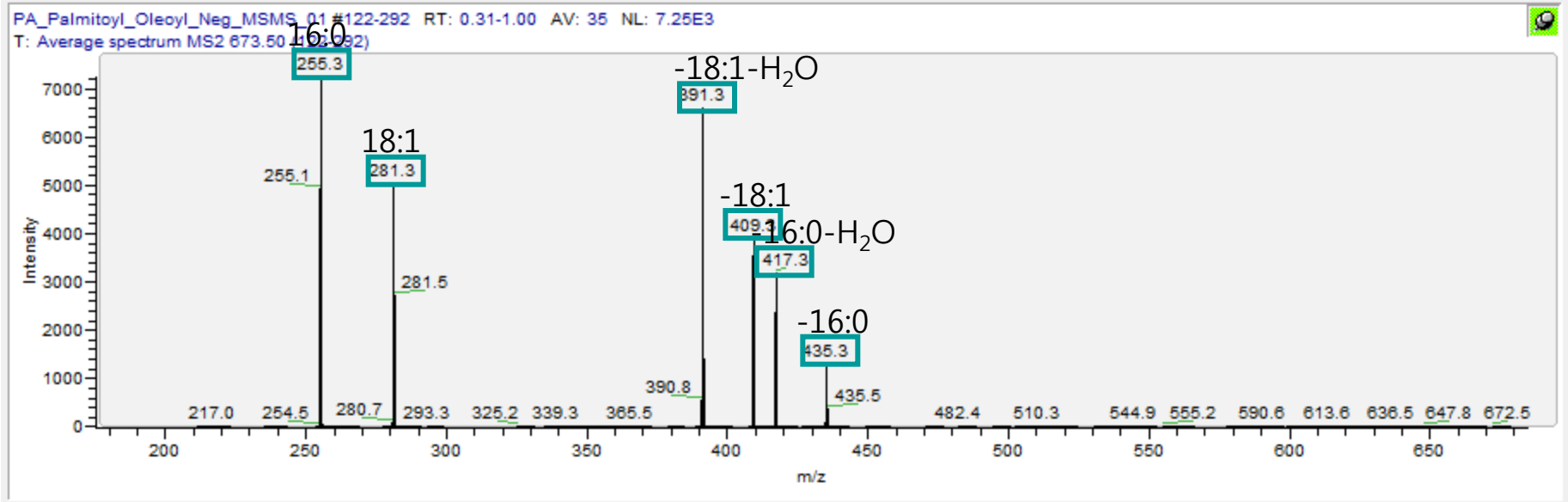
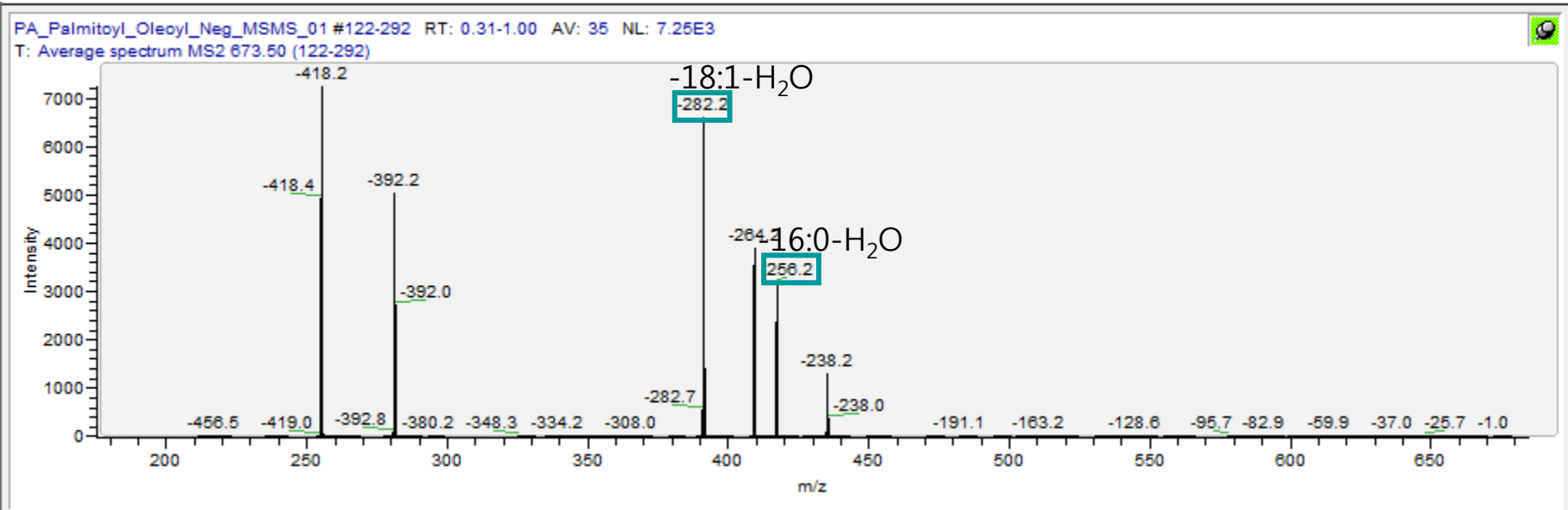


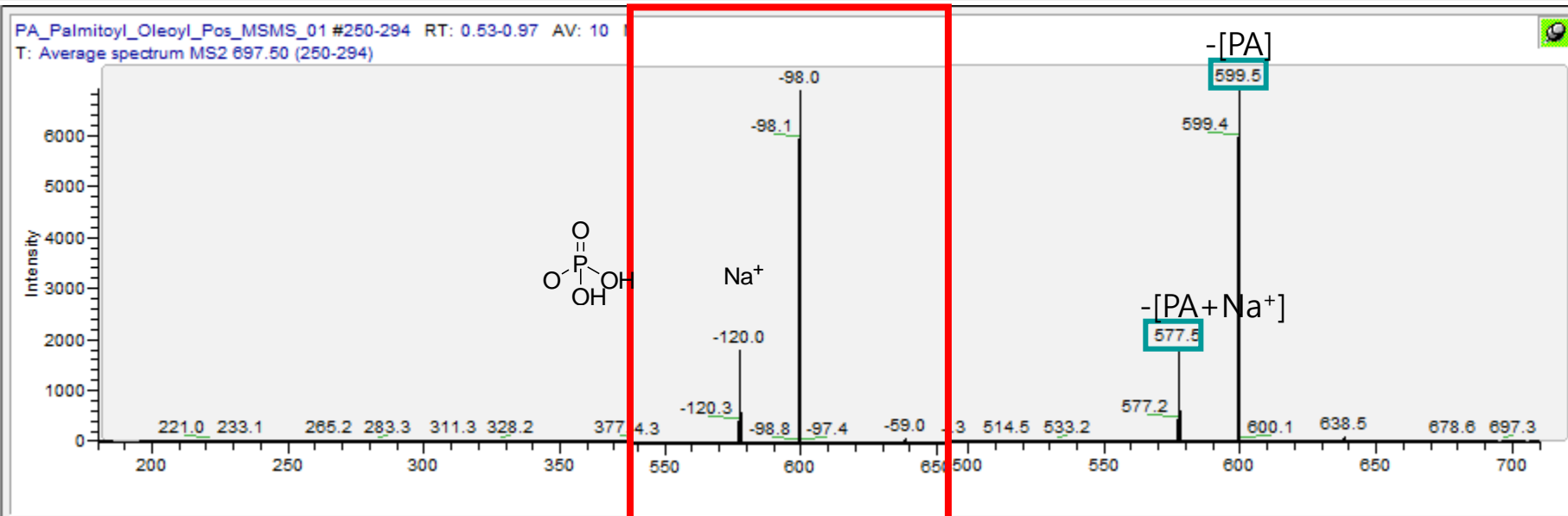
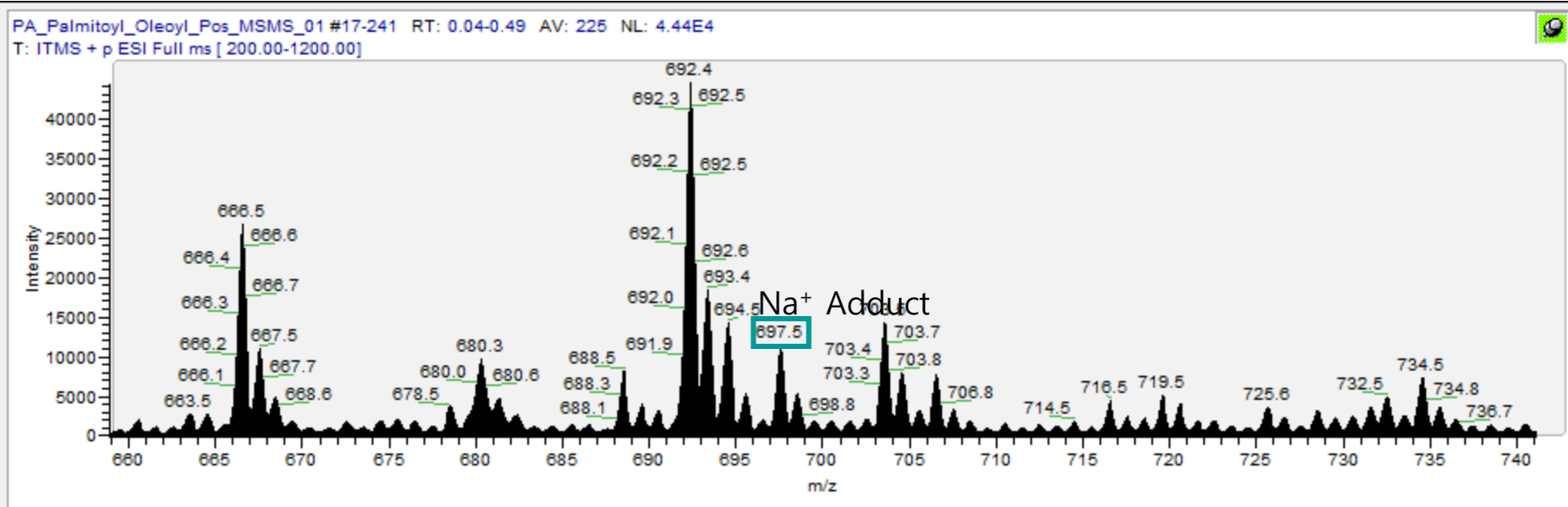
Phosphatidic acid ID

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

Neg. Mode



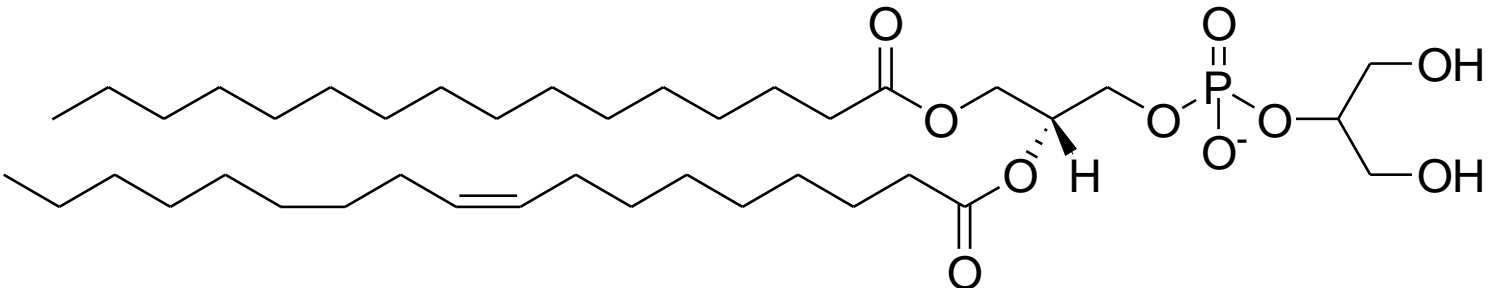




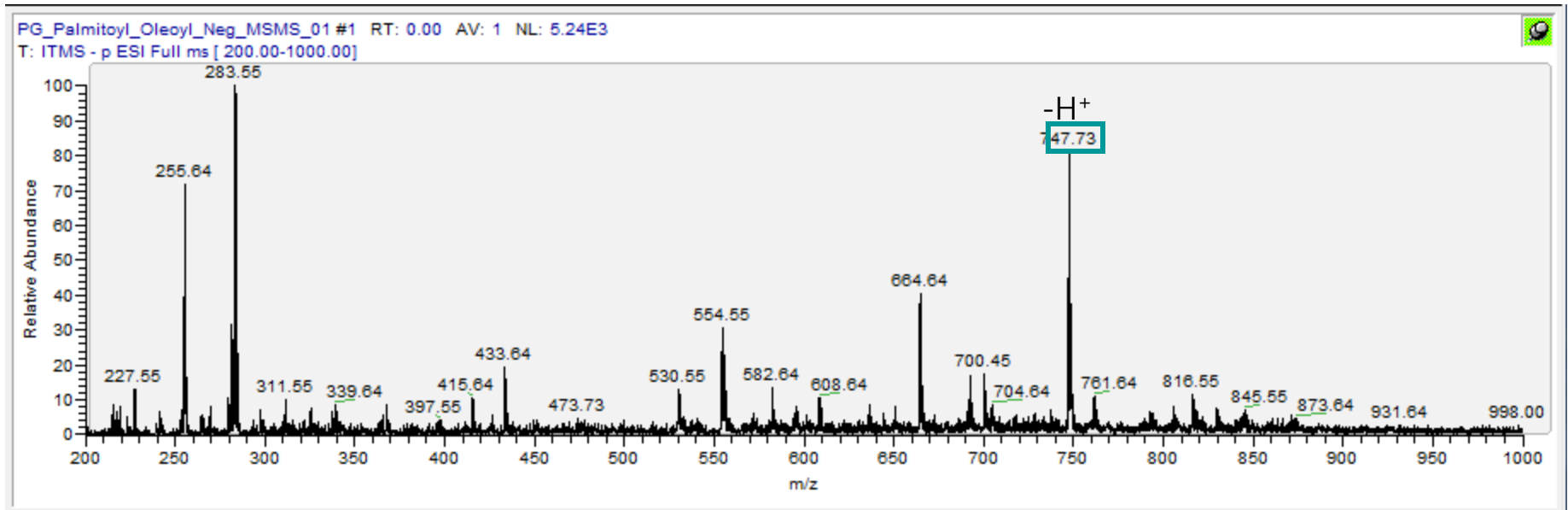
Phosphatidylglycerol ID

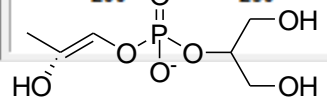
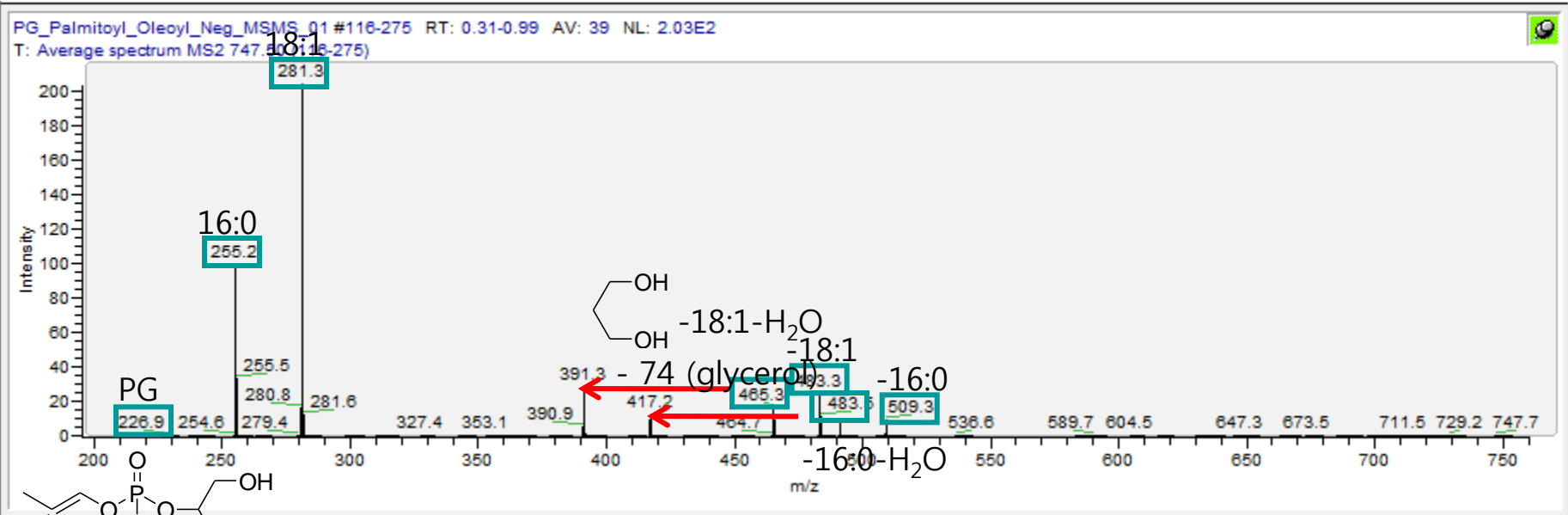
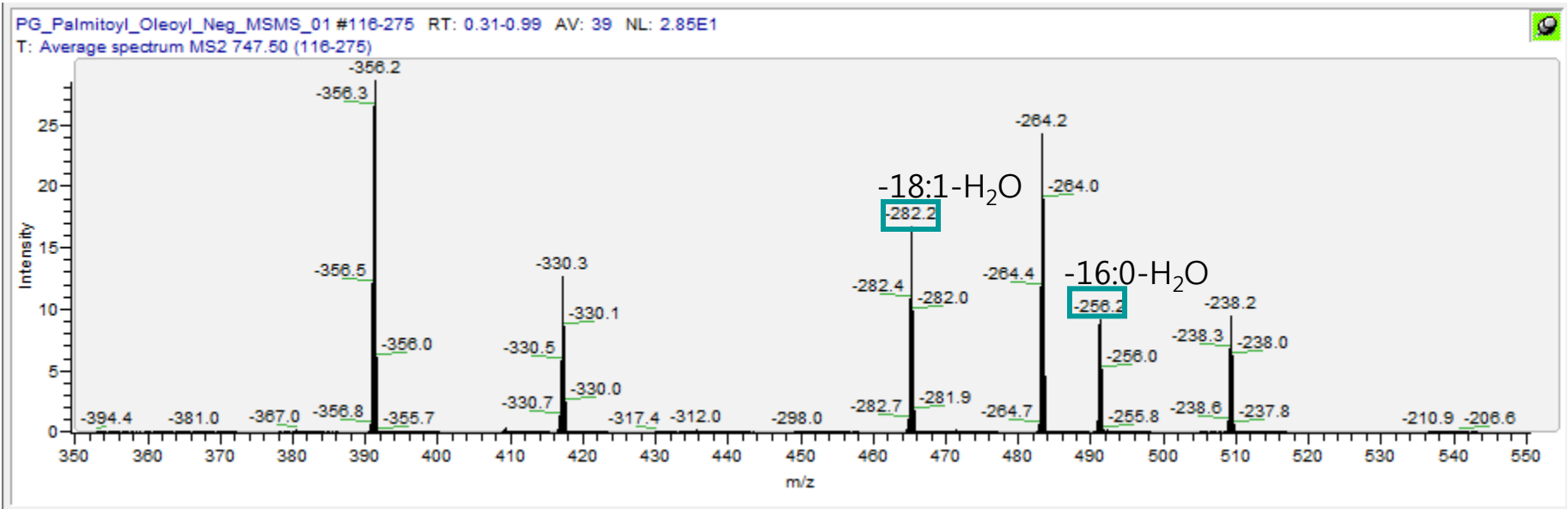
m/z 747.7 (PG 34:1 (16:0, 18:1))

Neg. Mode

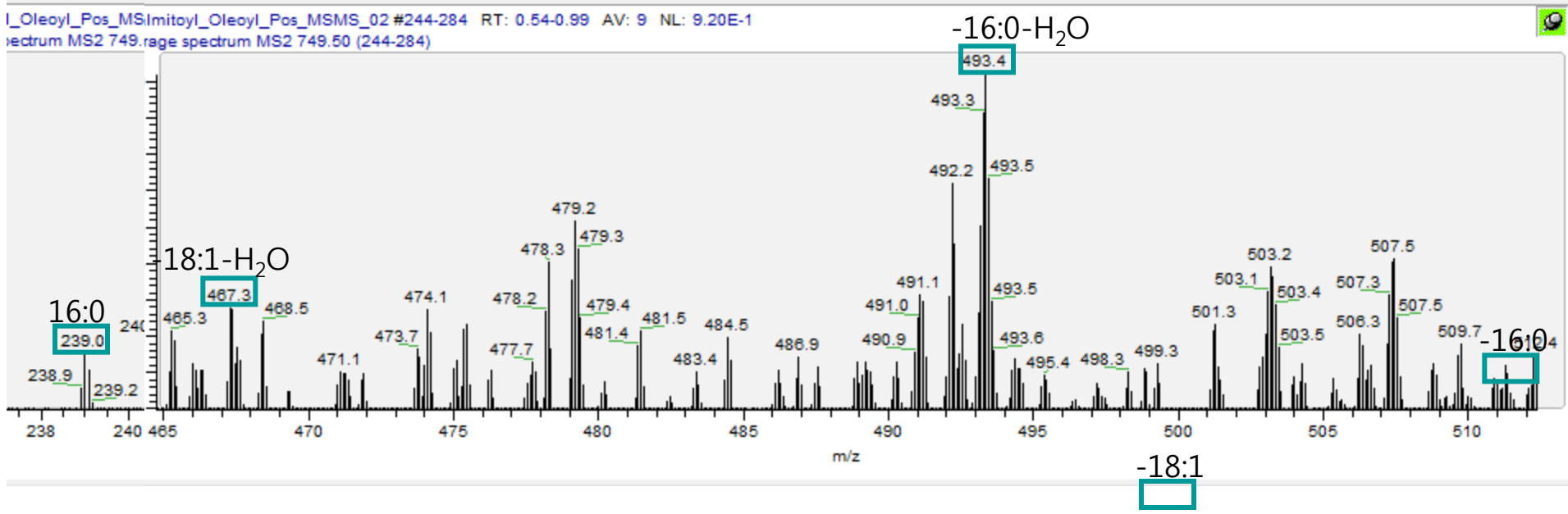
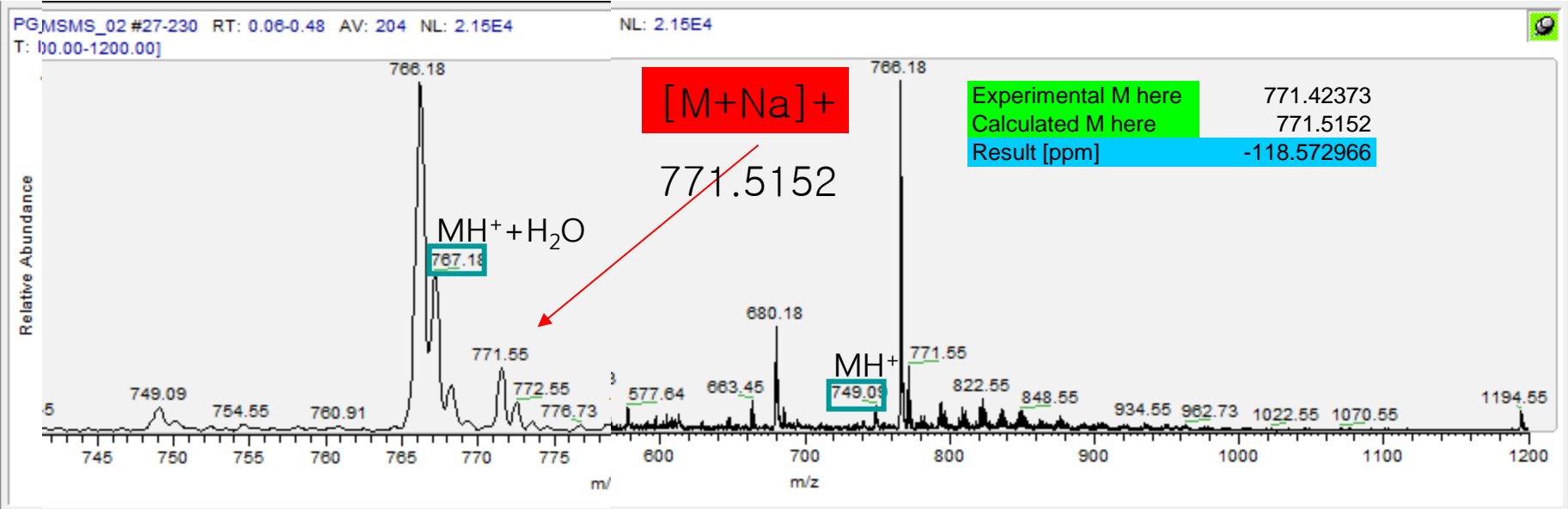


Exact Mass: 747.52





Exact Mass: 227.03



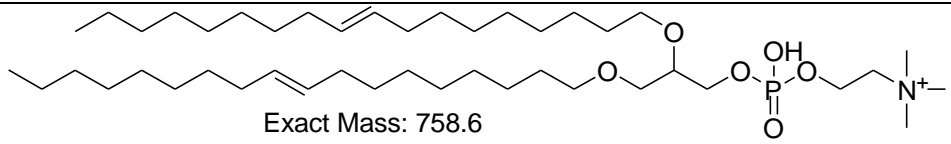
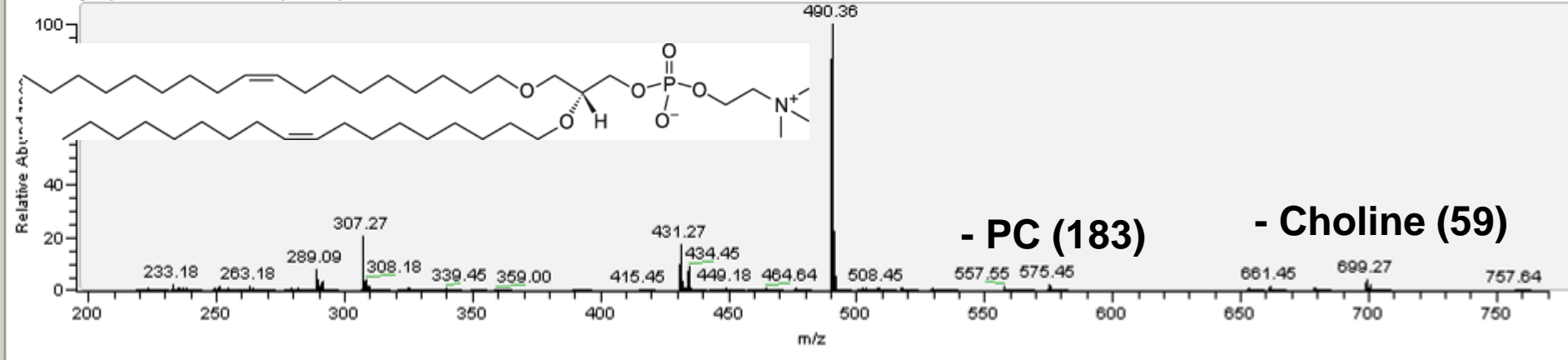
Phospholipids ID Collection B

Dr. KH LIU
UC Davis Metabolomics
LipidBlast

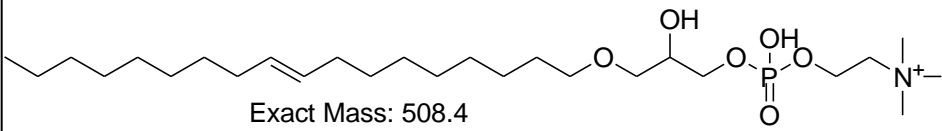
DLOPC (18:1, 18:1, diether form, m/z 758.8 [M+H]⁺)

090602_DLOPC_5ug_ml_Pos_CE35_01 #54-115 RT: 0.11-0.88 AV: 4 NL: 3.83E2
 T: Average spectrum MS2 758.81 (54-115)

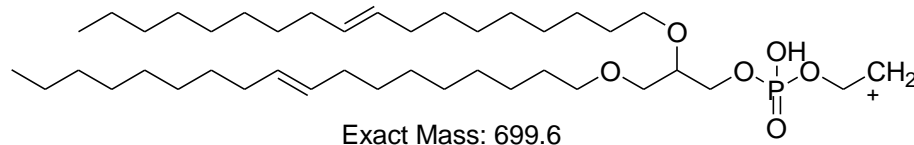
Positive mode



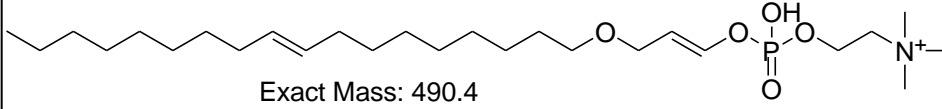
18:1 Diether PC (1,2-di-O-(9Z-octadecenyl)-sn-glycero-3-phosphocholine)



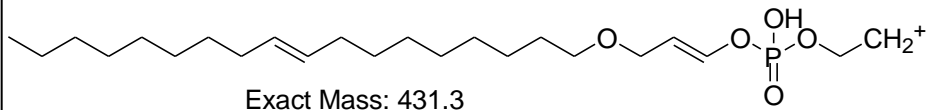
Exact Mass: 508.4



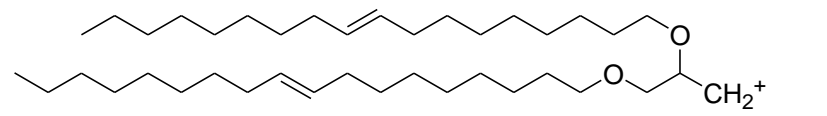
Exact Mass: 699.6



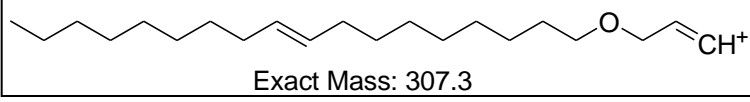
Exact Mass: 490.4



Exact Mass: 431.3



Exact Mass: 575.6

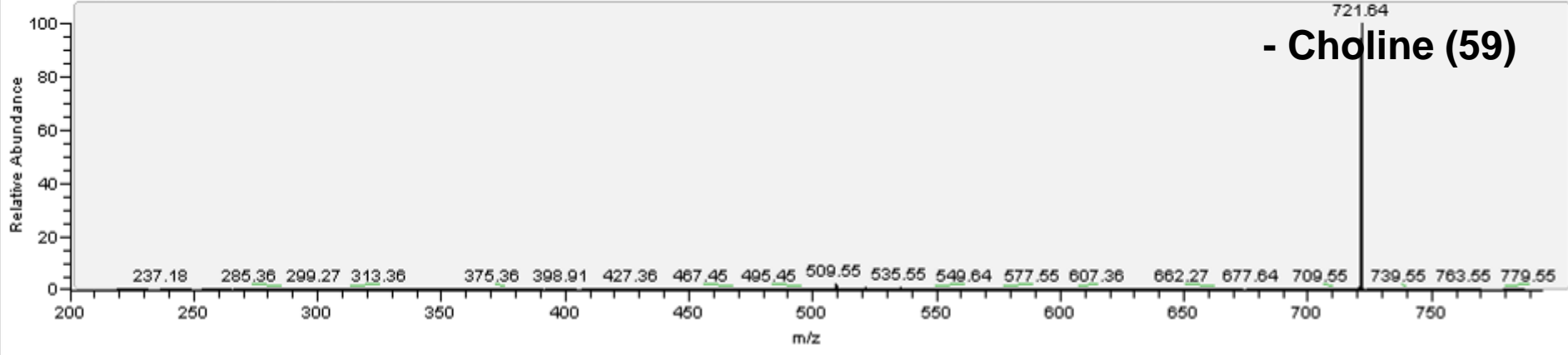


Exact Mass: 307.3

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

090602_DLOPC_5ug_ml_Pos_CE35_01 #57-118 RT: 0.14-0.91 AV: 4 NL: 1.17E4
T: Average spectrum MS2 780.64 (57-118)

Positive mode 

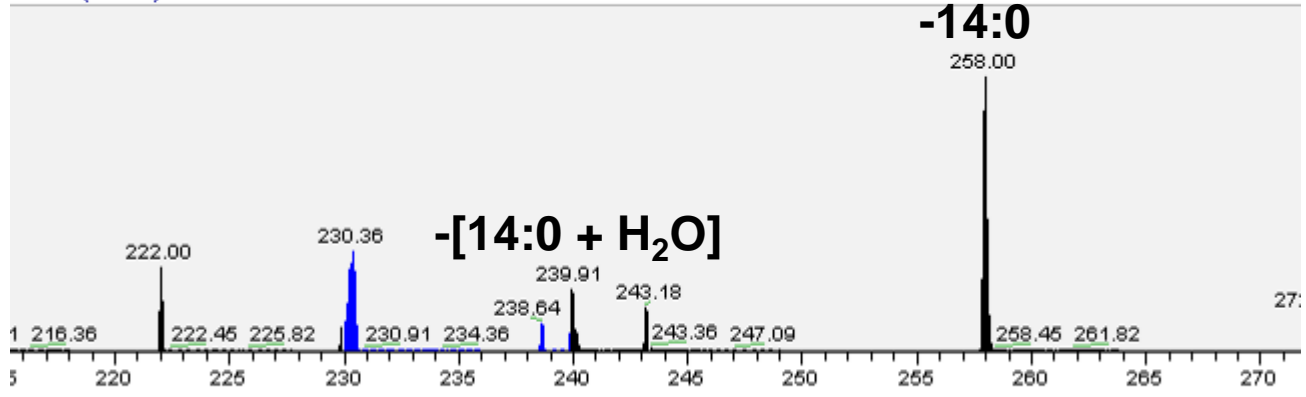
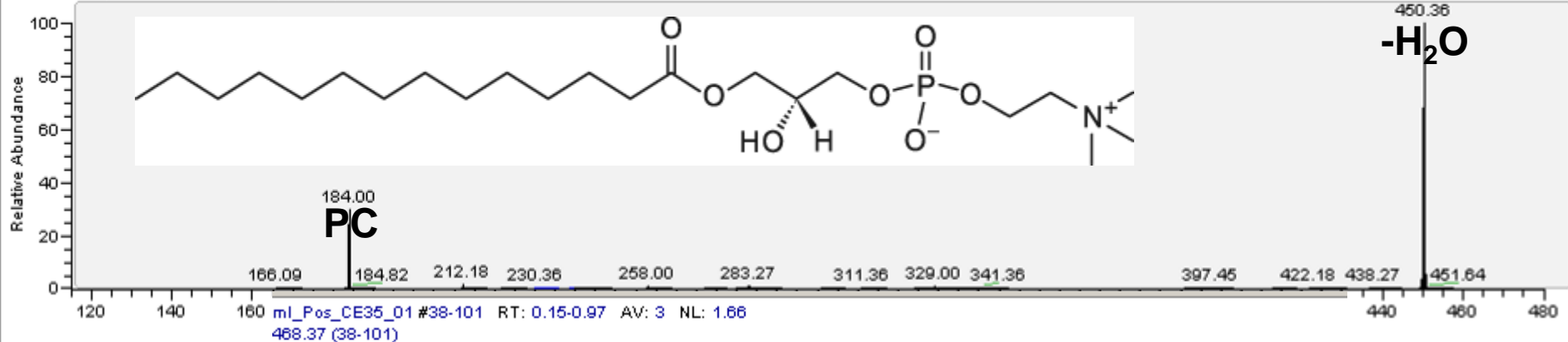


- Choline (59)

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

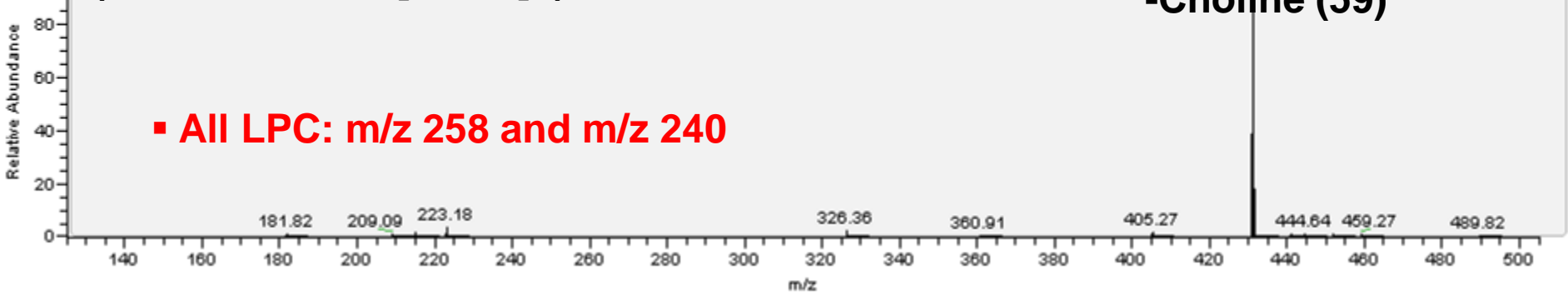
090623_LPL3Mix_2_5ug_ml_Pos_CE35_01 #38-101 RT: 0.15-0.97 AV: 3 NL: 1.22E2
T: Average spectrum MS2 468.37 (38-101)

Positive mode



090623_LPL3Mix_2_5ug_ml_Pos_CE35_01 #54 RT: 0.35 AV: 1 NL: 5.21E1
T: ITMS + p ESI d Full ms2 490.35@cid35.00 [125.00-505.00]

LPC (14:0, m/z 490.4 [M+Na]+)

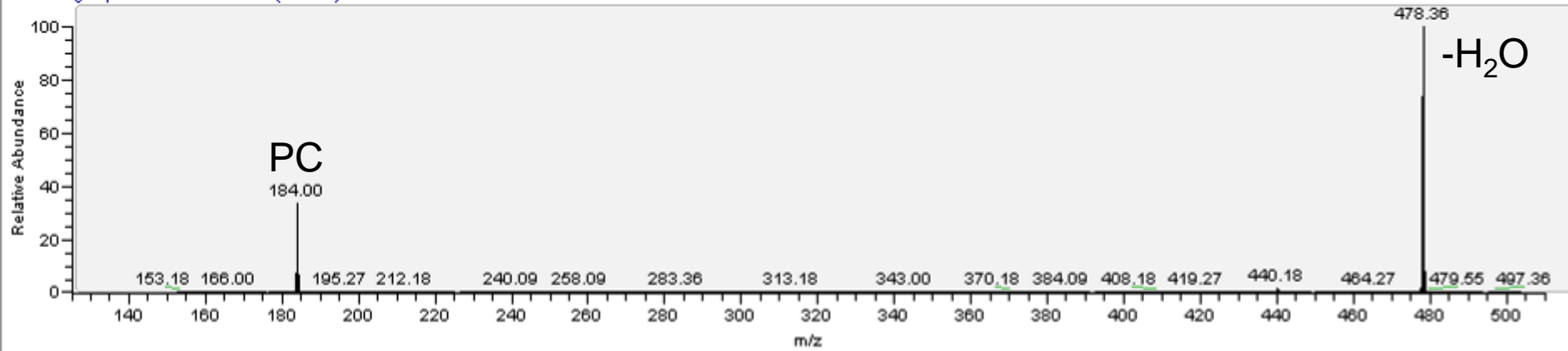


▪ All LPC: m/z 258 and m/z 240

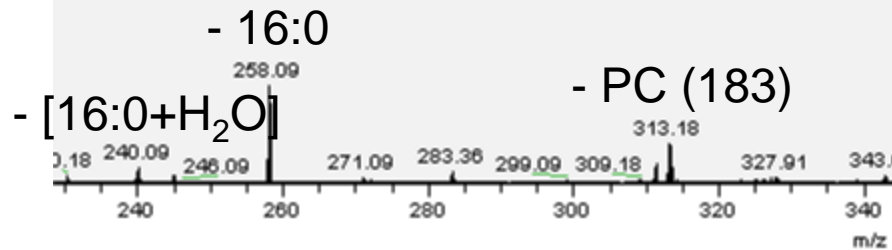
LPC 16:0 (m/z 496.4, [M+H]⁺)

090708_LPCs_EY_Pos_CE25_02 #56-117 RT: 0.11-0.86 AV: 4 NL: 1.39E4
T: Average spectrum MS2 496.46 (56-117)

Positive mode 

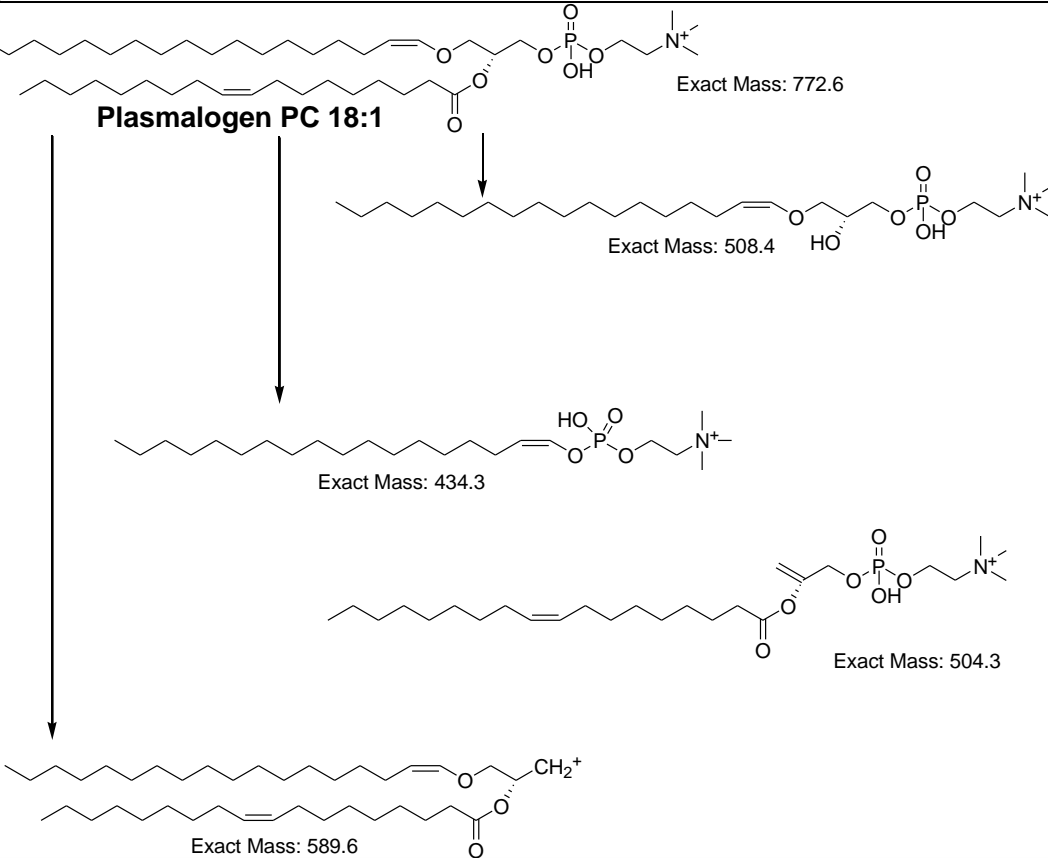
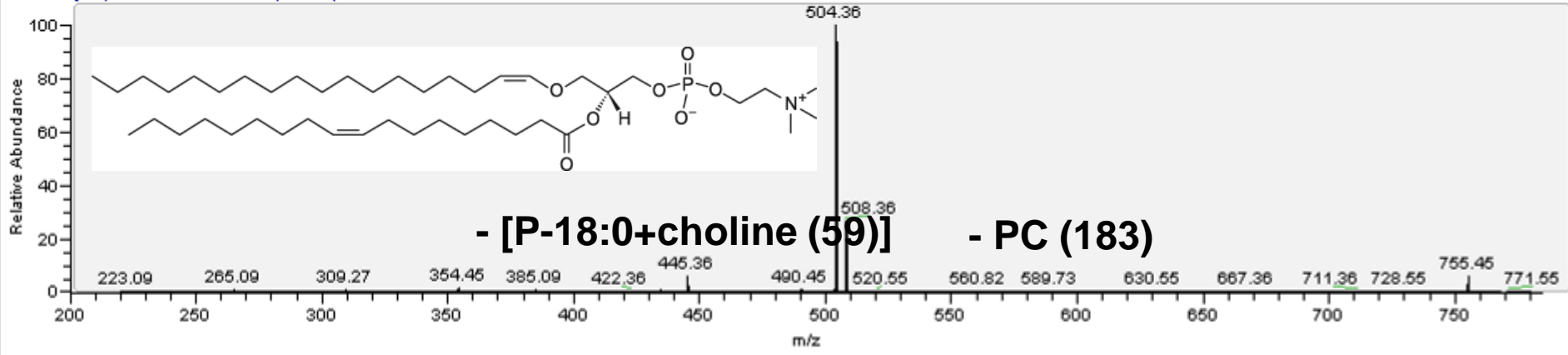


EY_Pos_CE25_02 #56-117 RT: 0.11-0.86 AV: 4 NL: 1.96E2
ctrum MS2 496.46 (56-117)



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

090624_PL_4Mix_3ug_mL_Pos_CE35_01 #54-116 RT: 0.11-0.89 AV: 4 NL: 9.33E2 - P-18:0 (268) Positive mode

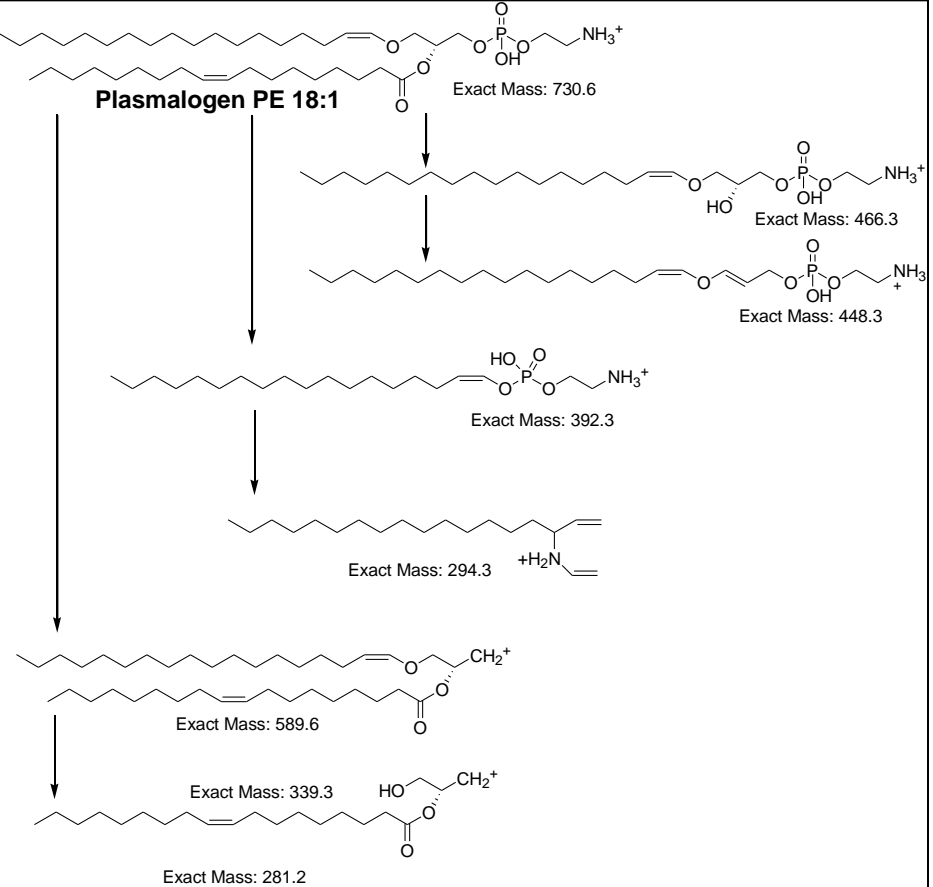
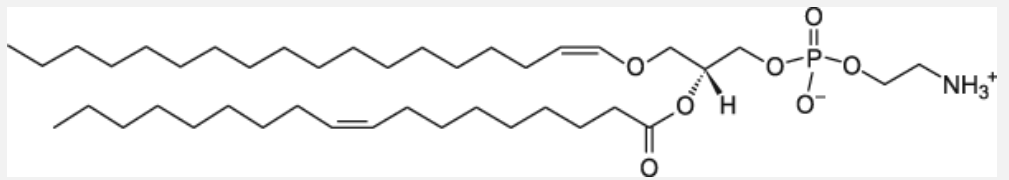
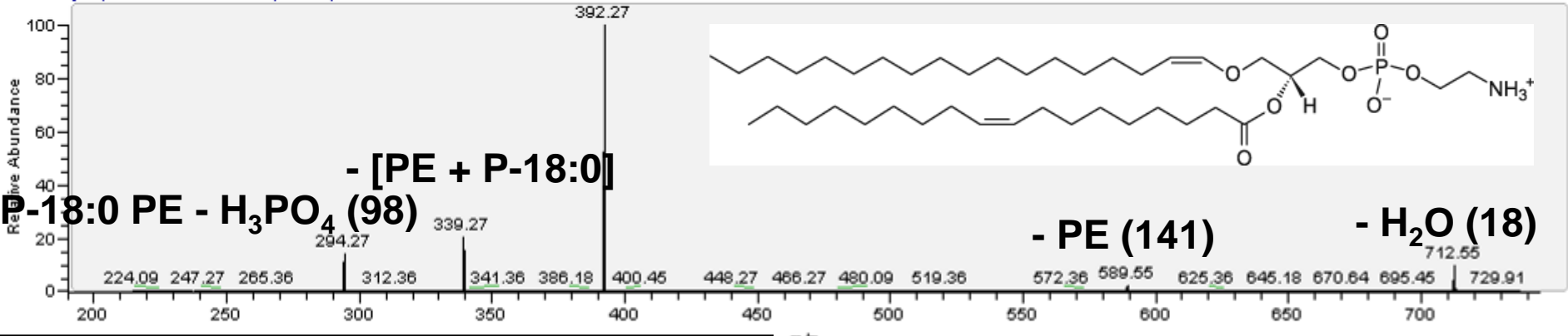


- Positive mode
- Characteristic ion of plasmalogen PC
 - P-18:0: loss of m/z 268 from MH⁺
 - P-18:1: loss of m/z 266 from MH⁺
 - P-16:0: loss of m/z 240 from MH⁺
 - P-16:1: loss of m/z 238 from MH⁺

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

090624_PL_4Mix_3ug_mL_Pos_CE35_01 #65-123 RT: 0.24-0.96 min. P-18:0 PE
 T: Average spectrum MS2 730.62 (65-123)

Positive mode

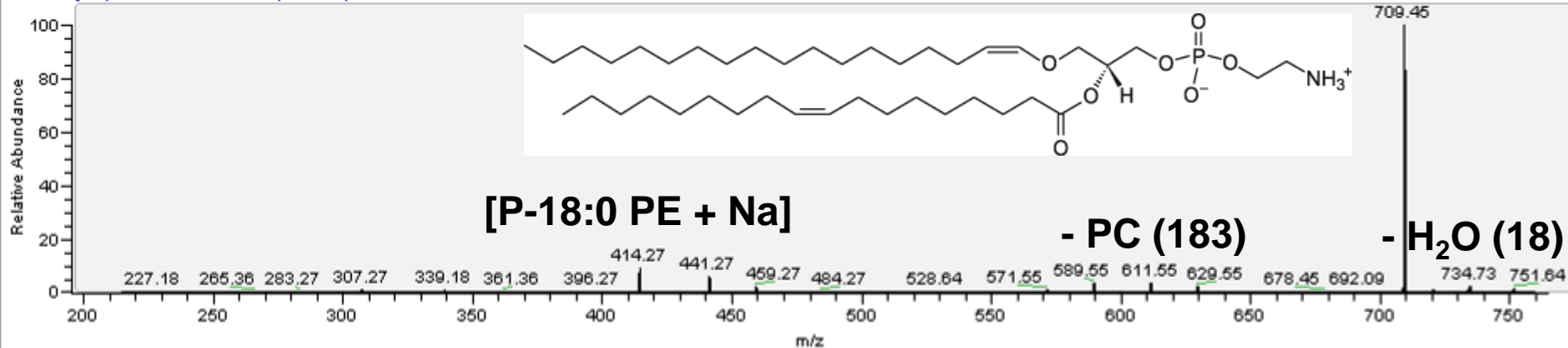


- Positive mode
- Characteristic ion of plasmalogen PE
 - P-20:0: m/z 420
 - P-20:1: m/z 418
 - P-18:0: m/z 392
 - P-18:1: m/z 390
 - P-16:0: m/z 364
 - P-16:1: m/z 362
 -

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

090624_PL_4Mix_3ug_mL_Pos_CE35_01 #101-162 RT: 0.70-1.47 AV: 2 NL: 1.74E3
T: Average spectrum MS2 752.69 (101-162)

Positive mode

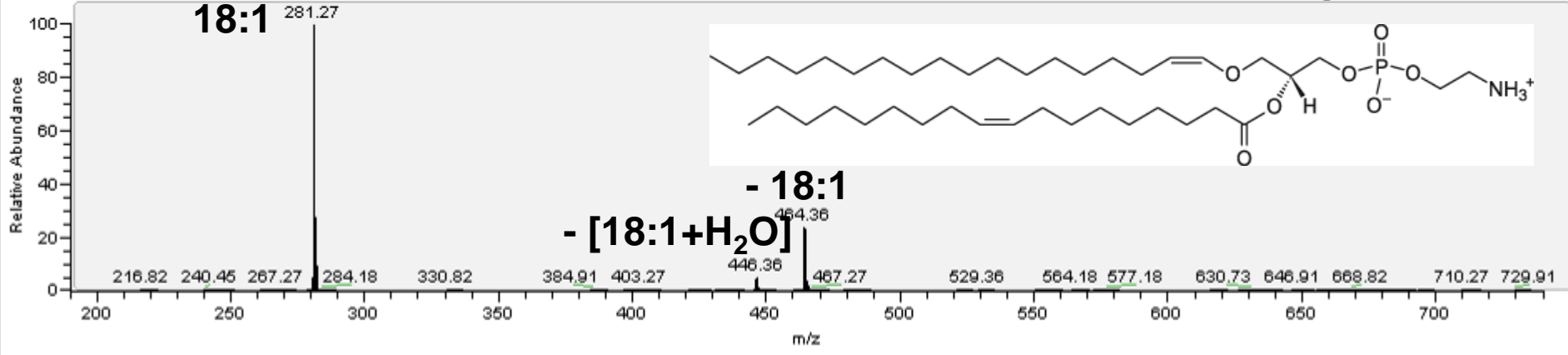


- Positive mode
- Characteristic ion of plasmalogen PE
 - P-20:0: m/z 442
 - P-20:1: m/z 440
 - P-18:0: m/z 414
 - P-18:1: m/z 412
 - P-16:0: m/z 386
 - P-16:1: m/z 384
 -

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

090624_PL_4Mix_3ug_mL_Neg_CE35_01 #115-226 RT: 0.46-0.98 AV: 5 NL: 3.53E3
T: Average spectrum MS2 728.84 (115-226)

Negative mode



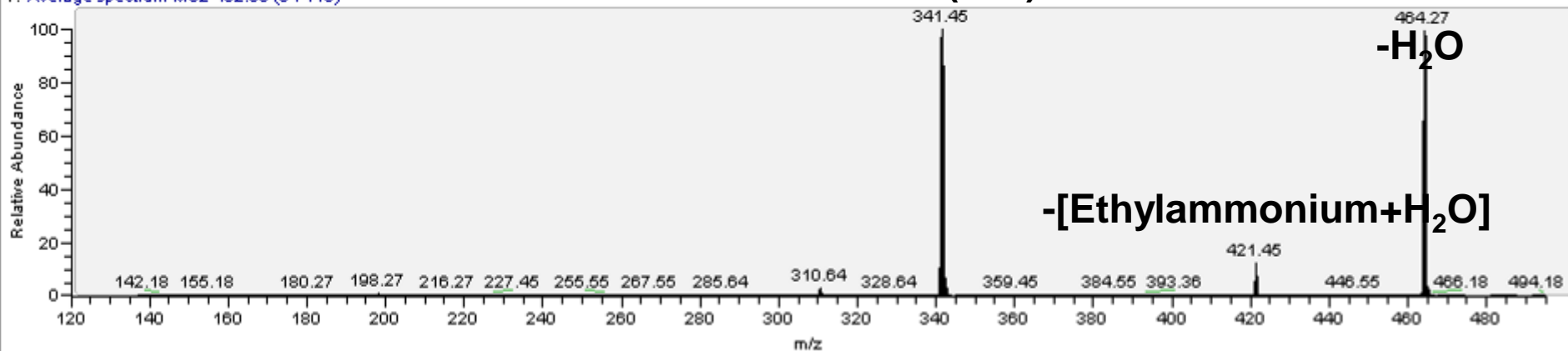
LPE (18:0, m/z 482.4 [M+H]⁺)

090708_LPEs_EY_Pos_CE35_01 #54-115 RT: 0.11-0.88 AV: 4 NL: 1.19E4

T: Average spectrum MS2 482.39 (54-115)

-PE (141)

Positive mode

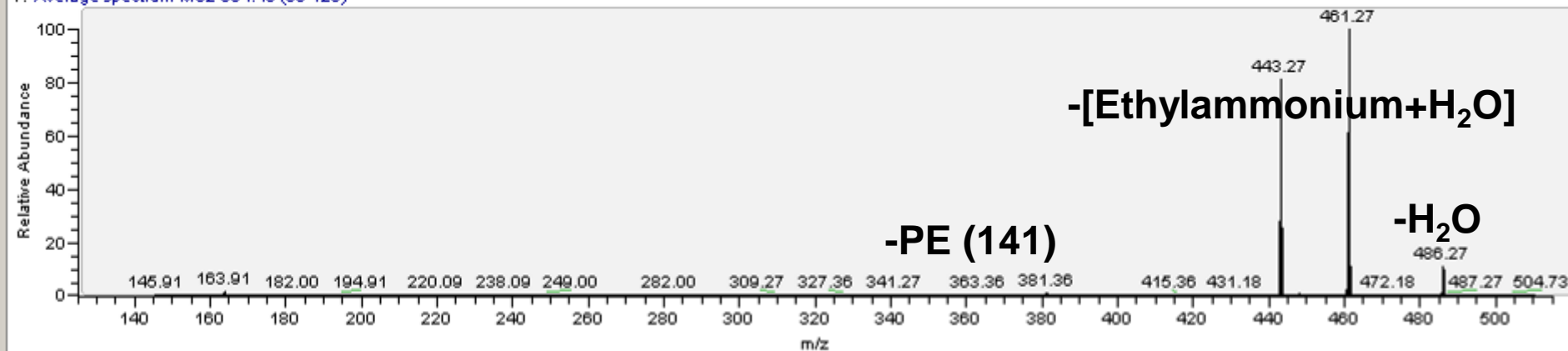


LPE (18:0, m/z 504.4 [M+Na]⁺)

090708_LPEs_EY_Pos_CE35_01 #65-123 RT: 0.23-0.97 AV: 2 NL: 4.47E3

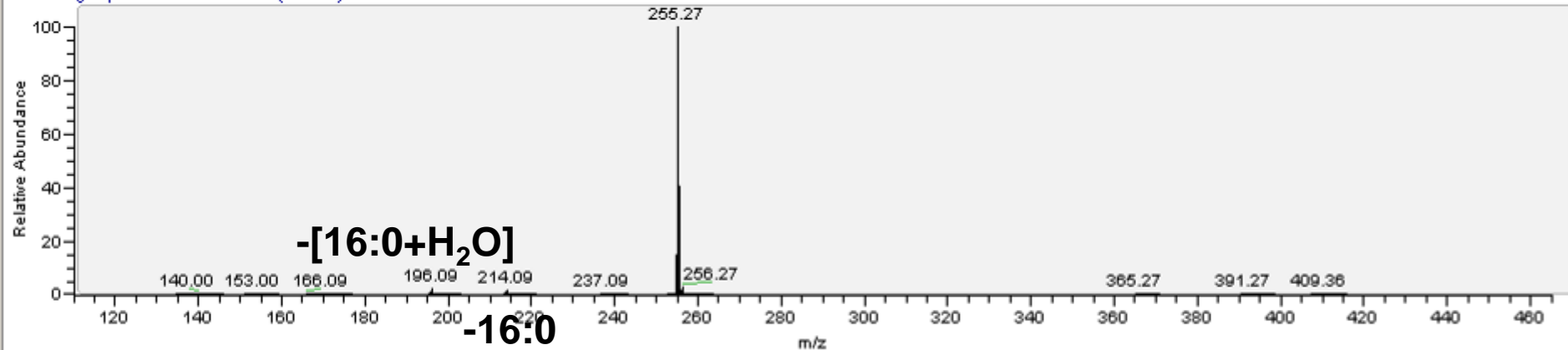
T: Average spectrum MS2 504.40 (65-123)

-Ethylammonium (43)



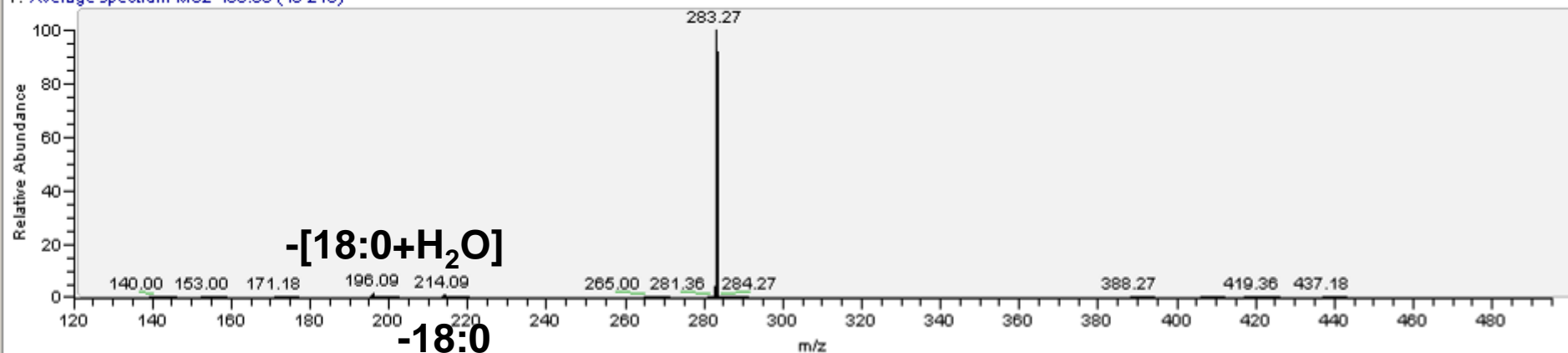
LPE (16:0, m/z 452.3 [M-H]-)

090708_LPEs_EY_Neg_CE35_01 #46-219 RT: 0.11-0.88 AV: 8 NL: 3.92E4 **16:0**
T: Average spectrum MS2 452.86 (46-219)



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

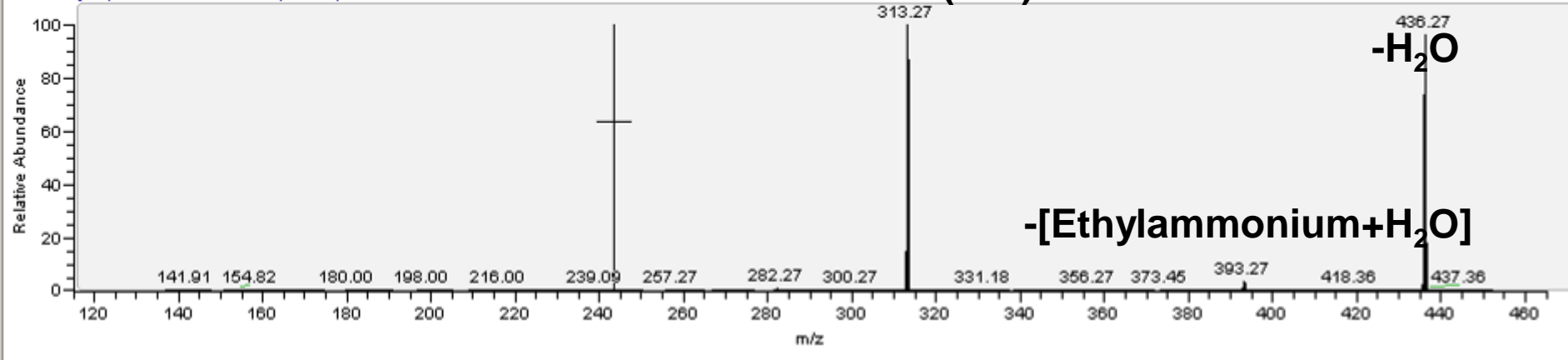
090708_LPEs_EY_Neg_CE35_01 #45-218 RT: 0.11-0.88 AV: 8 NL: 2.91E4 **18:0**
T: Average spectrum MS2 480.58 (45-218)



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

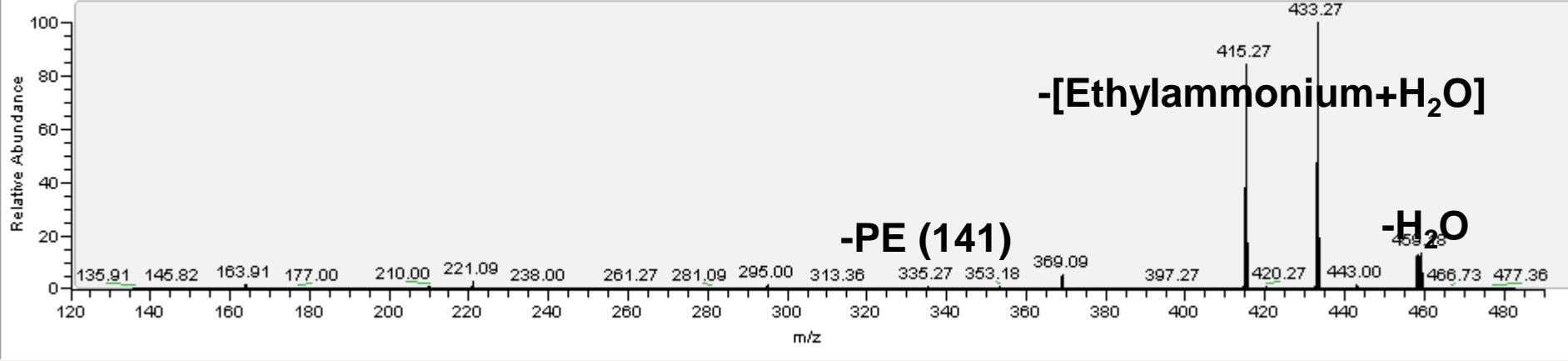
LPE (16:0, m/z 454.4 [M+H]+)

090708_LPEs_EY_Pos_CE35_01 #55-116 RT: 0.12-0.89 AV: 4 NL: 1.84E4
T: Average spectrum MS2 454.41 (55-116)



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

090708_LPEs_EY_Pos_CE35_01 #58-122 RT: 0.15-0.96 AV: 2 NL: 2.16E3
T: Average spectrum MS2 476.31 (58-122)

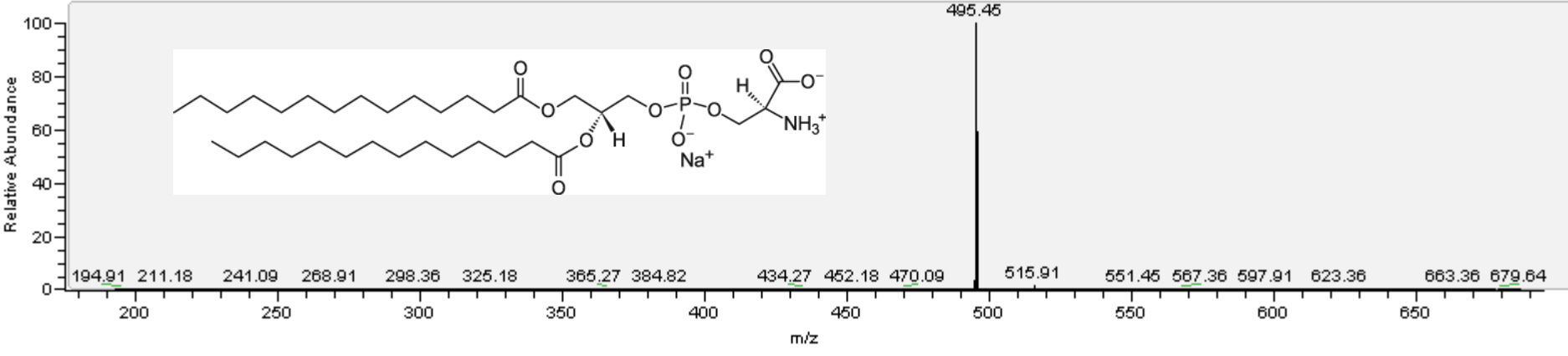


DMPS (14:0, 14:0, m/z 680.6 [M+H]⁺)

090623_PL5Mix_10ug_mL_Pos_CE35_01 #58-119 RT: 0.13-0.87 AV: 4 NL: 2.87E3
T: Average spectrum MS2 680.41 (58-119)

- PS (185)

Positive mode

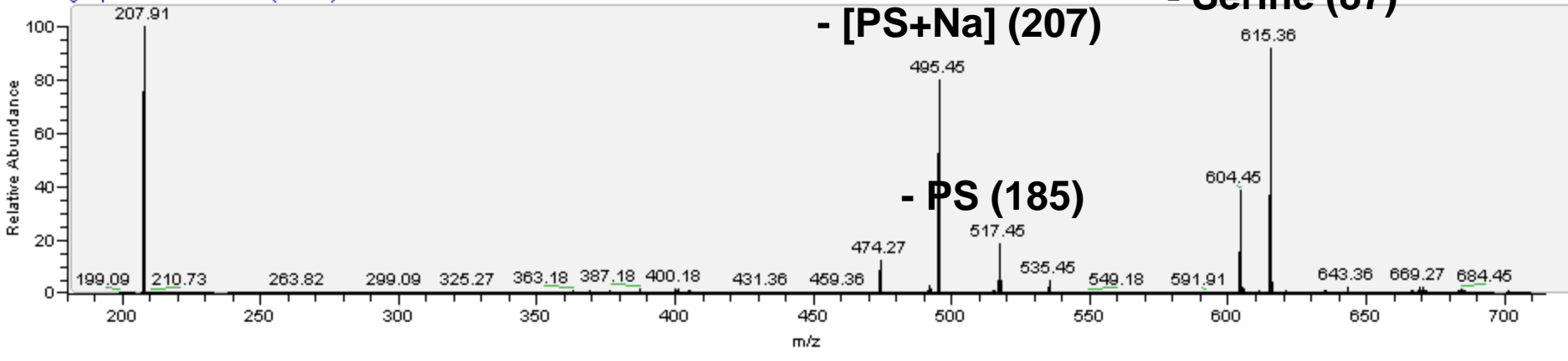


DMPS (14:0, 14:0, m/z 702.6 [M+Na]⁺)

090623_PL5Mix_10ug_mL_Pos_CE35_01 #79-133 RT: 0.37-1.03 AV: 2 NL: 7.24E2
T: Average spectrum MS2 702.59 (79-133)

- [PS+Na] (207)

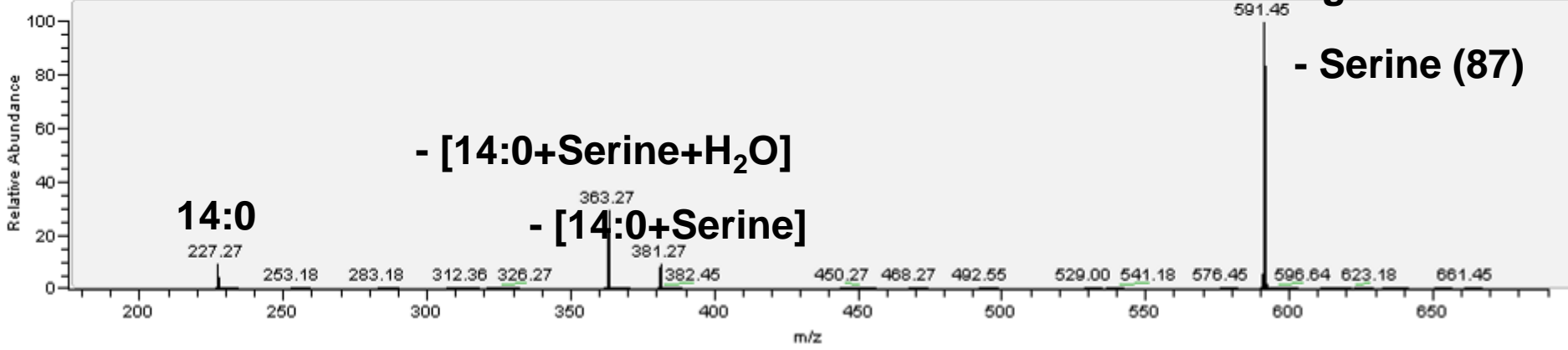
- Serine (87)



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

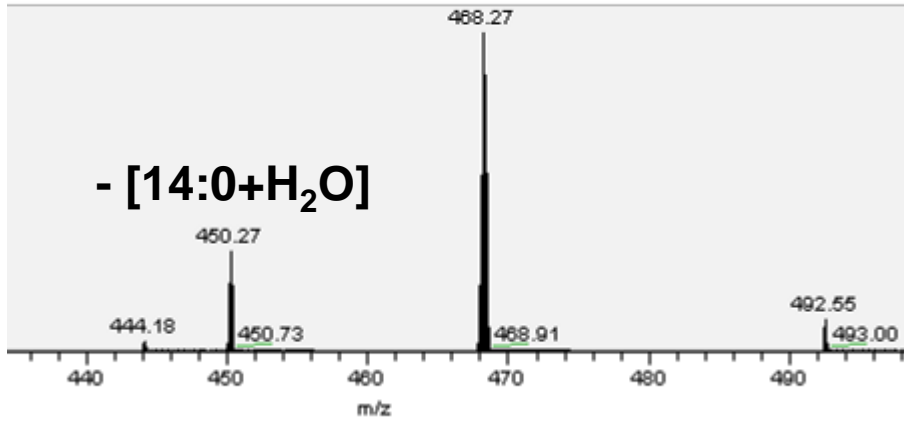
090623_PL5Mix_10ug_mL_Neg_CE35_01 #49-222 RT: 0.11-0.89 AV: 8 NL: 2.68E4

T: Average spectrum MS2 678.76 (49-222)



0.89 AV: 8 NL: 3.03E1

- 14:0

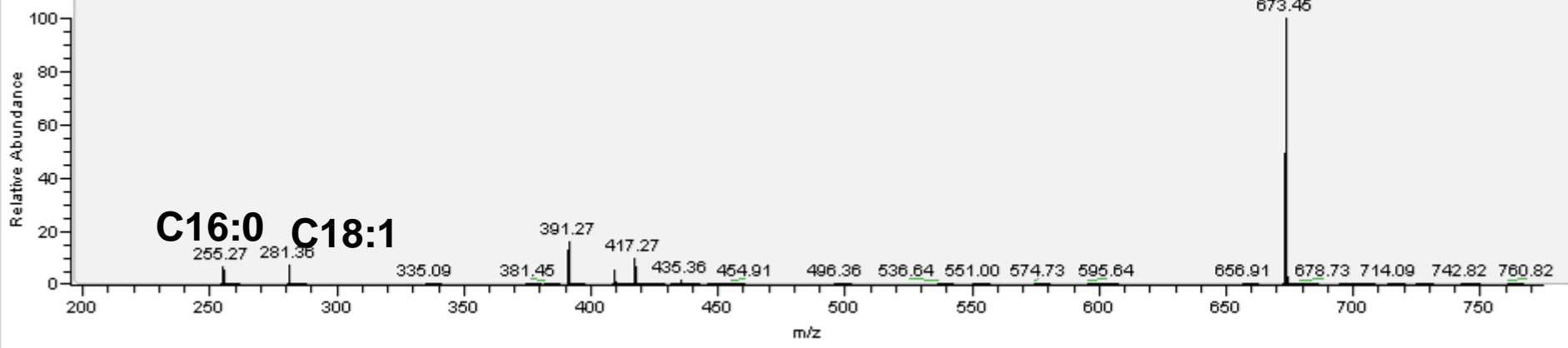


POPS (16:0, 18:1, m/z 760.7 [M-H]-)

090624_PL_4Mix_3ug_mL_Neg_CE35_01 #93-190 RT: 0.36-0.81 AV: 2 NL: 1.42E3

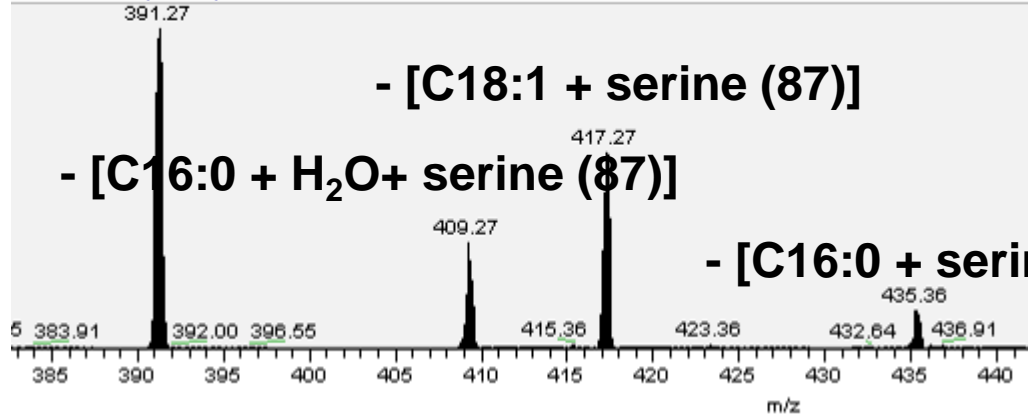
T: Average spectrum MS2 760.74 (93-190)

- Serine (87)



- [C18:1 + H₂O + serine (87)]

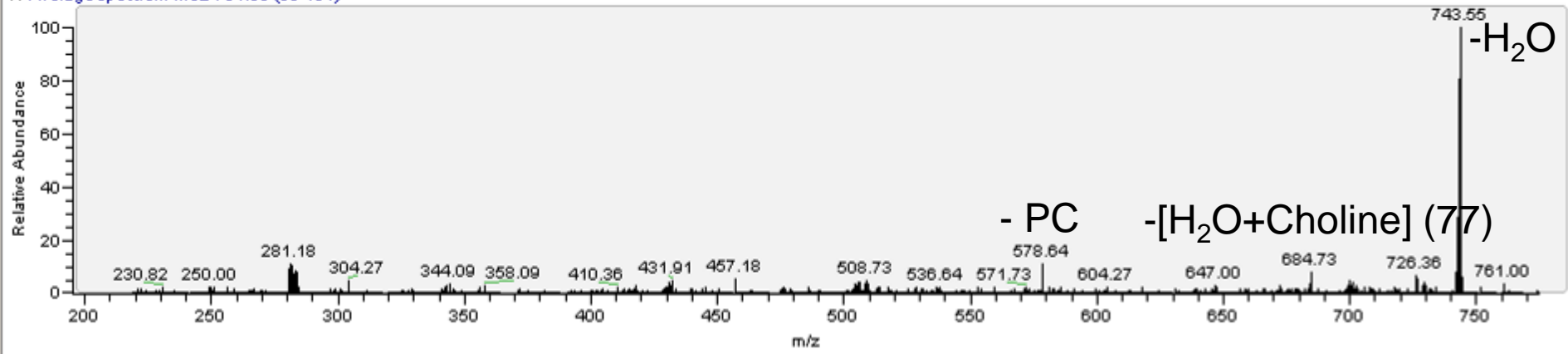
090624_PL_4Mix_3ug_mL_Neg_CE35_01 #93-190 RT: 0.36-0.81 AV: 2 NL: 2.24E2
MS2 760.74 (93-190)



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

090708_SMs_BB_Pos_CE35_01 #90-151 RT: 0.57-1.37 AV: 2 NL: 4.99E1
T: Average spectrum MS2 761.63 (90-151)

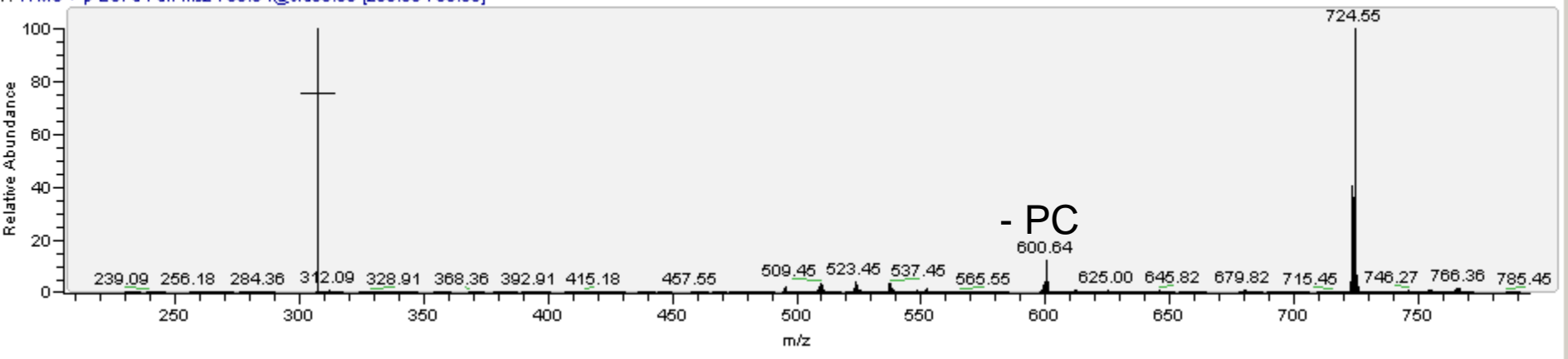
Positive mode



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

090708_SMs_BB_Pos_CE35_01 #102-102 RT: 0.73-0.73 AV: 2 NL: 4.10E2
T: ITMS + p ESI d Full ms2 783.64@cid35.00 [205.00-795.00]

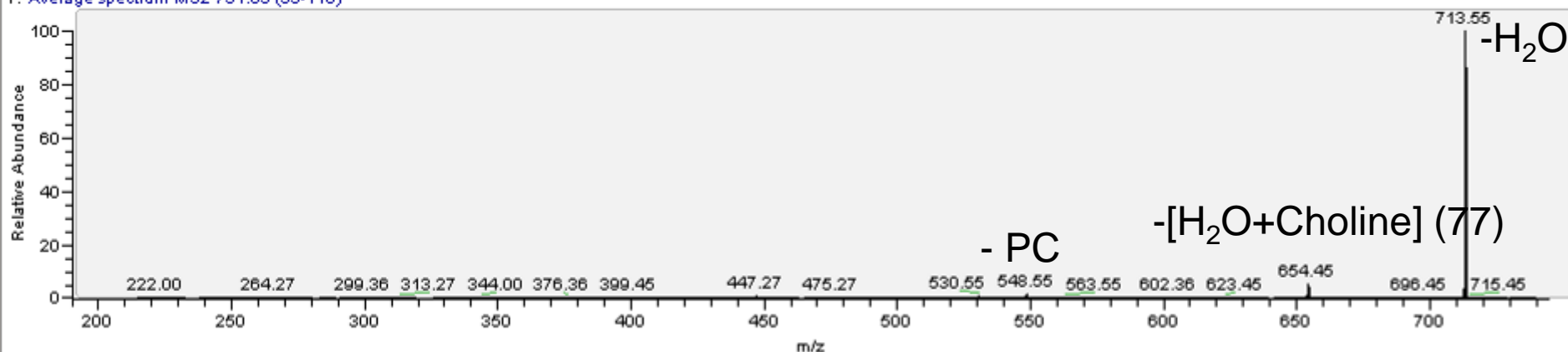
- Choline



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

090708_SMs_BB_Pos_CE35_01 #55-116 RT: 0.11-0.91 AV: 4 NL: 6.65E2
T: Average spectrum MS2 731.63 (55-116)

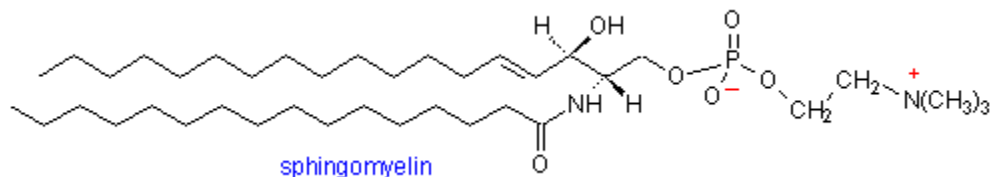
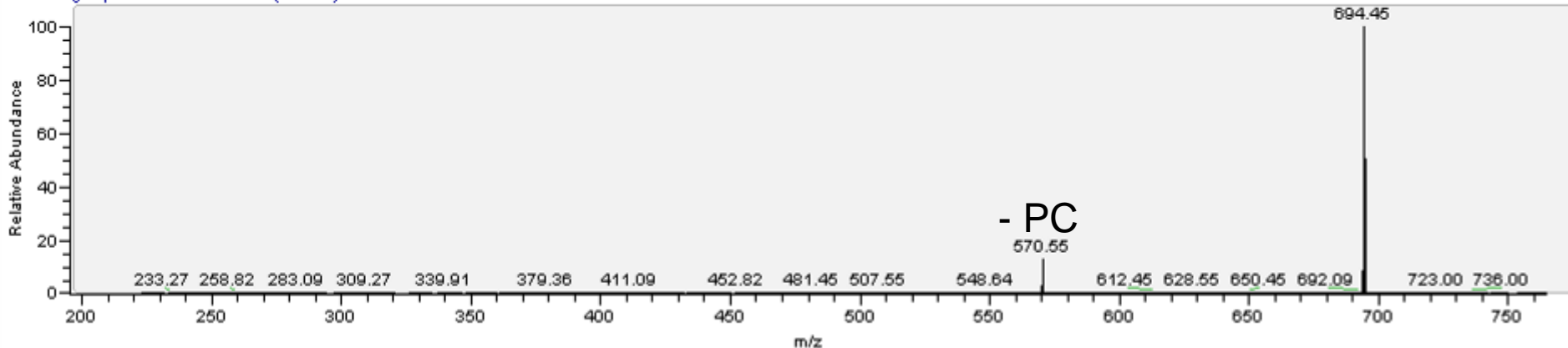
Positive mode



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

090708_SMs_BB_Pos_CE35_01 #65-122 RT: 0.23-0.98 AV: 2 NL: 7.97E3
T: Average spectrum MS2 753.57 (65-122)

- Choline



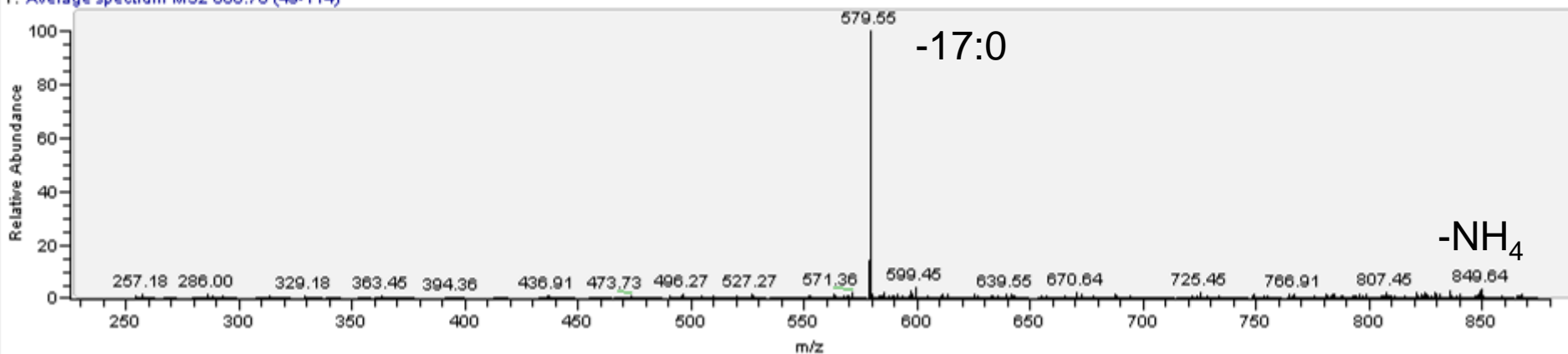
SM 34:1 (d18:1, 16:0)

TG 54:0 (17:0, 17:0, 17:0, m/z 866.8, [M+NH₄]+)

TG_17_0_1_074ug_ml_Pos_CE35_01 #49-114 RT: 0.11-0.92 AV: 8 NL: 1.62E1

T: Average spectrum MS2 866.78 (49-114)

Positive mode

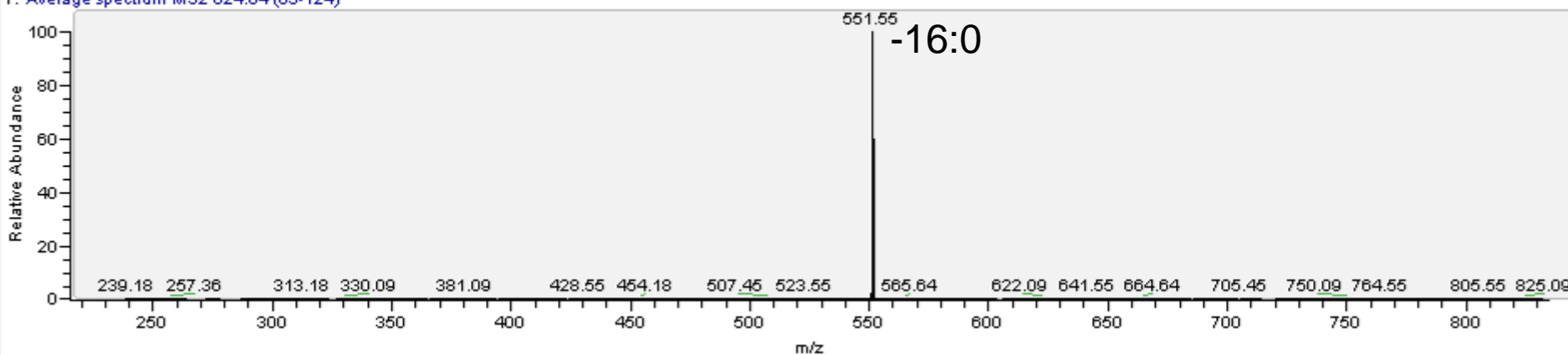


TG 48:0 (16:0, 16:0, 16:0, m/z 824.7, [M+NH₄]+)

090814_TG_TP_Pos_CE25_MSMS_400_1000_01 #63-124 RT: 0.11-0.89 AV: 4 NL: 5.22E3

T: Average spectrum MS2 824.64 (63-124)

Positive mode

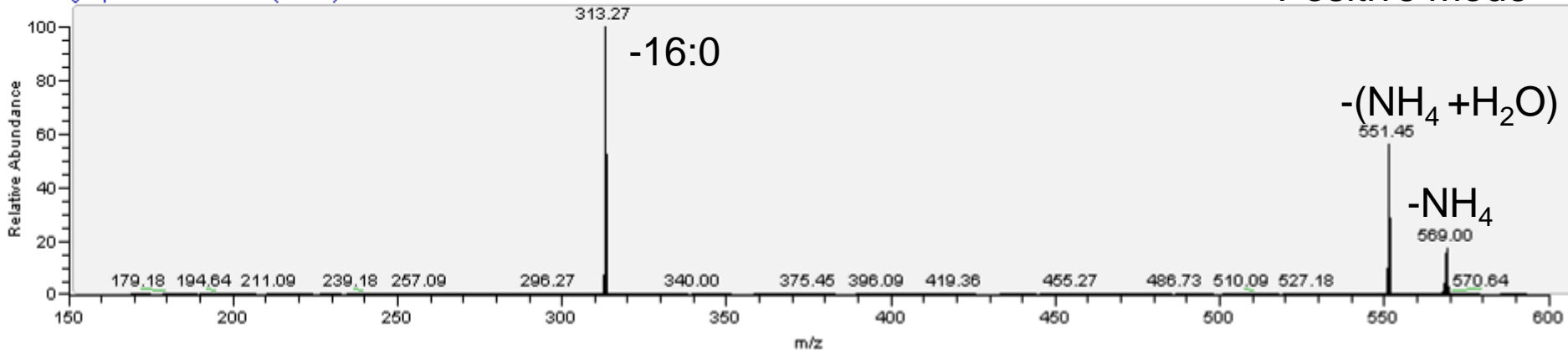


DG 32.0 (16:0, 16:0, m/z 586.6, [M+NH₄]+)

090814_DG_DP_Pos_CE35_MSMS_400_1000_01 #64-125 RT: 0.11-0.83 AV: 4 NL: 1.66E3

Positive mode

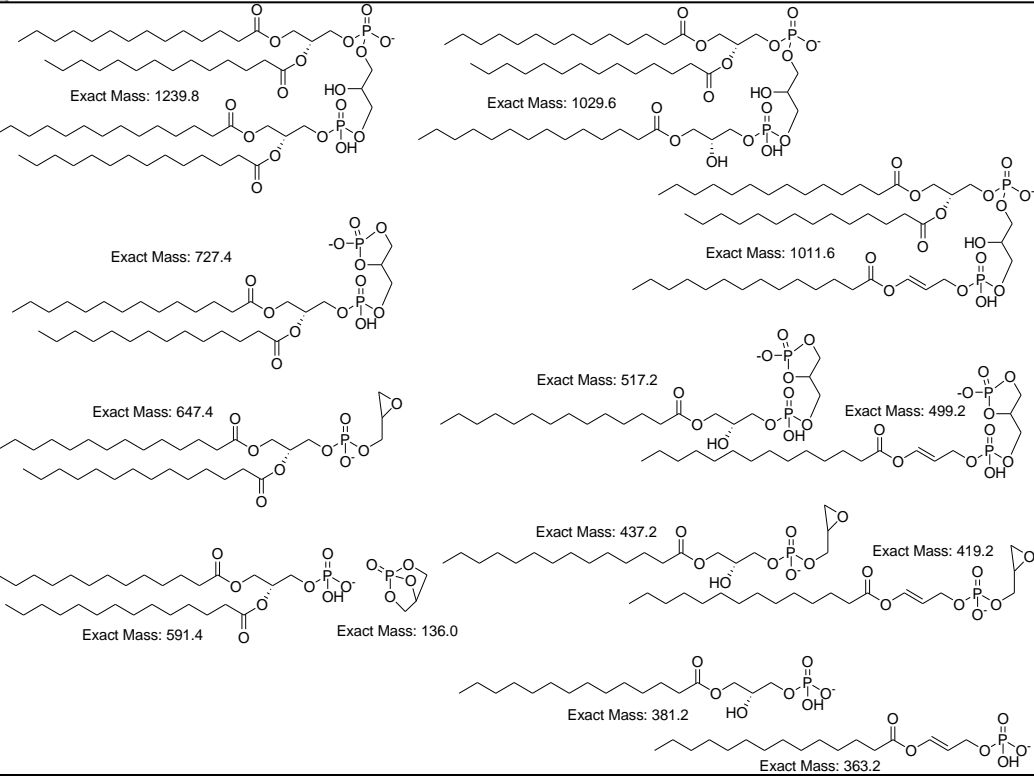
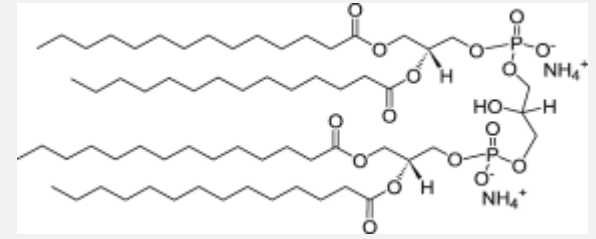
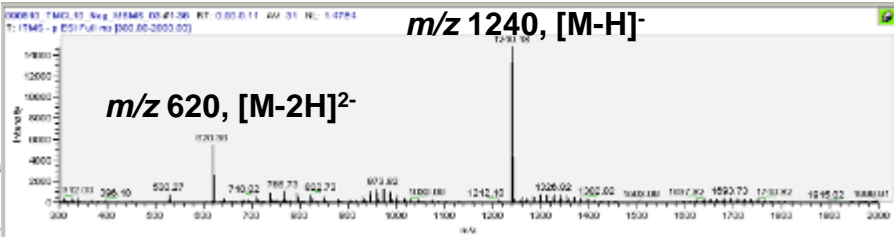
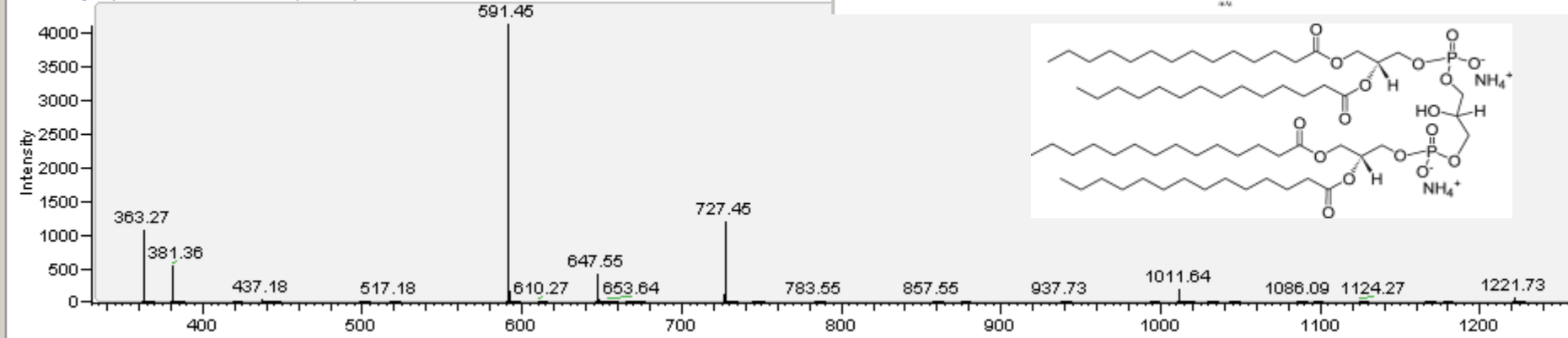
T: Average spectrum MS2 586.57 (64-125)



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

090810_TMCL10_Neg_MSMS_03 #36-200 RT: 0.13-0.90 AV: 4 NL: 4.12E3

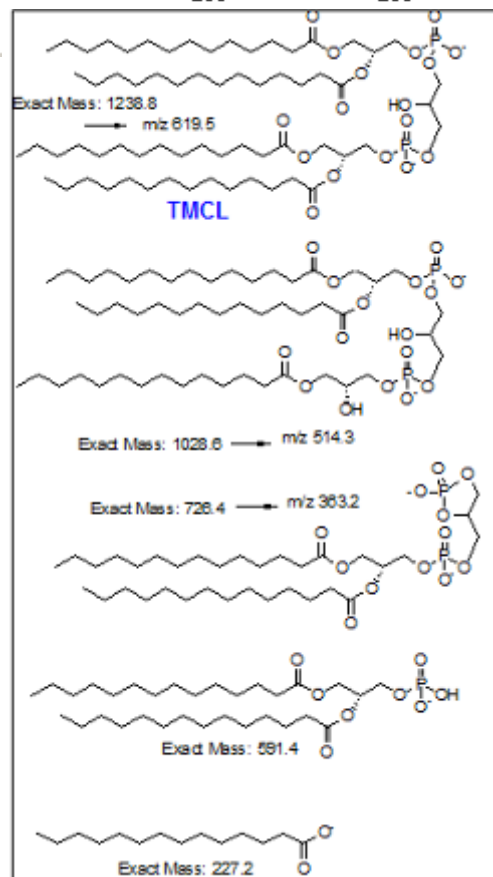
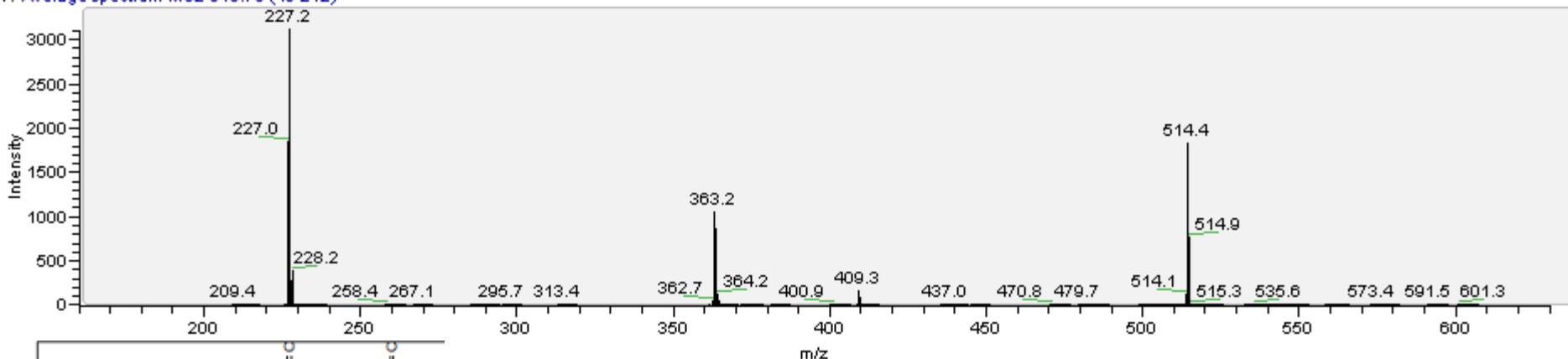
T: Average spectrum MS2 1240.16 (36-200)



- 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

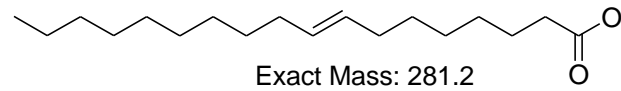
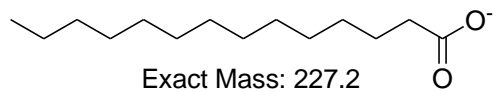
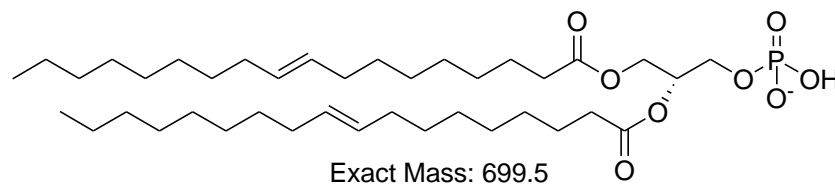
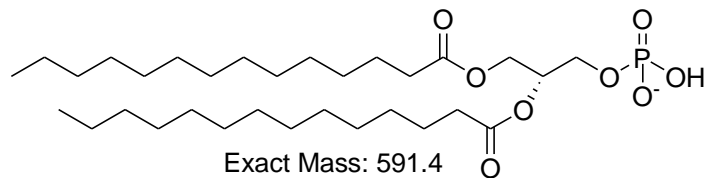
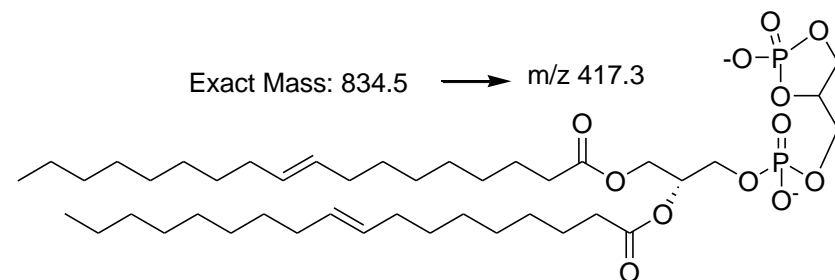
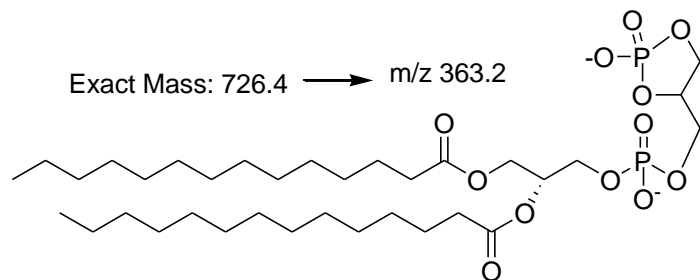
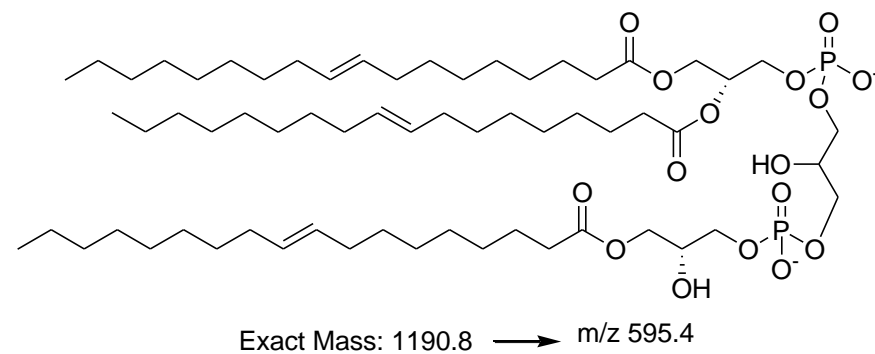
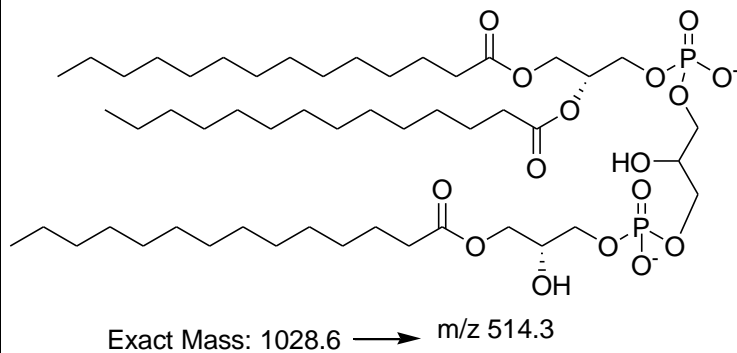
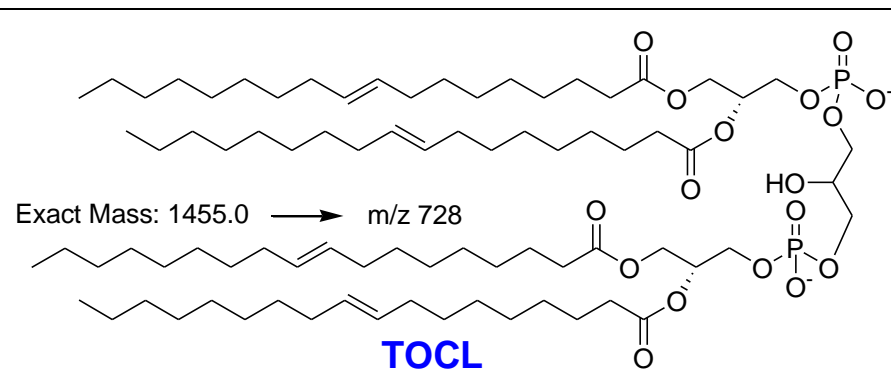
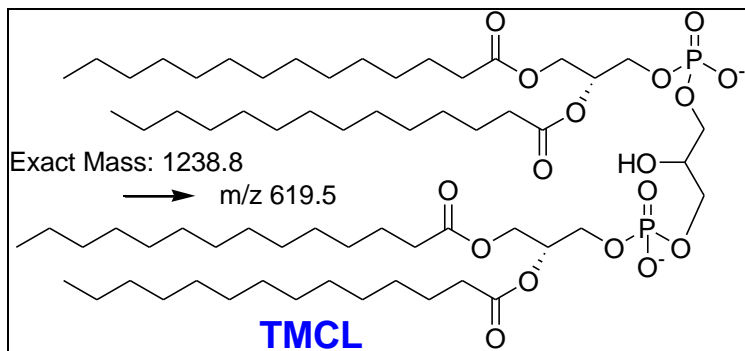
Cardiolipin 14:0 (CL 14:0, m/z 620, [M-2H]2-)

090810_TMCL10_Neg_MSMS_03 #45-212 RT: 0.16-0.96 AV: 3 NL: 3.11E3
T: Average spectrum MS2 619.79 (45-212)

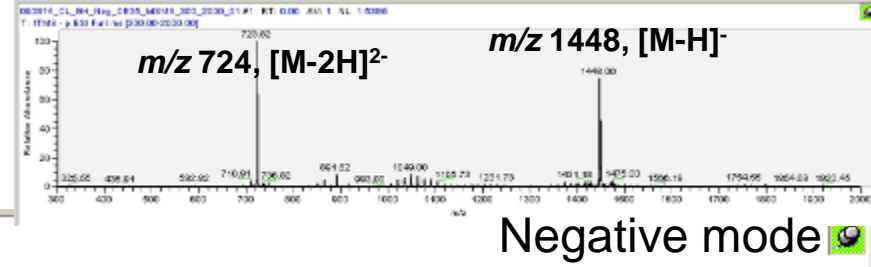


- Negative mode
- Characteristic ion
 - m/z 620: [M-2H]2-
 - m/z 514.4: loss of monoacyl group
 - m/z 363.2: loss of diacyl group
 - m/z 227.2: 14:0

✓ **Positive mode: No signal**

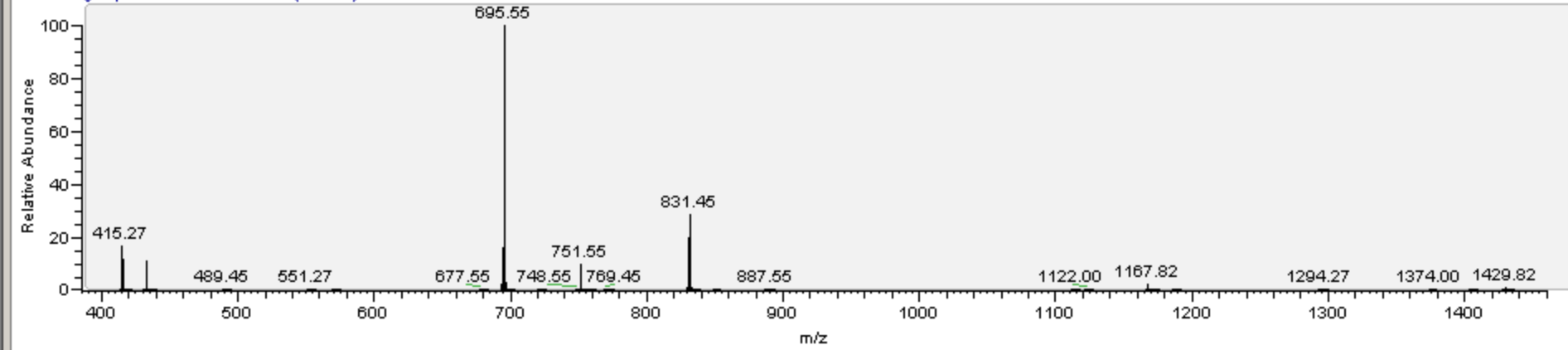


Cardiolipin 18:2 (CL 18:2, m/z 1448, [M-H]-)



Negative mode

090814_CL_BH_Neg_CE35_MSMS_300_2000_01#41-198 RT: 0.13-0.87 AV: 4 NL: 1.12E4
T: Average spectrum MS2 1448.11 (41-198)



- 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

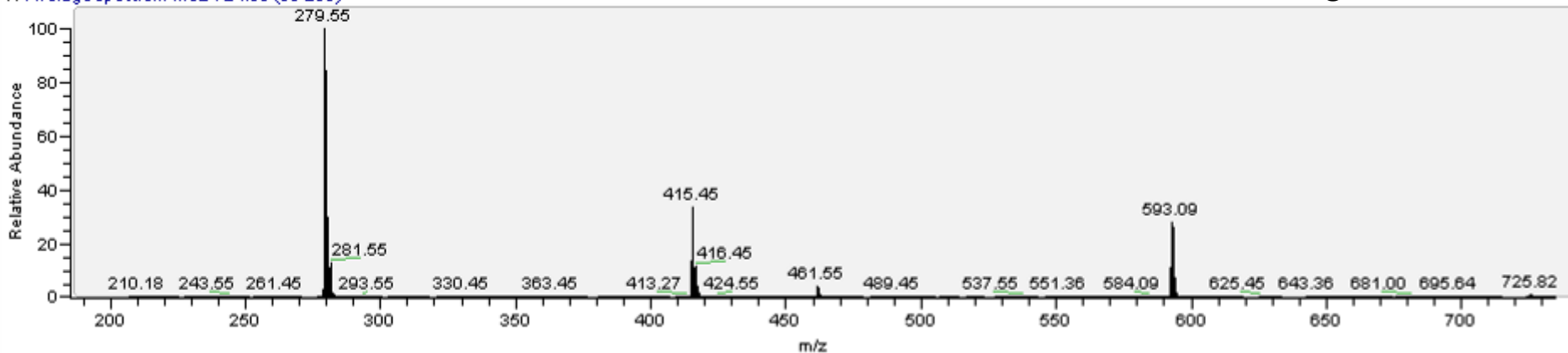
✓ Positive mode: No signal

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

Negative mode

090814_CL_BH_Neg_CE35_MSMS_300_2000_01 #39-200 RT: 0.12-0.87 AV: 4 NL: 1.56E4

T: Average spectrum MS2 724.58 (39-200)



- 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

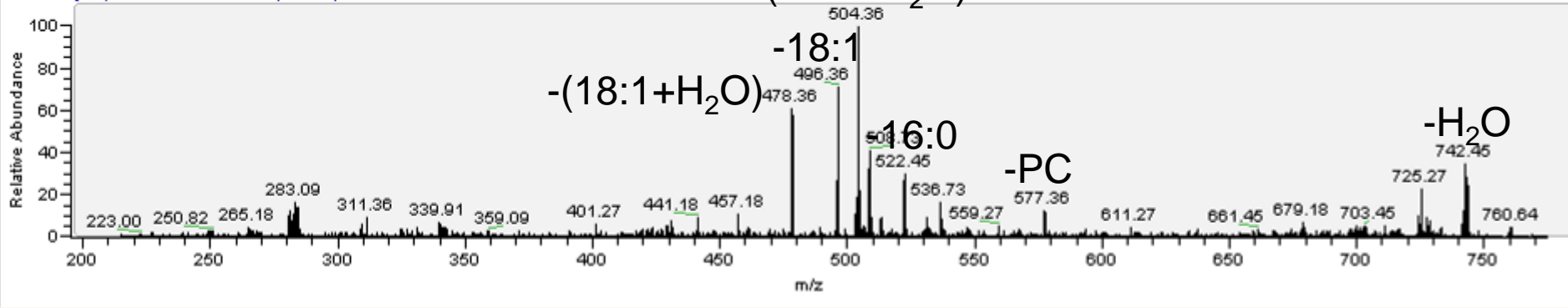
By adding LiOH in reconstitution solvent
(Final concentration of Li: 2 mM)

PLPC (16:0, 18:1, m/z 760.6, [M+H]⁺)

090813_PLPC_WO_Li_Pos_MSMS_01 #37-108 RT: 0.11-1.04 AV: 4 NL: 2.61E1
T: Average spectrum MS2 760.50 (37-108)

-(16:0+H₂O)

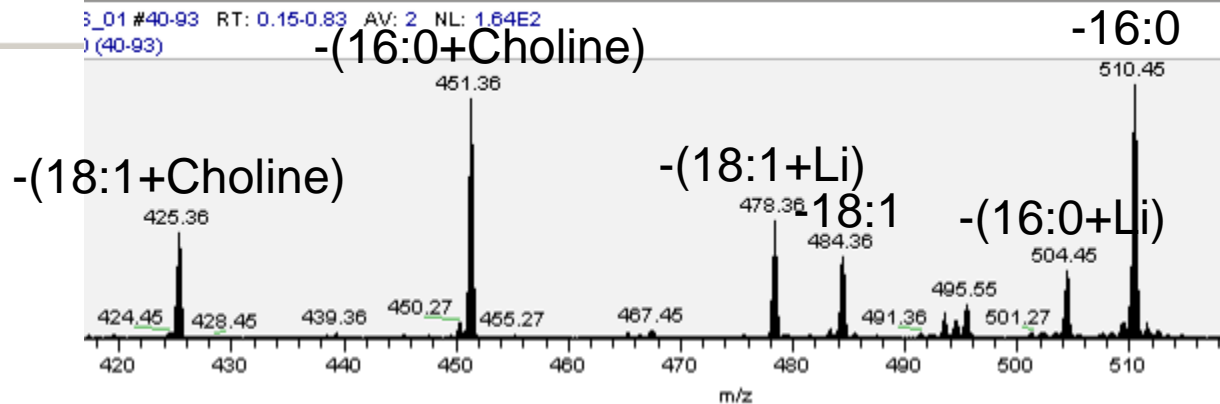
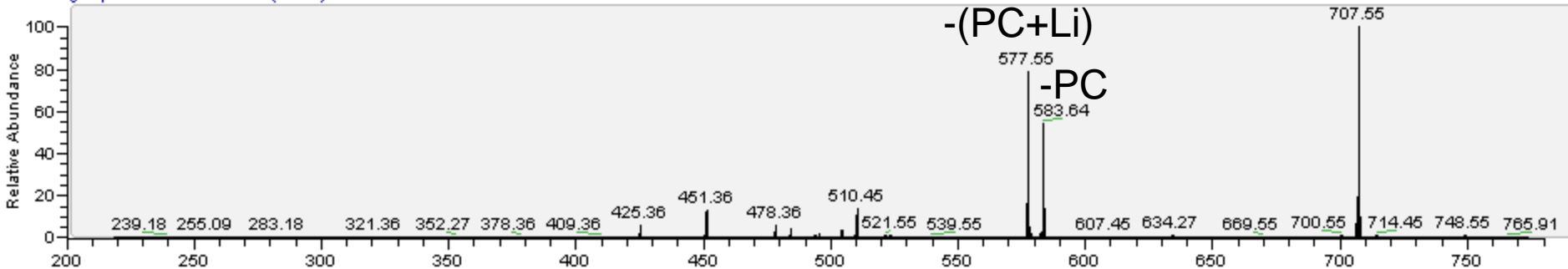
Positive mode



PLPC (16:0, 18:1, m/z 766.6, [M+Li]⁺)

090813_PLPC_W_Li_Pos_MSMS_01 #40-93 RT: 0.15-0.83 AV: 2 NL: 1.21E3
T: Average spectrum MS2 766.60 (40-93)

-Choline



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

NIST MS Search 2.0 - [Peptide, Presearch Default - empty]

File Search View Tools Options Window Help

MS m/z

1. Agilent 6530 QqTOF; [M+H]⁺

#	Src.	Name
22	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ;
23	A	Agilent 6520 Q-TOF; [M-H] ⁻ ;
24	A	Agilent 6530 QqTOF; [M+HCOO] ⁻ ;
25	A	Agilent 6530 QqTOF; [M+H] ⁺ ;
26	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
27	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
28	A	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TAG
29	A	Agilent LC/MSD 1100 Ion Trap ; [M-H] ⁻ ;
30	A	Agilent Ion Trap SL; [M+Na] ⁺ ;

Name: Agilent 6530 QqTOF; [M+H]⁺;
 MW: 786 ID#: 1366 DB: Text File
 Comment: PC 36:2 ; [M+H]⁺; 786.5987; Comprehensive blood plasma lipido
 2 largest peaks:
 184.0728 999.00 | 786.5987 800.00 |
 2 m/z Values and Intensities:
 184.0728 999.00 | 786.5987 800.00 |
 Synonyms:
 no synonyms.

(Text File) Agilent 6530 QqTOF; [M+H]⁺

lipidblast-neg; lipidblast-pos; 212516 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
---	---------	-------	-------------	-----------	---------	------

Difference Head to Tail Side by Side Subtraction

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

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 observed.

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 179 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF: [M+H]⁺

#	Src.	Name
22	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻
23	A	Agilent 6520 Q-TOF; [M-H] ⁻
24	A	Agilent 6530 QqTOF; [M+HCOO] ⁻
25	A	Agilent 6530 QqTOF; [M+H] ⁺
26	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
27	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
28	A	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TAG
29	A	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻
30	A	Agilent Ion Trap SL; [M+Na] ⁺

Names Structures Spec List

lipidblast-neg; lipidblast-pos; mmslib; custompc+hpos.msp; custompc+npos.msp; pc-ac-neg.msp; pc-form-neg.msp; 235420 total spectra

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: Agilent 6530 QqTOF; [M+H]⁺
 Mw: 786 ID#: 1366 DB: Text File
 Comment: PC 36:2; [M+H]⁺; 786.5987; Comprehensive blood plasma lipido
 2 largest peaks:
 184.0728 999.00 | 786.5987 800.00 |
 Synonyms:
 no synonyms.

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
2	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
3	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
4	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
5	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
6	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
7	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
8	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
9	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
10	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
11	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
12	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
13	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺
14	custompc+hpos.msp	7	737	0.61	737	PC 36:2; [M+H] ⁺

Names Structures Hit List

Agilent 6530 QqTOF; [M+H]⁺ Head to Tail MF=7 RMF=737 PC 36:2; [M+H]⁺; GPCho[18:1(11E)]/18:1(11E)

Difference Head to Tail Side by Side Subtraction 7 737R 0.61P

Plot/Text of Hit Plot of Hit

Name: PC 36:2; [M+H]⁺; GPCho[18:1(11E)]/18:1(11E)
 Mw: 786 ID#: 2569 DB: custompc+hpos.msp
 Comment: Parent=786.60126 Mz_exact=786.60126 ; PC 36:2; [M+H]⁺
 7 largest peaks:
 184.07387 999.00 | 504.34554 200.00 | 522.35610 200.00 | 603.53522 200.00 | 727.52776 200.00 | 786.59070 10.00 |
 7 m/z Values and Intensities:
 184.07387 999.00 fragment C5H15NO4P
 504.34554 200.00 [M+H]-sn1-H2O || [M+H]-sn2-H2O
 522.35610 200.00 [M+H]-sn1 || [M+H]-sn2
 603.53522 200.00 [M+H]-C5H14NO4P (-183)
 727.52776 200.00 [M+H]-C3H9N (-59)
 786.59070 10.00 [M+H]-H2O (-18)
 786.60126 200.00 [M+H]

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 24 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+HCOO]⁻

#	Src.	Name
22	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ;
23	A	Agilent 6520 Q-TOF; [M-H] ⁻ ;
24	A	Agilent 6530 QqTOF; [M+HCOO] ⁻ ;
25	A	Agilent 6530 QqTOF; [M+H] ⁺ ;
26	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
27	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
28	A	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TAG
29	A	Agilent LC/MSD 1100 Ion Trap ; [M-H] ⁻ ;
30	A	Agilent Ion Trap SL; [M+Na] ⁺ ;

Names Structures Spec List

(Text File) Agilent 6530 QqTOF; [M+HCOO]⁻

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: Agilent 6530 QqTOF; [M+HCOO]⁻;
MW: 830 ID#: 1367 DB: Text File
Comment: PC 36:2 ; [M+HCOO]⁻; 830.5966; Comprehensive blood plasma li
4 largest peaks:
770.5758 999.00 | 830.5966 250.00 | 279.2344 200.00 | 283.2645 10
4 m/z Values and Intensities:
279.2344 200.00 | 283.2645 100.00 | 770.5758 999.00 | 830.5966 25
Synonyms:
no synonyms.

lipidblast-neg; lipidblast-pos; 212516 total spectra

Agilent 6530 QqTOF; [M+HCOO]⁻; Head to Tail MF=79 RMF=281 PE 42:0; [M-H]⁻; GPEtn(18:0/24:0)
Difference Head to Tail Side by Side Subtraction 79 281R 15.5P

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	79	281	15.5	632	PE 42:0; [M-H] ⁻ ; I
2	lipidblast-neg	79	281	15.5	632	PE 42:0; [M-H] ⁻ ; I
3	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
4	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
5	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
6	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
7	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
8	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
9	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
10	lipidblast-pos	39	157	3.59	354	MGDG 38:1; [M+
11	lipidblast-neg	34	140	2.89	224	PS 40:8; [M-H] ⁻ ; I
12	lipidblast-neg	34	140	2.89	224	PS 40:8; [M-H] ⁻ ; I
13	lipidblast-neg	34	140	2.89	224	PS 40:8; [M-H] ⁻ ; I
14	lipidblast-neg	34	140	2.89	224	PS 40:8; [M-H] ⁻ ; I

Names Structures Hit List

Name: PE 42:0; [M-H]⁻; GPEtn(18:0/24:0)
MW: 830 ID#: 108480 DB: lipidblast-neg
Comment: Parent=830.66387 Mz_exact=830.66387 ; PE 42:0; [M-H]⁻; GPE
6 largest peaks:
283.26354 999.00 | 367.35738 999.00 | 480.30923 200.00 | 564.4030
546.39251 50.00 |
6 m/z Values and Intensities:
283.26354 999.00 sn1 FA
367.35738 999.00 sn2 FA
462.29867 50.00 [M-H]-sn2-H2O
480.30923 200.00 [M-H]-sn2
546.39251 50.00 [M-H]-sn1-H2O
564.40307 200.00 [M-H]-sn1

(lipidblast-neg) PE 42:0; [M-H]⁻; GPEtn(18:0/24:0)
Plot/Text of Hit Plot of Hit

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 394 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+HCOO]⁻

#	Src.	Name
22	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻
23	A	Agilent 6520 Q-TOF; [M-H] ⁻
24	A	Agilent 6530 QqTOF; [M+HCOO] ⁻
25	A	Agilent 6530 QqTOF; [M+H] ⁺
26	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
27	A	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
28	A	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TAG
29	A	Agilent LC/MSD 1100 Ion Trap ; [M-H] ⁻
30	A	Agilent Ion Trap SL; [M+Na] ⁺

Names Structures Spec List

(Text File) Agilent 6530 QqTOF; [M+HCOO]⁻

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: Agilent 6530 QqTOF; [M+HCOO]⁻
 MW: 830 ID#: 1367 DB: Text File
 Comment: PC 36:2 ; [M+HCOO]⁻; 830.5966; Comprehensive blood plasma li
 4 largest peaks:
 770.5758 999.00 | 830.5966 250.00 | 279.2344 200.00 | 283.2645 10
 4 m/z Values and Intensities:
 279.2344 200.00 | 283.2645 100.00 | 770.5758 999.00 | 830.5966 25
 Synonyms:
 no synonyms.

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; mmslib; pc-ac-neg.msp;
 pc-form-neg.msp; 235420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
2	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
3	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
4	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
5	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
6	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
7	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
8	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
9	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
10	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
11	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
12	pc-form-neg.msp	683	991	7.54	992	PC 36:2; [M+HCOO] ⁻
13	pc-form-neg.msp	83	838	0.07	951	PC 36:2; [M+HCOO] ⁻
14	pc-form-neg.msp	83	838	0.07	951	PC 36:2; [M+HCOO] ⁻

Names Structures Hit List

Agilent 6530 QqTOF; [M+HCOO]⁻ Head to Tail MF=683 RMF=991 PC 36:2; [M+HCOO]⁻; GPCho(18:0/18:2[2E,4E]
 Difference Head to Tail Side by Side Subtraction 683 991R 7.54P

Name: PC 36:2; [M+HCOO]⁻; GPCho(18:0/18:2[2E,4E])
 MW: 830 ID#: 2563 DB: pc-form-neg.msp
 Comment: Parent=830.59110 Mz_exact=830.59110 ; PC 36:2; [M+HCOO]⁻.
 4 largest peaks:
 770.56997 999.00 | 279.23226 100.00 | 283.26354 100.00 | 830.5911
 4 m/z Values and Intensities:
 279.23226 100.00 FA sn2
 283.26354 100.00 FA sn1
 770.56997 999.00 [M-CH3]⁻ (-15)
 830.59110 100.00 [M+HCOO]⁻ (M+44.9976)

(pc-form-neg.msp) PC 36:2; [M+HCOO]⁻; GPCho(18:0/18:2[2E,4E]
 Plot/Text of Hit Plot of Hit

Lib. Search Other Search Names Compare Librarian

Peptide Peptide



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:

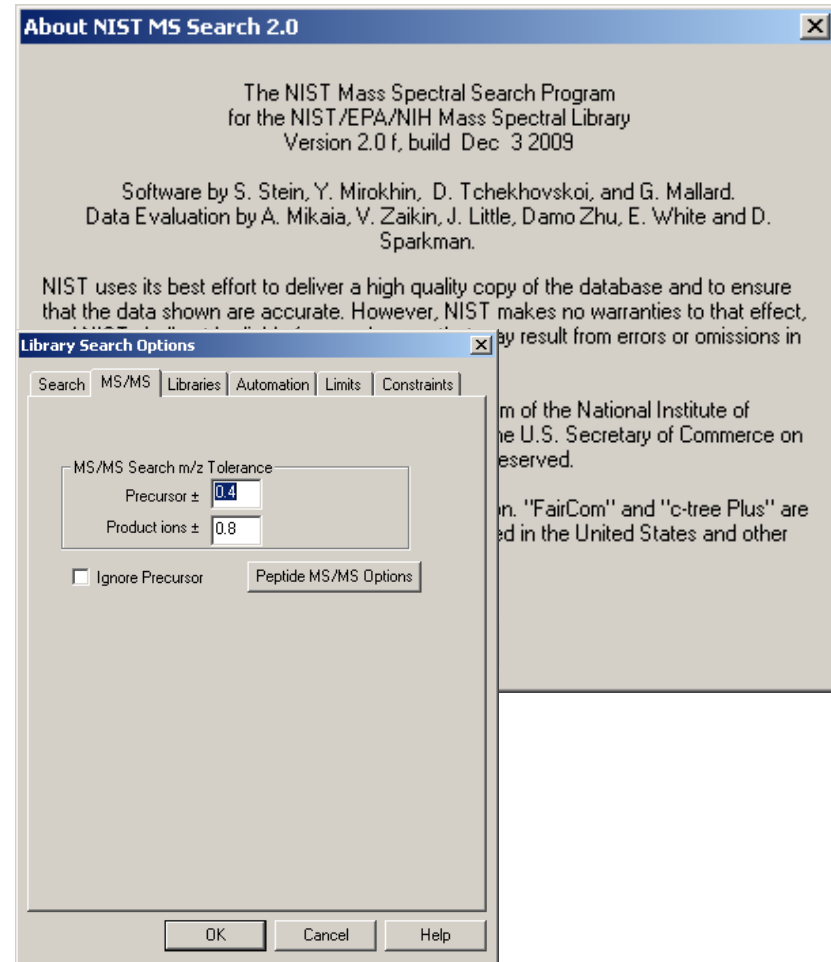
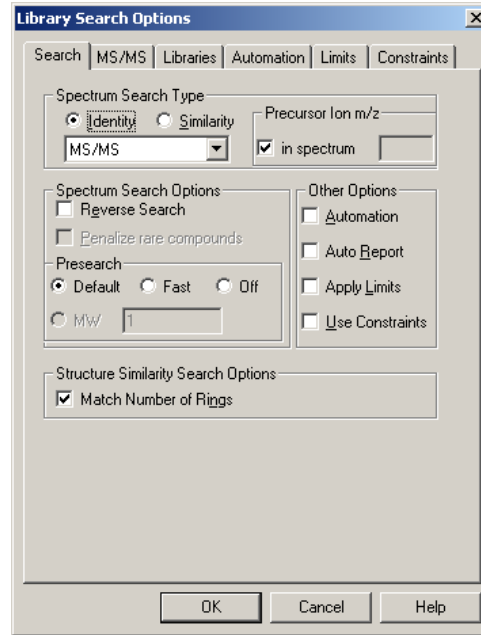
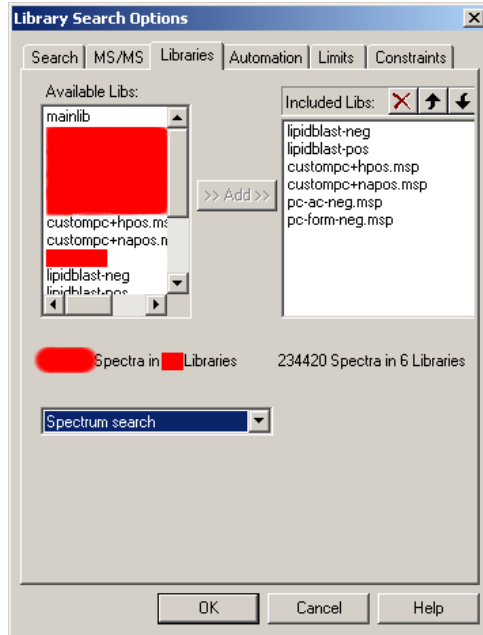
<http://fiehnlab.ucdavis.edu/projects/LipidBlast>

For questions please contact the curator: Dr. Tobias Kind

<http://fiehnlab.ucdavis.edu/staff/kind/>

NIST MS Search GUI – Search parameters

NIST MS PepSearch 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

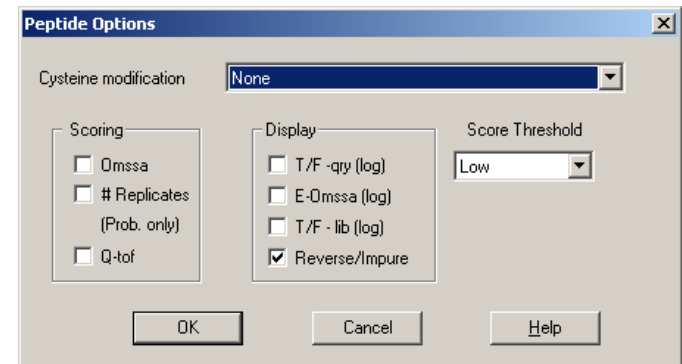
Version 2.0g 2011 produces slightly different hit scores.

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=LMSF>

NIST MS Search 2.0 - [Peptide, Presearch Default - 39 spectra]

File Search View Tools Options Window Help

MS m/z

1. ABI 4000 Q-Trap; [M-H]-; CerP(d18:1, 12:0)

#	Src.	Name
1	A	ABI 4000 Q-Trap; [M-H]-; CerP(d18:1/12:0)
2	A	ABI 4000 Q-Trap; [M+H]+; CerP(d18:1/12:0)
3	A	ABI QTRAP 4000; [M-H]-; Lipid A (dIPP-14-hexaacyl)
4	A	ABI 4000 Q-Trap; [M-H]-; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4]+; TG 52:3
6	A	ABI-API 4000 QTrap; [M-H]-; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M-H]-; GM2(d20:1/C18:0)
8	A	ABI 4700 MALDI-TOF/TOF; [M-H]-; Ac2PIM1(16:0/methyl-18:0)
9	A	ABI 4700 MALDI TOF/TOF; [M-H]-; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M-H]-; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M-H]-; CL 76:12
12	A	ABI QTRAP 4000; [M+H]+; CerP(d18:1/12:0)

Names Structures Spec List

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	149	761	63.8	762	CerP 30:1; [M-H]-; CerP(d18:1(4E)/12:0)
2	lipidblast-neg	55	517	5.22	649	CerP 30:1; [M-H]-; CerP(d14:1(4E)/16:0)
3	lipidblast-neg	55	517	5.22	649	CerP 30:1; [M-H]-; CerP(d16:1(4E)/14:0)
4	custompc+n...	19	261	1.29	422	PC 18:0; [M+Na]+; GPCho(6:0/12:0)
5	custompc+n...	19	261	1.29	422	PC 18:0; [M+Na]+; GPCho(12:0/6:0)
6	lipidblast-pos	5	91	0.80	150	PC 18:0; [M+Na]+; GPCho(6:0/12:0)
7	lipidblast-pos	5	91	0.80	150	PC 18:0; [M+Na]+; GPCho(12:0/6:0)
8	custompc+h...	1	24	0.68	122	PC 20:3; [M+H]+; GPCho(2:0/18:3(6Z,5Z,12Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Search Spectrum

Name: ABI 4000 Q-Trap; [M-H]-; CerP(d18:1/12:0)
 MW: 560 ID#: 281 DB: Text File
 Comment: Ceramide-phosphate CerP(d18:1/12:0); [M-H]-; Prec. m/z: 874.8;
 5 largest peaks:
 97.0 999.00 | 378.2 333.00 | 360.2 249.75 | 560.4 199.80 | 542.3 13
 5 m/z Values and Intensities:

Plot/Text of Hit

Name: CerP 30:1; [M-H]-; CerP(d18:1(4E)/12:0)
 MW: 560 ID#: 22881 DB: lipidblast-neg
 Comment: Parent=560.40801 Mz_exact=560.40801
 5 largest peaks:
 78.95851 999.00 | 96.96908 999.00 | 360.2 78.95851
 78.95851 999.00 ion P03- (78.95851)
 96.96908 999.00 ion H2P04- (96.96908)

Peptide Peptide

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=LMSF>

NIST MS Search 2.0 - [Peptide, Presearch Default - 70 spectra]

File Search View Tools Options Window Help

1. ABI 4000 Q-Trap; [M+H]⁺; CerP(d18:1/12:0)

#	Src.	Name
1	A	ABI 4000 Q-Trap; [M+H] ⁺ ; CerP(d18:1/12:0)
2	A	ABI 4000 Q-Trap; [M+H] ⁺ ; CerP(d18:1/12:0)
3	A	ABI QTRAP 4000; [M+H] ⁺ ; Lipid A (dIPP-14-hexaacyl)
4	A	ABI 4000 Q-Trap; [M+H] ⁺ ; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4] ⁺ ; TG 52:3
6	A	ABI-API 4000 QTrap; [M+H] ⁺ ; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M+H] ⁺ ; GM2(d20:1/C18:0)
8	A	ABI 4700 MALDI-TOF/TOF; [M+H] ⁺ ; Ac2PIM1(16:0/methyl-18:0)
9	A	ABI 4700 MALDI TOF/TOF; [M+H] ⁺ ; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M+H] ⁺ ; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M+H] ⁺ ; CL 76:12
12	A	ABI QTRAP 4000; [M+H] ⁺ ; PI 36:1

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	972	988	98.0	991	CerP 30:1; [M+H] ⁺ ; CerP(d18:1(4E)/12:0)
2	lipidblast-pos	504	715	0.97	835	CerP 30:1; [M+H] ⁺ ; CerP(d14:1(4E)/16:0)
3	lipidblast-pos	504	715	0.97	835	CerP 30:1; [M+H] ⁺ ; CerP(d16:1(4E)/14:0)
4	lipidblast-neg	113	297	0.00	451	plasmeyl-PE 24:0; [M+H] ⁺ ; PE(P-18:0/6:0)
5	lipidblast-neg	69	198	0.00	301	PE 23:1; [M+H] ⁺ ; GPEtn(6:0/17:1(SZ))
6	lipidblast-neg	69	198	0.00	301	PE 23:1; [M+H] ⁺ ; GPEtn(17:1(SZ)/6:0)
7	lipidblast-pos	52	154	0.00	327	PS 18:0; [M+Na] ⁺ ; GPSer(2:0/16:0)
8	lipidblast-pos	52	154	0.00	327	PS 18:0; [M+Na] ⁺ ; GPSer(3:0/15:0)

ABI 4000 Q-Trap; [M+H]⁺; CerP(d18:1/12:0)
 MW: 562 ID#: 280 DB: Text File
 Comment: Ceramide-phosphate CerP(d18:1/12:0); M+NH4; Prec. m/z: 874.8
 7 largest peaks:
 562.4 999.00 | 264.2 280.00 | 544.4 250.00 | 464.5 190.00 | 446.5 18
 482.2 170.00 | 530.3 50.00

CerP 30:1; [M+H]⁺; CerP(d18:1(4E)/12:0)
 MW: 562 ID#: 129 DB: lipidblast-pos
 Comment: Parent=562.42365 Mz_exact=562.4236
 6 largest peaks:
 562.42365 999.00 | 264.26896 599.40 | 544.4
 482.45732 399.60 |
 6 m/z Values and Intensities:
 264.26896 599.40 sn2 N

Lib. Search Other Search Names Compare Librarian MSMS

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. ABI QTRAP 4000; Lipid A (diPP-14-hc) [M-H]⁻

#	Src.	Name
1	A	4000 Q-Trap mass spectrometer; [M-H] ⁻
2	A	4000 Q-Trap mass spectrometer; M+H
3	A	ABI QTRAP 4000; Lipid A (diPP-14-hexaacyl); [M-H] ⁻
4	A	ABI 4000 Q-Trap mass spectrometer; [M-H] ⁻
5	A	4000 Q-Trap mass spectrometer; M+NH ₄
6	A	API 2000 triple quadrupole; [M-H] ⁻
7	A	ABI-QSTAR-Pulsar-Quadrupol-TOF PSer; [M-H] ⁻
8	A	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H] ⁻
9	A	Agilent 6520 Q-TOF; [M-H] ⁻
10	A	Agilent LC/MSD 1100 Ion Trap ; [M-H] ⁻
11	A	Agilent Ion Trap SL; [M+Na] ⁺
12	A	Agilent Ion Trap XCT; [M+H] ⁺

Names Structures

lipidblast-pos; lipidblast-neg: 184164 total spectra

#	Library	Score	Dot Prod...	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	25	136	0.25	370	LipidA PP [10/10/18/18/30-(14)/30-(14)]; [M-H] ⁻
2	lipidblast-neg	25	136	0.25	370	LipidA PP [12/12/14/18/30-(14)/30-(14)]; [M-H] ⁻
3	lipidblast-neg	25	136	0.25	370	LipidA PP [12/12/16/16/30-(14)/30-(14)]; [M-H] ⁻
4	lipidblast-neg	25	136	0.25	370	LipidA PP [12/12/18/14/30-(14)/30-(14)]; [M-H] ⁻
5	lipidblast-neg	25	136	0.25	370	LipidA PP [14/14/10/18/30-(14)/30-(14)]; [M-H] ⁻
6	lipidblast-neg	25	136	0.25	370	LipidA PP [14/14/12/16/30-(14)/30-(14)]; [M-H] ⁻
7	lipidblast-neg	25	136	0.25	370	LipidA PP [14/14/14/14/30-(14)/30-(14)]; [M-H] ⁻
8	lipidblast-neg	25	136	0.25	370	LipidA PP [14/14/16/12/30-(14)/30-(14)]; [M-H] ⁻
9	lipidblast-neg	25	136	0.25	370	LipidA PP [14/14/18/10/30-(14)/30-(14)]; [M-H] ⁻
10	lipidblast-neg	25	136	0.25	370	LipidA PP [16/16/10/14/30-(14)/30-(14)]; [M-H] ⁻
11	lipidblast-neg	25	136	0.25	370	LipidA PP [16/16/12/12/30-(14)/30-(14)]; [M-H] ⁻
12	lipidblast-neg	25	136	0.25	370	LipidA PP [16/16/14/10/30-(14)/30-(14)]; [M-H] ⁻
13	lipidblast-neg	25	136	0.25	370	LipidA PP [18/18/10/10/30-(14)/30-(14)]; [M-H] ⁻
14	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/14/18/30-(18)/30-(18)]; [M-H] ⁻
15	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/14/18/30-(18)/30-(14)]; [M-H] ⁻
16	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/16/16/30-(14)/30-(18)]; [M-H] ⁻
17	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/16/16/30-(18)/30-(14)]; [M-H] ⁻
18	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/16/18/30-(14)/30-(16)]; [M-H] ⁻
19	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/16/18/30-(16)/30-(14)]; [M-H] ⁻
20	lipidblast-neg	22	123	0.24	336	LipidA PP [10/10/18/14/30-(14)/30-(18)]; [M-H] ⁻

Names Structures

Hit List

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

Plot/Text of Search Spectrum

Name: ABI QTRAP 4000; Lipid A (diPP-14-hexaacyl); [M-H]⁻
MW: 1824 ID#: 296 DB: Text File
Comment: Accurate Mass should be 1824.24287; ELECTROPHORESIS, Volume 29, Issue 10 (p 2171-2181); Characterization of intact lipopolysaccharides
8 m/z Values and Intensities:
1272.4 180.00 | 1290.4 250.00 | 1308.6 180.00 | 1388.4 100.00 | 1449.0 50.00 | 1596.6 50.00 | 1824.9 500.00 |
Synonyms:
no synonyms.

Plot/Text of Spec List

Name: LipidA PP [14/14/14/14/30-(14)/30-(14)]; [M-H]⁻
MW: 1824 ID#: 64309 DB: lipidblast-neg
Comment: Parent=1824.24287 Mz_exact=1824.24287 ; LipidA PP [14/14/14/14/30-(14)/30-(14)]; [M-H]⁻
7 largest peaks:
1580.03915 999.00 | 1726.26597 600.00 | 1824.24287 500.00 |
1482.06225 250.00 | 1742.26089 500.00 |
7 m/z Values and Intensities:
1824.24287 500.00 [M-H]
1742.26089 50.00 [M-H]-PO3H
1726.26597 600.00 [M-H]-PO4H3
1596.03407 250.00 [M-H]-PO4H3-R2'-O-FA || [M-H]-PO4H3-R3'-O-F
1580.03915 999.00 [M-H]-R2 acyl FA || [M-H]-R3 acyl FA
1498.05717 300.00 [M-H]-PO4H3-R2'-O-FA || [M-H]-PO4H3-R3'-O-F
1482.06225 250.00 [M-H]-R2-PO4H3 || [M-H]-R3-PO4H3
Synonyms:
no synonyms.

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 65 spectra]

File Search View Tools Options Window Help

Go 1. ABI 4000 Q-Trap; [M-H]-; PI 36:1

#	Src.	Name
1	A	ABI 4000 Q-Trap; [M-H]-; CerP(d18:1/12:0)
2	A	ABI 4000 Q-Trap; [M-H]+; CerP(d18:1/12:0)
3	A	ABI QTRAP 4000; [M-H]-; Lipid A (dPP-14-hexaacyl)
4	A	ABI 4000 Q-Trap; [M-H]-; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4]+; TG 52:3
6	A	ABI-API 4000 QTrap; [M-H]-; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M-H]-; GM2(d20:1/C18:0)
8	A	ABI 4700 MALDI-TOF/TOF; [M-H]-; Ac2PIM1(16:0/methyl-18:0)
9	A	ABI 4700 MALDI TOF/TOF; [M-H]-; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M-H]-; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M-H]-; CL 76:12
12	A	ABI OCTAPOL... TOF/TOF; [M-H]-; PC 34:0

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(11E))
2	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(11Z))
3	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(13Z))
4	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(17Z))
5	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(4E))
6	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(6Z))
7	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(7Z))
8	lipidblast-neg	143	577	5.18	639	PI 36:1; [M-H]-; GPIs(18:0/18:1(9E))

Names Structures Spec List

Plot/Text of Search Spectrum

Name: ABI 4000 Q-Trap; [M-H]-; PI 36:1
Mw: 863 ID#: 278 DB: Text File
Comment: PI(18:0/18:1) (putative); [M-H]-; Prec. m/z: 863.6; Applied Biosyst
8 largest peaks:
283.3 999.00 | 281.3 570.00 | 863.6 300.00 | 410.1 200.00 | 309.1 10
403.4 50.00 | 581.0 50.00 | 297.0 10.00

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Plot/Text of Hit

Name: PI 36:1; [M-H]-; GPIs(18:0/18:1(11E))
Mw: 863 ID#: 119390 DB: lipidblast-neg
Comment: Parent=863.56493 Mz_exact=863.5649
8 largest peaks:
281.24790 999.00 | 283.26354 999.00 | 597.30413 100.00 | 419.25638 400.00 | 579.29357 200.00 | 581.30413 100.00
8 m/z Values and Intensities:
281.24790 999.00 sn2 FA

Plot/Text of Hit Plot of Hit

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 diacylglycerol next 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

NIST MS Search 2.0 - [Peptide, Presearch Default - 13 spectra]

File Search View Tools Options Window Help

Go 1. 4000 Q-Trap mass spectrometer; M+N

#	Src.	Name
1	A	4000 Q-Trap mass spectrometer; [M-H];
2	A	4000 Q-Trap mass spectrometer; M+H
3	A	ABI QTRAP 4000; Lipid A (diPP-14-hexaacyl); [M-H];
4	A	ABI 4000 Q-Trap mass spectrometer; [M-H];
5	A	4000 Q-Trap mass spectrometer; M+NH4
6	A	API 2000 triple quadrupole; [M-H];
7	A	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H];
8	A	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H];
9	A	Agilent 6520 Q-TOF; [M-H];
10	A	Agilent LC/MSD 1100 Ion Trap ; [M-H];
11	A	Agilent Ion Trap SL; [M+Na+];
12	A	Agilent Ion Trap XCT; [M+H];

Names Structures Spec List

lipidblast-pos; lipidblast-neg: 184164 total spectra

#	Library	Score	Dot Prod...	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	968	992	100.0	993	TG 52:3; [M+NH4]+; TG(16:0/18:1/18:2)
2	lipidblast-pos	159	444	0.00	713	TG 52:3; [M+NH4]+; TG(16:0/16:0/20:3)
3	lipidblast-pos	119	364	0.00	584	TG 52:3; [M+NH4]+; TG(16:0/16:1/20:2)
4	lipidblast-pos	119	364	0.00	584	TG 52:3; [M+NH4]+; TG(16:0/18:0/18:3)
5	lipidblast-pos	119	364	0.00	584	TG 52:3; [M+NH4]+; TG(16:1/18:0/18:2)
6	lipidblast-pos	119	364	0.00	584	TG 52:3; [M+NH4]+; TG(17:0/17:1/18:2)
7	lipidblast-pos	111	347	0.00	714	TG 52:3; [M+NH4]+; TG(16:1/18:1/18:1)
8	lipidblast-pos	111	347	0.00	714	TG 52:3; [M+NH4]+; TG(17:1/17:1/18:1)
9	lipidblast-pos	86	284	0.00	585	TG 52:3; [M+NH4]+; TG(17:0/17:2/18:1)
10	lipidblast-pos	2	12	0.00	140	TG 52:3; [M+NH4]+; TG(16:1/16:1/20:1)
11	lipidblast-pos	2	12	0.00	140	TG 52:3; [M+NH4]+; TG(17:0/17:0/18:3)
12	lipidblast-pos	2	10	0.00	115	TG 52:3; [M+NH4]+; TG(16:1/17:2/19:0)
13	lipidblast-pos	2	10	0.00	115	TG 52:3; [M+NH4]+; TG(17:1/17:2/18:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian

Name: 4000 Q-Trap mass spectrometer; M+NH4
 MW: 874 ID#: 294 DB: Text File
 Comment: TAG(16:0/18:1/18:2); M+NH4; Prec. m/z: 874
 5 m/z Values and Intensities:
 575.5 600.00 | 577.5 999.00 | 601.5 999.00 | 857.8
 Synonyms:
 no synonyms.

Name: TG 52:3; [M+NH4]+; TG(16:0/18:1/18:2)
 MW: 874 ID#: 71286 DB: lipidblast-pos
 Comment: Parent=874.78589 Mz_exact=874.78589 ; C55H10006; [M+NH4]
 4 largest peaks:
 601.51926 999.00 | 577.51926 999.00 | 575.50362 999.00 | 857.78
 4 m/z Values and Intensities:
 857.78315 199.80 [M+NH4]-17
 601.51926 999.00 [M+NH4]-sn1-18
 577.51926 999.00 [M+NH4]-sn3-18
 575.50362 999.00 [M+NH4]-sn2-18
 Synonyms:
 no synonyms.

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 2 spectra]

File Search View Tools Options Window Help

Go 1. ABI-API 4000 QTrap; [M-H]⁻; GM2(d18:1/C18:0)

#	Src.	Name
1	A	ABI 4000 Q-Trap; [M-H] ⁻ ; CerP(d18:1/12:0)
2	A	ABI 4000 Q-Trap; [M-H] ⁺ ; CerP(d18:1/12:0)
3	A	ABI QTRAP 4000; [M-H] ⁻ ; Lipid A (dIPP-14-hexaacyl)
4	A	ABI 4000 Q-Trap; [M-H] ⁻ ; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4] ⁺ ; TG 52:3
6	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d20:1/C18:0)
8	A	ABI 4700 MALDI-TOF/TOF; [M-H] ⁻ ; Ac2PIM1(16:0/methyl-18:0)
9	A	ABI 4700 MALDI-TOF/TOF; [M-H] ⁻ ; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M-H] ⁻ ; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
12	A	ABI QTRAP 4000; [M-H] ⁻ ; CerP(d18:1/12:0)

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	637	859	50.0	985	[glycan]-Cer 36:1; GM2(d18:1/18:0); [M-H] ⁻ ; GalNAc
2	lipidblast-neg	637	859	50.0	985	[glycan]-Cer 36:1; Ganglioside; [M-H] ⁻ ; NeuAcalpha2

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 M
10 largest peaks:
1383.0 999.00 | 1091.8 500.00 | 290.1 250.00 | 1075.0 200.00 | 888.7 200.00
564.6 90.00 | 726.6 80.00 | 1049.9 20.00 | 1184.9 20.00 | 1015.0 20.00

(Text File) ABI-API 4000 QT...

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: [glycan]-Cer 36:1; GM2(d18:1/18:0); [M-H]⁻
MW: 1382 ID#: 79299 DB: lipidblast-neg
Comment: Parent=1382.81601 Mz_exact=1382.81
5 largest peaks:
1382.81601 999.00 | 1091.72060 500.00 | 290.08759 400.00 ion C11H16NO8- (290.08759)
564.53523 200.00 ion ceramide

(lipidblast-neg) [glycan]-Cer 36:1; GM2(d18:1/18:0); [M-H]⁻

Plot/Text of Hit Plot of Hit

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

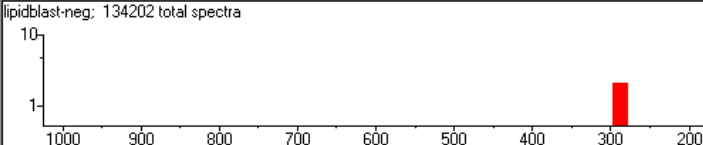
NIST MS Search 2.0 - [Peptide, Presearch Default - 2 spectra]

File Search View Tools Options Window Help

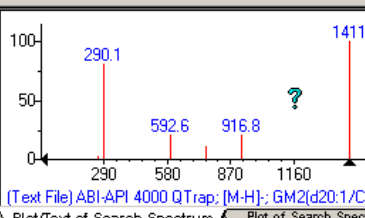
1. ABI-API 4000 QTrap; [M-H]⁻; GM2(d20:1/C18:0)

#	Src.	Name
4	A	ABI 4000 Q-Trap; [M-H] ⁻ ; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4] ⁺ ; TG 52:3
6	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GD1a
8	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d20:1/C18:0)
9	A	ABI 4700 MALDI-TOF/TOF; [M-H] ⁻ ; Ac2PIM1(16:0/methyl-18:0)
10	A	ABI 4700 MALDI TOF/TOF; [M-H] ⁻ ; Lipid A

lipidblast-neg: 134202 total spectra

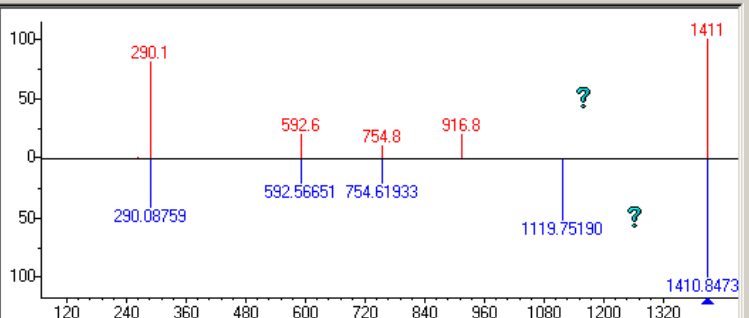


#	Library	Score	Dot Product	Pro...	Rev-Dot	Name
1	lipidblast-neg	282	622	50.0	793	[glycan]-Cer 38:1; Ganglioside
2	lipidblast-neg	282	622	50.0	793	[glycan]-Cer 38:1; GM2(d18:1/C18:0)

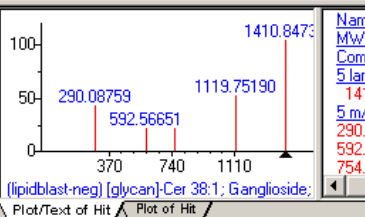


(Text File) ABI-API 4000 QTrap; [M-H]⁻; GM2(d20:1/C18:0)

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
7 largest peaks:
1411 999.00 | 290.1 800.00 | 119.8 600.0
754.8 100.00 | 265.2 10.00 |
7 m/z Values and Intensities:
119.8 600.00 | 265.2 10.00 | 290.1 800.0
916.8 200.00 | 1411 999.00 |



Head to Tail MF=282 RMF=622 [glycan]-Cer 38:1; Ganglioside; [M-H]⁻



Name: [glycan]-Cer 38:1; Ganglioside; [M-H]⁻; NeuAcap1
MW: 1410 ID#: 79716 DB: lipidblast-neg
Comment: Parent=1410.84731 Mz_exact=1410.84731 ;
5 largest peaks:
1410.84731 999.00 | 1119.75190 500.00 | 290.08759 400.00
5 m/z Values and Intensities:
290.08759 400.00 ion C11H16NO8- (290.08759)
592.56651 200.00 ion ceramide
754.61933 200.00 [M-H]-Cer-C6H1005

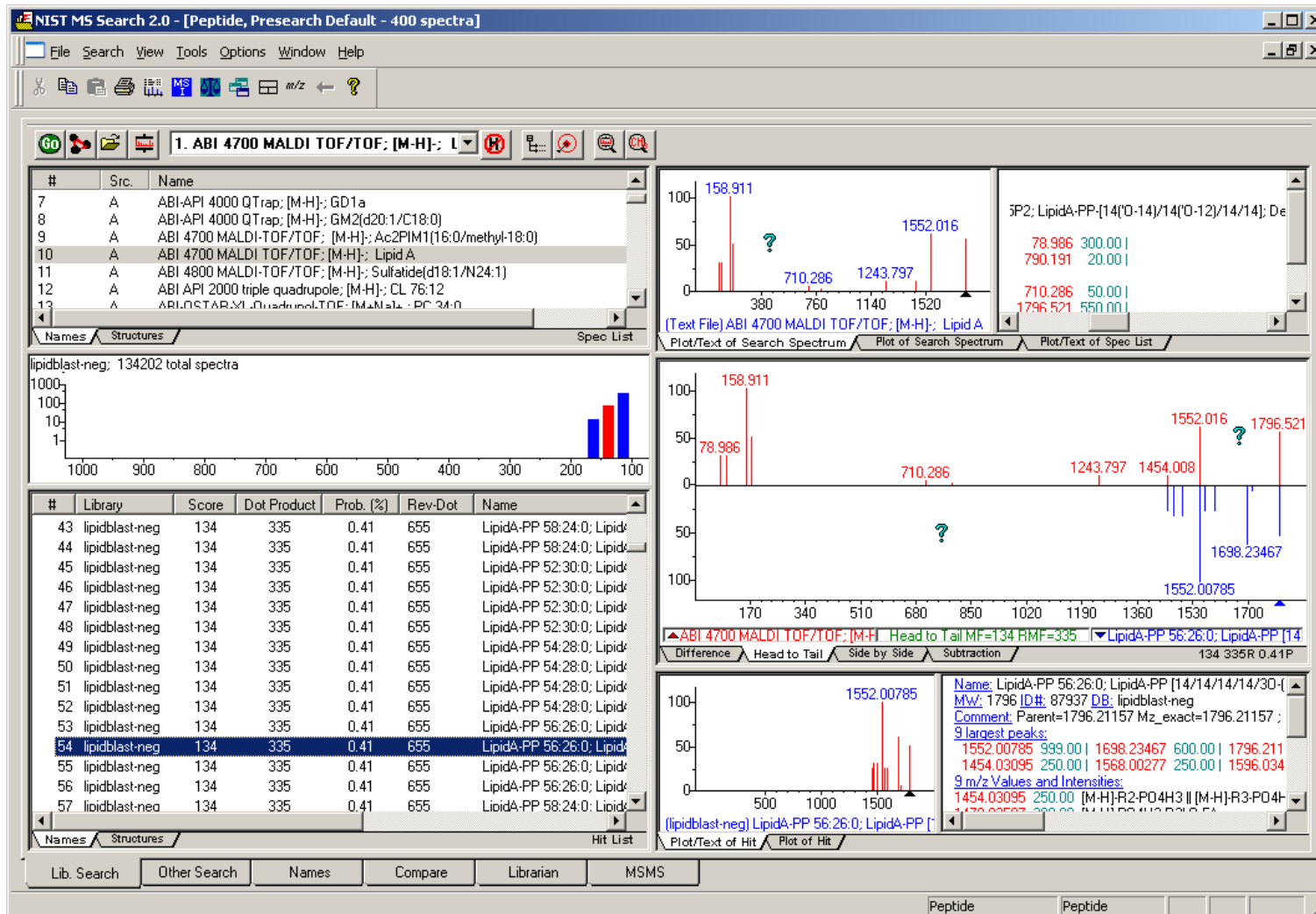
Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 multivariied 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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 175 spectra]

File Search View Tools Options Window Help

60 1. ABI 4800 MALDI-TOF/TOF; [M-H]⁻; S

#	Src.	Name
1	A	ABI 4000 Q-Trap; [M-H] ⁻ ; CerP(d18:1/12:0)
2	A	ABI 4000 Q-Trap; [M+H] ⁺ ; CerP(d18:1/12:0)
3	A	ABI QTRAP 4000; [M-H] ⁻ ; Lipid A (dIPP-14-hexaacyl)
4	A	ABI 4000 Q-Trap; [M-H] ⁻ ; PI 36:1
5	A	ABI 4000 Q-Trap; [M+NH4] ⁺ ; TG 52:3
6	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d18:1/C18:0)
7	A	ABI-API 4000 QTrap; [M-H] ⁻ ; GM2(d20:1/C18:0)
8	A	ABI 4700 MALDI-TOF/TOF; [M-H] ⁻ ; Ac2PIM1(16:0/methyl-18:0)
9	A	ABI 4700 MALDI TOF/TOF; [M-H] ⁻ ; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M-H] ⁻ ; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
12	A	ABI 4800 MALDI-TOF/TOF; [M-H] ⁻ ; PC 24:0

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	248	781	72.7	901	ST 42:2; [M-H] ⁻ ; Sulfatide(d18:1(4E)/24:1(15Z))
2	lipidblast-neg	137	633	4.59	807	ST 42:2; [M-H] ⁻ ; Sulfatide(d16:1(4E)/26:1(17Z))
3	custompc+n...	40	193	0.36	338	PC 42:4; [M+Na] ⁺ ; GPCho(18:3(6Z,9Z,12Z)/24:1
4	custompc+n...	40	193	0.36	338	PC 42:4; [M+Na] ⁺ ; GPCho(18:3(9Z,12Z,15Z)/24
5	custompc+n...	40	193	0.36	338	PC 42:4; [M+Na] ⁺ ; GPCho(24:1(15Z)/18:3(6Z,9Z
6	custompc+n...	40	193	0.36	338	PC 42:4; [M+Na] ⁺ ; GPCho(24:1(15Z)/18:3(9Z,12
7	pc-ac-neg.m...	24	127	0.20	243	PC 39:1; [M-Ac-H] ⁻ ; GPCho(15:0/24:1(15Z))
8	pc-ac-neg.m...	24	127	0.20	243	PC 39:1; [M-Ac-H] ⁻ ; GPCho(24:1(15Z)/15:0)

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:
888.67 999.00 | 97.09 400.00 | 119.17 90.00 | 241.16 50.00 |
522.46 50.00 | 540.47 50.00 | 59.14 10.00 | 300.44 10.00 |

Name: ST 42:2; [M-H]⁻; Sulfatide(d18:1(4E)/24:1(15Z))
MW: 888 ID#: 134173 DB: lipidblast-neg
Comment: Parent=888.62346 Mz_exact=888.6234
5 largest peaks:
96.95956 999.00 | 241.00181 999.00 | 522.27390 999.00 |
5 m/z Values and Intensities:
96.95956 999.00 ion S04H⁻ (96.95956)
241.00181 999.00 ion C6H9O8S⁻ (241.00181)

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

API 2000 triple quadrupole; [M-H]-;

Cardiolipin CL 76:12 (MIX from rat heart); [M-H]-; Prec. m/z: 1495.97;

Journal of Lipid Research Volume 46, 2005;

Quantitation of cardiolipin molecular species in spontaneously hypertensive heart failure rats using electrospray ionization mass spectrometry

NIST MS Search 2.0 - [Peptide, Presearch Default - 222 spectra]

File Search View Tools Options Window Help

1. API 2000 triple quadrupole; [M-H]-

#	Src.	Name
1	A	4000 Q-Trap mass spectrometer; [M-H]-
2	A	4000 Q-Trap mass spectrometer; M+H
3	A	ABI QTRAP 4000; Lipid A (diPP-14-hexaacyl); [M-H]-;
4	A	ABI 4000 Q-Trap mass spectrometer; [M-H]-
5	A	4000 Q-Trap mass spectrometer; M+NH4
6	A	API 2000 triple quadrupole; [M-H]-;
7	A	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H]-;
8	A	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H]-;
9	A	Agilent 6520 Q-ToF; [M-H]-;
10	A	Agilent LC/MSD 1100 Ion Trap ; [M-H]-;
11	A	Agilent Ion Trap SL; [M+Na]+;
12	A	Agilent Ion Trap XCT; [M+H]+;

Names Structures Spec List

lipidblast-pos; lipidblast-neg: 184164 total spectra

#	Library	Score	Dot Prod...	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	10	314	0.47	320	CL 76:12; [M-H]-; CL(16:0/22:6/18:2/20:4)
2	lipidblast-neg	10	314	0.47	320	CL 76:12; [M-H]-; CL(16:0/22:6/20:4/18:2)
3	lipidblast-neg	10	314	0.47	320	CL 76:12; [M-H]-; CL(18:2/20:4/22:6/16:0)
4	lipidblast-neg	10	314	0.47	320	CL 76:12; [M-H]-; CL(20:4/18:2/22:6/16:0)
5	lipidblast-neg	8	263	0.45	285	CL 76:12; [M-H]-; CL(18:2/20:4/18:2/20:4)
6	lipidblast-neg	8	263	0.45	285	CL 76:12; [M-H]-; CL(20:4/18:2/20:4/18:2)
7	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(16:0/18:2/20:4/22:6)
8	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(16:0/18:2/22:6/20:4)
9	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(16:0/20:4/18:2/22:6)
10	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(16:0/20:4/22:6/18:2)
11	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(18:2/16:0/20:4/22:6)
12	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(18:2/16:0/22:6/20:4)
13	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(18:2/22:6/20:4/16:0)
14	lipidblast-neg	8	257	0.45	262	CL 76:12; [M-H]-; CL(20:4/16:0/22:6/18:2)
15	lipidblast-neg	7	237	0.44	257	CL 76:12; [M-H]-; CL(18:2/20:4/20:4/18:2)
16	lipidblast-neg	6	229	0.44	248	CL 76:12; [M-H]-; CL(16:1/22:5/18:2/20:4)
17	lipidblast-neg	6	229	0.44	248	CL 76:12; [M-H]-; CL(16:1/22:5/20:4/18:2)
18	lipidblast-neg	6	229	0.44	248	CL 76:12; [M-H]-; CL(18:2/20:4/18:3/20:3)
19	lipidblast-neg	6	229	0.44	248	CL 76:12; [M-H]-; CL(18:2/20:4/20:3/18:3)
20	lipidblast-neg	6	229	0.44	248	CL 76:12; [M-H]-; CL(18:3/20:3/20:4/18:2)

Names Structures Hit List

Plot/Text of Search Spectrum

Name: API 2000 triple quadrupole; [M-H]-;
 MW: 1495 ID#: 293 DB: Text File
 Comment: Cardiolipin CL 76:12 (MIX from rat heart); [M-H]-
 5 m/z Values and Intensities:
 255.2 50.00 | 279.2 999.00 | 281.2 50.00 | 303.2
 Synonyms:
 no synonyms.

Plot/Text of Hit

Name: CL 76:12; [M-H]-; CL(16:0/22:6/18:2/20:4)
 MW: 1495 ID#: 7885 DB: lipidblast-neg
 Comment: Parent=1495.96441 Mz_exact=1495.96441 ; CL 76:12; [M-H]-
 10 largest peaks:
 719.46489 999.00 | 855.45744 300.00 | 463.22481 300.00 | 439
 457.23537 200.00 | 775.49110 100.00 | 327.23226 100.00 | 303
 12 m/z Values and Intensities:
 1239.72433 50.00 [M-H]-sn1
 855.45744 300.00 sn1+sn2+C6H11P2O8 (+272.9929) || sn3+sn4+
 775.49110 100.00 sn1+sn2+C6H10O5P (+193.026) || sn3+sn4+C6
 719.46489 999.00 sn1+sn2+C3H6PO4 (+137.00) || sn3+sn4+C3H6
 481.23537 200.00 sn2+C3H6PO4+H2O
 463.22481 300.00 sn2+C3H6PO4 (+137.00)
 457.23537 200.00 sn4+C3H6PO4+H2O
 439.22481 300.00 sn4+C3H6PO4 (+137.00)
 327.23226 100.00 sn2 Fd

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 327 spectra]

File Search View Tools Options Window Help

1. ABI-QSTAR-XL-Quadrupol-TOF; [M+N]

#	Src.	Name
12	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
13	A	ABI-QSTAR-XL-Quadrupol-TOF; [M+Na] ⁺ ; PC 34:0
14	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
16	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
18	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6

Names / Structures Spec List

lipidblast-neg; custompc+hpos.msp; custompc+napos.msp; lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	231	580	4.96	943	PC 34:0; [M+Na] ⁺ ; GPC
2	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
3	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
4	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
5	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
6	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
7	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
8	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
9	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
10	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
11	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
12	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
13	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
14	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC
15	lipidblast-pos	221	567	3.50	922	PC 34:0; [M+Na] ⁺ ; GPC

Names / Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Journal of Mass Spectrometry 293 (2010) 4550

(Text File) ABI-QSTAR-XL-Quadrupol-TOF; [M+Na]⁺; P

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

ABI-QSTAR-XL-Quadrupol-TOF; Head to Tail MF=231 RMF=580 PC 34:0; [M+Na]⁺; GPC

Difference Head to Tail Side by Side Subtraction 231 580R 4.96P

(lipidblast-pos) PC 34:0; [M+Na]⁺; GPC

Plot/Text of Hit Plot of Hit

Name: PC 34:0; [M+Na]⁺; GPC

MW: 784 ID#: 44465 DB: lipidblast-pos

Comment: Parent=784.58321 Mz_exact=784.58321 ; PC

5 largest peaks:

725.50971 999.00 | 601.51717 600.00 | 455.25399

5 m/z Values and Intensities:

455.25399 40.00 [M+Na]-59-sn1 || [M+Na]-59-sn2

514.32749 20.00 [M+Na]-sn1-H2O || [M+Na]-sn2-H2O

For Help, press F1

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 186 spectra]

File Search View Tools Options Window Help

1. ABI QSTAR-XL QTOF; [M-H]⁻; Sulfatide

#	Src.	Name
9	A	ABI 4700 MALDI TOF/TOF; [M-H] ⁻ ; Lipid A
10	A	ABI 4800 MALDI-TOF/TOF; [M-H] ⁻ ; Sulfatide(d18:1/N24:1)
11	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
12	A	ABI-QSTAR-XL-Quadrupol-TOF; [M+Na] ⁺ ; PC 34:0
13	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
14	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
16	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6
18	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; PI 38:4
19	A	ABI-QSTAR-Pulsar-Quadrupol-TOF PSer; [M-H] ⁻ ; PS 40:6

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	5	802	0.65	809	ST 40:1; [M-H] ⁻ ; Sulfatide(d18:1(4E)/22:0)
2	lipidblast-neg	4	785	0.63	794	ST 40:1; [M-H] ⁻ ; Sulfatide(d14:0/26:1(17Z))
3	lipidblast-neg	4	785	0.63	794	ST 40:1; [M-H] ⁻ ; Sulfatide(d14:1(4E)/26:0)
4	lipidblast-neg	4	785	0.63	794	ST 40:1; [M-H] ⁻ ; Sulfatide(d16:0/24:1(15Z))
5	lipidblast-neg	4	785	0.63	794	ST 40:1; [M-H] ⁻ ; Sulfatide(d16:1(4E)/24:0)
6	pc-ac-neg.m...	0	119	0.53	293	PC 37:0; [M-Ac-H] ⁻ ; GPCho(15:0/22:0)
7	pc-ac-neg.m...	0	119	0.53	293	PC 37:0; [M-Ac-H] ⁻ ; GPCho(22:0/15:0)
8	pc-form-neg....	0	119	0.53	293	PC 38:0; [M-HCOO] ⁻ ; GPCho(15:0/23:0)

Names Structures Spec List Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
96.9621 999.00 | 862.5729 500.00 | 241.0024 100.00 | 364.3579 100.00 | 522.2697 100.00 | 522.27389 100.00 | 844.59725 100.00

(Text File) ABI QSTAR-XL QTOF; [M-H]⁻; Sulfatide (d18:1/C22:0)

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

ABI QSTAR-XL QTOF; [M-H]⁻; Sulfatide (d18:1/C22:0) Head to Tail MF=5 RMF=802 ST 40:1; [M-H]⁻; Sulfatide(d18:1(4E)/22:0) 5 802R 0.65P

Difference Head to Tail Side by Side Subtraction

Name: ST 40:1; [M-H]⁻; Sulfatide(d18:1(4E)/22:0)
MW: 862 ID#: 134171 DB: lipidblast-neg
Comment: Parent=862.60781 Mz_exact=862.60781
5 largest peaks:
96.95956 999.00 | 241.00181 999.00 | 522.27389 100.00 | 844.59725 100.00 | 96.95956 999.00 ion SO4H- (96.95956) 241.00181 999.00 ion C6H9O8S- (241.00181)

(lipidblast-neg) ST 40:1; [M-H]⁻; Sulfatide(d18:1(4E)/22:0)

Plot/Text of Hit Plot of Hit

Name: ABI Sciex API III QQQ; [M-H]⁻; PE MIX

not found

MW: 750 ID#: 4234 DB: Text File

Comment: PE MIX; alkenyl/acyl PE(18:0/20:4) and PE(16:0/22:4); [M-H]⁻; Prec. m/z:750.3; JL Kerwin, AR Tuninga, and LH Ericsson; Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry; J. Lipid Res., Jun 1994; 35: 1102 - 1114.

NIST MS Search 2.0 - [Peptide, Presearch Default - 229 spectra]

File Search View Tools Options Window Help

1. ABI Sciex API III QQQ; [M-H]⁻; PE M

#	Src.	Name
12	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
13	A	ABI-QSTAR-XL-Quadrupol-TOF; [M+Na] ⁺ ; PC 34:0
14	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
16	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
18	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6

Names Structures Spec List

lipidblast-neg; custompc+hpos.msp; custompc+napos.msp; lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

[%]	Rev-Dot	Name
1.5	877	plasmeryl-PE 38:4; [M-H] ⁻ ; PE(P-16:0/22:4(7Z,10Z,13Z,16Z))
38	877	plasmeryl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4(5E,8E,11E,14E))
38	877	plasmeryl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4(5Z,8Z,11Z,14Z))
38	877	plasmeryl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4(7E,10E,13E,16E))
59	632	PE 37:5; [M-H] ⁻ ; GPEtn(15:1(9Z)/22:4(7Z,10Z,13Z,16Z))
59	632	PE 37:5; [M-H] ⁻ ; GPEtn(22:4(7Z,10Z,13Z,16Z)/15:1(9Z))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(17:1(9Z)/20:4(5E,8E,11E,14E))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(17:1(9Z)/20:4(5Z,8Z,11Z,14Z))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(17:1(9Z)/20:4(7E,10E,13E,16E))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(20:4(5E,8E,11E,14E)/17:1(9Z))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(20:4(5Z,8Z,11Z,14Z)/17:1(9Z))
26	632	PE 37:5; [M-H] ⁻ ; GPEtn(20:4(7E,10E,13E,16E)/17:1(9Z))
35	452	CL 76:9; [M-2H] ²⁻ ; CL(18:1/20:3/18:1/20:4)
35	452	CL 76:9; [M-2H] ²⁻ ; CL(18:2/20:1/18:2/20:4)
35	452	CL 76:9; [M-2H] ²⁻ ; CL(20:2/16:1/20:2/20:4)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Name: ABI Sciex API III QQQ; [M-H]⁻; PE MIX
MW: 750 ID#: 4234 DB: Text File
Comment: PE MIX; alkenyl/acyl PE(18:0/20:4)
3 largest peaks: 750.3 999.00 | 331.5 450.00 | 303.4 400.0
3 m/z Values and Intensities: 303.4 400.00 | 331.5 450.00 | 750.3 999.0
Synonyms: no synonyms

(Text File) ABI Sciex API III QQQ; [M-H]⁻; PE MIX

Name: plasmeryl-PE 38:4; [M-H]⁻; PE(P-16:0/22:4(7Z,10Z,13Z,16Z))
MW: 750 ID#: 123275 DB: lipidblast-neg
Comment: Parent=750.54375 Mz_exact=750.54375; pls
3 largest peaks: 331.26354 999.00 | 436.28295 250.00 | 418.27239
3 m/z Values and Intensities: 331.26354 999.00 sn2 FA
418.27239 50.00 [M-H]-sn2-H2O
166.00000 200.00000

(Lipidblast-neg) plasmeryl-PE 38:4; [M-H]⁻; PE(P-18:0/20:4(5E,8E,11E,14E))

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.

NIST MS Search 2.0 - [Peptide, Presearch Default - 256 spectra]

File Search View Tools Options Window Help

1. ABI Sciex API III QQQ; [M-H]⁻; PE 40

#	Src.	Name
12	A	ABI API 2000 triple quadrupole; [M-H] ⁻ ; CL 76:12
13	A	ABI-QSTAR-XL-Quadrupol-TOF; [M+Na] ⁺ ; PC 34:0
14	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
16	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
18	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6

lipidblast-neg; custompc+hpos.msp; custompc+napos.msp; lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	257	881	40.2	885	PE 40:6; [M-H] ⁻ ; GPEtn(18:0/22:6)
2	lipidblast-neg	257	881	40.2	885	PE 40:6; [M-H] ⁻ ; GPEtn(18:0/22:6)
3	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
4	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
5	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
6	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
7	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
8	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
9	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
10	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
11	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
12	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
13	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
14	lipidblast-neg	50	534	0.40	536	CL 82:11; [M-2H] ²⁻ ; CL
15	lipidblast-neg	25	361	0.12	452	CL 82:11; [M-2H] ²⁻ ; CL

(Text File) ABI Sciex API III QQQ; [M-H]⁻; PE 40:6

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
3 largest peaks:
283.4 999.00 | 327.5 550.00 | 790.4 500.00
3 m/z Values and Intensities:
283.4 999.00 | 327.5 550.00 | 790.4 500.00
Synonyms:
no synonyms

ABI Sciex API III QQQ; [M-H]⁻; PE 40:6; [M-H]⁻; GPEtn(18:0/22:6)

Name: PE 40:6; [M-H]⁻; GPEtn(18:0/22:6)(42.72.102.13)
MW: 790 ID#: 108478 DB: lipidblast-neg
Comment: Parent=790.53869 Mz_exact=790.53869; PE 40:6
6 largest peaks:
283.26354 999.00 | 327.23226 999.00 | 480.30917 506.26733 50.00 |
6 m/z Values and Intensities:
283.26354 999.00 sn1 FA
327.23226 999.00 sn1 FA

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Name: ABI Sciex API III QQQ; [M+H]⁺; PE MIX

MW: 752 ID#: 4232 DB: Text File

Comment: PE MIX; alkenyl/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

NIST MS Search 2.0 - [Peptide, Presearch Default - 295 spectra]

File Search View Tools Options Window Help

MS m/z

1. ABI Sciex API III QQQ; [M+H]⁺; PE MIX

#	Src.	Name
14	A	ABI QSTAR-XL QTOF; [M-]; Sulfatide (d18:1/C22:0)
15	A	ABI Sciex API III QQQ; [M-]; PE MIX
16	A	ABI Sciex API III QQQ; [M-]; PE 40:6
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
18	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6
19	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-]; PI 38:4
20	A	ABI-QSTAR-Pulsar-Quadrupol-TOF PS; [M+H] ⁺ ; PS 40:6

lipidblast-neg; custompc+hpos.msp; custompc+npos.msp; lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
2	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
3	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
4	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
5	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
6	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
7	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
8	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
9	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(1
10	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)
11	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)
12	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)
13	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)
14	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)
15	lipidblast-pos	72	397	1.68	997	PE 37:5; [M+H] ⁺ ; GPEtn(2)

(Text File) ABI Sciex API III QQQ; [M+H]⁺; PE MIX

Name: ABI Sciex API III QQQ; [M+H]⁺; PE MIX
MW: 752 ID#: 4232 DB: Text File
Comment: PE MIX; alkenyl/acyl PE(18:0/20:4)
4 largest peaks:
752.4 999.00 | 389.5 800.00 | 361.4 500.0
4 m/z Values and Intensities:
361.4 500.00 | 389.5 800.00 | 611.5 250.0
Synonyms:
no synonyms

ABI Sciex API III QQQ; [M+H]⁺; PE MIX Head to Tail MF=72 RMF=397 PE 37:5; [M+H]⁺; GPEtn(15:0/22:4) 72 397R 1.68P

Difference Head to Tail Side by Side Subtraction

(lipidblast-pos) PE 37:5; [M+H]⁺; GPEtn(15:0/22:4)

Name: PE 37:5; [M+H]⁺; GPEtn(15:0/22:5(42:72,102:1
MW: 752 ID#: 49070 DB: lipidblast-pos
Comment: Parent=752.52302 Mz_exact=752.52302; PE
8 largest peaks:
611.50392 999.00 | 225.22170 1.00 | 313.25298
510.29858 1.00 | 528.30914 1.00 | 734.51246
8 m/z Values and Intensities:
225.22170 1.00 sn1-0

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.

NIST MS Search 2.0 - [Peptide, Presearch Default - 273 spectra]

File Search View Tools Options Window Help

1. ABI Sciex API III QQQ; [M+H]⁺; PE 40:6

#	Src.	Name
14	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
16	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
18	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6
19	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; PI 38:4
20	A	ABI-QSTAR-Pulsar-Quadrupol-TOF PSar; [M-H] ⁻ ; PS 40:6

lipidblast-neg; custompc+hpos.msp; custompc+npos.msp; lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
75	lipidblast-pos	96	855	1.05	997	PE 40:6; [M+H] ⁺ ; GPEtn
76	lipidblast-pos	96	855	1.05	997	PE 40:6; [M+H] ⁺ ; GPEtn
77	lipidblast-pos	96	855	1.05	997	PE 40:6; [M+H] ⁺ ; GPEtn
78	lipidblast-pos	96	855	1.05	997	PE 40:6; [M+H] ⁺ ; GPEtn
79	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
80	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
81	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
82	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
83	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
84	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
85	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
86	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
87	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
88	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt
89	lipidblast-pos	15	458	0.11	534	PE 38:3; [M+Na] ⁺ ; GPEt

Plot of Search Spectrum

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]⁺; PE
3 largest peaks:
792.2 999.00 | 651.4 900.00 | 610.6 300.0
3 m/z Values and Intensities:
610.6 300.00 | 651.4 900.00 | 792.2 999.0
Synonyms:
no synonyms

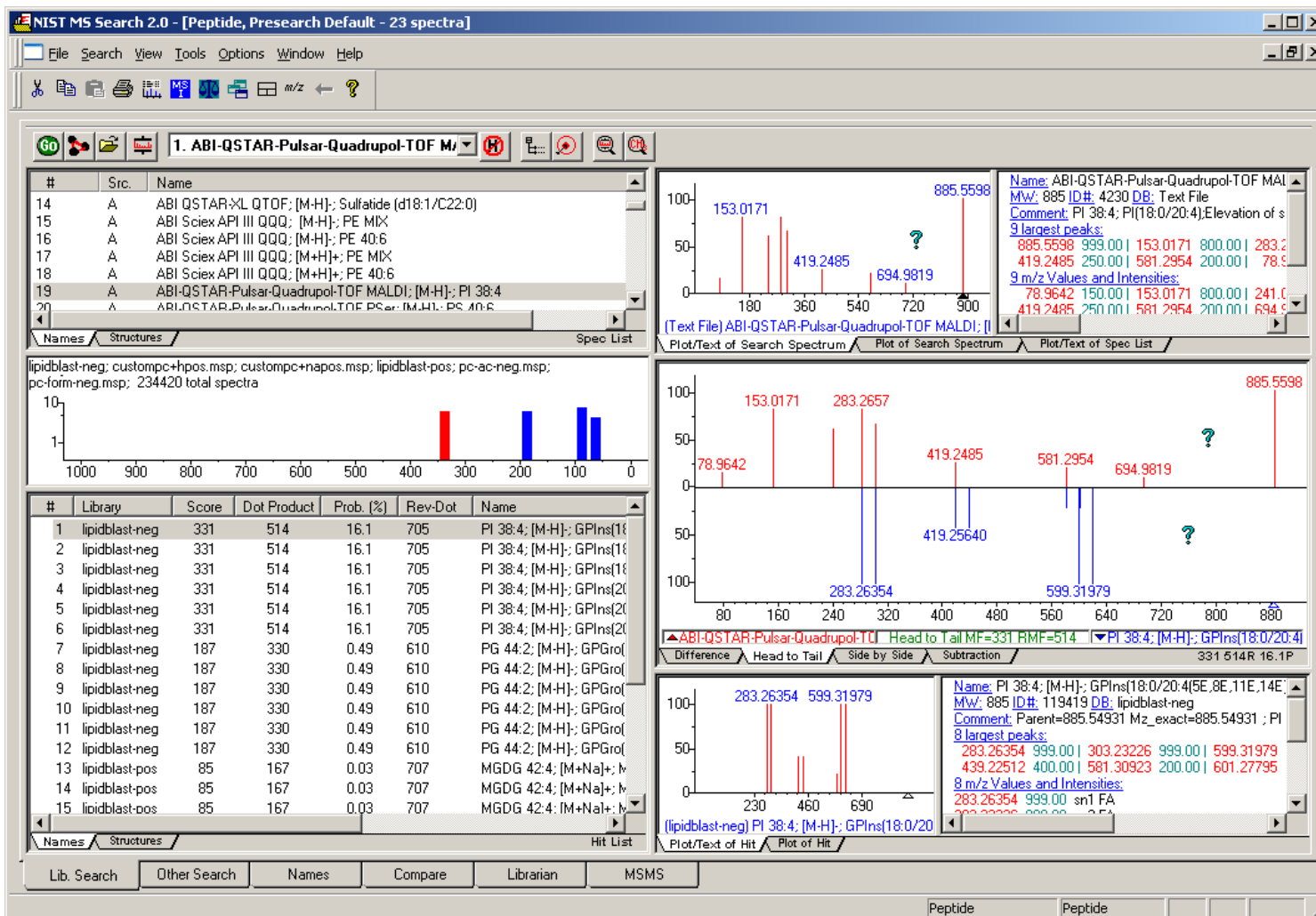
Plot of Search Spectrum

Name: PE 40:6; [M+H]⁺; GPEtn(22:6(42,72,102,132,162))
Mw: 792 ID#: 52657 DB: lipidblast-pos
Comment: Parent=792.55433 Mz_exact=792.55433 ; PE
8 largest peaks:
651.53523 999.00 | 267.26862 1.00 | 311.23734
508.28297 1.00 | 526.29353 1.00 | 774.54377
8 m/z Values and Intensities:
267.26862 1.00 sn2-D
311.23734 1.00

Plot of Hit

Lib. Search Other Search Names Compare Librarian MSMS

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

MS m/z

1. ABI-QSTAR-Pulsar-Quadrupol-TOF Pser

#	Src.	Name
13	A	ABI QSTAR-XL QTOF; [M-H] ⁻ ; Sulfatide (d18:1/C22:0)
14	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE MIX
15	A	ABI Sciex API III QQQ; [M-H] ⁻ ; PE 40:6
16	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE MIX
17	A	ABI Sciex API III QQQ; [M+H] ⁺ ; PE 40:6
18	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; PI 38:4
19	A	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H] ⁻ ; PS 40:6
20	A	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H] ⁻ ; SQDG 34:2
21	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; ST 34:1
22	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI3P 37:1
23	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI 34:1
24	A	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI 34:1

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	499	735	45.3	789	PS 40:6; [M-H] ⁻ ; GPSer(18:0/22:6)(4Z,7Z,10Z,13Z,16Z)
2	lipidblast-neg	499	735	45.3	789	PS 40:6; [M-H] ⁻ ; GPSer(22:6(4Z,7Z,10Z,13Z,16Z)
3	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:1(11E)/20:5(5Z,8Z,11Z)
4	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:1(11Z)/20:5(5Z,8Z,11Z)
5	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:1(13E)/20:5(5Z,8Z,11Z)
6	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:1(13Z)/20:5(5Z,8Z,11Z)
7	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:5(5Z,8Z,11Z,14Z,17Z)
8	lipidblast-neg	185	387	0.45	805	PS 40:6; [M-H] ⁻ ; GPSer(20:5(5Z,8Z,11Z,14Z,17Z)

Names Structures Spec List

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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
8 largest peaks:
419.35 999.00 | 283.33 950.00 | 153.03 450.00 | 747.67 400.00 | 437.327.30 250.00 | 834.75 200.00 | 463.33 100.00

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PS 40:6; [M-H]⁻; GPSer(18:0/22:6)(4Z,7Z,11Z,14Z,17Z)
MW: 834 ID#: 125128 DB: lipidblast-neg
Comment: Parent=834.52850 Mz_exact=834.52850
7 largest peaks:
747.49647 999.00 | 419.25639 200.00 | 437.21283.26354 100.00 | 327.23226 100.00 |
7 m/z Values and Intensities:
283.26354 100.00 sn1 FA

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 121 spectra]

File Search View Tools Options Window Help

MS m/z

1. ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H]-; SQDG 34:2

#	Src.	Name
13	A	ABI QSTAR-XL QTOF; [M-H]-; Sulfatide (d18:1/C22:0)
14	A	ABI Sciex API III QQQ; [M-H]-; PE MIX
15	A	ABI Sciex API III QQQ; [M-H]-; PE 40:6
16	A	ABI Sciex API III QQQ; [M+H]+; PE MIX
17	A	ABI Sciex API III QQQ; [M+H]+; PE 40:6
18	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H]-; PI 38:4
19	A	ABI-QSTAR-Pulsar-Quadrupol-TOF P5er; [M-H]-; P5 40:6
20	A	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H]-; SQDG 34:2
21	A	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H]-; ST 34:1
22	A	Agilent 6410 triple quadrupole MS; [M-H]-; PI3P 37:1
23	A	Agilent 6410 triple quadrupole MS; [M-H]-; PI 34:1
24	A	Agilent 6410 triple quadrupole MS; [M-H]-; PI 35:0

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[2E,4E])
2	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[6Z,9Z])
3	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[9E,10E])
4	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[9E,12E])
5	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[9Z,11Z])
6	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(16:0/18:2[9Z,12Z])
7	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(18:2[2E,4E]/16:0)
8	lipidblast-neg	474	794	8.22	997	SQDG 34:2; [M-H]-; SQDG(18:2[6Z,9Z]/16:0)

Names Structures Spec List

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);
8 largest peaks:
225.00 999.00 | 164.9 500.00 | 152.0 250.00 | 537.27 250.00 | 206.
561.27 200.00 | 255.23 100.00 | 279.23 100.00

(Text File) ABI-QSTAR-Pulsa

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: SQDG 34:2; [M-H]-; SQDG(16:0/18:2[2E,4E])
MW: 817 ID#: 129776 DB: lipidblast-neg
Comment: Parent=817.51358 Mz_exact=817.51358
5 largest peaks:
225.00690 999.00 | 537.27350 300.00 | 561.2
5 m/z Values and Intensities:
225.00690 999.00 fragment C6H9O7S
255.23226 100.00 sn1 FA

(lipidblast-neg) SQDG 34:2; [M-H]-; SQDG(16:0/18:2[2E,4E])

Plot/Text of Hit Plot of Hit

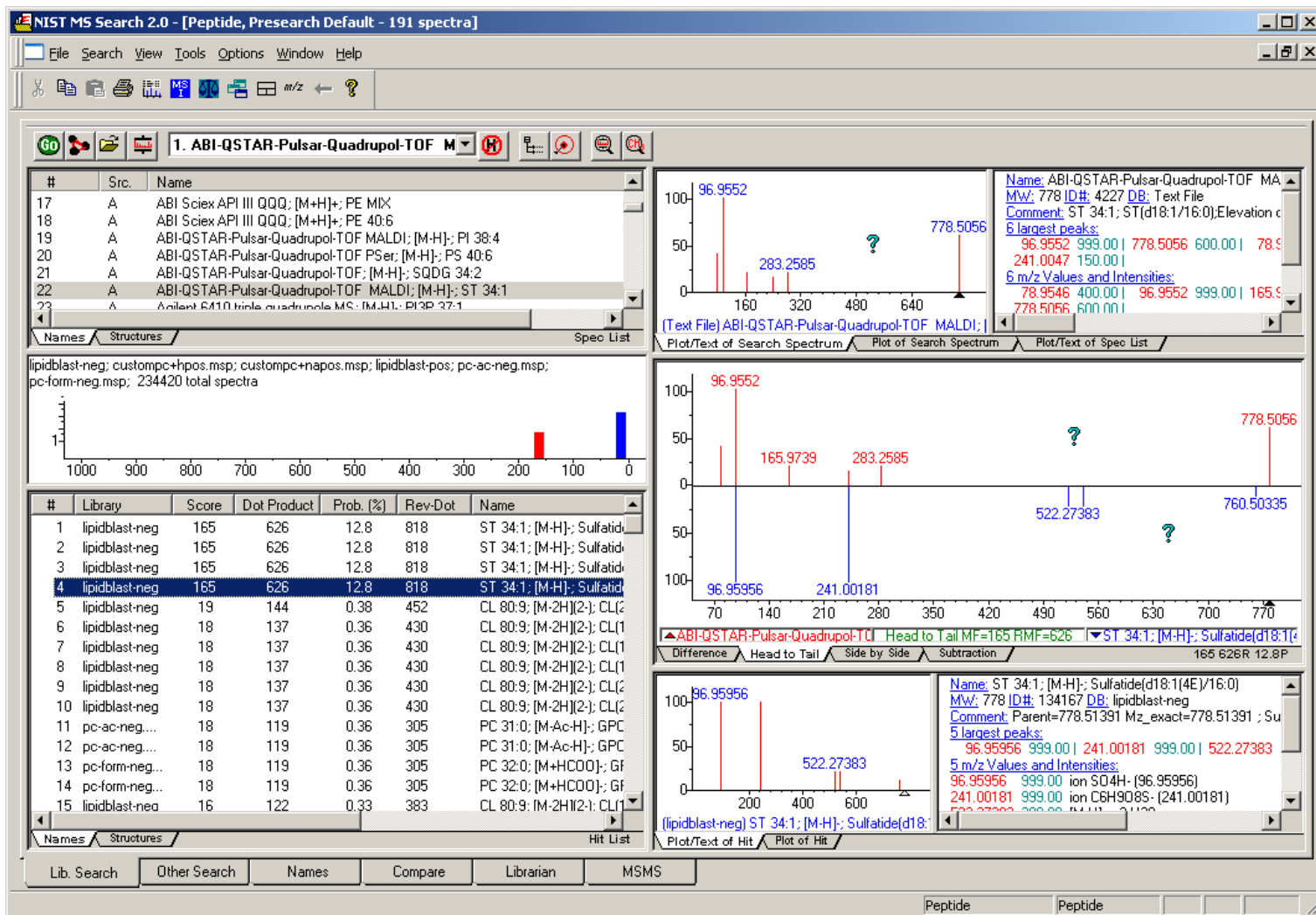
Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Name: ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H]⁻; ST 34:1

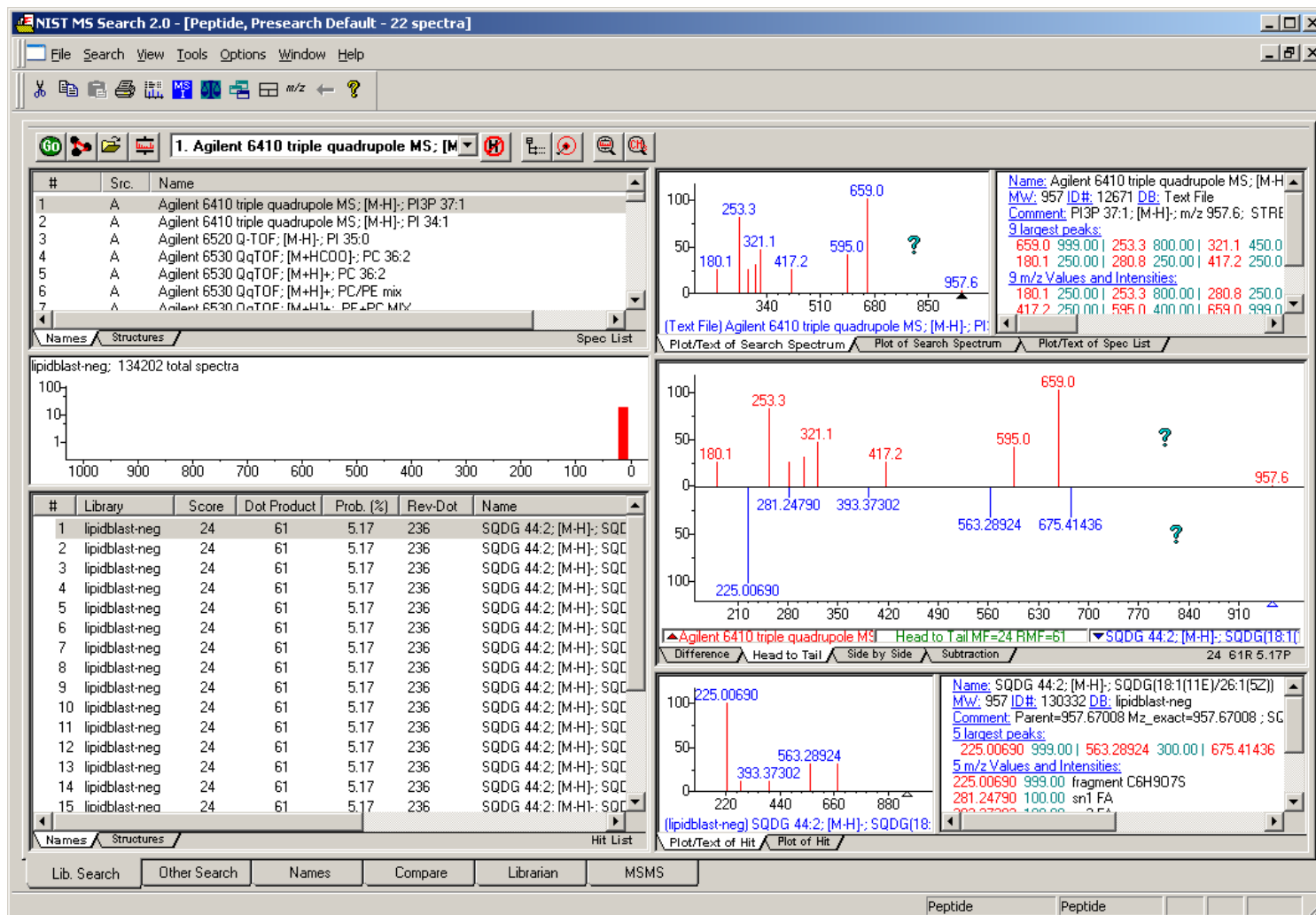
MW: 778 ID#: 4227 DB: Text File

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

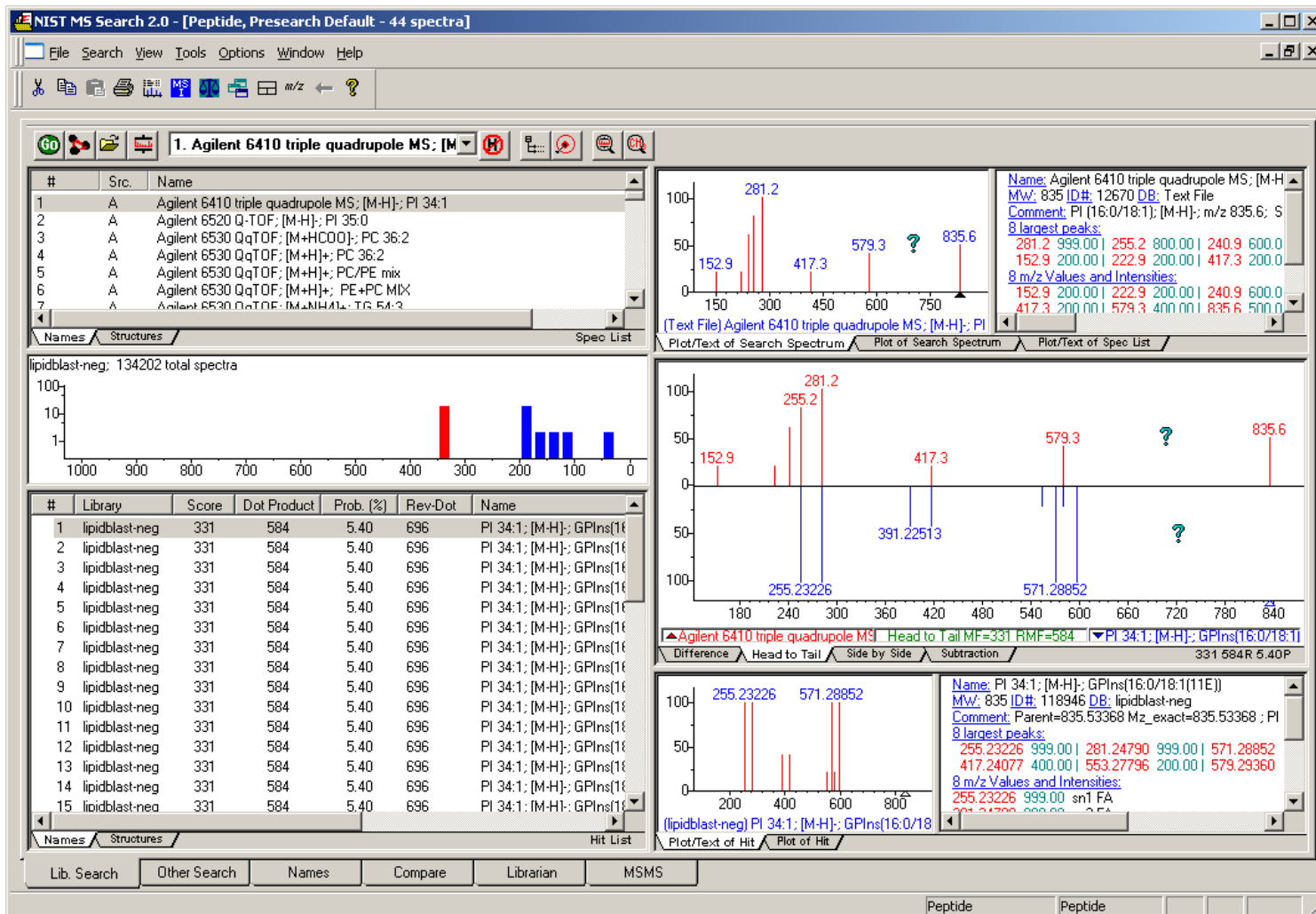


Name: Agilent 6410 triple quadrupole MS; [M-H]⁻; PI3P 37:1
 MW: 957 ID#: 12671 DB: Text File
 Comment: PI3P 37:1; [M-H]⁻; m/z 957.6; STRESS-INDUCED SYNTHESIS OF PHOSPHATIDYLINOSITOL 3-PHOSPHATE IN MYCOBACTERIA;
<http://www.jbc.org/cgi/doi/10.1074/jbc.M110.119263>
 9 largest peaks:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 24 spectra]

File Search View Tools Options Window Help

1. Agilent 6520 Q-TOF; [M-H]⁻; PI 35:0

#	Src.	Name
20	L	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H] ⁻ ; PS 40:6
21	L	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H] ⁻ ; SQDG 34:2
22	L	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; ST 34:1;
23	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI3P 37:1
24	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI 34:1
25	L	Agilent 6520 Q-TOF; [M-H] ⁻ ; PI 35:0
26	L	Agilent 6530 QqTOF; [M+HCOO] ⁻ ; PC 36:2
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	388	578	48.1	665	PI 35:0; [M-H] ⁻ ; GPIs(16:0/19:0)
2	lipidblast-neg	388	578	48.1	665	PI 35:0; [M-H] ⁻ ; GPIs(19:0/16:0)
3	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(15:0/26:2(5E,9Z))
4	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(15:0/26:2(5Z,9E))
5	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(15:0/26:2(5Z,9Z))
6	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(26:2(5E,9Z)/15:0)
7	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(26:2(5Z,9E)/15:0)
8	lipidblast-neg	180	322	0.48	707	MGDG 41:2; [M-H] ⁻ ; MGDG(26:2(5Z,9Z)/15:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
851.77 999.00 | 433.42 120.00 | 241.12 110.00 | 297.40 100.00 | 595.34 80.00

(Spec. List) Agilent 6520 Q-T

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PI 35:0; [M-H]⁻; GPIs(16:0/19:0)
MW: 851 ID#: 118965 DB: lipidblast-neg
Comment: Parent=851.56493 Mz_exact=851.56493
8 largest peaks:
255.23226 999.00 | 297.27918 999.00 | 571.28849 999.00 | 433.27202 400.00 | 553.27793 200.00 | 595.34 200.00

(lipidblast-neg) PI 35:0; [M-H]⁻; GPIs(16:0/19:0)

Plot/Text of Hit Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 191 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+HCOO]-; PC 36:2

#	Src.	Name
1	A	Agilent 6530 QqTOF; [M+HCOO]-; PC 36:2
2	A	Agilent 6530 QqTOF; [M+H]+; PC 36:2
3	A	Agilent 6530 QqTOF; [M+H]+; PC/PE mix
4	A	Agilent 6530 QqTOF; [M+H]+; PE+PC MIX
5	A	Agilent 6530 QqTOF; [M+NH4]+; TG 54:3
6	A	Agilent LC/MSD 1100 Ion Trap; [M-H]-; PE 34:1
7	A	Agilent Ion Trap SL; [M+Na]+; PC 34:1

lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; 145154 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
2	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
3	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
4	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
5	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
6	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
7	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
8	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
9	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
10	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
11	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
12	pc-form-neg...	683	991	7.62	992	PC 36:2; [M+HCOO]-; Gf
13	pc-form-neg...	83	838	0.07	951	PC 36:2; [M+HCOO]-; Gf
14	pc-form-neg...	83	838	0.07	951	PC 36:2; [M+HCOO]-; Gf
15	pc-form-neg...	83	838	0.07	951	PC 36:2; [M+HCOO]-; Gf

Agilent 6530 QqTOF; [M+HCOO]-; PC 36:2

770.5758

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:
770.5758 999.00 | 830.5966 250.00 | 279.2344 200.00 | 283.2645 100.00 | 770.5758 999.00
4 m/z Values and Intensities:
279.2344 200.00 | 283.2645 100.00 | 770.5758 999.00
Synonyms:
no synonyms

Agilent 6530 QqTOF; [M+HCOO]-; PC 36:2; [M+HCOO]-; GPCCho(18:0/18:2[2E,4E])

770.5758

830.5966

830.59110

770.56997

Name: PC 36:2; [M+HCOO]-; GPCCho(18:0/18:2[2E,4E])
MW: 830 ID#: 2563 DB: pc-form-neg.msp
Comment: Parent=830.59110 Mz_exact=830.59110 ; PC 36:2; [M+HCOO]-; GPCCho(18:0/18:2[2E,4E])
4 largest peaks:
770.56997 999.00 | 279.23226 100.00 | 283.26354 100.00
4 m/z Values and Intensities:
279.23226 100.00 FA sn2
283.26354 100.00 FA sn1
770.56997 999.00 FA sn3

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 179 spectra]

File Search View Tools Options Window Help

MS m/z

1. Agilent 6530 QqTOF; [M+H]⁺; PC 36:2

#	Src.	Name
20	L	ABI-QSTAR-Pulsar-Quadrupol-TOF PSe; [M-]; PS 40:6
21	L	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-]; SQDG 34:2
22	L	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-]; ST 34:1
23	L	Agilent 6410 triple quadrupole MS; [M-]; PI3P 37:1
24	L	Agilent 6410 triple quadrupole MS; [M-]; PI 34:1
25	L	Agilent 6520 Q-TOF; [M-]; PI 35:0
26	L	Agilent 6530 QqTOF; [M+HCOO] ⁻ ; PC 36:2
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hlic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmldformat; 365886 total spectra

Library Score Dot Product Prob. (%) Rev-Dot Name

1	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(11E))
2	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(11Z))
3	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(13Z))
4	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(17Z))
5	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(4E))
6	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(6Z))
7	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(7Z))
8	custompc+h...	7	737	0.61	737	PC 36:2; [M+H] ⁺ ; GPCho(18:1(11E)/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 lipidom
2 largest peaks:
184.0728 999.00 | 786.5987 800.00 |
2 m/z Values and Intensities:

(Spec. List) Agilent 6530 QqTOF

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 36:2; [M+H]⁺; GPCho(18:1(11E)/18:1(11E))
MW: 786 **ID#:** 2569 **DB:** custompc+hpos.msp
Comment: Parent=786.60126 Mz_exact=786.6012
7 largest peaks:
184.07387 999.00 | 504.34554 200.00 | 522.3...
786.60126 200.00 | 768.59070 10.00 |
7 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 36:2; [M+H]⁺; GPCho(18:1(11E)/18:1(11E))

Difference Head to Tail Side by Side Subtraction

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 66 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+H]⁺; PC/PE

#	Src.	Name
20	L	ABI-QSTAR-Pulsar-Quadrupol-TOF PSer; [M-]; PS 40:6
21	L	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-]; SQDG 34:2
22	L	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-]; ST 34:1
23	L	Agilent 6410 triple quadrupole MS; [M-]; PI3P 37:1
24	L	Agilent 6410 triple quadrupole MS; [M-]; PI 34:1
25	L	Agilent 6520 Q-TOF; [M-]; PI 35:0
26	L	Agilent 6530 QqTOF; [M+HCOO] ⁻ ; PC 36:2
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE 36:2

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5E,9Z])
2	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5Z,9E])
3	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5Z,9Z])
4	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(11:0/22:2[13Z,16Z])
5	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(13:0/20:2[11Z,14Z])
6	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(13:0/20:2[5Z,8Z])
7	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(15:0/18:2[2E,4E])
8	custompc+h...	19	621	1.72	676	PC 33:2; [M+H] ⁺ ; GPCho(15:0/18:2[6Z,9Z])

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
3 largest peaks:
184.0723 999.00 | 744.5864 500.00 | 603.5311 200.00 |
3 m/z Values and Intensities:

(Spec. List) Agilent 6530 Qq

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

▲ Agilent 6530 QqTOF; [M+H]⁺; PC; Head to Tail MF=19 RMF=621 ▼ PC 33:2; [M+H]⁺; GPCho(7:0/26:2
19 621R 1.72P

Difference Head to Tail Side by Side Subtraction

Name: PC 33:2; [M+H]⁺; GPCho(7:0/26:2[5E,9Z])
MW: 744 ID#: 1648 DB: custompc+hpos.msp
Comment: Parent=744.55433 Mz_exact=744.5543
9 largest peaks:
184.07387 999.00 | 352.18913 200.00 | 370.11
632.46557 200.00 | 685.48083 200.00 | 744.55433
9 m/z Values and Intensities:
184.07387 999.00 fragment C5H15N04P

(custompc+hpos.msp) PC 33:2; [M+H]⁺; GPCho(7:0/26:2

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 48 spectra]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+H]⁺; PC/PE

#	Src.	Name
20	L	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H] ⁻ ; PS 40:6
21	L	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H] ⁻ ; SQDG 34:2
22	L	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; ST 34:1
23	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI3P 37:1
24	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI 34:1
25	L	Agilent 6520 Q-TOF; [M-H] ⁻ ; PI 35:0
26	L	Agilent 6530 QqTOF; [M+HCOO] ⁻ ; PC 36:2
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE 36:2

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5E,9Z])
2	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5Z,9E])
3	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(7:0/26:2[5Z,9Z])
4	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(11:0/22:2[13Z,16Z])
5	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(13:0/20:2[11Z,14Z])
6	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(13:0/20:2[5Z,8Z])
7	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(15:0/18:2[2E,4E])
8	custompc+h...	19	621	2.08	676	PC 33:2; [M+H] ⁺ ; GPCho(15:0/18:2[6Z,9Z])

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

Name: Agilent 6530 QqTOF; [M+H]⁺; PE+PC MIX
MW: 744 ID#: 29 DB: Spec. L
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:
184.0723 999.00 | 744.5864
3 m/z Values and Intensities:

(Spec. List) Agilent 6530 QqTOF; [M+H]⁺; PE+PC MIX

Agilent 6530 QqTOF; [M+H]⁺; PE | Head to Tail MF=31 RMF=608 | PC 33:2; [M+H]⁺; GPCho(7:0/26:2[5E,9Z])

(custompc+hpos.msp) PC 33:2; [M+H]⁺; GPCho(7:0/26:2[5E,9Z])

Name: PC 33:2; [M+H]⁺; GPCho(7:0/26:2[5E,9Z])
MW: 744 ID#: 1648 DB: custompc+hpos.msp
Comment: Parent=744.55433 Mz_exact=744.55433
9 largest peaks:
184.07387 999.00 | 352.18913 200.00 | 370.18913 200.00 | 632.46557 200.00 | 685.48083 200.00 | 744.55433 200.00
9 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

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

NIST MS Search 2.0 - [Peptide, Presearch Default - empty]

File Search View Tools Options Window Help

1. Agilent 6530 QqTOF; [M+NH4]⁺; TG 54:3

#	Src.	Name
20	L	ABI-QSTAR-Pulsar-Quadrupol-TOF Pser; [M-H] ⁻ ; PS 40:6
21	L	ABI-QSTAR-Pulsar-Quadrupol-TOF; [M-H] ⁻ ; SQDG 34:2
22	L	ABI-QSTAR-Pulsar-Quadrupol-TOF MALDI; [M-H] ⁻ ; ST 34:1
23	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI3P 37:1
24	L	Agilent 6410 triple quadrupole MS; [M-H] ⁻ ; PI 34:1
25	L	Agilent 6520 Q-TOF; [M-H] ⁻ ; PI 35:0
26	L	Agilent 6530 QqTOF; [M+HCOO] ⁻ ; PC 36:2
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3

Names Structures Spec List

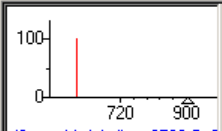
acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
---	---------	-------	-------------	-----------	---------	------

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List



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:
603.5315 999.00 |
1 m/z Values and Intensities:

Difference Head to Tail Side by Side Subtraction

Plot/Text of Hit Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 145 spectra]

File Search View Tools Options Window Help

Go 1. Agilent LC/MSD 1100 Ion Trap ; [M-H]⁻

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap ; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(11E))
2	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(11Z))
3	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(13Z))
4	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(17Z))
5	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(4E))
6	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(6Z))
7	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(7Z))
8	lipidblast-neg	236	851	5.38	881	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
281.2 999.00 | 255.2 500.00 | 716.5 100.00 | 140 55.00 | 196 55.00

5 m/z Values and Intensities:

Name: PE 34:1; [M-H]⁻; GPEtn(16:0/18:1(11E))
MW: 716 ID#: 107994 DB: lipidblast-neg
Comment: Parent=716.52306 Mz_exact=716.52306

6 largest peaks:
255.23226 999.00 | 281.24790 999.00 | 452.2 50.00 | 460.28298 50.00

6 m/z Values and Intensities:
255.23226 999.00 sn1 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 177 spectra]

File Search View Tools Options Window Help

1. Agilent Ion Trap SL; [M+Na]⁺; PC 34:1

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap.; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[2E,4
2	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[6Z,9
3	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9E,1
4	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9E,1
5	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9Z,1
6	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9Z,1
7	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[6Z,9Z])/18:2[2E,4
8	custompc+h...	90	431	1.09	446	PC 36:4; [M+H] ⁺ ; GPCho(18:2[6Z,9Z])/18:2[6Z,9

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
6 largest peaks:
723.3 999.00 | 599.4 900.00 | 577.5 70.00 | 478.2 30.00 | 504.2 20.00 | 651.3 10.00

(Spec. List) Agilent Ion Trap | Plot of Search Spectrum | Plot/Text of Spec List

Agilent Ion Trap SL; [M+Na]⁺; PC Head to Tail MF=90 RMF=431 PC 36:4; [M+H]⁺; GPCho(18:2[2E,4E])/18:2[6Z,9Z] 90 431R 1.09P

Difference Head to Tail Side by Side Subtraction

Name: PC 36:4; [M+H]⁺; GPCho(18:2[2E,4E])/18:2[6Z,9Z]
MW: 782 ID#: 2356 DB: custompc+hpos.msp
Comment: Parent=782.56995 Mz_exact=782.56995
7 largest peaks:
184.07387 999.00 | 502.32987 200.00 | 520.32987 200.00 | 764.55939 10.00 | 782.56995 200.00 | 764.55939 10.00 | 184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 36:4; [M+H]⁺; GPCho(18:2[2E,4E])/18:2[6Z,9Z] | Plot/Text of Hit | Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 265 spectra]

File Search View Tools Options Window Help

Go 1. Agilent Ion Trap XCT; [M+H]⁺; NA

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent LC/MSD 1100 Ion Trap; [M+H] ⁺ ; PE 33:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+naps; custompc+hpos.msp; custompc+naps.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(14:1(9Z)/24:4(5Z,8Z,11Z,13Z)
2	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(16:0/22:5(7Z,10Z,13Z)
3	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(16:0/22:5(7Z,10Z,13Z)
4	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(16:1(7Z)/22:4(7Z,10Z,13Z)
5	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(16:1(9Z)/22:4(7Z,10Z,13Z)
6	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(18:0/20:5(5Z,8Z,11Z,13Z)
7	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(18:1(11E)/20:4(5E,8E,11Z,13Z)
8	custompc+h...	49	432	0.63	433	PC 38:5; [M+H] ⁺ ; GPCho(18:1(11E)/20:4(5Z,8Z,11Z,13Z)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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;
3 largest peaks:
808.6 999.00 | 625.7 800.00 | 749.7 350.00 |
3 m/z Values and Intensities:

(Spec. List) Agilent Ion Trap; Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 38:5; [M+H]⁺; NA
MW: 808 ID#: 3047 DB: custompc+hpos.msp
Comment: Parent=808.58564 Mz_exact=808.58564
9 largest peaks:
184.07387 999.00 | 504.34556 200.00 | 522.31111 200.00 | 625.51960 200.00 | 749.51214 200.00 | 808.58564 200.00 | 184.07387 999.00
9 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 38:5; [M+H]⁺; GPCho(18:1(11E)/20:4(5E,8E,11Z,13Z)); Plot/Text of Hit Plot of Hit

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.bbali.2006.03.022

5 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 10 spectra]

File Search View Tools Options Window Help

Go 1. Agilent Ion Trap XCT ESI; [M-H]⁻; PI 38:4

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent LC/MSD 1100 Ion Trap; [M+H] ⁺ ; PC 36:2

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(18:0/20:4(5E,8E,11E,14E))
2	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(18:0/20:4(5Z,8Z,11Z,14Z))
3	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(18:0/20:4(7E,10E,13E,16E))
4	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(20:4(5E,8E,11E,14E))/18:(
5	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(20:4(5Z,8Z,11Z,14Z))/18:(
6	lipidblast-neg	37	331	12.2	438	PI 38:4; [M-H] ⁻ ; GPIs(20:4(7E,10E,13E,16E))/18:(
7	lipidblast-neg	24	239	7.89	707	MGDG 44:6; [M-H] ⁻ ; MGDG(22:2(13Z,16Z)/22:4)
8	lipidblast-neg	24	239	7.89	707	MGDG 44:6; [M-H] ⁻ ; MGDG(22:4(7Z,10Z,13Z,16Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 perit
5 largest peaks:
303.3 999.00 | 259.3 250.00 | 484.3 250.00 | 331.3 200.00 | 436.3 5
5 m/z Values and Intensities:

Name: PI 38:4; [M-H]⁻; GPIs(18:0/20:4(5E,8E,11E,14E))
MW: 885 ID#: 119419 DB: lipidblast-neg
Comment: Parent=885.54931 Mz_exact=885.5493
8 largest peaks:
283.26354 999.00 | 303.23226 999.00 | 599.3
439.22512 400.00 | 581.30923 200.00 | 601.2
8 m/z Values and Intensities:
283.26354 999.00 sn1 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 184 spectra]

File Search View Tools Options Window Help

Go 1. Agilent Ion Trap XCT ESI; [M+H]⁺; PE 34:2

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent LC/MSD 1100 Ion Trap; [M+H] ⁺ ; PE 33:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmdformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[2E,4E])
2	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[6Z,9Z])
3	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[9E,10E])
4	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[9E,12E])
5	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[9Z,11Z])
6	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(16:0/18:2[9Z,12Z])
7	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(18:2[2E,4E]/16:0)
8	lipidblast-neg	477	941	8.11	942	PE 34:2; [M-H] ⁻ ; GPEtn(18:2[6Z,9Z]/16:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 pe
4 largest peaks:
279.2 999.00 | 255.2 400.00 | 452.2 200.00 | 476.2 20.00 |
4 m/z Values and Intensities:

(Spec. List) Agilent Ion Trap

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PE 34:2; [M-H]⁻; GPEtn(16:0/18:2[2E,4E])
MW: 714 ID#: 108003 DB: lipidblast-neg
Comment: Parent=714.50738 Mz_exact=714.5073
6 largest peaks:
255.23226 999.00 | 279.23226 999.00 | 452.2
458.26730 50.00 |
6 m/z Values and Intensities:
255.23226 999.00 sn1 FA

(lipidblast-neg) PE 34:2; [M-H]⁻; GPEtn(16:0/18:2[2E,4E])

Plot/Text of Hit Plot of Hit

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 ion-trap mass spectrometry

http://dx.doi.org/10.1016/j.bbailp.2006.03.022

8 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 28 spectra]

File Search View Tools Options Window Help

1. Agilent Ion Trap XCT ESI; [M-H]⁻; PI 38:4

#	Src.	Name
27	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC 36:2
28	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PC/PE mix
29	L	Agilent 6530 QqTOF; [M+H] ⁺ ; PE+PC MIX
30	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
31	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
32	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
33	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
34	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
35	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
36	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hlic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(18:0/20:4(5E,8E,11E,14E
2	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(18:0/20:4(5Z,8Z,11Z,14Z
3	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(18:0/20:4(7E,10E,13E,16
4	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(20:4(5E,8E,11E,14E)/18:(
5	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(20:4(5Z,8Z,11Z,14Z)/18:(
6	lipidblast-neg	597	769	16.5	831	PI 38:4; [M-H] ⁻ ; GPlns(20:4(7E,10E,13E,16E)/18
7	lipidblast-neg	261	443	0.16	633	PG 44:2; [M-H] ⁻ ; GPGro(18:0/26:2(5E,9Z))
8	lipidblast-neg	261	443	0.16	633	PG 44:2; [M-H] ⁻ ; GPGro(18:0/26:2(5Z,9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 spec
8 largest peaks:
419.2 999.00 | 581.3 950.00 | 283.3 800.00 | 489.2 600.00 | 599.3 40
619.2 250.00 | 303.3 200.00 | 601.2 20.00 |

Name: PI 38:4; [M-H]⁻; GPlns(18:0/20:4(5E,8E,11E,14E)
MW: 885 ID#: 119419 DB: lipidblast-neg
Comment: Parent=885.54931 Mz_exact=885.54931
8 largest peaks:
283.26354 999.00 | 303.23226 999.00 | 599.3
439.22512 400.00 | 581.30923 200.00 | 601.2
8 m/z Values and Intensities:
283.26354 999.00 sn1 FA

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 ion-trap mass spectrometry

http://dx.doi.org/10.1016/j.bbali.2006.03.022

6 largest peaks:

NIST MS Search [Peptide, Presearch Default - 182 spectra]

File Search View Tools Options Window Help

1. Agilent Ion Trap XCT ESI; [M-H]⁻; PS 38:4

#	Src.	Name
1	A	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PS 38:4
2	L	ABI 4000 Q-Trap; [M-H] ⁻ ; CerP(d18:1/12:0)
3	L	ABI 4000 Q-Trap; [M-H] ⁺ ; CerP(d18:1/12:0)
4	L	ABI QTRAP 4000; [M-H] ⁻ ; Lipid A [dIPP-14-hexaacyl]
5	L	ABI 4000 Q-Trap; [M-H] ⁻ ; PI 36:1
6	L	ABI 4000 Q-Trap; [M+NH4] ⁺ ; TG 52:3
7	L	ABI-API 4000 Q Trap; [M-H] ⁻ ; GM2(d18:1/C18:0)
8	L	ABI-API 4000 Q Trap; [M-H] ⁻ ; GD1a
9	L	ABI-API 4000 Q Trap; [M-H] ⁻ ; GM2(d20:1/C18:0)
10	L	ABI 4700 MALDI-TOF/TOF; [M-H] ⁻ ; Ac2PIM1(16:0/methyl-18:0)
11	L	ABI 4700 MALDI TOF/TOF; [M-H] ⁻ ; Lipid A
12	L	ABI 4000 MALDI TOF/TOF; [M-H] ⁻ ; CerP(d18:1/12:0)

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; respectdbinmldformat; 365886 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(18:0/20:4[5E,8E,11E,14E,17E,20E])
2	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(18:0/20:4[5Z,8Z,11Z,14Z,17Z,20Z])
3	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(18:0/20:4[7E,10E,13E,16E,19E,22E])
4	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(20:4[5E,8E,11E,14E,17E,20E])
5	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(20:4[5Z,8Z,11Z,14Z,17Z,20Z])
6	lipidblast-neg	340	831	14.5	879	PS 38:4; [M-H] ⁻ ; GPSer(20:4[7E,10E,13E,16E,19E,22E])
7	lipidblast-neg	99	514	0.14	707	PS 38:4; [M-H] ⁻ ; GPSer(14:0/24:4[5Z,8Z,11Z,14Z,17Z,20Z])
8	lipidblast-neg	99	514	0.14	707	PS 38:4; [M-H] ⁻ ; GPSer(16:0/22:4[7Z,10Z,13Z,16Z,19Z,22Z])

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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 ion-trap mass spectrometry
6 largest peaks:
723.5 999.00 | 419.3 250.00 | 283.3 220.00 | 437.3 200.00 | 546.3 20.00 | 303.3 20.00

Name: PS 38:4; [M-H]⁻; GPSer(18:0/20:4[5E,8E,11E,14E,17E,20E])
MW: 810 ID#: 125117 DB: lipidblast-neg
Comment: Parent=810.52850 Mz_exact=810.52850
7 largest peaks:
723.49647 999.00 | 419.25639 200.00 | 437.25639 100.00 | 283.26354 100.00 | 303.23226 100.00 | 283.26354 100.00 sn1 FA

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](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

NIST MS Search 2.0 - [Peptide, Presearch Default - 118 spectra]

File Search View Tools Options Window Help

1. Agilent MSD 1100 single quadrupole

#	Src.	Name
31	L	Agilent 6530 QqTOF; [M+NH ₄] ⁺ ; TG 54:3
32	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
33	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
34	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
35	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
36	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H] ⁺ ; PE 32:0
40	L	Agilent QTOF; [M+NH ₄] ⁺ ; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H] ⁺ ; PC MIX
42	L	Bruker Esquire 3000 Ion Trap ESI; M+H+; PI 34; PD 50; 30:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; 359499 total spectra

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 pho
7 largest peaks:
692.5 999.00 | 551.5 200.00 | 663.4 50.00 | 686.6 50.00 | 282.3 3
313.2 30.00 | 371.2 30.00

(Spec. List) Agilent MSD 1100

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Agilent MSD 1100 single quadrupole MS; [M+H]⁺; PE 32:0
Head to Tail MF=19 RMF=84
PC 29:0; [M+H]⁺; GPCho(3:0/26:0)
Difference Head to Tail Side by Side Subtraction 19 84R 0.87P

(custompc+hpos.msp) PC 29:0; [M+H]⁺; GPCho(3:0/26:0)
Name: PC 29:0; [M+H]⁺; GPCho(3:0/26:0)
MW: 692 ID#: 1151 DB: custompc+hpos.msp
Comment: Parent=692.52302 Mz_exact=692.5230
9 largest peaks:
184.07387 999.00 | 296.12654 200.00 | 314.1
633.44952 200.00 | 636.49682 200.00 | 692.5
9 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(3:0/26:0)
2	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(4:0/25:0)
3	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(5:0/24:0)
4	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(6:0/23:0)
5	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(7:0/22:0)
6	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(8:0/21:0)
7	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(9:0/20:0)
8	custompc+h...	19	84	0.87	133	PC 29:0; [M+H] ⁺ ; GPCho(10:0/19:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 2 spectra]

File Search View Tools Options Window Help

1. Agilent QTOF; [M+NH4]+; TG

#	Src.	Name
31	L	Agilent 6530 QqTOF; [M+NH4]+; TG 54:3
32	L	Agilent LC/MSD 1100 Ion Trap; [M-H]-; PE 34:1
33	L	Agilent Ion Trap SL; [M+Na]+; PC 34:1
34	L	Agilent Ion Trap XCT; [M+H]+; NA
35	L	Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
36	L	Agilent Ion Trap XCT ESI; [M+H]+; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H]+; PE 32:0
40	L	Agilent QTOF; [M+NH4]+; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H]+; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI; [M+H]+; PE 50:20:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
359499 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	0	70	50.0	707	MGDG 44:1; [M-H]-; MGDG(22:0/22:1(13Z))
2	lipidblast-neg	0	70	50.0	707	MGDG 44:1; [M-H]-; MGDG(22:1(13Z)/22:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

Plot/Text of Search Spectrum

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 D
3 largest peaks:
599.5 999.00 | 263.2357 10.00 | 337.27 10.00 |
3 m/z Values and Intensities:

Plot/Text of Search Spectrum

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 D
3 largest peaks:
599.5 999.00 | 263.2357 10.00 | 337.27 10.00 |
3 m/z Values and Intensities:

Plot/Text of Hit

Name: MGDG 44:1; [M-H]-; MGDG(22:0/22:1(13Z))
MW: 895 ID#: 100111 DB: lipidblast-neg
Comment: Parent=895.72378 Mz_exact=895.7237
2 largest peaks:
337.31046 999.00 | 339.32610 999.00 |
2 m/z Values and Intensities:
337.31046 999.00 sn2 FA
339.32610 999.00 sn1 FA

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

PC -MIX

9 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 93 spectra]

File Search View Tools Options Window Help

1. Bruker DESI FTICR APEX-Q. [M+H]⁺

#	Src.	Name
31	L	Agilent 6530 QqTOF; [M+NH4] ⁺ ; TG 54:3
32	L	Agilent LC/MSD 1100 Ion Trap; [M-H] ⁻ ; PE 34:1
33	L	Agilent Ion Trap SL; [M+Na] ⁺ ; PC 34:1
34	L	Agilent Ion Trap XCT; [M+H] ⁺ ; NA
35	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
36	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H] ⁺ ; PE 32:0
40	L	Agilent QTOF; [M+NH4] ⁺ ; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H] ⁺ ; PC MIX
42	L	Bruker Esquire 3000 Ion Trap; [M+H] ⁺ ; PC 34:2

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos;
acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hiloc-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp;
359499 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(2E,4E))
2	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(6Z,9Z))
3	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(9E,10E))
4	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(9E,12E))
5	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(9Z,11Z))
6	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(16:0/18:2(9Z,12Z))
7	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(18:2(2E,4E)/16:0)
8	custompc+h...	115	207	6.64	429	PC 34:2; [M+H] ⁺ ; GPCho(18:2(6Z,9Z)/16:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
568.3400 999.00 | 542.3220 900.00 | 590.3217 800.00 | 520.3403 758.5694 120.00 | 496.3401 350.00 | 806.5686 150.00 | 780.5517 130.00 | 758.5694 120.00

Name: Bruker DESI FTICR APEX-Q, [M+H]⁺; GPCho(16:0/18:2(2E,4E))
MW: 758 ID#: 1857 DB: custompc+hpos.msp
Comment: Parent=758.56995 Mz_exact=758.5699
9 largest peaks:
184.07387 999.00 | 478.32987 200.00 | 496.3401 200.00 | 575.50391 200.00 | 699.49645 200.00 | 758.56995 200.00 | 184.07387 999.00 fragment C5H15NO4P

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 [14/14/14/14/30-(12)/30-(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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Bruker Esquire 3000 ion trap; ESI, [M-H]⁻

#	Src.	Name
36	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H] ⁺ ; PE 32:0
40	L	Agilent QTOF; [M+NH4] ⁺ ; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H] ⁺ ; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI, [M-H] ⁻ ; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI, [M-H] ⁻ ; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS, [M+H] ⁺ ; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4] ⁺ ; NA
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+H] ⁺ ; MGDG 30:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hlic-urine; lipidblast-neg; pc-ac-neg.msp; 359499 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [10/10/16/18/30-]
2	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [10/10/18/16/30-]
3	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [12/12/12/18/30-]
4	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [12/12/14/16/30-]
5	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [12/12/16/14/30-]
6	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [12/12/18/12/30-]
7	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [14/14/10/16/30-]
8	lipidblast-neg	79	172	0.44	370	LipidA-PP 54:28:0; LipidA-PP [14/14/12/14/30-]

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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 [14/14/14/14/30-(12)/30-(14)]; [M-H]⁻
10 largest peaks:
1796.2 999.00 | 1359.8 700.00 | 1506.0 400.00 | 1568.0 400.00 | 1488.2 400.00 | 1279.8 300.00 | 1716.2 300.00 | 1768.2 100.00 | 1688.2 50.00 | 1818.2 50.00

(Spec. List) Bruker Esquire 3000

▲ Bruker Esquire 3000 ion trap; ESI, Head to Tail MF=79 RMF=172 ▼ LipidA-PP 54:28:0; LipidA-PP [10/10/16/18/30-]
Difference Head to Tail Side by Side Subtraction 79 172R 0.44P

Name: LipidA-PP 54:28:0; LipidA-PP [10/10/16/18/30-]
MW: 1796 ID#: 80617 DB: lipidblast-neg
Comment: Parent=1796.21157 Mz_exact=1796.21157
7 largest peaks:
1608.07041 999.00 | 1698.23467 600.00 | 1796.21157 500.00 | 1568.00277 250.00 | 1714.22959 50.00 | 1470.02587 300.00 | 1470.02587 300.00 [M-H]⁻; PO4H3-R2'-O-FA II [M-H]⁻
7 m/z Values and Intensities:
1470.02587 300.00 [M-H]⁻; PO4H3-R2'-O-FA II [M-H]⁻

(lipidblast-neg) LipidA-PP 54:28:0; LipidA-PP [10/10/16/18/30-]

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 [14/14/14/14/30-(12)/30-(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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. Bruker Esquire 3000 ion trap; ESI, [M-]

#	Src.	Name
36	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H] ⁺ ; PE 32:0
40	L	Agilent QTOF; [M+NH4] ⁺ ; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H] ⁺ ; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI, [M-H] ⁻ ; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI, [M-H] ⁻ ; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS; [M+H] ⁺ ; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS; [M-H] ⁻ ; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS; [M+NH4] ⁺ ; NA
47	L	Bruker Esquire ion trap; ESI MS/MS; [M+H] ⁺ ; MGDG 30:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol+hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; 359499 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/10/18/30-(12)
2	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/10/18/30-(14)
3	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/12/16/30-(12)
4	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/12/16/30-(14)
5	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/14/14/30-(12)
6	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/14/14/30-(14)
7	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/16/12/30-(12)
8	lipidblast-neg	167	436	0.99	592	LipidA-PP 56:26:0; LipidA-PP [14/14/16/12/30-(14)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 [14/14/14/14/30-(12)/30-(14)]; [M-]
10 largest peaks:
1698.2 999.00 | 1470 400.00 | 1035.6 333.00 | 1243.8 333.00 | 1011.0 149.00
999.6 180.00 | 1225.8 100.00 | 1261.8 100.00 | 1454.0 50.00 | 1498.0 50.00

Name: LipidA-PP 56:26:0; LipidA-PP [14/14/14/14/30-(14)]
MW: 1796 ID#: 87941 DB: lipidblast-neg
Comment: Parent=1796.21157 Mz_exact=1796.21
9 largest peaks:
1552.00785 999.00 | 1698.23467 600.00 | 1796.21157 250.00
1454.03095 250.00 | 1568.00277 250.00 | 1598.00277 250.00
9 m/z Values and Intensities:
1454.03095 250.00 [M-H]⁻R2-PD4H3 || [M-H]⁻R3

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 117 spectra]

File Search View Tools Options Window Help

Go 1. Bruker Esquire ion trap; ESI MS/MS.

#	Src.	Name
36	L	Agilent Ion Trap XCT ESI; [M+H] ⁺ ; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H] ⁻ ; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H] ⁺ ; PE 32:0
40	L	Agilent QTOF; [M+NH4] ⁺ ; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H] ⁺ ; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI; [M-H] ⁻ ; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI; [M-H] ⁻ ; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS; [M+H] ⁺ ; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS; [M-H] ⁻ ; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS; [M+NH4] ⁺ ; NA
47	L	Bruker Esquire ion trap; ESI MS/MS; [M+H] ⁺ ; MDC 20:0

Names Structures Spec List

acylcoa+mol+hpos; acylcoa+mol-hneg; mainlib; acylcarnitine+custom+mol+hpos; acylcarnitine+mol+hpos; acylcarnitine+mol+napos; custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; 359499 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(11E))
2	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(11Z))
3	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(13Z))
4	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(17Z))
5	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(4E))
6	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(6Z))
7	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(7Z))
8	custompc+h...	2	700	0.89	700	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) 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:
 184.0 999.00 | 760.7 550.00 | 478.4 1.00 | 496.3 1.00 | 504.4 1.00

Bruker Esquire ion trap; ESI MS/MS; [M+H]⁺; GPCho(16:0/18:1(11E))
 MW: 760 ID#: 1927 DB: custompc+hpos.msp
 Comment: Parent=760.58564 Mz_exact=760.58564
 9 largest peaks:
 184.07387 999.00 | 478.32992 200.00 | 496.3 1.00 | 577.51960 200.00 | 701.51214 200.00 | 760.58564 1.00

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 chromatography positive electrospray tandem mass spectrometry, and application of developed methods in comprehensive analysis of low erucic acid rapeseed oil lipids

4 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 12 spectra]

File Search View Tools Options Window Help

1. Bruker Esquire ion trap; ESI MS/MS.

#	Src.	Name
36	L	Agilent Ion Trap XCT ESI; [M+H]+; PE 34:2
37	L	Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
38	L	Agilent Ion Trap XCT ESI; [M-H]-; PI 38:4
39	L	Agilent MSD 1100 single quadrupole MS; [M+H]+; PE 32:0
40	L	Agilent QTOF; [M+NH4]+; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H]+; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS, [M+H]+; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS, [M-H]-; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4]+; NA
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+H]+; MG(18:1)

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(11E)/0:0/0:0)
2	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(11Z)/0:0/0:0)
3	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(13Z)/0:0/0:0)
4	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(17Z)/0:0/0:0)
5	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(4E)/0:0/0:0)
6	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(6Z)/0:0/0:0)
7	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(7Z)/0:0/0:0)
8	lipidblast-pos	199	648	11.1	648	MG 18:1; [M+NH4]+; MG(18:1(9E)/0:0/0:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 chromatography positive electrospray tandem mass spectrometry, and application of developed methods in comprehensive analysis of low erucic acid rapeseed oil lipids
4 largest peaks: 339.3 999.00 | 357.3 800.00 | 283.3 50.00 | 374.3 5.00 |
4 m/z Values and Intensities:

(Spec. List) Bruker Esquire ion trap; ESI MS/MS, [M+NH4]+; NA

Name: MG 18:1; [M+NH4]+; MG(18:1(11E)/0:0/0:0)
MW: 374 ID#: 9590 DB: lipidblast-pos
Comment: Parent=374.32703 Mz_exact=374.32703
5 largest peaks: 339.31373 999.00 | 265.27679 400.00 | 283.28735 200.00 frag-sn1
5 m/z Values and Intensities:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 97 spectra]

File Search View Tools Options Window Help

1. Bruker Esquire ion trap; ESI MS/MS.

#	Src.	Name
39	L	Agilent MSD 1100 single quadrupole MS; [M+H]+; PE 32:0
40	L	Agilent QTOF; [M+NH4]+; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H]+; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS, [M+H]+; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS, [M-H]-; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4]+; NA
47	L	Bruker Esquire ion trap; ESI MS/MS, [M-H]-; MGDG 38:9
48	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na]+; MGDG 38:9
49	L	Bruker microTOF qQ-TOF; NA
50	L	Bruker microTOF qQ-TOF; NA

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	388	799	24.5	981	MGDG 38:9; [M-H]-; MGDG(18:4{6Z,9Z,12Z,15Z})
2	lipidblast-neg	388	799	24.5	981	MGDG 38:9; [M-H]-; MGDG(18:4{9E,11E,13E,15E})
3	lipidblast-neg	388	799	24.5	981	MGDG 38:9; [M-H]-; MGDG(20:5{5Z,8Z,11Z,14Z})
4	lipidblast-neg	388	799	24.5	981	MGDG 38:9; [M-H]-; MGDG(20:5{5Z,8Z,11Z,14Z})
5	lipidblast-neg	115	449	0.24	612	PG 38:5; [M-H]-; GPGro(18:0/20:5{5Z,8Z,11Z,14Z})
6	lipidblast-neg	115	449	0.24	612	PG 38:5; [M-H]-; GPGro(20:5{5Z,8Z,11Z,14Z})
7	lipidblast-neg	82	360	0.06	578	PG 38:5; [M-H]-; GPGro(18:4{6Z,9Z,12Z,15Z})
8	lipidblast-neg	82	360	0.06	578	PG 38:5; [M-H]-; GPGro(18:4{6Z,9Z,12Z,15Z})

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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:
301.5 999.00 | 275.5 450.00 | 537.5 400.00 | 795.5 200.00 | 511.0 184.47
447.4 150.00

(Spec. List) Bruker Esquire ion trap; ESI MS/MS, [M-H]-; MGDG 38:9

Plot/Text of Hit Plot of Hit

Name: MGDG 38:9; [M-H]-; MGDG(18:4{6Z,9Z,12Z,15Z})
MW: 795 ID#: 98850 DB: lipidblast-neg
Comment: Parent=795.50478 Mz_exact=795.50478
2 largest peaks:
275.20098 999.00 | 301.21662 999.00 |
2 m/z Values and Intensities:
275.20098 999.00 sn1 FA
301.21662 999.00 sn2 FA

(lipidblast-neg) MGDG 38:9; [M-H]-; MGDG(18:4{6Z,9Z,12Z,15Z})

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 16 spectra]

File Search View Tools Options Window Help

1. Bruker Esquire ion trap;ESI MS/MS, [M+Na]+; MGDG 38:9

#	Src.	Name
39	L	Agilent MSD 1100 single quadrupole MS; [M+H]+; PE 32:0
40	L	Agilent QTOF; [M+NH4]+; TG
41	L	Bruker DESI FTICR APEX-Q; [M+H]+; PC MIX
42	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
43	L	Bruker Esquire 3000 ion trap; ESI, [M-H]-; LipidA-PP 56:26:0
44	L	Bruker Esquire ion trap; ESI MS/MS, [M+H]+; PC 34:1
45	L	Bruker Esquire ion trap; ESI MS/MS, [M-H]-; DGDG 36:8
46	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4]+; NA
47	L	Bruker Esquire ion trap; ESI MS/MS, [M-H]-; MGDG 38:9
48	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na]+; MGDG 38:9
49	L	Bruker microTOF qQ-TOF; NA
50	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na]+; MGDG 38:9

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	131	944	22.4	949	MGDG 38:9; [M+Na]+; MGDG(18:4(6Z,9Z,12Z,15Z,18Z,21Z,24Z,27Z,30Z,33Z,36Z,39Z,42Z,45Z,48Z,51Z,54Z,57Z,60Z,63Z,66Z,69Z,72Z,75Z,78Z,81Z,84Z,87Z,90Z,93Z,96Z,99Z,102Z,105Z,108Z,111Z,114Z,117Z,120Z,123Z,126Z,129Z,132Z,135Z,138Z,141Z,144Z,147Z,150Z,153Z,156Z,159Z,162Z,165Z,168Z,171Z,174Z,177Z,180Z,183Z,186Z,189Z,192Z,195Z,198Z,201Z,204Z,207Z,210Z,213Z,216Z,219Z,222Z,225Z,228Z,231Z,234Z,237Z,240Z,243Z,246Z,249Z,252Z,255Z,258Z,261Z,264Z,267Z,270Z,273Z,276Z,279Z,282Z,285Z,288Z,291Z,294Z,297Z,300Z,303Z,306Z,309Z,312Z,315Z,318Z,321Z,324Z,327Z,330Z,333Z,336Z,339Z,342Z,345Z,348Z,351Z,354Z,357Z,360Z,363Z,366Z,369Z,372Z,375Z,378Z,381Z,384Z,387Z,390Z,393Z,396Z,399Z,402Z,405Z,408Z,411Z,414Z,417Z,420Z,423Z,426Z,429Z,432Z,435Z,438Z,441Z,444Z,447Z,450Z,453Z,456Z,459Z,462Z,465Z,468Z,471Z,474Z,477Z,480Z,483Z,486Z,489Z,492Z,495Z,498Z,501Z,504Z,507Z,510Z,513Z,516Z,519Z,522Z,525Z,528Z,531Z,534Z,537Z,540Z,543Z,546Z,549Z,552Z,555Z,558Z,561Z,564Z,567Z,570Z,573Z,576Z,579Z,582Z,585Z,588Z,591Z,594Z,597Z,600Z,603Z,606Z,609Z,612Z,615Z,618Z,621Z,624Z,627Z,630Z,633Z,636Z,639Z,642Z,645Z,648Z,651Z,654Z,657Z,660Z,663Z,666Z,669Z,672Z,675Z,678Z,681Z,684Z,687Z,690Z,693Z,696Z,699Z,702Z,705Z,708Z,711Z,714Z,717Z,720Z,723Z,726Z,729Z,732Z,735Z,738Z,741Z,744Z,747Z,750Z,753Z,756Z,759Z,762Z,765Z,768Z,771Z,774Z,777Z,780Z,783Z,786Z,789Z,792Z,795Z,798Z,801Z,804Z,807Z,810Z,813Z,816Z,819Z,822Z,825Z,828Z,831Z,834Z,837Z,840Z,843Z,846Z,849Z,852Z,855Z,858Z,861Z,864Z,867Z,870Z,873Z,876Z,879Z,882Z,885Z,888Z,891Z,894Z,897Z,900Z,903Z,906Z,909Z,912Z,915Z,918Z,921Z,924Z,927Z,930Z,933Z,936Z,939Z,942Z,945Z,948Z,951Z,954Z,957Z,960Z,963Z,966Z,969Z,972Z,975Z,978Z,981Z,984Z,987Z,990Z,993Z,996Z,999Z,1002Z,1005Z,1008Z,1011Z,1014Z,1017Z,1020Z,1023Z,1026Z,1029Z,1032Z,1035Z,1038Z,1041Z,1044Z,1047Z,1050Z,1053Z,1056Z,1059Z,1062Z,1065Z,1068Z,1071Z,1074Z,1077Z,1080Z,1083Z,1086Z,1089Z,1092Z,1095Z,1098Z,1101Z,1104Z,1107Z,1110Z,1113Z,1116Z,1119Z,1122Z,1125Z,1128Z,1131Z,1134Z,1137Z,1140Z,1143Z,1146Z,1149Z,1152Z,1155Z,1158Z,1161Z,1164Z,1167Z,1170Z,1173Z,1176Z,1179Z,1182Z,1185Z,1188Z,1191Z,1194Z,1197Z,1200Z,1203Z,1206Z,1209Z,1212Z,1215Z,1218Z,1221Z,1224Z,1227Z,1230Z,1233Z,1236Z,1239Z,1242Z,1245Z,1248Z,1251Z,1254Z,1257Z,1260Z,1263Z,1266Z,1269Z,1272Z,1275Z,1278Z,1281Z,1284Z,1287Z,1290Z,1293Z,1296Z,1299Z,1302Z,1305Z,1308Z,1311Z,1314Z,1317Z,1320Z,1323Z,1326Z,1329Z,1332Z,1335Z,1338Z,1341Z,1344Z,1347Z,1350Z,1353Z,1356Z,1359Z,1362Z,1365Z,1368Z,1371Z,1374Z,1377Z,1380Z,1383Z,1386Z,1389Z,1392Z,1395Z,1398Z,1401Z,1404Z,1407Z,1410Z,1413Z,1416Z,1419Z,1422Z,1425Z,1428Z,1431Z,1434Z,1437Z,1440Z,1443Z,1446Z,1449Z,1452Z,1455Z,1458Z,1461Z,1464Z,1467Z,1470Z,1473Z,1476Z,1479Z,1482Z,1485Z,1488Z,1491Z,1494Z,1497Z,1500Z,1503Z,1506Z,1509Z,1512Z,1515Z,1518Z,1521Z,1524Z,1527Z,1530Z,1533Z,1536Z,1539Z,1542Z,1545Z,1548Z,1551Z,1554Z,1557Z,1560Z,1563Z,1566Z,1569Z,1572Z,1575Z,1578Z,1581Z,1584Z,1587Z,1590Z,1593Z,1596Z,1599Z,1602Z,1605Z,1608Z,1611Z,1614Z,1617Z,1620Z,1623Z,1626Z,1629Z,1632Z,1635Z,1638Z,1641Z,1644Z,1647Z,1650Z,1653Z,1656Z,1659Z,1662Z,1665Z,1668Z,1671Z,1674Z,1677Z,1680Z,1683Z,1686Z,1689Z,1692Z,1695Z,1698Z,1701Z,1704Z,1707Z,1710Z,1713Z,1716Z,1719Z,1722Z,1725Z,1728Z,1731Z,1734Z,1737Z,1740Z,1743Z,1746Z,1749Z,1752Z,1755Z,1758Z,1761Z,1764Z,1767Z,1770Z,1773Z,1776Z,1779Z,1782Z,1785Z,1788Z,1791Z,1794Z,1797Z,1800Z,1803Z,1806Z,1809Z,1812Z,1815Z,1818Z,1821Z,1824Z,1827Z,1830Z,1833Z,1836Z,1839Z,1842Z,1845Z,1848Z,1851Z,1854Z,1857Z,1860Z,1863Z,1866Z,1869Z,1872Z,1875Z,1878Z,1881Z,1884Z,1887Z,1890Z,1893Z,1896Z,1899Z,1902Z,1905Z,1908Z,1911Z,1914Z,1917Z,1920Z,1923Z,1926Z,1929Z,1932Z,1935Z,1938Z,1941Z,1944Z,1947Z,1950Z,1953Z,1956Z,1959Z,1962Z,1965Z,1968Z,1971Z,1974Z,1977Z,1980Z,1983Z,1986Z,1989Z,1992Z,1995Z,1998Z,2001Z,2004Z,2007Z,2010Z,2013Z,2016Z,2019Z,2022Z,2025Z,2028Z,2031Z,2034Z,2037Z,2040Z,2043Z,2046Z,2049Z,2052Z,2055Z,2058Z,2061Z,2064Z,2067Z,2070Z,2073Z,2076Z,2079Z,2082Z,2085Z,2088Z,2091Z,2094Z,2097Z,2100Z,2103Z,2106Z,2109Z,2112Z,2115Z,2118Z,2121Z,2124Z,2127Z,2130Z,2133Z,2136Z,2139Z,2142Z,2145Z,2148Z,2151Z,2154Z,2157Z,2160Z,2163Z,2166Z,2169Z,2172Z,2175Z,2178Z,2181Z,2184Z,2187Z,2190Z,2193Z,2196Z,2199Z,2202Z,2205Z,2208Z,2211Z,2214Z,2217Z,2220Z,2223Z,2226Z,2229Z,2232Z,2235Z,2238Z,2241Z,2244Z,2247Z,2250Z,2253Z,2256Z,2259Z,2262Z,2265Z,2268Z,2271Z,2274Z,2277Z,2280Z,2283Z,2286Z,2289Z,2292Z,2295Z,2298Z,2301Z,2304Z,2307Z,2310Z,2313Z,2316Z,2319Z,2322Z,2325Z,2328Z,2331Z,2334Z,2337Z,2340Z,2343Z,2346Z,2349Z,2352Z,2355Z,2358Z,2361Z,2364Z,2367Z,2370Z,2373Z,2376Z,2379Z,2382Z,2385Z,2388Z,2391Z,2394Z,2397Z,2400Z,2403Z,2406Z,2409Z,2412Z,2415Z,2418Z,2421Z,2424Z,2427Z,2430Z,2433Z,2436Z,2439Z,2442Z,2445Z,2448Z,2451Z,2454Z,2457Z,2460Z,2463Z,2466Z,2469Z,2472Z,2475Z,2478Z,2481Z,2484Z,2487Z,2490Z,2493Z,2496Z,2499Z,2502Z,2505Z,2508Z,2511Z,2514Z,2517Z,2520Z,2523Z,2526Z,2529Z,2532Z,2535Z,2538Z,2541Z,2544Z,2547Z,2550Z,2553Z,2556Z,2559Z,2562Z,2565Z,2568Z,2571Z,2574Z,2577Z,2580Z,2583Z,2586Z,2589Z,2592Z,2595Z,2598Z,2601Z,2604Z,2607Z,2610Z,2613Z,2616Z,2619Z,2622Z,2625Z,2628Z,2631Z,2634Z,2637Z,2640Z,2643Z,2646Z,2649Z,2652Z,2655Z,2658Z,2661Z,2664Z,2667Z,2670Z,2673Z,2676Z,2679Z,2682Z,2685Z,2688Z,2691Z,2694Z,2697Z,2700Z,2703Z,2706Z,2709Z,2712Z,2715Z,2718Z,2721Z,2724Z,2727Z,2730Z,2733Z,2736Z,2739Z,2742Z,2745Z,2748Z,2751Z,2754Z,2757Z,2760Z,2763Z,2766Z,2769Z,2772Z,2775Z,2778Z,2781Z,2784Z,2787Z,2790Z,2793Z,2796Z,2799Z,2802Z,2805Z,2808Z,2811Z,2814Z,2817Z,2820Z,2823Z,2826Z,2829Z,2832Z,2835Z,2838Z,2841Z,2844Z,2847Z,2850Z,2853Z,2856Z,2859Z,2862Z,2865Z,2868Z,2871Z,2874Z,2877Z,2880Z,2883Z,2886Z,2889Z,2892Z,2895Z,2898Z,2901Z,2904Z,2907Z,2910Z,2913Z,2916Z,2919Z,2922Z,2925Z,2928Z,2931Z,2934Z,2937Z,2940Z,2943Z,2946Z,2949Z,2952Z,2955Z,2958Z,2961Z,2964Z,2967Z,2970Z,2973Z,2976Z,2979Z,2982Z,2985Z,2988Z,2991Z,2994Z,2997Z,3000Z,3003Z,3006Z,3009Z,3012Z,3015Z,3018Z,3021Z,3024Z,3027Z,3030Z,3033Z,3036Z,3039Z,3042Z,3045Z,3048Z,3051Z,3054Z,3057Z,3060Z,3063Z,3066Z,3069Z,3072Z,3075Z,3078Z,3081Z,3084Z,3087Z,3090Z,3093Z,3096Z,3099Z,3102Z,3105Z,3108Z,3111Z,3114Z,3117Z,3120Z,3123Z,3126Z,3129Z,3132Z,3135Z,3138Z,3141Z,3144Z,3147Z,3150Z,3153Z,3156Z,3159Z,3162Z,3165Z,3168Z,3171Z,3174Z,3177Z,3180Z,3183Z,3186Z,3189Z,3192Z,3195Z,3198Z,3201Z,3204Z,3207Z,3210Z,3213Z,3216Z,3219Z,3222Z,3225Z,3228Z,3231Z,3234Z,3237Z,3240Z,3243Z,3246Z,3249Z,3252Z,3255Z,3258Z,3261Z,3264Z,3267Z,3270Z,3273Z,3276Z,3279Z,3282Z,3285Z,3288Z,3291Z,3294Z,3297Z,3300Z,3303Z,3306Z,3309Z,3312Z,3315Z,3318Z,3321Z,3324Z,3327Z,3330Z,3333Z,3336Z,3339Z,3342Z,3345Z,3348Z,3351Z,3354Z,3357Z,3360Z,3363Z,3366Z,3369Z,3372Z,3375Z,3378Z,3381Z,3384Z,3387Z,3390Z,3393Z,3396Z,3399Z,3402Z,3405Z,3408Z,3411Z,3414Z,3417Z,3420Z,3423Z,3426Z,3429Z,3432Z,3435Z,3438Z,3441Z,3444Z,3447Z,3450Z,3453Z,3456Z,3459Z,3462Z,3465Z,3468Z,3471Z,3474Z,3477Z,3480Z,3483Z,3486Z,3489Z,3492Z,3495Z,3498Z,3501Z,3504Z,3507Z,3510Z,3513Z,3516Z,3519Z,3522Z,3525Z,3528Z,3531Z,3534Z,3537Z,3540Z,3543Z,3546Z,3549Z,3552Z,3555Z,3558Z,3561Z,3564Z,3567Z,3570Z,3573Z,3576Z,3579Z,3582Z,3585Z,3588Z,3591Z,3594Z,3597Z,3600Z,3603Z,3606Z,3609Z,3612Z,3615Z,3618Z,3621Z,3624Z,3627Z,3630Z,3633Z,3636Z,3639Z,3642Z,3645Z,3648Z,3651Z,3654Z,3657Z,3660Z,3663Z,3666Z,3669Z,3672Z,3675Z,3678Z,3681Z,3684Z,3687Z,3690Z,3693Z,3696Z,3699Z,3702Z,3705Z,3708Z,3711Z,3714Z,3717Z,3720Z,3723Z,3726Z,3729Z,3732Z,3735Z,3738Z,3741Z,3744Z,3747Z,3750Z,3753Z,3756Z,3759Z,3762Z,3765Z,3768Z,3771Z,3774Z,3777Z,3780Z,3783Z,3786Z,3789Z,3792Z,3795Z,3798Z,3801Z,3804Z,3807Z,3810Z,3813Z,3816Z,3819Z,3822Z,3825Z,3828Z,3831Z,3834Z,3837Z,3840Z,3843Z,3846Z,3849Z,3852Z,3855Z,3858Z,3861Z,3864Z,3867Z,3870Z,3873Z,3876Z,3879Z,3882Z,3885Z,3888Z,3891Z,3894Z,3897Z,3900Z,3903Z,3906Z,3909Z,3912Z,3915Z,3918Z,3921Z,3924Z,3927Z,3930Z,3933Z,3936Z,3939Z,3942Z,3945Z,3948Z,3951Z,3954Z,3957Z,3960Z,3963Z,3966Z,3969Z,3972Z,3975Z,3978Z,3981Z,3984Z,3987Z,3990Z,3993Z,3996Z,3999Z,4002Z,4005Z,4008Z,4011Z,4014Z,4017Z,4020Z,4023Z,4026Z,4029Z,4032Z,4035Z,4038Z,4041Z,4044Z,4047Z,4050Z,4053Z,4056Z,4059Z,4062Z,4065Z,4068Z,4071Z,4074Z,4077Z,4080Z,4083Z,4086Z,4089Z,4092Z,4095Z,4098Z,4101Z,4104Z,4107Z,4110Z,4113Z,4116Z,4119Z,4122Z,4125Z,4128Z,4131Z,4134Z,4137Z,4140Z,4143Z,4146Z,4149Z,4152Z,4155Z,4158Z,4161Z,4164Z,4167Z,4170Z,4173Z,4176Z,4179Z,4182Z,4185Z,4188Z,4191Z,4194Z,4197Z,4200Z,4203Z,4206Z,4209Z,4212Z,4215Z,4218Z,4221Z,4224Z,4227Z,4230Z,4233Z,4236Z,4239Z,4242Z,4245Z,4248Z,4251Z,4254Z,4257Z,4260Z,4263Z,4266Z,4269Z,4272Z,4275Z,4278Z,4281Z,4284Z,4287Z,4290Z,4293Z,4296Z,4299Z,4302Z,4305Z,4308Z,4311Z,4314Z,4317Z,4320Z,4323Z,4326Z,4329Z,4332Z,4335Z,4338Z,4341Z,4344Z,4347Z,4350Z,4353Z,4356Z,4359Z,4362Z,4365Z,4368Z,4371Z,4374Z,4377Z,4380Z,4383Z,4386Z,4389Z,4392Z,4395Z,4398Z,4401Z,4404Z,4407Z,4410Z,4413Z,4416Z,4419Z,4422Z,4425Z,4428Z,4431Z,4434Z,4437Z,4440Z,4443Z,4446Z,4449Z,4452Z,4455Z,4458Z,4461Z,4464Z,4467Z,4470Z,4473Z,4476Z,4479Z,4482Z,4485Z,4488Z,4491Z,4494Z,4497Z,4500Z,4503Z,4506Z,4509Z,4512Z,4515Z,4518Z,4521Z,4524Z,4527Z,4530Z,4533Z,4536Z,4539Z,4542Z,4545Z,4548Z,4551Z,4554Z,4557Z,4560Z,4563Z,4566Z,4569Z,4572Z,4575Z,4578Z,4581Z,4584Z,4587Z,4590Z,4593Z,4596Z,4599Z,4602Z,4605Z,4608Z,4611Z,4614Z,4617Z,4620Z,4623Z,4626Z,4629Z,4632Z,4635Z,4638Z,4641Z,4644Z,4647Z,4650Z,4653Z,4656Z,4659Z,4662Z,4665Z,4668Z,4671Z,4674Z,4677Z,4680Z,4683Z,4686Z,4689Z,4692Z,4695Z,4698Z,4701Z,4704Z,4707Z,4710Z,4713Z,4716Z,4719Z,4722Z,4725Z,4728Z,4731Z,4734Z,4737Z,4740Z,4743Z,4746Z,4749Z,4752Z,4755Z,4758Z,4761Z,4764Z,4767Z,4770Z,4773Z,4776Z,4779Z,4782Z,4785Z,4788Z,4791Z,4794Z,4797Z,4800Z,4803Z,4806Z,4809Z,4812Z,4815Z,4818Z,4821Z,4824Z,4827Z,4830Z,4833Z,4836Z,4839Z,4842Z,4845Z,4848Z,4851Z,4854Z,4857Z,4860Z,4863Z,4866Z,4869Z,4872Z,4875Z,4878Z,4881Z,4884Z,4887Z,4890Z,4893Z,4896Z,4899Z,4902Z,4905Z,4908Z,4911Z,4914Z,4917Z,4920Z,4923Z,4926Z,4929Z,4932Z,4935Z,4938Z,4941Z,4944Z,4947Z,4950Z,4953Z,4956Z,4959Z,4962Z,4965Z,4968Z,4971Z,4974Z,4977Z,4980Z,4983Z,4986Z,4989Z,4992Z,4995Z,4998Z,5001Z,5004Z,5007Z,5010Z,5013Z,5016Z,5019Z,5022Z,5025Z,5028Z,5031Z,5034Z,5037Z,5040Z,5043Z,5046Z,5049Z,5052Z,5055Z,5058Z,5061Z,5064Z,5067Z,5070Z,5073Z,5076Z,5079Z,5082Z,5085Z,5088Z,5091Z,5094Z,5097Z,5100Z,5103Z,5106Z,5109Z,5112Z,5115Z,5118Z,5121Z,5124Z,5127Z,5130Z,5133Z,5136Z,5139Z,5142Z,5145Z,5148Z,5151Z,5154Z,5157Z,5160Z,5163Z,5166Z,5169Z,5172Z,5175Z,5178Z,5181Z,5184Z,5187Z,5190Z,5193Z,5196Z,5199Z,5202Z,5205Z,5208Z,5211Z,5214Z,5217Z,5220Z,5223Z,5226Z,5229Z,5232Z,5235Z,5238Z,5241Z,5244Z,5247Z,5250Z,5253Z,5256Z,5259Z,5262Z,5265Z,5268Z,5271Z,5274Z,5277Z,5280Z,5283Z,5286Z,5289Z,5292Z,5295Z,5298Z,5301Z,5304Z,5307Z,5310Z,5313Z,5316Z,5319Z,5322Z,5325Z,5328Z,5331Z,5334Z,5337Z,5340Z,5343Z,5346Z,5349Z,5352Z,5355Z,5358Z,5361Z,5364Z,5367Z,5370Z,5373Z,5376Z,5379Z,5382Z,5385Z,5388Z,5391Z,5394Z,5397Z,5400Z,5403Z,5406Z,5409Z,5412Z,5415Z,5418Z,5421Z,5424Z,5427Z,5430Z,5433Z,5436Z,5439Z,5442Z,5445Z,5448Z,5451Z,5454Z,5457Z,5460Z,5463Z,5466Z,5469Z,5472Z,5475Z,5478Z,5481Z,5484Z,5487Z,5490Z,5493Z,5496Z,5499Z,5502Z,5505Z,5508Z,5511Z,5514Z,5517Z,5520Z,5523Z,5526Z,5529Z,5532Z,5535Z,5538Z,5541Z,5544Z,5547Z,5550Z,5553Z,5556Z,5559Z,5562Z,5565Z,5568Z,5571Z,5574Z,5577Z,5580Z,5583Z,5586Z,5589Z,5592Z,5595Z,5598Z,5601Z,5604Z,5607Z,5610Z,5613Z,5616Z,5619Z,5622Z,5625Z,5628Z,5631Z,5634Z,5637Z,5640Z,5643Z,5646Z,5649Z,5652Z,5655Z,5658Z,5661Z,5664Z,5667Z,5670Z,5673Z,5676Z,5679Z,5682Z,5685Z,5688Z,5691Z,5694Z,5697Z,5700Z,5703Z,5706Z,5709Z,5712Z,5715Z,5718Z,5721Z,5724Z,5727Z,5730Z,5733Z,5736Z,5739Z,5742Z,5745Z,5748Z,5751Z,5754Z,5757Z,5760Z,57

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-phosphatidylcholine; Hyphenated Tools for Lipidomics; Jan Willmann¹, Herbert Thiele², Dieter Leibfritz¹; HUPO 2007, Poster M-195

5 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 326 spectra]

File Search View Tools Options Window Help

Go 1. Bruker microTOF qQ-TOF: NA

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH ₄] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF/TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF/TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF/TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF/TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(11E))
2	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(11Z))
3	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(13Z))
4	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(17Z))
5	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(4E))
6	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(6Z))
7	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(7Z))
8	lipidblast-neg	86	676	2.37	700	PE 36:1; [M-H] ⁻ ; GPEtn(18:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 s
5 largest peaks:
281.0 999.00 | 480.1 400.00 | 744.4 150.00 | 506.1 100.00 | 462.1 50.00

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
6 largest peaks:
281.24790 999.00 | 283.26354 999.00 | 478.24790 50.00 | 462.29859 50.00

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 22 spectra]

File Search View Tools Options Window Help

Go 1. Bruker ultraflex II MALDI TOF/TOF: [H]

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DG DG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DG DG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DG DG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex extreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex extreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	230	753	24.0	765	SM 34:1; [M+Na] ⁺ ; SM(d14:1(4E)/20:0)
2	lipidblast-pos	230	753	24.0	765	SM 34:1; [M+Na] ⁺ ; SM(d16:0/18:1(9Z))
3	lipidblast-pos	230	753	24.0	765	SM 34:1; [M+Na] ⁺ ; SM(d16:1(4E)/18:0)
4	lipidblast-pos	230	753	24.0	765	SM 34:1; [M+Na] ⁺ ; SM(d18:1(4E)/16:0)
5	lipidblast-neg	3	397	0.24	438	PI 26:0; [M-H] ⁻ ; GPLns(12:0/14:0)
6	lipidblast-neg	3	397	0.24	438	PI 26:0; [M-H] ⁻ ; GPLns(14:0/12:0)
7	lipidblast-pos	0	38	0.21	175	DG 43:2; [M+Li] ⁺ ; DG(17:0/26:2/0:0)
8	lipidblast-pos	0	38	0.21	175	DG 43:2; [M+Li] ⁺ ; DG(17:1/26:1/0:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
542.5 999.00 | 666.5 800.00 | 725.6 300.00 | 147.0 50.00 |
4 m/z Values and Intensities:

(Spec. List) Bruker ultraflex II

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)
MW: 725 ID#: 70249 DB: lipidblast-pos
Comment: Parent=725.55733 Mz_exact=725.5573
2 largest peaks:
666.48383 999.00 | 542.49129 20.00 |
2 m/z Values and Intensities:
542.49129 20.00 [M+Na]⁺-C5H14NO4P (-183)
666.48383 999.00 [M+Na]⁺-C3H9N (-59)

(lipidblast-pos) SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 5 spectra]

File Search View Tools Options Window Help

1. Bruker UltraFlex II MALDI TOF-TOF; [M+Na]⁺; DGDG 30:0

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH ₄] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	71	548	59.4	707	DGDG 30:0; [M+Na] ⁺ ; DGDG(15:0/15:0)
2	lipidblast-neg	9	131	10.2	438	PI 38:3; [M-H] ⁻ ; GPIIns(18:3(6Z,9Z,12Z)/20:0)
3	lipidblast-neg	9	131	10.2	438	PI 38:3; [M-H] ⁻ ; GPIIns(18:3(9Z,12Z,15Z)/20:0)
4	lipidblast-neg	9	131	10.2	438	PI 38:3; [M-H] ⁻ ; GPIIns(20:0/18:3(6Z,9Z,12Z))
5	lipidblast-neg	9	131	10.2	438	PI 38:3; [M-H] ⁻ ; GPIIns(20:0/18:3(9Z,12Z,15Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
645.4 999.00 | 887.7 500.00 | 323.1 200.00 | 382.2 200.00 | 627.4 150.00 | 731.1 100.00

(Spec. List) Bruker UltraFlex II MALDI TOF-TOF; [M+Na]⁺; DGDG 30:0

Name: DGDG 30:0; [M+Na]⁺; DGDG(15:0/15:0)
MW: 887 **ID#:** 4747 **DB:** lipidblast-pos
Comment: Parent=887.57077 Mz_exact=887.57077
2 largest peaks:
483.29351 999.00 | 645.34633 999.00 |
2 m/z Values and Intensities:
483.29351 999.00 [M+Na]-sn1-C6H10O5 (-162) |
645.34633 999.00 [M+Na]-sn1 || [M+Na]-sn2

(lipidblast-pos) DGDG 30:0; [M+Na]⁺; DGDG(15:0/15:0)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 15 spectra]

File Search View Tools Options Window Help

1. Bruker UltraFlex II MALDI TOF-TOF; I

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	219	504	38.8	697	DGDG 31:0; [M+Na] ⁺ ; DGDG(15:0/16:0)
2	lipidblast-pos	219	504	38.8	697	DGDG 31:0; [M+Na] ⁺ ; DGDG(16:0/15:0)
3	lipidblast-pos	165	417	7.59	707	TG 54:6; [M+Na] ⁺ ; TG(16:0/16:0/22:6)
4	lipidblast-pos	125	340	1.76	577	TG 55:5; [M+Li] ⁺ ; TG(16:0/17:0/22:5)
5	lipidblast-pos	125	340	1.76	577	TG 55:5; [M+Li] ⁺ ; TG(16:0/17:1/22:4)
6	lipidblast-pos	125	340	1.76	577	TG 55:5; [M+Li] ⁺ ; TG(16:0/17:2/22:3)
7	lipidblast-pos	125	340	1.76	577	TG 55:5; [M+Li] ⁺ ; TG(16:0/19:0/20:5)
8	lipidblast-pos	125	340	1.76	577	TG 54:6; [M+Na] ⁺ ; TG(16:0/16:1/22:5)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
645.4 999.00 | 901.7 800.00 | 551.4 600.00 | 659.4 500.00 | 327.1 300.00 | 745.2 300.00 | 523.4 100.00 | 405.2 50.00

(Spec. List) Bruker UltraFlex II

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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:
645.4 999.00 | 901.7 800.00 | 551.4 600.00 | 659.4 500.00 | 327.1 300.00 | 745.2 300.00 | 523.4 100.00 | 405.2 50.00

▲ Bruker UltraFlex II MALDI TOF-TOF; Head to Tail MF=219 RMF=504 ▼ DGDG 31:0; [M+Na]⁺; DGDG(15:0/16:0)

Difference Head to Tail Side by Side Subtraction 219 504R 38.8P

Name: DGDG 31:0; [M+Na]⁺; DGDG(15:0/16:0)
MW: 901 ID#: 4749 DB: lipidblast-pos
Comment: Parent=901.58647 Mz_exact=901.5864
4 largest peaks:
483.29357 999.00 | 497.30921 999.00 | 645.3 999.00 | 497.30921 999.00
4 m/z Values and Intensities:
483.29357 999.00 [M+Na]-sn2-C6H10O5 (-162)
497.30921 999.00 [M+Na]-sn1-C6H10O5 (-162)

(lipidblast-pos) DGDG 31:0; [M+Na]⁺; DGDG(15:0/16:0)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 18 spectra]

File Search View Tools Options Window Help

1. Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH ₄] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	94	679	28.8	697	DGDG 32:0; [M+Na] ⁺ ; DGDG(15:0/17:0)
2	lipidblast-pos	94	679	28.8	697	DGDG 32:0; [M+Na] ⁺ ; DGDG(17:0/15:0)
3	lipidblast-pos	59	562	7.23	707	TG 56:5; [M+Li] ⁺ ; TG(17:0/17:0/22:5)
4	lipidblast-pos	40	459	3.51	577	TG 56:5; [M+Li] ⁺ ; TG(17:0/17:1/22:4)
5	lipidblast-pos	40	459	3.51	577	TG 56:5; [M+Li] ⁺ ; TG(17:0/17:2/22:3)
6	lipidblast-pos	40	459	3.51	577	TG 56:5; [M+Li] ⁺ ; TG(17:0/19:0/20:5)
7	lipidblast-pos	40	459	3.51	577	TG 55:6; [M+Na] ⁺ ; TG(16:0/17:0/22:6)
8	lipidblast-pos	40	459	3.51	577	TG 55:6; [M+Na] ⁺ ; TG(16:1/17:0/22:5)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
645.4 999.00 | 673.4 500.00 | 915.7 400.00 | 405.2 50.00 | 758.9 20.00
5 m/z Values and Intensities:

Name: DGDG 32:0; [M+Na]⁺; DGDG(15:0/17:0)
MW: 915 ID#: 4752 DB: lipidblast-pos
Comment: Parent=915.60207 Mz_exact=915.60207
4 largest peaks:
483.29353 999.00 | 511.32481 999.00 | 645.34635 999.00 | 673.4 500.00
4 m/z Values and Intensities:
483.29353 999.00 [M+Na]-sn2-C6H1005 (-162)
511.32481 999.00 [M+Na]-sn1-C6H1005 (-162)

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 266 spectra]

File Search View Tools Options Window Help

60 1. Bruker UltraFlex II MALDI TOF-TOF; [M+K]⁺; PC 36:1

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS, [M+NH4] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS, [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS, [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	146	537	2.08	657	PC 40:10; [M+H] ⁺ ; GPCho(20:5(5Z,8Z,11Z,14Z...
2	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(16:1(7Z)/22:6(4Z,7Z...
3	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(16:1(9Z)/22:6(4Z,7Z...
4	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(18:2(2E,4E)/20:5(5Z...
5	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(18:2(6Z,9Z)/20:5(5Z...
6	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(18:2(9E,10E)/20:5(5Z...
7	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(18:2(9E,12E)/20:5(5Z...
8	lipidblast-pos	126	531	0.95	754	PC 38:7; [M+Na] ⁺ ; GPCho(18:2(9Z,11Z)/20:5(5Z...

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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-C...
4 largest peaks:
767.4 999.00 | 163.1 700.00 | 826.3 600.00 | 184.2 300.00 |
4 m/z Values and Intensities:

(Spec. List) Bruker UltraFlex II

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 40:10; [M+H]⁺; GPCho(20:5(5Z,8Z,11Z,14Z...
MW: 826 ID#: 3546 DB: custompc+hpos.msp
Comment: Parent=826.53870 Mz_exact=826.5387
7 largest peaks:
184.07387 999.00 | 524.31426 200.00 | 542.3...
826.53870 200.00 | 808.52814 10.00 |
7 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 40:10; [M+H]⁺; GPCho(20:5(5Z...

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 6 spectra]

File Search View Tools Options Window Help

1. Bruker UltraFlex II MALDI TOF-TOF; [M+Na]⁺; SM(d18:1/16:0)

#	Src.	Name
45	L	Bruker Esquire ion trap; ESI MS/MS; [M+NH ₄] ⁺ ; NA
46	L	Bruker Esquire ion trap; ESI MS/MS; [M-H] ⁻ ; MGDG 38:9
47	L	Bruker Esquire ion trap; ESI MS/MS; [M+Na] ⁺ ; MGDG 38:9
48	L	Bruker microTOF qQ-TOF; NA
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflex Xtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	271	831	24.9	879	SM 34:1; [M+Na] ⁺ ; SM(d14:1(4E)/20:0)
2	lipidblast-pos	271	831	24.9	879	SM 34:1; [M+Na] ⁺ ; SM(d16:0/18:1(9Z))
3	lipidblast-pos	271	831	24.9	879	SM 34:1; [M+Na] ⁺ ; SM(d16:1(4E)/18:0)
4	lipidblast-pos	271	831	24.9	879	SM 34:1; [M+Na] ⁺ ; SM(d18:1(4E)/16:0)
5	lipidblast-neg	33	336	0.24	438	PI 26:0; [M-H] ⁻ ; GPIs(12:0/14:0)
6	lipidblast-neg	33	336	0.24	438	PI 26:0; [M-H] ⁻ ; GPIs(14:0/12:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Bruker UltraFlex II MALDI TOF-TOF; [M+Na]⁺; SM(d18:1/16:0)
 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;
 4 largest peaks:
 666.5 999.00 | 542.5 550.00 | 184.0 180.00 | 722.5 100.00 |
 4 m/z Values and Intensities:

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

(lipidblast-pos) SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)
 Name: SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)
 MW: 725 ID#: 70249 DB: lipidblast-pos
 Comment: Parent=725.55733 Mz_exact=725.55733
 2 largest peaks:
 666.48383 999.00 | 542.49129 20.00 |
 2 m/z Values and Intensities:
 542.49129 20.00 [M+Na]⁺-C5H14NO4P (-183)
 666.48383 999.00 [M+Na]⁺-C3H9N (-59)

▲ Bruker UltraFlex II MALDI TOF-TOF; Head to Tail MF=271 RMF=831 ▼ SM 34:1; [M+Na]⁺; SM(d14:1(4E))
 Difference Head to Tail Side by Side Subtraction 271 831R 24.9P

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.pdf
6 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 31 spectra]

File Search View Tools Options Window Help

60 1. Bruker ultrafleXtreme MALDI TOF/TO

#	Src.	Name
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	ISOL_MALDI_11104_11104_Tandem_MS_FAB_MALDI_DGDG_30:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
11	custompc+h...	121	581	6.83	737	PC 17:0; [M+H] ⁺ ; GPCho(12:0/5:0)
12	custompc+h...	121	581	6.83	737	PC 17:0; [M+H] ⁺ ; GPCho(13:0/4:0)
13	custompc+h...	121	581	6.83	737	PC 17:0; [M+H] ⁺ ; GPCho(14:0/3:0)
14	custompc+h...	121	581	6.83	737	PC 17:0; [M+H] ⁺ ; GPCho(15:0/2:0)
15	lipidblast-pos	51	374	0.99	481	lysoPC 18:0; [M+H] ⁺ ; PC(18:0/0:0)
16	lipidblast-pos	6	72	0.21	309	PC 17:0; [M+H] ⁺ ; GPCho(2:0/15:0)
17	lipidblast-pos	6	72	0.21	309	PC 17:0; [M+H] ⁺ ; GPCho(3:0/14:0)
18	lipidblast-pos	6	72	0.21	309	PC 17:0; [M+H] ⁺ ; GPCho(4:0/13:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

(Spec. List) Bruker ultrafleXtr

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 Perf
6 largest peaks:
184.08 999.00 | 104.10 600.00 | 524.38 300.00 | 487.10 200.00 | 258.341.25 100.00 |

(lipidblast-pos) lysoPC 18:0; [M+H]⁺; PC(18:0/0:0)

Name: lysoPC 18:0; [M+H]⁺; PC(18:0/0:0)
MW: 524 ID#: 9197 DB: lipidblast-pos
Comment: Parent=524.37159 Mz_exact=524.3715
4 largest peaks:
506.36103 999.00 | 184.07387 300.00 | 240.11
4 m/z Values and Intensities:
184.07387 300.00 C5H15NO4P m/z=184
240.10023 10.00 [M+H]⁺-sn1-H2O

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 187 spectra]

File Search View Tools Options Window Help

60 1. Bruker ultrafleXtreme MALDI TOF/TO

#	Src.	Name
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(8:0/26:1(5Z))
2	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(10:0/24:1(15Z))
3	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(12:0/22:1(13Z))
4	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(14:0/20:1(11E))
5	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(14:0/20:1(11Z))
6	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(14:0/20:1(13E))
7	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(14:0/20:1(13Z))
8	custompc+h...	25	683	0.93	737	PC 34:1; [M+H] ⁺ ; GPCho(14:1(9Z)/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Bruker ultrafleXtr

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]⁺; ultrafleXtrr
 8 largest peaks:
 184.06 999.00 | 146.97 100.00 | 577.33 100.00 | 760.59 100.00 | 104.301.26 20.00 | 379.06 20.00 | 467.19 20.00

(custompc+hpos.msp) PC 34:1; [M+H]⁺; GPCho(8:0/26:1(5Z))

Name: PC 34:1; [M+H]⁺; GPCho(8:0/26:1(5Z))
 MW: 760 ID#: 1918 DB: custompc+hpos.msp
 Comment: Parent=760.58564 Mz_exact=760.5856
 9 largest peaks:
 184.07387 999.00 | 366.20480 200.00 | 384.2634.48124 200.00 | 701.51214 200.00 | 760.58564 100.00
 9 m/z Values and Intensities:
 184.07387 999.00 fragment C5H15NO4P

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 297 spectra]

File Search View Tools Options Window Help

60 1. Bruker ultrafleXtreme MALDI TOF/TO

#	Src.	Name
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	ISOL_MALDI1104_11104_Tandem_MS_FAB_BALLI_DGDG_30:4

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[2E,4
2	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[6Z,9
3	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9E,1
4	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9E,1
5	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9Z,1
6	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[2E,4E])/18:2[9Z,1
7	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[6Z,9Z])/18:2[2E,4
8	custompc+h...	269	744	2.11	882	PC 36:4; [M+H] ⁺ ; GPCho(18:2[6Z,9Z])/18:2[6Z,9

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Bruker ultrafleXtr...

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]⁺; ultrafleXtr
 10 largest peaks:
 184.1 999.00 | 147.0 200.00 | 599.5 200.00 | 723.5 200.00 | 577.5 18
 782.6 150.00 | 614.2 100.00 | 86.1 50.00 | 198.1 20.00 | 467.3 2

▲ Bruker ultrafleXtreme MALDI TOF/... Head to Tail MF=269 RMF=744 ▼ PC 36:4; [M+H]⁺; GPCho(18:2[2E

Difference Head to Tail Side by Side Subtraction 269 744 R 2.11 P

Name: PC 36:4; [M+H]⁺; GPCho(18:2[2E,4E])/18:2
 MW: 782 ID#: 2356 DB: custompc+hpos.msp
 Comment: Parent=782.56995 Mz_exact=782.5699
 7 largest peaks:
 184.07387 999.00 | 502.32987 200.00 | 520.3
 782.56995 200.00 | 764.55939 10.00 |
 7 m/z Values and Intensities:
 184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 36:4; [M+H]⁺; GPCho(18:2[2E

Name: PC 36:4; [M+H]⁺; GPCho(18:2[2E,4E])/18:2
 MW: 782 ID#: 2356 DB: custompc+hpos.msp
 Comment: Parent=782.56995 Mz_exact=782.5699
 7 largest peaks:
 184.07387 999.00 | 502.32987 200.00 | 520.3
 782.56995 200.00 | 764.55939 10.00 |
 7 m/z Values and Intensities:
 184.07387 999.00 fragment C5H15NO4P

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 155 spectra]

File Search View Tools Options Window Help

60 1. Bruker ultrafleXtreme MALDI TOF/TO

#	Src.	Name
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(7:0/26:1(5Z))
2	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(9:0/24:1(15Z))
3	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(11:0/22:1(13Z))
4	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(13:0/20:1(11E))
5	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(13:0/20:1(11Z))
6	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(13:0/20:1(13E))
7	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(13:0/20:1(13Z))
8	lipidblast-pos	69	460	1.46	989	PE 33:1; [M+Na] ⁺ ; GPEtn(14:1(9Z)/19:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Bruker ultrafleXtr

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;
 6 largest peaks:
 164.0 999.00 | 726.5 500.00 | 683.5 450.00 | 563.5 300.00 | 585.5 300.00 | 121.0 100.00

(lipidblast-pos) PE 33:1; [M+Na]⁺; GPEtn(7:0/26:1(5Z))

Name: PE 33:1; [M+Na]⁺; GPEtn(7:0/26:1(5Z))
 MW: 726 ID#: 53889 DB: lipidblast-pos
 Comment: Parent=726.50497 Mz_exact=726.50497
 4 largest peaks:
 683.46277 999.00 | 585.48587 400.00 | 289.08193 3.00 | 553.36345 3.00
 4 m/z Values and Intensities:
 683.46277 999.00 [M+Na]⁺-43-SN2-H
 553.36345 3.00 [M+Na]⁺-43-SN1-H

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 32 spectra]

File Search View Tools Options Window Help

Go 1. Bruker ultrafleXtreme MALDI TOF/TO

#	Src.	Name
49	L	Bruker ultraflex II MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
50	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; DGDG 30:0
51	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 31:0
52	L	Bruker UltraFlex II MALDI TOF-TOF; DGDG 32:0
53	L	Bruker UltraFlex II MALDI TOF-TOF; [M+K] ⁺ ; PC 36:1
54	L	Bruker UltraFlex II MALDI TOF-TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	270	819	24.5	889	SM 34:1; [M+Na] ⁺ ; SM(d14:1(4E)/20:0)
2	lipidblast-pos	270	819	24.5	889	SM 34:1; [M+Na] ⁺ ; SM(d16:0/18:1(9Z))
3	lipidblast-pos	270	819	24.5	889	SM 34:1; [M+Na] ⁺ ; SM(d16:1(4E)/18:0)
4	lipidblast-pos	270	819	24.5	889	SM 34:1; [M+Na] ⁺ ; SM(d18:1(4E)/16:0)
5	lipidblast-neg	49	315	0.24	438	PI 26:0; [M-H] ⁻ ; GPLns(12:0/14:0)
6	lipidblast-neg	49	315	0.24	438	PI 26:0; [M-H] ⁻ ; GPLns(14:0/12:0)
7	lipidblast-pos	5	42	0.05	175	DG 43:2; [M+Li] ⁺ ; DG(17:0/26:2/0:0)
8	lipidblast-pos	5	42	0.05	175	DG 43:2; [M+Li] ⁺ ; DG(17:1/26:1/0:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

(Spec. List) Bruker ultrafleXtr

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
 10 largest peaks:
 666.6 999.00 | 542.53 500.00 | 725.6 300.00 | 86.11 200.00 | 168.198.09 10.00 | 320.84 10.00 | 429.62 10.00 | 502.47 10.00 | 630.5

(lipidblast-pos) SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)

Name: SM 34:1; [M+Na]⁺; SM(d14:1(4E)/20:0)
 MW: 725 ID#: 70249 DB: lipidblast-pos
 Comment: Parent=725.55733 Mz_exact=725.5573
 2 largest peaks:
 666.48383 999.00 | 542.49129 20.00 |
 2 m/z Values and Intensities:
 542.49129 20.00 [M+Na]⁺-C5H14NO4P (-183)
 666.48383 999.00 [M+Na]⁺-C3H9N (-59)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 58 spectra]

File Search View Tools Options Window Help

1. JEOL JMS-HX110A/110A Tandem MS

#	Src.	Name
55	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultraflexxtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU MALDI TOF; [M+H] ⁺ ; PC 36:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[2E,4E]
2	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[6Z,9E]
3	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[9E,9E]
4	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[9E,9E]
5	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[9Z,9Z]
6	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[2E,4E])/18:2[9Z,9Z]
7	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[6Z,9Z])/18:2[2E,4E]
8	lipidblast-neg	133	824	2.71	1e+3	DGDG 36:4; [M-H] ⁻ ; DGDG(18:2[6Z,9Z])/18:2[6Z,9Z]

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]⁻; DGDG 36:4

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:
 279 999.00 | 939 999.00 | 397 100.00 | 659 100.00 | 677 100.00 |
 21 50.00 | 179 50.00 | 415 50.00

(lipidblast-neg) DGDG 36:4; [M-H]⁻; DGDG(18:2[2E,4E])/18:2[2E,4E]

Name: DGDG 36:4; [M-H]⁻; DGDG(18:2[2E,4E])/18:2[2E,4E]
 MW: 939 ID#: 76174 DB: lipidblast-neg
 Comment: Parent=939.60448 Mz_exact=939.6044
 1 largest peaks:
 279.23226 999.00 |
 1 m/z Values and Intensities:
 279.23226 999.00 sn1 FA || sn2 FA
 Synonyms:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 1 spectrum]

File Search View Tools Options Window Help

Go 1. JEOL JMS-HX110A/110A Tandem MS

#	Src.	Name
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	116	374	100.0	824	[glycan]-Cer 34:1; GM3(d18:1/16:0); [M-H] ⁻ ; NeuAc

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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:
297.2 999.00 | 1151.7 999.00 | 295.2 500.00 | 468.1 200.00 | 599.3 200.00
860.8 120.00 | 536 100.00 | 698 100.00 | 1031.7 100.00

(Spec. List) JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]⁻; GM3

JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]⁻; GM3
Head to Tail MF=116 RMF=374
[glycan]-Cer 34:1; GM3(d18:1/16:0)
Difference Head to Tail Side by Side Subtraction 116 374R 100.0P

[glycan]-Cer 34:1; GM3(d18:1/16:0); [M-H]⁻
MW: 1151 ID#: 79290 DB: lipidblast-neg
Comment: Parent=1151.70534 Mz_exact=1151.70534
5 largest peaks:
1151.70534 999.00 | 860.60993 500.00 | 295.2 500.00
5 m/z Values and Intensities:
290.08759 400.00 ion C11H16NO8- (290.08759)
536.50395 200.00 ion ceramide

(lipidblast-neg) [glycan]-Cer 34:1; GM3(d18:1/16:0); [M-H]⁻

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 184 spectra]

File Search View Tools Options Window Help

Go 1. JEOL JMS-HX110A/110A Tandem M⁻

#	Src.	Name
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU MALDI-TOF; [M+H] ⁺ ; PC 33:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[2E,4E]
2	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[2E,4E]
3	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[9E,9E]
4	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[9E,9E]
5	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[9E,9E]
6	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[2E,4E])/18:2[9E,9E]
7	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[6Z,9Z])/18:2[2E,4E]
8	lipidblast-neg	46	912	1.53	1e+3	MGDG 36:4; [M-H] ⁻ ; MGDG(18:2[6Z,9Z])/18:2[2E,4E]

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

(Spec. List) JEOL JMS-HX110A/110A

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; St
 4 largest peaks:
 279 999.00 | 777 999.00 | 515 100.00 | 253 80.00 |
 4 m/z Values and Intensities:

JEOL JMS-HX110A/110A Tande

Name: MGDG 36:4; [M-H]⁻; MGDG(18:2[2E,4E])/18:2[2E,4E]
 MW: 777 ID#: 98235 DB: lipidblast-neg
 Comment: Parent=777.55168 Mz_exact=777.55168
 1 largest peaks:
 279.23226 999.00 |
 1 m/z Values and Intensities:
 279.23226 999.00 sn1 FA | sn2 FA
 Synonyms:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 12 spectra]

File Search View Tools Options Window Help

1. JEOL JMS-HX110A/110A Tandem MS

#	Src.	Name
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:6

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(19:0/20:4)(5E,8E,11E,14E)
2	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(19:0/20:4)(5Z,8Z,11Z,14Z)
3	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(19:0/20:4)(7E,10E,13E,16E)
4	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(20:4)(5E,8E,11E,14E)
5	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(20:4)(5Z,8Z,11Z,14Z)
6	lipidblast-neg	36	341	11.4	707	MGDG 39:4; [M-H] ⁻ ; MGDG(20:4)(7E,10E,13E,16E)
7	lipidblast-neg	26	269	8.03	559	PG 39:0; [M-H] ⁻ ; GPGro(19:0/20:0)
8	lipidblast-neg	26	269	8.03	559	PG 39:0; [M-H] ⁻ ; GPGro(20:0/19:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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);
6 largest peaks:
148 999.00 | 819 500.00 | 297 400.00 | 80 150.00 | 208 150.00 | 793 100.00

(Spec. List) JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H]⁻; NA

Name: SQDG 34:1; [M-H]⁻; SQDG(15:1)(9Z)/19:0
MW: 819 ID#: 129712 DB: lipidblast-neg
Comment: Parent=819.52923 Mz_exact=819.52923
5 largest peaks:
225.00690 999.00 | 521.24223 300.00 | 579.30000 100.00
5 m/z Values and Intensities:
225.00690 999.00 fragment C6H9O7S
239.20098 100.00 sn1 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 126 spectra]

File Search View Tools Options Window Help

60 1. Kratos MALDI-TOF AXIMA-CFR; [M-H]⁻

#	Src.	Name
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysoPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU MALDI TOF; [M+H] ⁺ ; PC 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [14/14/18/18/30-1
2	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [16/16/14/18/30-1
3	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [16/16/16/16/30-1
4	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [16/16/18/14/30-1
5	lipidblast-neg	13	117	0.85	198	LipidA-PP 68:32:0; LipidA-PP [16/16/18/18/30-1
6	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [18/18/10/18/30-1
7	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [18/18/12/16/30-1
8	lipidblast-neg	13	117	0.85	198	LipidA-PP 64:36:0; LipidA-PP [18/18/14/14/30-1

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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 Requ
 3 largest peaks:
 2048.6 999.00 | 2021.2 700.00 | 2071.1 300.00 |
 3 m/z Values and Intensities:

(Spec. List) Kratos MALDI-TOF

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: LipidA-PP 64:36:0; LipidA-PP [14/14/18/18/30-1
 MW: 2048 ID#: 88254 DB: lipidblast-neg
 Comment: Parent=2048.49327 Mz_exact=2048.49
 7 largest peaks:
 1804.28955 999.00 | 1950.51637 600.00 | 204
 1764.22191 250.00 | 1966.51129 50.00 |
 7 m/z Values and Intensities:
 1666.24501 300.00 [M-H]⁻; PO4H3-R2'-O-FA || [M-

(lipidblast-neg) LipidA-PP 64:36:0; LipidA-PP [14/14/18/18/30-1

Plot/Text of Hit Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 92 spectra]

File Search View Tools Options Window Help

MS m/z

1. SHIMADZU KRATOS MALDI TRAP TOF

#	Src.	Name
55	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; lysPC 18:0
56	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+H] ⁺ ; PC 34:1
57	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PC 36:1
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	682	922	35.7	923	SQDG 36:5; [M-H] ⁻ ; SQDG(16:0/20:5(5Z,8Z,11Z,14Z,17Z,20:4(7E,10E,13E,16E,19E)))
2	lipidblast-neg	682	922	35.7	923	SQDG 36:5; [M-H] ⁻ ; SQDG(20:5(5Z,8Z,11Z,14Z,17Z,20:4(7E,10E,13E,16E,19E)))
3	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(14:0/22:5(4Z,7Z,10Z,13Z,16Z,19Z,22:4(5E,8E,11E,14E,17E,20:4(7E,10E,13E,16E,19E))))
4	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(14:0/22:5(7Z,10Z,13Z,16Z,19Z,22:4(7Z,10Z,13Z,16Z,19Z,22:4(5E,8E,11E,14E,17E,20:4(7E,10E,13E,16E,19E))))
5	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(14:1(9Z)/22:4(7Z,10Z,13Z,16Z,19Z,22:4(5E,8E,11E,14E,17E,20:4(7E,10E,13E,16E,19E))))
6	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(16:1(7Z)/20:4(5E,8E,11E,14E,17E,20:4(7E,10E,13E,16E,19E)))
7	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(16:1(7Z)/20:4(5Z,8Z,11Z,14Z,17Z,20:4(7E,10E,13E,16E,19E)))
8	lipidblast-neg	148	491	0.35	745	SQDG 36:5; [M-H] ⁻ ; SQDG(16:1(7Z)/20:4(7E,10E,13E,16E,19E,22:4(5E,8E,11E,14E,17E,20:4(7E,10E,13E,16E,19E))))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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: 224.8 999.00 | 537.3 800.00 | 583.3 500.00 |
3 m/z Values and Intensities:

Name: SQDG 36:5; [M-H]⁻; SQDG(16:0/20:5(5Z,8Z,11Z,14Z,17Z,20:4(7E,10E,13E,16E,19E)))
MW: 839 ID#: 129799 DB: lipidblast-neg
Comment: Parent=839.49792 Mz_exact=839.49792
5 largest peaks: 225.00690 999.00 | 537.27348 300.00 | 583.27348 100.00 | 225.00690 999.00 fragment C6H9O7S
255.23226 100.00 sn1 FA

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 120 spectra]

File Search View Tools Options Window Help

Go 1. SHIMADZU LCMS-IT-TOF; [M-H]⁻; PS 32:0

#	Src.	Name
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	828	963	79.3	964	PS 32:0; [M-H] ⁻ ; GPSer(16:0/16:0)
2	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(6:0/26:0)
3	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(7:0/25:0)
4	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(8:0/24:0)
5	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(9:0/23:0)
6	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(10:0/22:0)
7	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(11:0/21:0)
8	lipidblast-neg	136	466	0.79	707	PS 32:0; [M-H] ⁻ ; GPSer(12:0/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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); Ident
4 largest peaks:
647.4381 999.00 | 391.2107 750.00 | 409.2167 300.00 | 255.2200 250.00
4 m/z Values and Intensities:

Name: PS 32:0; [M-H]⁻; GPSer(16:0/16:0)
MW: 734 ID#: 124637 DB: lipidblast-neg
Comment: Parent=734.49718 Mz_exact=734.4971
4 largest peaks:
647.46515 999.00 | 391.22507 200.00 | 409.2167 200.00
4 m/z Values and Intensities:
255.23226 100.00 sn1 FA || sn2 FA
391.22507 200.00 [M-H-87]-sn1 || [M-H-87]-sn2

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 Chloroplatic 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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 12 spectra]

File Search View Tools Options Window Help

1. SHIMADZU LCMS-IT-TOF; [M-H]⁻; SQDG 34:3

#	Src.	Name
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	147	619	23.1	619	SQDG 34:3; [M-H] ⁻ ; SQDG(16:0/18:3(6Z,9Z,12Z,15Z)/16:1)
2	lipidblast-neg	147	619	23.1	619	SQDG 34:3; [M-H] ⁻ ; SQDG(16:0/18:3(9Z,12Z,15Z)/16:1)
3	lipidblast-neg	147	619	23.1	619	SQDG 34:3; [M-H] ⁻ ; SQDG(18:3(6Z,9Z,12Z)/16:1)
4	lipidblast-neg	147	619	23.1	619	SQDG 34:3; [M-H] ⁻ ; SQDG(18:3(9Z,12Z,15Z)/16:1)
5	lipidblast-neg	23	181	1.07	250	PG 40:9; [M-H] ⁻ ; GPGro(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z))
6	lipidblast-neg	23	181	1.07	250	PG 40:9; [M-H] ⁻ ; GPGro(18:3(9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z))
7	lipidblast-neg	23	181	1.07	250	PG 40:9; [M-H] ⁻ ; GPGro(22:6(4Z,7Z,10Z,13Z,16Z))
8	lipidblast-neg	23	181	1.07	250	PG 40:9; [M-H] ⁻ ; GPGro(22:6(4Z,7Z,10Z,13Z,16Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 Chloroplatic UDP-Glucose Pyrophosphorylase from Arabidopsis Is the Committed Enzyme for the First Step of Sulfolipid Biosynthesis; Plant Cell Okazaki et al. 21: 892 ;
3 largest peaks:
537.267 999.00 | 559.258 600.00 | 255.009 300.00 |
3 m/z Values and Intensities:

Name: SQDG 34:3; [M-H]⁻; SQDG(16:0/18:3(6Z,9Z,12Z,15Z)/16:1)
MW: 815 ID#: 129782 DB: lipidblast-neg
Comment: Parent=815.49792 Mz_exact=815.49792
5 largest peaks:
225.00690 999.00 | 537.27348 300.00 | 559.27348 100.00 | 255.23226 100.00 | sn1 FA
5 m/z Values and Intensities:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 51 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan DecaXP ion trap; [M+Na]⁺

#	Src.	Name
58	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; PE 33:1
59	L	Bruker ultrafleXtreme MALDI TOF/TOF; [M+Na] ⁺ ; SM(d18:1/16:0)
60	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; DGDG 36:4
61	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEOL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(11E))
2	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(11Z))
3	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(13Z))
4	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(17Z))
5	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(4E))
6	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(6Z))
7	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(7Z))
8	lipidblast-pos	33	709	3.26	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

Plot/Search Spectrum Plot/Text of Spec List

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:
 659.23 999.00 | 685.32 280.00 | 365.10 10.00 | 497.46 10.00 | 603.07 10.00

(lipidblast-pos) DGDG 34:1; [M+Na]⁺; DGDG(16:0/18:1

Plot/Text of Hit Plot of Hit

Name: DGDG 34:1; [M+Na]⁺; DGDG(16:0/18:1(11E))
 MW: 941 ID#: 4904 DB: lipidblast-pos
 Comment: Parent=941.61777 Mz_exact=941.6177
 4 largest peaks:
 497.30923 999.00 | 523.32487 999.00 | 659.30923 999.00 | 685.37769 999.00
 4 m/z Values and Intensities:
 497.30923 999.00 [M+Na]⁺-sn2-C6H10O5 (-162)
 523.32487 999.00 [M+Na]⁺-sn1-C6H10O5 (-162)

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Thermo Fisher Exactive Orbitrap; [M-H]⁻

#	Src.	Name
61	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDG 36:4

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	385	648	42.1	845	PS 40:6; [M-H] ⁻ ; GPSer(18:0/22:6(4Z,7Z,10Z,13Z,16Z))
2	lipidblast-neg	385	648	42.1	845	PS 40:6; [M-H] ⁻ ; GPSer(22:6(4Z,7Z,10Z,13Z,16Z))
3	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:1(11E)/20:5(5Z,8Z,11Z))
4	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:1(11Z)/20:5(5Z,8Z,11Z))
5	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:1(13E)/20:5(5Z,8Z,11Z))
6	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:1(13Z)/20:5(5Z,8Z,11Z))
7	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:5(5Z,8Z,11Z,14Z,17Z))
8	lipidblast-neg	193	414	0.61	773	PS 40:6; [M-H] ⁻ ; GPSer(20:5(5Z,8Z,11Z,14Z,17Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
255.2332 999.00 | 747.4981 750.00 | 419.2576 700.00 | 834.5299 300.00
437.2680 200.00 | 792.5774 185.00 | 621.4589 150.00 | 480.3100 100.00

(Spec. List) Thermo Fisher Exactive Orbitrap; [M-H]⁻; PS MIX

Name: PS 40:6; [M-H]⁻; GPSer(18:0/22:6(4Z,7Z,11Z))
MW: 834 ID#: 125128 DB: lipidblast-neg
Comment: Parent=834.52850 Mz_exact=834.52850

7 largest peaks:
747.49647 999.00 | 419.25639 200.00 | 437.26354 100.00 | 327.23226 100.00 | 283.26354 100.00 sn1 FA

7 m/z Values and Intensities:
283.26354 100.00 sn1 FA

(lipidblast-neg) PS 40:6; [M-H]⁻; GPSer(18:0/22:6(4Z,7Z,11Z))

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 phospholipids 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)

NIST MS Search 2.0 - [Peptide, Presearch Default - 30 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Finnigan LCQ ion trap; ESI; [M+NH4]⁺; DGDG 36:4

#	Src.	Name
61	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDG 36:4

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	19	340	5.67	707	TG 58:6; [M+Na] ⁺ ; TG(18:3/18:3/22:0)
2	lipidblast-pos	14	277	4.57	577	TG 59:5; [M+Li] ⁺ ; TG(17:0/20:5/22:0)
3	lipidblast-pos	14	277	4.57	577	TG 59:5; [M+Li] ⁺ ; TG(17:1/20:4/22:0)
4	lipidblast-pos	14	277	4.57	577	TG 59:5; [M+Li] ⁺ ; TG(17:2/20:3/22:0)
5	lipidblast-pos	14	277	4.57	577	TG 58:6; [M+Na] ⁺ ; TG(16:1/20:5/22:0)
6	lipidblast-pos	12	240	4.22	500	DGDG 35:0; [M+Na] ⁺ ; DGDG(13:0/22:0)
7	lipidblast-pos	12	240	4.22	500	DGDG 35:0; [M+Na] ⁺ ; DGDG(22:0/13:0)
8	lipidblast-neg	11	223	4.05	452	SQDG 44:2; [M-H] ⁻ ; SQDG(22:0/22:2(13Z,16Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Plot of Search Spectrum

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; Sir
10 largest peaks:
681.3 999.00 | 617.3 350.00 | 506.6 50.00 | 339.2 20.00 | 425.4 2
519.1 20.00 | 591.9 20.00 | 797.5 20.00 | 933.0 20.00 | 682.1 1

Plot of Hit

Name: DGDG 35:0; [M+Na]⁺; DGDG(13:0/22:0)
MW: 957 ID#: 4568 DB: lipidblast-pos
Comment: Parent=957.64907 Mz_exact=957.6490
4 largest peaks:
455.26233 999.00 | 581.40309 999.00 | 617.3
4 m/z Values and Intensities:
455.26233 999.00 [M+Na]⁺-sn1-C6H1005 (-162)
581.40309 999.00 [M+Na]⁺-sn1-C6H1005 (-162)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap; [M-H]⁻; Lipid A

#	Src.	Name
61	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; GM3
62	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; MGDG 36:4
63	L	JEDL JMS-HX110A/110A Tandem MS; FAB; [M-H] ⁻ ; NA
64	L	Kratos MALDI-TOF AXIMA-CFR; [M-H] ⁻ ; Lipid A
65	L	SHIMADZU KRATOS MALDI TRAP TOF; [M-H] ⁻ ; SQDG 36:5
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	696	902	20.0	985	LipidA-PP 54:28:0; LipidA-PP [14/14/10/16/30]-
2	lipidblast-neg	696	902	20.0	985	LipidA-PP 54:28:0; LipidA-PP [14/14/12/14/30]-
3	lipidblast-neg	696	902	20.0	985	LipidA-PP 54:28:0; LipidA-PP [14/14/14/12/30]-
4	lipidblast-neg	696	902	20.0	985	LipidA-PP 54:28:0; LipidA-PP [14/14/16/10/30]-
5	lipidblast-neg	597	857	1.51	926	LipidA-PP 56:26:0; LipidA-PP [14/14/10/18/30]-
6	lipidblast-neg	597	857	1.51	926	LipidA-PP 56:26:0; LipidA-PP [14/14/10/18/30]-
7	lipidblast-neg	597	857	1.51	926	LipidA-PP 56:26:0; LipidA-PP [14/14/12/16/30]-
8	lipidblast-neg	597	857	1.51	926	LipidA-PP 56:26:0; LipidA-PP [14/14/12/16/30]-

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

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
 10 largest peaks:
 1552.2 999.00 | 1698.2 550.00 | 1796.3 500.00 | 1454.2 250.00 | 147.2 1356.00
 1568.1 200.00 | 1470.2 150.00 | 1226.0 50.00 | 1324.0 50.00 | 1356.0 50.00

(lipidblast-neg) LipidA-PP 54:28:0; LipidA-PP [14/14/10/16/30]-

Name: LipidA-PP 54:28:0; LipidA-PP [14/14/10/16/30]-
MW: 1796 **ID#:** 87717 **DB:** lipidblast-neg
Comment: Parent=1796.21157 Mz_exact=1796.21157
 7 largest peaks:
 1552.00785 999.00 | 1698.23467 600.00 | 1796.21157 500.00
 1568.00277 250.00 | 1714.22959 50.00
 7 m/z Values and Intensities:
 1454.03095 250.00 [M-H]⁻;R2-PD4H3 || [M-H]⁻;R3

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 phospholipids molecular species in avocado (Persea americana Mill) fruit; <http://dx.doi.org/10.1016/j.chroma.2006.10.022>
 6 largest peaks:

MGDG MIX

NIST MS Search 2.0 - [Peptide, Presearch Default - 100 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Finnigan LCQ ion trap; ESI; [M+NH4]⁺

#	Src.	Name
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDGD MIX
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	24	207	1.68	283	PA 43:1; [M-H] ⁻ ; GPA(19:0/24:1(15Z))
2	lipidblast-neg	24	207	1.68	632	PA 43:1; [M-H] ⁻ ; GPA(21:0/22:1(13Z))
3	lipidblast-neg	24	207	1.68	632	PA 43:1; [M-H] ⁻ ; GPA(22:1(13Z)/21:0)
4	lipidblast-neg	24	207	1.68	283	PA 43:1; [M-H] ⁻ ; GPA(24:1(15Z)/19:0)
5	lipidblast-neg	24	207	1.68	632	PE 40:1; [M-H] ⁻ ; GPEtn(18:0/22:1(13Z))
6	lipidblast-neg	24	207	1.68	632	PE 40:1; [M-H] ⁻ ; GPEtn(22:1(13Z)/18:0)
7	lipidblast-pos	14	130	1.18	395	MGDG 38:2; [M+NH4-CO] ⁺ ; MGDG(18:2(2E,4E))
8	lipidblast-pos	14	130	1.18	395	MGDG 38:2; [M+NH4-CO] ⁺ ; MGDG(18:2(6Z,9Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

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]⁺;
 6 largest peaks:
 519.2 999.00 | 337.3 200.00 | 498.4 200.00 | 521.1 200.00 | 728.7 15
 594.0 100.00

Thermo Finnigan LCQ ion trap; ESI; Head to Tail MF=14 RMF=130 MGDG 38:2; [M+NH4-CO]⁺; MGDG(18:2(2E,4E))

(lipidblast-pos) MGDG 38:2; [M+NH4-CO]⁺; MGDG(18:2(2E,4E))

Name: MGDG 38:2; [M+NH4-CO]⁺; MGDG(18:2(2E,4E))
 MW: 800 ID#: 17528 DB: lipidblast-pos
 Comment: Parent=800.66155 Mz_exact=800.6615
 6 largest peaks:
 308.29552 999.00 | 340.35808 999.00 | 488.35891 100.00 | 311.29482 374.62 |
 279.23226 374.62 sn1 FA

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 153 spectra]

File Search View Tools Options Window Help

1. Thermo LCQ iontrap ESI; [M+NH4]+

#	Src.	Name
66	L	SHIMADZU LCMS-IT-TOF; [M-H]; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H]; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na]+; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H]; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4]+; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H]; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4]+; MGDGD MIX
73	L	Thermo LCQ iontrap ESI; [M+NH4]+; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4]+; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4]+; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H]; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H]; PIM2 35:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	117	930	12.9	932	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
2	lipidblast-pos	11	534	0.86	584	TG 52:2; [M+NH4]+; TG(14:0/18:1/20:1)
3	lipidblast-pos	11	534	0.86	584	TG 52:2; [M+NH4]+; TG(16:1/18:0/18:1)
4	lipidblast-pos	11	534	0.86	584	TG 52:2; [M+NH4]+; TG(17:0/17:1/18:1)
5	lipidblast-pos	4	310	0.66	674	TG 52:2; [M+NH4]+; TG(16:0/16:0/20:2)
6	custompc+n...	3	278	0.63	305	PC 41:3; [M+Na]+; GPCho(15:1(SZ)/26:2(5E,9Z)
7	custompc+n...	3	278	0.63	305	PC 41:3; [M+Na]+; GPCho(15:1(SZ)/26:2(5Z,9E)
8	custompc+n...	3	278	0.63	305	PC 41:3; [M+Na]+; GPCho(15:1(SZ)/26:2(5Z,9Z)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
577.4 999.00 | 859.7 350.00 | 603.5 200.00 | 876.9 200.00 |

4 m/z Values and Intensities:

Name: TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
MW: 876 ID#: 76056 DB: lipidblast-pos
Comment: Parent=876.80153 Mz_exact=876.80153

3 largest peaks:
577.51926 999.00 | 603.53490 999.00 | 859.79879 999.00 |

3 m/z Values and Intensities:
577.51926 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn1-18
603.53490 999.00 [M+NH4]-sn1-18

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 113 spectra]

File Search View Tools Options Window Help

Go 1. Thermo LCQ iontrap ESI; [M+NH4]⁺

#	Src.	Name
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDGD MIX
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	908	981	98.2	982	TG 48:1; [M+NH4] ⁺ ; TG(14:0/16:0/18:1)
2	lipidblast-pos	147	476	0.98	714	TG 48:1; [M+NH4] ⁺ ; TG(16:0/16:0/16:1)
3	lipidblast-pos	101	371	0.20	585	TG 48:1; [M+NH4] ⁺ ; TG(14:0/16:1/18:0)
4	lipidblast-pos	78	308	0.07	707	TG 48:1; [M+NH4] ⁺ ; TG(15:0/18:1/15:0)
5	custompc+n...	45	196	0.01	309	PC 37:2; [M+Na] ⁺ ; GPCho(11:0/26:2(5E,SZ))
6	custompc+n...	45	196	0.01	309	PC 37:2; [M+Na] ⁺ ; GPCho(11:0/26:2(5Z,9E))
7	custompc+n...	45	196	0.01	309	PC 37:2; [M+Na] ⁺ ; GPCho(11:0/26:2(5Z,SZ))
8	custompc+n...	45	196	0.01	309	PC 37:2; [M+Na] ⁺ ; GPCho(26:2(5E,SZ)/11:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Search Spectrum

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:
 549.5 999.00 | 577.5 900.00 | 523.5 400.00 | 822.6 300.00 | 805.7 25

Plot/Text of Hit

Name: TG 48:1; [M+NH4]⁺; TG(14:0/16:0/18:1)
 MW: 822 ID#: 75692 DB: lipidblast-pos
 Comment: Parent=822.75461 Mz_exact=822.75461
 4 largest peaks:
 523.47234 999.00 | 549.48798 999.00 | 577.51926 999.00 | 805.75187 999.00
 4 m/z Values and Intensities:
 523.47234 999.00 [M+NH4]⁺-sn3-18
 549.48798 999.00 [M+NH4]⁺-sn2-18

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 108 spectra]

File Search View Tools Options Window Help

1. Thermo LCQ iontrap ESI; [M+NH4]⁺

#	Src.	Name
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDGD MIX
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	83	934	8.97	936	TG 54:1; [M+NH4] ⁺ ; TG(18:0/18:0/18:1)
2	lipidblast-pos	7	533	1.13	584	TG 54:1; [M+NH4] ⁺ ; TG(16:0/18:0/20:1)
3	lipidblast-pos	7	533	1.13	584	TG 54:1; [M+NH4] ⁺ ; TG(16:1/18:0/20:0)
4	lipidblast-pos	7	533	1.13	584	TG 54:1; [M+NH4] ⁺ ; TG(17:1/18:0/19:0)
5	lipidblast-pos	2	247	0.91	579	TG 54:1; [M+NH4] ⁺ ; TG(16:0/18:1/20:0)
6	lipidblast-pos	2	247	0.91	579	TG 54:1; [M+NH4] ⁺ ; TG(17:0/18:1/19:0)
7	lipidblast-pos	2	247	0.91	579	TG 55:8; [M+NH4] ⁺ ; TG(17:2/18:1/20:5)
8	custompc+h...	0	23	0.84	133	PC 45:5; [M+H] ⁺ ; GPCho(20:5[52,82,112,142,1

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

(Spec. List) Thermo LCQ iontrap ESI; [M+NH4]⁺; TG 54:1
 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)
 4 largest peaks:
 605.7 999.00 | 607.7 200.00 | 906.7 200.00 | 889.8 120.00 |
 4 m/z Values and Intensities:

Name: TG 54:1; [M+NH4]⁺; TG(18:0/18:0/18:1)
 MW: 906 ID#: 76980 DB: lipidblast-pos
 Comment: Parent=906.84845 Mz_exact=906.8484
 3 largest peaks:
 605.55054 999.00 | 607.56618 999.00 | 889.84571 120.00 |
 3 m/z Values and Intensities:
 605.55054 999.00 [M+NH4]⁺-sn1-18 || [M+NH4]⁺-sn1-18 ||
 607.56618 999.00 [M+NH4]⁺-sn3-18

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-myoinositol 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 | 999.00 |

NIST MS Search 2.0 - [Peptide, Presearch Default - 61 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap;

#	Src.	Name
66	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; PS 32:0
67	L	SHIMADZU LCMS-IT-TOF; [M-H] ⁻ ; SQDG 34:3
68	L	Thermo Finnigan DecaXP ion trap; [M+Na] ⁺ ; DGDG 34:1
69	L	Thermo Fisher Exactive Orbitrap; [M-H] ⁻ ; PS MIX
70	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; DGDG 36:4
71	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; Lipid A
72	L	Thermo Finnigan LCQ ion trap; ESI; [M+NH4] ⁺ ; MGDGD MIX
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

Library Score Dot Product Prob. (%) Rev-Dot Name

1	lipidblast-neg	422	627	39.0	797	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM1(16:0/19:0)
2	lipidblast-neg	422	627	39.0	797	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM1(16:0/methyl-18:0)
3	lipidblast-neg	392	598	10.8	759	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM1(19:0/16:0)
4	lipidblast-neg	392	598	10.8	759	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM1(methyl-18:0/16:0)
5	lipidblast-pos	171	328	0.10	628	DGDG 39:0; [M+Na] ⁺ ; DGDG(16:0/23:0)
6	lipidblast-pos	171	328	0.10	628	DGDG 39:0; [M+Na] ⁺ ; DGDG(23:0/16:0)
7	lipidblast-pos	123	249	0.02	674	TG 62:4; [M+NH4] ⁺ ; TG(18:2/22:1/22:1)
8	lipidblast-pos	103	213	0.01	577	TG 63:5; [M+Li] ⁺ ; TG(19:0/22:0/22:5)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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, Struct

10 largest peaks:
757 999.00 | 433 700.00 | 715 550.00 | 1013.7 500.00 | 4
775 300.00 | 733 200.00 | 995 200.00 | 385 100.00 | 3

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Finnigan LCQ DECA ion trap; Head to Tail MF=392 RMF=598 Ac2PIM2 35:0; [M-H]⁻; Ac2PIM1(19:0/16:0) Difference Head to Tail Side by Side Subtraction 392 598R 10.8P

Name: Ac2PIM2 35:0; [M-H]⁻; Ac2PIM1(19:0/16:0)
MW: 1013 ID#: 63 DB: lipidblast-neg
Comment: Parent=1013.61778 Mz_exact=1013.61

9 largest peaks:
715.33078 999.00 | 689.51214 600.00 | 101
391.22514 400.00 | 433.27206 400.00 | 75
9 m/z Values and Intensities:
255.23226 400.00 sn2 FA

(lipidblast-neg) Ac2PIM2 35:0; [M-H]⁻; Ac2PIM1(19:0/16:0)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 8 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap;

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+NH4] ⁺ ; TG 52:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	410	702	24.8	854	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(16:0/19:0)
2	lipidblast-neg	410	702	24.8	854	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(16:0/methyl-18:0)
3	lipidblast-neg	410	702	24.8	854	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(19:0/16:0)
4	lipidblast-neg	410	702	24.8	854	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(methyl-18:0/16:0)
5	lipidblast-neg	30	96	0.24	293	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(15:0/20:0)
6	lipidblast-neg	30	96	0.24	293	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(17:0/18:0)
7	lipidblast-neg	30	96	0.24	293	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(18:0/17:0)
8	lipidblast-neg	30	96	0.24	293	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(20:0/15:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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, Struct...

10 largest peaks:

919	999.00	877	700.00	565	300.00	433	250.00	6
937	150.00	1013	100.00	1175.6	100.00	485	50.00	5

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: Ac2PIM2 35:0; [M-H]⁻; Ac2PIM2(16:0/19:0)
MW: 1175 ID#: 174 DB: lipidblast-neg
Comment: Parent=1175.67061 Mz_exact=1175.67

7 largest peaks:

877.38361	999.00	919.43053	999.00	25
1175.67061	100.00	1013.61779	50.00	

7 m/z Values and Intensities:

255.23226	400.00	sn1	FA	
-----------	--------	-----	----	--

(lipidblast-neg) Ac2PIM2 35:0; [M-H]⁻; Ac2PIM2(16:0/19:0)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 52 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap; [M-H]⁻; PIM2 51:0

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	441	799	41.7	837	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(16:0/19:0/16:0)
2	lipidblast-neg	441	799	41.7	837	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(16:0/methyl-18:
3	lipidblast-neg	386	760	8.08	796	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(19:0/16:0/16:0)
4	lipidblast-neg	386	760	8.08	796	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(methyl-18:0/16:
5	lipidblast-neg	210	573	0.15	716	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(16:0/16:0/19:0)
6	lipidblast-neg	210	573	0.15	716	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(16:0/16:0/meth
7	lipidblast-neg	146	463	0.02	537	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(15:0/20:0/16:0)
8	lipidblast-neg	146	463	0.02	537	Ac3PIM2 51:0; [M-H] ⁻ ; Ac3PIM2(17:0/18:0/16:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 T
10 largest peaks:
1157 999.00 | 803 450.00 | 1115 400.00 | 859 200.00 |
1175 100.00 | 723 50.00 | 877 50.00 | 1251 50.00 |

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 T
10 largest peaks:
1157 999.00 | 803 450.00 | 1115 400.00 | 859 200.00 |
1175 100.00 | 723 50.00 | 877 50.00 | 1251 50.00 |

Name: Ac3PIM2 51:0; [M-H]⁻; Ac3PIM2(16:0/19:0/16:0)
MW: 1413 ID#: 639 DB: lipidblast-neg
Comment: Parent=1413.90027 Mz_exact=1413.90027
10 largest peaks:
1157.66019 999.00 | 1115.61327 500.00 | 255.23226 400.00 | 859.37319 200.00 | 1413.90027 200.00 | 113.07343 100.00 |
10 m/z Values and Intensities:
255.23226 400.00 sn1 FA ll sn3 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap;

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	563	763	10.7	870	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/19:0
2	lipidblast-neg	563	763	10.7	870	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/16:1
3	lipidblast-neg	563	763	10.7	870	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/16:1
4	lipidblast-neg	563	763	10.7	870	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/meth
5	lipidblast-neg	544	748	5.20	854	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:1/19:0/16:0
6	lipidblast-neg	544	748	5.20	854	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:1/19:0/18:1
7	lipidblast-neg	544	748	5.20	854	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:1/methyl-18:
8	lipidblast-neg	544	748	5.20	854	Ac4PIM2 69:2; [M-H] ⁻ ; Ac4PIM2(16:1/methyl-18:

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
10 largest peaks:
1419.9 999.00 | 1421.9 650.00 | 1377.8 400.00 | 1676.1 400.00 | 1067.7 250.00 | 1393.6 250.00 | 1405.8 150.00 | 1081.7 120.00 | 1087.7 120.00 | 1087.7 120.00

Name: Ac4PIM2 69:2; [M-H]⁻; Ac4PIM2(16:0/18:1/19:0/16:1)
MW: 1676 ID#: 6836 DB: lipidblast-neg
Comment: Parent=1676.12994 Mz_exact=1676.12994
10 largest peaks:
1419.88986 999.00 | 1377.84294 500.00 | 1393.6 250.00 | 281.24790 400.00 | 1067.59229 300.00 | 1067.7 250.00 | 255.23226 400.00 sn1 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

60 1. Thermo Finnigan LCQ DECA ion trap;

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/16:0
2	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/18:1
3	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/16:0
4	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/16:0
5	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/19:0
6	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/18:1/meth
7	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18:
8	lipidblast-neg	36	211	0.56	435	Ac4PIM2 69:1; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18:

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
1421 999.00 | 1379 400.00 | 1678.1 400.00 | 1067 300.00 | 14
1083 50.00 | 1123 50.00 | 1395 50.00 | 1515 50.00 | 13

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Finnigan LCQ DECA ion trap; Head to Tail MF=36 RMF=211 Ac4PIM2 69:1; [M-H]⁻; Ac4PIM2(16:0/19:0/16:0) 36 211R 0.56P

Difference Head to Tail Side by Side Subtraction

Name: Ac4PIM2 69:1; [M-H]⁻; Ac4PIM2(16:0/19:0/16:0)
MW: 1678 ID#: 6226 DB: lipidblast-neg
Comment: Parent=1678.14559 Mz_exact=1678.14

10 largest peaks:
1421.90551 999.00 | 1379.85859 500.00 | 1395.00000 50.00 | 1067.59230 300.00 | 1083.62358 300.00 | 1678.14559 400.00 | 255.23226 400.00 sn1 FA

(lipidblast-neg) Ac4PIM2 69:1; [M-H]⁻; Ac4PIM2(16:0/19:0/16:0)

Plot/Text of Hit Plot of Hit

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 Guirin by multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization. II. Monoacyl- and Diacyl-PIMs

10 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 389 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LCQ DECA ion trap;

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/16:0)
2	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/16:0)
3	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/19:0)
4	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/19:0/methyl-18)
5	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18)
6	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18)
7	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18)
8	lipidblast-neg	353	811	10.4	837	Ac4PIM2 70:0; [M-H] ⁻ ; Ac4PIM2(16:0/methyl-18)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
10 largest peaks:
1437.9 999.00 | 1083.7 350.00 | 1395.9 350.00 | 1694.2 200.00 | 1139.7 100.00 | 1455.9 70.00 | 1157.7 30.00 | 1532.1 20.00 | 1065.6 1.00 | 1293.7 1.00

Name: Ac4PIM2 70:0; [M-H]⁻; Ac4PIM2(16:0/19:0/16:0)
MW: 1694 ID#: 6222 DB: lipidblast-neg
Comment: Parent=1694.17689 Mz_exact=1694.17689
7 largest peaks:
1437.93681 999.00 | 1395.88989 500.00 | 1694.17689 200.00 | 1139.64981 100.00 | 255.23226 400.00 sn1 FA

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-myoinositol 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

NIST MS Search 2.0 - [Peptide, Presearch Default - empty]

File Search View Tools Options Window Help

Go 1. Thermo Finnigan LCQ DECA ion trap; [M-H]⁻; PIM3(19:0/16:0)

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

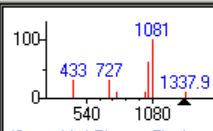
Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
---	---------	-------	-------------	-----------	---------	------

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS



Plot/Text of Search Spectrum

Plot of Search Spectrum

Plot/Text of Spec List

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, Struct
7 largest peaks:
1081 999.00 | 1039 600.00 | 433 300.00 | 727 300.00 | 7
1013 100.00 | 1337.9 100.00

Difference Head to Tail Side by Side Subtraction

Plot/Text of Hit

Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 65 spectra]

File Search View Tools Options Window Help

1. Thermo LCQ Deca XP MAX ion trap; [M+Na]⁺; DGDG 34:1

#	Src.	Name
73	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 52:2
74	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 48:1
75	L	Thermo LCQ iontrap ESI; [M+NH4] ⁺ ; TG 54:1
76	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM1 35:0
77	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 35:0
78	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 51:0
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(11E))
2	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(11Z))
3	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(13Z))
4	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(17Z))
5	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(4E))
6	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(6Z))
7	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(7Z))
8	lipidblast-pos	33	709	2.85	717	DGDG 34:1; [M+Na] ⁺ ; DGDG(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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; Mz_exact=941.41777
6 largest peaks:
659.23 999.00 | 685.32 280.00 | 365.10 10.00 | 497.46 10.00 | 603.07 10.00 | 779.23 10.00

(Spec. List) Thermo LCQ Deca XP MAX ion trap; [M+Na]⁺; DGDG 34:1

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: DGDG 34:1; [M+Na]⁺; DGDG(16:0/18:1(11E))
MW: 941 ID#: 4904 DB: lipidblast-pos
Comment: Parent=941.61777 Mz_exact=941.61777
4 largest peaks:
497.30923 999.00 | 523.32487 999.00 | 659.36205 999.00 | 779.23 10.00

(lipidblast-pos) DGDG 34:1; [M+Na]⁺; DGDG(16:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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 chromatography tandem mass spectrometry

;http://dx.doi.org/10.1016/j.chroma.2010.01.006

5 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

60 1. Thermo LCQ Deca XP MAX ion trap ESI

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[2E,4E])
2	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[6Z,9Z])
3	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[9E,10E])
4	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[9E,12E])
5	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[9Z,11Z])
6	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:0/18:2[9Z,12Z])
7	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:2[2E,4E]/18:0)
8	lipidblast-pos	325	752	7.99	752	PC 36:2; [M+H] ⁺ ; GPCho(18:2[6Z,9Z]/18:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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
5 largest peaks: 502.4 999.00 | 523.8 603.00 | 506.6 330.00 | 604.2 200.00 | 520.6 500.00
5 m/z Values and Intensities:

(Spec. List) Thermo LCQ Deca XP MAX ion trap ESI; [M+H]⁺; NA

Plot/Search Spectrum Plot/Text of Spec List

Name: PC 36:2; [M+H]⁺; GPCho(18:0/18:2[2E,4E])
MW: 786 ID#: 39583 DB: lipidblast-pos
Comment: Parent=786.60126 Mz_exact=786.60126
7 largest peaks: 727.52776 999.00 | 502.32990 600.00 | 506.32990 600.00 | 603.53522 400.00 | 768.59070 400.00
7 m/z Values and Intensities: 502.32990 600.00 [M+H]⁺-sn1-H2O

(lipidblast-pos) PC 36:2; [M+H]⁺; GPCho(18:0/18:2[2E,4E])

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. Thermo LTQ; [M+H]⁺; PC 34:1

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-]; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DG DG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+npos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(11E))
2	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(11Z))
3	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(13Z))
4	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(17Z))
5	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(4E))
6	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(6Z))
7	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(7Z))
8	lipidblast-pos	866	941	5.49	984	PC 34:1; [M+H] ⁺ ; GPCho(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo LTQ; [M+H]⁺; PC 34:1

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));
 10 largest peaks:
 701.314 999.00 | 504.335 808.51 | 496.299 576.85 | 478.313 496.75 |
 577.407 346.84 | 522.283 199.91 | 700.322 180.94 | 743.178 75.22 |

(Spec. List) Thermo LTQ; [M+H]⁺; PC 34:1

Name: PC 34:1; [M+H]⁺; GPCho(16:0/18:1(11E))
 MW: 760 ID#: 38947 DB: lipidblast-pos
 Comment: Parent=760.58564 Mz_exact=760.58564
 7 largest peaks:
 701.51214 999.00 | 478.32992 600.00 | 496.32992 600.00 |
 577.51960 400.00 | 742.57508 400.00 |
 7 m/z Values and Intensities:
 478.32992 600.00 [M+H]-sn2-H2O

Thermo LTQ; [M+H]⁺; PC 34:1; Head to Tail MF=866 RMF=941 PC 34:1; [M+H]⁺; GPCho(16:0/18:1(11E))

Difference Head to Tail Side by Side Subtraction 866 941R 5.49P

(lipidblast-pos) PC 34:1; [M+H]⁺; GPCho(16:0/18:1(11E))

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 221 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Finnigan LTQ linear ion trap; [M+Na]⁺; TG 52:1

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ DecaXP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ DecaXP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	604	803	97.5	986	TG 52:1; [M+Na] ⁺ ; TG(16:0/18:0/18:1)
2	lipidblast-pos	435	674	2.18	963	TG 54:7; [M+Li] ⁺ ; TG(16:0/18:3/20:4)
3	lipidblast-pos	357	598	0.25	816	TG 53:0; [M+Li] ⁺ ; TG(16:0/18:0/19:0)
4	lipidblast-pos	284	515	0.03	1e+3	TG 54:7; [M+Li] ⁺ ; TG(18:1/18:3/18:3)
5	lipidblast-pos	213	420	0.00	816	TG 54:7; [M+Li] ⁺ ; TG(16:1/18:3/20:3)
6	lipidblast-pos	182	373	0.00	707	TG 53:0; [M+Li] ⁺ ; TG(16:0/16:0/21:0)
7	lipidblast-pos	182	373	0.00	707	TG 52:1; [M+Na] ⁺ ; TG(16:0/16:0/20:1)
8	lipidblast-pos	173	358	0.00	707	TG 53:0; [M+Li] ⁺ ; TG(17:0/18:0/18:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

Name: Thermo Finnigan LTQ linear ion trap; [M+Na]⁺; TG 52:1
 MW: 883 ID#: 86 DB: Spec. List
 Comment: TAG(16:0/18:1/18:0); [M+Na]⁺; Prec. m/z: 883.6; Electrospray Ionization
 7 largest peaks:
 627 999.00 | 599 920.00 | 605 500.00 | 577 450.00 | 601 450.00
 579 250.00 | 883.6 170.00 |

Thermo Finnigan LTQ linear ion trap; Head to Tail MF=604 RMF=803 TG 52:1; [M+Na]⁺; TG(16:0/18:0/18:1)

Name: TG 52:1; [M+Na]⁺; TG(16:0/18:0/18:1)
 MW: 883 ID#: 73179 DB: lipidblast-pos
 Comment: Parent=883.77257 Mz_exact=883.77257
 3 largest peaks:
 599.50121 999.00 | 601.51685 999.00 | 627.51685 999.00
 3 m/z Values and Intensities:
 599.50121 999.00 [M+Na]-sn2+Na
 601.51685 999.00 [M+Na]-sn3+Na

(lipidblast-pos) TG 52:1; [M+Na]⁺; TG(16:0/18:0/18:1)

Name: TG 52:1; [M+Na]⁺; TG(16:0/18:0/18:1)
 MW: 883 ID#: 73179 DB: lipidblast-pos
 Comment: Parent=883.77257 Mz_exact=883.77257
 3 largest peaks:
 599.50121 999.00 | 601.51685 999.00 | 627.51685 999.00
 3 m/z Values and Intensities:
 599.50121 999.00 [M+Na]-sn2+Na
 601.51685 999.00 [M+Na]-sn3+Na

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 215 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LTQ linear ion trap;

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1;
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	833	958	94.1	960	TG 52:1; [M+NH4] ⁺ ; TG(16:0/18:0/18:1)
2	lipidblast-pos	139	425	0.94	674	TG 52:1; [M+NH4] ⁺ ; TG(16:1/18:0/18:0)
3	lipidblast-pos	133	414	0.73	674	TG 52:1; [M+NH4] ⁺ ; TG(16:0/16:0/20:1)
4	lipidblast-pos	120	386	0.47	612	MGDG 42:5; [M+NH4] ⁺ ; MGDG(20:5(5Z,8Z,11Z)
5	lipidblast-pos	120	386	0.47	612	MGDG 42:5; [M+NH4] ⁺ ; MGDG(22:0/20:5(5Z,8Z)
6	lipidblast-pos	106	352	0.29	559	TG 52:1; [M+NH4] ⁺ ; TG(17:0/17:1/18:0)
7	lipidblast-pos	102	343	0.25	559	TG 52:1; [M+NH4] ⁺ ; TG(16:0/16:1/20:0)
8	lipidblast-pos	102	343	0.25	559	TG 52:1; [M+NH4] ⁺ ; TG(16:0/17:1/19:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

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
 6 largest peaks:
 577 999.00 | 605 950.00 | 579 550.00 | 878.7 180.00 | 861 10
 846 50.00 |

(lipidblast-pos) TG 52:1; [M+NH4]⁺; TG(16:0/18:0/18:1)

Name: TG 52:1; [M+NH4]⁺; TG(16:0/18:0/18:1)
 MW: 878 ID#: 75819 DB: lipidblast-pos
 Comment: Parent=878.81717 Mz_exact=878.8171
 4 largest peaks:
 577.51926 999.00 | 579.53490 999.00 | 605.5
 4 m/z Values and Intensities:
 577.51926 999.00 [M+NH4]⁺-sn2-18
 579.53490 999.00 [M+NH4]⁺-sn3-18

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 77 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LTQ linear ion trap;

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	766	927	98.9	985	TG 52:1; [M+Li] ⁺ ; TG(16:0/18:0/18:1)
2	lipidblast-pos	367	693	0.98	816	TG 51:2; [M+Na] ⁺ ; TG(16:0/17:2/18:0)
3	lipidblast-pos	261	578	0.06	802	TG 51:2; [M+Na] ⁺ ; TG(16:0/17:1/18:1)
4	lipidblast-pos	160	426	0.00	707	TG 52:1; [M+Li] ⁺ ; TG(16:1/18:0/18:0)
5	lipidblast-pos	158	422	0.00	707	TG 52:1; [M+Li] ⁺ ; TG(16:0/16:0/20:1)
6	lipidblast-pos	120	348	0.00	577	TG 52:1; [M+Li] ⁺ ; TG(17:0/17:1/18:0)
7	lipidblast-pos	120	348	0.00	577	TG 51:2; [M+Na] ⁺ ; TG(16:1/17:1/18:0)
8	lipidblast-pos	119	345	0.00	577	TG 52:1; [M+Li] ⁺ ; TG(16:0/16:1/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
583 999.00 | 611 980.00 | 585 450.00 | 867.6 200.00 | 605 15
577 80.00 | 579 80.00

(Spec. List) Thermo Finnigan

Name: TG 52:1; [M+Li]⁺; TG(16:0/18:0/18:1)
MW: 867 ID#: 70539 DB: lipidblast-pos
Comment: Parent=867.79881 Mz_exact=867.79881
3 largest peaks:
583.52745 999.00 | 585.54309 999.00 | 611.54309 999.00
3 m/z Values and Intensities:
583.52745 999.00 [M+Li]⁺-sn2+Li
585.54309 999.00 [M+Li]⁺-sn3+Li

(lipidblast-pos) TG 52:1; [M+Li]⁺; TG(16:0/18:0/18:1)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 354 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan LTQ linear ion trap

#	Src.	Name
79	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:2
80	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 69:1
81	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM2 70:0
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DG DG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	169	895	16.1	949	TG 50:1; [M+Li] ⁺ ; TG(16:0/16:0/18:1)
2	lipidblast-pos	169	895	16.1	949	TG 50:1; [M+Li] ⁺ ; TG(16:0/16:0/18:1)
3	lipidblast-pos	34	596	0.61	707	TG 49:2; [M+Na] ⁺ ; TG(16:0/16:0/17:2)
4	lipidblast-pos	22	487	0.40	577	TG 50:1; [M+Li] ⁺ ; TG(16:0/16:1/18:0)
5	lipidblast-pos	22	487	0.40	577	TG 50:1; [M+Li] ⁺ ; TG(16:0/17:0/17:1)
6	lipidblast-pos	22	487	0.40	577	TG 49:2; [M+Na] ⁺ ; TG(16:0/16:1/17:1)
7	lipidblast-neg	12	344	0.28	408	SQDG 36:5; [M-H] ⁻ ; SQDG(16:0/20:5(5Z,8Z,11Z
8	lipidblast-neg	12	344	0.28	408	SQDG 36:5; [M-H] ⁻ ; SQDG(20:5(5Z,8Z,11Z,14Z

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 Ion
6 largest peaks:
583 899.00 | 557 250.00 | 839 200.00 | 577 120.00 | 551 30.00 |
821 10.00 |

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: TG 50:1; [M+Li]⁺; TG(16:0/16:0/18:1)
MW: 839 ID#: 70432 DB: lipidblast-pos
Comment: Parent=839.76753 Mz_exact=839.7675
2 largest peaks:
557.51181 999.00 | 583.52745 999.00 |
2 m/z Values and Intensities:
557.51181 999.00 [M+Li]-sn3+Li
583.52745 999.00 [M+Li]-sn1+Li || [M+Li]-sn2+Li

(lipidblast-pos) TG 50:1; [M+Li]⁺; TG(16:0/16:0/18:1)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 52 spectra] SciFinder - Reference Answer Set

File Search View Tools Options Window Help

1. Thermo Finnigan LTQ linear ion trap;

#	Src.	Name
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 60:12
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 40:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	3	978	2.17	1e+3	TG 60:12; [M+Li] ⁺ ; TG(20:4/20:4/20:4)
2	lipidblast-pos	0	621	1.91	632	TG 59:5; [M+Li] ⁺ ; TG(19:0/20:1/20:4)
3	lipidblast-pos	0	621	1.91	632	TG 58:6; [M+Na] ⁺ ; TG(18:1/20:1/20:4)
4	lipidblast-pos	0	564	1.91	577	TG 59:5; [M+Li] ⁺ ; TG(17:0/20:4/22:1)
5	lipidblast-pos	0	564	1.91	577	TG 59:5; [M+Li] ⁺ ; TG(17:1/20:4/22:0)
6	lipidblast-pos	0	564	1.91	577	TG 59:5; [M+Li] ⁺ ; TG(18:1/20:4/21:0)
7	lipidblast-pos	0	564	1.91	577	TG 60:12; [M+Li] ⁺ ; TG(18:2/20:4/22:6)
8	lipidblast-pos	0	564	1.91	577	TG 60:12; [M+Li] ⁺ ; TG(18:3/20:4/22:5)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Search Spectrum

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 Ion
7 largest peaks:
653 999.00 | 957.6 200.00 | 311 10.00 | 361 10.00 | 483 1
647 10.00 | 939 10.00

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Finnigan LTQ linear ion trap; Head to Tail MF=3 RMF=978 TG 60:12; [M+Li]⁺; TG(20:4/20:4/20:4); Difference Head to Tail Side by Side Subtraction 3 978R 2.17P

Plot/Text of Hit

Name: TG 60:12; [M+Li]⁺; TG(20:4/20:4/20:4)
MW: 957 ID#: 72815 DB: lipidblast-pos
Comment: Parent=957.75189 Mz_exact=957.75189
1 largest peaks:
653.51181 999.00 |
1 m/z Values and Intensities:
653.51181 999.00 [M+Li]-sn1+Li || [M+Li]-sn2+Li
Synonyms:

(lipidblast-pos) TG 60:12; [M+Li]⁺; TG(20:4/20:4/20:4)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 2 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Fisher LTQ-FT; [M-H]⁻; GM2-α

#	Src.	Name
82	L	Thermo Finnigan LCQ DECA ion trap; [M-H] ⁻ ; PIM3(19:0/16:0)
83	L	Thermo LCQ Deca XP MAX ion trap; [M+Na] ⁺ ; DGDG 34:1
84	L	Thermo LCQ Deca XP MAX ion trap ESI; [M+H] ⁺ ; NA
85	L	Thermo LTQ; [M+H] ⁺ ; PC 34:1
86	L	Thermo Finnigan LTQ linear ion trap; [M+Na] ⁺ ; TG 52:1
87	L	Thermo Finnigan LTQ linear ion trap; [M+NH4] ⁺ ; TG 52:1
88	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 52:1
89	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 50:1
90	L	Thermo Finnigan LTQ linear ion trap; [M+Li] ⁺ ; TG 60:12
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 40:3

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	168	436	50.0	617	[glycan]-Cer 34:1; GM2(d18:1/16:0); [M-H] ⁻ ; GalNAc
2	lipidblast-neg	168	436	50.0	617	[glycan]-Cer 34:1; Ganglioside; [M-H] ⁻ ; NeuAcalpha2

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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; M
9 largest peaks:
1063.5 999.00 | 860.5 950.00 | 698.4 200.00 | 1156.5 200.00 | 536.4
680.4 150.00 | 1336.5 100.00 | 1198.6 50.00 | 1021.3 30.00

(Spec. List) Thermo Fisher LTQ-FT; [M-H]⁻; GM2-alpha

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Fisher LTQ-FT; [M-H]⁻; GM2-alpha Head to Tail MF=168 RMF=436 [glycan]-Cer 34:1; GM2(d18:1/16:0); [M-H]⁻ 168 436R 50.0P

Difference Head to Tail Side by Side Subtraction

Name: [glycan]-Cer 34:1; GM2(d18:1/16:0); [M-H]⁻
MW: 1354 ID#: 79298 DB: lipidblast-neg
Comment: Parent=1354.78471 Mz_exact=1354.78471
5 largest peaks:
1354.78471 999.00 | 1063.68930 500.00 | 290.08759 400.00
5 m/z Values and Intensities:
290.08759 400.00 ion C11H16NO8- (290.08759)
536.50395 200.00 ion ceramide

(lipidblast-neg) [glycan]-Cer 34:1; GM2(d18:1/16:0); [M-H]⁻

Plot/Text of Hit Plot of Hit

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.bbali.2009.10.009

7 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 347 spectra]

File Search View Tools Options Window Help

1. Thermo Fisher LTQ-FT; [M-H]; PG 36:2

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H]; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H]; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H]; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4]+; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H]; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H]; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H]; PS 36:1
102	L	Thermo LTQ Orbitrap; [M-H]; GM 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(11E))
2	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(11Z))
3	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(13Z))
4	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(17Z))
5	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(4E))
6	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(6Z))
7	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(7Z))
8	lipidblast-neg	246	872	1.22	978	PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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.bbali.2009.10.009

7 largest peaks:
281 999.00 | 283 200.00 | 279 100.00 | 417 100.00 | 509 100.00
491 50.00 | 415 20.00

(Spec. List) Thermo Fisher LTQ-FT

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(11E))
MW: 773 ID#: 113988 DB: lipidblast-neg
Comment: Parent=773.53326 Mz_exact=773.5332

4 largest peaks:
281.24790 999.00 | 417.24076 200.00 | 491.24076 200.00 | 415.24076 200.00

4 m/z Values and Intensities:
281.24790 999.00 sn1 FA || sn2 FA
417.24076 200.00 [M-H]-sn1-C3H8O3 || [M-H]-sn2

(lipidblast-neg) PG 36:2; [M-H]; GPGro(18:1(11E)/18:1(11E))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 14 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Fisher LTQ-FT; [M+NH4]+; TG 48:2

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H]; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H]; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H]; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4]+; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H]; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H]; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H]; PS 36:1
102	L	Thermo LTQ Orbitrap; [M-H]; GM 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	138	410	63.0	709	TG 48:2; [M+NH4]+; TG(16:0/16:1/16:1)
2	lipidblast-pos	115	362	23.0	581	TG 48:2; [M+NH4]+; TG(14:0/16:1/18:1)
3	lipidblast-neg	59	215	4.38	408	SQDG 34:0; [M-H]; SQDG(15:0/19:0)
4	lipidblast-neg	59	215	4.38	408	SQDG 34:0; [M-H]; SQDG(19:0/15:0)
5	lipidblast-neg	25	103	1.12	196	PI 33:1; [M-H]; GPlns(14:1(SZ)/19:0)
6	lipidblast-neg	25	103	1.12	196	PI 33:1; [M-H]; GPlns(19:0/14:1(SZ))
7	lipidblast-pos	1	6	0.37	126	DG 49:2; [M+NH4]+; DG(23:0/26:2/0:0)
8	lipidblast-pos	1	6	0.37	126	DG 49:2; [M+NH4]+; DG(26:2/23:0/0:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot of Search Spectrum

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:
575.5021 999.00 | 547.4704 860.00 | 523.4705 720.00 | 803.7133 303.00

4 m/z Values and Intensities:

Plot of Search Spectrum

Plot of Hit

Name: TG 48:2; [M+NH4]+; TG(16:0/16:1/16:1)
MW: 820 ID#: 75731 DB: lipidblast-pos
Comment: Parent=820.73897 Mz_exact=820.73897

3 largest peaks:
547.47234 999.00 | 549.48798 999.00 | 803.7133 303.00

3 m/z Values and Intensities:

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 7 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Fisher LTQ-FT; [M+NH4]⁺; TG 50:2

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; GM1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	568	941	97.3	941	TG 50:2; [M+NH4] ⁺ ; TG(16:0/16:1/18:1)
2	lipidblast-pos	78	506	0.97	674	TG 50:2; [M+NH4] ⁺ ; TG(16:0/16:0/18:2)
3	lipidblast-pos	78	506	0.97	674	TG 50:2; [M+NH4] ⁺ ; TG(16:0/17:1/17:1)
4	lipidblast-pos	56	420	0.38	559	TG 50:2; [M+NH4] ⁺ ; TG(16:0/17:0/17:2)
5	lipidblast-pos	34	299	0.15	674	TG 50:2; [M+NH4] ⁺ ; TG(16:1/16:1/18:0)
6	lipidblast-pos	26	248	0.11	559	TG 50:2; [M+NH4] ⁺ ; TG(14:1/16:1/20:0)
7	lipidblast-pos	26	248	0.11	559	TG 50:2; [M+NH4] ⁺ ; TG(16:1/17:0/17:1)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
3 largest peaks: 575.5017 999.00 | 549.4861 420.00 | 577.5176 350.00 |
3 m/z Values and Intensities:

(Spec. List) Thermo Fisher LTQ-FT; [M+NH4]⁺; TG 50:2

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: TG 50:2; [M+NH4]⁺; TG(16:0/16:1/18:1)
MW: 848 ID#: 75736 DB: lipidblast-pos
Comment: Parent=848.77025 Mz_exact=848.77025
4 largest peaks: 549.48798 999.00 | 575.50362 999.00 | 577.5176 350.00 |
4 m/z Values and Intensities:

(lipidblast-pos) TG 50:2; [M+NH4]⁺; TG(16:0/16:1/18:1)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. Thermo MALDI LTQ ion trap; [M-H]⁻

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH ₄] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH ₄] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH ₄] ⁺ ; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; GM1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	412	564	6.13	814	LipidA-PP 56:28:0; LipidA-PP [14/14/10/18/30-]
2	lipidblast-neg	412	564	6.13	814	LipidA-PP 56:28:0; LipidA-PP [14/14/12/16/30-]
3	lipidblast-neg	412	564	6.13	814	LipidA-PP 56:28:0; LipidA-PP [14/14/14/14/30-]
4	lipidblast-neg	412	564	6.13	814	LipidA-PP 56:28:0; LipidA-PP [14/14/16/12/30-]
5	lipidblast-neg	412	564	6.13	814	LipidA-PP 56:28:0; LipidA-PP [14/14/18/10/30-]
6	lipidblast-neg	367	518	1.30	747	LipidA-PP 52:32:0; LipidA-PP [14/14/10/14/30-]
7	lipidblast-neg	367	518	1.30	747	LipidA-PP 52:32:0; LipidA-PP [14/14/10/14/30-]
8	lipidblast-neg	367	518	1.30	747	LipidA-PP 54:30:0; LipidA-PP [14/14/10/16/30-]

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo MALDI LTQ ion trap; [M-H]⁻; Lipid A

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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:

1253.5	999.00	1579.5	999.00	1481.5	800.00	1271.5	700.00	1599.00	1726.8	400.00	1027.4	300.00	1045.4	300.00	1351.5	300.00	718.4
--------	--------	--------	--------	--------	--------	--------	--------	---------	--------	--------	--------	--------	--------	--------	--------	--------	-------

(lipidblast-neg) LipidA-PP 56:28:0; LipidA-PP [14/14/10/18/30-]

Plot/Text of Hit Plot of Hit

Name: LipidA-PP 56:28:0; LipidA-PP [14/14/10/18/30-]
 MW: 1824 ID#: 87742 DB: lipidblast-neg
 Comment: Parent=1824.24287 Mz_exact=1824.24
 7 largest peaks:

1580.03915	999.00	1726.26597	600.00	1824.24287	1596.03407	250.00	1742.26089	50.00
------------	--------	------------	--------	------------	------------	--------	------------	-------

7 m/z Values and Intensities:
 1482.06225 250.00 [M-H]⁻;R2-P04H3 [M-H]⁻;R3

Peptide Peptide

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 Gialvalisco, and Lothar Willmitzer; dx.doi.org/10.1007/978-90-481-2863-1_20
3 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 56 spectra]

File Search View Tools Options Window Help

1. Thermo LTQ Orbitrap; ???; MGDG 34

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ ion trap; MALDI; CL 36:10

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z)/20:
2	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z)/20:
3	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z)/20:
4	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z)/20:
5	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(9Z,12Z,15Z)/21:
6	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(9Z,12Z,15Z)/21:
7	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(9Z,12Z,15Z)/21:
8	lipidblast-pos	32	310	2.88	408	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(9Z,12Z,15Z)/21:

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
3 largest peaks:
769.48 999.00 | 492.3545 300.00 | 520.3710 200.00 |
3 m/z Values and Intensities:

(Spec. List) Thermo LTQ Orb

Name: PA 38:4; [M+Na2H]⁺; GPA(18:3(6Z,9Z,12Z)/20:
MW: 769 ID#: 28925 DB: lipidblast-pos
Comment: Parent=769.47605 Mz_exact=769.4760
4 largest peaks:
459.18905 999.00 | 491.25161 999.00 | 460.1:
4 m/z Values and Intensities:
459.18905 999.00 [M+Na2H]⁺-sn2-H
460.19687 500.00 [M+Na2H]⁺-sn2

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 145 spectra]

File Search View Tools Options Window Help

1. Thermo LTQ Orbitrap; [M+NH4]⁺; TG 52:2

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2 ;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2 ;

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	766	980	78.2	992	TG 52:2; [M+NH4] ⁺ ; TG(16:0/18:1/18:1)
2	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4] ⁺ ; TG(14:0/18:1/20:1)
3	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4] ⁺ ; TG(16:1/18:0/18:1)
4	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4] ⁺ ; TG(17:0/17:1/18:1)
5	lipidblast-pos	49	440	0.66	713	TG 52:2; [M+NH4] ⁺ ; TG(16:0/16:0/20:2)
6	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na] ⁺ ; GPCho(15:1(9Z)/26:2(5E,9Z)
7	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na] ⁺ ; GPCho(15:1(9Z)/26:2(5Z,9E)
8	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na] ⁺ ; GPCho(15:1(9Z)/26:2(5Z,9Z)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

(Spec. List) Thermo LTQ Orb

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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; Cc
 4 largest peaks:
 876.7995 999.00 | 577.5180 500.00 | 603.5335 300.00 | 859.774 100
 4 m/z Values and Intensities:

(lipidblast-pos) TG 52:2; [M+NH4]⁺; TG(16:0/18:1/18:1)

Plot/Text of Hit Plot of Hit

Name: TG 52:2; [M+NH4]⁺; TG(16:0/18:1/18:1)
 MW: 876 ID#: 76056 DB: lipidblast-pos
 Comment: Parent=876.80153 Mz_exact=876.8015
 3 largest peaks:
 577.51926 999.00 | 603.53490 999.00 | 859.774 100
 3 m/z Values and Intensities:
 577.51926 999.00 [M+NH4]⁺-sn2-18 || [M+NH4]⁺-sn1-18
 603.53490 999.00 [M+NH4]⁺-sn1-18

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 21 spectra]

File Search View Tools Options Window Help

1. Thermo LTQ Orbitrap; [M-H]⁻; PC 32:0

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 50:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	pc-ac-neg.m...	0	912	4.76	913	PC 32:0; [M-Ac-H] ⁻ ; GPCho(16:0/16:0)
2	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(6:0/26:0)
3	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(7:0/25:0)
4	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(8:0/24:0)
5	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(9:0/23:0)
6	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(10:0/22:0)
7	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(11:0/21:0)
8	pc-ac-neg.m...	0	876	4.76	877	PC 32:0; [M-Ac-H] ⁻ ; GPCho(12:0/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Peptide Peptide

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
1 largest peaks:
718.53778 999.00 |
1 m/z Values and Intensities:

(Spec. List) Thermo LTQ Orb

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 32:0; [M-Ac-H]⁻; GPCho(16:0/16:0)
MW: 792 ID#: 1583 DB: pc-ac-neg.msp
Comment: Parent=792.57544 Mz_exact=792.5754
3 largest peaks:
718.53866 999.00 | 255.23226 100.00 | 792.57544
3 m/z Values and Intensities:
255.23226 100.00 FA sn1 || FA sn2
718.53866 999.00 [M-CH3]⁻ (-15)

(pc-ac-neg.msp) PC 32:0; [M-Ac-H]⁻; GPCho(16:0/16:0)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 145 spectra]

File Search View Tools Options Window Help

MS m/z ← ?

1. Thermo LTQ Orbitrap ; TG 52:2

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H]; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H]; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4]+; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H]; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6
97	L	Thermo LTQ Orbitrap; [M+NH4]+; TG 52:2 ;
98	L	Thermo LTQ Orbitrap; [M-H]; -PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H]; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H]; PS 36:1
102	L	Thermo LTQ Orbitrap; [M-H]; GM 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	766	980	78.2	992	TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
2	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4]+; TG(14:0/18:1/20:1)
3	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4]+; TG(16:1/18:0/18:1)
4	lipidblast-pos	53	460	0.78	585	TG 52:2; [M+NH4]+; TG(17:0/17:1/18:1)
5	lipidblast-pos	49	440	0.66	713	TG 52:2; [M+NH4]+; TG(16:0/16:0/20:2)
6	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na]+; GPCho(15:1(9Z)/26:2(5E,9E)
7	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na]+; GPCho(15:1(9Z)/26:2(5Z,9E)
8	custompc+n...	42	258	0.50	310	PC 41:3; [M+Na]+; GPCho(15:1(9Z)/26:2(5Z,9Z)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
876.7995 999.00 | 577.5180 500.00 | 603.5335 300.00 | 859.774 100.00
4 m/z Values and Intensities:

Name: TG 52:2; [M+NH4]+; TG(16:0/18:1/18:1)
MW: 876 ID#: 76056 DB: lipidblast-pos
Comment: Parent=876.80153 Mz_exact=876.80153
3 largest peaks:
577.51926 999.00 | 603.53490 999.00 | 859.774 100.00
3 m/z Values and Intensities:
577.51926 999.00 [M+NH4]-sn2-18 II [M+NH4]-sn1-18
603.53490 999.00 [M+NH4]-sn1-18

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. Dutta, Alice M.

Delvolv1, Amina S. Woods1.; ASMS2010;

http://www.asms.org/asms10pdf/ASMS201020798.0375VER.4.pdf

10 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 57 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Orbitrap Velos ESI ; [M-H]⁻; GM1(d18:1/18:0)

#	Src.	Name
91	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; GM2-alpha
92	L	Thermo Fisher LTQ-FT; [M-H] ⁻ ; PG 36:2
93	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 48:2
94	L	Thermo Fisher LTQ-FT; [M+NH4] ⁺ ; TG 50:2
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 36:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

Thermo Orbitrap Velos ESI ; [M-H]⁻; GM1(d18:1/18:0); Head to Tail MF=446 RMF=651 [glycan]-Cer 36:1; GM1(d18:1/18:0); [M-H]⁻; Gal

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; Ganglioside; [M-H] ⁻ ; NeuAcalp
2	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; GM1(d18:1/18:0); [M-H] ⁻ ; Gal
3	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; cis GM1, GM1b(d18:1/18:0); [M-H] ⁻
4	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; GM1alpha(d18:1/18:0); [M-H] ⁻
5	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; sialyl-lactotetraosylceramide(d1
6	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; sialyl(2-6)lactotetraosylceramid
7	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; Ganglioside; [M-H] ⁻ ; Galbeta1:
8	lipidblast-neg	446	651	10.8	938	[glycan]-Cer 36:1; Ganglioside; [M-H] ⁻ ; NeuAcalp

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Name: [glycan]-Cer 36:1; GM1(d18:1/18:0); [M-H]⁻
MW: 1544 ID#: 79307 DB: lipidblast-neg
Comment: Parent=1544.86883 Mz_exact=1544.8683
5 largest peaks:
1544.86883 999.00 | 1253.77342 500.00 | 290.08759 400.00
5 m/z Values and Intensities:
290.08759 400.00 ion C11H16NO8- (290.08759) ion ceramide
564.53523 200.00

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. Thermo Fisher LTQ with DESI; [M-H]⁻

#	Src.	Name
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; -PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; Phospholipid PE 38:4

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(11E))
2	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(11Z))
3	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(13Z))
4	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(17Z))
5	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(4E))
6	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(6Z))
7	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(7Z))
8	lipidblast-neg	75	863	1.70	866	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
6 largest peaks:
701.2 999.00 | 788.2 350.00 | 419.2 170.00 | 283.3 80.00 | 437.2 3
281 20.00 |

(Spec. List) Thermo Fisher LTQ

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Fisher LTQ with DESI; [M-H]⁻; Head to Tail MF=75 RMF=863 PS 36:1; [M-H]⁻; GPSer(18:0/18:1(11E))

Difference Head to Tail Side by Side Subtraction 75 863R 1.70P

Name: PS 36:1; [M-H]⁻; GPSer(18:0/18:1(11E))
MW: 788 ID#: 125088 DB: lipidblast-neg
Comment: Parent=788.54418 Mz_exact=788.5441
7 largest peaks:
701.51215 999.00 | 417.24079 200.00 | 419.2
281.24790 100.00 | 283.26354 100.00 |
7 m/z Values and Intensities:
281.24790 100.00 sn2 FA

(lipidblast-neg) PS 36:1; [M-H]⁻; GPSer(18:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 254 spectra]

File Search View Tools Options Window Help

1. Thermo LXQ iontrap; [M-H]⁻; CL 76:10

#	Src.	Name
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2 ;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	248	458	17.4	625	CL 76:10; [M-H] ⁻ ; CL(18:1/18:2/22:5/18:2)
2	lipidblast-neg	227	430	7.42	587	CL 76:10; [M-H] ⁻ ; CL(18:1/18:2/18:2/22:5)
3	lipidblast-neg	227	430	7.42	587	CL 76:10; [M-H] ⁻ ; CL(18:2/18:1/22:5/18:2)
4	lipidblast-neg	224	425	6.55	580	CL 76:10; [M-H] ⁻ ; CL(16:0/20:3/22:5/18:2)
5	lipidblast-neg	224	425	6.55	580	CL 76:10; [M-H] ⁻ ; CL(16:1/20:2/22:5/18:2)
6	lipidblast-neg	224	425	6.55	580	CL 76:10; [M-H] ⁻ ; CL(18:0/18:3/22:5/18:2)
7	lipidblast-neg	224	425	6.55	580	CL 76:10; [M-H] ⁻ ; CL(18:3/18:0/22:5/18:2)
8	lipidblast-neg	224	425	6.55	580	CL 76:10; [M-H] ⁻ ; CL(20:2/16:1/22:5/18:2)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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 I
10 largest peaks:
697.7 999.00 | 415.3 800.00 | 744.6 600.00 | 800.4 500.00 | 1462.9 320.00
1499.8 400.00 | 629.8 300.00 | 1097.2 300.00 | 279.3 100.00 | 320.00 100.00

(Spec. List) Thermo LXQ iontrap

Plot of Search Spectrum Plot/Text of Search Spectrum Plot/Text of Spec List

Name: CL 76:10; [M-H]⁻; CL(18:1/18:2/22:5/18:2)
Mw: 1499 ID#: 34784 DB: lipidblast-neg
Comment: Parent=1499.99571 Mz_exact=1499.99571
10 largest peaks:
697.48053 999.00 | 745.48053 999.00 | 415.2 433.23537 200.00 | 279.23226 100.00 | 281.2 100.00
279.23226 100.00 sn2 FA II sn4 FA

(lipidblast-neg) CL 76:10; [M-H]⁻; CL(18:1/18:2/22:5/18:2)

Plot/Text of Hit Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

Go 1. Thermo LXQ iontrap; ESI; [M-H]-; PS

#	Src.	Name
95	L	Thermo MALDI LTQ ion trap; [M-H]-; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4]+; TG 52:2 ;
98	L	Thermo LTQ Orbitrap; [M-H]-; PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H]-; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H]-; PS 36:1
102	L	Thermo LXQ iontrap; [M-H]-; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H]-; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H]-; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H]-; NA
106	L	Thermo LTQ Orbitrap; [M-H]-; PS 38:4

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(18:0/20:4)(5E,8E,11E,14
2	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(18:0/20:4)(5Z,8Z,11Z,14
3	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(18:0/20:4)(7E,10E,13E,1
4	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(20:4)(5E,8E,11E,14E)/18
5	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(20:4)(5Z,8Z,11Z,14Z)/18
6	lipidblast-neg	542	784	14.7	811	PS 38:4; [M-H]-; GPSer(20:4)(7E,10E,13E,16E)/1
7	lipidblast-neg	152	355	0.14	503	CL 84:5; [M-2H](2-); CL(22:0/18:0/22:0/22:5)
8	lipidblast-neg	142	338	0.10	479	CL 84:5; [M-2H](2-); CL(18:0/22:0/22:0/22:5)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
419.3 999.00 | 723.6 700.00 | 283.3 600.00 | 437.4 500.00 | 153.0 200.00 | 303.3 200.00 | 810.5 200.00

(Spec. List) Thermo LXQ iontrap

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo LXQ iontrap; ESI; [M-H]-; Head to Tail MF=542 RMF=784 PS 38:4; [M-H]-; GPSer(18:0/20:4)(5E,8E,11E,14E)/18 542 784R 14.7P

Difference Head to Tail Side by Side Subtraction

Name: PS 38:4; [M-H]-; GPSer(18:0/20:4)(5E,8E,11E,14E)/18
MW: 810 ID#: 125117 DB: lipidblast-neg
Comment: Parent=810.52850 Mz_exact=810.52850

7 largest peaks:
723.49647 999.00 | 419.25639 200.00 | 437.2 200.00 | 283.26354 100.00 | 303.23226 100.00

7 m/z Values and Intensities:
283.26354 100.00 sn1 FA

(lipidblast-neg) PS 38:4; [M-H]-; GPSer(18:0/20:4)(5E,8E,11E,14E)/18

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 291 spectra]

File Search View Tools Options Window Help

Go 1. Thermo LXQ iontrap; ESI; [M-H]⁻; PS

#	Src.	Name
95	L	Thermo MALDI LTQ ion trap; [M-H] ⁻ ; Lipid A
96	L	Thermo LTQ Orbitrap; ???; MGDG 34:6;
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2 ;
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap ; TG 52:2
100	L	Thermo Orbitrap Velos ESI ; [M-H] ⁻ ; GM1(d18:1/18:0);
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(11E)/24:1(15Z))
2	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(11Z)/24:1(15Z))
3	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(13Z)/24:1(15Z))
4	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(17Z)/24:1(15Z))
5	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(4E)/24:1(15Z))
6	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(6Z)/24:1(15Z))
7	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(7Z)/24:1(15Z))
8	lipidblast-neg	459	706	5.53	809	PS 42:2; [M-H] ⁻ ; GPSer(18:1(9E)/24:1(15Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo LXQ iontrap

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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:
 783.8 999.00 | 501.3 800.00 | 365.3 600.00 | 153.0 200.00 | 283.3 200.00 | 419.3 200.00 | 519.4 200.00 | 870.5 200.00 | 437.3 100.00 | 747.6 100.00

(lipidblast-neg) PS 42:2; [M-H]⁻; GPSer(18:1(11E)/24:1(15Z))

Plot/Text of Hit Plot of Hit

Name: PS 42:2; [M-H]⁻; GPSer(18:1(11E)/24:1(15Z))
 Mw: 870 ID#: 125205 DB: lipidblast-neg
 Comment: Parent=870.62243 Mz_exact=870.6224
 7 largest peaks:
 783.59040 999.00 | 417.24084 200.00 | 435.24084 200.00 | 281.24790 100.00 | 365.34174 100.00 | 281.24790 100.00 sn1 FA

Difference Head to Tail Side by Side Subtraction

459 706R 5.53P

For Help, press F1

Peptide Peptide

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)

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Thermo LTQ Orbitrap; [M-H]⁻; NA

#	Src.	Name
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmenyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+L] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 triple quadrupole; [M+L] ⁺ ; CL 60:3

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	362	522	17.2	724	CL 80:15; [M-2H] ²⁻ ; CL(18:1/18:2/22:6/22:6)
2	lipidblast-neg	362	522	17.2	724	CL 80:15; [M-2H] ²⁻ ; CL(18:2/18:1/22:6/22:6)
3	lipidblast-neg	347	506	10.4	769	CL 80:15; [M-2H] ²⁻ ; CL(22:6/18:1/22:6/18:2)
4	lipidblast-neg	325	482	4.11	733	CL 80:15; [M-2H] ²⁻ ; CL(18:1/22:6/18:2/22:6)
5	lipidblast-neg	325	482	4.11	733	CL 80:15; [M-2H] ²⁻ ; CL(18:1/22:6/22:6/18:2)
6	lipidblast-neg	325	482	4.11	733	CL 80:15; [M-2H] ²⁻ ; CL(18:2/22:6/22:6/18:1)
7	lipidblast-neg	305	458	1.87	775	CL 80:15; [M-2H] ²⁻ ; CL(18:2/22:5/18:2/22:6)
8	lipidblast-neg	300	453	1.51	870	PE 38:1; [M-H] ⁻ ; GPEtn(18:1(11E)/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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
10 largest peaks:
281.25 999.00 | 279.23 800.00 | 329.25 580.00 | 462.3 450.00 | 283.327.23 400.00 | 311.29 380.00 | 309.28 350.00 | 772.5 250.00 | 109.07

(Spec. List) Thermo LTQ Orb

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo LTQ Orbitrap; [M-H]⁻; NA Head to Tail MF=300 RMF=453 PE 38:1; [M-H]⁻; GPEtn(18:1(11E)/20:0 Difference Head to Tail Side by Side Subtraction 300 453R 1.51P

Name: PE 38:1; [M-H]⁻; GPEtn(18:1(11E)/20:0
MW: 772 ID#: 108532 DB: lipidblast-neg
Comment: Parent=772.58562 Mz_exact=772.58562
6 largest peaks:
281.24790 999.00 | 311.29482 999.00 | 478.2490.32990 50.00 |
6 m/z Values and Intensities:
281.24790 999.00 sn1 FA

(lipidblast-neg) PE 38:1; [M-H]⁻; GPEtn(18:1(11E)/20:0

Plot/Text of Hit Plot of Hit

Peptide Peptide

Name: Thermo LTQ Orbitrap; [M-H]⁻; plasmeyl-PE 38:4

MW: 750 ID#: 176 DB: Text File

Comment: plasmeyl-PE 18:0-20:4 (plasmeylethanolamine); [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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 258 spectra]

File Search View Tools Options Window Help

Go 1. Thermo LTQ Orbitrap; [M-H]⁻; plasmei

#	Src.	Name
97	A	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
98	A	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	A	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
100	A	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	A	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	A	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	A	Thermo LXQ iontrap ESI; [M-H] ⁻ ; PS 38:4
104	A	Thermo LXQ iontrap w ESI; [M-H] ⁻ ; PS 42:2 MIX
105	A	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	A	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmeyl-PE 38:4
107	A	Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li] ⁺ ; DG 34:1
108	A	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M+Li] ⁺ ; CL 60:3

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	413	937	30.1	998	plasmeyl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4)(5E,8E)
2	lipidblast-neg	413	937	30.1	998	plasmeyl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4)(5Z,8E)
3	lipidblast-neg	413	937	30.1	998	plasmeyl-PE 38:4; [M-H] ⁻ ; PE(P-18:0/20:4)(7E,11E)
4	lipidblast-neg	84	661	0.30	704	PE 37:5; [M-H] ⁻ ; GPEtn(17:1)(9Z)/20:4(5E,8E,11E)
5	lipidblast-neg	84	661	0.30	704	PE 37:5; [M-H] ⁻ ; GPEtn(17:1)(9Z)/20:4(5Z,8Z,11Z)
6	lipidblast-neg	84	661	0.30	704	PE 37:5; [M-H] ⁻ ; GPEtn(17:1)(9Z)/20:4(7E,10E,13E)
7	lipidblast-neg	84	661	0.30	704	PE 37:5; [M-H] ⁻ ; GPEtn(20:4)(5E,8E,11E,14E)/17
8	lipidblast-neg	84	661	0.30	704	PE 37:5; [M-H] ⁻ ; GPEtn(20:4)(5Z,8Z,11Z,14Z)/17

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Name: Thermo LTQ Orbitrap; [M-H]⁻; plasmeyl-PE 38:4
MW: 750 ID#: 176 DB: Text File
Comment: plasmeyl-PE 18:0-20:4 (plasmeylethanolamine); [M-H]⁻; Prec. m/z: 750.54
8 largest peaks:
303.23 999.00 | 464.31 300.00 | 750.45 180.00 | 259.24 160.00 | 446.31 205.20 | 10.00 | 285.22 10.00 | 284.90 1.00 |

Name: plasmeyl-PE 38:4; [M-H]⁻; PE(P-18:0/20:4)
MW: 750 ID#: 123341 DB: lipidblast-neg
Comment: Parent=750.54375 Mz_exact=750.5437
3 largest peaks:
303.23226 999.00 | 464.31423 250.00 | 446.31423 50.00 |
3 m/z Values and Intensities:
303.23226 999.00 sn2 FA
446.30367 50.00 [M-H]⁻-sn2-H2O

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 64 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan TSQ-7000 triple qua

#	Src.	Name
97	L	Thermo LTQ Orbitrap; [M+NH4] ⁺ ; TG 52:2
98	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; PC 32:0
99	L	Thermo LTQ Orbitrap; TG 52:2
100	L	Thermo Orbitrap Velos ESI; [M-H] ⁻ ; GM1(d18:1/18:0)
101	L	Thermo Fisher LTQ with DESI; [M-H] ⁻ ; PS 36:1
102	L	Thermo LXQ iontrap; [M-H] ⁻ ; CL 76:10
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmenyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M+Li] ⁺ ; CL 60:3

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	496	598	48.9	988	DG 34:1; [M+Li] ⁺ ; DG(16:0/18:1/0:0)
2	lipidblast-pos	496	598	48.9	988	DG 34:1; [M+Li] ⁺ ; DG(18:1/16:0/0:0)
3	lipidblast-pos	155	217	0.48	562	DG 34:1; [M+Li] ⁺ ; DG(14:1/20:0/0:0)
4	lipidblast-pos	155	217	0.48	562	DG 34:1; [M+Li] ⁺ ; DG(20:0/14:1/0:0)
5	lipidblast-pos	143	201	0.32	579	DG 34:1; [M+Li] ⁺ ; DG(12:0/22:1/0:0)
6	lipidblast-pos	143	201	0.32	579	DG 34:1; [M+Li] ⁺ ; DG(22:1/12:0/0:0)
7	lipidblast-neg	61	90	0.03	559	PG 24:4; [M-H] ⁻ ; GPGro(4:0/20:4(5E,8E,11E,14E
8	lipidblast-neg	61	90	0.03	559	PG 24:4; [M-H] ⁻ ; GPGro(4:0/20:4(5Z,8Z,11Z,14Z

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

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:
 57.3 999.00 | 81.3 800.00 | 289.2 800.00 | 94.4 600.00 | 601.7 601.70
 263.2 580.00 | 363.3 500.00 | 109.0 400.00 | 313.4 400.00 | 337.0 400.00

Name: DG 34:1; [M+Li]⁺; DG(16:0/18:1/0:0)
 MW: 601 ID#: 605 DB: lipidblast-pos
 Comment: Parent=601.53801 Mz_exact=601.53801
 8 largest peaks:
 263.25609 999.00 | 289.27173 999.00 | 601.53801 601.53801
 345.29793 400.00 | 363.30849 400.00 | 583.53801 400.00
 8 m/z Values and Intensities:
 263.25609 999.00 sn1+Li

(lipidblast-pos) DG 34:1; [M+Li]⁺; DG(16:0/18:1/0:0)

Name: DG 34:1; [M+Li]⁺; DG(16:0/18:1/0:0)
 MW: 601 ID#: 605 DB: lipidblast-pos
 Comment: Parent=601.53801 Mz_exact=601.53801
 8 largest peaks:
 263.25609 999.00 | 289.27173 999.00 | 601.53801 601.53801
 345.29793 400.00 | 363.30849 400.00 | 583.53801 400.00
 8 m/z Values and Intensities:
 263.25609 999.00 sn1+Li

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 160 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan MAT TSQ 7000 Trip

#	Src.	Name
107	A	Thermo Finnigan TSQ-7000 triple quadrupole; [M+L] ⁺ ; DG 34:1
108	A	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	A	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	A	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	A	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	A	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	A	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	A	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	A	Waters micro QTOF; [M+Na] ⁺ ; MGDG 38:4
116	A	Waters Micromass Q-ToF Micro; [M-H] ⁻ ; PG 44:12
117	A	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	A	Waters Q-ToF triple quadrupole; [M+H] ⁺ ; PC 34:1

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	368	584	35.3	604	CL 68:3; [M-H] ⁻ ; CL(16:0/18:1/18:1/16:0)
2	lipidblast-neg	366	582	32.6	607	CL 68:3; [M-H] ⁻ ; CL(16:0/18:1/16:1/18:1)
3	lipidblast-neg	336	549	9.06	584	CL 68:3; [M-H] ⁻ ; CL(16:0/18:1/18:2/16:0)
4	lipidblast-neg	333	545	8.00	569	CL 68:3; [M-H] ⁻ ; CL(16:0/18:1/18:1/16:1)
5	lipidblast-neg	306	515	2.35	549	CL 68:3; [M-H] ⁻ ; CL(16:1/18:0/16:1/18:1)
6	lipidblast-neg	306	515	2.35	549	CL 68:3; [M-H] ⁻ ; CL(18:0/16:1/16:1/18:1)
7	lipidblast-neg	302	510	1.99	548	CL 68:3; [M-H] ⁻ ; CL(16:0/18:1/16:0/18:2)
8	lipidblast-neg	301	509	1.91	542	CL 68:3; [M-H] ⁻ ; CL(14:0/20:1/16:1/18:1)

Names Structures Spec List

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:
10 largest peaks:
281 999.00 | 417 950.00 | 435 500.00 | 729 250.00 | 253 200.00 |
727 200.00 | 807 200.00 | 809 180.00 | 153 150.00 | 255 150.00 |

(Text File) Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H]⁻; CL 68:3

Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H]⁻; CL 68:3; [M-H]⁻; CL(16:0/18:1/16:1/18:1)
Head to Tail MF=366 RMF=582
Difference Head to Tail Side by Side Subtraction 366 582R 32.6P

(lipidblast-neg) CL 68:3; [M-H]⁻; CL(16:0/18:1/16:1/18:1)

Name: CL 68:3; [M-H]⁻; CL(16:0/18:1/16:1/18:1)
MW: 1401 ID#: 27285 DB: lipidblast-neg
Comment: Parent=1401.98006 Mz_exact=1401.98006
10 largest peaks:
671.46489 999.00 | 673.48053 999.00 | 417.2 435.25101 200.00 | 253.21662 100.00 | 255.2 253.21662 100.00 | sn3 FA

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 88 spectra]

File Search View Tools Options Window Help

60 1. Thermo Finnigan MAT TSQ 7000 Trip

#	Src.	Name
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmeyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+L] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+L] ⁺ ; DG 34:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370
 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	70	813	10.3	814	CL 72:8; [M-H] ⁻ ; CL(18:2/18:2/18:2/18:2)
2	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(16:0/20:4/18:2/18:2)
3	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(16:1/20:3/18:2/18:2)
4	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(18:1/18:3/18:2/18:2)
5	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(18:2/18:2/18:3/18:1)
6	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(18:2/18:2/20:3/16:1)
7	lipidblast-neg	39	702	2.81	702	CL 72:8; [M-H] ⁻ ; CL(18:2/18:2/20:4/16:0)
8	lipidblast-neg	34	669	2.26	710	CL 72:8; [M-H] ⁻ ; CL(16:0/20:4/16:0/20:4)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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]⁻; Pr
 3 largest peaks:
 695.2 999.00 | 751.2 200.00 | 415.3 150.00 |
 3 m/z Values and Intensities:

(lipidblast-neg) CL 72:8; [M-H]⁻; CL(18:2/18:2/18:2/18:2)

Plot/Text of Hit Plot of Hit

Name: CL 72:8; [M-H]⁻; CL(18:2/18:2/18:2/18:2)
 Mw: 1447 ID#: 33273 DB: lipidblast-neg
 Comment: Parent=1447.96441 Mz_exact=1447.96
 7 largest peaks:
 695.46489 999.00 | 415.22481 300.00 | 831.45744 100.00 |
 751.49110 100.00 | 1167.72433 50.00 |
 7 m/z Values and Intensities:
 279.23226 100.00 sn1 FA || sn2 FA || sn3 FA || s

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 108 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan MAT TSQ 7000 Trip

#	Src.	Name
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmenyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Water AutoSample injection system; MS; [M+H] ⁺ ; DG 34:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	714	863	81.6	882	CL 68:2; [M-H] ⁻ ; CL(16:0/18:1/18:1/16:0)
2	lipidblast-neg	665	834	16.8	883	CL 68:2; [M-H] ⁻ ; CL(16:0/18:1/16:0/18:1)
3	lipidblast-neg	509	724	0.43	767	CL 68:2; [M-H] ⁻ ; CL(16:0/18:1/16:1/18:0)
4	lipidblast-neg	509	724	0.43	767	CL 68:2; [M-H] ⁻ ; CL(16:0/18:1/18:0/16:1)
5	lipidblast-neg	509	724	0.43	767	CL 68:2; [M-H] ⁻ ; CL(16:0/18:1/20:1/14:0)
6	lipidblast-neg	490	709	0.21	756	CL 68:2; [M-H] ⁻ ; CL(14:0/20:1/16:0/18:1)
7	lipidblast-neg	456	680	0.05	842	CL 68:2; [M-H] ⁻ ; CL(18:1/16:0/18:1/16:0)
8	lipidblast-neg	363	590	0.00	731	CL 68:2; [M-H] ⁻ ; CL(14:0/20:1/18:1/16:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

(Spec. List) Thermo Finnigan

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
 10 largest peaks:
 281 999.00 | 417 700.00 | 673 500.00 | 435 400.00 | 255 350.00 |
 809 200.00 | 153 150.00 | 391 150.00 | 729 150.00 | 409 100.00 |

Thermo Finnigan MAT TSQ 7000 Head to Tail MF=456 RMF=680 CL 68:2; [M-H]⁻; CL(18:1/16:0/18:1/16:0) 456 680R 0.05P

Name: CL 68:2; [M-H]⁻; CL(18:1/16:0/18:1/16:0)
 MW: 1403 ID#: 31993 DB: lipidblast-neg
 Comment: Parent=1403.99571 Mz_exact=1403.99571
 8 largest peaks:
 673.48053 999.00 | 391.22481 300.00 | 809.47308 100.00 |
 281.24790 100.00 | 729.50674 100.00 | 1121.73999 100.00 |
 8 m/z Values and Intensities:
 255.23226 100.00 sn2 FA || sn4 FA

(lipidblast-neg) CL 68:2; [M-H]⁻; CL(18:1/16:0/18:1/16:0)

Name: CL 68:2; [M-H]⁻; CL(18:1/16:0/18:1/16:0)
 MW: 1403 ID#: 31993 DB: lipidblast-neg
 Comment: Parent=1403.99571 Mz_exact=1403.99571
 8 largest peaks:
 673.48053 999.00 | 391.22481 300.00 | 809.47308 100.00 |
 281.24790 100.00 | 729.50674 100.00 | 1121.73999 100.00 |
 8 m/z Values and Intensities:
 255.23226 100.00 sn2 FA || sn4 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 140 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan TSQ Quantum Triple

#	Src.	Name
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmeyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+L] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	...

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	custompc+h...	0	796	0.71	801	PC 32:0; [M+H] ⁺ ; GPCho(16:0/16:0)
2	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(6:0/26:0)
3	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(7:0/25:0)
4	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(8:0/24:0)
5	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(9:0/23:0)
6	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(10:0/22:0)
7	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(11:0/21:0)
8	custompc+h...	0	663	0.71	674	PC 32:0; [M+H] ⁺ ; GPCho(12:0/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
6 largest peaks:
184.2 999.00 | 734.8 20.00 | 478.7 10.00 | 496.7 10.00 | 103.9
125 5.00 |

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Finnigan TSQ Quantum Triple Quadrupole; Head to Tail MF=0 RMF=796
PC 32:0; [M+H]⁺; GPCho(16:0/16:0)
0 796R 0.71P

Difference Head to Tail Side by Side Subtraction

Name: PC 32:0; [M+H]⁺; GPCho(16:0/16:0)
MW: 734 ID#: 1583 DB: custompc+hpos.msp
Comment: Parent=734.56995 Mz_exact=734.56995
7 largest peaks:
184.07387 999.00 | 478.32987 200.00 | 496.3
734.56995 200.00 | 716.55939 10.00 |
7 m/z Values and Intensities:
184.07387 999.00 fragment C5H15NO4P

(custompc+hpos.msp) PC 32:0; [M+H]⁺; GPCho(16:0/16:0)

Plot/Text of Hit Plot of Hit

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 78 spectra]

File Search View Tools Options Window Help

MS m/z

1. Thermo Finnigan TSQ Quantum Triple

#	Src.	Name
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmeyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	...

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	474	725	93.1	934	PI 32:0; [M-H] ⁻ ; GPIs(16:0/16:0)
2	lipidblast-neg	177	388	0.93	707	MGDG 38:2; [M-H] ⁻ ; MGDG(16:0/22:2(13Z,16Z))
3	lipidblast-neg	177	388	0.93	707	MGDG 38:2; [M-H] ⁻ ; MGDG(22:2(13Z,16Z)/16:0)
4	lipidblast-pos	99	245	0.10	707	MGDG 36:0; [M+Na] ⁺ ; MGDG(16:0/20:0)
5	lipidblast-pos	99	245	0.10	707	MGDG 36:0; [M+Na] ⁺ ; MGDG(20:0/16:0)
6	lipidblast-pos	99	245	0.10	707	TG 48:2; [M+Li] ⁺ ; TG(16:0/16:1/16:1)
7	lipidblast-neg	99	245	0.10	707	MGDG 38:2; [M-H] ⁻ ; MGDG(12:0/26:2(5E,9Z))
8	lipidblast-neg	99	245	0.10	707	MGDG 38:2; [M-H] ⁻ ; MGDG(12:0/26:2(5Z,9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 a
10 largest peaks:
255.3 999.00 | 809.7 600.00 | 241.0 500.00 | 391.5 400.00 | 553.3 40
152.9 350.00 | 223.1 200.00 | 571.4 200.00 | 297.2 100.00 | 258.8 5

(Spec. List) Thermo Finnigan

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PI 32:0; [M-H]⁻; GPIs(16:0/16:0)
MW: 809 ID#: 118939 DB: lipidblast-neg
Comment: Parent=809.51800 Mz_exact=809.5180
4 largest peaks:
255.23226 999.00 | 571.28848 999.00 | 391.22509 400.00 | 297.2 100.00

(lipidblast-neg) PI 32:0; [M-H]⁻; GPIs(16:0/16:0)

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Thermo Finnigan TSQ Quantum Triple

#	Src.	Name
103	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 38:4
104	L	Thermo LXQ iontrap; ESI; [M-H] ⁻ ; PS 42:2 MIX
105	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; NA
106	L	Thermo LTQ Orbitrap; [M-H] ⁻ ; plasmeyl-PE 38:4
107	L	Thermo Finnigan TSQ-7000 triple quadrupole; [M+Li] ⁺ ; DG 34:1
108	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:3
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2

Names Structures Spec List

custompc+npos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(11E))
2	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(11Z))
3	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(13Z))
4	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(17Z))
5	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(4E))
6	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(6Z))
7	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(7Z))
8	lipidblast-neg	682	882	1.22	918	PS 36:2; [M-H] ⁻ ; GPser(18:1(11E)/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Thermo Finnigan

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
 7 largest peaks:
 417.2 999.00 | 699.6 800.00 | 281.3 500.00 | 435.2 400.00 | 152.7 200.00
 786.8 100.00 | 79.2 20.00

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H]⁻; PS 36:2; [M-H]⁻; GPser(18:1(11E))
 Difference Head to Tail Side by Side Subtraction
 682 882R 1.22P

(lipidblast-neg) PS 36:2; [M-H]⁻; GPser(18:1(11E)/18:1(11E))

Name: PS 36:2; [M-H]⁻; GPser(18:1(11E)/18:1(11E))
 MW: 786 ID#: 125162 DB: lipidblast-neg
 Comment: Parent=786.52850 Mz_exact=786.52850
 4 largest peaks:
 699.49647 999.00 | 417.24075 200.00 | 435.24075 200.00
 4 m/z Values and Intensities:
 281.24790 100.00 sn1 FA || sn2 FA
 417.24075 200.00 [M-H-87]-sn1 || [M-H-87]-sn2

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 96 spectra]

File Search View Tools Options Window Help

1. Waters AutoSpec magnetic sector MS

#	Src.	Name
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-]; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-]; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-]; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-]; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	L	Waters micro QTOF; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro; [M-]; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-]; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-]; GM1
119	L	Waters QTOF Premier; [M-]; Ac2PIM2
120	L	Waters QTOF Premier; [M-]; BA 24:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	236	514	72.4	633	PC 24:0; [M+H] ⁺ ; GPCho(12:0/12:0)
2	custompc+h...	186	407	14.7	486	PC 24:0; [M+H] ⁺ ; GPCho(12:0/12:0)
3	lipidblast-pos	138	355	3.05	612	MGDG 23:0; [M+NH4] ⁺ ; MGDG(11:0/12:0)
4	lipidblast-pos	138	355	3.05	612	MGDG 23:0; [M+NH4] ⁺ ; MGDG(12:0/11:0)
5	lipidblast-pos	79	229	0.55	395	MGDG 25:0; [M+NH4-CO] ⁺ ; MGDG(12:0/13:0)
6	lipidblast-pos	79	229	0.55	395	MGDG 25:0; [M+NH4-CO] ⁺ ; MGDG(13:0/12:0)
7	lipidblast-neg	61	183	0.28	316	PS 24:0; [M-]; GPSer(7:0/17:0)
8	lipidblast-neg	61	183	0.28	316	PS 24:0; [M-]; GPSer(17:0/7:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 sp
5 largest peaks:
622.7 999.00 | 422.6 620.00 | 440.3 600.00 | 644.6 600.00 | 585.5 10
5 m/z Values and Intensities:

(Spec. List) Waters AutoSpec

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 24:0; [M+H]⁺; GPCho(12:0/12:0)
Mw: 622 ID#: 37601 DB: lipidblast-pos
Comment: Parent=622.44477 Mz_exact=622.4447
5 largest peaks:
563.37127 999.00 | 422.26725 600.00 | 440.2
422.26725 600.00 [M+H]-sn1-H2O || [M+H]-sn2+
439.37873 400.00 [M+H]-C5H14NO4P (-183)

(lipidblast-pos) PC 24:0; [M+H]⁺; GPCho(12:0/12:0)

Plot/Text of Hit Plot of Hit

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 Ionization Quadrupole Time-of-Flight Tandem Mass
Spectrometry

10 largest peaks:

NIST MS Search 2.0 - [Peptide, Presearch Default - 94 spectra]

File Search View Tools Options Window Help

Go 1. Waters micro QTOF : [M+Na]⁺; MGDG 38:4

#	Src.	Name
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-ToF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M+H] ⁺ ; BA 24:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(6Z,9Z,12Z)/
2	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(6Z,9Z,12Z)/
3	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(6Z,9Z,12Z)/
4	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(6Z,9Z,12Z)/
5	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(9Z,12Z,15Z)/
6	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(9Z,12Z,15Z)/
7	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(9Z,12Z,15Z)/
8	lipidblast-pos	170	298	5.67	957	MGDG 38:4; [M+Na] ⁺ ; MGDG(18:3(9Z,12Z,15Z)/

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 Ionization Quadrupole Time-of-Flight Tandem Mass Spectrometry

10 largest peaks:
333.4 999.00 | 783.8 999.00 | 243.2 700.00 | 315.3 600.00 | 293.2 500.00
335.4 400.00 | 341.4 400.00 | 829.9 400.00 | 519.5 350.00 | 830.9 300.00

(Spec. List) Waters micro QT

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Waters micro QTOF ; [M+Na]⁺; MGDG 38:4; [M+Na]⁺; MGDG(18:3(6Z,9Z,12Z)/

Difference Head to Tail Side by Side Subtraction 170 298R 5.67P

Name: MGDG 38:4; [M+Na]⁺; MGDG(18:3(6Z,9Z,12Z)/

MW: 829 ID#: 12497 DB: lipidblast-pos
Comment: Parent=829.58057 Mz_exact=829.58057

2 largest peaks:
519.29357 999.00 | 551.35613 999.00

2 m/z Values and Intensities:
519.29357 999.00 [M+Na]⁺-sn2
551.35613 999.00 [M+Na]⁺-sn1

(lipidblast-pos) MGDG 38:4; [M+Na]⁺; MGDG(18:3(6Z,9Z,12Z)/

Plot/Text of Hit Plot of Hit

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]⁻; m/z=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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 16 spectra]

File Search View Tools Options Window Help

1. Waters Micromass Q-TOF Micro ; [M-H]⁻

#	Src.	Name
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M+H] ⁺ ; BA 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	135	785	67.1	933	PG 44:12; [M-H] ⁻ ; GPGro(22:6(4Z,7Z,10Z,13Z,16Z,19Z))
2	lipidblast-neg	53	570	6.84	707	DGDG 31:6; [M-H] ⁻ ; DGDG(9:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
3	lipidblast-neg	53	570	6.84	707	DGDG 31:6; [M-H] ⁻ ; DGDG(22:6(4Z,7Z,10Z,13Z,16Z,19Z))
4	lipidblast-neg	37	481	3.94	571	PI 37:7; [M-H] ⁻ ; GPIs(15:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
5	lipidblast-neg	37	481	3.94	571	PI 37:7; [M-H] ⁻ ; GPIs(22:6(4Z,7Z,10Z,13Z,16Z,19Z))
6	lipidblast-neg	14	250	1.43	620	PI 36:0; [M-H] ⁻ ; GPIs(18:0/18:0)
7	lipidblast-neg	13	247	1.38	302	SQDG 38:6; [M-H] ⁻ ; SQDG(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
8	lipidblast-neg	13	247	1.38	302	SQDG 38:6; [M-H] ⁻ ; SQDG(22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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]⁻; m/z=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:
327.222 999.00 | 865.336 300.00 | 283.217 250.00 | 229.175 50.00 |
209.052 30.00 | 463.256 30.00 | 537.311 30.00 | 555.274 30.00 |

(Spec. List) Waters Micromass Q-TOF Micro ; [M-H]⁻; PG 44:12

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PG 44:12; [M-H]⁻; GPGro(22:6(4Z,7Z,10Z,13Z,16Z,19Z))
MW: 865 ID#: 116988 DB: lipidblast-neg
Comment: Parent=865.50195 Mz_exact=865.50195
4 largest peaks:
327.23226 999.00 | 463.22509 200.00 | 537.23226 200.00 | 555.27243 200.00 |

(lipidblast-neg) PG 44:12; [M-H]⁻; GPGro(22:6(4Z,7Z,10Z,13Z,16Z,19Z))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 249 spectra]

File Search View Tools Options Window Help

MS m/z

1. Waters MicroMass QqQ triple quadrupole

#	Src.	Name
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	L	Waters micro QTOF; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-ToF Micro; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M+H] ⁺ ; PA 24:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	64	426	3.01	922	SQDG 30:0; [M-H] ⁻ ; SQDG(14:0/16:0)
2	lipidblast-neg	64	426	3.01	922	SQDG 30:0; [M-H] ⁻ ; SQDG(16:0/14:0)
3	lipidblast-neg	45	342	1.46	845	SQDG 30:0; [M-H] ⁻ ; SQDG(15:0/15:0)
4	lipidblast-neg	41	319	1.23	775	SQDG 30:0; [M-H] ⁻ ; SQDG(12:0/18:0)
5	lipidblast-neg	41	319	1.23	775	SQDG 30:0; [M-H] ⁻ ; SQDG(18:0/12:0)
6	lipidblast-neg	38	302	1.09	745	SQDG 30:0; [M-H] ⁻ ; SQDG(4:0/26:0)
7	lipidblast-neg	38	302	1.09	745	SQDG 30:0; [M-H] ⁻ ; SQDG(5:0/25:0)
8	lipidblast-neg	38	302	1.09	745	SQDG 30:0; [M-H] ⁻ ; SQDG(6:0/24:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(Spec. List) Waters MicroMa

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

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
 10 largest peaks:
 81.19 999.00 | 165.20 400.00 | 225.32 300.00 | 765.97 150.00 | 227.
 243.13 20.00 | 255.53 20.00 | 283.35 10.00 | 509.71 10.00 | 537.

(lipidblast-neg) SQDG 30:0; [M-H]⁻; SQDG(14:0/16:0)

Plot/Text of Hit Plot of Hit

Name: SQDG 30:0; [M-H]⁻; SQDG(14:0/16:0)
 Mw: 765 ID#: 129464 DB: lipidblast-neg
 Comment: Parent=765.48228 Mz_exact=765.4822
 5 largest peaks:
 225.00690 999.00 | 509.24220 300.00 | 537.2
 5 m/z Values and Intensities:
 225.00690 999.00 fragment C6H9O7S
 227.20098 100.00 sn1 FA

Peptide Peptide

Name: Waters QqQ triple quadrupole 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

NIST MS Search 2.0 - [Peptide, Presearch Default - 31 spectra]

File Search View Tools Options Window Help

1. Waters QqQ triple quadrupole VG Quattro II

#	Src.	Name
109	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 72:8
110	L	Thermo Finnigan MAT TSQ 7000 Triple Quadrupole; [M-H] ⁻ ; CL 68:2
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+H] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+H] ⁺ ; PC 24:0
115	L	Waters micro QTOF; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M+H] ⁺ ; DA 24:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; Ganglioside; [M-H] ⁻ ; NeuAcalp
2	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; GM1(d18:1/20:0); [M-H] ⁻ ; Gall
3	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; cis GM1, GM1b(d18:1/20:0); [M-H] ⁻
4	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; GM1alpha(d18:1/20:0); [M-H] ⁻
5	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; sialyl-lactotetraosylceramide(d18:1/20:0); [M-H] ⁻
6	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; sialyl(2-6)lactotetraosylceramide(d18:1/20:0); [M-H] ⁻
7	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; Ganglioside; [M-H] ⁻ ; Galbeta1-4
8	lipidblast-neg	353	659	10.9	895	[glycan]-Cer 38:1; Ganglioside; [M-H] ⁻ ; NeuAcalp

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

Name: Waters QqQ triple quadrupole 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:
290.1 999.00 | 1572.5 999.00 | 916.5 500.00 | 1574.6 500.00 | 916.5 500.00 | 1575.6 200.00 | 754.4 180.00 | 592.5 120.00 | 736.5 120.00 | 916.5 500.00

(Spec. List) Waters QqQ triple quadrupole VG Quattro II

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: [glycan]-Cer 38:1; GM1(d18:1/20:0); [M-H]⁻
MW: 1572 ID#: 79308 DB: lipidblast-neg
Comment: Parent=1572.90013 Mz_exact=1572.90013

5 largest peaks:
1572.90013 999.00 | 1281.80472 500.00 | 290.08759 400.00 | 592.56651 200.00 | 1281.80472 500.00

5 m/z Values and Intensities:
290.08759 400.00 ion C11H16NO8- [290.08759]
592.56651 200.00 ion ceramide

(lipidblast-neg) [glycan]-Cer 38:1; GM1(d18:1/20:0); [M-H]⁻

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - Peptide Research Default - 8 spectra

ChemMate
http://128.120.136.66:8080/compound-repository/homePage/index

1. Waters QTOF Premier; [M-H]⁻; Ac2PIM2

#	Src.	Name
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+] ⁺ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+] ⁺ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+] ⁺ ; PC 24:0
115	L	Waters micro QTOF; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro; [M+] ⁺ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M+] ⁺ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M+] ⁺ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M+] ⁺ ; PE 34:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	382	595	24.8	782	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(16:0/19:0)
2	lipidblast-neg	382	595	24.8	782	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(16:0/methyl-18:0)
3	lipidblast-neg	382	595	24.8	782	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(19:0/16:0)
4	lipidblast-neg	382	595	24.8	782	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(methyl-18:0/16:0)
5	lipidblast-neg	47	105	0.24	263	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(15:0/20:0)
6	lipidblast-neg	47	105	0.24	263	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(17:0/18:0)
7	lipidblast-neg	47	105	0.24	263	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(18:0/17:0)
8	lipidblast-neg	47	105	0.24	263	Ac2PIM2 35:0; [M-H] ⁻ ; Ac2PIM2(20:0/15:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
297.2748 999.00 | 1175.6753 700.00 | 621.1405 500.00 | 255.2326 392.2321 350.00 | 639.1478 300.00 | 500 200.00 | 919.4312

(Spec. List) Waters QTOF Premier

Waters QTOF Premier; [M-H]⁻; Ac2PIM2

Name: Ac2PIM2 35:0; [M-H]⁻; Ac2PIM2(methyl-18:0/16:0)
MW: 1175 ID#: 279 DB: lipidblast-neg
Comment: Parent=1175.67061 Mz_exact=1175.67061

7 largest peaks:
877.38361 999.00 | 919.43053 999.00 | 255.23226 1175.67061 100.00 | 1013.61779 50.00 | 255.23226 400.00 sn2 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 9 spectra]

File Search View Tools Options Window Help

Go 1. Waters QTOF Premier; [M-H]-; Gangli...

#	Src.	Name
118	A	Waters QqQ triple quadrupole VG Quattro II; [M-H]-; GM1
119	A	Waters QTOF Premier; [M-H]-; Ac2PIM2
120	A	Waters QTOF Premier; [M-H]-; Ganglioside; [glycan]-Cer(d18:1, C24:1)
121	A	Waters QTOF Premier; [M-H]-; Ganglioside; [glycan]-Cer(d18:1, C16:0)
122	A	Waters QTOF Premier; [M-H]-; PA 34:1
123	A	Waters QTOF Premier; [M-H]-; NA
124	A	Waters QTOF Premier; [M-H]-; PE 34:0
125	A	Waters QTOF Premier; [M-H]-; PE 34:1
126	A	Waters QTOF Premier; [M-H]-; PG 34:1
127	A	Waters QTOF Premier; [M-H]-; NA
128	A	Waters QTOF Premier; [M-H]-; PS 34:1
129	A	Waters QTOF Premier; [M-H]-; PC 34:1

lipidblast-neg; lipidblast-pos; custompc+hpos.msp; custompc+napos.msp; pc-ac-neg.msp; pc-form-neg.msp; 234420 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; Ganglioside; [M-H]-; NeuAcalp
2	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; GM1(d18:1/24:1); [M-H]-; Gal
3	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; cis GM1, GM1b(d18:1/24:1); [M-H]-; Gal
4	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; GM1 alpha(d18:1/24:1); [M-H]-; Gal
5	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; sialyl-lactotetraosylceramide(d18:1/24:1); [M-H]-; Gal
6	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; sialyl(2-6)lactotetraosylceramide(d18:1/24:1); [M-H]-; Gal
7	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; Ganglioside; [M-H]-; Galbeta1-
8	lipidblast-neg	65	806	11.1	834	[glycan]-Cer 42:2; Ganglioside; [M-H]-; NeuAcalp

Names Structures Spec List

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;
 10 largest peaks:
 290.16 999.00 | 1627.1 400.00 | 1335.95 133.00 | 970.81 37.00 |
 1173.89 31.00 | 1155.90 18.00 | 646.68 12.00 | 470.23 1.00

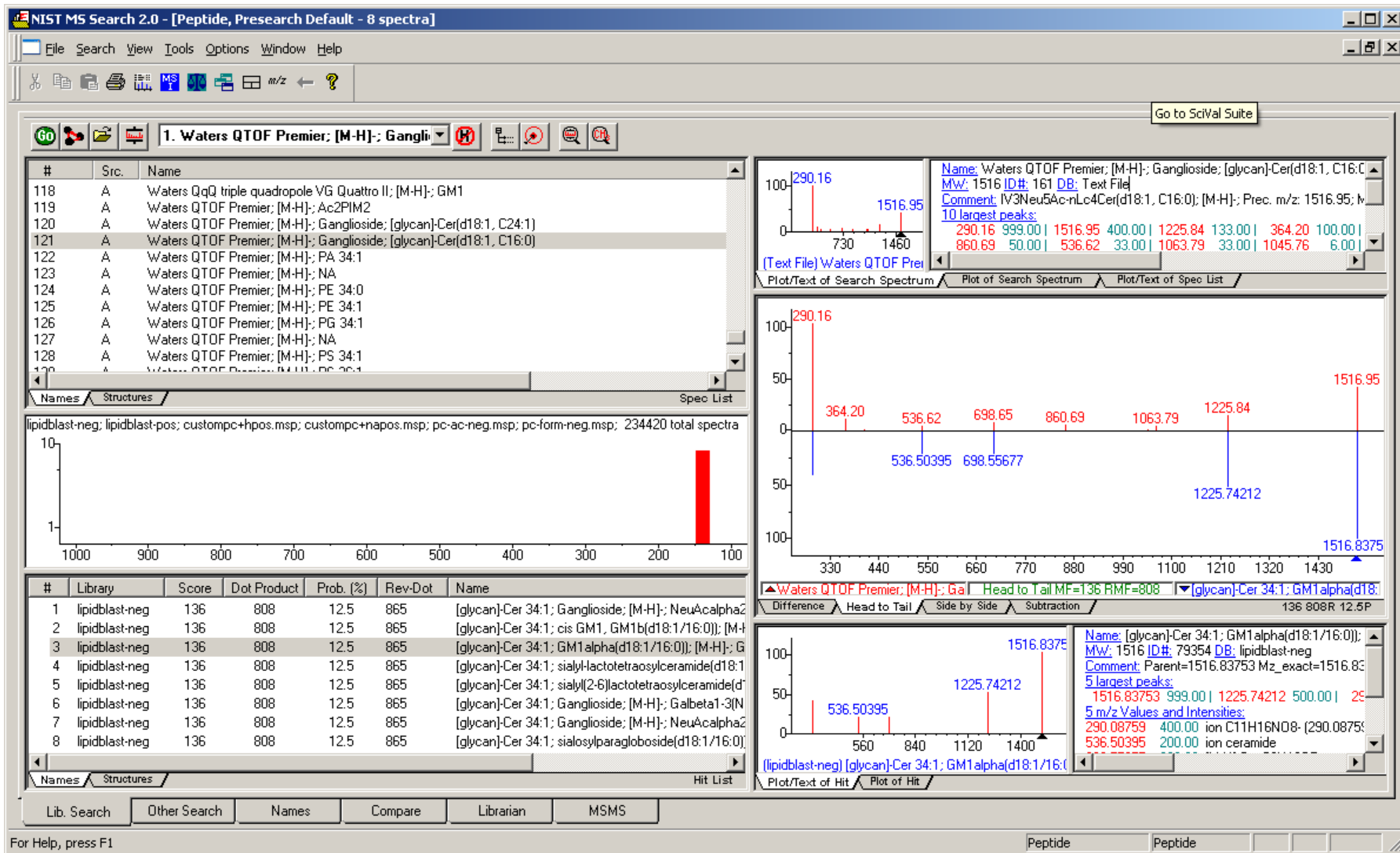
Waters QTOF Premier; [M-H]-; Gal Head to Tail MF=65 RMF=806 [glycan]-Cer 42:2; GM1(d18:1/24:1); [M-H]-; Gal
 65 806R 11.1P

(lipidblast-neg) [glycan]-Cer 42:2; GM1(d18:1/24:1); [M-H]-; Gal
 MW: 1626 ID#: 79312 DB: lipidblast-neg
 Comment: Parent=1626.94708 Mz_exact=1626.94708
 5 largest peaks:
 1626.94708 999.00 | 1335.85167 500.00 | 290.08759 400.00
 5 m/z Values and Intensities:
 290.08759 400.00 ion C11H16NO8- (290.08759) ion ceramide
 646.61343 200.00 ion ceramide

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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
 Reviews/Volume 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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 80 spectra]

File Search View Tools Options Window Help

Go 1. Waters QTOF Premier; [M-H]⁻; PA 34:1

#	Src.	Name
111	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M+] ⁺ ; PC 32:0
112	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PI 32:0
113	L	Thermo Finnigan TSQ Quantum Triple Quadrupole; [M-H] ⁻ ; PS 36:2
114	L	Waters AutoSpec magnetic sector MS; [M+] ⁺ ; PC 24:0
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PC 34:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(11E))
2	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(11Z))
3	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(13Z))
4	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(17Z))
5	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(4E))
6	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(6Z))
7	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(7Z))
8	lipidblast-neg	509	708	5.50	860	PA 34:1; [M-H] ⁻ ; GPA(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
152.9608 999.00 | 255.1864 999.00 | 281.2081 950.00 | 391.1979 500.00
436.2561 200.00 | 170.9940 100.00 | 673.4825 100.00

(Spec. List) Waters QTOF Premier; [M-H]⁻; PA 34:1

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Waters QTOF Premier; [M-H]⁻; PA 34:1 Head to Tail MF=509 RMF=708 PA 34:1; [M-H]⁻; GPA(16:0/18:1(11E))

Difference Head to Tail Side by Side Subtraction 509 708R 5.50P

Name: PA 34:1; [M-H]⁻; GPA(16:0/18:1(11E))
MW: 673 ID#: 102518 DB: lipidblast-neg
Comment: Parent=673.48083 Mz_exact=673.48083
6 largest peaks:
255.23226 999.00 | 281.24790 999.00 | 409.23567 50.00 | 417.24075 50.00
6 m/z Values and Intensities:
255.23226 999.00 sn1 FA

(lipidblast-neg) PA 34:1; [M-H]⁻; GPA(16:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 197 spectra] <https://scifinder.cas.org/>

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; NA

#	Src.	Name
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PC 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(14:0/20:1(11E))
2	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(14:0/20:1(11Z))
3	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(14:0/20:1(13E))
4	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(14:0/20:1(13Z))
5	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(20:1(11E)/14:0)
6	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(20:1(11Z)/14:0)
7	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(20:1(13E)/14:0)
8	lipidblast-neg	29	556	0.99	657	PE 34:1; [M-H] ⁻ ; GPEtn(20:1(13Z)/14:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
4 largest peaks:
227.1755 999.00 | 281.2328 400.00 | 506.3202 10.00 | 716.5045
4 m/z Values and Intensities:

(Spec. List) Waters QTOF Premier

Name: PE 34:1; [M-H]⁻; GPEtn(14:0/20:1(11E))
MW: 716 ID#: 107719 DB: lipidblast-neg
Comment: Parent=716.52306 Mz_exact=716.5230
6 largest peaks:
227.20098 999.00 | 309.27918 999.00 | 424.24662 50.00 | 488.31426 50.00 |
6 m/z Values and Intensities:
227.20098 999.00 sn1 FA

(lipidblast-neg) PE 34:1; [M-H]⁻; GPEtn(14:0/20:1(11E))

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 109 spectra] <https://scifinder.cas.org/>

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PE 34:0

#	Src.	Name
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	70	864	6.16	960	PE 34:0; [M-H] ⁻ ; GPEtn(17:0/17:0)
2	lipidblast-pos	4	268	0.97	306	MGDG 32:1; [M+NH4-CD] ⁺ ; MGDG(15:1(9Z)/17
3	lipidblast-pos	4	268	0.97	306	MGDG 32:1; [M+NH4-CD] ⁺ ; MGDG(17:0/15:1(9
4	lipidblast-pos	3	206	0.93	500	MGDG 32:1; [M+NH4-CD] ⁺ ; MGDG(15:0/17:1(9
5	lipidblast-pos	3	206	0.93	500	MGDG 32:1; [M+NH4-CD] ⁺ ; MGDG(17:1(9Z)/15
6	custompc+h...	3	100	0.93	262	PC 31:1; [M+H] ⁺ ; GPCho(14:1(9Z)/17:0)
7	custompc+h...	3	100	0.93	262	PC 31:1; [M+H] ⁺ ; GPCho(17:0/14:1(9Z))
8	lipidblast-neg	2	196	0.89	224	PS 31:1; [M-H] ⁻ ; GP5er(14:1(9Z)/17:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
269.2297 999.00 | 718.4834 800.00 | 719.1092 500.00 | 269.6114 220.00
5 m/z Values and Intensities:

(Spec. List) Waters QTOF Premier; [M-H]⁻; PE 34:0

Waters QTOF Premier; [M-H]⁻; PE 34:0
MW: 718 ID#: 108212 DB: lipidblast-neg
Comment: Parent=718.53869 Mz_exact=718.53869
3 largest peaks:
269.24790 999.00 | 466.29353 200.00 | 448.28297 50.00
3 m/z Values and Intensities:
269.24790 999.00 sn1 FA || sn2 FA
448.28297 50.00 [M-H]-sn1-H2O || [M-H]-sn2-H2O

Waters QTOF Premier; [M-H]⁻; PE 34:0; [M-H]⁻; GPEtn(17:0/17:0)
Difference Head to Tail Side by Side Subtraction 70 864 R 6.16 P

(lipidblast-neg) PE 34:0; [M-H]⁻; GPEtn(17:0/17:0)

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 202 spectra] <https://scifinder.cas.org/>

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PE 34:1

#	Src.	Name
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(11E))
2	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(11Z))
3	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(13Z))
4	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(17Z))
5	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(4E))
6	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(6Z))
7	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(7Z))
8	lipidblast-neg	404	895	5.50	923	PE 34:1; [M-H] ⁻ ; GPEtn(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
281.2205 999.00 | 255.2099 600.00 | 140.0014 100.00 | 452.2726 50.00

5 m/z Values and Intensities:

(Spec. List) Waters QTOF Premier

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PE 34:1; [M-H]⁻; GPEtn(16:0/18:1(11E))
MW: 716 ID#: 107994 DB: lipidblast-neg
Comment: Parent=716.52306 Mz_exact=716.52306

6 largest peaks:
255.23226 999.00 | 281.24790 999.00 | 452.2726 50.00 | 460.28298 50.00

6 m/z Values and Intensities:
255.23226 999.00 sn1 FA

(lipidblast-neg) PE 34:1; [M-H]⁻; GPEtn(16:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 222 spectra]

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PG 34:1

#	Src.	Name
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1

Names / Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(11E))
2	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(11Z))
3	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(13Z))
4	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(17Z))
5	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(4E))
6	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(6Z))
7	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(7Z))
8	lipidblast-neg	559	781	5.43	896	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(9E))

Names / Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 ph
8 largest peaks:
281.1957 999.00 | 255.1864 800.00 | 747.4617 700.00 | 152.9698 500
391.2051 300.00 | 483.2516 300.00 | 491.2730 200.00 |

(Spec. List) Waters QTOF Pr

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PG 34:1; [M-H]⁻; GPGro(16:0/18:1(11E))
MW: 747 ID#: 113470 DB: lipidblast-neg
Comment: Parent=747.51763 Mz_exact=747.5176
8 largest peaks:
255.23226 999.00 | 281.24790 999.00 | 391.2
483.27247 200.00 | 491.27755 200.00 | 509.2
255.23226 999.00 sn1 FA

(lipidblast-neg) PG 34:1; [M-H]⁻; GPGro(16:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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,Prezni,Ryan,Rainville,Baker; 720001756EN; 10 largest peaks:

Unknown wrongly assigned FA missing

NIST MS Search 2.0 - [Peptide, Presearch Default - 328 spectra]

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PS 40:1

#	Src.	Name
115	L	Waters micro QTOF ; [M+Na] ⁺ ; MGDG 38:4
116	L	Waters Micromass Q-TOF Micro ; [M-H] ⁻ ; PG 44:12
117	L	Waters MicroMass QqQ triple quadrupole; [M-H] ⁻ ; SQDG 30:0
118	L	Waters QqQ triple quadrupole VG Quattro II; [M-H] ⁻ ; GM1
119	L	Waters QTOF Premier; [M-H] ⁻ ; Ac2PIM2
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(11E)
2	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(11Z)
3	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(13Z)
4	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(17Z)
5	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(4E)
6	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(6Z)
7	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(7Z)
8	pc-ac-neg.m...	113	506	1.07	655	PC 36:2; [M-Ac-H] ⁻ ; GPCho(18:1(11E))/18:1(9E)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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

10 largest peaks:
281.2476 999.00 | 282.2514 220.00 | 303.2322 188.00 | 770.5710 180
766.5373 98.00 | 844.6067 79.00 | 506.3250 74.00 | 304.2348 50

(Spec. List) Waters QTOF Premier; [M-H]⁻; PS 40:1

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: PC 36:2; [M-Ac-H]⁻; GPCho(18:1(11E))/18:1
MW: 844 **ID#:** 2569 **DB:** pc-ac-neg.msp
Comment: Parent=844.60675 Mz_exact=844.6067

3 largest peaks:
770.56997 999.00 | 281.24790 100.00 | 844.60675 50

3 m/z Values and Intensities:
281.24790 100.00 FA sn1 || FA sn2
770.56997 999.00 [M-CH3]⁻ (-15)

(pc-ac-neg.msp) PC 36:2; [M-Ac-H]⁻; GPCho(18:1(11E))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 400 spectra]

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PS 34:1

#	Src.	Name
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(11E))
2	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(11Z))
3	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(13Z))
4	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(17Z))
5	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(4E))
6	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(6Z))
7	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(7Z))
8	lipidblast-neg	639	772	5.54	843	PS 34:1; [M-H] ⁻ ; GPSer(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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:
391.1833 999.00 | 255.2158 900.00 | 152.9790 800.00 | 281.2390 800.00
417.2129 600.00 | 435.2339 200.00 | 153.9870 10.00 | 760.5132 10.00

(Spec. List) Waters QTOF Premier; [M-H]⁻; PS 34:1

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Waters QTOF Premier; [M-H]⁻; PS 34:1; Head to Tail MF=639 RMF=772 PS 34:1; [M-H]⁻; GPSer(16:0/18:1(11E))

Difference Head to Tail Side by Side Subtraction 639 772R 5.64P

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

7 largest peaks:
673.48084 999.00 | 391.22512 200.00 | 409.22512 100.00 | 281.24790 100.00

7 m/z Values and Intensities:
255.23226 100.00 | 391.22512 200.00 | 409.22512 100.00 | 673.48084 999.00

(lipidblast-neg) PS 34:1; [M-H]⁻; GPSer(16:0/18:1(11E))

Plot/Text of Hit Plot of Hit

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 397 spectra]

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M-H]⁻; PS 36:1

#	Src.	Name
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2
131	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(11E))
2	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(11Z))
3	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(13Z))
4	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(17Z))
5	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(4E))
6	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(6Z))
7	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(7Z))
8	lipidblast-neg	572	715	5.45	845	PS 36:1; [M-H] ⁻ ; GPSer(18:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 phot
9 largest peaks:
419.2157 999.00 | 283.2244 900.00 | 701.4664 900.00 | 152.9698 700.00
417.2129 500.00 | 437.2410 500.00 | 438.2578 200.00 | 788.5463 100.00

Name: PS 36:1; [M-H]⁻; GPSer(18:0/18:1(11E))
MW: 788 ID#: 125088 DB: lipidblast-neg
Comment: Parent=788.54418 Mz_exact=788.5441
7 largest peaks:
701.51215 999.00 | 417.24079 200.00 | 419.2157 100.00
281.24790 100.00 | 283.26354 100.00 |
281.24790 100.00 sn2 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 100 spectra]

Tools : Nature Lipidomics Gateway
http://www.lipidmaps.org/tools/structuredrawing/StrDraw.pl

File Search View Tools Options Window Help

1. Waters QTOF Premier; [M+Na]⁺; MGC

#	Src.	Name
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	167	615	15.5	699	DGDG 22:3; [M+Na] ⁺ ; DGDG(4:0/18:3(6Z,9Z,12Z))
2	lipidblast-pos	167	615	15.5	699	DGDG 22:3; [M+Na] ⁺ ; DGDG(4:0/18:3(9Z,12Z,15Z))
3	lipidblast-pos	167	615	15.5	699	DGDG 22:3; [M+Na] ⁺ ; DGDG(18:3(6Z,9Z,12Z))
4	lipidblast-pos	167	615	15.5	699	DGDG 22:3; [M+Na] ⁺ ; DGDG(18:3(9Z,12Z,15Z))
5	lipidblast-pos	79	407	1.35	577	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z))/20:
6	lipidblast-pos	79	407	1.35	577	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z))/20:
7	lipidblast-pos	79	407	1.35	577	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z))/20:
8	lipidblast-pos	79	407	1.35	577	PA 38:4; [M+Na2H] ⁺ ; GPA(18:3(6Z,9Z,12Z))/20:

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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:
491.2625 999.00 | 769.4885 800.00 | 770.4918 600.00 | 519.2942 550.00
771.4944 200.00 | 607.4341 20.00 |

(Spec. List) Waters QTOF Premier; [M+Na]⁺; MGDG 34:6

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: DGDG 22:3; [M+Na]⁺; DGDG(4:0/18:3(6Z,9Z,12Z))
MW: 769 ID#: 3883 DB: lipidblast-pos
Comment: Parent=769.39867 Mz_exact=769.39867

4 largest peaks:
329.12141 999.00 | 491.17423 999.00 | 519.2942 999.00 | 681.34627 999.00

(lipidblast-pos) DGDG 22:3; [M+Na]⁺; DGDG(4:0/18:3(6Z,9Z,12Z))

Plot/Text of Hit Plot of Hit

Peptide Peptide

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 218 spectra]

Tools : Nature Lipidomics Gateway
<http://www.lipidmaps.org/tools/structuredrawing/StrDraw.pl>

File Search View Tools Options Window Help

Go 1. Waters QTOF Premier; [M-H]⁻; PG 34:1

#	Src.	Name
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2
131	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

Plot/Text of Search Spectrum

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:
281.2436 999.00 | 255.23226 500.00 | 747.5078 400.00 | 152.9957 250.00 | 227.0278 20.00

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Waters QTOF Premier; [M-H]⁻; PG 34:1 Head to Tail MF=190 RMF=696 PG 34:1; [M-H]⁻; GPGro(16:0/18:1) 190 696R 4.63P

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(11E))
2	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(11Z))
3	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(13Z))
4	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(17Z))
5	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(4E))
6	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(6Z))
7	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(7Z))
8	lipidblast-neg	190	696	4.63	779	PG 34:1; [M-H] ⁻ ; GPGro(16:0/18:1(9E))

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Plot/Text of Hit Plot of Hit

Name: PG 34:1; [M-H]⁻; GPGro(16:0/18:1(11E))
MW: 747 ID#: 113470 DB: lipidblast-neg
Comment: Parent=747.51763 Mz_exact=747.51763
8 largest peaks:
255.23226 999.00 | 281.24790 999.00 | 391.22513 200.00 | 483.27247 200.00 | 491.27755 200.00 | 509.22513 200.00 | 255.23226 999.00 sn1 FA

Peptide Peptide

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

NIST MS Search 2.0 - [Peptide, Presearch Default - 123 spectra]

File Search View Tools Options Window Help

Go 1. Waters QTOF Premier; [M-H]⁻; SQDG

#	Src.	Name
120	L	Waters QTOF Premier; [M-H] ⁻ ; PA 34:1
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2
131	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[2E,4E])
2	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[6Z,9Z])
3	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[9E,10E])
4	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[9E,12E])
5	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[9Z,11Z])
6	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(16:0/18:2[9Z,12Z])
7	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(18:2[2E,4E]/16:0)
8	lipidblast-neg	755	985	8.19	993	SQDG 34:2; [M-H] ⁻ ; SQDG(18:2[6Z,9Z]/16:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Peptide Peptide

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 characteri
8 largest peaks:
225.0061 999.00 | 817.5167 600.00 | 818.5209 400.00 | 537.2714 250.00
819.5173 200.00 | 279.2322 50.00 | 255.2292 40.00 |

Name: SQDG 34:2; [M-H]⁻; SQDG(16:0/18:2[2E,4E]
MW: 817 ID#: 129776 DB: lipidblast-neg
Comment: Parent=817.51358 Mz_exact=817.5135
5 largest peaks:
225.00690 999.00 | 537.27350 300.00 | 561.2
5 m/z Values and Intensities:
225.00690 999.00 fragment C6H9O7S
255.23226 100.00 sn1 FA

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:

NIST MS Search 2.0 - [Peptide, Presearch Default - 208 spectra]

File Search View Tools Options Window Help

MS m/z

1. Waters Synapt HDMS; [M+Na]⁺; PC 32:0

#	Src.	Name
121	L	Waters QTOF Premier; [M-H] ⁻ ; NA
122	L	Waters QTOF Premier; [M-H] ⁻ ; PE 34:0
123	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
124	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
125	L	Waters QTOF Premier; [M-H] ⁻ ; PS 40:1
126	L	Waters QTOF Premier; [M-H] ⁻ ; PS 34:1
127	L	Waters QTOF Premier; [M-H] ⁻ ; PS 36:1
128	L	Waters QTOF Premier; [M+Na] ⁺ ; MGDG 34:6
129	L	Waters QTOF Premier; [M-H] ⁻ ; PG 34:1
130	L	Waters QTOF Premier; [M-H] ⁻ ; SQDG 34:2
131	L	Waters Synapt HDMS; [M+Na] ⁺ ; PC 32:0

Names Structures Spec List

custompc+hpos.msp; custompc+napos.msp; hilic-urine; lipidblast-neg; pc-ac-neg.msp; pc-form-neg.msp; lipidblast-pos; 235370 total spectra

#	Library	Score	Dot Product	Prob. (%)	Rev-Dot	Name
1	lipidblast-pos	393	635	12.1	974	PC 32:0; [M+Na] ⁺ ; GPCho(16:0/16:0)
2	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(6:0/26:0)
3	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(7:0/25:0)
4	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(8:0/24:0)
5	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(9:0/23:0)
6	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(10:0/22:0)
7	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(11:0/21:0)
8	lipidblast-pos	369	611	4.04	946	PC 32:0; [M+Na] ⁺ ; GPCho(12:0/20:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian MSMS

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
9 largest peaks:
756.5524 999.00 | 146.9827 680.00 | 697.4801 510.00 | 573.4851 500.00
86.0943 200.00 | 184.0753 150.00 | 478.3405 22.00 | 500.3149 20.00

(Spec. List) Waters Synapt H

Plot/Text of Search Spectrum Plot of Search Spectrum Plot/Text of Spec List

Name: Waters Synapt HDMS; [M+Na]⁺; PC 32:0
MW: 756 ID#: 131 DB: Spec. List
Comment: Parent=756.55190 Mz_exact=756.55190
5 largest peaks:
697.47840 999.00 | 573.48586 600.00 | 441.23832 40.00 | 500.31182 20.00 | [M+Na]-sn1-H2O || [M+Na]-sn1

Waters Synapt HDMS; [M+Na]⁺; Head to Tail MF=393 RMF=635 PC 32:0; [M+Na]⁺; GPCho(16:0/16:0) 393 635R 12.1P

Difference Head to Tail Side by Side Subtraction

Name: PC 32:0; [M+Na]⁺; GPCho(16:0/16:0)
MW: 756 ID#: 44079 DB: lipidblast-pos
Comment: Parent=756.55190 Mz_exact=756.55190
5 largest peaks:
697.47840 999.00 | 573.48586 600.00 | 441.23832 40.00 | 500.31182 20.00 | [M+Na]-sn1-H2O || [M+Na]-sn1

(lipidblast-pos) PC 32:0; [M+Na]⁺; GPCho(16:0/16:0)

Plot/Text of Hit Plot of Hit

Peptide Peptide

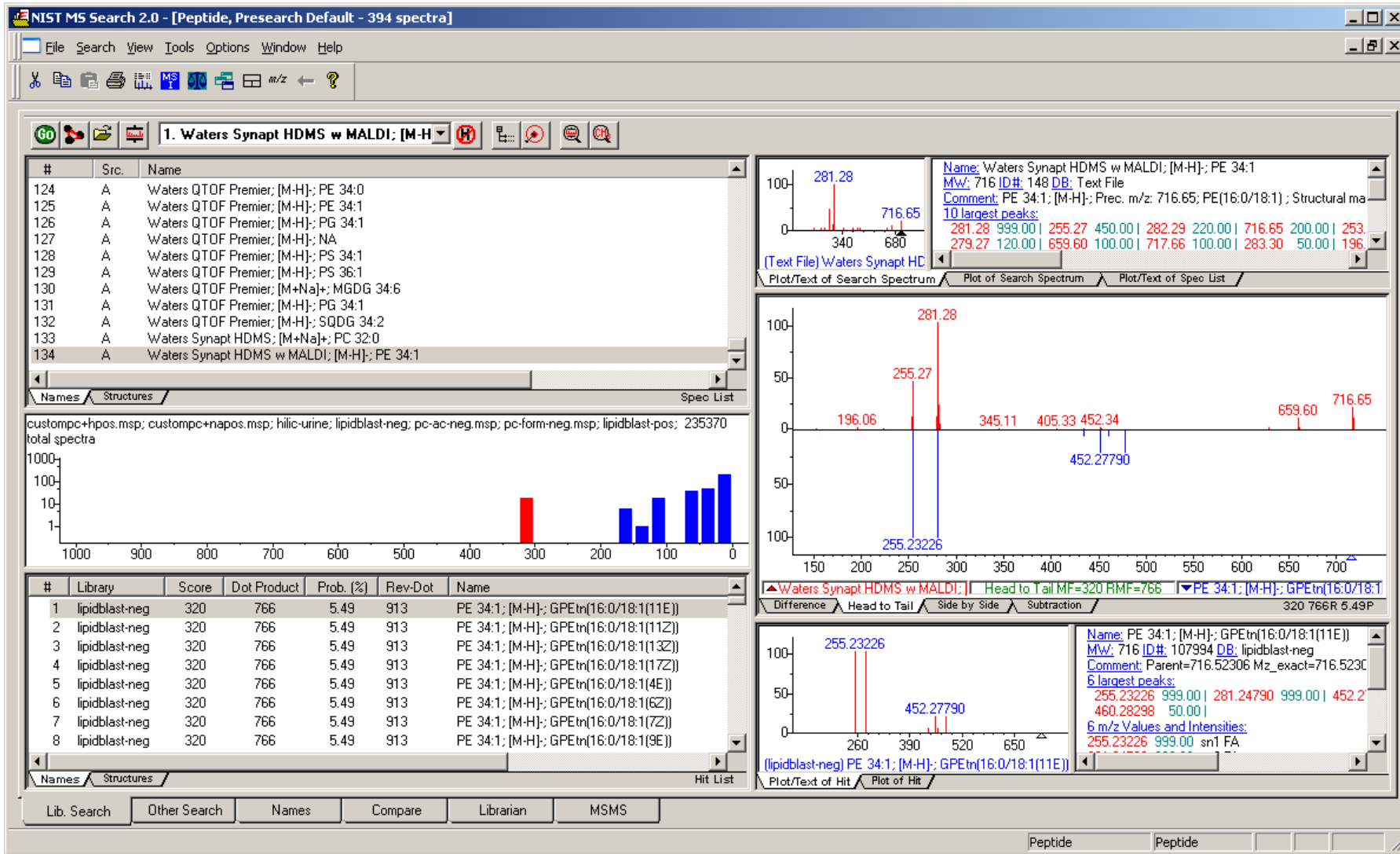
Name: Waters Synapt HDMS w MALDI; [M-H]⁻; PE 34:1

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 Vijaykrishnan, 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

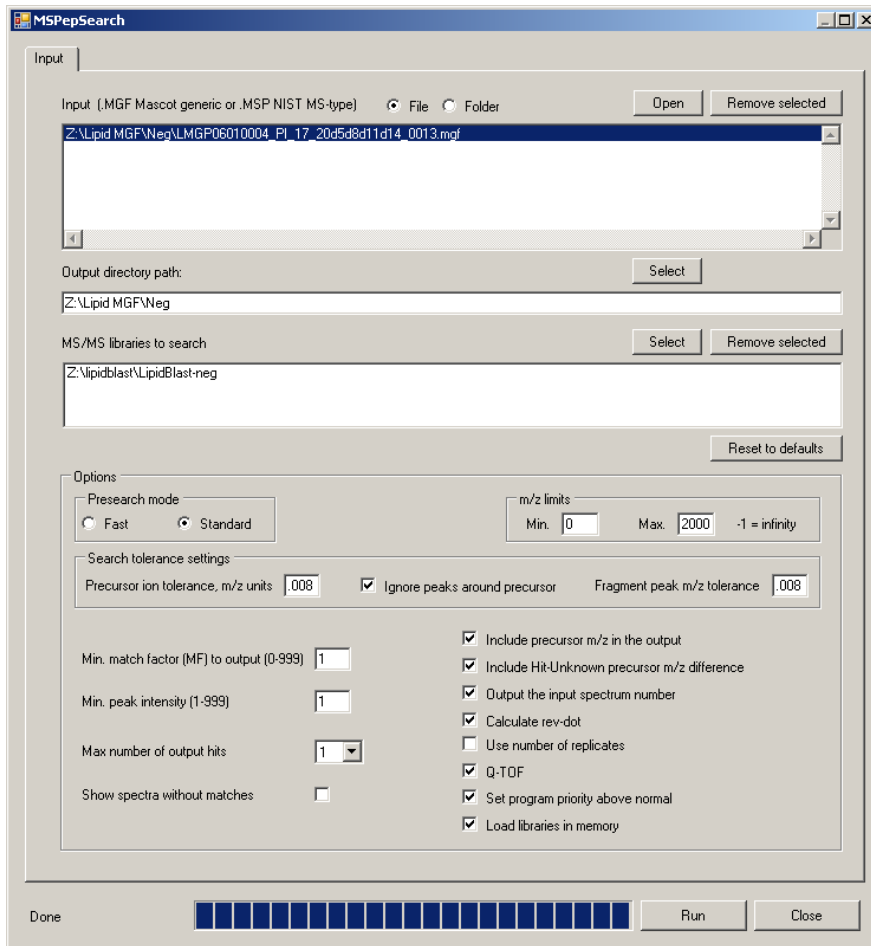
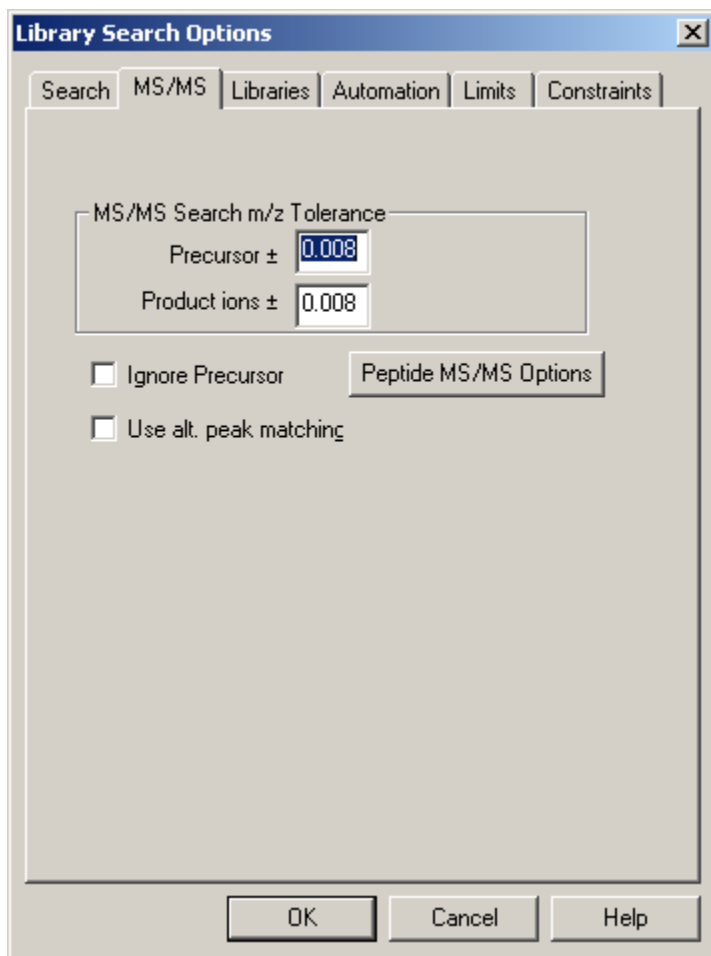
<http://fiehnlab.ucdavis.edu/projects/LipidBlast>

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;



MS PepSearch

Input

Input (.MGF Mascot generic or .MSP NIST MS-type) File Folder Open Remove selected

Z:\Lipid MGF\Pos\A852758_PlasmeylPE_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. Max. -1 = infinity

Search tolerance settings

Precursor ion tolerance, m/z units Ignore peaks around precursor Fragment peak m/z tolerance

Min. match factor (MF) to output (0-999)

Min. peak intensity (1-999)

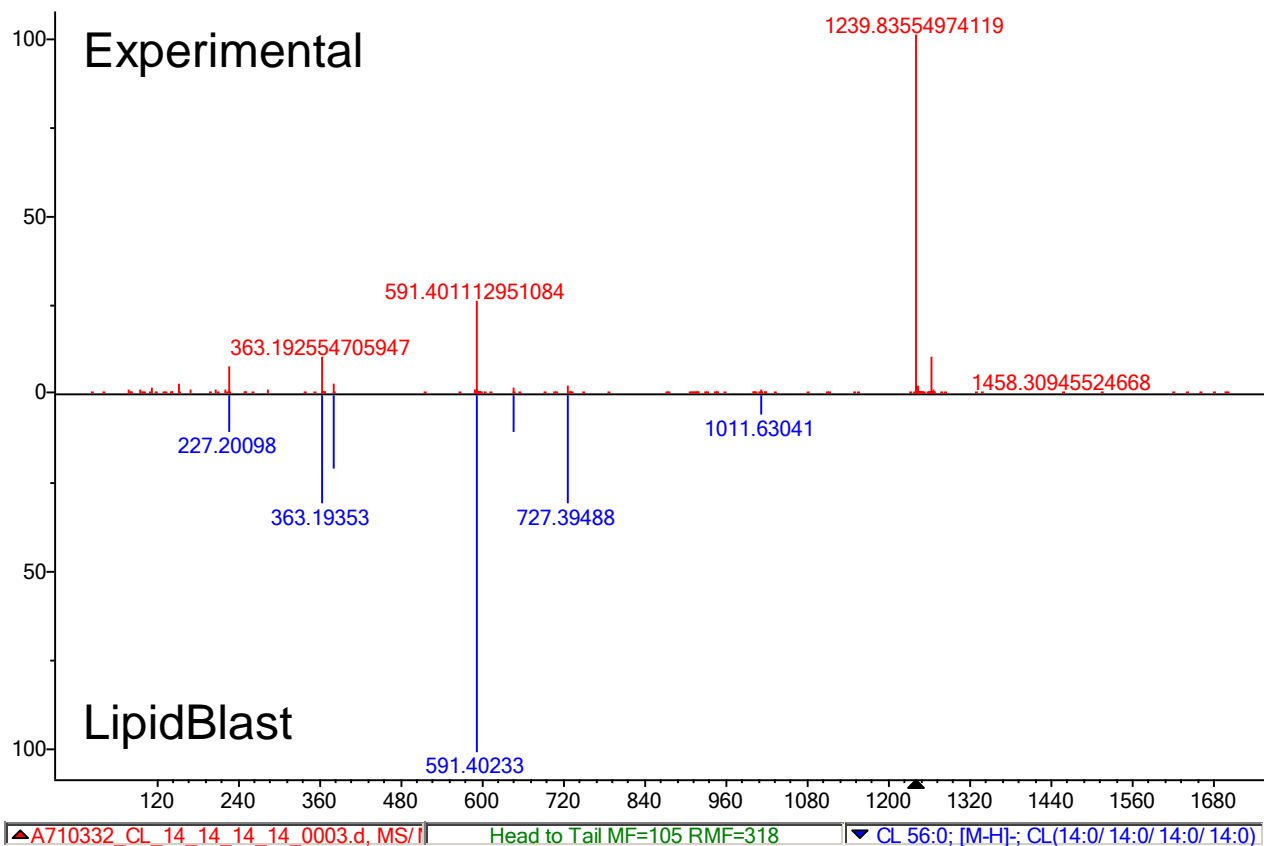
Max number of output hits

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

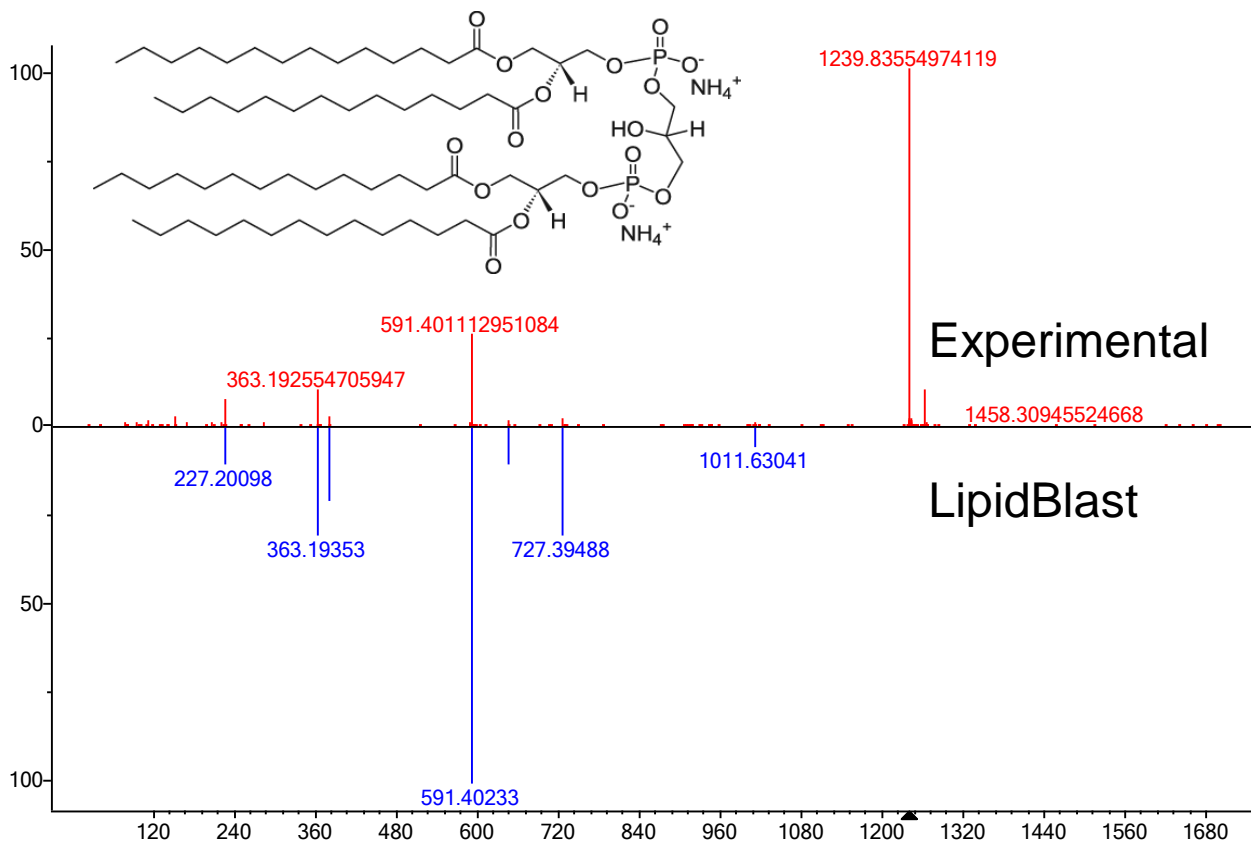
Name: CL 56:0; [M-H]-; CL(14:0/14:0/14:0/14:0)

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

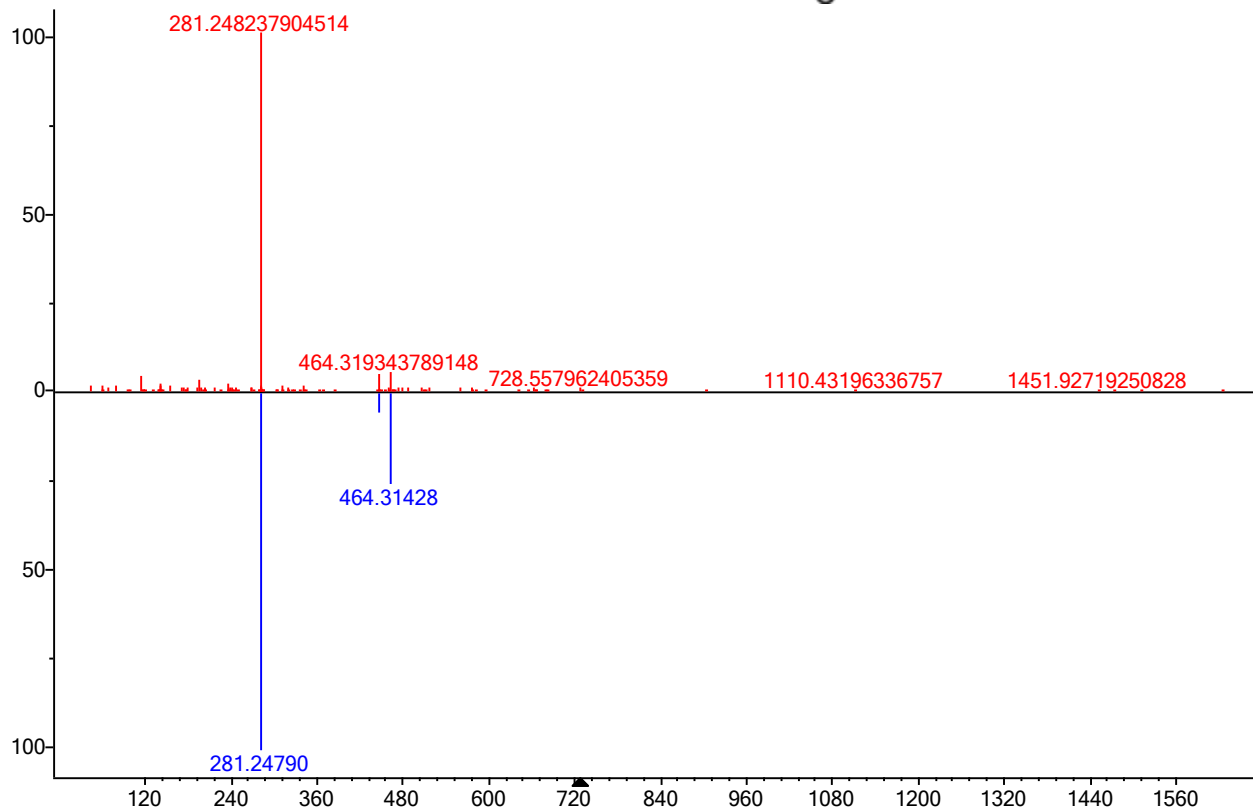
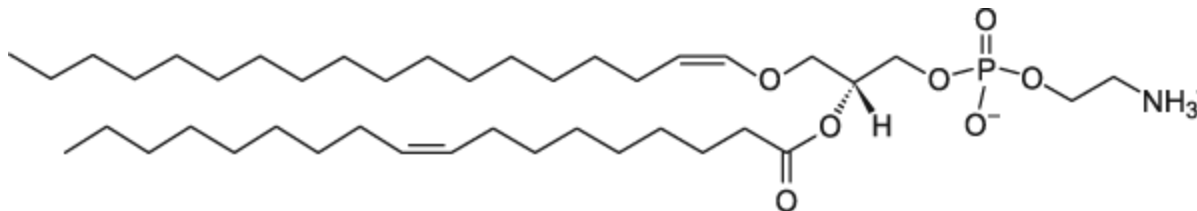
Automatic LipidBlast explanation of fragments: Cardiolipin CL(1'-[14:0/14:0],3'-[14:0/14:0]); C₆₅H₁₃₂N₂O₁₇P₂



▲ A710332_CL_14_14_14_14_0003.d, MS/ | Head to Tail MF=105 RMF=318 | ▼ CL 56:0; [M-H]⁻; CL(14:0/14:0/14:0/14:0)

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

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



▲ A852758_PlasmenylPE_18_18d9_0005.d, Head to Tail MF=175 RMF=566 ▼ plasmenyl-PE 36:1; [M-H]⁻; PE(P-18:0/18:1)

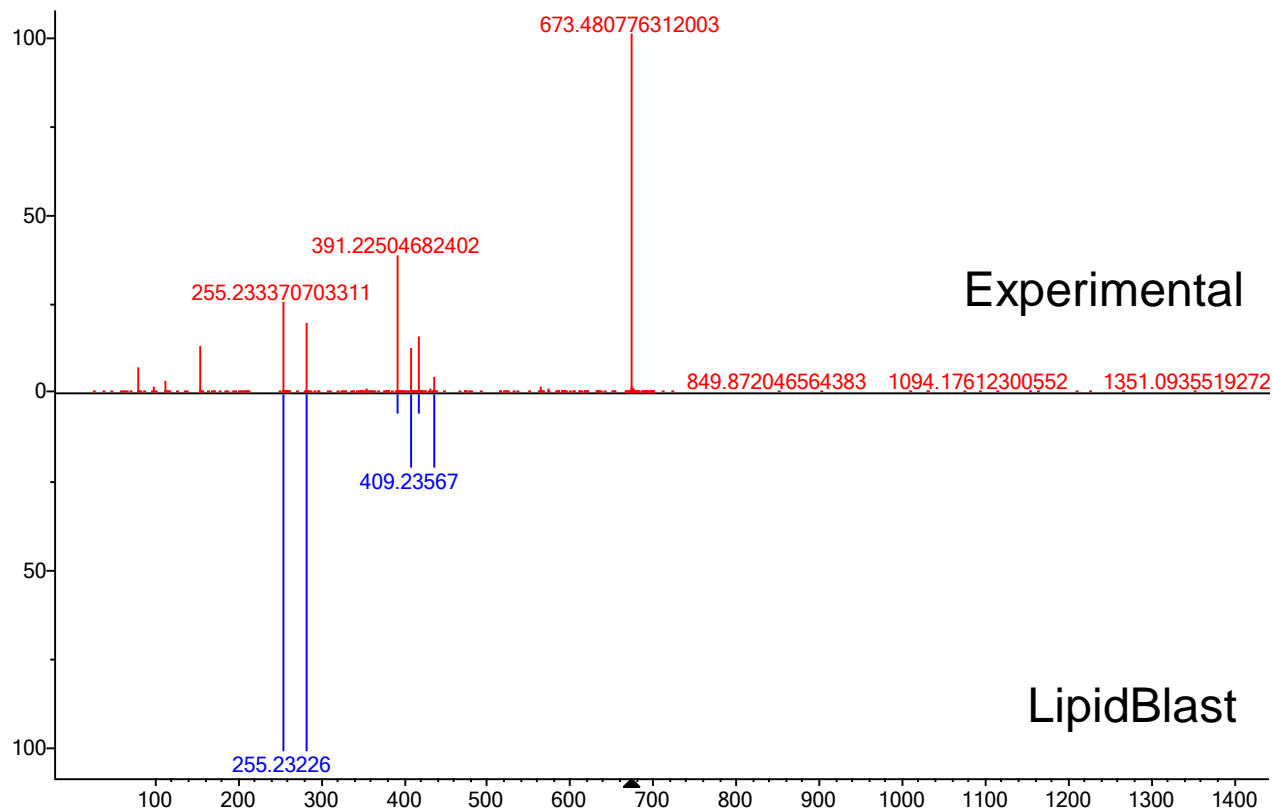
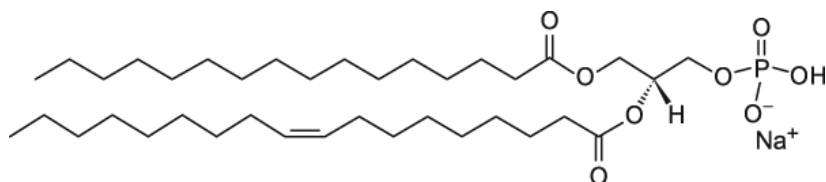
ID in LipidBlast – First HIT

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(-)



▲ A840857_PA_16_18d9_0010.d, MS/MS o | Head to Tail MF=123 RMF=399 | ▼ PA 34:1; [M-H]⁻; GPA(16:0/18:1(11E))

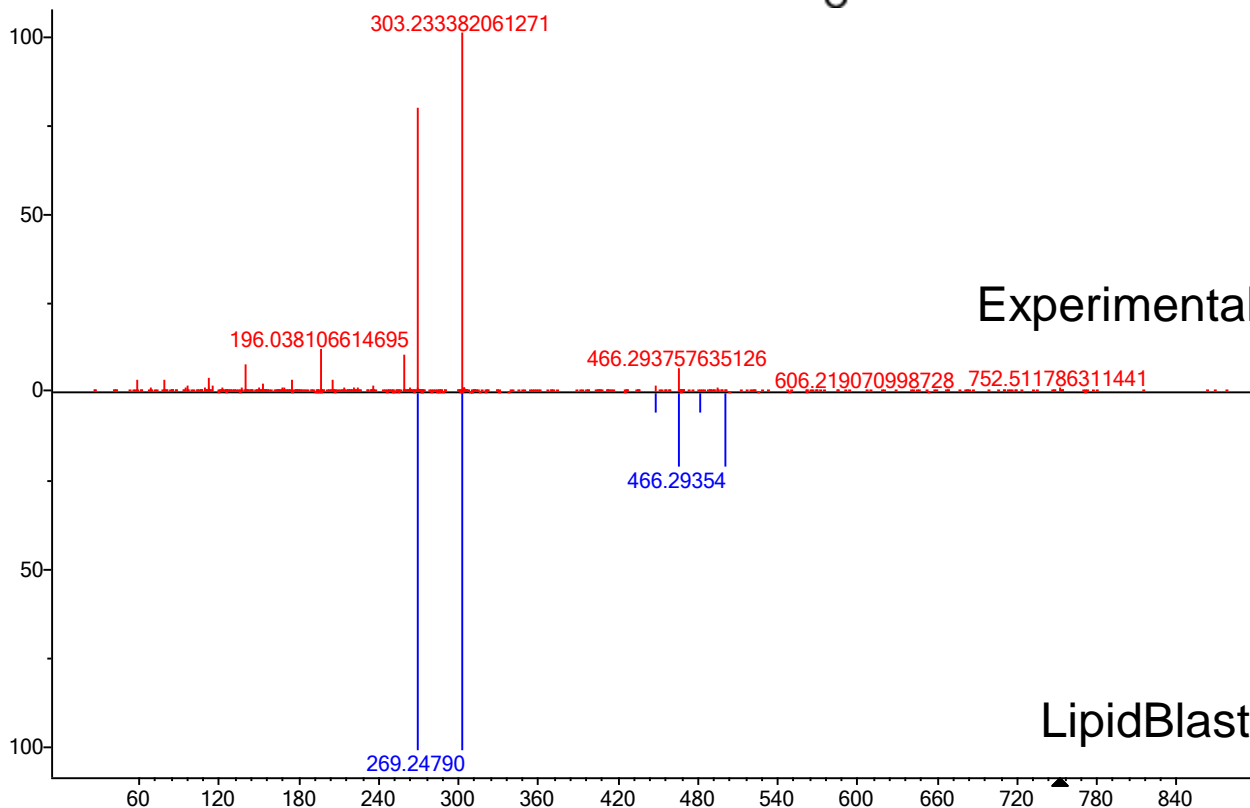
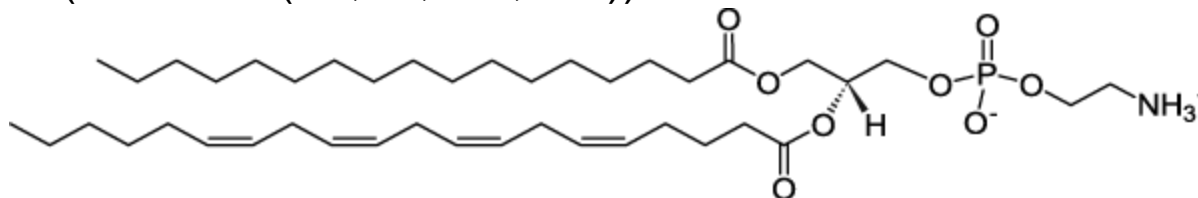
ID in LipidBlast – First HIT

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))



▲ LMGP02010003_PE_17_20d5d8d11d14_0
 ▼ Head to Tail MF=474 RMF=768
 ▼ PE 37:4; [M-H]⁻; GPEtn(17:0/20:4(5E,8E,11E,14E))

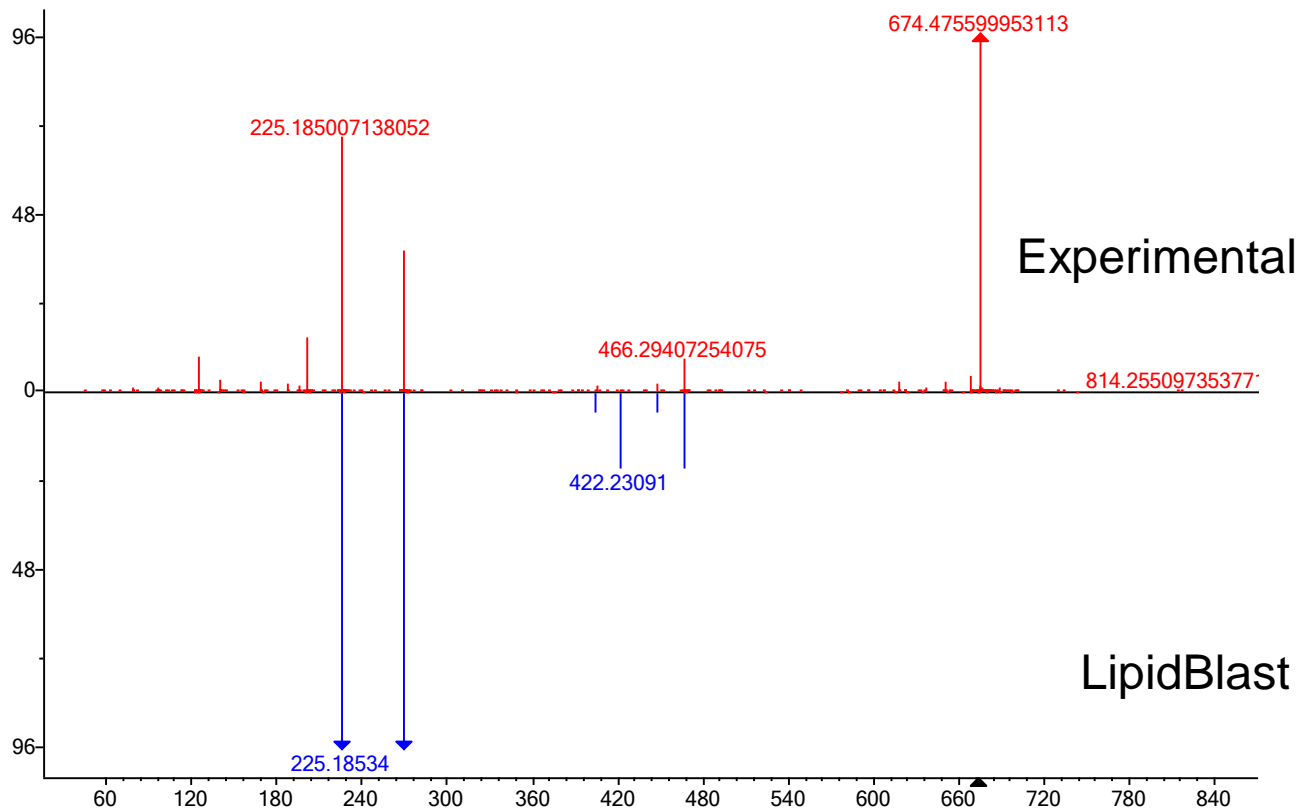
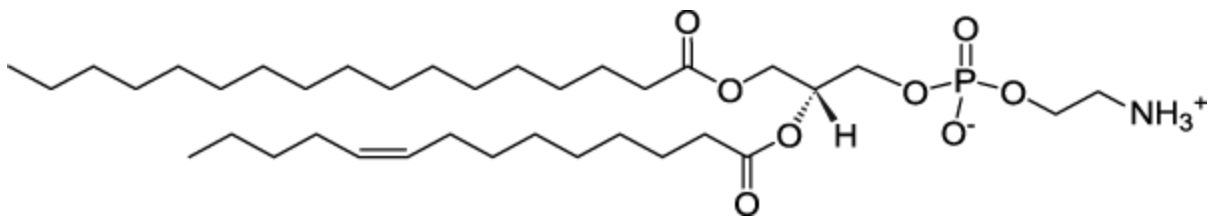
ID in LipidBlast – First HIT

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))



▲LMGP02010005_PE_17d10_14d9_0022.d Head to Tail MF=169 RMF=447 ▼ PE 31:1; [M-H]⁻; GPEtn(14:1(9Z)/17:0)

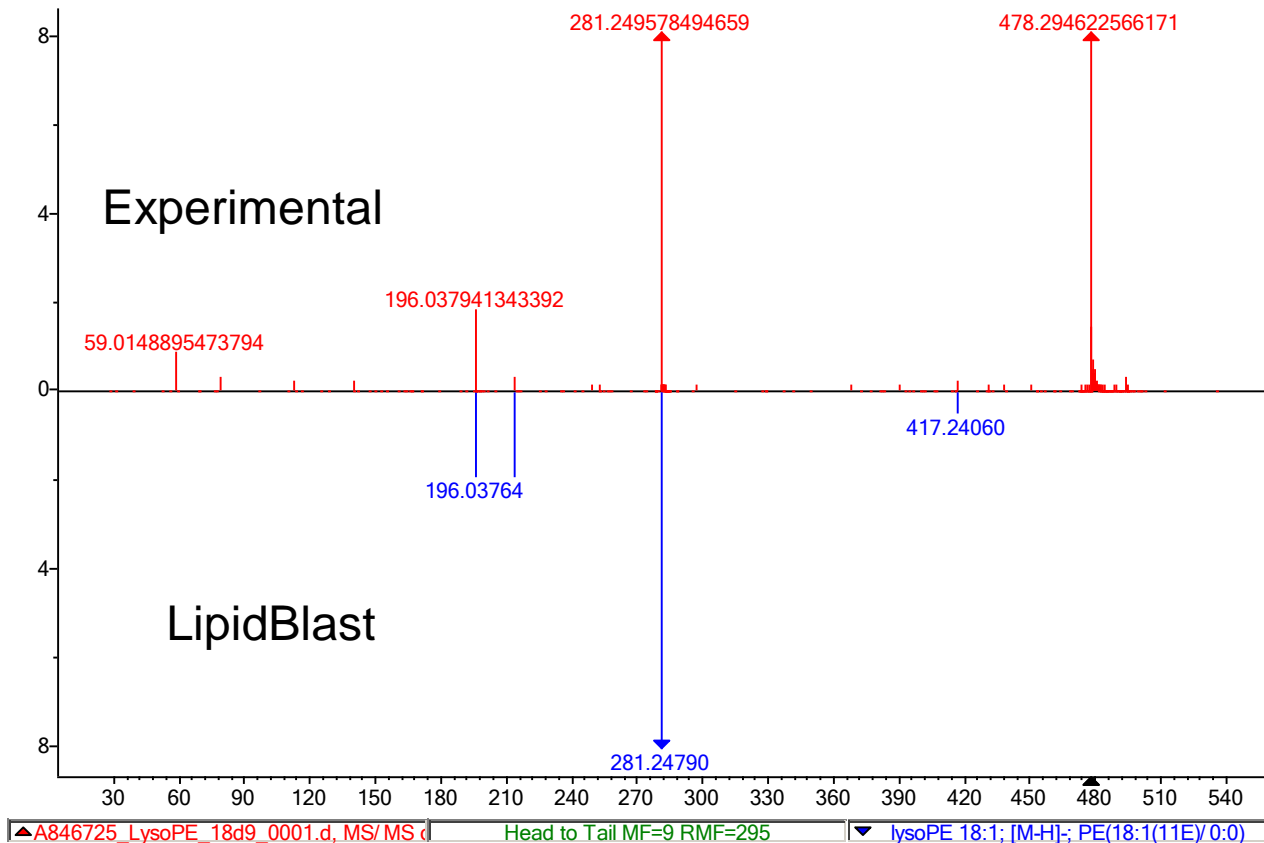
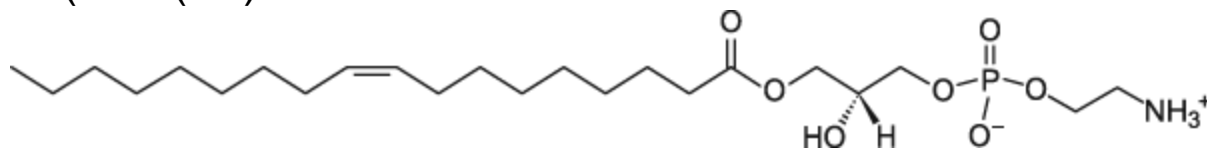
ID in LipidBlast – First HIT

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

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



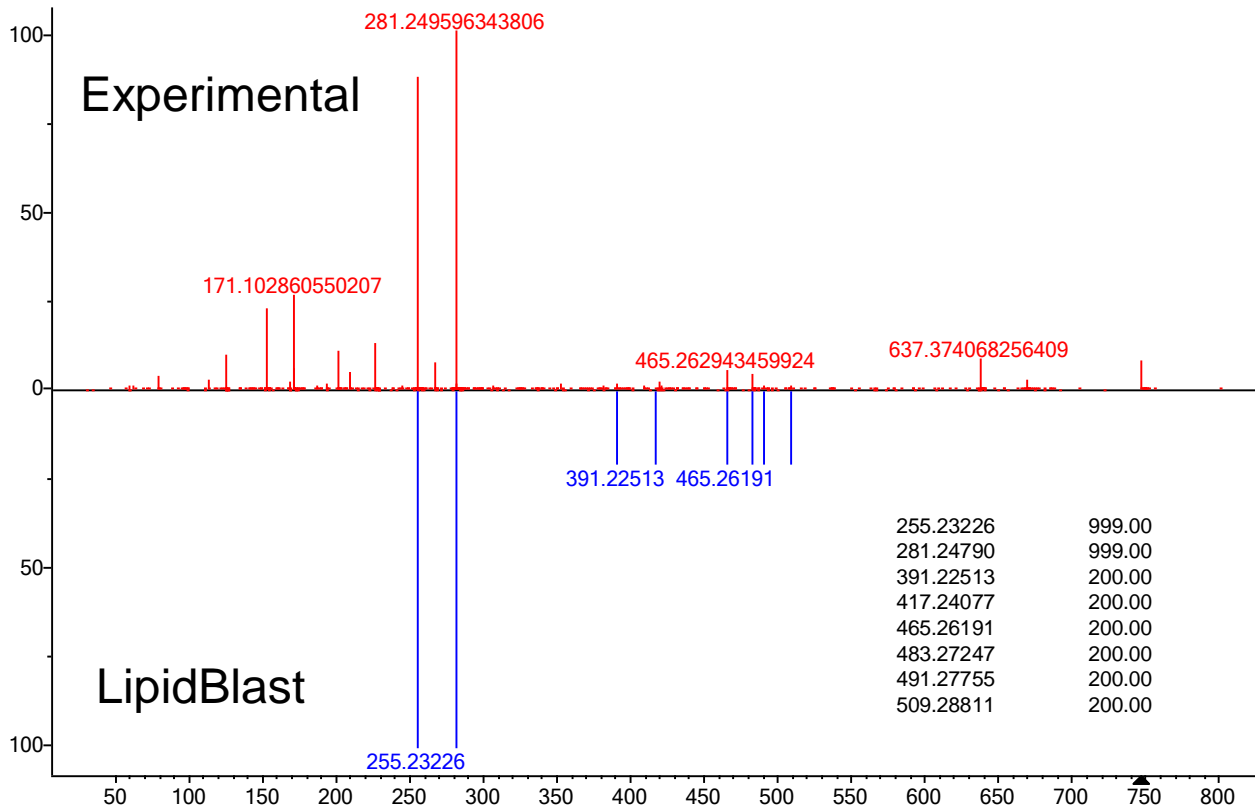
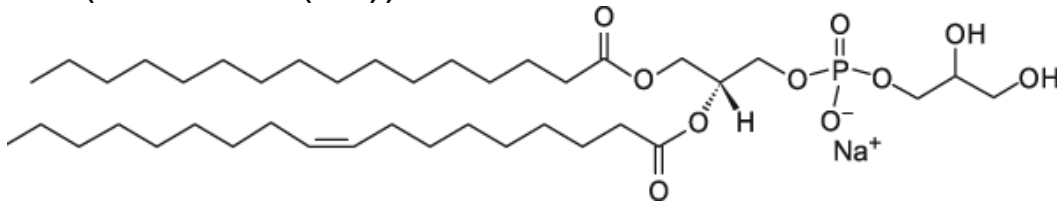
ID in LipidBlast – First HIT

Name: lysoPE 18:1; [M-H]-; PE(18:1(11E)/0:0)

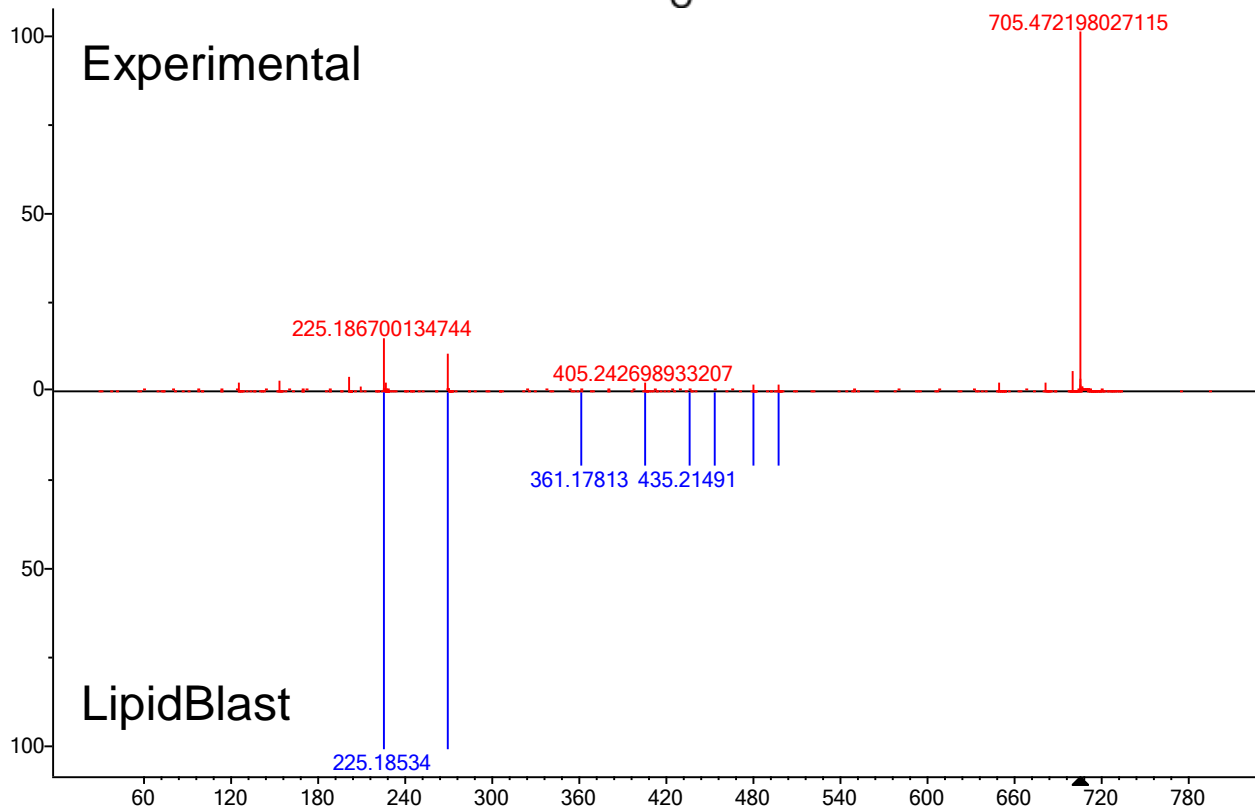
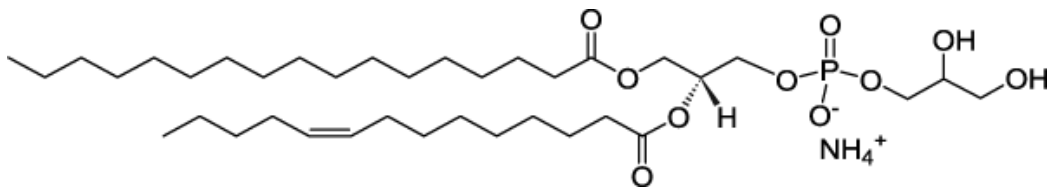
MW: 478 ID#: 95782 DB: lipidblast-neg

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))



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



▲ LMGPO4010007_PG_17_14d1_0014.d, M | Head to Tail MF=53 RMF=324 | ▼ PG 31:1; [M-H]⁻; GPGro(14:1(9Z)/17:0)

ID in LipidBlast – First HIT

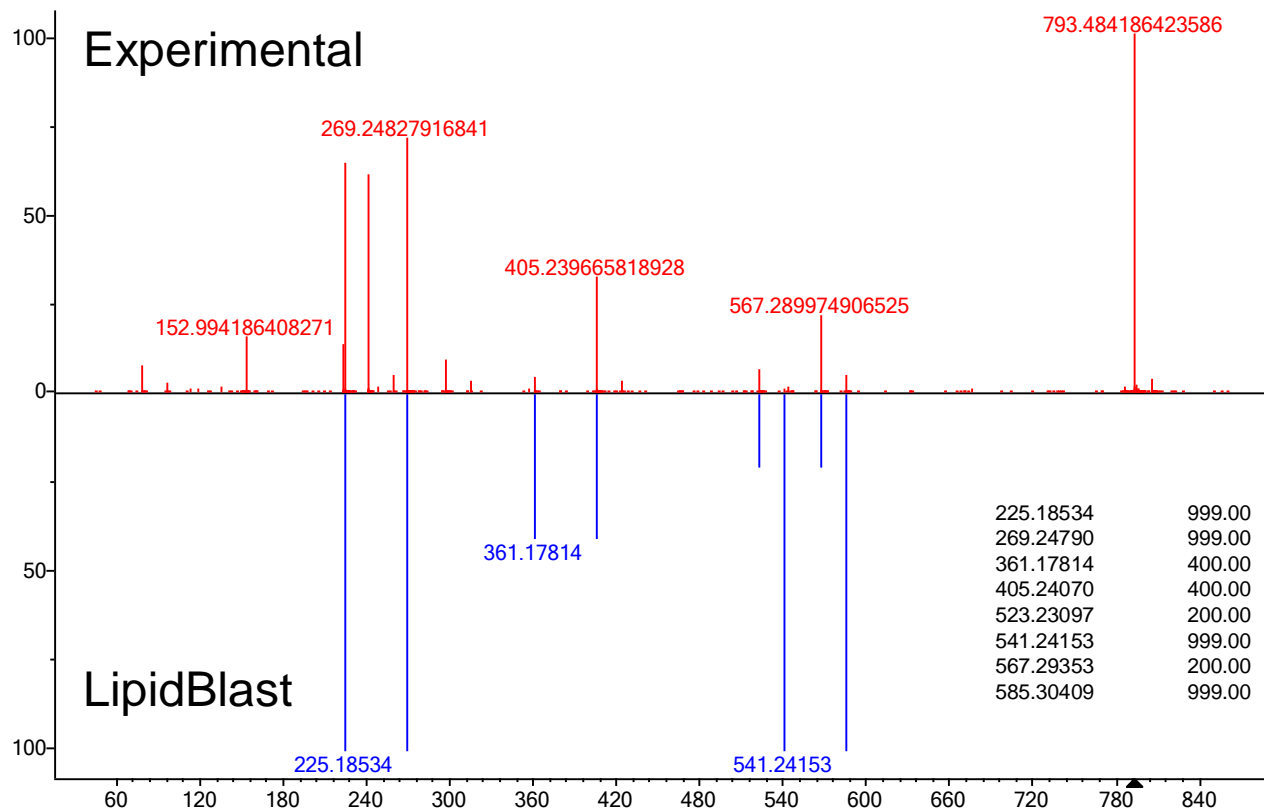
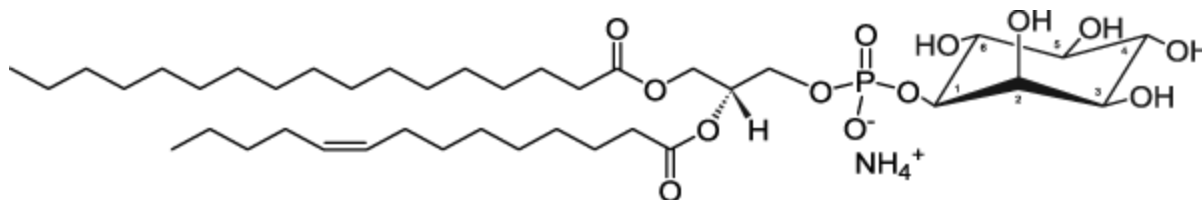
Name: PG 31:1; [M-H]⁻; GPGro(14:1(9Z)/17:0)

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]-sn2
585.30409	999.00	[M-H]-sn1-H2O
		[M-H]-sn1

▲ LMGPO6010006_PI_17_14d9_0017.d, MS | Head to Tail MF=344 RMF=524 | ▼ PI 31:1; [M-H]-; GPIns(14:1(9Z)/17:0)

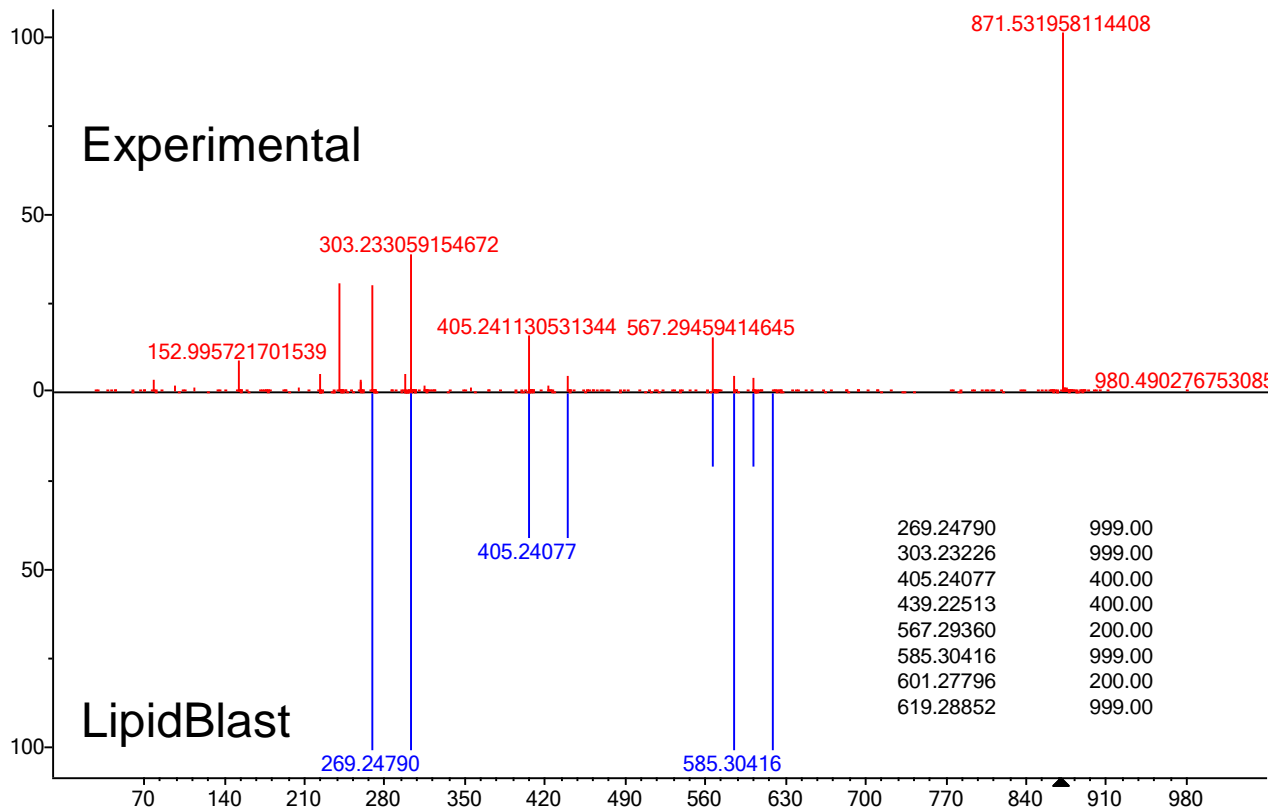
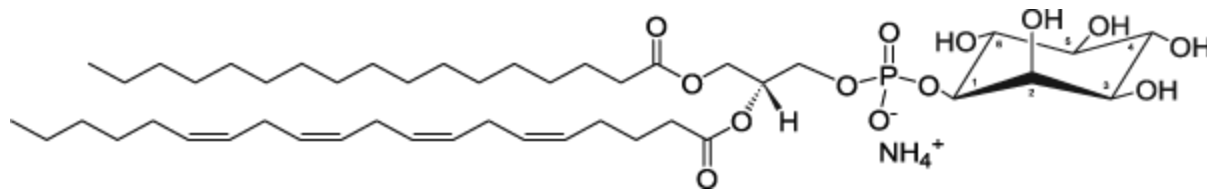
ID in LipidBlast – First HIT

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))



▲LMGP06010004_PI_17_20d5d8d11d14_0 Head to Tail MF=76 RMF=328 ▼PI 37:4; [M-H]-; GPIs(17:0/20:4(5E,8E,11E,14E))

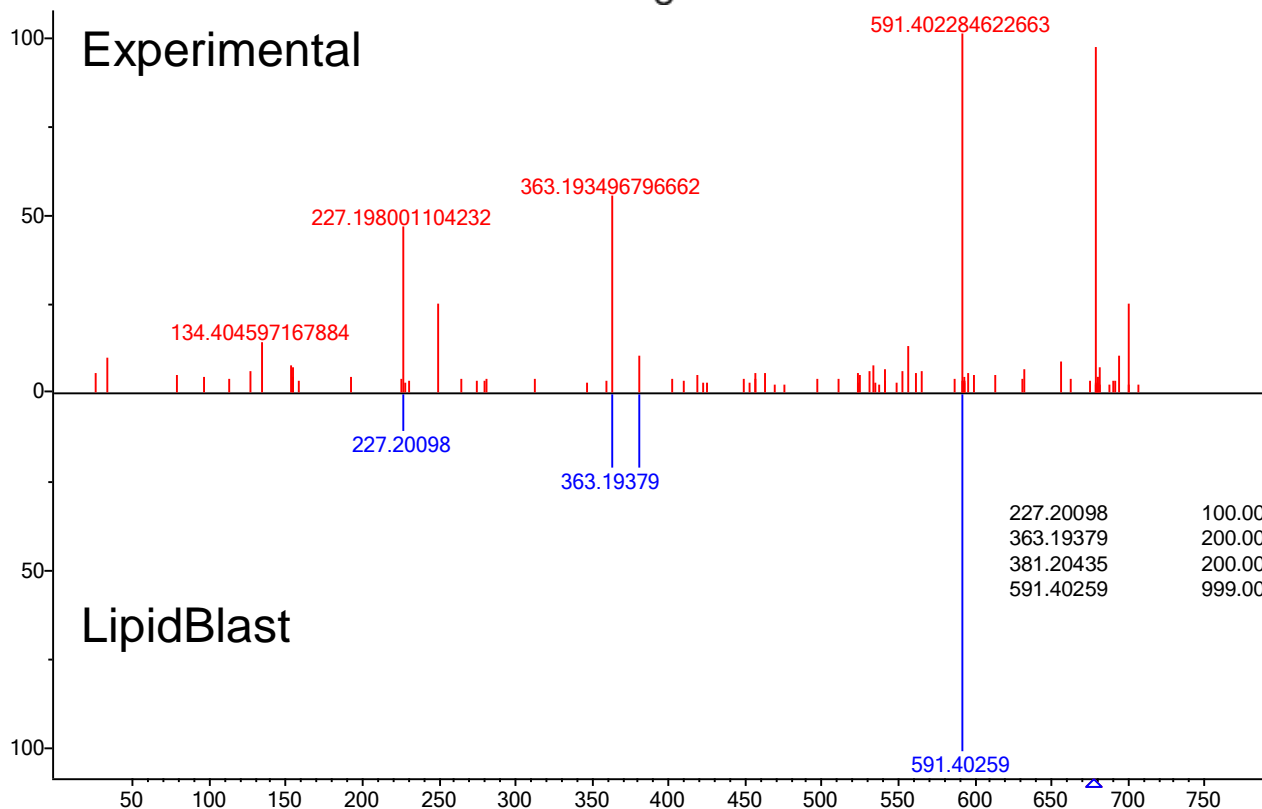
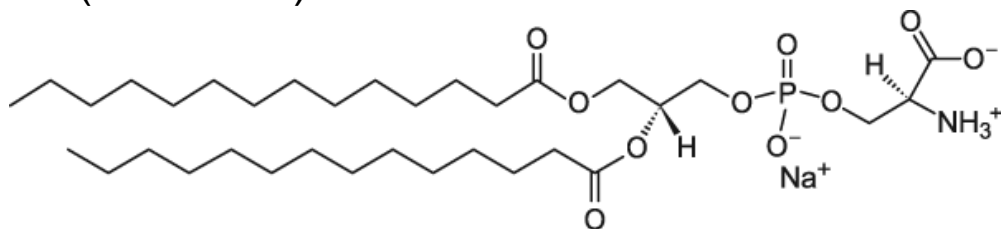
ID in LipidBlast – First HIT

Name: PI 37:4; [M-H]-; GPIs(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]-; GPIs(17:0/20:4(5E,8E,11E,14E)); C46H81O13P

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



227.20098	100.00
363.19379	200.00
381.20435	200.00
591.40259	999.00

sn1 FA || sn2 FA
 [M-H-87]-sn1 || [M-H-87]-sn2
 [M-H-87]-sn1+H2O || [M-H-87]-sn2+H2O
 [M-H]-C3H5NO2 (-87)

▲ A840033_PS_14_14_0002.d, MS/MS of 6 | Head to Tail MF=266 RMF=504 | ▼ PS 28:0; [M-H]-; GPSer(14:0/14:0)

ID in LipidBlast – First HIT

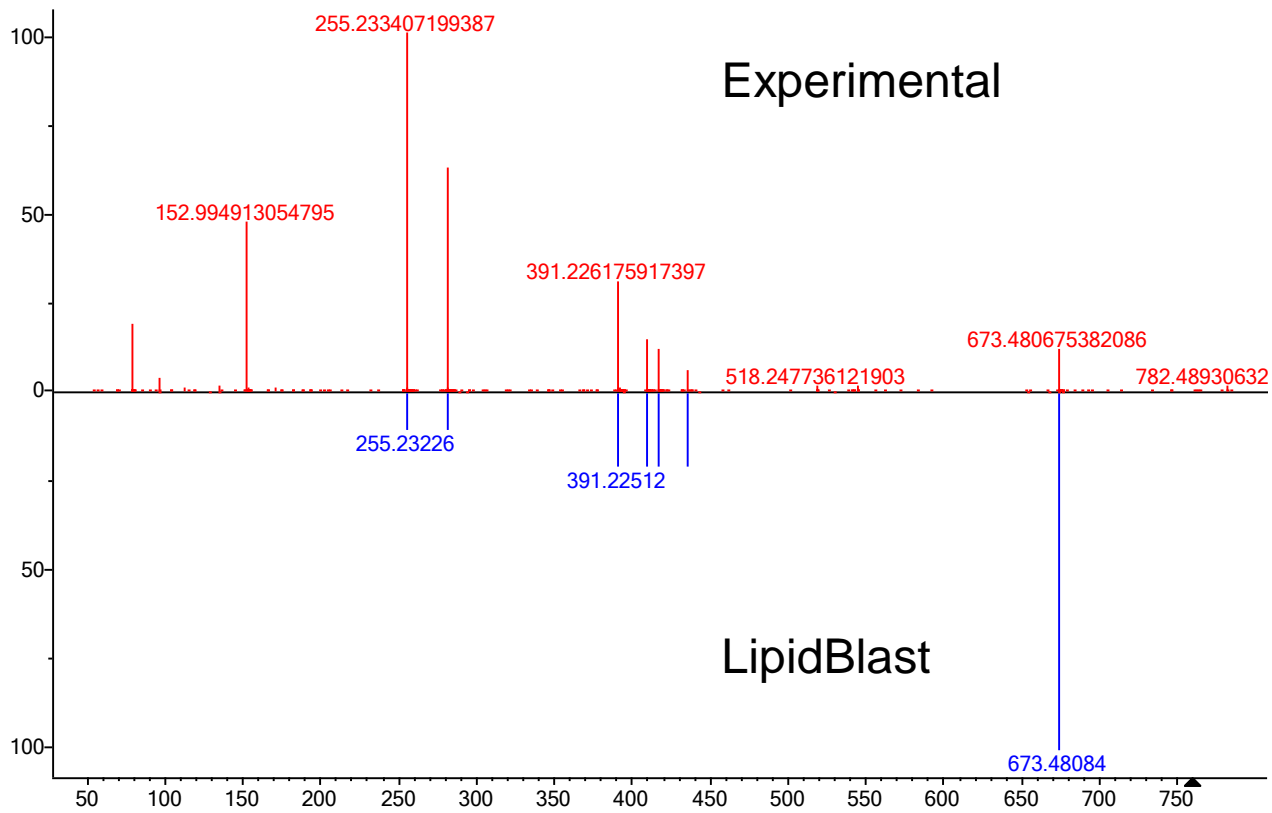
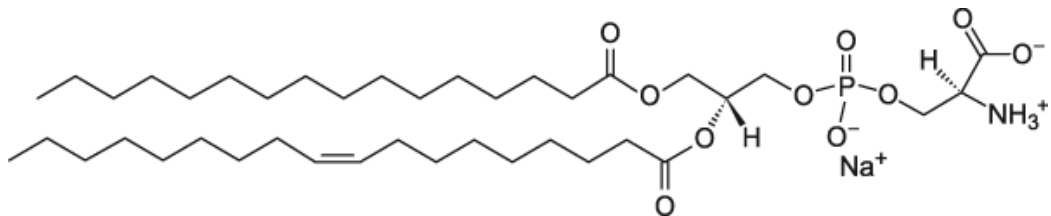
Name: PS 28:0; [M-H]-; GPSer(14:0/14:0)

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))



▲ A840034_PS_16_18d9_0009.d, MS/MS o | Head to Tail MF=444 RMF=666 | ▼ PS 34:1; [M-H]-; GPSer(16:0/18:1(11E))

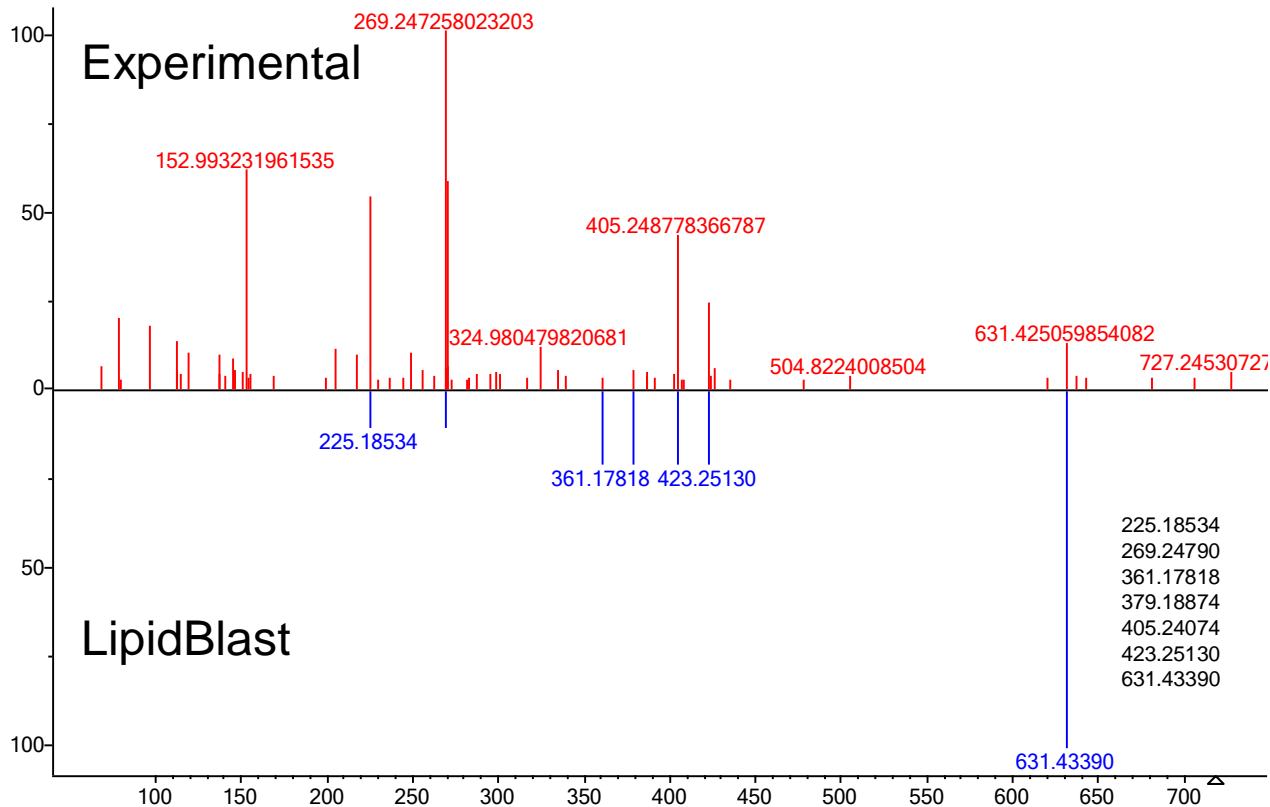
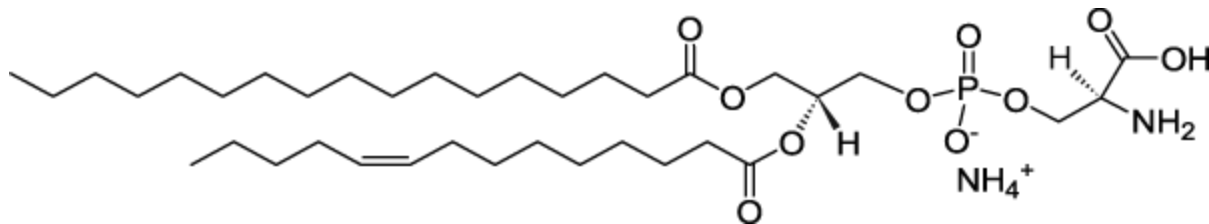
ID in LipidBlast – First HIT

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)

▲ LMGP03010006_PS_17_14d9_0018.d, MS | Head to Tail MF=358 RMF=455 | ▼ PS 31:1; [M-H]-; GPser(17:0/14:1(9Z))

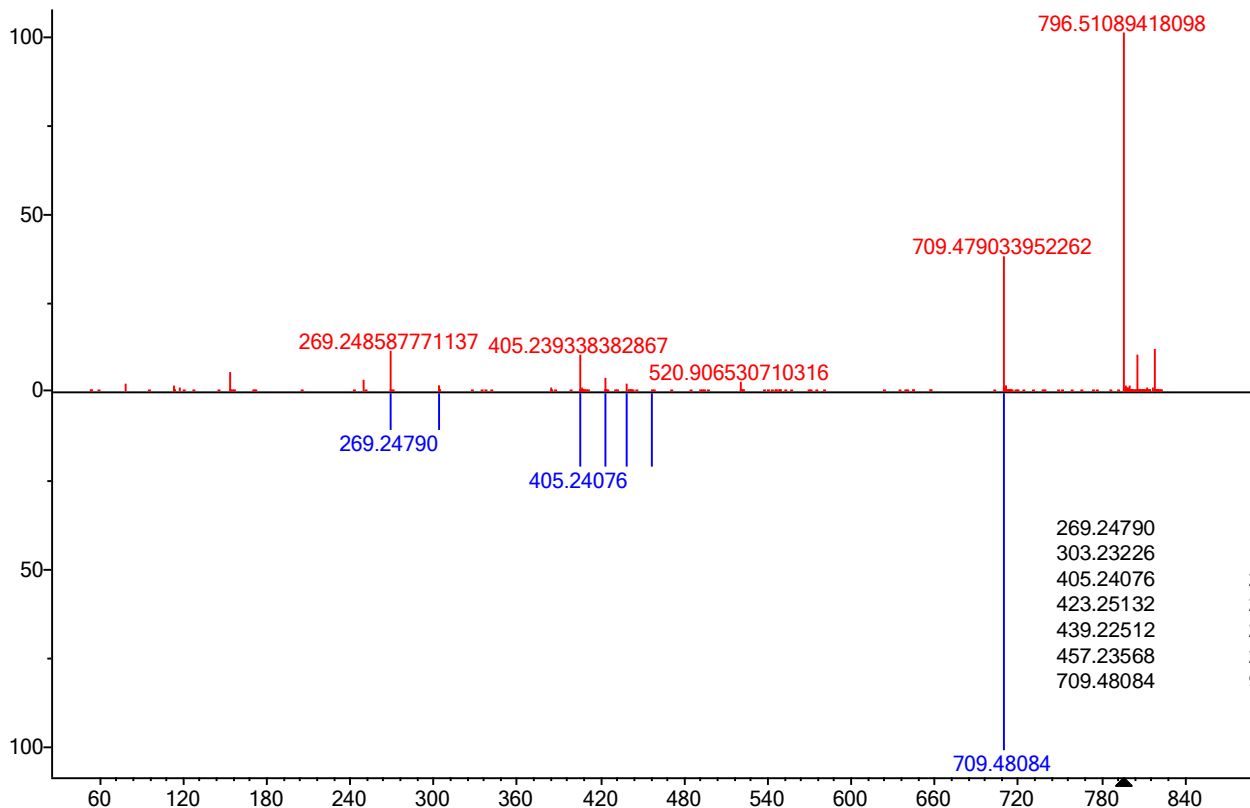
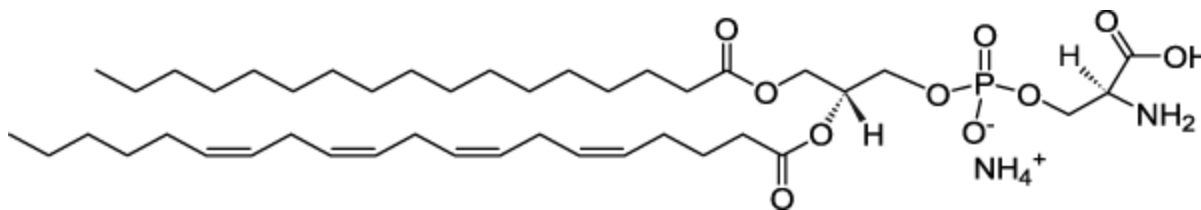
ID in LipidBlast – First HIT

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))



LMGP03010003_PS_17_20d5d8d11d14_() Head to Tail MF=295 RMF=610 PS 37:4; [M-H]-; GPSer(17:0/20:4(5E,8E,11E,14E))

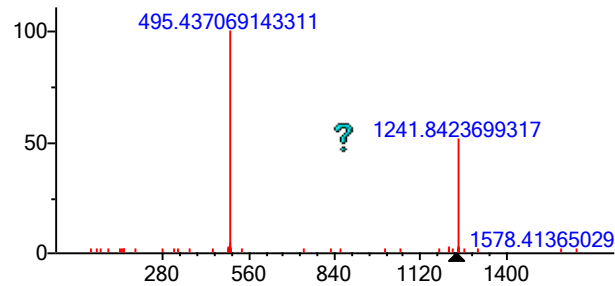
ID in LipidBlast – First HIT

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(+)

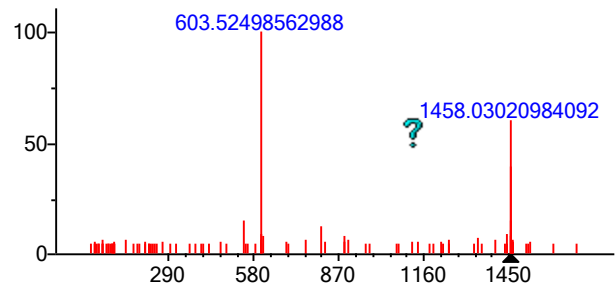


(Text File) A710332_CL_14_14_14_14_0003.d, MS/MS of 1241.8

Cardiolipin

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

double negative charge, usually measured in negative mode.



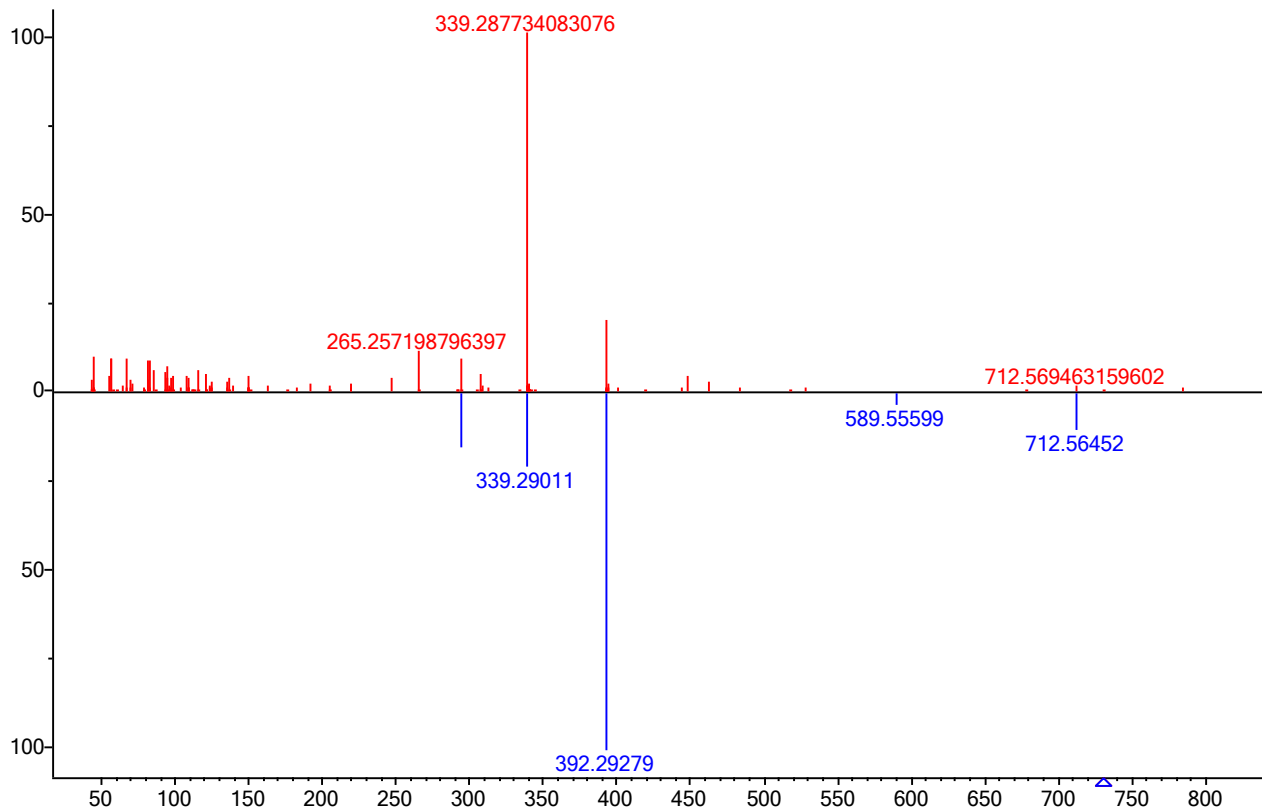
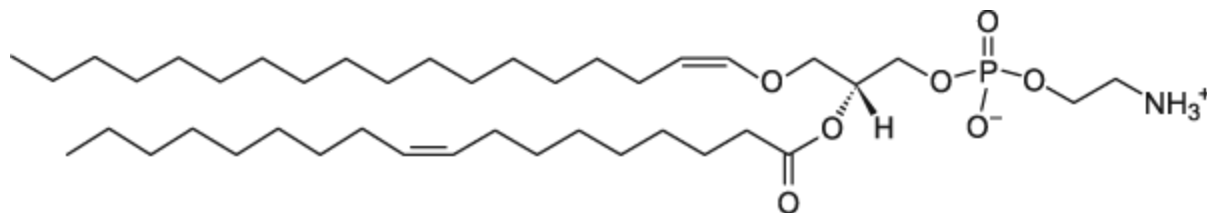
(Text File) A710335_CL_18d1_18d1_18d1_18d1_0012.d, MS/MS

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))



▲ A852758_PlasmenylPE_18_18d9_0005.d, Head to Tail MF=140 RMF=481 ▼ plasmenyl-PE 36:1; [M+H]⁺; PE(P-18:0/18:

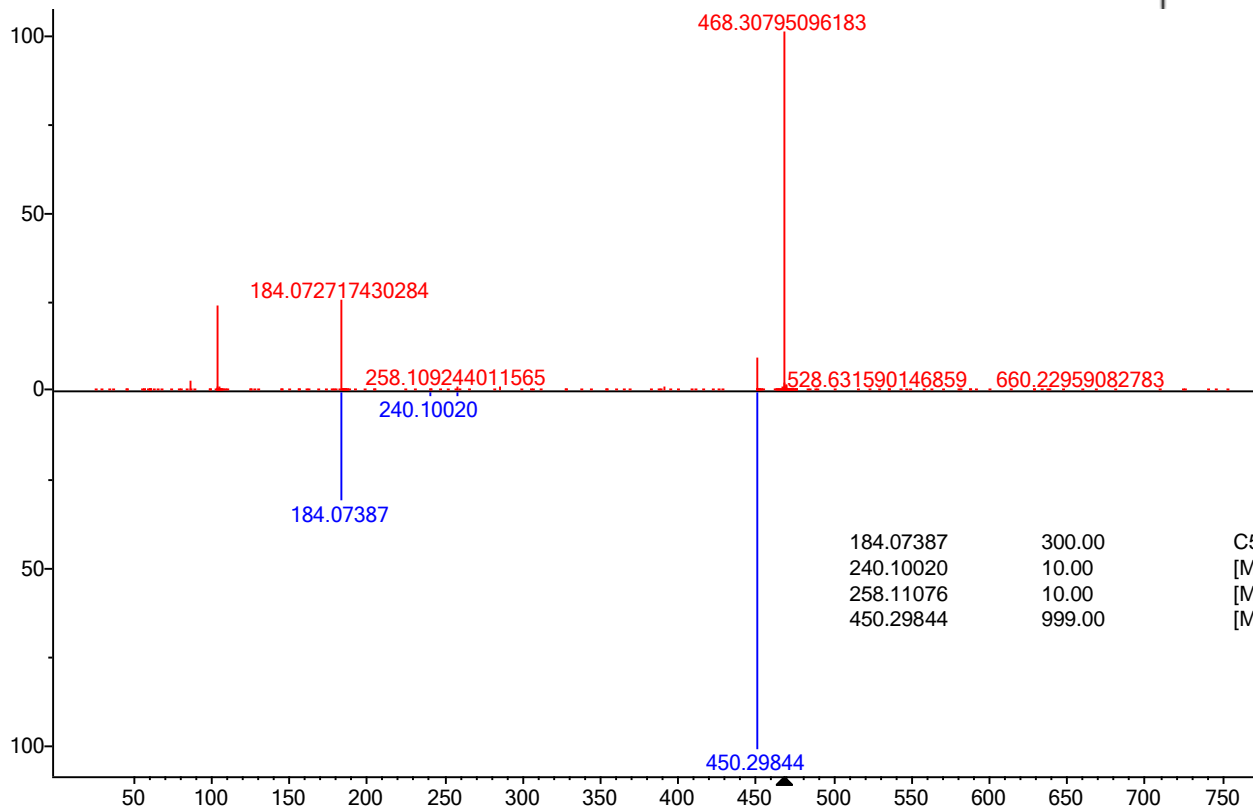
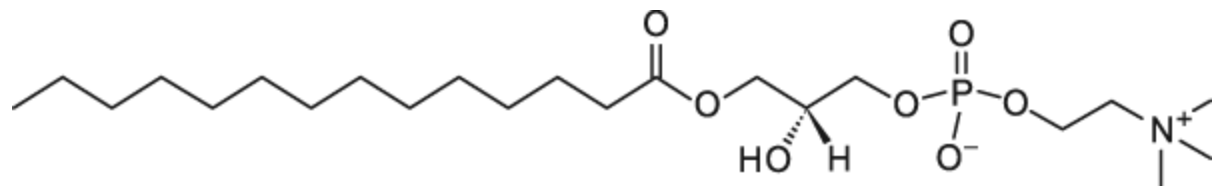
ID in LipidBlast – First HIT – issue with batch version

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)



184.07387	300.00	C5H15NO4P m/z=184
240.10020	10.00	[M+H]-sn1-H2O
258.11076	10.00	[M+H]-sn1
450.29844	999.00	[M+H]-H2O (-18)

▲ A855575_LysoPC_14_0004.d, MS/MS of 4 Head to Tail MF=35 RMF=257 ▼ lysoPC 14:0; [M+H]⁺; PC(14:0/0:0)

ID in LipidBlast – First HIT

Name: lysoPC 14:0; [M+H]⁺; PC(14:0/0:0)

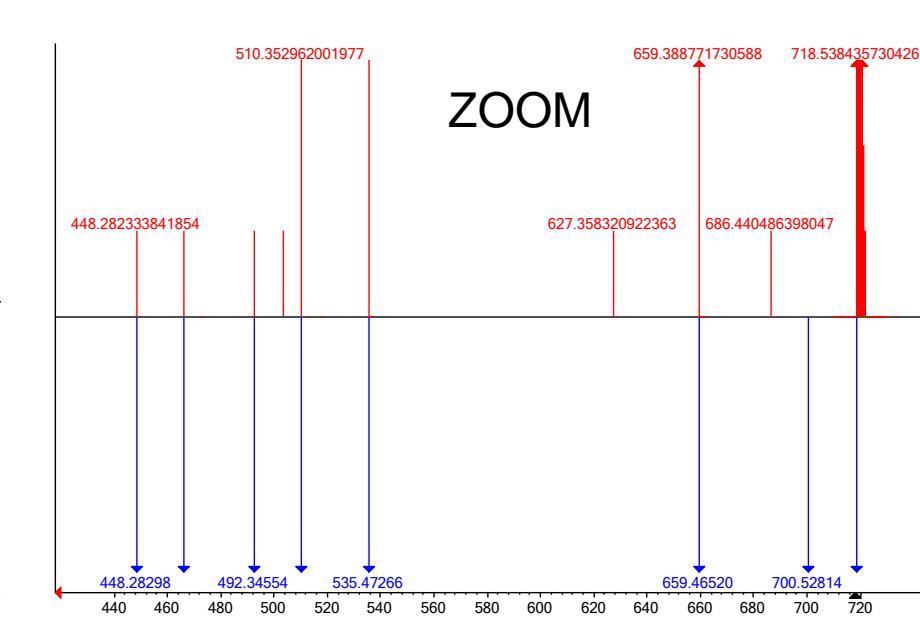
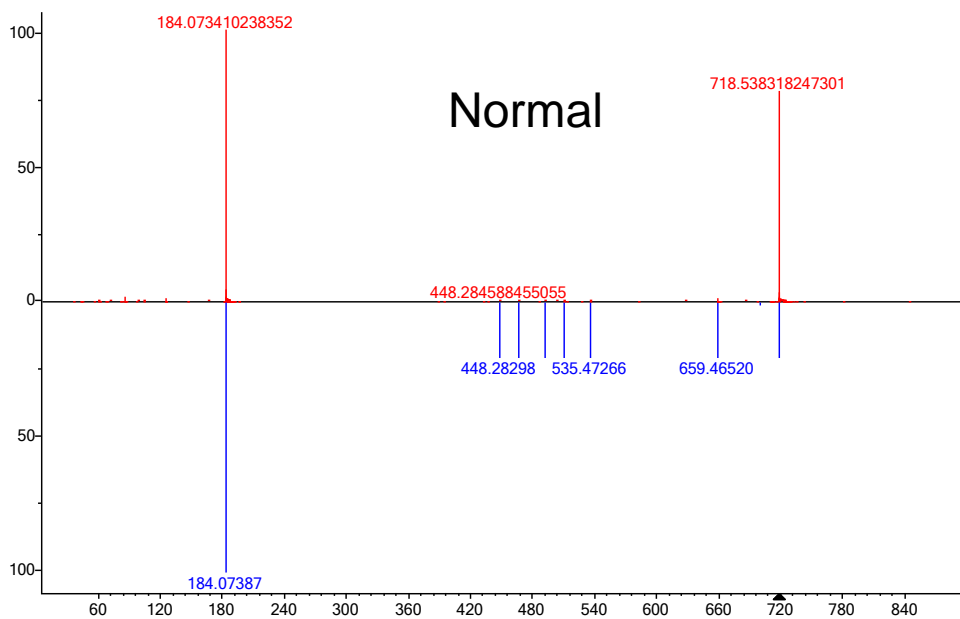
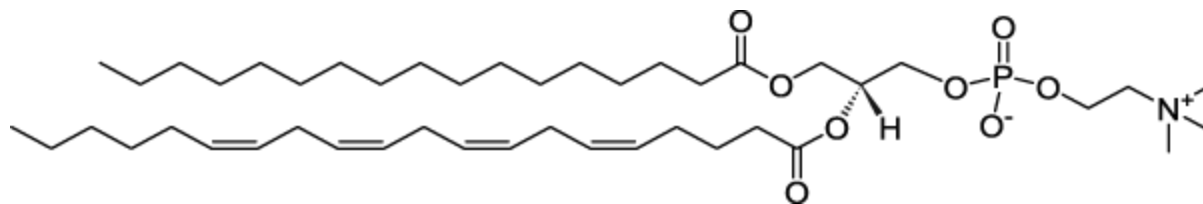
MW: 468 ID#: 9185 DB: lipidblast-pos

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))



▲ LMGP01010008_PC_17_14d9_0020.d.MS Head to Tail MF=164 RMF=598 ▼ PC 31:1; [M+H]⁺; GPCho(14:1(9Z)/17:0)

▲ LMGP01010008_PC_17_14d9_0020.d.MS Head to Tail MF=174 RMF=591 ▼ PC 31:1; [M+H]⁺; GPCho(14:1(9Z)/17:0)

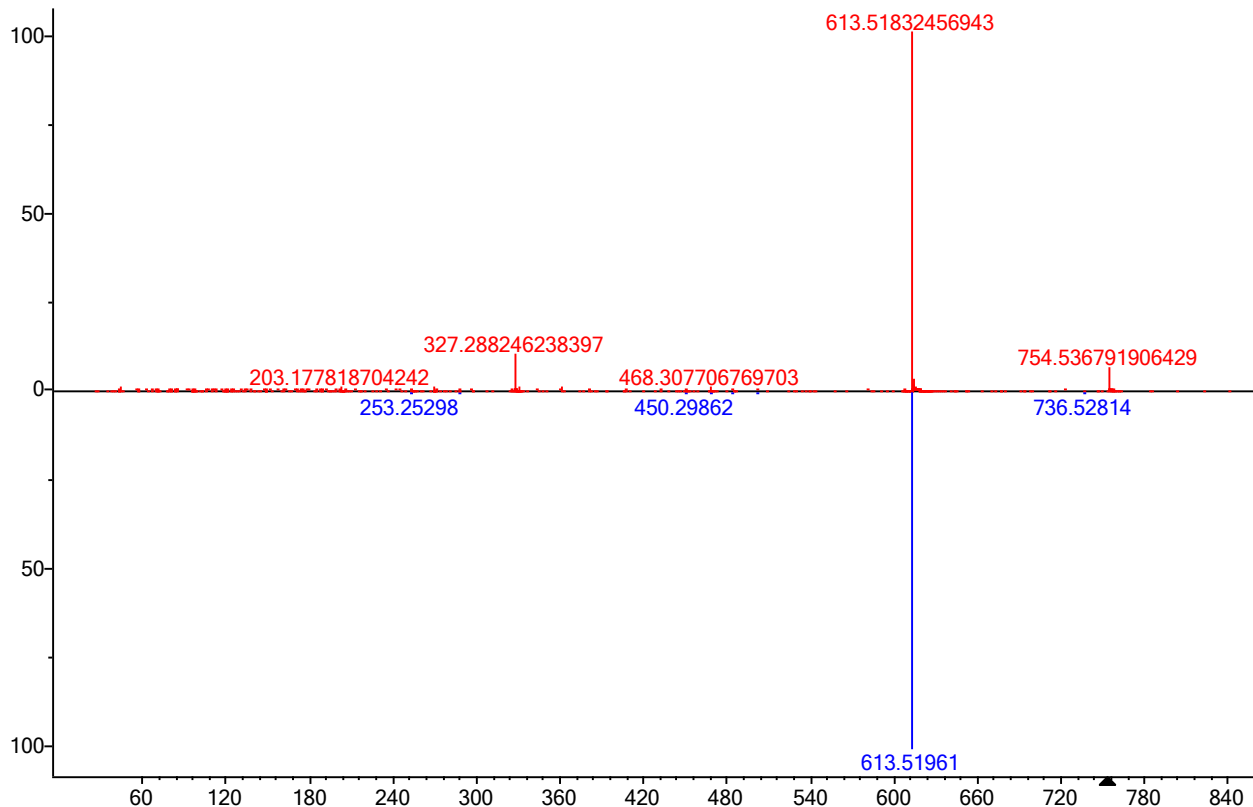
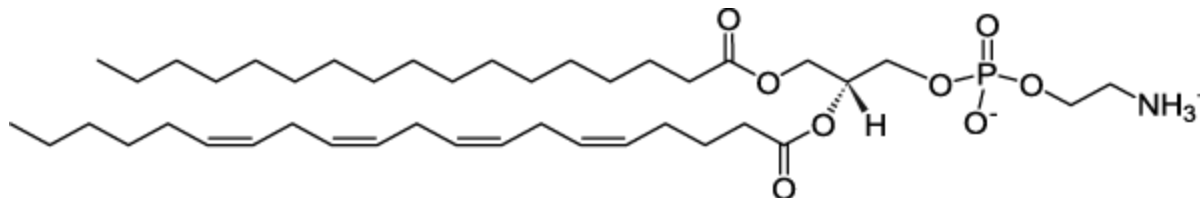
ID in LipidBlast – First HIT

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))



▲LMGP02010003_PE_17_20d5d8d11d14_(Head to Tail MF=37 RMF=923 ▼PE 37:4; [M+H]⁺; GPEtn(17:0/20:4(5E,8E,

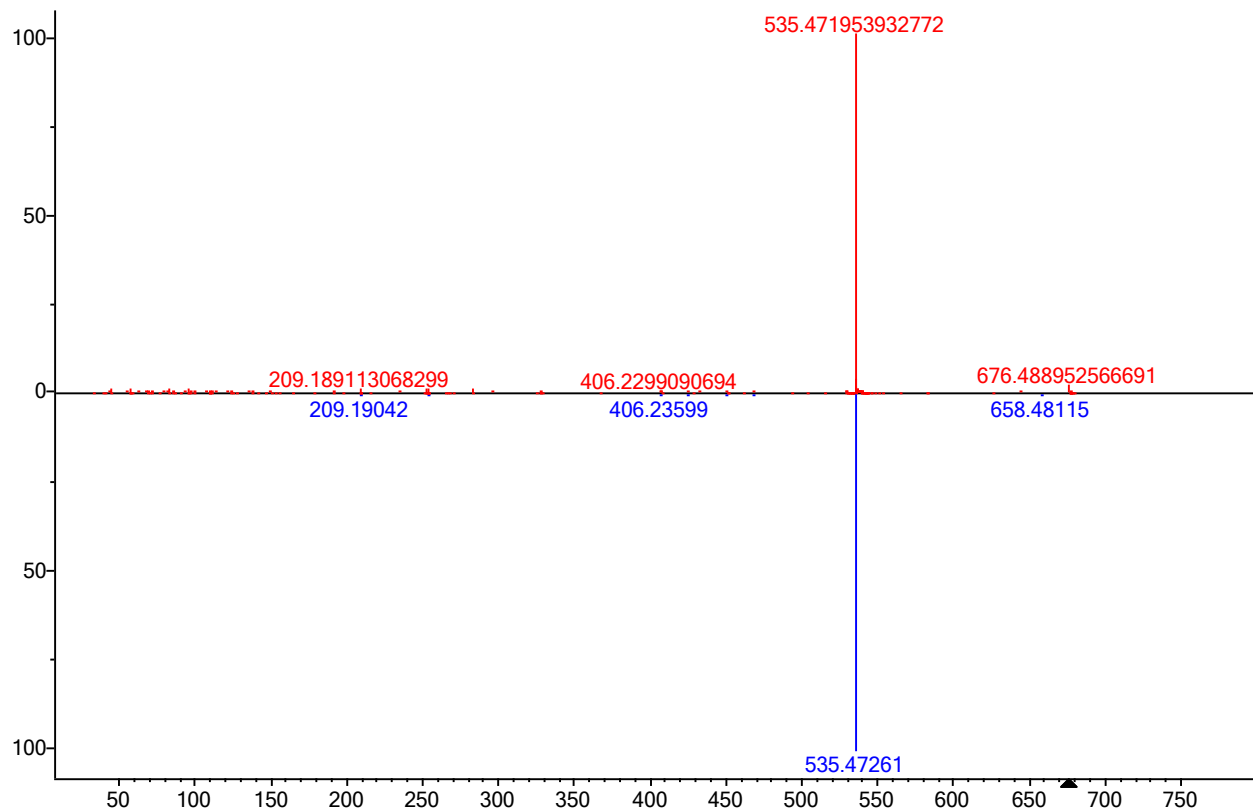
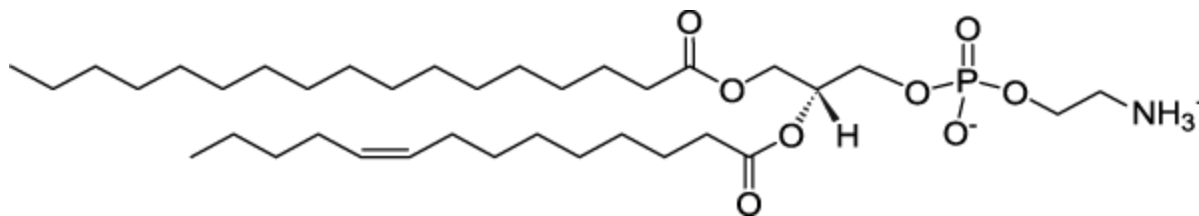
ID in LipidBlast – First HIT

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))



▲ LMGP02010005_PE_17d10_14d9_0022.d | Head to Tail MF=25 RMF=938 | ▼ PE 31:1; [M+H]⁺; GPEtn(14:1(9Z)/17:0)

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

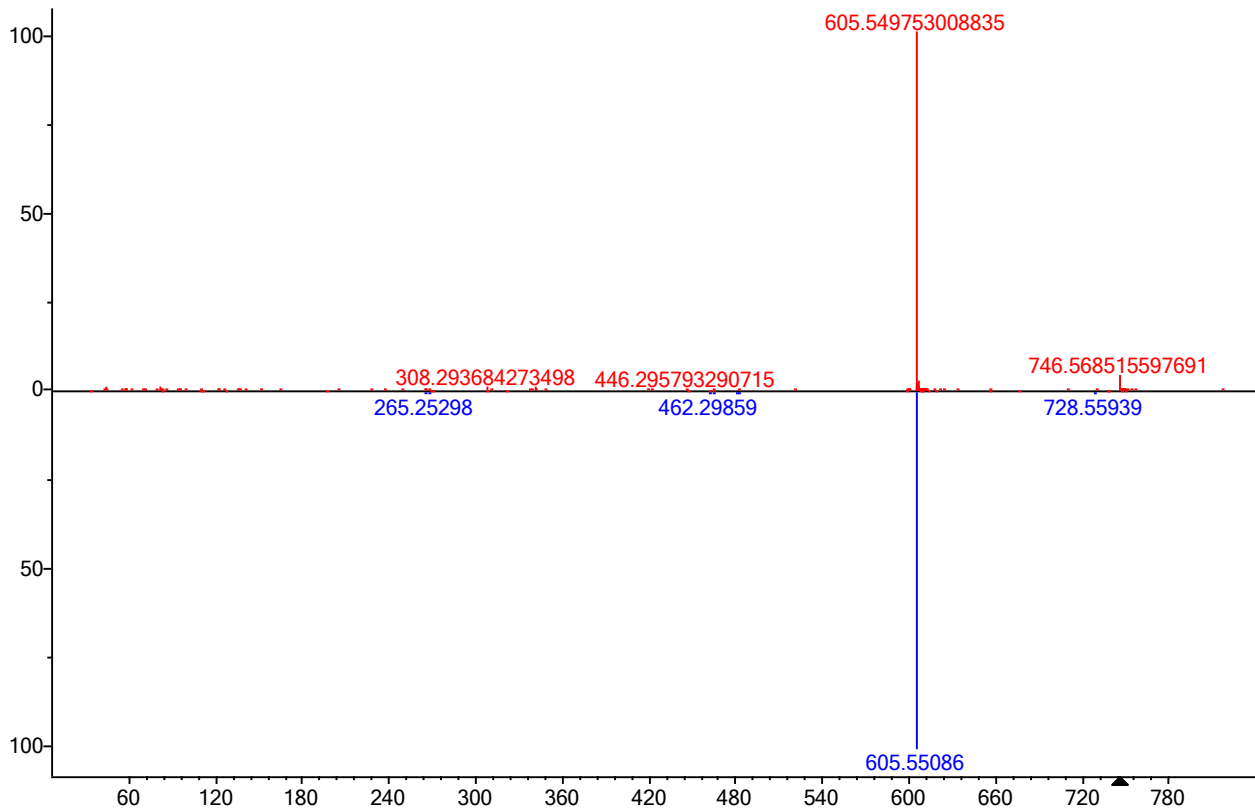
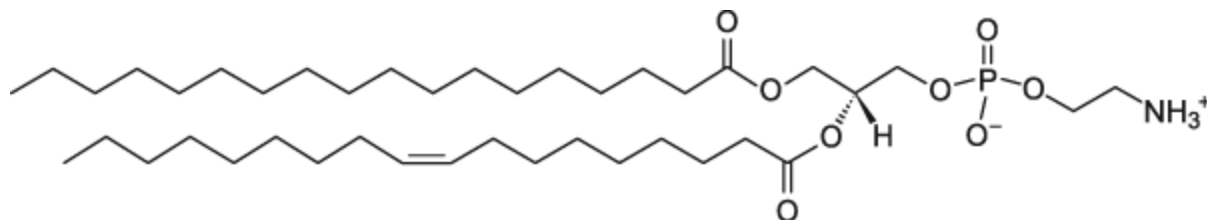
Name: PE 31:1; [M+H]⁺; GPEtn(14:1(9Z)/17:0)

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); C₃₆H₇₀N₀O₈P

8 largest peaks:

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



▲ A850758_PE_18_18d9_0011.d, MS/MS o | Head to Tail MF=35 RMF=924 | ▼ PE 36:1; [M+H]⁺; GPEtn(18:0/18:1(11E))

ID in LipidBlast – First HIT

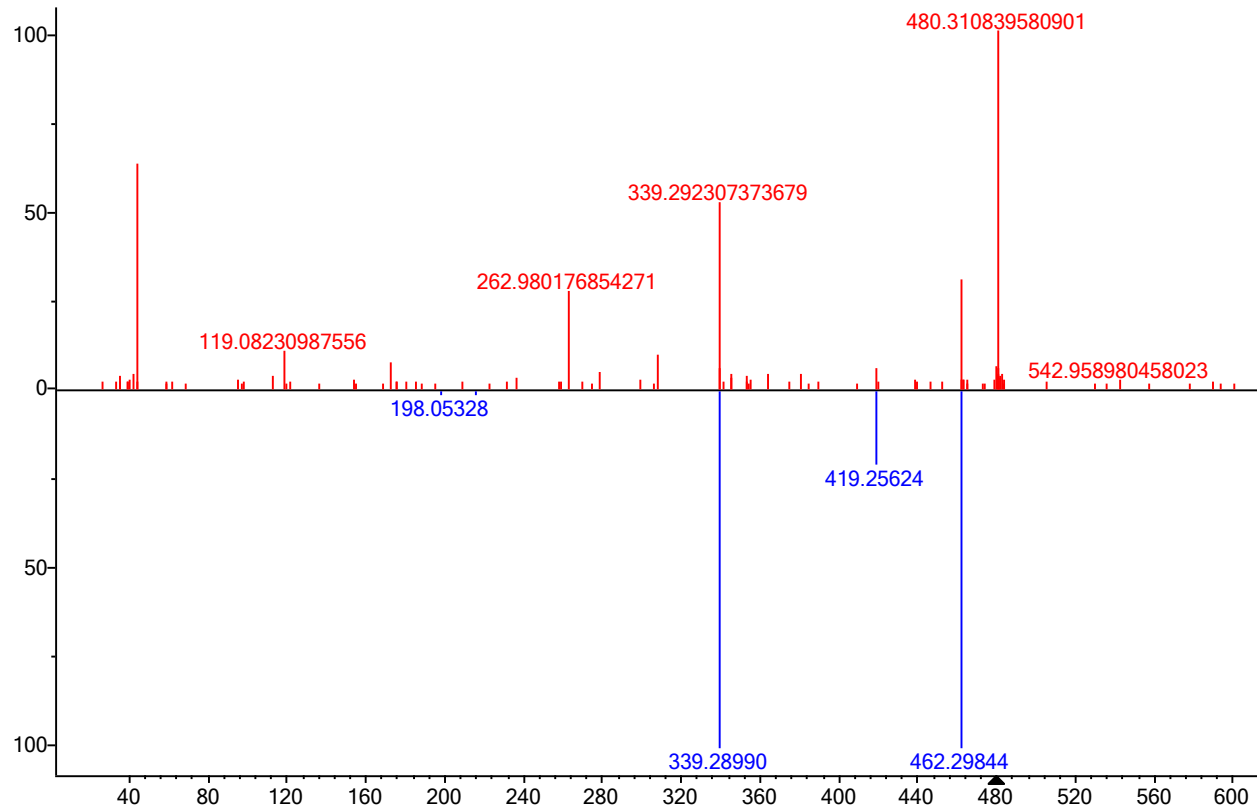
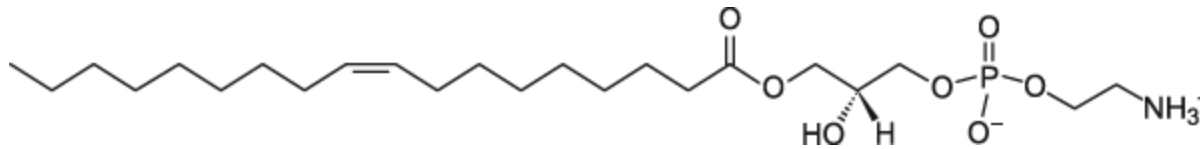
Name: PE 36:1; [M+H]⁺; GPEtn(18:0/18:1(11E))

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)); C₄₁H₈₀N₀O₈P

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



▲A846725_LysoPE_18d9_0001.d, MS/MS d Head to Tail MF=290 RMF=436 ▼ lysoPE 18:1; [M+H]⁺; PE(18:1(11E)/0:0)

ID in LipidBlast – First HIT

Name: lysoPE 18:1; [M+H]⁺; PE(18:1(11E)/0:0)

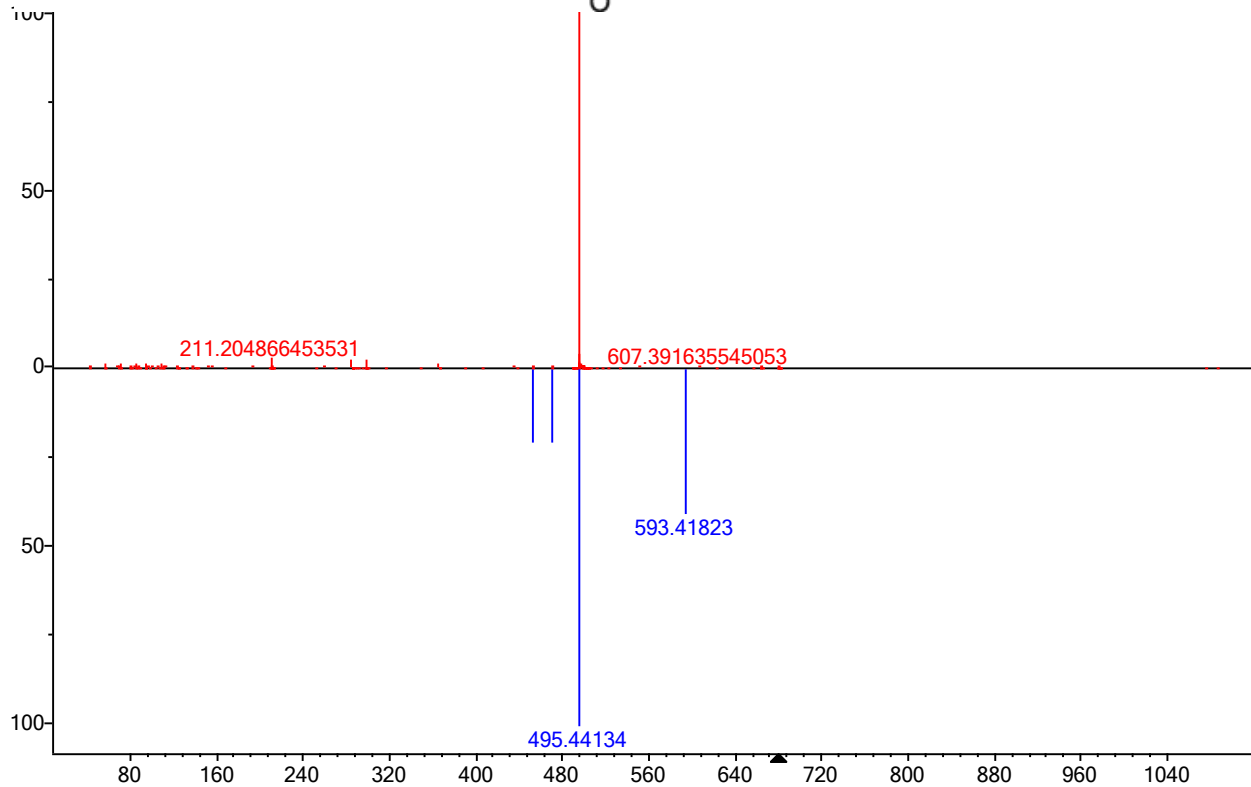
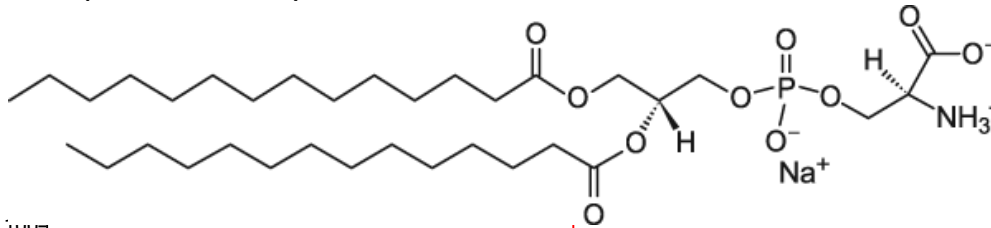
MW: 480 ID#: 9360 DB: lipidblast-pos

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)



▲ A840033_PS_14_14_0002.d, MS/MS of 6 | Head to Tail MF=5 RMF=788 | ▼ PS 28:0; [M+H]⁺; GPSer(14:0/14:0)

ID in LipidBlast – First HIT

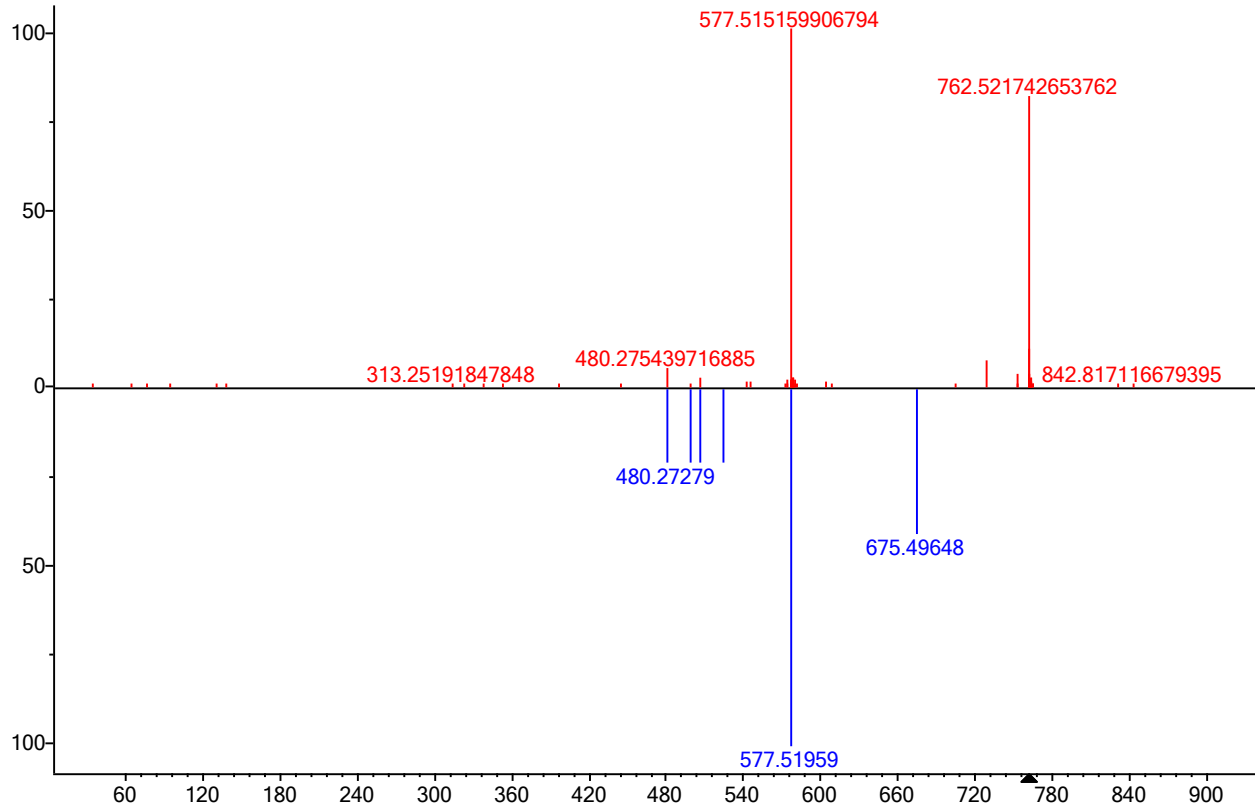
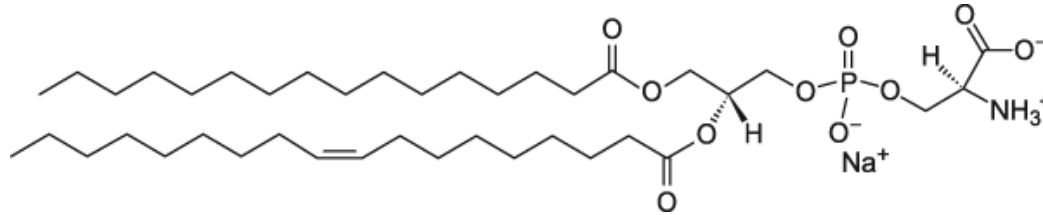
Name: PS 28:0; [M+H]⁺; GPSer(14:0/14:0)

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))



▲ A840034_PS_16_18d9_0009.d, MS/MS o | Head to Tail MF=95 RMF=609 | ▼ PS 34:1; [M+H]⁺; GPSer(16:0/18:1(11E))

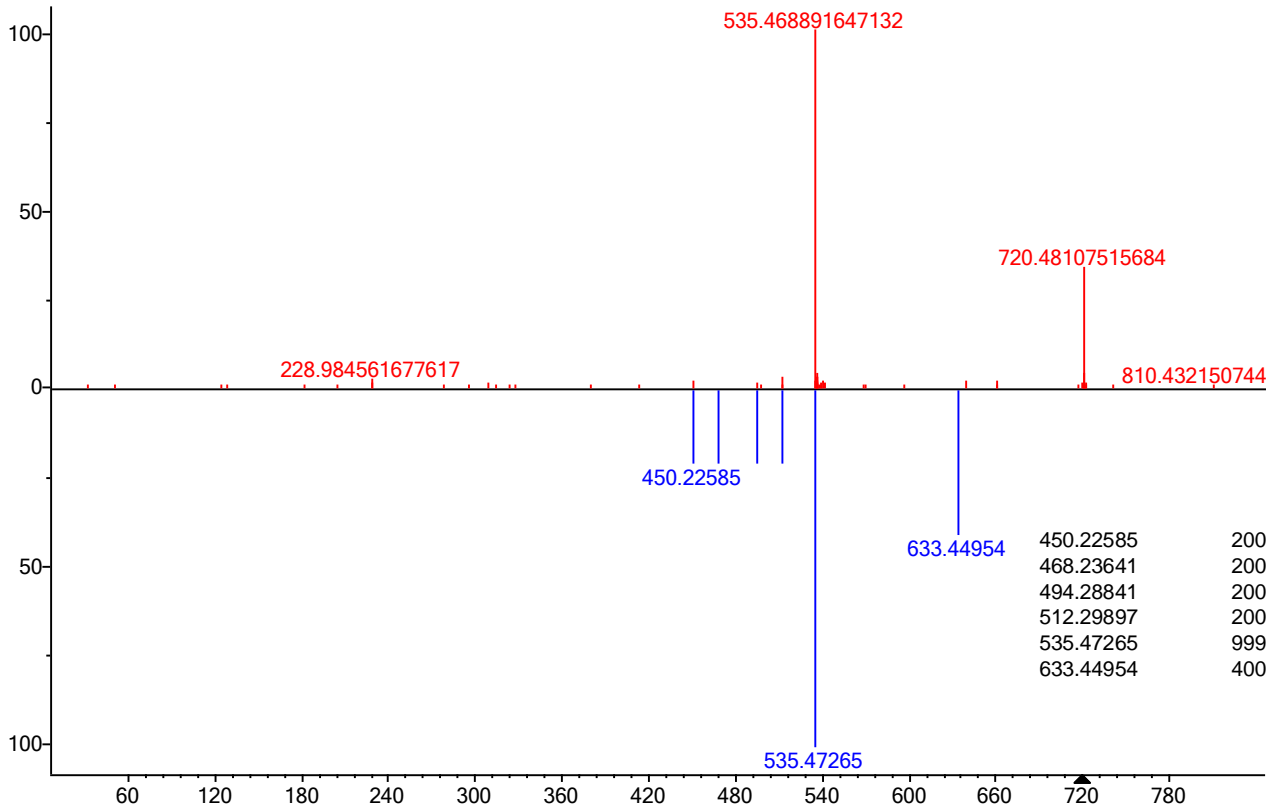
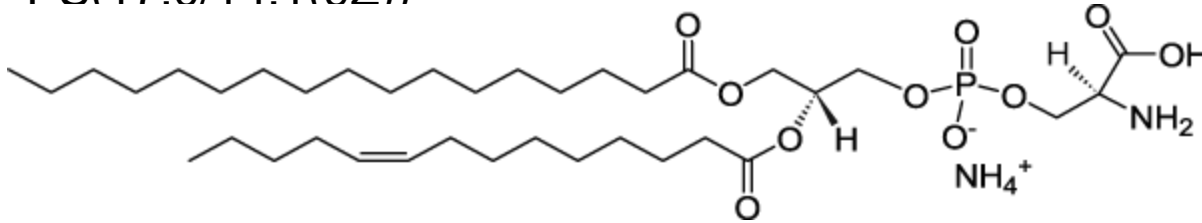
ID in LipidBlast – First HIT

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)

▲ LMGPO3010006_PS_17_14d9_0018.d, M\$ Head to Tail MF=72 RMF=647 ▼ PS 31:1; [M+H]⁺; GPSer(14:1(9Z)/17:0)

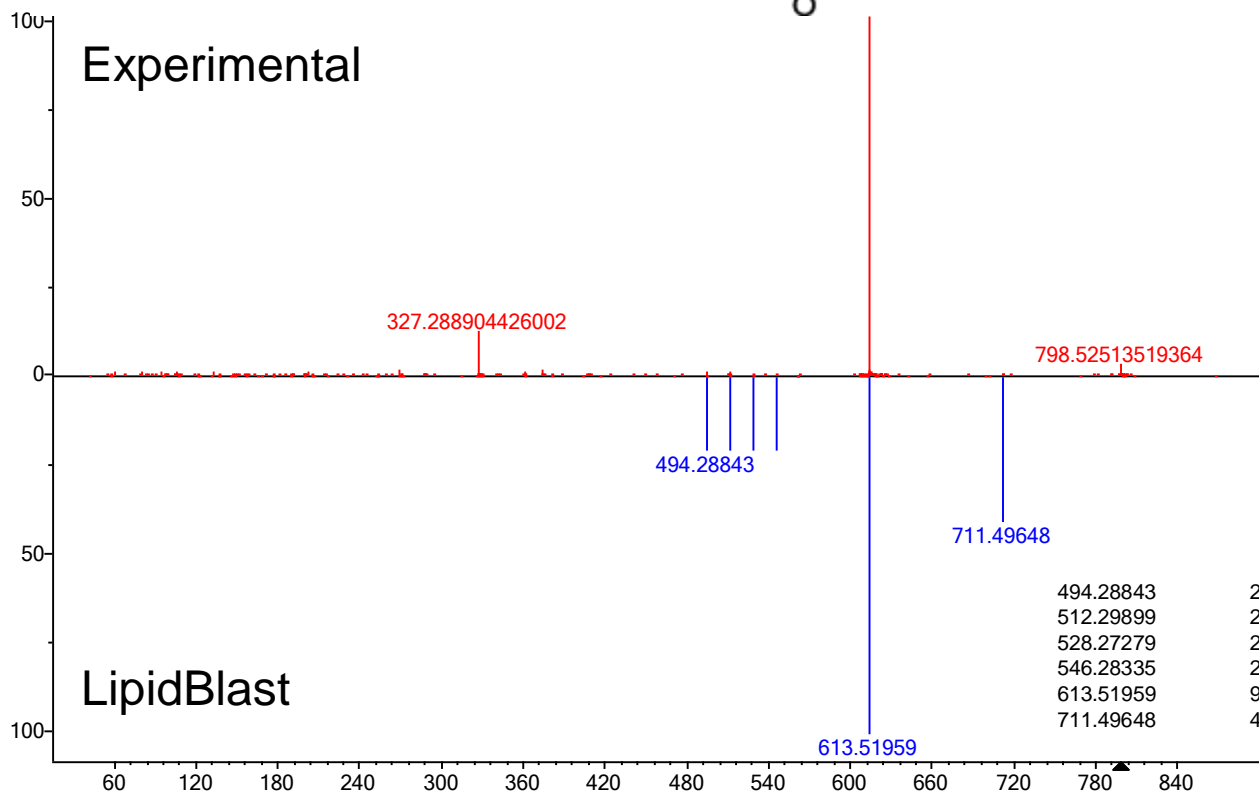
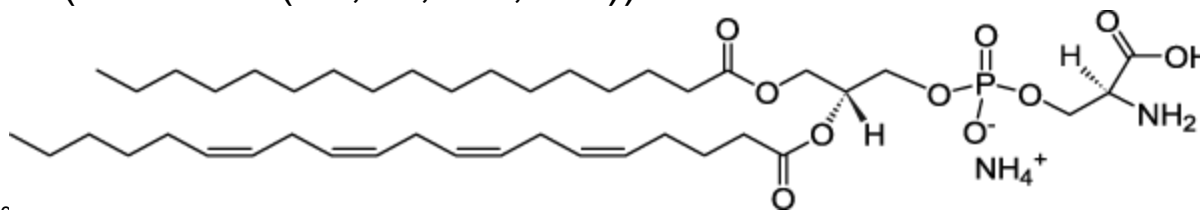
ID in LipidBlast – First HIT

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))



494.28843	200.00	[M+H]-sn2-H2O
512.29899	200.00	[M+H]-sn2
528.27279	200.00	[M+H]-sn1-H2O
546.28335	200.00	[M+H]-sn1
613.51959	999.00	[M+H]-C3H8NO6P (-185)
711.49648	400.00	[M+H]-C3H5NO2 (-87)

▲LMGP03010003_PS_17_20d5d8d11d14_() Head to Tail MF=7 RMF=788 ▼PS 37:4; [M+H]⁺; GPSer(17:0/20:4(5E,8E,

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

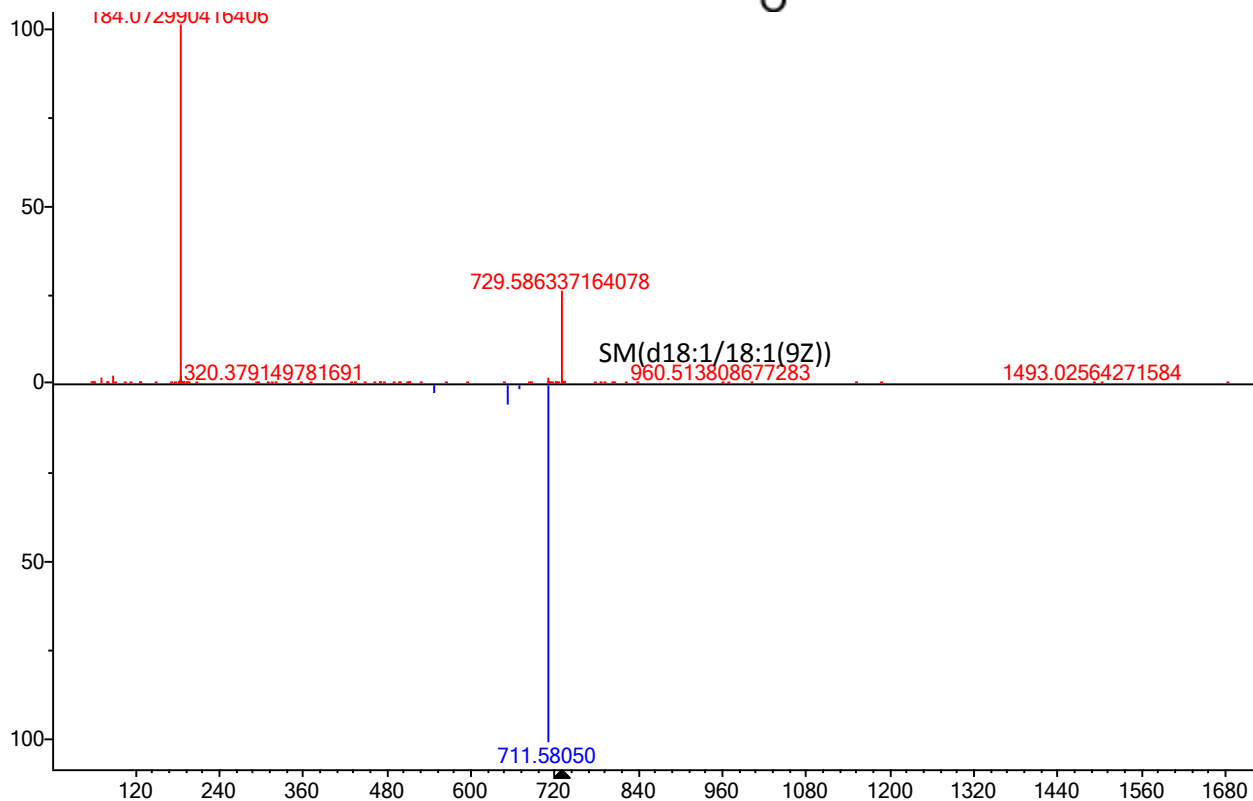
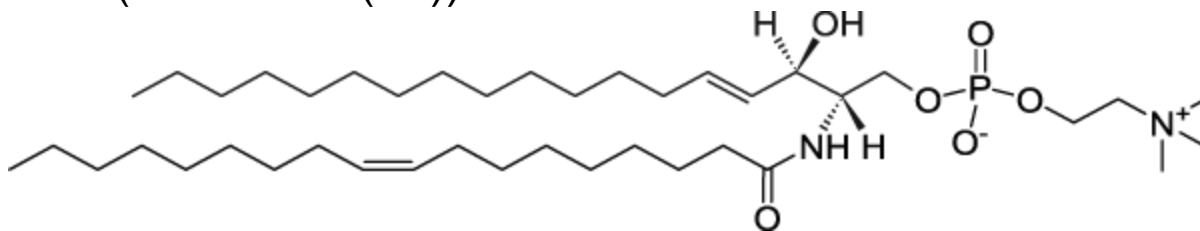
Comment: Parent=798.52851 Mz_exact=798.52851 ; PS 37:4; [M+H]⁺;

GPSer(17:0/20:4(5E,8E,11E,14E)); C43H76NO10P

6 largest peaks:

29) Standard sphingomyeine – ESI(+)

SM(d18:1/18:1(9Z))



▲ A860587_SM_18d9_18d9_0008.d, MS/M\$ Head to Tail MF=14 RMF=174 ▼ SM 36:2; [M]⁺; SM(d18:1(4E)/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.

Phospholipids in general
[1-45]

Phosphatidylcholine (PC)
[46-49]

Phosphatidylethanolamine (PE)
[50-52]

Phosphatidylglycerol (PG)
[53]

Phosphatidylinositol (PI)
[54-57]

Phosphatidic Acid (PA)
[58]

Plasmalogens and lysophospholipids
[59, 60]

Fatty Acids and Acyls
[61-65]

Ceramides (Cer)
[66-74]

Cardiolipins (CL)
[75-81]

MAG-DAG-TAG Mono-Di-Triacylglycerides
[82-96]

Gangliosides + Sulfatides
[97-103]

General lipid MS/MS identification and lipid analysis
[104-122]

Plant Lipids

[123-127]

Algal Lipids and viral and bacterial lipids

[128-144]

Yeast and fungal lipids

[145-148]

Decoy DBs

[149, 150]

LipidMaps

[151]

LipidSearch (online service)

[152]

Historic

[153-155]

Biocrates + ABI Kit

[156]

Chlorinated Lipids

[157]

Odd Number of carbons in fatty acids

[158-160]

FT-ICR accurate mass and time tag

[161, 162]

Glycolipids and Galactolipids - MGDG, DGDG, SQDG

[163-182]

Lipid A – complex lipids

[183-203]

Oxy-Lipids

[204-217]

Computer-Programs and tools and databases

[24, 104, 218-260]

Mass Spectrometer Types

[261, 262]

MALDI, FAB and ion mobility and others like DESI, FI, FD, SIMS

[58, 263-269]

References

1. Mitchell TW: **The effect of exercise and diet on rat skeletal muscle phospholipid molecular species profile: an electrospray ionisation mass spectrometric analysis.** *University of Wollongong Thesis Collection* 2004:585.
2. Brügger B, Erben G, Sandhoff R, Wieland FT, Lehmann WD: **Quantitative analysis of biological membrane lipids at the low picomole level by nano-electrospray ionization tandem mass spectrometry.** *Proceedings of the National Academy of Sciences of the United States of America* 1997, **94**(6):2339.
3. Larsen A, Hvattumh E: **Analysis of Phospholipids by Liquid Chromatography Coupled with On-Line Electrospray Ionization Mass Spectrometry and Tandem Mass Spectrometry.** *Modern Methods for Lipid Analysis by Liquid Chromatography/mass Spectrometry and Related Techniques* 2005:19.
4. Duffin K, Obukowicz M, Raz A, Shieh JJ: **Electrospray/tandem mass spectrometry for quantitative analysis of lipid remodeling in essential fatty acid deficient mice.** *Analytical Biochemistry* 2000, **279**(2):179-188.
5. Ekroos K: **Characterization of Molecular Glycerophospholipids by Quadrupole Time-of-Flight Mass Spectrometry.** 2003.
6. Retra K: **Schistosomal lysophosphatidylserine:an immunomodulatory factor.** 2007.
7. Erickson MC: **Phospholipids: Structures and Physicochemical Activities.** *Lipid analysis and lipidomics: new techniques and applications* 2006:399.
8. Byrdwell WC: **Modern methods for lipid analysis by liquid chromatography/mass spectrometry and related techniques:** AOCS press Champaign, IL (USA); 2005
9. Schürenberg M, Fuchs B, Bischoff A, Süß R, Anders U, Suckau D, Morlock G, Schiller J: **High Resolution Lipid Profiling and Identification by Hyphenated HPTLC-MALDI-TOF/TOF.** 2010.
10. Pelizzi N, Catinella S, Barbosa S, Zanol M: **Different electrospray tandem mass spectrometric approaches for rapid characterization of phospholipid classes of Curosurf®, a natural pulmonary surfactant.** *Rapid Communications in Mass Spectrometry* 2002, **16**(24):2215-2220.
11. Wang C, Xie S, Yang J, Yang Q, Xu G: **Structural identification of human blood phospholipids using liquid chromatography/quadrupole-linear ion trap mass spectrometry.** *Analytica Chimica Acta* 2004, **525**(1):1-10.
12. Oursel D, Loutelier-Bourhis C, Orange N, Chevalier S, Norris V, Lange CM: **Lipid composition of membranes of Escherichia coli by liquid chromatography/tandem mass spectrometry using negative electrospray ionization.** *Rapid Communications in Mass Spectrometry* 2007, **21**(11):1721-1728.
13. Yang K, Zhao Z, Gross RW, Han X: **Shotgun lipidomics identifies a paired rule for the presence of isomeric ether phospholipid molecular species.** *PLoS ONE* 2007, **2**(12).
14. Crone C, Genin E, Muenster H: **Analysis of whole lipid extracts using on-line high resolution LC-MS.** 2009.

15. Yu S, Cho K, Kim YH, Park S, Kim J, Oh HB: **Identification of Phospholipid Molecular Species in Porcine Brain Extracts Using High Mass Accuracy of 4.7 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry.** *Notes* 2006, **27**(5):793.
16. Ishida M, Yamaguchi S, Taniguchi J, Iida J, Miseki K, Nishimura O, Shimizu T, Taguchi R: **Precise Identification of Molecular Species of Phosphatidylethanolamine and Phosphatidylserine by Neutral Loss Survey with MS3 and Accurate Mass Measurement;**
17. Shinzawa-Itoh K, Aoyama H, Muramoto K, Terada H, Kurauchi T, Tadehara Y, Yamasaki A, Sugimura T, Kurono S, Tsujimoto K: **Structures and physiological roles of 13 integral lipids of bovine heart cytochrome c oxidase.** *the EMBO Journal* 2007, **26**(6):1713.
18. Buyukpamukcu E, Hau J, Fay LB, Dionisi F: **Analysis of phospholipids using electrospray ionisation tandem mass spectrometry.** *Lipid Technology* 2007, **19**(6):136-138.
19. Moehring T, Scigelova M, Ejsing CS, Schwudke D, Shevchenko A: **Essential Lipidomics Experiments Using the LTQ Orbitrap Hybrid Mass Spectrometer;**
20. Milne SB, Forrester JS, Ivanova PT, Armstrong MD, Brown HA: **Multiplexed Lipid Arrays of Anti-Immunoglobulin M-Induced Changes in the Glycerophospholipid Composition of WEHI-231 Cells.** *AfCS Research Reports I: I* 2003.
21. Yin C: **ESI-MS quantitation of increased sphingomyelin in Niemann-Pick disease type B HDL.** *The Journal of Lipid Research* 2005:M500011.
22. Wang C, Yang J, Gao P, Lu X, Xu G: **Identification of phospholipid structures in human blood by direct-injection quadrupole-linear ion-trap mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2005, **19**(17):2443-2453.
23. Jain S, Jayasimhulu K, Clark JF: **Metabolomic analysis of molecular species of phospholipids from normotensive and preeclamptic human placenta electrospray ionization mass spectrometry.** *Frontiers in Bioscience* 2004, **9**:3167-3175.
24. Ivanova PT, Milne SB, Forrester JS, Brown HA: **Lipid arrays: new tools in the understanding of membrane dynamics and lipid signaling.** *Molecular Interventions* 2004, **4**(2):86.
25. Ishida M, Yamazaki T, Houjou T, Imagawa M, Harada A, Inoue K, Taguchi R: **High-resolution analysis by nano-electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry for the identification of molecular species of phospholipids and their oxidized metabolites.** *Rapid Communications in Mass Spectrometry* 2004, **18**(20):2486-2494.
26. Jungalwala FB, Evans JE, McCluer RH: **Compositional and molecular species analysis of phospholipids by high performance liquid chromatography coupled with chemical ionization mass spectrometry.** *The Journal of Lipid Research* 1984, **25**(7):738.
27. Sommerer D, Süß R, Hammerschmidt S, Wirtz H, Arnold K, Schiller J: **Analysis of the phospholipid composition of bronchoalveolar lavage (BAL) fluid from**

- man and minipig by MALDI-TOF mass spectrometry in combination with TLC. *Journal of pharmaceutical and biomedical analysis* 2004, **35**(1):199-206.
28. Isaac G: **Development of Enhanced Analytical Methodology for Lipid Analysis from Sampling to Detection.** 2005.
 29. **LC-MS analysis of lipids and phospholipids.** In: *Liquid Chromatography-Mass Spectrometry, Third Edition.* vol. null: CRC Press; 2009.
 30. Watkins SM, Lin TY, Davis RM, Ching JR, DePeters EJ, Halpern GM, Walzem RL, German JB: **Unique phospholipid metabolism in mouse heart in response to dietary docosahexaenoic or -linolenic acids.** *Lipids* 2001, **36**(3):247-254.
 31. Han X, Gross RW: **Shotgun lipidomics: electrospray ionization mass spectrometric analysis and quantitation of cellular lipidomes directly from crude extracts of biological samples.** *Mass spectrometry reviews* 2004, **24**(3):367-412.
 32. Kerwin JL, Tuininga AR, Ericsson LH: **Identification of molecular species of glycerophospholipids and sphingomyelin using electrospray mass spectrometry.** *The Journal of Lipid Research* 1994, **35**(6):1102.
 33. Pulfer M, Murphy RC: **Electrospray mass spectrometry of phospholipids.** *Mass spectrometry reviews* 2003, **22**(5):332-364.
 34. Wang-Sattler R, Yu Y, Mittelstrass K, Lattka E, Altmaier E, Gieger C, Ladwig KH, Dahmen N, Weinberger KM, Hao P: **Metabolic profiling reveals distinct variations linked to nicotine consumption in humans—first results from the KORA study.** *PLoS One* 2008, **3**(12).
 35. Pietiläinen KH, Sysi-Aho M, Rissanen A, Seppänen-Laakso T, Yki-Järvinen H, Kaprio J, Oreši M: **Acquired obesity is associated with changes in the serum lipidomic profile independent of genetic effects—a monozygotic twin study.** *PLoS One* 2007, **2**(2).
 36. Kallury KMR, Ghaemmaghami V, Krull UJ, Thompson M, Davies MC: **Immobilization of phospholipids on silicon, platinum, indium/tin oxide and gold surfaces with characterization by X-ray photoelectron spectroscopy and time-of-flight secondary-ion mass spectrometry.** *Analytica Chimica Acta* 1989, **225**:369-389.
 37. Schwudke D, Hannich JT, Surendranath V, Grimard V, Moehring T, Burton L, Kurzchalia T, Shevchenko A: **Top-down lipidomic screens by multivariate analysis of high-resolution survey mass spectra.** *Anal Chem* 2007, **79**(11):4083-4093.
 38. Ekroos K, Chernushevich IV, Simons K, Shevchenko A: **Quantitative profiling of phospholipids by multiple precursor ion scanning on a hybrid quadrupole time-of-flight mass spectrometer.** *Anal Chem* 2002, **74**(5):941-949.
 39. Fridriksson EK, Shipkova PA, Sheets ED, Holowka D, Baird B, McLafferty FW: **Quantitative Analysis of Phospholipids in Functionally Important Membrane Domains from RBL-2H3 Mast Cells Using Tandem High-Resolution Mass Spectrometry†.** *Biochemistry* 1999, **38**(25):8056-8063.
 40. Ivanova PT, Milne SB, Byrne MO, Xiang Y, Brown HA: **Glycerophospholipid identification and quantitation by electrospray ionization mass spectrometry.** *Methods in enzymology* 2007:21-57.

41. Thomas MC, Mitchell TW, Blanksby SJ: **A comparison of the gas phase acidities of phospholipid headgroups: experimental and computational studies.** *Journal of the American Society for Mass Spectrometry* 2005, **16**(6):926-939.
42. Hsu FF, Turk J: **Structural Characterization of Unsaturated Glycerophospholipids by Multiple-Stage Linear Ion-Trap Mass Spectrometry with Electrospray Ionization.** *Journal of the American Society for Mass Spectrometry* 2008, **19**(11):1681-1691.
43. Dennis EA: **Lipidomics joins the omics evolution.** *Proceedings of the National Academy of Sciences* 2009, **106**(7):2089.
44. Kaddurah-Daouk R, Krishnan KRR: **Metabolomics: a global biochemical approach to the study of central nervous system diseases.** *Neuropsychopharmacology* 2008, **34**(1):173-186.
45. Matyash V, Liebisch G, Kurzchalia TV, Shevchenko A, Schwudke D: **Lipid extraction by methyl tert-butyl ether for high-throughput lipidomics.** *The Journal of Lipid Research* 2008:D700041.
46. Zhang X, Reid GE: **Multistage tandem mass spectrometry of anionic phosphatidylcholine lipid adducts reveals novel dissociation pathways.** *International Journal of Mass Spectrometry* 2006, **252**(3):242-255.
47. Domingues P, Domingues MRM, Amado FML, Ferrer-Correia AJ: **Characterization of sodiated glycerol phosphatidylcholine phospholipids by mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2001, **15**(10):799-804.
48. Zirrolli JA, Clay KL, Murphy RC: **Tandem mass spectrometry of negative ions from choline phospholipid molecular species related to platelet activating factor.** *Lipids* 1991, **26**(12):1112-1116.
49. Houjou T, Yamatani K, Nakanishi H, Imagawa M, Shimizu T, Taguchi R: **Rapid and selective identification of molecular species in phosphatidylcholine and sphingomyelin by conditional neutral loss scanning and MS3.** *Rapid Communications in Mass Spectrometry* 2004, **18**(24):3123-3130.
50. Raith K: **BEITRÄGE ZUR ANWENDUNG DER MASSENSPEKTROMETRIE IN DER LIPIDANALYTIK.** 1999.
51. Hsu FF, Turk J: **Characterization of phosphatidylethanolamine as a lithiated adduct by triple quadrupole tandem mass spectrometry with electrospray ionization.** *Journal of Mass Spectrometry* 2000, **35**(5):595-606.
52. Han X, Gross RW: **Structural determination of picomole amounts of phospholipids via electrospray ionization tandem mass spectrometry.** *Journal of the American Society for Mass Spectrometry* 1995, **6**(12):1202-1210.
53. Cabrera GM, Murga MLF, de Valdez GF, Seldes AM: **Direct analysis by electrospray ionization tandem mass spectrometry of mixtures of phosphatidylglycerols from Lactobacillus.** *Journal of Mass Spectrometry* 2001, **35**(12):1452-1459.
54. Valero-Guillén PL, Yagüe G, Segovia M: **Characterization of acyl-phosphatidylinositol from the opportunistic pathogen Corynebacterium amycolatum.** *Chemistry and physics of lipids* 2005, **133**(1):17-26.

55. Coté GG, Crain RC: **Why do plants have phosphoinositides?** *BioEssays* 2005, **16**(1):39-46.
56. Wenk MR: **The emerging field of lipidomics.** *Nature Reviews Drug Discovery* 2005, **4**(7):594-610.
57. Wenk MR, Lucast L, Di Paolo G, Romanelli AJ, Suchy SF, Nussbaum RL, Cline GW, Shulman GI, McMurray W, De Camilli P: **Phosphoinositide profiling in complex lipid mixtures using electrospray ionization mass spectrometry.** *Nature biotechnology* 2003, **21**(7):813-817.
58. Ham BM, Jacob JT, Cole RB: **MALDI-TOF MS of phosphorylated lipids in biological fluids using immobilized metal affinity chromatography and a solid ionic crystal matrix.** *Anal Chem* 2005, **77**(14):4439-4447.
59. DaTorre SD, Creer MH: **Differential turnover of polyunsaturated fatty acids in plasmalogen and diacyl glycerophospholipids of isolated cardiac myocytes.** *The Journal of Lipid Research* 1991, **32**(7):1159.
60. Barroso B, Bischoff R: **LC-MS analysis of phospholipids and lysophospholipids in human bronchoalveolar lavage fluid.** *Journal of Chromatography B* 2005, **814**(1):21-28.
61. Rawlings BJ: **Biosynthesis of fatty acids and related metabolites.** *Natural product reports* 1998, **15**(3):275-308.
62. Esch SW, Tamura P, Sparks AA, Roth MR, Devaiah SP, Heinz E, Wang X, Williams TD, Welti R: **Rapid characterization of the fatty acyl composition of complex lipids by collision-induced dissociation time-of-flight mass spectrometry.** *The Journal of Lipid Research* 2007, **48**(1):235.
63. Bergé JP, Barnathan G: **Fatty acids from lipids of marine organisms: molecular biodiversity, roles as biomarkers, biologically active compounds, and economical aspects.** *Marine biotechnology I* 2005:49-125.
64. Leblond JD, Chapman PJ: **Lipid class distribution of highly unsaturated long chain fatty acids in marine dinoflagellates.** *Journal of Phycology* 2000, **36**(6):1103-1108.
65. Poerschmann J, Carlson R: **New fractionation scheme for lipid classes based on.** *Journal of Chromatography A* 2006, **1127**(1-2):18-25.
66. Gu M, Kerwin JL, Watts JD, Aebersold R: **Ceramide profiling of complex lipid mixtures by electrospray ionization mass spectrometry.** *Analytical biochemistry* 1997, **244**(2):347-356.
67. Valsecchi M, Mauri L, Casellato R, Prioni S, Loberto N, Prinetti A, Chigorno V, Sonnino S: **Ceramide and sphingomyelin species of fibroblasts and neurons in culture.** *The Journal of Lipid Research* 2007, **48**(2):417.
68. Raith K, Neubert RHH: **Structural studies on ceramides by electrospray tandem mass spectrometry.** *Rapid Communications in Mass Spectrometry* 1998, **12**(14):935-938.
69. Colsch B, Afonso C, Popa I, Portoukalian J, Fournier F, Tabet JC, Baumann N: **Characterization of the ceramide moieties of sphingoglycolipids from mouse brain by ESI-MS/MS: identification of ceramides containing sphingadienine.** *The Journal of Lipid Research* 2004, **45**(2):281.
70. Shaner RL, Allegood JC, Park H, Wang E, Kelly S, Haynes CA, Cameron Sullards M: **Quantitative analysis of sphingolipids for lipidomics using triple**

- quadrupole and quadrupole linear ion trap mass spectrometers.** *The Journal of Lipid Research* 2008:D800051.
71. Hurme R: **Lipidomics-A new era for personalized medicine?;**
72. Sullards MC, Allegood JC, Kelly S, Wang E, Haynes CA, Park H, Chen Y, Merrill Jr AH: **Structure-Specific, Quantitative Methods for Analysis of Sphingolipids by Liquid Chromatography-Tandem Mass Spectrometry.** *Methods in enzymology* 2007:83-115.
73. Merrill AH: **Sphingolipidomics: high-throughput, structure-specific, and quantitative analysis of sphingolipids by liquid chromatography tandem mass spectrometry.** *Methods* 2005, **36**(2):207-224.
74. Pettus BJ, Bielawska A, Kroesen BJ, Moeller PDR, Szulc ZM, Hannun YA, Busman M: **Observation of different ceramide species from crude cellular extracts by normal-phase high-performance liquid chromatography coupled to atmospheric pressure chemical ionization mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2003, **17**(11):1203-1211.
75. Tyurina YY, Tyurin VA, Epperly MW, Greenberger JS, Kagan VE: **Oxidative lipidomics of [gamma]-irradiation-induced intestinal injury.** *Free Radical Biology and Medicine* 2008, **44**(3):299-314.
76. Hsu FF, Turk J, Rhoades ER, Russell DG, Shi Y, Groisman EA: **Structural characterization of cardiolipin by tandem quadrupole and multiple-stage quadrupole ion-trap mass spectrometry with electrospray ionization.** *Journal of the American Society for Mass Spectrometry* 2005, **16**(4):491-504.
77. Sparagna GC, Johnson CA, McCune SA, Moore RL, Murphy RC: **Quantitation of cardiolipin molecular species in spontaneously hypertensive heart failure rats using electrospray ionization mass spectrometry.** *The Journal of Lipid Research* 2005, **46**(6):1196.
78. Beckedorf AI, Schäffer C, Messner P, Peter K, cacute J: **Mapping and sequencing of cardiolipins from Geobacillus stearothermophilus NRS 2004/3a by positive and negative ion nanoESI-QTOF-MS and MS/MS.** *Journal of Mass Spectrometry* 2002, **37**(10):1086-1094.
79. Han X, Yang K, Yang J, Cheng H, Gross RW: **Shotgun lipidomics of cardiolipin molecular species in lipid extracts of biological samples.** *The Journal of Lipid Research* 2006, **47**(4):864.
80. Berger A, Gershwin ME, German JB: **Effects of various dietary fats on cardiolipin acyl composition during ontogeny of mice.** *Lipids* 1992, **27**(8):605-612.
81. Hsu FF, Turk J: **Characterization of Cardiolipin as the Sodiated Ions by Positive-Ion Electrospray Ionization with Multiple Stage Quadrupole Ion-Trap Mass Spectrometry.** *Journal of the American Society for Mass Spectrometry* 2006, **17**(8):1146-1157.
82. Ham BM, Jacob JT, Keese MM, Cole RB: **Identification, quantification and comparison of major non-polar lipids in normal and dry eye tear lipidomes by electrospray tandem mass spectrometry.** *Journal of mass spectrometry: JMS* 2004, **39**(11):1321.
83. Kalo PJ, Ollilainen V, Rocha JM, Malcata FX: **Identification of molecular species of simple lipids by normal phase liquid chromatography-positive**

- electrospray tandem mass spectrometry, and application of developed methods in comprehensive analysis of low erucic acid rapeseed oil lipids.** *International Journal of Mass Spectrometry* 2006, **254**(1-2):106-121.
84. Weil DA, Woodman M, Ball C: **Maximizing Detection of Complex Hydrophobic Lipids: Optimization Efficiency and Nano-Chromatography;**
85. Cvac ka J, Kofronová E: **Computer-assisted interpretation of triacylglycerols mass spectra.** *Methods in molecular biology (Clifton, NJ)* 2009, **580**:295.
86. Malone M, Evans JJ: **Running Title: Determining the Relative Amounts of Positional Isomers in Complex Mixtures of Triglycerides Using Reverse-Phase HPLC-MS-MS.**
87. ALLMAIER G, Stübiger G:
LASERFLUGZEITMASSENSPEKTROMETRIE ZUR CHARAKTERISIERUNG VON LIPIDEN UNTER BESONDERER BERÜCKSICHTIGUNG VON PFLANZENÖLTRIACYLGLYCEROLEN. 2006.
88. Facciotti D, Knauf V: **Triglycerides As Products of Photosynthesis. Genetic Engineering, Fatty Acid Composition and Structure of Triglycerides.** *Lipids in Photosynthesis: Structure, Function and Genetics* 1998:225-248.
89. Ha KS, Thompson Jr GA: **Diacylglycerol Metabolism in the Green Alga Dunaliella salina under Osmotic Stress: Possible Role of Diacylglycerols in Phospholipase C-Mediated Signal Transduction.** *Plant physiology* 1991, **97**(3):921.
90. Mottram HR, Woodbury SE, Evershed RP: **Identification of triacylglycerol positional isomers present in vegetable oils by high performance liquid chromatography/atmospheric pressure chemical ionization mass spectrometry.** *Rapid Communications in Mass Spectrometry* 1997, **11**(12):1240-1252.
91. Hvattum E: **Analysis of triacylglycerols with non-aqueous reversed-phase liquid chromatography and positive ion electrospray tandem mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2001, **15**(3):187-190.
92. Hsu FF, Turk J: **Structural characterization of triacylglycerols as lithiated adducts by electrospray ionization mass spectrometry using low-energy collisionally activated dissociation on a triple stage quadrupole instrument.** *Journal of the American Society for Mass Spectrometry* 1999, **10**(7):587-599.
93. Murphy RC, James PF, McAnoy AM, Krank J, Duchoslav E, Barkley RM: **Detection of the abundance of diacylglycerol and triacylglycerol molecular species in cells using neutral loss mass spectrometry.** *Analytical biochemistry* 2007, **366**(1):59-70.
94. Han X, Cheng H, Mancuso DJ, Gross RW: **Caloric restriction results in phospholipid depletion, membrane remodeling, and triacylglycerol accumulation in murine myocardium.** *Biochemistry* 2004, **43**(49):15584-15594.
95. Byrdwell WC, Neff WE: **Dual parallel electrospray ionization and atmospheric pressure chemical ionization mass spectrometry(MS), MS/MS and MS/MS/MS for the analysis of triacylglycerols and triacylglycerol**

- oxidation products.** *Rapid Communications in Mass Spectrometry* 2002, **16**(4):300-319.
96. Cai SS, Syage JA: **Comparison of atmospheric pressure photoionization, atmospheric pressure chemical ionization, and electrospray ionization mass spectrometry for analysis of lipids.** *Anal Chem* 2006, **78**(4):1191-1199.
97. He H, Emmett MR, Nilsson CL, Schaub TM, Conrad CA, Li Y, Marshal AG: **Profiling of Polar Membrane Lipids by On-Line Liquid Chromatography Electrospray Ionization FT-ICR Mass Spectrometry.** 2007.
98. Chen Y, Allegood J, Liu Y, Merrill AH, Sullards MC: **Imaging MALDI Mass Spectrometry of Sphingolipids Using an Oscillating Capillary Nebulizer (OCN) Matrix Application System;**
99. Allegood JC, Wang E, Sullards MC, Jr AHM: **Comparison of QTrap and chip-based nanospray Q-ToF for identification of sulfatides in complex mixtures;**
100. Chen Y, Allegood J, Liu Y, Wang E, Cachon-Gonzalez B, Cox TM, Merrill Jr AH, Sullards MC: **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):2780-2788.
101. Serb A, Schiopu C, Flangea C, Sisu E, Zamfir AD: **Top-down glycolipidomics: fragmentation analysis of ganglioside oligosaccharide core and ceramide moiety by chip-nanoelectrospray collision-induced dissociation MS2-MS6.** *Journal of Mass Spectrometry* 2009, **44**(10):1434-1442.
102. Eckhardt M: **The role and metabolism of sulfatide in the nervous system.** *Molecular Neurobiology* 2008, **37**(2):93-103.
103. Scandroglio F, Loberto N, Valsecchi M, Chigorno V, Prinetti A, Sonnino S: **Thin layer chromatography of gangliosides.** *Glycoconjugate Journal* 2009, **26**(8):961-973.
104. Yetukuri L, Katajamaa M, Medina-Gomez G, Seppänen-Laakso T, Vidal-Puig A, Oreši M: **Bioinformatics strategies for lipidomics analysis: characterization of obesity related hepatic steatosis.** *BMC Systems Biology* 2007, **1**(1):12.
105. Benning C, Ohlrogge J: **Current Advances in the Biochemistry and Cell Biology of Plant Lipids.** 2006.
106. Josephs JL, Sanders M, Shipkova P, Langish RA, Whitney J, Phillips JJ: **Detection and Characterization of Pharmaceutical Metabolites, Degradants and Impurities by the Application of MS/MS Software Algorithms.** 2003.
107. Böcker S: **Computational Mass Spectrometry.** 2009
108. Gurr MI, Harwood JL, Frayn KN, Gurr MI, Harwood JL, Frayn KN: **Lipid biochemistry - Lipids in cellular structures.** 2008.
109. Guschina IA, Harwood JL: **Lipids: Chemical Diversity.** 2008.
110. Bamba T, Shimonishi N, Matsubara A, Hirata K, Nakazawa Y, Kobayashi A, Fukusaki E: **High throughput and exhaustive analysis of diverse lipids by using supercritical fluid chromatography-mass spectrometry for metabolomics.** *Journal of bioscience and bioengineering* 2008, **105**(5):460-469.

111. Lemaire R, Wisztorski M, Desmons A, Tabet JC, Day R, Salzet M, Fournier I: **MALDI-MS direct tissue analysis of proteins: Improving signal sensitivity using organic treatments.** *Anal Chem* 2006, **78**(20):7145-7153.
112. Wishart DS, Lewis MJ, Morrissey JA, Flegel MD, Jeroncic K, Xiong Y, Cheng D, Eisner R, Gautam B, Tzur D: **The human cerebrospinal fluid metabolome.** *Journal of Chromatography B* 2008, **871**(2):164-173.
113. Liebisch G: **Hochdurchsatz-Lipid Profiling mit Tandem-Massenspektrometrie;**
114. **LIPID MAPS MASS SPECTROMETRY METHODS CHAPTERS;**
115. Watson AD: **Lipidomics: a global approach to lipid analysis in biological systems.** *The Journal of Lipid Research* 2006:R600022.
116. Milne S, Ivanova P, Forrester J, Alex Brown H: **Lipidomics: an analysis of cellular lipids by ESI-MS.** *Methods* 2006, **39**(2):92-103.
117. Watkins SM, Reifsnyder PR, Pan H, German JB, Leiter EH: **Lipid metabolome-wide effects of the peroxisome proliferator-activated receptor gamma agonist rosiglitazone.** *The Journal of Lipid Research* 2002:200169200.
118. Murphy RC: **Challenges in the Analysis of Glyceryl Lipids as Molecular Species.** 2005.
119. Van den Berg JDJ: **Analytical chemical studies on traditional linseed oil paints.** *University of Amsterdam* 2002.
120. Houjou T, Yamatani K, Imagawa M, Shimizu T, Taguchi R: **A shotgun tandem mass spectrometric analysis of phospholipids with normal-phase and/or reverse-phase liquid chromatography/electrospray ionization mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2005, **19**(5):654-666.
121. Hicks AM, DeLong CJ, Thomas MJ, Samuel M, Cui Z: **Unique molecular signatures of glycerophospholipid species in different rat tissues analyzed by tandem mass spectrometry.** *Biochimica et Biophysica Acta (BBA)-Molecular and Cell Biology of Lipids* 2006, **1761**(9):1022-1029.
122. Manicke NE, Wiseman JM, Ifa DR, Cooks RG: **Desorption electrospray ionization (DESI) mass spectrometry and tandem mass spectrometry (MS/MS) of phospholipids and sphingolipids: ionization, adduct formation, and fragmentation.** *Journal of the American Society for Mass Spectrometry* 2008, **19**(4):531-543.
123. Morton J: **Characterization of a lipase in Arabidopsis defense.** 2007.
124. Welti R, Wang X: **Lipid species profiling: a high-throughput approach to identify lipid compositional changes and determine the function of genes involved in lipid metabolism and signaling.** *Current opinion in plant biology* 2004, **7**(3):337-344.
125. Wanjie SW, Welti R, Moreau RA, Chapman KD: **Identification and Quantification of Lipid Metabolites in Cotton Fibers: Reconciliation with Metabolic Pathway Predictions from DNA Databases.** *Lipids* 2005, **40**(8):773-785.
126. Gounaris K, Barber J, Harwood JL: **The thylakoid membranes of higher plant chloroplasts.** *Biochemical Journal* 1986, **237**(2):313.

127. Wang X, Li W, Li M, Welti R: **Profiling lipid changes in plant response to low temperatures.** *Physiologia Plantarum* 2006, **126**(1):90-96.
128. Guschina IA, Harwood JL: **Lipids and lipid metabolism in eukaryotic algae.** *Progress in Lipid Research* 2006, **45**(2):160-186.
129. Khotimchenko SV: **Lipids from the marine alga *Gracilaria verrucosa*.** *Chemistry of Natural Compounds* 2005, **41**(3):285-288.
130. Harwood J: **Membrane lipids in algae.** *Lipids in Photosynthesis: Structure, Function and Genetics* 1998:53-64.
131. Wada H, Murata N: **Membrane lipids in cyanobacteria.** *Lipids in Photosynthesis: Structure, Function and Genetics* 1998:65-81.
132. Sheehan J, Dunahay T, Benemann J, Roessler P: **A look back at the US Department of Energy's aquatic species program—biodiesel from algae.** *National Renewable Energy Laboratory, Golden, CO* 1998, **80401**:580-24190.
133. Thomas WH, Tornabene TG, Weissman J: **Screening for lipid yielding microalgae: activities for 1983. Final subcontract report.** In.: SERI/STR-231-2207, Solar Energy Research Inst., Golden, CO (USA); 1984.
134. Li Q, Du W, Liu D: **Perspectives of microbial oils for biodiesel production.** *Applied microbiology and biotechnology* 2008, **80**(5):749-756.
135. Reisser W: **The Hidden Life of Algae Underground.** *Algae and Cyanobacteria in Extreme Environments*:47-58.
136. Ikawa M: **Algal polyunsaturated fatty acids and effects on plankton ecology and other organisms.** *UNH Center for Freshwater Biology Research* 2004, **6**(2):17-44.
137. Ravishankar GA: **Comparative study of lipid composition of two halotolerant alga, *Dunaliella bardawil* and *Dunaliella salina*.** *International Journal of Food Sciences and Nutrition* 2007, **58**(5):373-382.
138. Pick U, Gounaris K, Weiss M, Barber J: **Tightly bound sulpholipids in chloroplast CF0-CF1.** *Biochimica et Biophysica Acta (BBA)-Bioenergetics* 1985, **808**(3):415-420.
139. Sturt HF, Summons RE, Smith K, Elvert M, Hinrichs KU: **Intact polar membrane lipids in prokaryotes and sediments deciphered by high-performance liquid chromatography/electrospray ionization multistage mass spectrometry—new biomarkers for biogeochemistry and microbial ecology.** *Rapid Communications in Mass Spectrometry* 2004, **18**(6):617-628.
140. Zepke HD, Heinz E, Radunz A, Linscheid M, Pesch R: **Combination and positional distribution of fatty acids in lipids from blue-green algae.** *Archives of Microbiology* 1978, **119**(2):157-162.
141. Khotimchenko SV: **Distribution of glyceroglycolipids in marine algae and grasses.** *Chemistry of Natural Compounds* 2002, **38**(3):223-229.
142. Crews FT, McElhaney MR, Klepner CA, Lippa AS: **Lipids are major components of human immunodeficiency virus (HIV): Modification of HIV lipid composition, membrane organization, and protein conformation by AL-721®.** *Drug Development Research* 2004, **14**(1):31-44.
143. Brügger B, Glass B, Haberkant P, Leibrecht I, Wieland FT, Kräusslich HG: **The HIV lipidome: a raft with an unusual composition.** *Proceedings of the National Academy of Sciences* 2006, **103**(8):2641.

144. Los DA, Murata N: **Responses to cold shock in cyanobacteria.** *J Mol Microbiol Biotechnol* 1999, **1**(2):221-230.
145. Tosch W, Lanthaler K, Boote V, Stretz D, Robson GD, Geiger E, Drucker DB: **Molecular species of phosphatidylethanolamine from continuous cultures of *Saccharomyces pastorianus* syn. *carlsbergensis* strains.** *Yeast* 2006, **23**(2):75-82.
146. Bruneteau M, Fournol F, Gandon C, Becchi M, Pivot V: **Isolation and characterization of inositol sphingophospholipids from *Phytophthora parasitica* Dastur.** *Lipids* 1997, **32**(4):359-362.
147. Schneider R, Brugger B, Sandhoff R, Zellnig G, Leber A, Lampl M, Athenstaedt K, Hrastnik C, Eder S, Daum G: **Electrospray ionization tandem mass spectrometry (ESI-MS/MS) analysis of the lipid molecular species composition of yeast subcellular membranes reveals acyl chain-based sorting/remodeling of distinct molecular species en route to the plasma membrane.** *Journal of Cell Biology* 1999, **146**(4):741.
148. Ejsing CS, Sampaio JL, Surendranath V, Duchoslav E, Ekroos K, Klemm RW, Simons K, Shevchenko A: **Global analysis of the yeast lipidome by quantitative shotgun mass spectrometry.** *Proceedings of the National Academy of Sciences* 2009, **106**(7):2136.
149. Elias JE, Gygi SP: **Target-decoy search strategy for increased confidence in large-scale protein identifications by mass spectrometry.** *Nature methods* 2007, **4**(3):207-214.
150. Wishart DS, Tzur D, Knox C, Eisner R, Guo AC, Young N, Cheng D, Jewell K, Arndt D, Sawhney S: **HMDB: the human metabolome database.** *Nucleic acids research* 2007, **35**(Database issue):D521.
151. Fahy E, Subramaniam S, Murphy RC, Nishijima M, Raetz CRH, Shimizu T, Spener F, van Meer G, Wakelam MJO, Dennis EA: **Update of the LIPID MAPS comprehensive classification system for lipids.** *The Journal of Lipid Research* 2009, **50**(Supplement):S9.
152. Yokoi Y, Aoshima K, Yanagisawa K, Yamazaki T, Ishida M, Houjou T, Nakanishi H, Oda Y, Taguchi R: **Construction of Automated Identification System for Lipidome.** 2005.
153. Barbieri A: **Non-existence of Free or Combined Lecithins in the Yolk of Eggs and in Biological Structures.** *Abstracts of chemical papers* 1912.
154. Working EB, Andrews AC: **The Structure of the Phospholipids.** *Chemical Reviews* 1941, **29**(2):245-256.
155. Gamgee A, Blankenhorn E: **On Protagon.** *The Journal of Physiology* 1879, **2**(2):113.
156. Snijders H: **Understanding Small Molecule Biomarker Patterns by Targeted and Non-Targeted Metabolomics using LC/MS/MS;**
157. Pitt A, Spickett C: **Mass spectrometric analysis of HOCl- and free-radical-induced damage to lipids and proteins.** *Biochemical Society Transactions* 2008, **36**:1077-1082.
158. Ekroos K, Ejsing CS, Bahr U, Karas M, Simons K, Shevchenko A: **Charting molecular composition of phosphatidylcholines by fatty acid scanning and ion trap MS3 fragmentation.** *The Journal of Lipid Research* 2003, **44**(11):2181.

159. Cassel DL, Ragona DG, Carriedo L, Kempe JA, Conner RL: **Metabolism of odd-numbered, normal fatty acids in *Tetrahymena pyriformis* W.** *Biochimica et Biophysica Acta (BBA)-Lipids and Lipid Metabolism* 1981, **663**(1):121-133.
160. Lichtfouse E, Derenne S, Mariotti A, Largeau C: **Possible algal origin of long chain odd n-alkanes in immature sediments as revealed by distributions and carbon isotope ratios.** *Organic Geochemistry* 1994, **22**(6):1023-1027.
161. Sorensen CM, Ding J, Zhang Q, Mueller PW, Smith RD, Metz TO: **Application of the accurate mass and time tag approach in lipidomics studies of type 1 diabetes mellitus.** 2008.
162. Ding J, Sorensen CM, Jaitly N, Jiang H, Orton DJ, Monroe ME, Moore RJ, Smith RD, Metz TO: **Application of the accurate mass and time tag approach in studies of the human blood lipidome.** *Journal of Chromatography B* 2008, **871**(2):243-252.
163. Herrero M, Vicente MJ, Cifuentes A, Ibañez E: **Characterization by high-performance liquid chromatography/electrospray ionization quadrupole time-of-flight mass spectrometry of the lipid fraction of *Spirulina platensis* pressurized ethanol extract.** 2007.
164. Naumann I, Darsow KH, Walter C, Lange HA, Buchholz R: **Identification of sulfoglycolipids from the alga *Porphyridium purpureum* by matrix-assisted laser desorption/ionisation quadrupole ion trap time-of-flight mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2007, **21**(19):3185-3192.
165. Vieler A, Wilhelm C, Goss R, Süß R, Schiller J: **The lipid composition of the unicellular green alga *Chlamydomonas reinhardtii* and the diatom *Cyclotella meneghiniana* investigated by MALDI-TOF MS and TLC.** *Chemistry and physics of lipids* 2007, **150**(2):143-155.
166. Yao H, Shi Y, Gao R, Zhang G, Zhang R, Zheng C, Xu B: **Isolation of lipids from photosystem I complex and its characterization with high performance liquid chromatography/electrospray ionization mass spectrometry.** *Journal of Chromatography B* 2006, **837**(1-2):101-107.
167. Gray CG, Lasiter AD, Leblond JD: **Mono- and digalactosyldiacylglycerol composition of dinoflagellates. III. Four cold-adapted, peridinin-containing taxa and the presence of trigalactosyldiacylglycerol as an additional glycolipid.** *European Journal of Phycology* 2009, **99999**(1):1-7.
168. Devaiah SP, Roth MR, Baughman E, Li M, Tamura P, Jeannotte R, Welti R, Wang X: **Quantitative profiling of polar glycerolipid species from organs of wild-type *Arabidopsis* and a PHOSPHOLIPASE D [alpha] 1 knockout mutant.** *Phytochemistry* 2006, **67**(17):1907-1924.
169. Moreau RA, Doehlert DC, Welti R, Isaac G, Roth M, Tamura P, Nun ez A: **The identification of mono-, di-, tri-, and tetragalactosyl-diacylglycerols and their natural estolides in oat kernels.** *Lipids* 2008, **43**(6):533-548.
170. Naumann I: **Sulfoquinovosyldiacylglyceride-antiviral aktive Substanzen;** 2009
171. Guella G, Frassanito R, Mancini I: **A new solution for an old problem: the regiochemical distribution of the acyl chains in galactolipids can be established by electrospray ionization tandem mass spectrometry.** *Rapid Communications in Mass Spectrometry* 2003, **17**(17):1982-1994.

172. Gray CG, Lasiter AD, Li C, Leblond JD: **Mono- and digalactosyldiacylglycerol composition of dinoflagellates. I. Peridinin-containing taxa.** *European Journal of Phycology* 2009, **44**(2):191-197.
173. Healthcare I: **Mono- and digalactosyldiacylglycerol composition of dinoflagellates. II. Lepidodinium chlorophorum, Karenia brevis, and Kryptoperidinium foliaceum, three dinoflagellates with aberrant plastids.** *European Journal of Phycology* 2009, **44**(2):199-205.
174. Frassanito R, Mancini I, Guella G: **Chimica e biologia a confronto: pigmenti e altri metaboliti secondari prodotti da dinoflagellati del Lago di Tovel.** 2006.
175. Welti R, Wang X, Williams TD: **Electrospray ionization tandem mass spectrometry scan modes for plant chloroplast lipids.** *Analytical biochemistry* 2003, **314**(1):149-152.
176. Yamauchi R: **Analysis of Molecular Species of Plant Glycolipids by HPLC/APCI-MS.** *Modern Methods for Lipid Analysis by Liquid Chromatography/mass Spectrometry and Related Techniques* 2005:431.
177. Siegenthaler PA: **Molecular organization of acyl lipids in photosynthetic membranes of higher plants.** *Lipids in Photosynthesis: Structure, Function and Genetics* 1998:119-144.
178. Al-Fadhli A, Wahidulla S, D'Souza L: **Glycolipids from the red alga Chondria armata (Kütz.) Okamura.** *Glycobiology* 2006, **16**(10):902.
179. Naumann I: **Antiviral active Sulfoquinovosyldiacylglycerides from Phototrophic Microorganisms;**
180. Lynch DV, Gundersen RE, Thompson Jr GA: **Separation of galactolipid molecular species by high-performance liquid chromatography.** *Plant Physiology* 1983, **72**(3):903.
181. Dörmann P, Benning C: **Galactolipids rule in seed plants.** *Trends in plant science* 2002, **7**(3):112-118.
182. Roughan PG, Batt RD: **Quantitative analysis of sulfolipid (sulfoquinovosyl diglyceride) and galactolipids (monogalactosyl and digalactosyl diglycerides) in plant tissues.** *Analytical biochemistry* 1968, **22**(1):74-88.
183. Lukasiewicz J, Jachymek W, Niedziela T, Kenne L, Lugowski C: **Structural analysis of the lipid A isolated from Hafnia alvei 32 and PCM 1192 lipopolysaccharides.** *The Journal of Lipid Research* 2009, **51**(3):564.
184. Zhou P, Chandan V, Liu X, Chan K, Altman E, Li J: **Microwave-assisted sample preparation for rapid and sensitive analysis of H. pylori lipid A applicable to a single colony.** *The Journal of Lipid Research* 2009, **50**(9):1936.
185. Ting Y, Malmstroem L, Shaffer SA, Ng WV, Goodlett DR: **Characterization of Lipid A Species by Computational Analysis of Mass Spectrometry Data.** 2008.
186. Phillips NJ, Schilling B, McLendon MK, Apicella MA, Gibson BW: **Novel modification of lipid A of Francisella tularensis.** *Infection and immunity* 2004, **72**(9):5340.
187. Price NP, Jeyaretnam B, Carlson RW, Kadrmas JL, Raetz CR, Brozek KA: **Lipid A biosynthesis in Rhizobium leguminosarum: role of a 2-keto-3-deoxyoctulosonate-activated 4'phosphatase.** *Proceedings of the National Academy of Sciences of the United States of America* 1995, **92**(16):7352.

188. Sweet CR, Preston A, Toland E, Ramirez SM, Cotter RJ, Maskell DJ, Raetz CRH: **Relaxed acyl chain specificity of Bordetella UDP-N-acetylglucosamine acyltransferases.** *Journal of Biological Chemistry* 2002, **277**(21):18281.
189. Que NLS, Lin S, Cotter RJ, Raetz CRH: **Purification and mass spectrometry of six lipid A species from the bacterial endosymbiont Rhizobium etli.** *Journal of Biological Chemistry* 2000, **275**(36):28006.
190. Somerville Jr JE, Cassiano L, Bainbridge B, Cunningham MD, Darveau RP: **A novel Escherichia coli lipid A mutant that produces an antiinflammatory lipopolysaccharide.** *Journal of Clinical Investigation* 1996, **97**(2):359.
191. Jones JW, Shaffer SA, Ernst RK, Goodlett DR, Turek F: **Determination of pyrophosphorylated forms of lipid A in Gram-negative bacteria using a multivariate mass spectrometric approach.** *Proceedings of the National Academy of Sciences* 2008, **105**(35):12742.
192. Schilling B, McLendon MK, Phillips NJ, Apicella MA, Gibson BW: **Characterization of lipid A acylation patterns in Francisella tularensis, Francisella novicida, and Francisella philomiragia using multiple-stage mass spectrometry and matrix-assisted laser desorption/ionization on an intermediate vacuum source linear ion trap.** *Anal Chem* 2007, **79**(3):1034-1042.
193. Mikhail I, Yildirim HH, Lindahl ECH, Schweda EKH: **Structural characterization of lipid A from nontypeable and type f Haemophilus influenzae: Variability of fatty acid substitution.** *Analytical biochemistry* 2005, **340**(2):303-316.
194. Dzieciatkowska M, Schweda EKH, Moxon ER, Richards JC, Li J: **Characterization of intact lipopolysaccharides from the Haemophilus influenzae strain RM 118 using electrophoresis-assisted open-tubular liquid chromatography-mass spectrometry.** *Electrophoresis* 2008, **29**(10):2171-2181.
195. Feulner JA, Lu M, Shelton JM, Zhang M, Richardson JA, Munford RS: **Identification of acyloxyacyl hydrolase, a lipopolysaccharide-detoxifying enzyme, in the murine urinary tract.** *Infection and immunity* 2004, **72**(6):3171.
196. Klein G, Lindner B, Brabetz W, Brade H, Raina S: **Escherichia coli K-12 Suppressor-free Mutants Lacking Early Glycosyltransferases and Late Acyltransferases.** *Journal of Biological Chemistry* 2009, **284**(23):15369.
197. Lee CS, Kim YG, Joo HS, Kim BG: **Structural analysis of lipid A from Escherichia coli O157: H7: K-using thin-layer chromatography and ion-trap mass spectrometry.** *Journal of Mass Spectrometry* 2004, **39**(5):514-525.
198. Wang X, Ribeiro AA, Guan Z, Raetz CRH: **Identification of undecaprenyl phosphate- -D-galactosamine in Francisella novicida and its function in lipid A modification.** *Biochemistry* 2009, **48**(6):1162.
199. Montminy SW, Khan N, McGrath S, Walkowicz MJ, Sharp F, Conlon JE, Fukase K, Kusumoto S, Sweet C, Miyake K: **Virulence factors of Yersinia pestis are overcome by a strong lipopolysaccharide response.** *Nature immunology* 2006, **7**(10):1066-1073.
200. John CM, Liu M, Jarvis GA: **Natural Phosphoryl and Acyl Variants of Lipid A from Neisseria meningitidis Strain 89I Differentially Induce Tumor Necrosis**

- Factor- α in Human Monocytes.** *Journal of Biological Chemistry* 2009, **284**(32):21515.
201. Volk AS, Krasikova IN, Anastyuk SD, Dmitrenok PS, Solov'eva TF: **Structure of lipid A from the marine gram-negative bacterium *Pseudoalteromonas nigrifaciens* IAM 13010 T.** *Chemistry of Natural Compounds* 2007, **43**(5):519-524.
202. Sforza S, Silipo A, Molinaro A, Marchelli R, Parrilli M, Lanzetta R: **Determination of fatty acid positions in native lipid A by positive and negative electrospray ionization mass spectrometry.** *Journal of Mass Spectrometry* 2004, **39**(4):378-383.
203. Long X, Deng S, Mattner J, Zang Z, Zhou D, McNary N, Goff RD, Teyton L, Bendelac A, Savage PB: **Synthesis and evaluation of stimulatory properties of Sphingomonadaceae glycolipids.** *Nature chemical biology* 2007, **3**(9):559-564.
204. Domingues MRM, Reis A, Domingues P: **Mass spectrometry analysis of oxidized phospholipids.** *Chemistry and Physics of Lipids* 2008, **156**(1-2):1-12.
205. Tyurina YY, Tyurin VA, Kapralova VI, Amoscato AA, Epperly MW, Greenberger JS, Kagan VE: **Mass-spectrometric characterization of phospholipids and their hydroperoxide derivatives in vivo: effects of total body irradiation.** *Methods in molecular biology (Clifton, NJ)* 2009, **580**:153.
206. Peterson B, Stovall K, Monian P, Franklin JL, Cummings BS: **Alterations in phospholipid and fatty acid lipid profiles in primary neocortical cells during oxidant-induced cell injury.** *Chemico-biological interactions* 2008, **174**(3):163-176.
207. Zemski Berry KA, Murphy RC: **Free radical oxidation of plasmalogen glycerophosphocholine containing esterified docosahexaenoic acid: structure determination by mass spectrometry.** *Antioxidants & Redox Signaling* 2005, **7**(1-2):157-169.
208. Sjövall O, Kuksis A, Kallio H: **Analysis of molecular species of peroxide adducts of triacylglycerols following treatment of corn oil with tert-butyl hydroperoxide.** *Lipids* 2001, **36**(12):1347-1356.
209. Newman JW, Morisseau C, Hammock BD: **Epoxide hydrolases: their roles and interactions with lipid metabolism.** *Progress in lipid research* 2005, **44**(1):1-51.
210. Ahmed Z, Ravandi A, Maguire GF, Emili A, Draganov D, Du BNL, Kuksis A, Connelly PW: **Apolipoprotein AI promotes the formation of phosphatidylcholine core aldehydes that are hydrolyzed by paraoxonase (PON-1) during high density lipoprotein oxidation with a peroxynitrite donor.** *Journal of Biological Chemistry* 2001, **276**(27):24473.
211. Mesaros AC: **Epoxy phospholipids: Total synthesis, generation and in vivo detection of a new class of oxidatively truncated lipids.** 2005.
212. Brouwers J, Gadella BM: **In situ detection and localization of lipid peroxidation in individual bovine sperm cells.** *Free Radical Biology and Medicine* 2003, **35**(11):1382-1391.
213. Kuksis A, Suomela JP, Tarvainen M, Kallio H: **Lipidomic Analysis of Glycerolipid and Cholesteryl Ester Autooxidation Products.** *Molecular biotechnology* 2009, **42**(2):224-268.

214. Subbanagounder G, Leitinger N, Schwenke DC, Wong JW, Lee H, Rizza C, Watson AD, Faull KF, Fogelman AM, Berliner JA: **Determinants of bioactivity of oxidized phospholipids: specific oxidized fatty acyl groups at the sn-2 position.** *Arteriosclerosis, thrombosis, and vascular biology* 2000, **20**(10):2248.
215. Thomas MC, Mitchell TW, Harman DG, Deeley JM, Murphy RC, Blanksby SJ: **Elucidation of double bond position in unsaturated lipids by ozone electrospray ionization mass spectrometry.** *Anal Chem* 2007, **79**(13):5013-5022.
216. Watson AD, Leitinger N, Navab M, Faull KF, Hörkkö S, Witztum JL, Palinski W, Schwenke D, Salomon RG, Sha W: **Structural identification by mass spectrometry of oxidized phospholipids in minimally oxidized low density lipoprotein that induce monocyte/endothelial interactions and evidence for their presence in vivo.** *Journal of Biological Chemistry* 1997, **272**(21):13597.
217. Nonas S, Miller I, Kawkitinarong K, Chatchavalvanich S, Gorshkova I, Bochkov VN, Leitinger N, Natarajan V, Garcia JGN, Birukov KG: **Oxidized phospholipids reduce vascular leak and inflammation in rat model of acute lung injury.** *American journal of respiratory and critical care medicine* 2006, **173**(10):1130.
218. Hübner G, Crone C, Lindner B: **lipID-a software tool for automated assignment of lipids in mass spectra.** *Journal of Mass Spectrometry* 2009, **44**(12):1676-1683.
219. Ejsing CS, Duchoslav E, Sampaio J, Simons K, Bonner R, Thiele C, Ekroos K, Shevchenko A: **Automated identification and quantification of glycerophospholipid molecular species by multiple precursor ion scanning.** *Anal Chem* 2006, **78**(17):6202-6214.
220. Song H, Hsu FF, Ladenson J, Turk J: **Algorithm for processing raw mass spectrometric data to identify and quantitate complex lipid molecular species in mixtures by data-dependent scanning and fragment ion database searching.** *Journal of the American Society for Mass Spectrometry* 2007, **18**(10):1848-1858.
221. Haimi P, Uphoff A, Hermansson M, Somerharju P: **Software tools for analysis of mass spectrometric lipidome data.** *Analytical Chemistry-Columbus* 2006, **78**(24):8324-8331.
222. Yetukuri L, Ekroos K, Vidal-Puig A, Oreši M: **Informatics and computational strategies for the study of lipids.** *Molecular BioSystems* 2008, **4**(2):121-127.
223. Schwudke D, Oegema J, Burton L, Entchev E, Hannich JT, Ejsing CS, Kurzchalia T, Shevchenko A: **Lipid profiling by multiple precursor and neutral loss scanning driven by the data-dependent acquisition.** *Anal Chem* 2006, **78**(2):585-595.
224. Leavell MD, Leary JA: **Fatty acid analysis tool (FAAT): an FT-ICR MS lipid analysis algorithm.** *Anal Chem* 2006, **78**(15):5497-5503.
225. Maass K, Ranzinger R, Geyer H, von der Lieth CW, Geyer R: **"Glycopeakfinder"-de novo composition analysis of glycoconjugates.** *Proteomics* 2007, **7**(24):4435-4444.
226. Lapadula AJ, Hatcher PJ, Hanneman AJ, Ashline DJ, Zhang H, Reinhold VN: **Congruent strategies for carbohydrate sequencing. 3. OSCAR: an algorithm**

- for assigning oligosaccharide topology from MSn data. *Anal Chem* 2005, **77**(19):6271-6279.
227. Yang K, Cheng H, Gross RW, Han X: **Automated Lipid Identification and Quantification by Multidimensional Mass Spectrometry-Based Shotgun Lipidomics.** *Analytical chemistry* 2009.
228. Watanabe K, Yasugi E, Oshima M: **How to Search the Glycolipid data in "LIPID _{BANK} for Web", the Newly Developed Lipid Database in Japan.** *Trends in Glycoscience and Glycotechnology* 2000, **12**(65):175-184.
229. Serhan CN, Hong S, Lu Y: **Lipid mediator informatics-lipidomics: novel pathways in mapping resolution.** *The AAPS Journal* 2006, **8**(2):284-297.
230. Herzog R, Schwudke D, Schroeder M, Shevchenko A: **LipidX: a truly platform independent lipid analysis suite.** In: 207.
231. **LipidBank Service -** <http://lipidbank.jp>; [<http://lipidbank.jp>]
232. Huang N, Siegel MM, Kruppa GH, Laukien FH: **Automation of a Fourier transform ion cyclotron resonance mass spectrometer for acquisition, analysis, and e-mailing of high-resolution exact-mass electrospray ionization mass spectral data.** *Journal of the American Society for Mass Spectrometry* 1999, **10**(11):1166-1173.
233. Frank AM, Bandeira N, Shen Z, Tanner S, Briggs SP, Smith RD, Pevzner PA: **Clustering millions of tandem mass spectra.** *Journal of proteome research* 2008, **7**(1):113.
234. Jaitly N, Mayampurath A, Littlefield K, Adkins J, Anderson G, Smith R: **Decon2LS: An open-source software package for automated processing and visualization of high resolution mass spectrometry data.** *BMC bioinformatics* 2009, **10**(1):87.
235. **NIST MS Search 2.0** [<http://peptide.nist.gov/>]
236. Stein SE, Rudnick PA: **NIST Peptide Mass Spectral Libraries. Human Peptide Mass Spectral Reference Data, H. sapiens, ion trap, Official Build Date: Feb. 4, 2009.** National Institute of Standards and Technology, Gaithersburg, MD, 20899; [<http://peptide.nist.gov.>]
237. Song H, Ladenson J, Turk J: **Algorithms for automatic processing of data from mass spectrometric analyses of lipids.** *Journal of Chromatography B* 2009, **877**(26):2847-2854.
238. Forrester JS, Milne SB, Ivanova PT, Brown HA: **Computational lipidomics: a multiplexed analysis of dynamic changes in membrane lipid composition during signal transduction.** *Molecular pharmacology* 2004, **65**(4):813.
239. Kind T: **Lipid Analysis with GC-MS, LC-MS, FT-MS — Metabolomics Fiehn Lab;** [<http://fiehnlab.ucdavis.edu/staff/kind/Metabolomics/LipidAnalysis/>]
240. Biemann K, Gapp G, Seibl J: **Application of mass spectrometry to structure problems. I. Amino acid sequence in peptides.** *Journal of the American Chemical Society* 1959, **81**(9):2274-2275.
241. Lam H, Deutsch EW, Eddes JS, Eng JK, King N, Stein SE, Aebersold R: **Development and validation of a spectral library searching method for peptide identification from MS/MS.** *Proteomics* 2007, **7**(5):655-667.

242. Sadygov RG, Cociorva D, Yates JR: **Large-scale database searching using tandem mass spectra: looking up the answer in the back of the book.** *Nature Methods* 2004, **1**(3):195-202.
243. Halket JM, Waterman D, Przyborowska AM, Patel RKP, Fraser PD, Bramley PM: **Chemical derivatization and mass spectral libraries in metabolic profiling by GC/MS and LC/MS/MS.** *Journal of experimental botany* 2005, **56**(410):219.
244. An HJ, Tillinghast JS, Woodruff DL, Rocke DM, Lebrilla CB: **A new computer program (GlycoX) to determine simultaneously the glycosylation sites and oligosaccharide heterogeneity of glycoproteins.** *Journal of proteome research* 2006, **5**(10):2800-2808.
245. Ceroni A, Maass K, Geyer H, Geyer R, Dell A, Haslam SM: **GlycoWorkbench: a tool for the computer-assisted annotation of mass spectra of glycans.** *Journal of proteome research* 2008, **7**(4):1650.
246. Hill DW, Kertesz TM, Fontaine D, Friedman R, Grant DF: **Mass Spectral Metabonomics beyond Elemental Formula: Chemical Database Querying by Matching Experimental with Computational Fragmentation Spectra.** *Analytical chemistry* 2008, **80**:5574-5582.
247. Zhang H, Singh S, Reinhold VN: **Congruent strategies for carbohydrate sequencing. 2. FragLib: an MSn spectral library.** *Anal Chem* 2005, **77**(19):6263-6270.
248. Frank AM, Savitski MM, Nielsen ML, Zubarev RA, Pevzner PA: **De novo peptide sequencing and identification with precision mass spectrometry.** *J Proteome Res* 2007, **6**(1):114-123.
249. **LipidInspector 0.9 - for lipid profiling by multiple precursor and neutral loss scanning;** [<http://www.scionics.de/>]
250. Sud M, Fahy E, Cotter D, Brown A, Dennis EA, Glass CK, Merrill Jr AH, Murphy RC, Raetz CRH, Russell DW: **LMSD: LIPID MAPS structure database.** *Nucleic Acids Research* 2007, **35**(Database issue):D527.
251. Fahy E, Sud M, Cotter D, Subramaniam S: **LIPID MAPS online tools for lipid research.** *Nucleic Acids Research* 2007.
252. Song CM, Bernardo PH, Chai CLL, Tong JC: **CLEVER: pipeline for designing in silico chemical libraries.** *Journal of Molecular Graphics and Modelling* 2009, **27**(5):578-583.
253. Schüller A, Hähnke V, Schneider G: **SmiLib v2. 0: A Java-Based Tool for Rapid Combinatorial Library Enumeration.** *QSAR & Combinatorial Science* 2006, **26**(3):407-410.
254. Sud M: **MayaChemTools;** [<http://www.mayachemtools.org>]
255. Pirok G, Máté N, Varga J, Szegezdi J, Vargyas M, Dorant S, Csizmadia F: **Making" Real" Molecules in Virtual Space.** *Journal of chemical information and modeling* 2006, **46**(2):563-568.
256. Salmi J, Nyman TA, Nevalainen OS, Aittokallio T: **Filtering strategies for improving protein identification in high-throughput MS/MS studies.** *Proteomics* 2009, **9**(4):848-860.

257. Baker C, Kanagasabai R, Ang W, Veeramani A, Low HS, Wenk M: **Towards ontology-driven navigation of the lipid bibliosphere.** *BMC bioinformatics* 2008, **9**(Suppl 1):S5.
258. Mortensen P, Gouw JW, Olsen JV, Ong SE, Rigbolt KTG, Bunkenborg J, Cox J, Foster L, Heck AJR, Blagoev B: **MSQuant, an open source platform for mass spectrometry-based quantitative proteomics.** *Journal of Proteome Research* 2009.
259. Mayampurath AM, Jaitly N, Purvine SO, Monroe ME, Auberry KJ, Adkins JN, Smith RD: **DeconMSn: a software tool for accurate parent ion monoisotopic mass determination for tandem mass spectra.** *Bioinformatics* 2008, **24**(7):1021.
260. Frank A: **MS-Clustering - CSE Computational Mass Spectrometry;** [<http://proteomics.ucsd.edu/Software/MSClustering.html>]
261. Gelpí E: **From large analogical instruments to small digital black boxes: 40 years of progress in mass spectrometry and its role in proteomics. Part I 1965-1984.** *Journal of Mass Spectrometry* 2008, **43**(4):419-435.
262. Gelpí E: **From large analogical instruments to small digital black boxes: 40 years of progress in mass spectrometry and its role in proteomics. Part II 1985-2000.** *Journal of Mass Spectrometry* 2009, **44**(8):1137-1161.
263. Schiller J, Süß R, Arnhold J, Fuchs B, Lessig J, Müller M, Petkovic M, Spalteholz H, Zschörnig O, Arnold K: **Matrix-assisted laser desorption and ionization time-of-flight (MALDI-TOF) mass spectrometry in lipid and phospholipid research.** *Progress in Lipid Research* 2004, **43**(5):449-488.
264. Jackson SN, Ugarov M, Post JD, Egan T, Langlais D, Schultz JA, Woods AS: **A Study of Phospholipids by Ion Mobility TOFMS.** *Journal of the American Society for Mass Spectrometry* 2008, **19**(11):1655-1662.
265. Marto JA, White FM, Seldomridge S, Marshall AG: **Structural characterization of phospholipids by matrix-assisted laser desorption/ionization Fourier transform ion cyclotron resonance mass spectrometry.** *Analytical chemistry* 1995, **67**(21):3979-3984.
266. Cole MJ, Enke CG: **Fast atom bombardment tandem mass spectrometry employing ion-molecule reactions for the differentiation of phospholipid classes.** *Journal of the American Society for Mass Spectrometry* 1991, **2**(6):470-475.
267. Pacholski ML, Cannon DM, Ewing AG, Winograd N: **Static time-of-flight secondary ion mass spectrometry imaging of freeze-fractured, frozen-hydrated biological membranes.** *Rapid Communications in Mass Spectrometry* 1998, **12**(18):1232-1235.
268. Wood GW, Morrow G, Schmidt Jr DE, Tuebner J: **Field desorption mass spectrometry of phospholipids. III. Survey of structural types.** *Chemistry and physics of lipids* 1977, **18**(3-4):316.
269. McFarland MA, Marshall AG, Hendrickson CL, Nilsson CL, Fredman P, Månsson JE: **Structural characterization of the GM1 ganglioside by infrared multiphoton dissociation, electron capture dissociation, and electron detachment dissociation electrospray ionization FT-ICR MS/MS.** *Journal of the American Society for Mass Spectrometry* 2005, **16**(5):752-762.

End of supplement