**Electronic Supplementary Material\_2; Data file S1** 

Sequential lipidomic, metabolomic and proteomic analyses of serum, liver and heart tissue specimens from peroxisomal biogenesis factor 11α knockout mice

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# Details on lipid identification and relative-quantification by LipidSearch (v4.2.23) software<sup>1,2</sup>

# Manual curation criteria

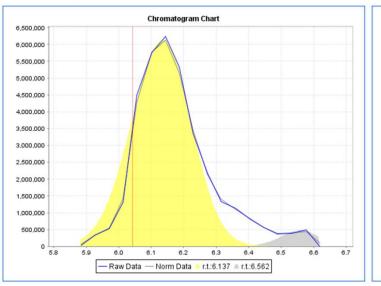
- Mass accuracy (MS  $\leq$  5 ppm and MS/MS  $\leq$  5 ppm)
- Confirmation of lipid identifications with multiple ion adducts and their diagnostic fragment ions (lipid class-specific fragments and lipid species-specific fragments) in both positive- and negative-ion mode<sup>3-5</sup>
- Fragmentation grade (identification level A, B and/or C)
- Base retention time window of lipid classes (as shown in ESM\_1; Fig. S4)
- Isotopic profile and fatty acid distribution pattern
- Peak shape and quality
- Chromatographic peak integration and reassignment
- Fragmentation match score (m-score), c-score and t-score
- Area relative standard deviation (as shown in ESM\_1; Fig. S3) and signal-to-noise ratio

# References

- 1. Peake DA et al., Processing of a complex lipid dataset for the NIST inter-laboratory comparison exercise for lipidomics measurements in human serum and plasma. ASMS 2015 Poster
- 2. Kiyonami R, Peake DA et al., Large scale lipid profiling of a human serum lipidome using a high-resolution accurate-mass LC/MS/MS approach. LIPID MAPS Annual Meeting 2015 Poster

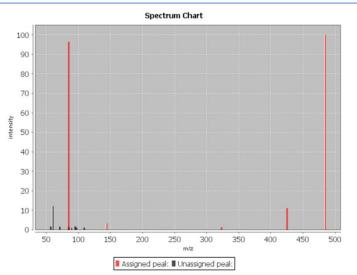
- 3. Murphy RC. Tandem mass spectrometry of lipids: molecular analysis of complex lipids. Royal Society of Chemistry, 2014
- 4. Lipidomics Standards Initiative guidelines (<u>https://lipidomics-standards-initiative.org/guidelines</u>)
- 5. Xu LN et al., Assessment of potential false positives via orbitrap-based untargeted lipidomics from rat tissues. Talanta 2018, 178, 287-293

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● AcCa(22:0)+H	32.9	0.2	82.2	



## Match Detail

ObsMz	Туре	It.(%)	Frag.	Delta(Da)
57.0708	MS2	1.699	-	-
60.0817	MS2	12.188	-	-
71.0864	MS2	1.596	-	-
85.0069	MS2	1.224	-	-
85.0291	MS2	96.426	NL[FA(22:0)-N(	0.0007
85.0497	MS2	1.516	-	-
85.1019	MS2	1.053	-	-
89.0604	MS2	1.004	-	-
95.086	MS2	1.772	-	-
97.1016	MS2	1.14	-	-
109.1017	MS2	1.128	-	-
144.1021	MS2	3.24	NL[FA(22:0)]	0.0002
323.3316	MS2	1.356	FA(22:0)-OH	0.0008
425.3631	MS2	11.138	M+H-N(CH3)3	0.0005
484.4365	MS2	100	M+H	0.0005

# Acylcarnitines or Carnitine esters (AcCa)

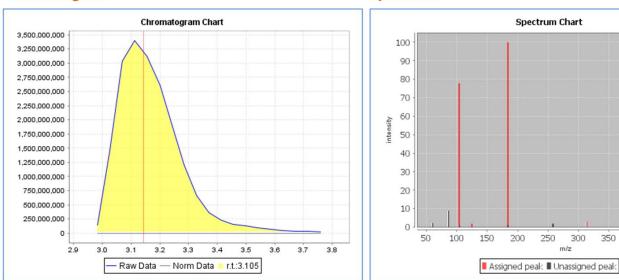
# **Information**

- Ionization: Positive-ion mode
- > Main ion adduct used for identification:  $[M+H]^+$
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of acylcarnitines or carnitine esters (AcCa) identification information obtained with LipidSearch software

e.g. [AcCa(22:0)+H]<sup>+</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• LPC(16:0)+H	44	0.1	87.9	
OPC(8:0e_8:0)+H	35.2	0.1	87.9	8
OPC(10:0e_6:0)+H	35.2	0.1	87.9	

Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
60.0818	MS2	2.233	-	-
86.0973	MS2	8.918	-	-
104.1076	MS2	77.821	C5H14N1O1	0.0007
104.137	MS2	1.047	-	-
125.0002	MS2	1.896	C2H6O4P1	0.0004
184.0738	MS2	100	(P-Cho)+H	0.0005
184.1428	MS2	1.101	-	-
258.111	MS2	1.925	-	-
313.2747	MS2	2.973	M+H-PC	0.001
478.3304	MS2	9.807	-	-
496.3411	MS2	14.628	M+H	0.0013

400

450

500

# Lysophosphatidylcholine (LPC)

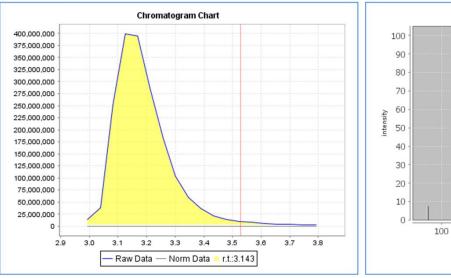
# Information

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup>, [M+Na]<sup>+</sup> and [M+K]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of lysophosphatidylcholine (LPC) identification information obtained with LipidSearch software

e.g. [LPC(16:0)+H]<sup>+</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LPC(16:0)+HCOO	46.5	0	93	
OPC(8:0e_8:0)+HCOO	5.8	0	19.2	
OPC(10:0e_6:0)+HCOO	5.8	0	19.2	

Match Detail

150

200

250

Assigned peak Unassigned peak

300

m/z

350

400

450

500

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
78.9573	MS2	7.528	-	-
152.9947	MS2	2.436	GP-H3O	-0.0012
168.042	MS2	3.925	(P-Cho)-CH3-H	-0.0011
224.0689	MS2	8.675	M-FA(16:0)-CH3	-0.0005
242.0801	MS2	2.178	-	-
255.233	MS2	100	FA(16:0)-H	0.0001
480.3102	MS2	14.119	M-CH3	0.0007

Spectrum Chart

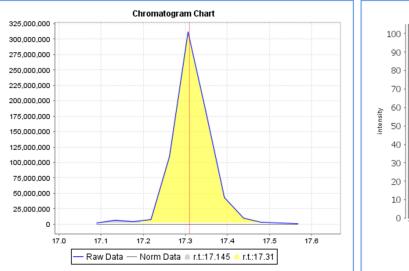
# Lysophosphatidylcholine (LPC)

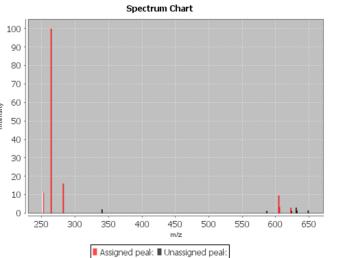
# **Information**

- Ionization: Negative-ion mode
- Main ion adducts used for identification: [M+HCOO]<sup>-</sup> and [M-CH<sub>3</sub>]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M+HCOO]<sup>-</sup>

Representation of lysophosphatidylcholine (LPC) identification information obtained with LipidSearch software e.g. [LPC(16:0)+HCOO]<sup>-</sup>

## Spectrum





## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• Cer(d18:1_22:0)+H	37.5	0.7	93.8	
○ Cer(t18:0_22:0)+H-H2O	25.5	1.4	85.1	
○ Cer(d17:0_23:1)+H	3.2	0.7	16.1	
Ocer(m17:1_23:0+0)+H	3.2	0.7	16.1	
○ Cer(d22:0_18:1)+H	2	0.7	10	
Ocer(m22:1_18:0+0)+H	2	0.7	10	

## Match Detail

<

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
252.2692	MS2	11.168	SPH(d18:1)+H-H2O-CH2O	0.0006
264.2691	MS2	100	SPH(d18:1)+H-2H2O	0.0006
282.2799	MS2	16.076	SPH(d18:1)+H-H2O	0.0007
340.3584	MS2	2.077	-	-
586.5937	MS2	1.283	-	-
604.6048	MS2	9.587	NL[H2O]	0.0021
605.6079	MS2	3.334	NL[H2O] [isotope]	1.0052
622.6149	MS2	2.921	M+H	0.0016
623.6176	MS2	1.264	-	-
630.6202	MS2	3.034	-	-
631.6215	MS2	1.418	-	-
648.6301	MS2	1.506	-	-

>

Сору

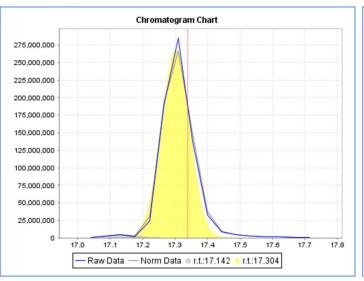
# **Ceramides** (Cer)

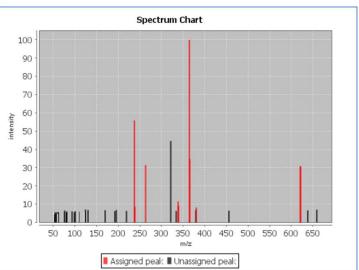
## **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup>, [M+H-H<sub>2</sub>O]<sup>+</sup> and [M+H-2H<sub>2</sub>O]<sup>+</sup>
- Identification (fragmentation) grade: A, B and C
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of ceramides (Cer) identification information obtained with LipidSearch software e.g. [Cer(d40:1)+H]<sup>+</sup>

#### Spectrum





## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• Cer(d18:1_22:0)+HCOO	35.7	0	59.5	
O Cer(d16:0_24:1)+HCOO	19.9	0	49.8	8
Ocer(d15:0_25:1)+HCOO	7.3	0	36.4	
Ocer(d15:1_25:0)+HCOO	7.3	0	36.4	
O Cer(d18:0_22:1)+HCOO	6.4	0	21.2	
O Cer(d24:0_16:1)+HCOO	4.7	0	23.3	8
Ocer(d22:0_18:1)+HCOO	3.9	0	19.7	8
O Cer(d24:1_16:0)+HCOO	3.9	0	19.7	
O Cer(d17:1_23:0)+HCOO	3	0	15.2	
Ocer(m18:1_22:0+0)+HCOO	2.6	0	12.9	

## Match Detail

ObsMz	Туре	It.(%)	Frag.	Delta(Da)	
195.5036	MS2	6.801	-	-	
218.9571	MS2	6.297	-	-	
237.2228	MS2	55.795	Frag[d18:1]-H	0.0004	
238.2263	MS2	8.554	Frag[d18:1]-H [i	1.004	
263.2387	MS2	31.44	NL[H2O,FAmide	0.0006	
321.3167	MS2	44.586	-	-	
333.8749	MS2	6.308	-	-	
338.3446	MS2	11.552	FAmide(22:0)-H	0.0017	
339.3287	MS2	8.98	FAmide(22:0)-H	0.9859	
364.36	MS2	100	NL[d18:1,H2O]	0.0015	
365.363	MS2	34.747	NL[d18:1,H2O]	1.0046	
379.3787	MS2	6.797	-	-	
380.3534	MS2	8.25	NL[d18:1,H2]	0	
455.8556	MS2	6.503	-	-	
620.6018	MS2	30.8	M-H	0.0031	•

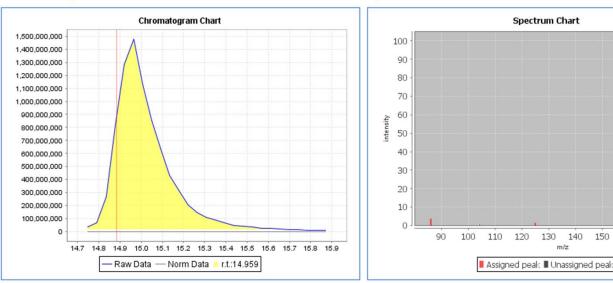
# **Ceramides** (Cer)

## **Information**

- Ionization: Negative-ion mode
- Main ion adducts used for identification: [M+HCOO]<sup>-</sup> and [M-H]<sup>-</sup>
- ➢ Identification (fragmentation) grade: A, B and C
- ➤ Main ion adduct used for quantification: [M+HCOO]<sup>-</sup>

Representation of ceramides (Cer) identification information obtained with LipidSearch software e.g. [Cer(d40:1)+HCOO]<sup>-</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
○ SM(d16:0_24:1)+H	39.6	0.9	99	
○ SM(d16:1_24:0)+H	39.6	0.9	99	
○ SM(d17:0_23:1)+H	39.6	0.9	99	
○ SM(d17:1_23:0)+H	39.6	0.9	99	
○ SM(d18:0_22:1)+H	39.6	0.9	99	
● SM(d18:1_22:0)+H	39.6	0.9	99	
○ SM(d19:0_21:1)+H	39.6	0.9	99	
○ SM(d19:1_21:0)+H	39.6	0.9	99	8
○ SM(d20:0_20:1)+H	39.6	0.9	99	
○ SM(d20:1_20:0)+H	39.6	0.9	99	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
86.097	MS2	3.697	C5H12N1	0.0006
104.1073	MS2	1.009	C5H14N1O1	0.0003
125	MS2	1.469	C2H6O4P1	0.0001
184.0037	MS2	1.098	-	-
184.0733	MS2	100	(P-Cho)+H	0

130 140

m/z

150 160 170

180 190

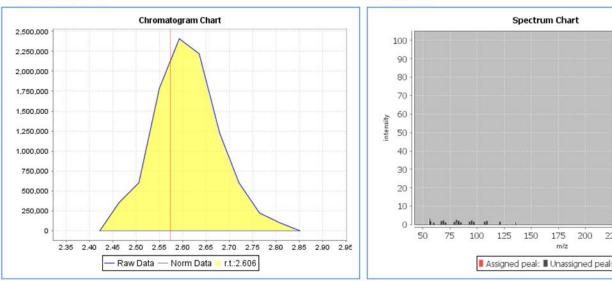
# Sphingomyelin (SM)

# **Information**

- Ionization: Positive- and negative-ion mode  $\geq$
- Main ion adducts used for identification:  $[M+H]^+$ ,  $\succ$  $[M+Na]^+$  and  $[M+HCOO]^-$
- Identification (fragmentation) grade: A, B and C  $\succ$
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of sphingomyelin (SM) identification information obtained with LipidSearch software e.g. [SM(d40:1)+H]<sup>+</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• SPH(d18:1)+H	23.7	0.5	78.9	
○ SPH(t18:0)+H-H2O	23.7	0.8	78.9	

## Match Detail

	Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
	-	-	1.17	MS2	82.0659
	-	-	2.128	MS2	83.0863
	-	-	1.221	MS2	85.1019
	-	-	1.686	MS2	93.0705
	-		2.244	MS2	95.0861
	-	-	1.607	MS2	97.1018
	-	-	1.629	MS2	107.0861
	-	-	2.036	MS2	109.1017
			1.62	MS2	121.1015
	-	-	1.154	MS2	135.1171
	0.0005	NL[CH2O+H2O	15.355	MS2	252.269
	0.0004	NL[2H2O]	9.23	MS2	264.269
	-	-	1.064	MS2	282.1546
	0.0006	NL[H2O]	100	MS2	282.2797
~	0.0009	M+H	1.239	MS2	300.2906

150

175 200

m/z

250 275 300

225

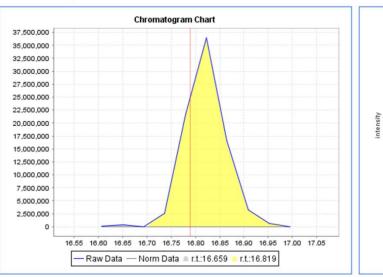
# **Sphingosine (SPH)**

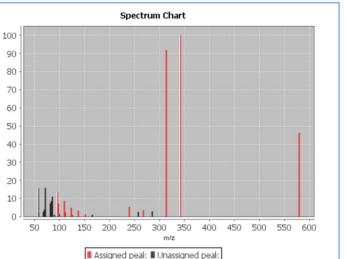
# Information

- Ionization: Positive-ion mode  $\geq$
- Main ion adducts used for identification: [M+H]<sup>+</sup> and  $\geq$  $[M+H-H_2O]^+$
- Identification (fragmentation) grade: A, B and C  $\geq$
- $\blacktriangleright$  Main ion adduct used for quantification:  $[M+H]^+$

Representation of sphingosine (SPH) identification information obtained with LipidSearch software e.g. [SPH(d18:1)+H]<sup>+</sup>

## Spectrum





## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• DG(18:0_16:0)+NH4	40.1	0.3	79	
OTG(12:0e_6:0_16:0)+NH4	16.3	0.3	53	
O DG(10:0_24:0)+NH4	2.6	0.3	24.3	
O DG(11:0_23:0)+NH4	2.6	0.3	24.3	
O DG(12:0_22:0)+NH4	2.6	0.3	24.3	
O DG(13:0_21:0)+NH4	2.6	0.3	24.3	
O DG(20:0_14:0)+NH4	2.6	0.3	24.3	
O DG(15:0_19:0)+NH4	2.6	0.3	24.3	
O DG(17:0_17:0)+NH4	2.6	0.3	24.3	
ODG(26:0_8:0)+NH4	2.6	0.3	24.3	
O DG(28:0_6:0)+NH4	2.6	0.3	24.3	
OTG(12:0e_8:0_14:0)+NH4	2.6	0.3	24.3	
OTG(12:0e_10:0_12:0)+NH4	2.6	0.3	24.3	

## Match Detail

Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
-	-	1.52	MS2	99.1174
0.0005	C8H13	8.773	MS2	109.1016
0.0005	C8H15	2.568	MS2	111.1173
0.0003	C9H15	4.979	MS2	123.1172
0.0003	C9H17	1.117	MS2	125.1328
0.0002	C10H17	3.304	MS2	137.1326
0.0001	C11H19	1.463	MS2	151.1482
-	-	1.116	MS2	165.164
0.0003	FA(16:0)-OH	5.447	MS2	239.2372
-	-	2.623	MS2	257.2477
0.0006	FA(18:0)-OH	3.644	MS2	267.2688
-	-	2.978	MS2	285.279
0.0005	NL[FA(18:0)-H+	91.874	MS2	313.2743
0.0005	NL[FA(16:0)-H+	100	MS2	341.3055
0.0005	M-OH	46.208	MS2	579.5352

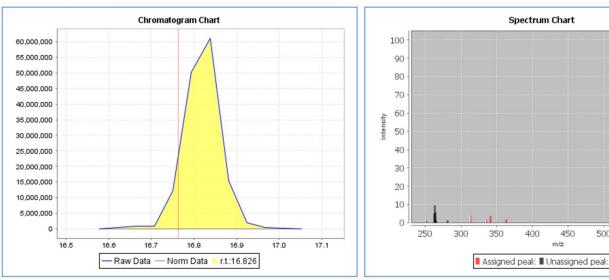
# **Diglyceride (DG)**

## **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+Na]<sup>+</sup>, [M+NH<sub>4</sub>]<sup>+</sup>, [M+H]<sup>+</sup> and [M+K]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adducts used for quantification: [M+NH<sub>4</sub>]<sup>+</sup> and [M+Na]<sup>+</sup>

Representation of diglyceride (DG) identification information obtained with LipidSearch software e.g.  $[DG(34:0)+NH_4]^+$ 

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St
● DG(18:0_16:0)+Na	12.8	0.8	32.1	8
O DG(16:0_20:3)+H	3.3	1.6	16.3	
ODG(18:0_18:3)+H	3.1	1.6	15.7	•
○ TG(12:0e_6:0_16:0)+Na	3.1	0.8	15.4	8
○ TG(12:0e_6:0_18:3)+H	2.1	1.6	10.3	

Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
251.2563	MS2	1.115	-	-
262.2532	MS2	5.038	-	-
263.2568	MS2	9.553	-	-
264.2603	MS2	5.706	-	-
265.263	MS2	1.215	-	-
281.2671	MS2	1.297	-	-
313.2745	MS2	3.979	NL[FA(18:0)-H+	0.0007
335.2566	MS2	1.897	NL[FA(18:0)]	0.001
341.3055	MS2	3.64	NL[FA(16:0)-H+	0.0005
363.288	MS2	1.777	NL[FA(16:0)]	0.001
619.5273	MS2	100	M+Na	0.0001

Spectrum Chart

450

400 m/z 550

500

600

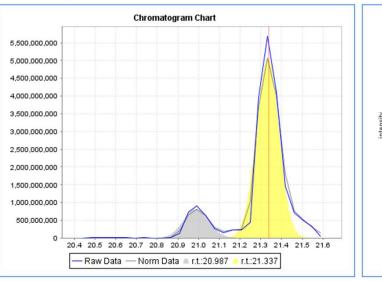
# **Diglyceride** (DG)

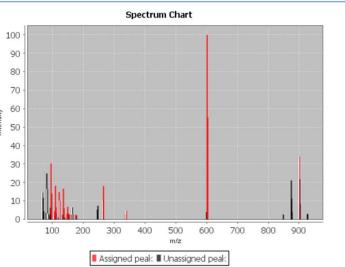
## Information

- Ionization: Positive-ion mode
- $\succ$  Main ion adducts used for identification: [M+Na]<sup>+</sup>,  $[M+NH_4]^+$ ,  $[M+H]^+$  and  $[M+K]^+$
- Identification (fragmentation) grade: A and B
- Main ion adducts used for quantification: [M+Na]<sup>+</sup> and  $\succ$  $[M+NH_4]^+$

Representation of diglyceride (DG) identification information obtained with LipidSearch software e.g. [DG(34:0)+Na]+

## Spectrum





#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• TG(18:1_18:1_18:2)+NH4	58.7	0.1	64.2	
OTG(18:0_18:2_18:2)+NH4	29.4	0.1	41.2	
OTG(18:0_18:1_18:3)+NH4	21.4	0.1	51.7	0
OTG(26:1_10:1_18:2)+NH4	16.9	0.1	40.9	0
OTG(16:0_18:1_20:3)+NH4	16	0.1	51	
OTG(16:1_18:1_20:2)+NH4	16	0.1	51	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
245.2268	MS2	5.321	-	-	~
247.2429	MS2	7.425	-	-	
263.2376	MS2	10.285	FA(18:2)-OH	0.0007	
265.2533	MS2	18.099	FA(18:1)-OH	0.0007	
337.2746	MS2	2.817	MG(18:2)-OH	0.0009	
339.2901	MS2	4.735	MG(18:1)-OH	0.0007	
599.5042	MS2	3.917	-	-	
601.5206	MS2	100	NL[FA(18:1)-H+NH4]	0.0016	
603.5363	MS2	55.323	NL[FA(18:2)-H+NH4]	0.0017	
848.7728	MS2	2.673	Ξ.	-	
874.7882	MS2	21.143	-	-	
875.7919	MS2	11.172	-	-	
876.7922	MS2	3.992	-	-	
900.8035	MS2	34.146	M+NH4	0.0021	~
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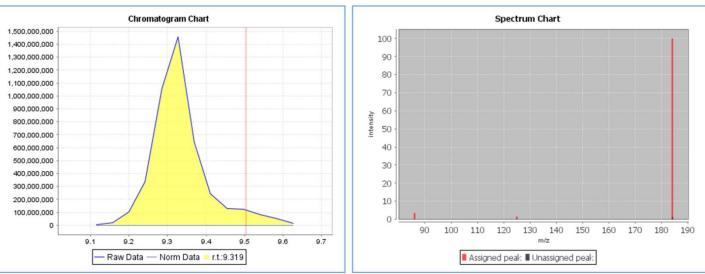
# Triglyceride (TG)

## **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+NH<sub>4</sub>]<sup>+</sup>, [M+Na]<sup>+</sup>, [M+H]<sup>+</sup> and [M+K]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+NH_4]^+$

Representation of triglyceride (TG) identification information obtained with LipidSearch software e.g.  $[TG(54:4)+NH_4]^+$ 

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
O PC(8:0_24:1)+H	29.7	1	98.8	
O PC(9:0_23:1)+H	29.7	1	98.8	
O PC(10:0_22:1)+H	29.7	1	98.8	
O PC(11:0_21:1)+H	29.7	1	98.8	
OPC(20:1_12:0)+H	29.7	1	98.8	
Opc(19:1_13:0)+H	29.7	1	98.8	
OPC(18:1_14:0)+H	29.7	1	98.8	
Opc(17:1_15:0)+H	29.7	1	98.8	
● PC(16:0_16:1)+H	29.7	1	98.8	
O PC(18:0_14:1)+H	29.7	1	98.8	
OPC(20:0_12:1)+H	29.7	1	98.8	
OPC(22:0_10:1)+H	29.7	1	98.8	
OPC(26:1_6:0)+H	29.7	1	98.8	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
86.0971	MS2	3.497	C5H12N	0.0007
125.0001	MS2	1.568	C2H6O4P1	0.0002
184.0735	MS2	100	(P-Cho)+H	0.0002
184.1413	MS2	1.274	-	-

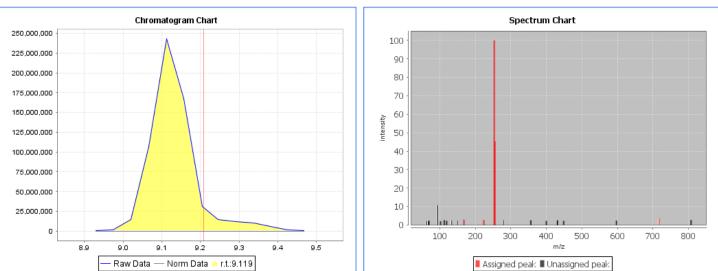
# Phosphatidylcholine (PC)

# **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup>, [M+Na]<sup>+</sup> and [M+K]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of phosphatidylcholine (PC) identification information obtained with LipidSearch software e.g. [PC(32:1)+H]<sup>+</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• PC(16:0_16:1)+HCOO	37.9	0.2	75.7	
OPS(16:0_19:0)-H	2.2	3.9	22.2	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
132.4829	MS2	2.5	-	-	~
148.0111	MS2	2.442	-	-	
168.0422	MS2	2.92	(P-Cho)-CH3-H	-0.001	
224.0696	MS2	2.699	M-FA1-FA2+H2O-CH3	0.0002	
253.2175	MS2	100	FA(16:1)-H	0.0002	
255.2332	MS2	45.333	FA(16:0)-H	0.0002	
277.44	MS2	2.631	-	-	
356.3354	MS2	2.599	-	-	
400.0869	MS2	2.231	-	-	
430.5109	MS2	2.553	-	-	
431.0115	MS2	2.515	-	-	
448.7605	MS2	2.318	-	-	
597.5173	MS2	2.442	-	-	
716.5259	MS2	3.786	M-CH3	0.0023	~
<				>	

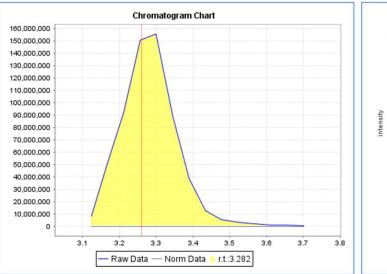
# Phosphatidylcholine (PC)

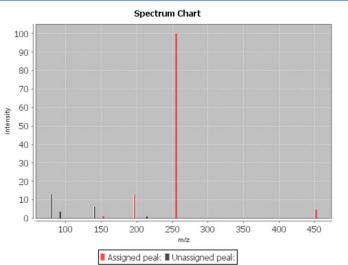
# **Information**

- Ionization: Negative-ion mode
- Main ion adducts used for identification: [M+HCOO]<sup>-</sup> and [M-CH<sub>3</sub>]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➢ Main ion adduct used for quantification: [M+HCOO]<sup>−</sup>

Representation of phosphatidylcholine (PC) identification information obtained with LipidSearch software e.g. [PC(32:1)+HCOO]<sup>-</sup>

#### Spectrum





## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LPE(16:0)-H	24.8	0.4	82.7	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
78.9573	MS2	12.949	-	-	
92.1398	MS2	3.562	-	-	
140.0104	MS2	6.261	-	-	
152.9947	MS2	1.16	GP-H3O	-0.0011	
196.0372	MS2	12.623	M-FA(16:0)-H	-0.0008	
214.0479	MS2	1.048	-	-	
255.233	MS2	100	FA(16:0)-H	0	
452.2785	MS2	4.611	M-H	0.0002	

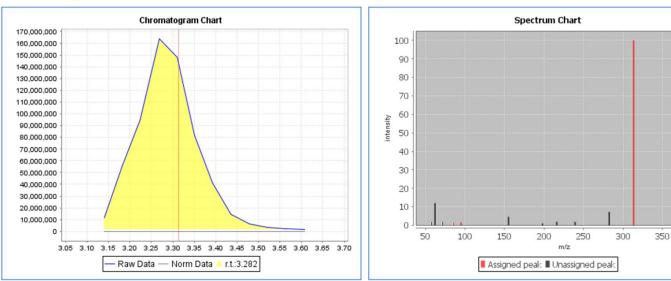
# Lysophosphatidylethanolamine (LPE)

## **Information**

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

Representation of lysophosphatidylethanolamine (LPE) identification information obtained with LipidSearch software e.g. [LPE(16:0)-H]<sup>-</sup>

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LPE(16:0)+H	7.7	0.1	75.1	
OPE(8:0e_8:0)+H	7.7	0.1	75.1	8
OPE(10:0e_6:0)+H	7.7	0.1	75.1	

Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
57.0709	MS2	1.906	-	-
62.061	MS2	12.064	-	-
71.0865	MS2	1.912	-	-
85.1018	MS2	1.44	C6H13	0.0007
95.0861	MS2	1.586	C7H11	0.0006
155.0107	MS2	4.634	-	-
198.0529	MS2	1.089	-	-
216.0636	MS2	1.901	-	-
239.2374	MS2	1.886	-	-
282.2799	MS2	7.291	-	-
313.2746	MS2	100	NL[PE]	0.0009
393.2404	MS2	1.477	-	-

# Lysophosphatidylethanolamine (LPE)

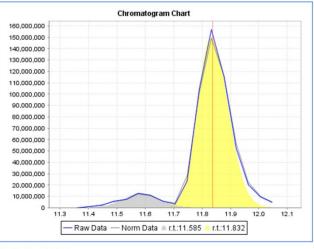
# **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup> and [M+Na]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+H]^+$

Representation of lysophosphatidylethanolamine (LPE) identification information obtained with LipidSearch software

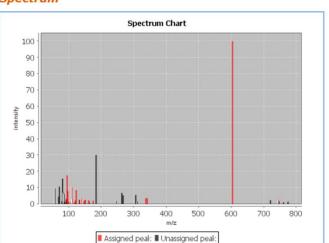
e.g. [LPE(16:0)+H]<sup>+</sup>





#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• PE(18:0_18:2)+H	18.5	0.2	58.8	
O PC(15:0_18:2)+H	7.4	3	34.4	
O PE(12:0_24:2)+H	6.5	0.2	56.5	
O PE(14:0_22:2)+H	6.5	0.2	56.5	
O PE(16:0_20:2)+H	6.5	0.2	56.5	
O PE(16:1_20:1)+H	6.5	0.2	56.5	
O PE(17:1_19:1)+H	6.5	0.2	56.5	
O PE(18:1_18:1)+H	6.5	0.2	56.5	
O PE(22:0_14:2)+H	6.5	0.2	56.5	
O PE(22:1_14:1)+H	6.5	0.2	56.5	
O PE(24:0_12:2)+H	6.5	0.2	56.5	0
O PE(24:1_12:1)+H	6.5	0.2	56.5	
O PE(26:0_10:2)+H	6.5	0.2	56.5	
O PE(25:0_11:2)+H	6.5	0.2	56.5	8
O PE(25:1_11:1)+H	6.5	0.2	56.5	
OPE(26:1_10:1)+H	6.5	0.2	56.5	



#### Match Detail

MS2       2.258       C12H17       0.0004         63.1485       MS2       1.28       -       -         75.1486       MS2       1.942       C13H19       0.0005         84.0737       MS2       30.077       -       -         75.1486       MS2       1.758       -       -         76.2688       MS2       6.749       -       -         76.72688       MS2       5.231       -       -         70.066.28       MS2       5.466       -       -         71.0864       MS2       1.585       -       -         73.72746       MS2       3.55       MG(18:2)-OH       0.0006         73.05308       MS2       3.444       MG(18:0)-OH       0.0006         744.5525       MS2       2.228       -       -         744.5525       MS2       2.598       M+H       -0.0013       90.0811         70.9018       MS2       1.462       1.147       97.1019       MS2       1.462         70.0501       MS2       3.268       -       -       -       90.0811       1.401         91.0548       MS2       1.041       91.0548       MS2	MS2       2.258       C12H17       0.0004         63.1485       MS2       1.28       -       -         175.1486       MS2       1.942       C13H19       0.0005       e.g. [PE(36:2)+H         84.0737       MS2       30.077       -       -       -         963.2376       MS2       1.758       -       -       -         967.2688       MS2       5.231       -       -       -         967.2688       MS2       5.466       -       -       -         906.28       MS2       5.466       -       -       -         910.3115       MS2       3.55       MG(18:2)-OH       0.0008       83.0863 MS2       6.121         93.0726       MS2       3.444       MG(18:0)-OH       0.0006       91.0548 MS2       1.141         93.0706 MS2       1.141       92.1468 MS2       1.141         93.0706 MS2       3.286 C7H9				Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
661.1329       MS2       2.258       C12H17       0.0004         63.1485       MS2       1.28       -       -         175.1486       MS2       1.942       C13H19       0.0005         88.0737       MS2       30.077       -       -         445.2269       MS2       1.758       -       -         67.2688       MS2       5.231       -       -         67.2688       MS2       5.231       -       -         67.2688       MS2       5.466       -       -         60.28       MS2       1.585       -       -         810.3115       MS2       3.55       MG(18:2)-OH       0.0008         81.0707       MS2       3.444       MG(18:0)-OH       0.0006         93.5358       MS2       2.228       -       -         70.0561       MS2       1.342       1.145         90.051       MS2       1.288       -       -         70.0561       MS2       2.228       -       -         70.0561       MS2       2.228       -       -         90.051       MS2       2.598       M+H       -0.0013 <td< td=""><td>MS2       2.258       C12H17       0.0004         63.1485       MS2       1.28       -       -         175.1486       MS2       1.942       C13H19       0.0005       e.g. [PE(36:2)+H         84.0737       MS2       30.077       -       -       -         963.2376       MS2       1.758       -       -       -         967.2688       MS2       5.231       -       -       -         967.2688       MS2       5.466       -       -       -         906.28       MS2       5.466       -       -       -         910.3115       MS2       3.55       MG(18:2)-OH       0.0008       83.0863 MS2       6.121         93.0726       MS2       3.444       MG(18:0)-OH       0.0006       91.0548 MS2       1.141         93.0706 MS2       1.141       92.1468 MS2       1.141         93.0706 MS2       3.286 C7H9</td><td>resentatio</td><td>Rer</td><td></td><td>0.0004</td><td>C11H19</td><td>2.341</td><td>MS2</td><td>151.1485</td></td<>	MS2       2.258       C12H17       0.0004         63.1485       MS2       1.28       -       -         175.1486       MS2       1.942       C13H19       0.0005       e.g. [PE(36:2)+H         84.0737       MS2       30.077       -       -       -         963.2376       MS2       1.758       -       -       -         967.2688       MS2       5.231       -       -       -         967.2688       MS2       5.466       -       -       -         906.28       MS2       5.466       -       -       -         910.3115       MS2       3.55       MG(18:2)-OH       0.0008       83.0863 MS2       6.121         93.0726       MS2       3.444       MG(18:0)-OH       0.0006       91.0548 MS2       1.141         93.0706 MS2       1.141       92.1468 MS2       1.141         93.0706 MS2       3.286 C7H9	resentatio	Rer		0.0004	C11H19	2.341	MS2	151.1485
663.1485       MS2       1.28       -       -         175.1486       MS2       1.942       C13H19       0.0005       e.g. [PE(36:2)+H         184.0737       MS2       30.077       -       -         163.2376       MS2       1.758       -       -         163.2376       MS2       6.749       -       -         167.2688       MS2       5.231       -       -         106.28       MS2       5.466       -       -         101.3115       MS2       3.55       MG(18:2)-OH       0.0008         101.3115       MS2       3.55       MG(18:2)-OH       0.0006         137.2746       MS2       3.444       MG(18:0)-OH       0.0006         1720.5909       MS2       2.228       -       -         120.5909       MS2       2.228       -       -         120.5909       MS2       2.598       M+H       -0.0013	663.1485       MS2       1.28       -       -         75.1486       MS2       1.942       C13H19       0.0005         84.0737       MS2       30.077       -       -         845.2269       MS2       1.758       -       -         963.2376       MS2       6.749       -       -         967.2688       MS2       5.231       -       -         906.28       MS2       5.466       -       -         910.3115       MS2       3.55       MG(18:2)-OH       0.0008         937.2746       MS2       3.444       MG(18:0)-OH       0.0006         93.5358       MS2       100       NL[PE]       0.0011		-	-	0.0004	C12H17	2.258	MS2	161.1329
MS2       30.077       -       -         V45.2269       MS2       1.758       -       -         V63.2376       MS2       6.749       -       -         V67.2688       MS2       5.231       -       -         V67.2688       MS2       5.466       -       -         V10.3115       MS2       5.466       -       -         V10.3115       MS2       3.55       MG(18:2)-OH       0.0008         V11.3056       MS2       3.444       MG(18:0)-OH       0.0006         V20.5909       MS2       2.228       -       -         V44.5525       MS2       2.598       M+H       -0.0013       -         V20.5009       MS2       2.598       M+H       -0.0013       -         V20.5009       MS2       2.598       M+H       -0.0013       -         V20.501       MS2       1.047       -       -         V11.1174       MS2       2.598       -       -         V20.509       MS2       2.598       M+H       -0.0013       -         V20.509       MS2       2.598       M+H       -0.0013       -         V20.501	MS2         30.077         -         -           245.2269         MS2         1.758         -         -           263.2376         MS2         6.749         -         -           267.2688         MS2         5.231         -         -           266.28         MS2         5.466         -         -           267.2688         MS2         5.466         -         -           267.2687         MS2         1.585         -         -           267.2688         MS2         5.231         -         -           267.2688         MS2         5.466         -         -           267.2746         MS2         3.55         MG(18:2)-OH         0.0008           37.2746         MS2         3.55         MG(18:0)-OH         0.0006           303.5358         MS2         100         NLIPEJ         0.0011				-	-	1.28	MS2	163.1485
NAS2         1.758         -         -           V45.2269         MS2         6.749         -         -         -         -         -         -         -         5.0552         MS2         1.147         -           V67.2688         MS2         5.231         - </td <td>MS2         1.758         -         -         -         ObsMz         Type         It.(%)         Frag.           263.2376         MS2         6.749         -         -         -         55.0552         MS2         9.491         -         -         -         -         55.0552         MS2         9.491         -</td> <td>[PE(36:2)</td> <td>e.g.</td> <td></td> <td>0.0005</td> <td>C13H19</td> <td>1.942</td> <td>MS2</td> <td>175.1486</td>	MS2         1.758         -         -         -         ObsMz         Type         It.(%)         Frag.           263.2376         MS2         6.749         -         -         -         55.0552         MS2         9.491         -         -         -         -         55.0552         MS2         9.491         -	[PE(36:2)	e.g.		0.0005	C13H19	1.942	MS2	175.1486
445.2269       MS2       1.758       -       -         63.2376       MS2       6.749       -       -         67.2688       MS2       5.231       -       -         667.2688       MS2       5.466       -       -         610.3115       MS2       1.585       -       -         610.3115       MS2       3.55       MG(18:2)-OH       0.0008         810.3115       MS2       3.55       MG(18:2)-OH       0.0008         837.2746       MS2       3.55       MG(18:0)-OH       0.0006         91.0548       MS2       1.14       -       -         803.5358       MS2       100       NL[PE]       0.0011       91.0548       MS2       1.14         92.1468       MS2       2.722       -       -       -       -       93.0706       MS2       3.286       CH9         93.0706       MS2       2.228       -       -       -       -       99.0811       MS2       1.146         92.1468       MS2       2.722       -       -       -       -       -       -       -       -       -       -       -       -       -       -	A45.2269       MS2       1.758       -       -       55.0552 M52       1.147         A63.2376       MS2       6.749       -       -       57.0709 M52       9.491         A67.2688       MS2       5.231       -       -       -       69.0708 M52       1.147         A67.2688       MS2       5.231       -       -       -       71.0864 M52       10.618         A66.28       MS2       5.466       -       -       -       81.0707 M52       15.508         A10.3115       MS2       1.585       -       -       -       83.0863 M52       6.949         A37.2746       MS2       3.55       MG(18:2)-OH       0.0008       85.102 M52       1.141         91.0548 M52       1.14       91.0548 M52       1.141       91.0548 M52       1.141         92.1468 M52       2.722       93.0706 M52       3.286 C7H9			×	-	-	30.077	MS2	184.0737
263.2376       MS2       6.749       -       -       -       57.0709       MS2       9.491         267.2688       MS2       5.231       -       -       -       -       69.0708       MS2       4.477         267.2688       MS2       5.231       -       -       -       -       71.0864       MS2       1.611         267.2688       MS2       5.466       -       -       -       83.0863       MS2       1.611         2006.28       MS2       1.585       -       -       -       83.0863       MS2       1.611         201.3115       MS2       1.585       -       -       -       83.0863       MS2       1.611         203.72746       MS2       3.55       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         91.0548       MS2       2.228       0.0011       92.1468       MS2       2.722         93.0706       MS2       2.289       M+H       -0.0013       99.0811       MS2       1.402         99.0811       MS2       2.598       M+H       -0.0013       109.1018       MS2       1.0269       C8H13         111.1174       MS2 <td< td=""><td>MS2         6.749         -         -         -         57.0709 M52         9.491         -         -         57.0709 M52         9.491         -         -         -         -         57.0709 M52         9.491         -         <th< td=""><td></td><td></td><td></td><td></td><td></td><td>1 750</td><td>MCO</td><td>245 2260</td></th<></td></td<>	MS2         6.749         -         -         -         57.0709 M52         9.491         -         -         57.0709 M52         9.491         -         -         -         -         57.0709 M52         9.491         - <th< td=""><td></td><td></td><td></td><td></td><td></td><td>1 750</td><td>MCO</td><td>245 2260</td></th<>						1 750	MCO	245 2260
103.2370       M32       0.749       -       -         1067.2688       MS2       5.231       -       -         106.28       MS2       5.466       -       -         101.3115       MS2       1.585       -       -         103.72746       MS2       3.55       MG(18:2)-OH       0.0008         103.7358       MS2       3.444       MG(18:0)-OH       0.0006         120.5909       MS2       2.228       -       -         120.5909       MS2       2.598       M+H       -0.0013         109.013       MS2       1.0269       CH11         109.013       MS2       1.046       CH11         99.0811       MS2       1.040       CH11         99.0811       MS2       1.040       CH11         99.0811       MS2       1.046       CH11         99.0811       MS2       1.0269       CH13         111.1174       MS2       2.869       CH13         111.1174       MS2       2.869       CH13         111.1174       MS2       2.869       CH13         111.1174       MS2       2.869       CH13         111.1174	MS2         6.749         Image: Second secon				-	=/	1.750	WIJZ	245.2209
MS2       5.231       -       -       -       71.0864       MS2       10.618       .         M06.28       MS2       5.466       -       -       .       81.0707       MS2       1.611       .         M10.3115       MS2       1.585       -       -       .       83.0863       MS2       6.949         M37.2746       MS2       3.55       MG(18:2)-OH       0.0008       85.102       MS2       1.401         M41.3056       MS2       3.444       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         93.5558       MS2       100       NL[PE]       0.0011       91.0548       MS2       3.286       CPH9         720.5909       MS2       2.228       -       -       -       93.0706       MS2       3.286       CPH9         92.0468       MS2       2.598       M+H       -0.0013       91.018       MS2       1.046       C8H11         109.018       MS2       1.0269       C8H13       111.1174       MS2       2.869       C8H15         111.1174       MS2       2.869       C8H15       133.1016       MS2       2.2545       C9H13       133.1016       MS2	MS2         5.231         -         -         71.0864 M52         10.618           006.28         MS2         5.466         -         -         79.0551 M52         1.611           010.3115         MS2         1.585         -         -         -         83.0863 M52         6.5499           037.2746         MS2         3.55         MG(18:2)-OH         0.0008         85.102 M52         1.14           91.0548 M52         1.14         99.10548 M52         1.14           93.0706 M52         100         NL[PE]         0.0011         93.0706 M52         3.286 C7H9				-	-	6.749	MS2	263.2376
MS2         5.466         -         -           M0.0.28         MS2         5.466         -         -           M10.3115         MS2         1.585         -         -           M37.2746         MS2         3.55         MG(18:2)-OH         0.0008         83.0863         MS2         6.949           M41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548         MS2         1.14           92.0550         MS2         100         NL[PE]         0.0011         91.0548         MS2         3.286         C/H9           720.5909         MS2         2.228         -         -         93.0706         MS2         3.286         C/H11           744.5525         MS2         2.598         M+H         -0.0013         99.0811         MS2         1.046         C8H11           111.1174         MS2         2.869         C8H15         107.0861         MS2         1.047           111.1174         MS2         2.869         C8H15         119.0862         MS2         1.046         C8H11           111.1174         MS2         2.869         C8H15         133.1016         MS2         2.545         119.0862         MS	MS2         5.466         -         -         79.0551 MS2         1.611           N10.3115         MS2         1.585         -         -         81.0707 M52         15.508           N10.3115         MS2         1.585         -         -         -         83.0863 M52         6.949           N37.2746         MS2         3.55         MG(18:2)-OH         0.0008         86.0972 M52         1.401           91.0548 M52         1.14         -         91.0548 M52         2.722           93.0706 M52         100         NL[PE]         0.0011         93.0706 M52         3.286 C7H9						5 004		007 0000
006.28       MS2       5.466       -       -       81.070       MS2       15.508       15.508         010.3115       MS2       1.585       -       -       83.0863       MS2       6.949         037.2746       MS2       3.55       MG(18:2)-OH       0.0008       85.102       MS2       1.101         041.3056       MS2       3.444       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         92.1468       MS2       2.272       93.0706       MS2       2.288       CH9         720.5909       MS2       2.228       -       -       97.1019       MS2       7.943       C7H13         744.5525       MS2       2.598       M+H       -0.0013       107.0661       MS2       1.0269       C8H13         107.0861       MS2       1.0269       C8H13       111.1174       MS2       2.869       C8H15       119.0862       MS2       1.047       121.1018       MS2       2.253       C9H3         111.1174       MS2       2.253       C9H3       133.1016       MS2       2.545       133.1016       MS2       2.545         1133.1016       MS2       2.5455       133.3016       MS2	MS2         5.466         -         -         81.0707         MS2         15.508           M10.3115         MS2         1.585         -         -         83.0863         MS2         6.949           M37.2746         MS2         3.55         MG(18:2)-OH         0.0008         85.02         6.121           M41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548         MS2         1.14           92.1468         MS2         2.722         93.0706         93.026         53.286         C7H9				-	-	5.231	MSZ	267.2688
MS2       1.585       -       -       83.0863       MS2       6.949       .         M37.2746       MS2       3.55       MG(18:2)-OH       0.0008       85.102       MS2       1.401         M41.3056       MS2       3.444       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         92.1468       MS2       2.722       93.0706       MS2       2.286       C7H9         720.5909       MS2       2.228       -       -       95.0862       MS2       1.7.943       C7H13         944.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.0269       CH11         109.1018       MS2       1.0269       CH13       119.0862       MS2       1.047       111.1174       MS2       2.869       CH13         111.1174       MS2       2.869       CH13       119.0862       MS2       1.047       111.1174       MS2       2.869       CH13         113.1016       MS2       2.02476       CH113       113.1172       MS2       2.446       CH14         113.1172       MS2       2.446       CH13       113.1172       MS2       2.446       CH14 <t< td=""><td>MS2         1.585         -         -         83.0863         MS2         6.949         -           X37.2746         MS2         3.55         MG(18:2)-OH         0.0008         85.102         MS2         6.121           X41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548         MS2         1.14           92.1468         MS2         2.722         93.0706         93.0706         MS2         3.286         C7H9</td><td></td><td></td><td></td><td>-</td><td>-</td><td>5.466</td><td>MS2</td><td>306.28</td></t<>	MS2         1.585         -         -         83.0863         MS2         6.949         -           X37.2746         MS2         3.55         MG(18:2)-OH         0.0008         85.102         MS2         6.121           X41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548         MS2         1.14           92.1468         MS2         2.722         93.0706         93.0706         MS2         3.286         C7H9				-	-	5.466	MS2	306.28
1.303       M32       1.303       Control       85       85       100       1.303       1.401       1.401         137.2746       MS2       3.55       MG(18:2)-OH       0.0008       91.0548       MS2       1.401         141.3056       MS2       3.444       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         92.1468       MS2       2.228       0.0011       93.0706       MS2       3.286       C7H9         95.0862       MS2       2.288       -       -       95.0862       MS2       1.14         97.1019       MS2       2.288       HH       -0.0013       99.0811       MS2       1.0269       CH11         99.0811       MS2       1.0269       CH13       109.1018       MS2       1.0269       CH13         109.1018       MS2       1.0269       CH13       111.1174       MS2       2.869       CH13         111.1174       MS2       2.846       CH13       103.1016       MS2       1.047       111.1174       MS2       2.846       CH13         111.1174       MS2       2.846       CH13       113.1016       MS2       2.545       1119.0862       MS2       1.047	MS2         N.000         MS2         S.55         MG(18:2)-OH         0.0008         85.02         MS2         6.121           M41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548         MS2         1.14           92.1468         MS2         2.722         93.0706         MS2         3.286         C7H9						4 505		240 2445
MS2       3.444       MG(18:0)-OH       0.0006       91.0548       MS2       1.14         903.5358       MS2       100       NL[PE]       0.0011       93.0706       MS2       3.286       C7H9         920.5909       MS2       2.228       0.0011       95.0862       MS2       1.14         944.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.45         100       NLIPE       -0.0013       0.0014       91.0548       MS2       1.42       C7H1         99.0811       MS2       2.598       M+H       -0.0013       0.011       99.0811       MS2       1.46       C8H11         109.1018       MS2       1.0269       C8H13       10.269       C8H13       111.1174       MS2       2.869       C8H15         111.1174       MS2       2.869       C8H15       119.0862       MS2       2.545       CH15         133.1016       MS2       2.545       CH15       133.1016       MS2       2.545       CH15         133.1016       MS2       2.476       CH11       137.1328       MS2       3.336       CH15	M41.3056         MS2         3.444         MG(18:0)-OH         0.0006         91.0548 M52         1.14           92.1468 M52         2.722         93.0706 M52         3.286 C7H9				-	-	1.585	WI52	310.3115
441.3056       MS2       3.444       MG(18:0)-OH       0.0006       92.1468       MS2       2.722         503.5358       MS2       100       NL[PE]       0.0011       95.0862       MS2       3.286       C7H9         720.5909       MS2       2.228       -       -       95.0862       MS2       7.442       C7H11         744.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.46       C8H11         109.1018       MS2       1.0269       C8H13       111.1174       MS2       2.869       C8H15         111.1174       MS2       2.253       C9H13       112.31172       MS2       2.646       C9H15         133.1016       MS2       2.545       C114       1137.1328       MS2       3.336       C10H15	MS2         3.444         MG(18:0)-OH         0.0006         92.1468         MS2         2.722           \$03.5358         MS2         100         NL[PE]         0.0011         93.0706         MS2         3.286         C7H9				0.0008	MG(18:2)-OH	3.55	MS2	337.2746
303.5358       MS2       100       NL[PE]       0.0011       93.0706       MS2       3.286       C7H2         '20.5909       MS2       2.228       -       -       95.0862       MS2       17.492       C7H11         '24.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.155         '107.0861       MS2       1.0269       CBH11       109.1018       MS2       10.269       CBH13         '111.1174       MS2       2.2593       M+H       -0.0013       111.1174       MS2       2.869       C8H13         '121.1018       MS2       1.0269       C8H13       119.0862       MS2       1.047         '121.1018       MS2       2.2535       C9H13       123.1172       MS2       8.486       C9H13         '133.1016       MS2       2.2545       C1141       137.1328       MS2       3.336       C10H11	03.5358 MS2 100 NL[PE] 0.0011 93.0706 M52 3.286 C7H9	152 1.14	91.0548 N		0.0000	MC(49-0) OH	2 4 4 4	MCO	244 2056
Kaling         Kaling<		1S2 2.722	92.1468 N		0.0006	MG(18.0)-OH	3.444	WI52	341.3050
22.5909       MS2       2.228       -       -       97.1019       MS2       7.943       C7H13         '44.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.155       107.0861       MS2       1.46       C8H11         '109.1018       MS2       10.269       C8H13       111.1174       MS2       2.869       C8H15         '119.0862       MS2       1.047       119.0862       2.253       C9H13         '121.1018       MS2       2.253       C9H13       123.1172       MS2       2.869       C8H15         '131.016       MS2       2.2545       C9H13       123.1172       MS2       2.476       C10H11         '137.1328       MS2       3.336       C10H11       137.1328       MS2       3.336       C10H11					0.0011	NL[PE]	100	MS2	603.5358
'44.5525       MS2       2.598       M+H       -0.0013       99.0811       MS2       1.155         '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.013       '00.016       MS2       1.155       '00.0269       C8H13         '111.1174       MS2       2.869       C8H15       '119.0862       MS2       1.047         '121.1018       MS2       2.253       C9H13       '123.1172       MS2       8.486       C9H15         '133.1016       MS2       2.2545       '133.1016       MS2       2.2476       C10H11         '137.1328       MS2       3.336       C10H11       '137.1328       MS2       3.336       C10H11							0.000	MCO	700 5000
44.5525         MS2         2.598         M+H         -0.0013         107.0861         MS2         1.46         C8H11           Copy           Copy           111.1174         MS2         2.869         C8H13           111.1174         MS2         2.869         C8H13           111.018         MS2         2.047           121.018         MS2         2.253         C9H13           123.1172         MS2         8.486         C9H13           133.1016         MS2         2.2545           135.1172         MS2         2.476         C10H11           137.1328         MS2         3.336         C10H11					-	-	2.228	WI52	720.5909
Copy         109.1018         MS2         10.269         C8H13           111.1174         MS2         2.869         C8H15           119.0862         MS2         1.047           121.1018         MS2         2.253         C9H13           123.1172         MS2         8.486         C9H15           133.016         MS2         2.545         135.1172           137.1328         MS2         3.336         C10H11	(44 5525 MS2 2 598 M+H -0.0013			~	-0.0013	M+H	2.598	MS2	744.5525
Copy         111.1174         MS2         2.869         C8H15           119.0862         MS2         1.047         111.0174         1000         1000           121.1018         MS2         2.253         C9H13         123.1172         MS2         8.486         C9H15           133.1016         MS2         2.545         135.1172         MS2         2.476         C10H11           137.1328         MS2         3.336         C10H11         137.1328         MS2         3.336         C10H11					Section Sections				
119.0862       MS2       1.047         121.1018       MS2       2.253       C9H13         123.1172       MS2       8.486       C9H15         133.1016       MS2       2.545       135.1172       MS2       2.476       C10H11         137.1328       MS2       3.336       C10H11       137.1328       MS2       3.336       C10H11	Conv			(Copy )					
121.1018       MS2       2.253       C9H13         123.1172       MS2       8.486       C9H15         133.1016       MS2       2.545          135.1172       MS2       2.476       C10H11         137.1328       MS2       3.336       C10H11									
133.1016     MS2     2.545       135.1172     MS2     2.476       137.1328     MS2     3.336									
135.1172         MS2         2.476         C10H1           137.1328         MS2         3.336         C10H1	123.1172 MS2 8.486 C9H15	1S2 8.486	123.1172 N						
137.1328 MS2 3.336 C10H1	133.1016 MS2 2.545	1S2 2.545	133.1016 N						
	135.1172 MS2 2.476 C10H1	1S2 2.476	135.1172 N						
147 1172 MS2 1 258 C11H1									
149.1328 MS2 2.355 C11H1	147.1172 MS2 1.258 C11H1								

## **Phosphatidylethanolamine (PE)**

## Information

 $\triangleright$ Ionization: Positive-ion mode

Delta(Da)

0.0007

0.0007

0.0007

0.0006

0.0006

0.0006

0.0006

0.0004

0.0004

0.0003

0.0003

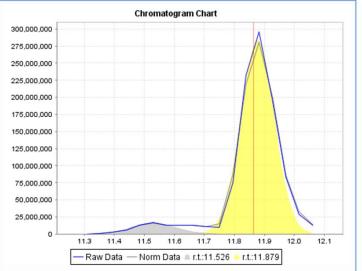
0.0003

- Main ion adducts used for identification:  $[M+H]^+$  and  $\geq$  $[M+Na]^+$
- $\geq$ Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M+H]<sup>+</sup>

ion of phosphatidylethanolamine (PE) identification obtained with LipidSearch software 2)+H]+

1	7	

## Spectrum





LipidIon	M-Sc.	T-Sc.	Occ.	St.
● PE(18:0_18:2)-H	35.8	0.3	89.5	
OdMePE(16:0_18:2)-H	12.5	2.3	62.5	
O PC(16:0_18:2)-CH3	12.5	2.4	62.5	

Spectrum Chart 100 90 80  $\succ$ 70 60 ⋧ 50  $\geq$ 40 30 20  $\geq$ 10 0 50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 m/z

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
78.9572	MS2	8.905	-	-
121.9995	MS2	1.463	-	-
140.0103	MS2	9.641	-	-
196.0371	MS2	4.923	M-FA1-FA2+H2O-H	-0.0009
279.2329	MS2	100	FA(18:2)-H	0
280.2363	MS2	18.164	FA(18:2)-H [isotope]	1.0033
283.2642	MS2	40.118	FA(18:0)-H	-0.0001
284.2677	MS2	6.708	FA(18:0)-H [isotope]	1.0035
480.3096	MS2	1.391	LPE(18:0)-H	0
742.5389	MS2	1.778	M-H	-0.0004

Assigned peak Unassigned peak

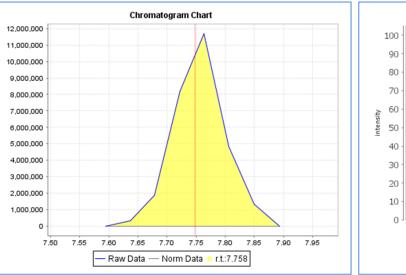
# **Phosphatidylethanolamine (PE)**

# Information

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

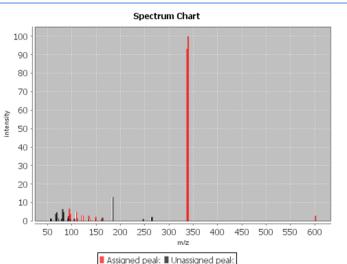
Representation of phosphatidylethanolamine (PE) identification information obtained with LipidSearch software e.g. [PE(36:2)-H]<sup>-</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• PG(18:1_18:2)+NH4	25.1	2.3	80.6	
Ops(18:0_18:1)+H	5.2	9.1	46.8	



## Match Dotail

latch De	tall					Repre
ObsMz	Туре	lt.(%)	Frag.	Delta(Da)		inform
123.1172	MS2	2.902	C9H15	0.0004		e.g. [P
133.1014	MS2	1.043	-	-	$\left( \right)$	0.g. [1
135.1171	MS2	2.909	C10H15	0.0003		ObsMz
137.1328	MS2	1.088	C10H17	0.0003		55.0552
147.1171	MS2	1,188	C11H15	0.0002		57.0345 57.0709
149.1328	MS2	2.24	C11H17	0.0004		67.0551
						69.0707
161.1329	MS2	1.197	C12H17	0.0004		71.0864
163.1483	MS2	1.804	-	-		72.0816
184.0737	MS2	13.011	-	-		79.0551 81.0707
247.2427	MS2	1.124	-	-		83.0862
263.2375	MS2	2.107	_			92.1458
			-	_		93.0706
265.2532	MS2	2.25	-	-		95.0862
337.2745	MS2	93.162	MG(18:2)-OH	8000.0		97.0654 97.1018
339.2902	MS2	100	MG(18:1)-OH	0.0008		105.0704
601.5166	MS2	2.903	NL[PG,+NH4]+H	-0.0025	$\sim$	107.0862
001.0100		2.000		0.0020		109.1017
				C	ору	111.1174
						121.1016

# **Phosphatidylglycerol (PG)**

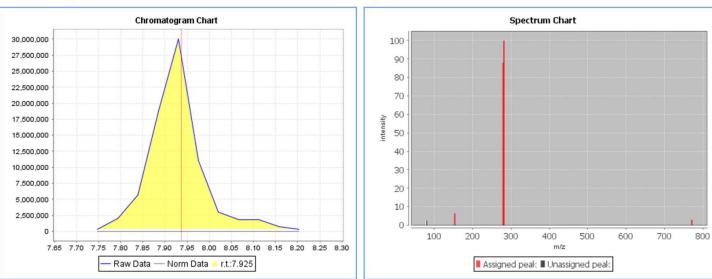
# Information

- Ionization: Positive-ion mode  $\geq$
- Main ion adducts used for identification:  $[M+NH_4]^+$ ,  $\geq$  $[M+H]^+$  and  $[M+Na]^+$
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+NH_4]^+$

sentation of phosphatidylglycerol (PG) identification nation obtained with LipidSearch software  $PG(36:3) + NH_{4}]^{+}$ 

	ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
4	55.0552	MS2	1.308		
	57.0345	MS2	1.18		
	57.0709	MS2	1.428		
	67.0551	MS2	3.905		
	69.0707	MS2	4.744		
	71.0864	MS2	1.462		
	72.0816	MS2	1.034		
	79.0551	MS2	1.282		
	81.0707	MS2	6.478		
	83.0862	MS2	4.832		
	92.1458	MS2	1.347		
	93.0706	MS2	2.643		
	95.0862	MS2	6.72	C7H11	0.0006
	97.0654		1.085		
	97.1018	-	3.848	C7H13	0.0006
	105.0704		1.191		
~	107.0862	-		C8H11	0.0006
_	109.1017	MS2	5.017	C8H13	0.0005
	111.1174			C8H15	0.0006
	121.1016	MS2	3.011	C9H13	0.0004

#### Spectrum



#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● PG(18:1_18:2)-H	29.6	1.5	98.8	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
78.9574	MS2	2.434	-	-
152.9947	MS2	6.327	GP-H3O	-0.0012
279.2334	MS2	87.976	FA(18:2)-H	0.0004
281.249	MS2	100	FA(18:1)-H	0.0004
771.5175	MS2	2.927	M-H	-0.0006

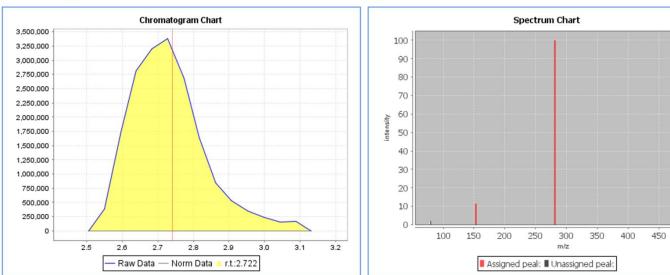
# Phosphatidylglycerol (PG)

## **Information**

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

Representation of phosphatidylglycerol (PG) identification information obtained with LipidSearch software e.g. [PG(36:3)-H]<sup>-</sup>

#### Spectrum



#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LPG(18:1)-H	19.6	0.3	98.2	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
78.9572	MS2	2.099	-	-	
152.9946	MS2	11.447	GP-H3O	-0.0012	
281.2489	MS2	100	FA(18:1)-H	0.0003	
509.29	MS2	3.48	M-H	0.0015	

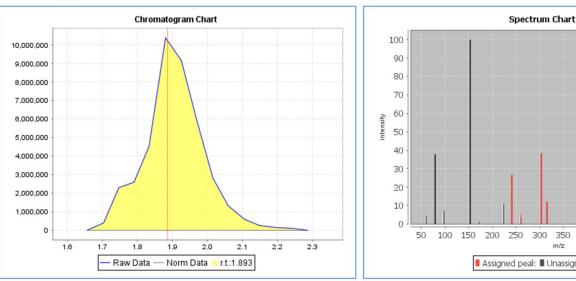
# Lysophosphatidylglycerol (LPG)

# Information

- ➢ Ionization: Negative- and positive-ion mode
- Main ion adducts used for identification: [M-H]<sup>-</sup>,  $\geq$  $[M+NH_4]^+$  and  $[M+H]^+$
- Identification (fragmentation) grade: A and B
- ➢ Main ion adduct used for quantification: [M-H]<sup>−</sup>

Representation of lysophosphatidylglycerol (LPG) identification information obtained with LipidSearch software e.g. [LPG(18:1)-H]<sup>-</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc	. T-Sc.	Occ.	St.
● LPI(20:4)-H	11.6	1	33.3	
O PI(8:0e_12:4)-H	4.9	1	16.4	
○ РІ(8:0р_12:3)-Н	4.9	1	16.4	
○ PI(8:1e_12:3)-H	4.9	1	16.4	
O PI(10:0e_10:4)-H	4.9	1	16.4	
○ PI(10:0p_10:3)-H	4.9	1	16.4	
○ PI(10:1e_10:3)-H	4.9	1	16.4	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
59.012	MS2	4.502	-	-
78.9572	MS2	37.906	-	-
96.9678	MS2	7.343	-	-
152.9944	MS2	100	-	-
171.0054	MS2	1.182	-	-
223.0007	MS2	10.776	-	-
241.0116	MS2	26.716	PH(inositol)-H20	-0.0003
259.0225	MS2	3.357	-	-
259.2433	MS2	5.341	FA(20:4)-H-CO2	0.0002
303.2331	MS2	38.454	FA(20:4)-H	0.0001
315.049	MS2	12.231	M-FA(20:4)-H	0.0003
390.1433	MS2	1.035	-	-
619.2891	MS2	15.299	M-H	0.0002

m/z

Assigned peak Unassigned peak

Spectrum Chart

# Lysophosphatidylinositol (LPI)

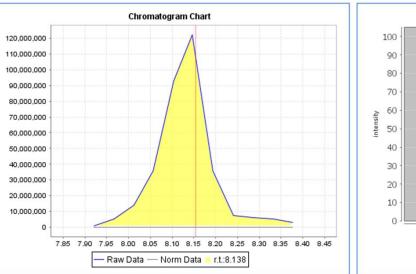
# **Information**

- Ionization: Negative- and positive-ion mode  $\succ$
- Main ion adducts used for identification: [M-H]<sup>-</sup>,  $\succ$  $[M+H]^+$  and  $[M+NH_4]^+$
- Identification (fragmentation) grade: A and B  $\succ$
- Main ion adduct used for quantification: [M-H]<sup>-</sup>  $\geq$

Representation of lysophosphatidylinositol (LPI) identification information obtained with LipidSearch software e.g. [LPI(20:4)-H]<sup>-</sup>

400 450 500 550 600 650

## Spectrum



# Spectrum Chart

#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● PI(18:1_20:4)-H	48.9	0.1	65.2	
○ PI(16:0_22:5)-H	6.2	0.1	20.7	
O PI(16:1_22:4)-H	6.2	0.1	20.7	
○ PI(18:0_20:5)-H	6.2	0.1	20.7	
O PI(20:3_18:2)-H	6.2	0.1	20.7	
O PI(18:3_20:2)-H	6.2	0.1	20.7	
O PI(18:4_20:1)-H	6.2	0.1	20.7	
O PI(24:1_14:4)-H	6.2	0.1	20.7	
O PI(24:2_14:3)-H	6.2	0.1	20.7	
O PI(26:1_12:4)-H	6.2	0.1	20.7	
○ рі(27:1_11:4)-н	6.2	0.1	20.7	
O PI(28:1_10:4)-H	6.2	0.1	20.7	1

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
193.89	MS2	1.24	-	-	/
223.0008	MS2	14.71	PH(inositol)-2H2O-H	-0.0006	
241.0116	MS2	55.524	PH(inositol)-H2O-H	-0.0003	
242.1822	MS2	1.226	-	-	
259.0224	MS2	5.982	IP	0	
259.2432	MS2	6.788	FA(20:4)-H-CO2	0.0001	
281.2487	MS2	100	FA(18:1)-H	0.0001	
297.0378	MS2	4.706	-	-	
303.2331	MS2	42.824	FA(20:4)-H	0.0001	
315.0498	MS2	1.672	-	-	
417.2404	MS2	7.655	LPA(18:1)-H3O	-0.0008	
428.7987	MS2	1.391	-	-	
579.2956	MS2	6.538	LPI(18:1)-H2O-H	0.0017	
883.5342	MS2	28.895	M-H	0	•
<				>	

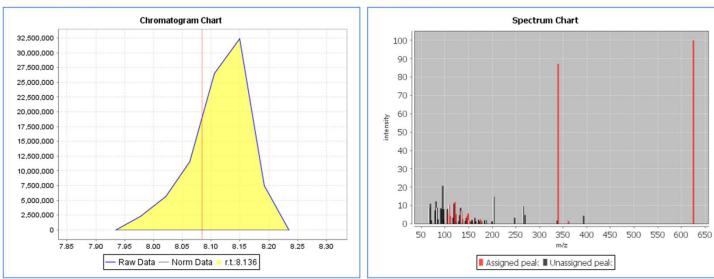
# **Phosphatidylinositol (PI)**

# **Information**

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

Representation of phosphatidylinositol (PI) identification information obtained with LipidSearch software e.g. [PI(38:5)-H]<sup>-</sup>

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• PI(18:1_20:4)+NH4	17.2	0.4	55.3	
O PI(20:3_18:2)+NH4	7.7	0.4	36.3	
O PI(16:0_22:5)+NH4	4	0.4	35.9	
O PI(16:1_22:4)+NH4	4	0.4	35.9	
O PI(18:0_20:5)+NH4	4	0.4	35.9	
O PI(18:3_20:2)+NH4	4	0.4	35.9	
O PI(18:4_20:1)+NH4	4	0.4	35.9	
O PI(24:1_14:4)+NH4	4	0.4	35.9	
O PI(24:2_14:3)+NH4	4	0.4	35.9	
O PI(26:1_12:4)+NH4	4	0.4	35.9	
O PI(27:1_11:4)+NH4	4	0.4	35.9	
O PI(28:1_10:4)+NH4	4	0.4	35.9	

#### Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
184.0736	MS2	1.935	-	-	~
185.1331	MS2	1.895	_	-	
187.1487	MS2	1.936	-	-	
199.1486	MS2	1.269	-	-	
201.1642	MS2	1.5	-	-	
203.1801	MS2	14.867	-	-	
247.2429	MS2	3.324	-	-	
265.2535	MS2	9.52	-	-	
269.2272	MS2	4.808	-	-	
337.2743	MS2	1.79	-	-	
339.2905	MS2	87.173	MG(18:1)-OH	0.0011	
361.2748	MS2	1.54	MG(20:4)-OH	0.0011	
393.3015	MS2	4.379	-	-	
625.5202	MS2	100	NL[PI,+NH4]+H	0.0012	~
<					>

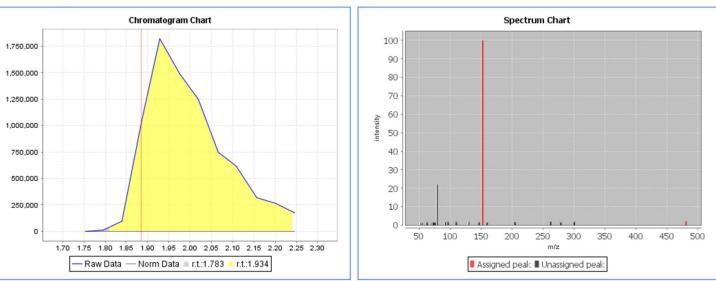
# **Phosphatidylinositol (PI)**

# **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup>, [M+Na]<sup>+</sup>, [M+K]<sup>+</sup> and [M+NH<sub>4</sub>]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- > Main ion adduct used for quantification:  $[M+NH_4]^+$

Representation of phosphatidylinositol (PI) identification information obtained with LipidSearch software e.g. [PI(38:5)+NH<sub>4</sub>]<sup>+</sup>

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LPS(22:6)-H	13.4	0.8	66.9	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da	ı)
78.9573	MS2	22.01	-	-	~
91.8837	MS2	1.591	-	-	
92.1582	MS2	1.629	-	-	
96.9682	MS2	1.832	-	-	
110.261	MS2	1.719	-	-	
130.0197	MS2	1.919	-	-	
147.2038	MS2	1.599	-	-	
152.9947	MS2	100	GP-H3O	-0.0011	
160.1281	MS2	1.488	-	-	
205.06	MS2	1.672	-	-	
262.7444	MS2	1.934	-	-	
279.1598	MS2	1.549	-	-	
300.7773	MS2	1.826	-	-	
481.2378	MS2	2.152	M-Serine+H2O-H	0.0017	~
<					>

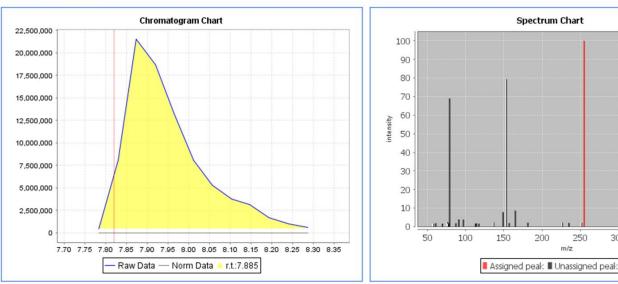
# Lysophosphatidylserine (LPS)

# **Information**

- Ionization: Negative- and positive-ion mode
- Main ion adducts used for identification: [M-H]<sup>-</sup>, [M+H]<sup>+</sup> and [M+NH<sub>4</sub>]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

Representation of lysophosphatidylserine (LPS) identification information obtained with LipidSearch software e.g. [LPS(22:6)-H]<sup>-</sup>

#### Spectrum



#### Match Lipid

LipidIon	M-So	:. T-Sc	Occ.	St.
• PS(16:0_22:6)-H	10	0.6	33.2	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
149.0084	MS2	7.884	-	-	~
152.9945	MS2	79.355	-	-	
156.9806	MS2	1.946	-	-	
165.0397	MS2	8.666	-	-	
181.5265	MS2	2.147	-	-	
226.4443	MS2	2.178	-	-	
235.3255	MS2	2.008	-	-	
251.8229	MS2	2.036	-	-	
255.233	MS2	100	FA(16:0)-H	0.0001	
321.593	MS2	2.095	-	-	
327.2328	MS2	2.593	FA(22:6)-H	-0.0001	
376.2403	MS2	2.324	-	-	
391.2271	MS2	3.867	LPS(16:0)-Serine-H	0.0016	
406.8138	MS2	2.288	-	-	~
<				2	>

# **Phosphatidylserine (PS)**

# **Information**

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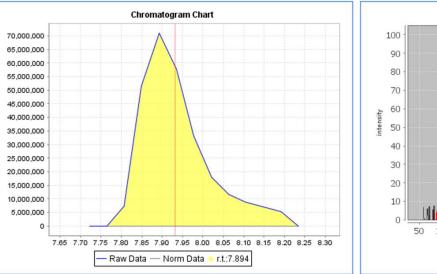
300

350

- Ionization: Negative-ion mode  $\geq$
- Main ion adduct used for identification: [M-H]<sup>-</sup>  $\geq$
- Identification (fragmentation) grade: A and B  $\triangleright$
- ➤ Main ion adduct used for quantification: [M-H]<sup>-</sup>

Representation of phosphatidylserine (PS) identification information obtained with LipidSearch software e.g. [PS(38:6)-H]<sup>-</sup>

## Spectrum



# Spectrum Chart

## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● PS(16:0_22:6)+H	10.3	0.7	33	
Ops(16:0_20:3)+Na	6.9	5.6	32.4	
Ops(16:1_22:5)+H	3.4	0.7	30.1	
Ops(18:1_20:5)+H	3.4	0.7	30.1	
Ops(18:2_20:4)+H	3.4	0.7	30.1	8
Ops(18:3_20:3)+H	3.4	0.7	30.1	
Ops(18:4_20:2)+H	3.4	0.7	30.1	
Ops(14:0_22:3)+Na	3.4	5.6	30.1	
Ops(16:1_20:2)+Na	3.4	5.6	30.1	
Ops(18:0_18:3)+Na	3.4	5.6	30.1	
Ops(18:1_18:2)+Na	3.4	5.6	30.1	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
161.1326	MS2	1.694	C12H17	0.0002	
169.1013	MS2	1.215	-	-	
171.1168	MS2	1.812	-	-	$\backslash$
173.1325	MS2	1.193	-	-	
184.0052	MS2	1.106	-	-	
184.0734	MS2	100	-	-	
185.0766	MS2	10.281	-	-	
186.0777	MS2	4.657	-	-	
201.1637	MS2	1.341	-	-	
239.237	MS2	5.072	-	-	
313.274	MS2	7.193	MG(16:0)-OH	0.0003	
326.269	MS2	1.652	-	-	
385.2733	MS2	1.941	MG(22:6)-OH	-0.0004	
398.2693	MS2	1.333	-	-	
623.5031	MS2	41.97	NL[PS]	-0.0003	$\sim$

# **Phosphatidylserine (PS)**

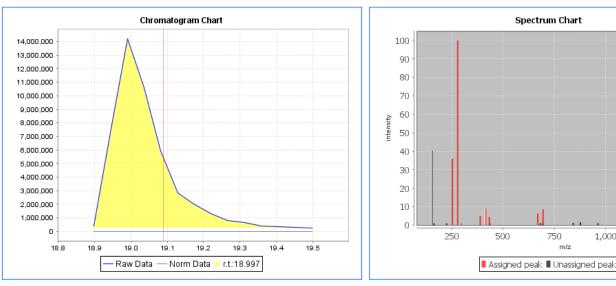
# Information

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+H]<sup>+</sup>, [M+NH<sub>4</sub>]<sup>+</sup> and [M+Na]<sup>+</sup>
- Identification (fragmentation) grade: A and B
- Main ion adducts used for quantification: [M+H]<sup>+</sup> and [M+NH<sub>4</sub>]<sup>+</sup>

Representation of phosphatidylserine (PS) identification information obtained with LipidSearch software e.g. [PS(38:6)+H]<sup>+</sup>

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
57.0708	MS2	7.011		
60.0817	MS2	1.011		
67.055	MS2	6.142		
69.0707	MS2	2.589		
71.0863	MS2	7.392		
79.0549	MS2	5.635		
81.0706	MS2	7.758		
83.0862	MS2	4.109	C6H11	0.0006
85.1018	MS2	4.962	C6H13	0.0007
86.097	MS2	4.023	C6H13 [isoto	0.9959
88.0398	MS2	2.347		
91.0548	MS2	5.657		
93.0703	MS2	5.669	C7H9	0.0005
95.0861	MS2	10.301	C7H11	0.0005
97.1017	M52	2.291	C7H13	0.0005
105.0703	MS2	4.069		
107.0859	MS2	3.644	C8H11	0.0004
109.1015	MS2	6.104	C8H13	0.0004
117.0701	MS2	3.778		
119.0858	MS2	4.671		
121.1015	MS2	2.482	C9H13	0.0003
123.1171	MS2	2.414	C9H15	0.0002
125.0001	MS2	1.595		
129.07	M52	1.934		
131.0857	MS2	5.502		
133.1013	MS2	3.127		
135.1168	MS2	1.44	C10H15	0
137.1326	MS2	1.224	C10H17	0.0001
143.0856	MS2	1.908		
145.1012	MS2	3.285		
147.1169	MS2	2.214	C11H15	0
155.0104	MS2	1.53		
157.1013	M52	1.612		
159.1168	MS2	2.321		

#### Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• CL(18:2_18:2_18:2_16:1)-H	103.7	0.6	74.1	
ОсL(18:2_16:1_18:2_18:2)-н	96.3	0.6	74.1	
О CL(18:2_16:1_16:1_20:3)-Н	66.7	0.6	74.1	
Ocl(12:3_24:1_18:2_16:1)-H	59.3	0.6	74.1	
ОсL(22:4_14:0_18:2_16:1)-Н	59.3	0.6	74.1	
О CL(20:4_16:0_18:2_16:1)-Н	59.3	0.6	74.1	
Ocl(18:3_18:1_18:2_16:1)-H	59.3	0.6	74.1	
Ocl(18:4_18:0_18:2_16:1)-H	59.3	0.6	74.1	
О CL(22:3_14:1_18:2_16:1)-Н	59.3	0.6	74.1	

## Match Detail

ObsMz	Туре	lt.(%)	Frag.	Delta(Da)	
253.2172	MS2	35.984	FA(16:1)-H	-0.0001	
279.2329	MS2	100	FA(18:2)-H	-0.0001	
294.3091	MS2	1.134	-	-	
389.2102	MS2	4.998	LPA(16:1)-H3O	0.0003	
415.2253	MS2	9.087	LPA(18:2)-H3O	-0.0003	
433.236	MS2	4.458	LPA(18:2)-H	-0.0001	
435.4289	MS2	1.093	-	-	
669.4474	MS2	6.323	PA(18:2/16:1)-F	-0.0027	
682.466	MS2	1.132	-	-	
695.1216	MS2	1.011	-	-	
695.4684	MS2	8.591	PA(18:2/18:2)-F	0.0026	
842.0308	MS2	1.259	-	-	
876.8726	MS2	1.58	-	-	
963.2915	MS2	1.119	-	-	
1421.9425	MS2	10.015	M-H	-0.0068	
				(	Сору

1,000

1,250

1,500

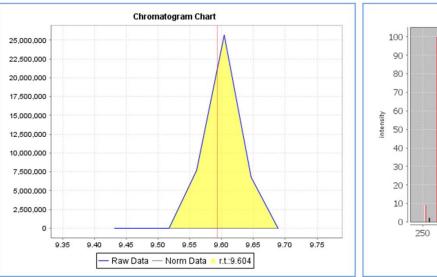
# **Cardiolipin** (CL)

# Information

- Ionization: Negative- and positive-ion mode
- Main ion adducts used for identification: [M-H]<sup>-</sup>, [M- $\geq$  $2H^{-}$  and  $[M+H]^{+}$
- Identification (fragmentation) grade: A and B  $\succ$
- Main ion adduct used for quantification: [M-H]<sup>-</sup>  $\geq$

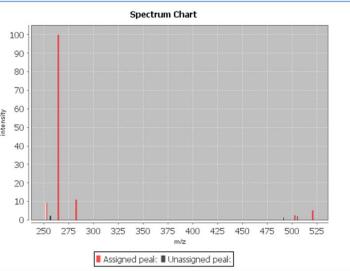
Representation of cardiolipin (CL) identification information obtained with LipidSearch software e.g. [CL(70:7)-H]<sup>-</sup>

## Spectrum



## Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• Hex1Cer(d18:1_16:0)+H	47.9	0.3	95.7	
OHex1Cer(t18:0_16:0)+H-H20	37.5	3.6	93.8	8
O Hex1Cer(d17:0_17:1)+H	3.8	0.3	12.7	8
O Hex1Cer(m17:1_17:0+0)+H	3.8	0.3	12.7	
O Hex1Cer(d16:0_18:1)+H	2.3	0.3	7.5	
OHex1Cer(d17:0_17:0+0) +H-H20	2.2	3.6	10.9	



## Match Detail

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ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
252.2693	MS2	9.295	SPH(d18:1)-H2O-CH2O	0.0008
256.2642	MS2	2.283	-	-
264.2694	MS2	100	SPH(d18:1)-2H2O	8000.0
282.28	MS2	11.052	SPH(d18:1)-H2O	8000.0
490.4992	MS2	1.387	-	-
502.4993	MS2	2.513	NL[G1,H2O]	0.001
504.515	MS2	2.081	-	-
520.5099	MS2	5.247	NL[G1]	0.0011

# Hexosylceramide (Hex1Cer)

# **Information**

>

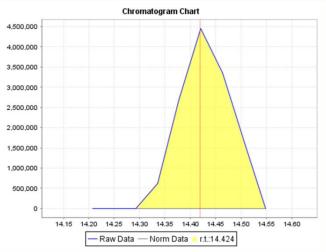
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- Ionization: Positive- and negative-ion mode
- > Main ion adducts used for identification:  $[M+H]^+$ ,  $[M+H-H_2O]^+$ ,  $[M+H-2H_2O]^+$  and  $[M+HCOO]^-$
- Identification (fragmentation) grade: A, B and C
- Main ion adduct used for quantification: [M+H]<sup>+</sup> and [M+HCOO]<sup>-</sup>

Representation of hexosylceramide (Hex1Cer) identification information obtained with LipidSearch software e.g. [Hex1Cer(d34:1)+H]<sup>+</sup>

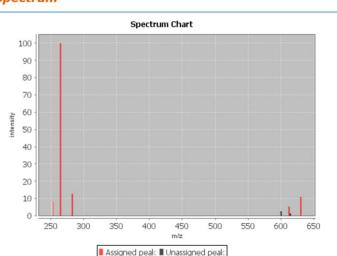
Match Lipid

## Spectrum



# Match Det

LipidIon	M-Sc	. T-Sc.	Occ.	St.
• Hex2Cer(d18:1_24:1)+H	48.6	0.1	97.1	
O Hex2Cer(t18:0_24:1)+H-H20	37.3	1.1	93.3	
O Hex2Cer(d19:2_23:0)+H	24.7	0.1	82.3	
O Hex2Cer(d18:1_24:0+0) +H-H20	15.7	1.1	78.5	
O Hex2Cer(t18:0_24:0+0) +H-2H2O	7.1	3.1	70.7	
O Hex2Cer(d17:0_25:2)+H	5.2	0.1	17.4	
OHex2Cer(d16:0_26:2)+H	2.3	0.1	11.6	
OHex2Cer(d16:1_26:1)+H	2.3	0.1	11.6	
OHex2Cer(d16:2_26:0)+H	2.3	0.1	11.6	
OHex2Cer(d17:1_25:1)+H	2.3	0.1	11.6	
OHex2Cer(d18:0_24:2)+H	2.3	0.1	11.6	
OHex2Cer(d18:2_24:0)+H	2.3	0.1	11.6	
OHex2Cer(d20:0_22:2)+H	2.3	0.1	11.6	
O Hex2Cer(d20:1_22:1)+H	2.3	0.1	11.6	
OHex2Cer(d20:2 22:0)+H	2.3	0.1	11.6	



## Match Detail

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ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
252.2687	MS2	8.262	SPH(d18:1)-H2O-CH2C	0.0001
264.2688	MS2	100	SPH(d18:1)-2H2O	0.0002
282.2794	MS2	12.723	SPH(d18:1)-H2O	0.0002
600.6071	MS2	2.656	-	-
612.6077	MS2	5.385	NL[G2,H2O]	-0.0001
614.625	MS2	1.407	-	-
630.6184	MS2	10.962	NL[G2]	0.0001

Сору

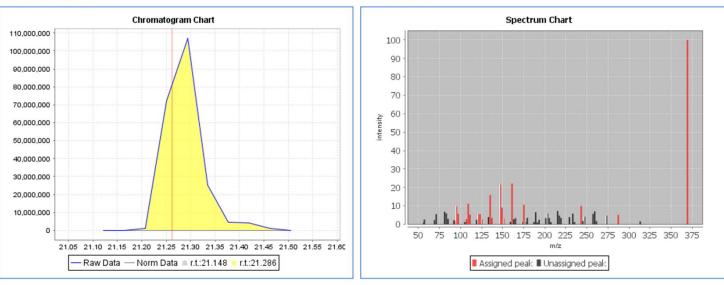
# Hexosylceramide (Hex2Cer)

# **Information**

- Ionization: Positive- and negative-ion mode
- > Main ion adducts used for identification:  $[M+H]^+$ ,  $[M+H-H_2O]^+$ ,  $[M+H-2H_2O]^+$  and  $[M+HCOO]^-$
- Identification (fragmentation) grade: A, B and C
- Main ion adduct used for quantification: [M+H]<sup>+</sup> and [M+HCOO]<sup>-</sup>

Representation of hexosylceramide (Hex2Cer) identification information obtained with LipidSearch software e.g. [Hex2Cer(d42:2)+H]<sup>+</sup>

## Spectrum



#### Match Lipid

LipidIon	м	-Sc.	T-Sc.	Occ.	. St.
ChE(20:5)+NH4	18	9.5	20.2	66.1	
	ObsMz	Туре	It.(%)	Frag.	Delta(Da)
	55.0552		1.004		
	57.0709		2.642		
	69.0707		2.234		
	71.0864 81.0707		5.522		
	81.0707 83.0863		6.788		
	83.0863		2.932		
	92.1486		2.932		
	93.0706			C7H9	0.0007
	95.0862			C7H11	0.0007
	97.1018			C7H13	0.0007
	105.0704		1.261		0.0007
	107.0861			C8H11	0.0006
	109.1017			C8H13	0.0005
	111.1174			C8H15	0.0005
	119.086	MS2	2.49		
	121.1016	MS2	5.533	C9H13	0.0005
	123.1172	MS2	5.516	C9H15	0.0004
	125.1329	MS2	2.767	C9H17	0.0004
	133.1015	MS2	3.914		
	135.1171	MS2	15.943	C10H15	0.0003
	137.1328	MS2	3.364	C10H17	0.0003
	147.1171			C11H15	0.0003
	149.1328			C11H17	0.0003
	151.1485			C11H19	0.0003
	159.1172		1.313		0.0000
	161.1327			C12H17	0.0003
	163.1484		2.78		
	165.1641 173.1328		1.165		
	175.1484			C13H19	0.0003
	175.1464		1.47		0.0003
	179.1798		3.49		
	187.1486		1.278		
	189.1641		6.55		
	191.1796		1.032		
	193.1954		2.454		
	201.1641		3.414		
	203.1798		5.868		
	205.1955	MS2	3.364		
	207.2111	MS2	1.231		
	215.1799	MS2	7.241		

## Match Detail

	Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
	-	-	4.769	MS2	217.1956
	-	-	3.436	MS2	219.2113
	-	-	3.879	MS2	229.1957
	-	-	5.77	MS2	233.2269
	-	-	1.257	MS2	235.2425
	0.0005	C18H27	10.034	MS2	243.2112
	-	-	1.782	MS2	245.2269
	-	-	4.11	MS2	247.2426
	-	-	5.634	MS2	257.227
	-	-	7.04	MS2	259.2427
	-	-	1.757	MS2	261.2585
	-	-	4.769	MS2	273.2584
	0.0007	C21H35	5.072	MS2	287.274
	-	-	1.542	MS2	313.2901
~	0.0008	M-FA	100	MS2	369.3523

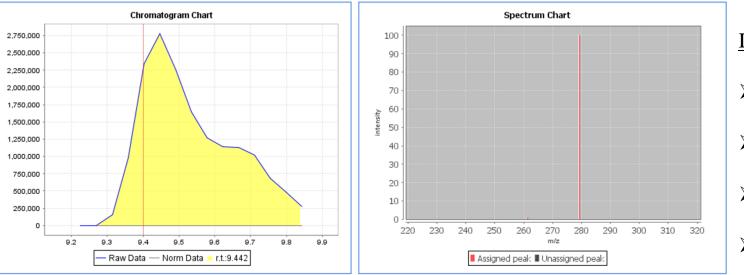
# Cholesteryl esters and Cholesterol (ChE)

# **Information**

- Ionization: Positive-ion mode
- Main ion adducts used for identification: [M+NH<sub>4</sub>]<sup>+</sup>, [M+H-H<sub>2</sub>O]<sup>+</sup> and [M+H]<sup>+</sup>
- Identification (fragmentation) grade: A, B and C
- Main ion adducts used for quantification: [M+NH<sub>4</sub>]<sup>+</sup> in the case of cholesteryl esters [M+H-H<sub>2</sub>O]<sup>+</sup> in the case of cholesterol

Representation of cholesteryl esters (ChE) identification information obtained with LipidSearch software e.g.  $[ChE(20:5)+NH_4]^+$ 

#### Spectrum



#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● FA(18:2)-H	10	6.1	100	

## Match Detail

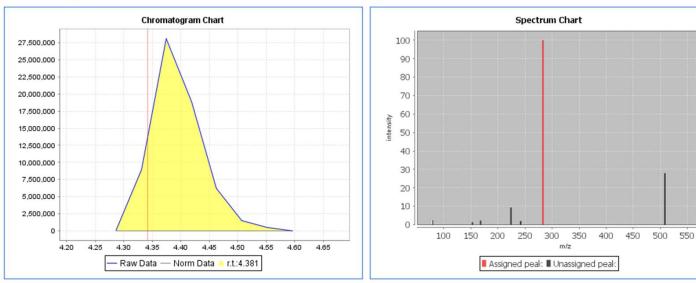
ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
261.2226	MS2	1.046	FA(18:2)-H3O	0.0003
279.2329	MS2	100	M-H	-0.0001

# Fatty acids (FA)

# **Information**

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A, B and C
- Note: A minimal number of free fatty acid species were identified with very low confidence (doesn't meet filtering criteria including diagnostic fragment ions, base retention time, etc.) and they were ignored for further analysis

#### Spectrum



#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
• CerG2GNAc1(d18:1_18:0)-H	6.8	5.3	68.1	

#### Match Detail

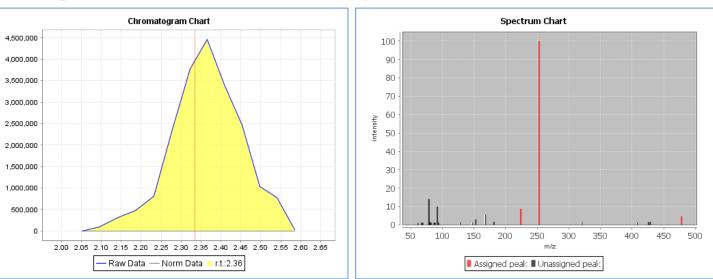
ObsMz	Туре	lt.(%)	Frag.	Delta(Da)
78.9572	MS2	2.434	-	-
152.9943	MS2	1.381	-	-
168.0418	MS2	2.267	-	-
224.0689	MS2	9.384	-	-
242.0795	MS2	1.991	-	-
283.2642	MS2	100	FA(18:0)-H	-0.0001
508.3404	MS2	27.939	-	-
568.3603	MS2	1.368	-	-

# Simple Glc series (CerG2GNAc1)

## **Information**

- ➢ Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- ➢ Identification (fragmentation) grade: A, B and C
- Note: A minimal number of CerG2GNAc1 species were identified with very low confidence (no diagnostic fragment ions) and they were ignored for further analysis

#### Spectrum



#### Match Lipid

LipidIon	M-Sc.	T-Sc.	Occ.	St.
● LdMePE(16:1)-H	13.2	0.1	66	
O LPC(16:1)-CH3	6.1	0.1	60.6	

## Match Detail

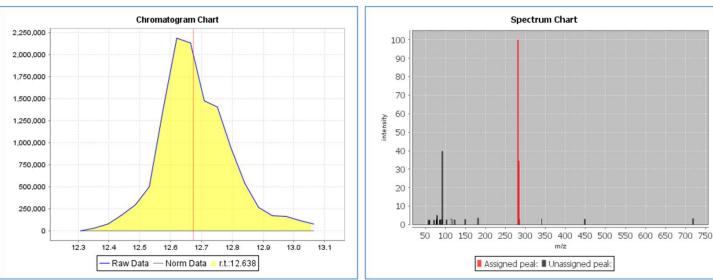
	Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
	-	-	1.311	MS2	88.2889
	-	-	9.991	MS2	92.1381
	-	-	1.372	MS2	94.2195
	-	-	1.466	MS2	127.8928
	-	-	1.304	MS2	147.4395
	-	-	3.023	MS2	152.9945
	-	-	5.703	MS2	168.0419
	-	-	1.65	MS2	181.6368
	-0.0002	LdMeGPE-H3O	8.763	MS2	224.0692
	0	FA(16:1)-H	100	MS2	253.2173
	-	-	1.603	MS2	320.3389
	-	-	1.384	MS2	407.8658
	-	-	1.479	MS2	426.0836
	-	-	1.662	MS2	428.7619
~	0.0027	M-H	4.743	MS2	478.2966

# Lysodimethylphosphatidylethanolamine (LdMePE)

# **Information**

- Ionization: Negative-ion mode
- ➤ Main ion adduct used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A, B and C
- Note: LdMePE lipid species share the same retention time and approximate equivalent abundance ratio values with identical acyl-chain length of LPC species. Possibly, in-source fragments [i.e., LPC-CH<sub>3</sub>] and they were ignored for further analysis<sup>5</sup>

## Spectrum



#### Match Lipid

LipidIon	M-Sc	T-Sc.	Occ.	St.
● dMePE(18:0_18:1)-H	11.3	0	56.6	
Opc(18:0_18:1)-CH3	11.3	0.2	56.6	
OPE(20:0_18:1)-H	4.2	2.3	42.1	

## Match Detail

	Delta(Da)	Frag.	lt.(%)	Туре	ObsMz
	-	-	2.799	MS2	87.1767
	-	-	2.904	MS2	91.7059
	-	-	39.864	MS2	92.1372
	-	-	2.763	MS2	102.5491
	-	-	3.185	MS2	114.3476
	-	-	2.846	MS2	115.1927
	-	-	2.75	MS2	122.8362
	-	-	2.997	MS2	149.2936
	-	-	3.7	MS2	181.5578
	0.0002	FA(18:1)-H	100	MS2	281.2488
	-0.0002	FA(18:0)-H	34.533	MS2	283.2641
	-	-	3.062	MS2	283.9593
	-	-	3.275	MS2	338.8096
	-	-	3.15	MS2	448.3401
~	-	-	3.42	MS2	719.0166

# Dimethylphosphatidylethanolamine (dMePE)

## Information

- Ionization: Negative-ion mode
- ➤ Main ion adducts used for identification: [M-H]<sup>-</sup>
- Identification (fragmentation) grade: A, B and C
- Note: dMePE lipid species share the same retention time and approximate equivalent abundance ratio values with identical acyl-chain length of PC species. Possibly, in-source fragments [i.e., PC-CH<sub>3</sub>] and they were ignored for further analysis<sup>5</sup>