Electronic Supplementary Information (ESI) for Direct analysis of lipids and small metabolites in mouse brain tissue by AP IR-MALDI and reactive LAESI mass spectrometry

Bindesh Shrestha,[a] Peter Nemes,[b] Javad Nazarian,[b] Yetrib Hathout,[b] Eric P. Hoffman,[b] and Akos Vertes [*,a]

[a]*Department of Chemistry, W. M. Keck Institute for Proteomics Technology and Applications, George Washington University, Washington, DC 20052*
[b]*Research Center for Genetic Medicine, Children's National Medical Center, Washington, DC 20010*
** Corresponding author. Phone: +1(202)994-2717, Fax: +1(202)994-5873, Email: vertes@gwu.edu*

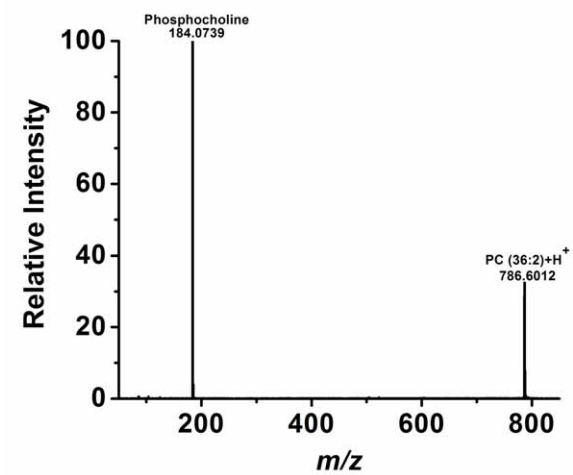
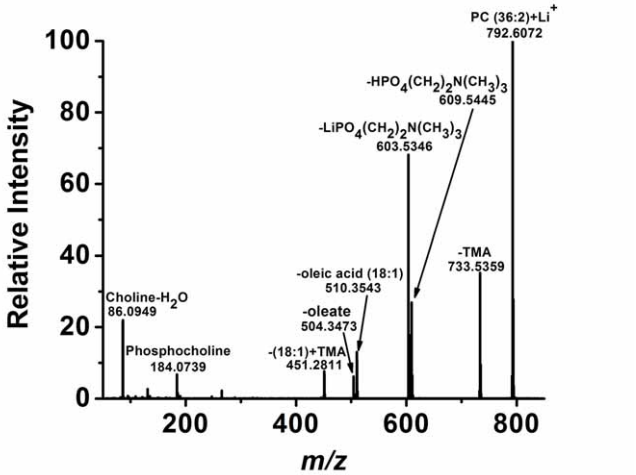


Figure S1. Tandem MS of the protonated PC(18:1/18:1) generated by LAESI produced a single fragment.



Figures S2. Tandem MS of the lithiated PC(18:1/18:1) generated by reactive LAESI produced structure-specific fragments.

LAESI vs. reactive LAESI tandem MS of DOPC

Except for the following modifications, all experimental conditions were the same as in the main section. In the LAESI experiments, a nanospray source was used. The source featured a tapered tip stainless steel emitter (i.d. 50 µm, MT320-50-5-5, New Objective, Woburn, MA), held at 2.8 kV high voltage. It sprayed methanol/water (1:1) mixture containing 0.1% (v/v) acetic acid at 200 nl/min flow rate. The mid-IR laser beam was focused with a 150 mm focal length CaF_2 lens (Infrared Optical Products, Farmingdale, NY). The >99% purity 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC), corresponding to PC(18:1/18:1) in the LIPID MAPS nomenclature,[1] was obtained from Sigma Aldrich, St. Louis, MO, and used without further purification.

This model lipid was used to illustrate the utility of reactive LAESI for the determination of the acyl chain lengths and double bond counts in the PC. The CAD fragmentation of the protonated DOPC ion, at *m/z* 786.6012, produced a single fragment, the phosphocholine ion at *m/z* 184.0739 (see Figure S1). This showed the presence of the phosphocholine headgroup, sufficient to assign the compound as PC(36:2), but lacked any information on the length of the individual acyl chains and the distribution of double bonds. In reactive LAESI with 500 µM Li_2SO_4 in the electrospray solution, in addition to the protonated DOPC, the formation of lithiated DOPC at *m/z* 792.6072 was also observed. The tandem mass spectrum of the lithiated DOPC, obtained with CAD at 20-25 eV collision energy, showed the phosphocholine ion, and the ions due to the losses of trimethylamine (TMA), $HPO_4(CH_2)_2N(CH_3)_3$, $LiPO_4(CH_2)_2N(CH_3)_3$, oleic acid (18:1), oleate, and oleic acid + TMA from the lithiated molecule (Figure S2 and Table S1). The first four fragments indicated the presence of a phosphocholine headgroup and the last three fragments indicated the nature of the acyl chains. Thus, reactive LAESI using Li^+ as a reactant in combination with CAD revealed that the standard DOPC molecule indeed had a PC(18:1/18:1) structure.

Table S1. Mass accuracy of fragment ions produced by CAD of lithiated DOPC generated by reactive LAESI.

Fragment ions	Chemical formula[a]	m/z calc.	m/z meas.	△m (mDa)	ppm
PC(18:1/18:1) + Li^+	$C_{44}H_{84}NO_8PLi^+$	792.6094	792.6072	-2.2	-2.8
PC(18:1/18:1) – TMA + Li^+	$C_{41}H_{75}O_8PLi^+$	733.5359	733.5359	0	0.0
PC(18:1/18:1) – $HPO_4(CH_2)_2N(CH_3)_3$ + Li^+	$C_{39}H_{70}O_4Li^+$	609.5434	609.5445	1.1	1.8
PC(18:1/18:1) – Li $PO_4(CH_2)_2N(CH_3)_3$ + H^+	$C_{39}H_{71}O_4^+$	603.5353	603.5346	-0.7	-1.2
PC(18:1/18:1) – oleic acid + Li^+	$C_{26}H_{50}NO_6PLi^+$	510.3536	510.3543	0.7	1.4
PC(18:1/18:1) – oleate + H^+	$C_{26}H_{51}NO_6P^+$	504.3454	504.3473	1.9	3.8
PC(18:1/18:1) – (oleic acid + TMA) + Li^+	$C_{23}H_{41}O_6PLi^+$	451.2801	451.2811	1	2.2
phosphocholine	$C_5H_{15}NO_4P^+$	184.0739	184.0739	0	0.0
choline – H_2O	$C_5H_{12}N^+$	86.0970	86.0949	-2.1	-24.4

[a] The monoisotopic masses were calculated using the NIST Isotope Calculator package (ISOFORM, Version 1.02), and the measured *m/z* values were obtained from a typical mass spectrum.

Table S2. Tentative peak assignments for ions in the AP IR-MALDI mass spectrum of normal mouse brain tissue.

Metabolites and Lipids[a]	Chemical formula	Ion	m/z calc.	m/z meas.	Δm (mDa)	ppm
pyrrolidinone	C_4H_7NO	$M+H^+$	86.0606	86.0597	-0.9	-10.5
alanine	$C_3H_7NO_2$	$M+H^+$	90.0555	90.0551	-0.4	-4.4
γ-aminobutyric acid	$C_4H_9NO_2$	$M+H^+$	104.0712	104.0731	1.9	18.3
choline	$C_5H_{14}NO^+$	(+)	104.1075	104.1075	0	0.0
creatine	$C_4H_9N_3O_2$	$M+H^+$	132.0773	132.0775	0.2	1.5
hypoxanthine	$C_5H_4N_4O$	$M+H^+$	137.0463	137.0459	-0.4	-2.9
phosphoethanolamine	$C_2H_8NO_4P$	$M+H^+$	142.0269	142.0302	3.3	23.2
spermidine	$C_7H_{19}N_3$	$M+H^+$	146.1657	146.1690	3.3	22.6
imidazolone propionic acid	$C_6H_8N_2O_3$	$M+H^+$	157.0613	157.0642	2.9	18.5
dihydroorotate	$C_5H_6N_2O_4$	$M+H^+$	159.0406	159.0291	-11.5	-72.3
dihydroxymandelaldehyde	$C_8H_8O_4$	$M+H^+$	169.0501	169.0591	9	53.2
furoylglycine	$C_7H_7NO_4$	$M+H^+$	170.0453	170.0362	-9.1	-53.5
arginine	$C_6H_{14}N_4O_2$	$M+H^+$	175.1195	175.1199	0.4	2.3
methyltryptamine	$C_{11}H_{14}N_2$	$M+H^+$	175.1235	175.1199	-3.6	-20.6
hydroxytryptophan	$C_{11}H_{12}N_2O_3$	$M+H^+$	221.0926	221.0950	2.4	10.9
carnosine	$C_9H_{14}N_4O_3$	$M+H^+$	227.1144	227.1126	-1.8	-7.9
homocarnosine	$C_{10}H_{16}N_4O_3$	$M+H^+$	241.1301	241.1284	-1.7	-7.1
glycerophosphocholine	$C_8H_{20}NO_6P$	$M+H^+$	258.1106	258.1133	2.7	10.5
inosine	$C_{10}H_{12}N_4O_5$	$M+H^+$	269.0886	269.0917	3.1	11.5
		$M+K^+$	307.0445	307.0462	1.7	5.5
aminoimidazole ribonucleotide	$C_8H_{14}N_3O_7P$	$M+H^+$	296.0648	296.0662	1.4	4.7
arachidonic acid	$C_{20}H_{32}O_2$	$M+H^+$	305.2481	305.2340	-14.1	-46.2
cholesterol	$C_{27}H_{46}O$	$M-H_2O+H^+$	369.3521	369.3540	1.9	5.1
		$M+Na^+$	409.3446	409.3487	4.1	10.0
		$M+K^+$	425.3186	425.3221	3.5	8.2
N-arachidonoyl D-serine	$C_{23}H_{37}NO_4$	$M+H^+$	392.2801	392.2833	3.2	8.2
hydroxycholesterol	$C_{27}H_{46}O_2$	$M+K^+$	441.3135	441.3259	12.4	28.1
PC(O-16:1)	$C_{24}H_{50}NO_6P$	$M+K^+$	518.3013	518.3072	5.9	11.4
PC(16:0)	$C_{24}H_{50}NO_7P$	$M+K^+$	534.2962	534.3058	9.6	18.0
PC(20:4)	$C_{28}H_{50}NO_7P$	$M+H^+$	544.3403	544.3317	-8.6	-15.8
PC(18:1)	$C_{26}H_{52}NO_7P$	$M+Na^+$	544.3379	544.3317	-6.2	-11.4
Cer(d18:1/18:0)	$C_{36}H_{71}NO_3$	$M+Na^+$	588.5331	588.5372	4.1	7.0
		$M+K^+$	604.5071	604.5123	5.2	8.6
DG(34:1)	$C_{37}H_{70}O_5$	$M+Na^+$	617.5120	617.5239	11.9	19.3
DG(36:1)	$C_{39}H_{74}O_5$	$M+Na^+$	645.5433	645.5369	-6.4	-9.9
		$M+K^+$	661.5173	661.5209	3.6	5.4
DG(38:4)	$C_{41}H_{72}O_5$	$M+Na^+$	667.5277	667.5402	12.5	18.7
PA(34:1)	$C_{37}H_{71}O_8P$	$M+Na^+$	697.4784	697.4857	7.3	10.5
		$M+K^+$	713.4524	713.4602	7.8	10.9
PA(36:2)	$C_{39}H_{73}O_8P$	$M+Na^+$	723.4940	723.5016	7.6	10.5
		$M+K^+$	739.4680	739.4800	12	16.2
SM(18:0)	$C_{41}H_{84}N_2O_6P^+$	(+)	731.6067	731.6086	1.9	2.6
		$M-H+Na^+$	753.5886	753.5836	-5	-6.6
		$M-H+K^+$	769.5626	769.5598	-2.8	-3.6
PC(32:0)	$C_{40}H_{80}NO_8P$	$M+H^+$	734.5700	734.5776	7.6	10.3
		$M+Na^+$	756.5519	756.5523	0.4	0.5
		$M+K^+$	772.5258	772.5313	5.5	7.1
PC(34:1)	$C_{42}H_{82}NO_8P$	$M+H^+$	760.5856	760.5878	2.2	2.9
		$M+Na^+$	782.5675	782.5671	-0.4	-0.5
		$M+K^+$	798.5415	798.5445	3	3.8
PE(38:4)	$C_{43}H_{78}NO_8P$	$M+H^+$	768.5543	768.5493	-5	-6.5
		$M+Na^+$	790.5363	790.5342	-2.1	-2.7
PE(36:1)	$C_{41}H_{80}NO_8P$	$M+Na^+$	768.5519	768.5493	-2.6	-3.4
SM(24:0)	$C_{42}H_{84}NO_6P$	$M+K^+$	768.5673	768.5632	-4.1	-5.3

PC(36:4)	$C_{44}H_{80}NO_8P$	$M+H^+$	782.5700	782.5671	-2.9	-3.7
PC(O-34:1)	$C_{42}H_{84}NO_7P$	$M+K^+$	784.5622	784.5659	3.7	4.7
PS(36:2)	$C_{42}H_{78}NO_{10}P$	$M+H^+$	788.5441	788.5528	8.7	11.0
PC(O-36:5)	$C_{44}H_{80}NO_7P$	$M+Na^+$	788.5566	788.5528	-3.8	-4.8
PE(40:6)	$C_{45}H_{78}NO_8P$	$M+H^+$	792.5543	792.5460	-8.3	-10.5
PC(O-36:3)	$C_{44}H_{84}NO_7P$	$M+K^+$	808.5622	808.5589	-3.3	-4.1
		$M+Na^+$	814.5363	814.5339	-2.4	-2.9
		$M+K^+$	830.5101	830.5212	11.1	13.4
PG(36:0)	$C_{42}H_{83}O_{10}P$	$M+H^+$	801.5621	801.5630	0.9	1.1
		$M+Na^+$	817.5361	817.5458	9.7	11.9
PC(36:1)	$C_{44}H_{86}NO_8P$	$M+Na^+$	810.5989	810.6011	2.2	2.7
		$M+K^+$	826.5728	826.5813	8.5	10.3
PC(38:4)	$C_{46}H_{84}NO_8P$	$M+H^+$	810.6012	810.6011	-0.1	-0.1
		$M+Na^+$	832.5831	832.5697	-13.4	-16.1
PC(O-38:5)	$C_{46}H_{84}NO_7P$	$M+K^+$	832.5622	832.5697	7.5	9.0
PC(38:3)	$C_{46}H_{86}NO_8P$	$M+Na^+$	834.5989	834.5854	-13.5	-16.2
PC(O-38:4)	$C_{46}H_{86}NO_7P$	$M+K^+$	834.5779	834.5854	7.5	9.0
PC(38:6)	$C_{46}H_{80}NO_8P$	$M+Na^+$	828.5519	828.5660	14.1	17.0
		$M+K^+$	844.5258	844.5347	8.9	10.5
PS(36:0)	$C_{42}H_{82}NO_{10}P$	$M+K^+$	830.5313	830.5212	-10.1	-12.2
SM(24:1)	$C_{47}H_{94}N_2O_6P$	$M-H+K^+$	851.6408	851.6492	8.4	9.9
PC(40:6)	$C_{48}H_{84}NO_8P$	$M+Na^+$	856.5831	856.5961	13	15.2
		$M+K^+$	872.5571	872.5673	10.2	11.7
PC(40:1)	$C_{48}H_{94}NO_8P$	$M+Na^+$	866.6614	866.6537	-7.7	-8.9
PC(40:1)	$C_{48}H_{94}NO_8P$	$M+K^+$	882.6354	882.6407	5.3	6.0

[a]DG, PA, PC, PE, PS, PG, and SM species are identified by the total length of the acyl chain(s) and the number of double bonds in parentheses.

Table S3. Tentative peak assignments for ions in the LAESI mass spectrum of normal mouse brain tissue.

Metabolites and Lipids[a]	Chemical formula[c]	Ion	m/z calc.	m/z meas.	Δm (mDa)	ppm
pyrrolidine	C_4H_9N	$M+H^+$	72.0813	72.0835	2.2	30.5
aminoimidazole	$C_3H_5N_3$	$M+H^+$	84.0562	84.0470	-9.2	-109.5
ethanolamine	C_2H_7NO	$M+Na^+$	84.0425	84.0470	4.5	53.5
dehydroalanine	$C_3H_5NO_2$	$M+H^+$	88.0399	88.0458	5.9	67.0
γ-aminobutyric acid	$C_4H_9NO_2$	$M+H^+$	104.0712	104.0664	-4.8	-46.1
choline	$C_5H_{14}NO^+$	(+)	104.1075	104.1098	2.3	22.1
diaminopropionic acid	$C_3H_8N_2O_2$	$M+H^+$	105.0664	105.0714	5	47.6
diaminobutyric acid	$C_4H_{10}N_2O_2$	$M+H^+$	119.0821	119.0887	6.6	55.4
creatine	$C_4H_9N_3O_2$	$M+H^+$	132.0773	132.0828	5.5	41.6
hydroxyhexanoic acid	$C_6H_{12}O_3$	$M+H^+$	133.0865	133.0992	12.7	95.4
ornithine	$C_5H_{12}N_2O_2$	$M+H^+$	133.0977	133.0992	1.5	11.3
adenine	$C_5H_5N_5$	$M+H^+$	136.0623	136.0766	14.3	105.1
octenoic acid	$C_8H_{14}O_2$	$M+H^+$	143.1072	143.0955	-11.7	-81.8
spermidine	$C_7H_{19}N_3$	$M+H^+$	146.1657	146.1695	3.8	26.0
oxooctanoic acid	$C_8H_{14}O_3$	$M+H^+$	159.1021	159.1010	-1.1	-6.9
pyridoxamine	$C_8H_{12}N_2O_2$	$M+H^+$	169.0977	169.1058	8.1	47.9
furoylglycine	$C_7H_7NO_4$	$M+H^+$	170.0453	170.0464	1.1	6.5
arginine	$C_6H_{14}N_4O_2$	$M+H^+$	175.1195	175.1228	3.3	18.8
methyltryptamine	$C_{11}H_{14}N_2$	$M+H^+$	175.1235	175.1228	-0.7	-4.0
phosphoethanolamine	$C_2H_8NO_4P$	$M+K^+$	179.9828	179.9967	13.9	77.2
phosphocholine	$C_5H_{15}NO_4P^+$	(+)	184.0739	184.0665	-7.4	-40.2
metanephrine	$C_{10}H_{15}NO_3$	$M+H^+$	198.1130	198.1074	-5.6	-28.3
decenedioic acid	$C_{10}H_{16}O_4$	$M+H^+$	201.1127	201.1186	5.9	29.3
spermine	$C_{10}H_{26}N_4$	$M+H^+$	203.2236	203.2302	6.6	32.5
hydroxytryptophan	$C_{11}H_{12}N_2O_3$	$M+H^+$	221.0926	221.0905	-2.1	-9.5
acetylspermidine	$C_9H_{21}N_3O$	$M+K^+$	226.1322	226.1362	4	17.7
carnosine	$C_9H_{14}N_4O_3$	$M+H^+$	227.1144	227.1110	-3.4	-15.0
oxo-heneicosanoic acid	$C_{21}H_{40}O_3$	$M+H^+$	341.3056	341.3123	6.7	19.6
MG(18:0)	$C_{21}H_{42}O_4$	$M-H_2O+H^+$	341.3056	341.3123	6.7	19.6
methyl-eicosanoic acid	$C_{21}H_{42}O_2$	$M+K^+$	365.2822	365.2884	6.2	17.0
docosahexaenoic acid (DHA)	$C_{22}H_{32}O_3$	$M+K^+$	383.1989	383.1981	-0.8	-2.1
MG(22:6)	$C_{25}H_{38}O_4$	$M-H_2O+H^+$	385.2743	385.2793	5	13.0
FA(22:0)	$C_{22}H_{44}O_5$	$M+H^+$	389.3267	389.3127	14	-36.0
MG(22:4)	$C_{25}H_{42}O_4$	$M-H_2O+H^+$	389.3056	389.3127	7.1	18.2
N-palmitoyl dopamine (PALDA)	$C_{24}H_{41}NO_3$	$M+H^+$	392.3165	392.3029	-13.6	-34.7
dihydro PGF-1alpha	$C_{20}H_{38}O_5$	$M+K^+$	397.2356	397.2298	-5.8	-14.6
PC(16:0)	$C_{24}H_{50}NO_7P$	$M+H^+$	496.3403	496.3457	5.4	10.9
DG(O-32:2)	$C_{35}H_{66}O_4$	$M+H^+$	551.5039	551.5150	11.1	20.1
DG(34:1)	$C_{37}H_{70}O_5$	$M-H_2O+H^+$	577.5196	577.5279	8.3	14.4
		$M-H_2O+Na^+$	599.5015	599.5099	8.4	14.0
DG(36:4)	$C_{39}H_{68}O_5$	$M-H_2O+H^+$	599.5040	599.5099	5.9	9.8
DG(36:1)	$C_{39}H_{74}O_5$	$M-H_2O+H^+$	605.5509	605.5587	7.8	12.9
		$M-H_2O+Na^+$	627.5328	627.5398	7	11.2
DG(38:6)	$C_{41}H_{68}O_5$	$M-H_2O+H^+$	623.5040	623.5137	9.7	15.6
DG(38:5)	$C_{41}H_{70}O_5$	$M-H_2O+H^+$	625.5196	625.5303	10.7	17.1
DG(O-36:4)	$C_{39}H_{70}O_4$	$M+Na^+$	625.5172	625.5303	13.1	20.9
DG(38:4)	$C_{41}H_{72}O_5$	$M-H_2O+H^+$	627.5353	627.5398	4.5	7.2
PC(26:0)	$C_{34}H_{68}NO_8P$	$M+H^+$	650.4761	650.4668	-9.3	-14.3
PA(36:4)	$C_{39}H_{69}O_8P$	$M+H^+$	697.4808	697.4922	11.4	16.3
PA(34:1)	$C_{37}H_{71}O_8P$	$M+Na^+$	697.4784	697.4922	13.8	19.8
		$M+K^+$	713.4524	713.4468	-5.6	-7.8
PE(O-36:5)	$C_{41}H_{76}NO_7P$	$M+H^+$	724.5281	724.5334	5.3	7.3
PE(O-34:0)	$C_{39}H_{80}NO_7P$	$M+Na^+$	728.5570	728.5477	-9.3	-12.8
SM(24:0)	$C_{42}H_{84}NO_6P$	$M+H^+$	730.6114	730.5981	-13.3	-18.2
		$M+K^+$	768.5673	768.5632	-4.1	-5.3

SM(18:0)	$C_{41}H_{84}N_2O_6P^+$	(+)	731.6067	731.6075	0.8	1.1
PC(32:0)	$C_{40}H_{80}NO_8P$	$M+H^+$	734.5700	734.5739	3.9	5.3
		$M+K^+$	772.5258	772.5371	11.3	14.6
PA(36:2)	$C_{39}H_{73}O_8P$	$M+K^+$	739.4680	739.4753	7.3	9.9
PE(O-34:0)	$C_{39}H_{80}NO_7P$	$M+K^+$	744.5309	744.5372	6.3	8.5
PE(36:1)	$C_{41}H_{80}NO_8P$	$M+H^+$	746.5700	746.5798	9.8	13.1
		$M+Na^+$	768.5519	768.5632	11.3	14.7
PE(O-38:7)	$C_{43}H_{74}NO_7P$	$M+H^+$	748.5281	748.5361	8	10.7
PE(O-36:4)	$C_{41}H_{76}NO_7P$	$M+Na^+$	748.5257	748.5361	10.4	13.9
PE(O-38:5)	$C_{43}H_{78}NO_7P$	$M+H^+$	752.5594	752.5632	3.8	5.0
		$M+Na^+$	774.5413	774.5345	-6.8	-8.8
PE(O-36:2)	$C_{41}H_{80}NO_7P$	M+Na+	752.5570	752.5632	6.2	8.2
PC(34:1)	$C_{42}H_{82}NO_8P$	$M+H^+$	760.5856	760.5885	2.9	3.8
		$M+Na^+$	782.5675	782.5789	11.4	14.6
		$M+K^+$	798.5415	798.5381	-3.4	-4.3
PE(38:4)	$C_{43}H_{78}NO_8P$	$M+H^+$	768.5543	768.5632	8.9	11.6
PE(O-40:6)	$C_{45}H_{78}NO_7P$	$M+H^+$	776.5594	776.5668	7.4	9.5
PC(36:4)	$C_{44}H_{80}NO_8P$	$M+H^+$	782.5700	782.5789	8.9	11.4
PC(36:2)	$C_{44}H_{84}NO_8P$	$M+H^+$	786.6012	786.5970	-4.2	-5.3
		$M+Na^+$	808.5831	808.5852	2.1	2.6
PC(36:1)	$C_{44}H_{86}NO_8P$	$M+H^+$	788.6169	788.6199	3	3.8
		$M+Na^+$	810.5989	810.6104	11.5	14.2
PS(36:0)	$C_{42}H_{82}NO_{10}P$	$M+H^+$	792.5754	792.5665	-8.9	-11.2
PE(40:6)	$C_{45}H_{78}NO_8P$	$M+H^+$	792.5543	792.5665	12.2	15.4
PC(O-36:1)	$C_{44}H_{88}NO_7P$	$M+Na^+$	796.6196	796.6061	-13.5	-16.9
PC(O-36:2)	$C_{44}H_{88}NO_6P$	$M+K^+$	796.5986	796.6061	7.5	9.4
[glycan]Cer(d18:0/20:0)	$C_{44}H_{87}NO_8$	$M+K^+$	796.6068	796.6061	-0.7	-0.9
PC(38:6)	$C_{46}H_{80}NO_8P$	$M+H^+$	806.5700	806.5676	-2.4	-3.0
PC(36:3)	$C_{44}H_{82}NO_8P$	$M+Na^+$	806.5675	806.5676	0.1	0.1
PC(38:5)	$C_{46}H_{82}NO_8P$	$M+H^+$	808.5856	808.5852	-0.4	-0.5
PC(36:3)	$C_{44}H_{84}NO_8P$	$M+Na^+$	808.5831	808.5852	2.1	2.6
PC(38:4)	$C_{46}H_{84}NO_8P$	$M+H^+$	810.6012	810.6104	9.2	11.3
		$M+Na^+$	832.5831	832.5750	-8.1	-9.7
PC(40:7)	$C_{48}H_{82}NO_8P$	$M+H^+$	832.5856	832.5750	-10.6	-12.7
PC(O-38:5)	$C_{46}H_{84}NO_7P$	$M+K^+$	832.5622	832.5750	12.8	15.4
PC(40:6)	$C_{48}H_{84}NO_8P$	$M+H^+$	834.6012	834.6118	10.6	12.7
PC(38:3)	$C_{46}H_{86}NO_8P$	$M+Na^+$	834.5989	834.6118	12.9	15.5

[a]DG, PA, PC, PE, PS, PG, and SM species are identified by the total length of the acyl chain(s) and the number of double bonds in parentheses.

Reference:

1. E. Fahy, S. Subramaniam, R. C. Murphy, M. Nishijima, C. R. H. Raetz, T. Shimizu, F. Spener, G. van Meer, M. J. O. Wakelam and E. A. Dennis, *J. Lipid Res.*, 2009, **50**, S9-14.