

Lipidomics of Brain Tissues in Rats Fed Human Milk from Chinese Mothers or Commercial Infant Formula

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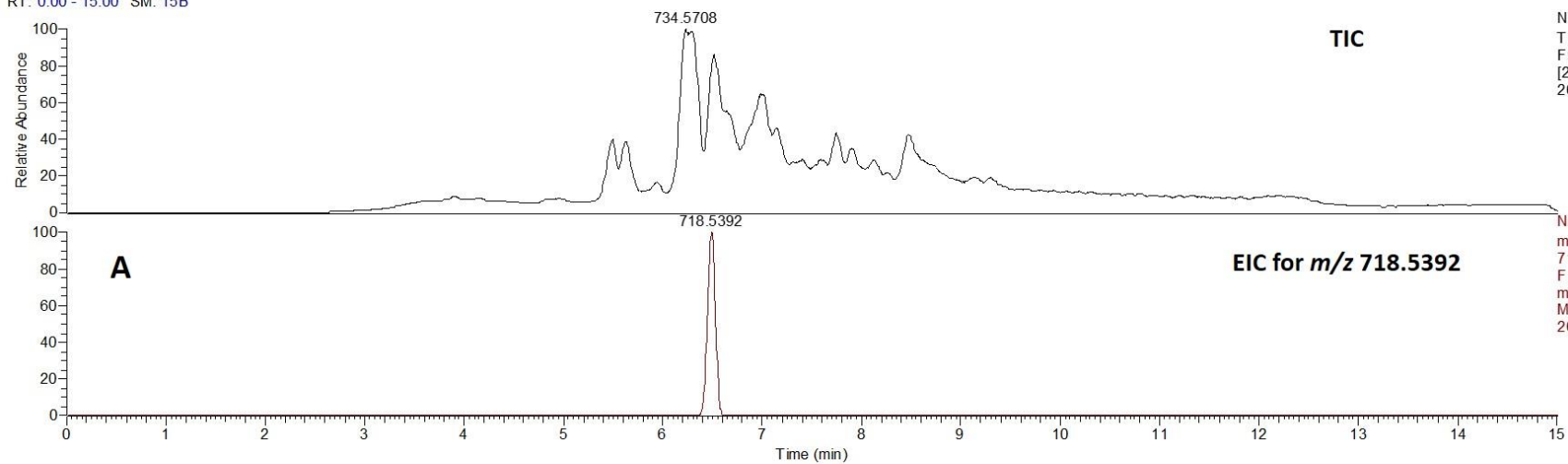
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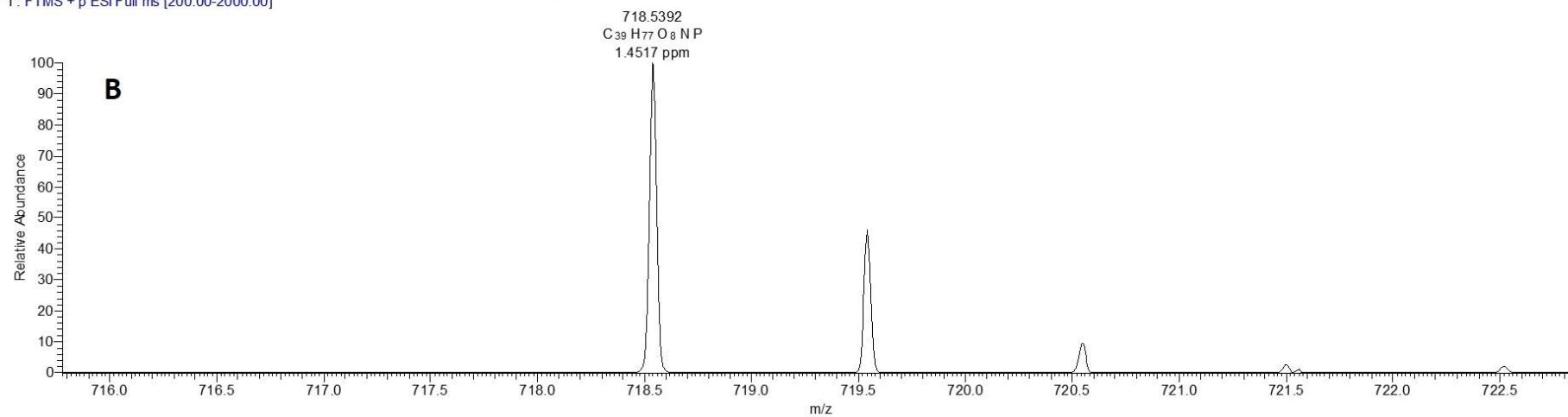
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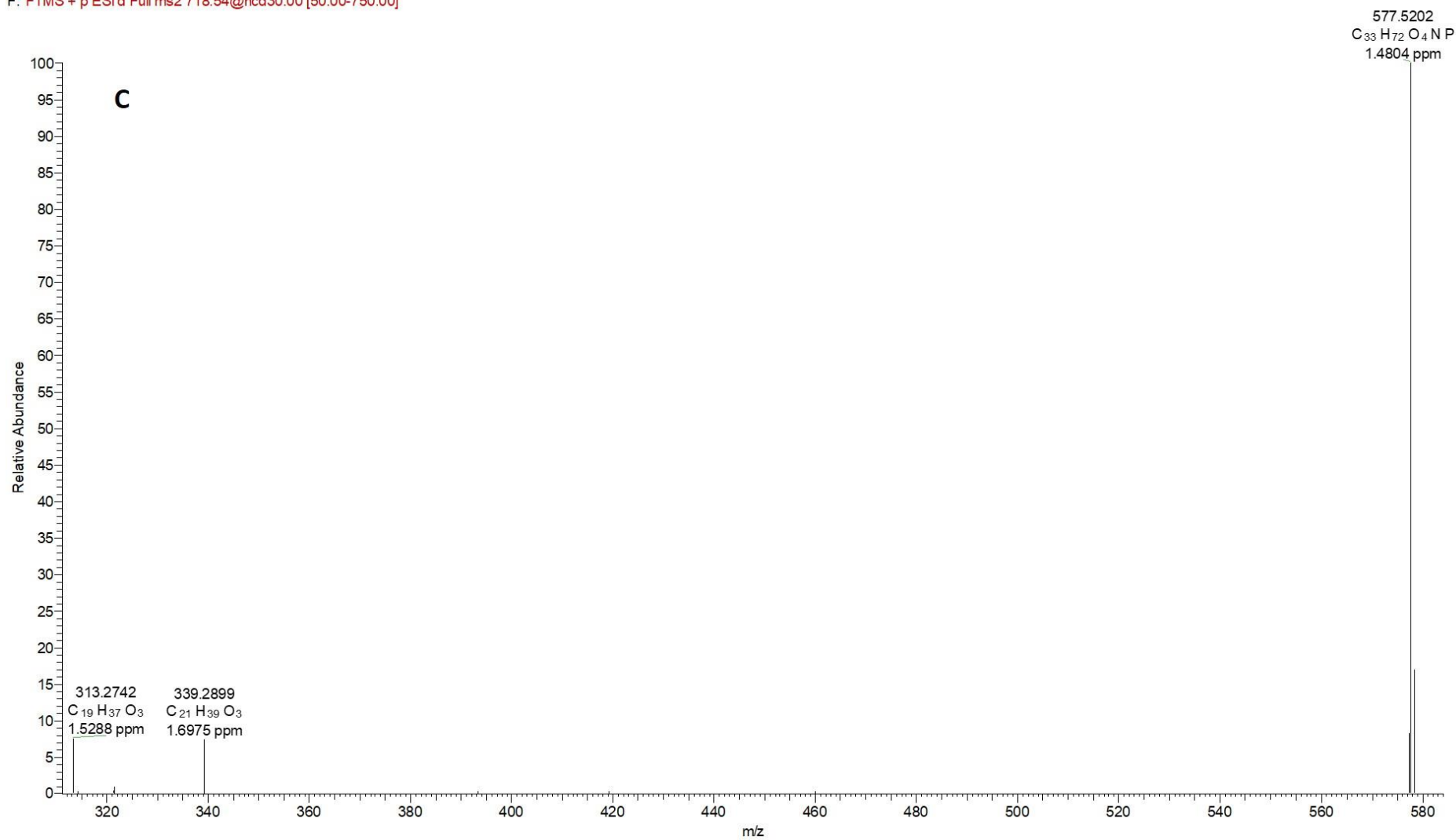
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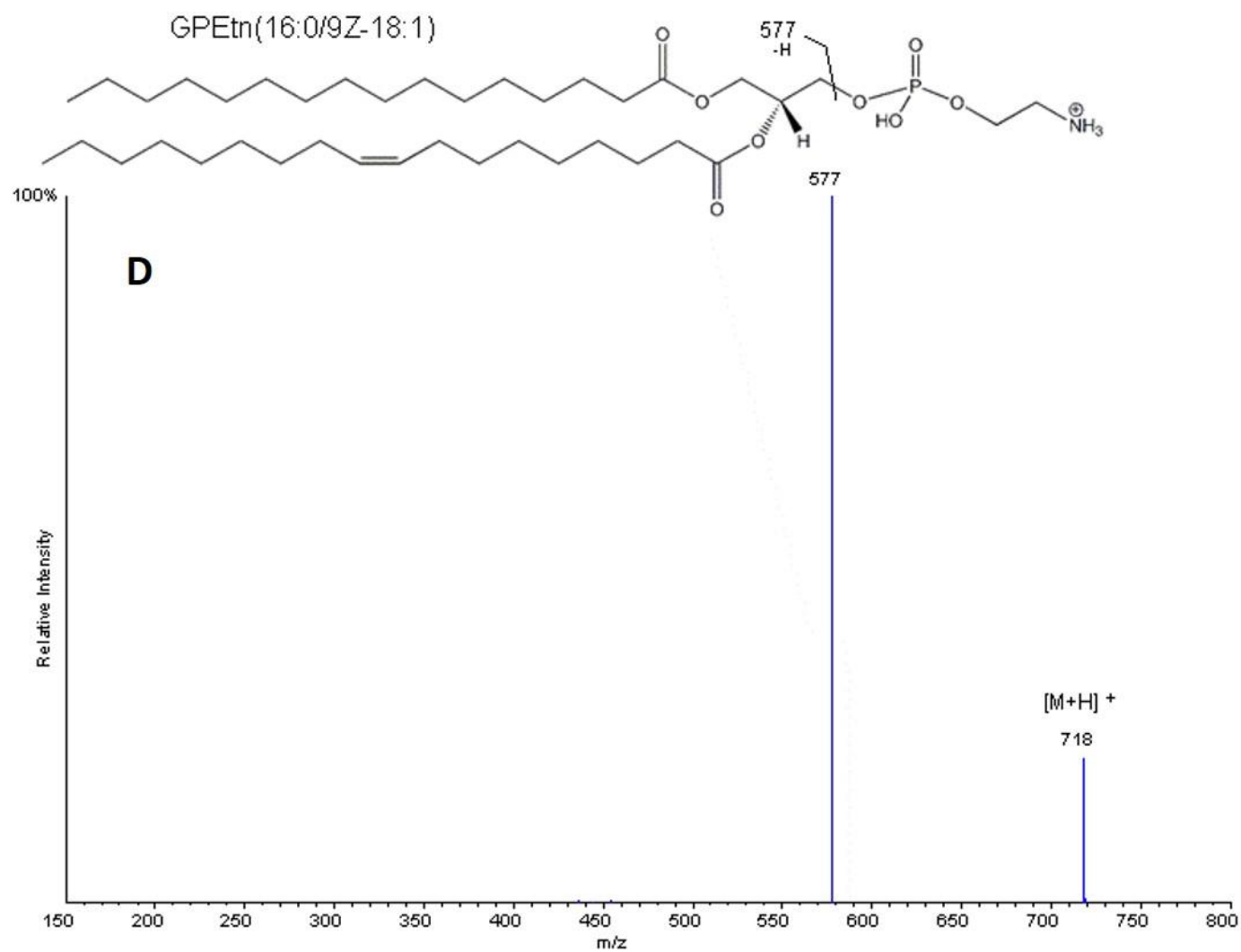


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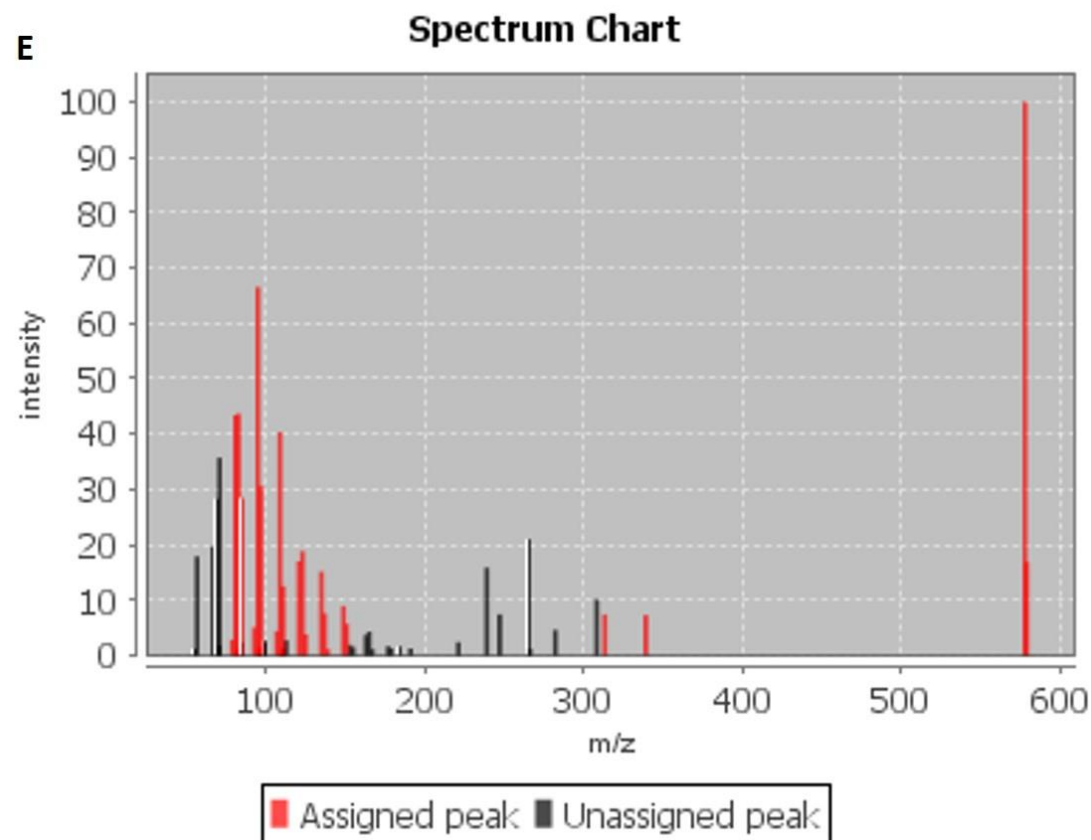


Figure S1. Identification of PE(16:0/18:1)+H where (A) shows an EIC corresponding to the parent ion m/z 718.5392, (B) shows elemental composition of m/z 718.5392 corresponding to the molecular formula of PE(16:0/18:1)+H, (C) shows the ddMS2 spectrum for m/z 718.54 @ CE of 30 eV, (D) shows principal product ions of an analytical standard of PE(16:0/18:1)+H from the LipidMaps database, and (E) shows the theoretical mass spectrum of MS2 product ions of m/z 718.5392.

Table S1. Tentative product/fragment ions of PE(16:0/18:1)+H and their corresponding observed m/z values generated by LipidSearch™.

Observed m/z	Tentative product/fragment ions
79.0548	C ₆ H ₇
81.0705	C ₆ H ₉
83.0862	C ₆ H ₁₁
85.1018	C ₆ H ₁₃
93.0704	C ₇ H ₉
95.0861	C ₇ H ₁₁
97.1017	C ₇ H ₁₃
107.086	C ₈ H ₁₁
109.1016	C ₈ H ₁₃
111.1172	C ₈ H ₁₅
121.1015	C ₉ H ₁₃
123.1171	C ₉ H ₁₅
125.1328	C ₉ H ₁₇
135.117	C ₁₀ H ₁₅
137.1325	C ₁₀ H ₁₇
139.1483	C ₁₀ H ₁₉
149.1327	C ₁₁ H ₁₇
151.1484	C ₁₁ H ₁₉
313.2741	(16:0)-OH
339.2897	(18:1)-OH
577.5199	NL[PE]

NL[PE] refers to the neutral loss of m/z 141 diagnostic of PE

Table S2. Putative combinations of fatty acids and adducts corresponding to PE(34:1) and their m-scores generated by LipidSearch™.

Lipid ion	m-score*
PE(16:0/18:1)+H	29.8
PE(18:1/16:0)+H	29.8
PE(10:0/24:1)+H	15.1
PE(12:0/22:1)+H	15.1
PE(14:0/20:1)+H	15.1
PE(15:1/19:0)+H	15.1
PE(16:1/18:0)+H	15.1
PE(17:1/17:0)+H	15.1
PE(18:0/16:1)+H	15.1
PE(19:1/15:0)+H	15.1
PE(20:0/14:1)+H	15.1
PE(20:1/14:0)+H	15.1
PE(22:1/12:0)+H	15.1
PE(24:1/10:0)+H	15.1
PE(26:1/8:0)+H	15.1
PE(16:0e/19:4)+Li	15.1
PE(16:0p/19:3)+Li	15.1
PE(16:1e/19:3)+Li	15.1
PE(16:1p/19:2)+Li	15.1
PE(18:0p/17:3)+Li	15.1

*The score calculated based on the number of matches with product ion peaks in the spectrum.

Table S3. List of 163 lipid species identified in the current study by LipidSearch software (based on ddMS²) and matched with the final data matrix (XCMS) in positive and negative ionisation modes, with average normalised peak intensities $\pm$ SE in brain samples from rats fed human milk or infant formula ($n=12$).

Lipid Ion	<i>m/z</i>	RT (secs)	Ion Formula	Class	Fatty Acid	Average peak intensity $\pm$ SE	
						Human milk	Infant formula
Positive ionisation mode							
Ceramides							
Cer(d18:1/16:0)+H	538.5194	381.28	C ₃₄ H ₆₈ O ₃ N	Cer	(d18:1/16:0)	23390237 $\pm$ 849340	22968114 $\pm$ 849277
Cer(d18:2/18:0)+H	564.535	386.52	C ₃₆ H ₇₀ O ₃ N	Cer	(d18:2/18:0)	70383939 $\pm$ 3456659	71824796 $\pm$ 3092380
Cer(d18:1/18:0)+H	566.5507	427.14	C ₃₆ H ₇₂ O ₃ N	Cer	(d18:1/18:0)	471871680 $\pm$ 27081731	468352547 $\pm$ 18724515
Cer(d20:1/18:0)+H	594.582	472	C ₃₈ H ₇₆ O ₃ N	Cer	(d20:1/18:0)	46137740 $\pm$ 1586564	41710459 $\pm$ 2727779
Cer(d18:1/22:0)+H	622.6133	515.04	C ₄₀ H ₈₀ O ₃ N	Cer	(d18:1/22:0)	7542913 $\pm$ 384422	6753847 $\pm$ 453905
Cer(d18:1/24:1)+H	648.6289	512.34	C ₄₂ H ₈₂ O ₃ N	Cer	(d18:1/24:1)	47623616 $\pm$ 2526683	43930662 $\pm$ 2659910
Cer(d18:1/24:0)+H	650.6446	555.02	C ₄₂ H ₈₄ O ₃ N	Cer	(d18:1/24:0)	7193849 $\pm$ 424658	6287841 $\pm$ 405475
CerG1(d18:1/18:0)+H	728.6035	386.54	C ₄₂ H ₈₂ O ₈ N	CerG1	(d18:1/18:0)	47372243 $\pm$ 1804599	42712717 $\pm$ 2622198
CerG1(d18:1/18:0+O)+H	744.5984	375.48	C ₄₂ H ₈₂ O ₉ N	CerG1	(d18:1/18:0+O)	21766753 $\pm$ 1159251	17850453 $\pm$ 1365347
CerG1(d18:1/20:0+O)+H	772.6297	417.6	C ₄₄ H ₈₆ O ₉ N	CerG1	(d18:1/20:0+O)	21766753 $\pm$ 1159251	17850453 $\pm$ 1365347

CerG1(d38:1)+H	756.6348	431	C ₄₄ H ₈₆ O ₈ N	CerG1	(d38:1)	23059911 ± 1296903	19095985 ± 1694169
CerG1(d18:1/22:1)+H	782.6504	464.2	C ₄₆ H ₈₈ O ₈ N	CerG1	(d18:1/22:1)	14325563 ± 647307	11579016 ± 920522
CerG1(d18:1/22:0)+H	784.6661	472.5	C ₄₆ H ₉₀ O ₈ N	CerG1	(d18:1/22:0)	32200872 ± 1694967	26462477 ± 2670847
CerG1(d40:0+O)+H	802.6767	480.66	C ₄₆ H ₉₂ O ₉ N	CerG1	(d40:0+O)	22680879 ± 1843054	17708949 ± 2024657
CerG1(d18:1/24:2)+H	808.6661	462.38	C ₄₈ H ₉₀ O ₈ N	CerG1	(d18:1/24:2)	12171501 ± 575191	9687452 ± 811384
CerG1(d18:2/24:1)+H	808.6661	433.88	C ₄₈ H ₉₀ O ₈ N	CerG1	(d18:2/24:1)	5069266 ± 242880	4440493 ± 374297
CerG1(d18:1/24:1)+H	810.6817	472.22	C ₄₈ H ₉₂ O ₈ N	CerG1	(d18:1/24:1)	166696157 ± 8407145	135403339 ± 13946084
CerG1(d42:1)+H	812.6974	516.16	C ₄₈ H ₉₄ O ₈ N	CerG1	(d42:1)	121747728 ± 7099915	104824272 ± 9976147
CerG1(d18:0/24:1)+H	812.6974	485.84	C ₄₈ H ₉₄ O ₈ N	CerG1	(d18:0/24:1)	7223754 ± 374450	5339250 ± 655133
CerG1(d18:0/24:0)+H	814.713	530.82	C ₄₈ H ₉₆ O ₈ N	CerG1	(d18:0/24:0)	11089637 ± 495319	8292721 ± 894933
CerG1(d42:0+O)+H	830.708	521.86	C ₄₈ H ₉₆ O ₉ N	CerG1	(d42:0+O)	56064641 ± 2745368	41254337 ± 3995143
CerG1(d18:1/26:1)+H	838.713	512.7	C ₅₀ H ₉₆ O ₈ N	CerG1	(d18:1/26:1)	10855874 ± 673048	9145632 ± 793104
CerG1(d44:1)+H	840.7287	554.86	C ₅₀ H ₉₈ O ₈ N	CerG1	(d44:1)	7331391 ± 511900	6021735 ± 514105
Diacylglycerol							
DG(18:0/16:0)+NH ₄	614.5718	502.76	C ₃₇ H ₇₆ O ₅ N	DG	(18:0/16:0)	14683932 ± 442610	13057723 ± 589684
DG(18:0/18:1)+NH ₄	640.5875	506.04	C ₃₉ H ₇₈ O ₅ N	DG	(18:0/18:1)	10987111 ± 849163	9072100 ± 1031855

DG(18:0/18:0)+NH ₄	642.6031	541.98	C ₃₉ H ₈₀ O ₅ N	DG	(18:0/18:0)	38458623 ± 1660750	35287483 ± 1280747
DG(18:0/20:4)+NH ₄	662.5718	461.2	C ₄₁ H ₇₆ O ₅ N	DG	(18:0/20:4)	27261396 ± 2594638	24747622 ± 2644507
Phosphatidylethanolamine							
PE(16:0p/16:0)+H	676.5276	407.82	C ₃₇ H ₇₅ O ₇ NP	PE	(16:0p/16:0)	5297000 ± 223815	4618677 ± 232877
PE(16:0p/18:1)+H	702.5432	412.7	C ₃₉ H ₇₇ O ₇ NP	PE	(16:0p/18:1)	229567636 ± 9557431	198310814 ± 13014100
PE(18:0p/16:0)+H	704.5589	451.78	C ₃₉ H ₇₉ O ₇ NP	PE	(18:0p/16:0)	13159539 ± 550477	11404356 ± 658703
PE(16:0e/18:1)+H	704.5589	417.32	C ₃₉ H ₇₉ O ₇ NP	PE	(16:0e/18:1)	31287163 ± 900958	26701141 ± 1669861
PE(16:0/18:1)+H	718.5381	387.28	C ₃₉ H ₇₇ O ₈ NP	PE	(16:0/18:1)	92758254 ± 2504884	87335358 ± 3773007
PE(18:0/16:0)+H	720.5538	426.64	C ₃₉ H ₇₉ O ₈ NP	PE	(18:0/16:0)	16058191 ± 694886	14978929 ± 715916
PE(16:0p/20:4)+H	724.5276	367.12	C ₄₁ H ₇₅ O ₇ NP	PE	(16:0p/20:4)	103670452 ± 5357121	100137061 ± 4827411
PE(18:1p/18:1)+H	728.5589	414.84	C ₄₁ H ₇₉ O ₇ NP	PE	(18:1p/18:1)	303861858 ± 11694492	261609275 ± 19165290
PE(18:0p/18:1)+H	730.5745	452.26	C ₄₁ H ₈₁ O ₇ NP	PE	(18:0p/18:1)	197605140 ± 10075566	162970118 ± 12751155
PE(18:0e/18:1)+H	732.5902	462.42	C ₄₁ H ₈₃ O ₇ NP	PE	(18:0e/18:1)	25168614 ± 1166438	19952740 ± 1647797
PE(16:0/20:4)+H	740.5225	345.86	C ₄₁ H ₇₅ O ₈ NP	PE	(16:0/20:4)	44849131 ± 2441902	45055266 ± 2221239
PE(18:0/18:1)+H	746.5694	431.88	C ₄₁ H ₈₁ O ₈ NP	PE	(18:0/18:1)	129706948 ± 4988478	111512912 ± 6619286
PE(16:0p/22:6)+H	748.5276	353.7	C ₄₃ H ₇₅ O ₇ NP	PE	(16:0p/22:6)	164904737 ± 9020185	154992902 ± 7949434

PE(18:1p/20:1)+H	756.5902	452.3	C ₄₃ H ₈₃ O ₇ NP	PE	(18:1p/20:1)	49049516 ± 3583071	36536204 ± 3374387
PE(18:0p/20:1)+H	758.6058	491.34	C ₄₃ H ₈₅ O ₇ NP	PE	(18:0p/20:1)	33159888 ± 1940875	26517580 ± 2609547
PE(16:0/22:6)+H	764.5225	335.18	C ₄₃ H ₇₅ O ₈ NP	PE	(16:0/22:6)	240338921 ± 11822540	236126020 ± 12061883
PE(18:1/20:4)+H	766.5381	350.64	C ₄₃ H ₇₇ O ₈ NP	PE	(18:1/20:4)	50382385 ± 2540264	47897491 ± 2319392
PE(18:0/20:3)+H	770.5694	408.54	C ₄₃ H ₈₁ O ₈ NP	PE	(18:0/20:3)	8264646 ± 392065	7540929 ± 447905
PE(18:1p/22:6)+H	774.5432	356.76	C ₄₅ H ₇₇ O ₇ NP	PE	(18:1p/22:6)	60366085 ± 3482997	55840385 ± 2930860
PE(18:0/20:1)+H	774.6007	470.12	C ₄₃ H ₈₅ O ₈ NP	PE	(18:0/20:1)	12210565 ± 694558	9356541 ± 923806
PE(18:0p/22:6)+H	776.5589	399.84	C ₄₅ H ₇₉ O ₇ NP	PE	(18:0p/22:6)	471166520 ± 16679831	449560071 ± 21016084
PE(18:1/22:6)+H	790.5381	337.32	C ₄₅ H ₇₇ O ₈ NP	PE	(18:1/22:6)	57122632 ± 3073425	55167080 ± 2665150
PE(18:0/22:6)+H	792.5538	380.92	C ₄₅ H ₇₉ O ₈ NP	PE	(18:0/22:6)	740366682 ± 20173629	710290814 ± 27968280
PE(18:0/22:5)+H	794.5694	404	C ₄₅ H ₈₁ O ₈ NP	PE	(18:0/22:5)	27531820 ± 1259669	23731642 ± 1059150
PE(18:0/22:4)+H	796.5851	421.82	C ₄₅ H ₈₃ O ₈ NP	PE	(18:0/22:4)	105666250 ± 3876693	98916103 ± 4576959
Sphingomyelins							
SM(d34:1)+H	703.5749	325.24	C ₃₉ H ₈₀ O ₆ N ₂ P	SM	(d34:1)	50764155 ± 2154145	49620160 ± 3589264
SM(d36:2)+H	729.5905	327.32	C ₄₁ H ₈₂ O ₆ N ₂ P	SM	(d36:2)	53108203 ± 1908169	49520389 ± 2910627
SM(d36:1)+H	731.6062	370.2	C ₄₁ H ₈₄ O ₆ N ₂ P	SM	(d36:1)	595682085 ± 14313611	568798967 ± 25111132

SM(d36:0)+H	733.6218	386.58	C ₄₁ H ₈₆ O ₆ N ₂ P	SM	(d36:0)	18506329 ± 702414	16668164 ± 830403
SM(d38:1)+H	759.6375	413.62	C ₄₃ H ₈₈ O ₆ N ₂ P	SM	(d38:1)	95973869 ± 3355740	87308842 ± 5576838
SM(d40:2)+H	785.6531	416.98	C ₄₅ H ₉₀ O ₆ N ₂ P	SM	(d40:2)	6802675 ± 417663	5215207 ± 495856
SM(d40:1)+H	787.6688	461	C ₄₅ H ₉₂ O ₆ N ₂ P	SM	(d40:1)	17145771 ± 1023207	14014343 ± 1328073
SM(d42:2)+H	813.6844	455.84	C ₄₇ H ₉₄ O ₆ N ₂ P	SM	(d42:2)	54735931 ± 3364245	44368485 ± 4268536
SM(d42:1)+H	815.7001	503.46	C ₄₇ H ₉₆ O ₆ N ₂ P	SM	(d42:1)	17883630 ± 971659	15212062 ± 1275012
Phosphatidylcholine							
PC(30:0)+H	706.5381	328.84	C ₃₈ H ₇₇ O ₈ NP	PC	(30:0)	268743924 ± 8859790	256007242 ± 13918027
PC(32:1e)+H	718.5745	395.32	C ₄₀ H ₈₁ O ₇ NP	PC	(32:1e)	26293990 ± 1075666	25697721 ± 1125782
PC(31:0)+H	720.5538	348.6	C ₃₉ H ₇₉ O ₈ NP	PC	(31:0)	18534715 ± 1118875	18851214 ± 1063688
PC(32:0e)+H	720.5902	397.54	C ₄₀ H ₈₃ O ₇ NP	PC	(32:0e)	38882741 ± 1825303	35659901 ± 1668226
PC(32:1)+H	732.5538	331.72	C ₄₀ H ₇₉ O ₈ NP	PC	(32:1)	251701301 ± 20931185	212956463 ± 11679169
PC(32:0)+H	734.5694	371.66	C ₄₀ H ₈₁ O ₈ NP	PC	(32:0)	3244692833 ± 94953762	3187938505 ± 100957320
PC(33:1)+H	746.5694	354.24	C ₄₁ H ₈₁ O ₈ NP	PC	(33:1)	16886949 ± 817511	16347720 ± 877657
PC(34:1e)+H	746.6058	402.26	C ₄₂ H ₈₅ O ₇ NP	PC	(34:1e)	240570825 ± 9683638	203695792 ± 14676231
PC(33:0)+H	748.5851	393.22	C ₄₁ H ₈₃ O ₈ NP	PC	(33:0)	26432770 ± 810261	26836742 ± 1395662

PC(34:0e)+H	748.6215	443.12	C ₄₂ H ₈₇ O ₇ NP	PC	(34:0e)	10409157 ± 443582	9174314 ± 546908
PC(34:1)+H	760.5851	375.36	C ₄₂ H ₈₃ O ₈ NP	PC	(34:1)	4739634496 ± 141951176	4599586978 ± 148321696
PC(34:0)+H	762.6007	415.52	C ₄₂ H ₈₅ O ₈ NP	PC	(34:0)	820034285 ± 30492265	760280516 ± 36554903
PC(34:2)+H	758.5694	342	C ₄₂ H ₈₁ O ₈ NP	PC	(34:2)	126887348 ± 8463306	142243771 ± 9037323
PC(36:2p)+H	770.6058	397.12	C ₄₄ H ₈₅ O ₇ NP	PC	(36:2p)	19167159 ± 856519	16758444 ± 1223754
PC(36:2e)+H	772.6215	406.2	C ₄₄ H ₈₇ O ₇ NP	PC	(36:2e)	42520517 ± 1420102	36506460 ± 2722413
PC(35:1)+H	774.6007	395.3	C ₄₃ H ₈₅ O ₈ NP	PC	(35:1)	46644505 ± 1241858	44110089 ± 2605718
PC(36:1e)+H	774.6371	444.94	C ₄₄ H ₈₉ O ₇ NP	PC	(36:1e)	23954908 ± 1318883	20255337 ± 1738660
PC(36:4)+H	782.5694	335.8	C ₄₄ H ₈₁ O ₈ NP	PC	(36:4)	1044886321 ± 53040058	1041344788 ± 49769789
PC(36:3)+H	784.5851	347.92	C ₄₄ H ₈₃ O ₈ NP	PC	(36:3)	22507124 ± 1136685	25113913 ± 1624553
PC(36:2)+H	786.6007	379.78	C ₄₄ H ₈₅ O ₈ NP	PC	(36:2)	414842931 ± 25380771	386298512 ± 24150022
PC(36:1)+H	788.6164	418.98	C ₄₄ H ₈₇ O ₈ NP	PC	(36:1)	1585506946 ± 52130483	1388590719 ± 78159047
PC(36:0)+H	790.632	458.34	C ₄₄ H ₈₉ O ₈ NP	PC	(36:0)	13729129 ± 664620	11278022 ± 808573
PC(37:4)+H	796.5851	356.72	C ₄₅ H ₈₃ O ₈ NP	PC	(37:4)	5036477 ± 318402	5163877 ± 310847
PC(38:6)+H	806.5694	325.1	C ₄₆ H ₈₁ O ₈ NP	PC	(16:0/22:6)	728839570 ± 44568585	708650922 ± 84262687
PC(38:5)+H	808.5851	352.3	C ₄₆ H ₈₃ O ₈ NP	PC	(38:5)	216968566 ± 13381802	204598735 ± 9959614

PC(38:4)+H	810.6007	384.86	C ₄₆ H ₈₅ O ₈ NP	PC	(38:4)	684023657 ± 21587197	663037581 ± 24328338
PC(38:3)+H	812.6164	395.72	C ₄₆ H ₈₇ O ₈ NP	PC	(38:3)	24989121 ± 1013201	23418016 ± 1113299
PC(38:2)+H	814.632	418.78	C ₄₆ H ₈₉ O ₈ NP	PC	(38:2)	42225775 ± 1550380	35738330 ± 2619357
PC(38:1)+H	816.6477	461.9	C ₄₆ H ₉₁ O ₈ NP	PC	(38:1)	62456377 ± 3339235	47281498 ± 4307697
PC(40:7)+H	832.5851	328.16	C ₄₈ H ₈₃ O ₈ NP	PC	(40:7)	355461192 ± 10797655	325922338 ± 17770318
PC(40:6)+H	834.6007	366.18	C ₄₈ H ₈₅ O ₈ NP	PC	(40:6)	255127030 ± 10697665	232849482 ± 12389867
PC(40:5)+H	836.6164	377.5	C ₄₈ H ₈₇ O ₈ NP	PC	(40:5)	27630236 ± 536462	26569780 ± 1463193
PC(40:4)+H	838.632	402.94	C ₄₈ H ₈₉ O ₈ NP	PC	(40:4)	53960384 ± 2131427	47504750 ± 2775447
PC(40:2)+H	842.6633	461.36	C ₄₈ H ₉₃ O ₈ NP	PC	(40:2)	17655500 ± 1140947	12829565 ± 1345492
PC(40:1)+H	844.679	502.7	C ₄₈ H ₉₅ O ₈ NP	PC	(40:1)	35394473 ± 2489364	26074984 ± 2441450
PC(42:10)+H	854.5694	288.94	C ₅₀ H ₈₁ O ₈ NP	PC	(42:10)	4732431 ± 303338	4470863 ± 281836
PC(42:8)+H	858.6007	329.24	C ₅₀ H ₈₅ O ₈ NP	PC	(42:8)	12192990 ± 352407	11197324 ± 634872
PC(41:1)+H	858.6946	524.56	C ₄₉ H ₉₇ O ₈ NP	PC	(41:1)	6367321 ± 496274	4569069 ± 460865
PC(42:7)+H	860.6164	367.12	C ₅₀ H ₈₇ O ₈ NP	PC	(42:7)	7249447 ± 302313	6141924 ± 371527
PC(42:1)+H	872.7103	539.62	C ₅₀ H ₉₉ O ₈ NP	PC	(42:1)	22880015 ± 1745326	17619307 ± 1691091
Phosphatidylserine							

PS(18:1/18:1)+H	788.5436	339.7	C ₄₂ H ₇₉ O ₁₀ NP	PS	(18:1/18:1)	30550480 ± 1191362	28036407 ± 1829513
PS(18:0/18:1)+H	790.5593	379.78	C ₄₂ H ₈₁ O ₁₀ NP	PS	(18:0/18:1)	176364612 ± 6595837	157774854 ± 9710268
PS(18:0/22:6)+H	836.5436	325.3	C ₄₆ H ₇₉ O ₁₀ NP	PS	(18:0/22:6)	375426076 ± 12434005	338561370 ± 20017339
PS(18:0/22:5)+H	838.5593	356.36	C ₄₆ H ₈₁ O ₁₀ NP	PS	(18:0/22:5)	14585049 ± 752127	13074054 ± 628191
PS(18:0/22:4)+H	840.5749	372.04	C ₄₆ H ₈₃ O ₁₀ NP	PS	(18:0/22:4)	43962289 ± 1111539	41412780 ± 1930131
PS(22:4/22:6)+H	884.5436	286.62	C ₅₀ H ₇₉ O ₁₀ NP	PS	(22:4/22:6)	5942725 ± 276206	5433577 ± 350357
Phosphatidylinositol							
PI(16:0/20:4)+NH ₄	876.5597	292.92	C ₄₅ H ₈₃ O ₁₃ NP	PI	(16:0/20:4)	8898107 ± 423108	8397330 ± 426502
PI(18:1/20:4)+NH ₄	902.5753	292.34	C ₄₇ H ₈₅ O ₁₃ NP	PI	(18:1/20:4)	5297353 ± 270342	5002631 ± 278596
PI(18:0/20:4)+NH ₄	904.591	333.18	C ₄₇ H ₈₇ O ₁₃ NP	PI	(18:0/20:4)	69548865 ± 2528047	63415266 ± 2948773
Negative ionisation mode							
Lysophosphatidylethanolamine							
LPE(18:0)-H	480.3096	146.28	C ₂₃ H ₄₇ O ₇ NP	LPE	(18:0)	12494183 ± 340750	11719958 ± 827898
LPE(22:6)-H	524.2783	39.9	C ₂₇ H ₄₃ O ₇ NP	LPE	(22:6)	5259986 ± 627249	4603514 ± 406515
Phosphatidylethanolamine							
PE(16:0p/16:0)-H	674.513	407.16	C ₃₇ H ₇₃ O ₇ NP	PE	(16:0p/16:0)	6051977 ± 175405	5426539 ± 313374

PE(16:0/18:1)-H	716.5236	388.48	C ₃₉ H ₇₅ O ₈ NP	PE	(16:0/18:1)	71714002 ± 939916	63409138 ± 4916605
PE(16:0p/20:4)-H	722.513	365.36	C ₄₁ H ₇₃ O ₇ NP	PE	(16:0p/20:4)	110292352 ± 2987477	102374043 ± 9190520
PE(16:0e/20:4)-H	724.5287	374.5	C ₄₁ H ₇₅ O ₇ NP	PE	(16:0e/20:4)	11655518 ± 644457	10540862 ± 1043294
PE(18:1p/18:1)-H	726.5443	413.9	C ₄₁ H ₇₇ O ₇ NP	PE	(18:1p/18:1)	262311977 ± 6282014	221888578 ± 15989372
PE(18:0e/18:1)-H	730.5756	462.84	C ₄₁ H ₈₁ O ₇ NP	PE	(18:0e/18:1)	30283301 ± 1190623	25295601 ± 1800753
PE(16:0/20:4)-H	738.5079	346.74	C ₄₁ H ₇₃ O ₈ NP	PE	(16:0/20:4)	76434748 ± 1463504	72329402 ± 6337640
PE(36:4)-H	738.5079	648.66	C ₄₁ H ₇₃ O ₈ NP	PE	(36:4)	7909748 ± 263045	7228706 ± 703078
PE(18:1/18:2)-H	740.5236	357.3	C ₄₁ H ₇₅ O ₈ NP	PE	(18:1/18:2)	4996178 ± 226106	5160839 ± 509008
PE(18:1/18:1)-H	742.5392	390.42	C ₄₁ H ₇₇ O ₈ NP	PE	(18:1/18:1)	78948705 ± 2011445	68797773 ± 5024460
PE(18:0/18:1)-H	744.5549	432.34	C ₄₁ H ₇₉ O ₈ NP	PE	(18:0/18:1)	188602257 ± 3737102	167059069 ± 8136023
PE(16:0p/22:6)-H	746.513	352.54	C ₄₃ H ₇₃ O ₇ NP	PE	(16:0p/22:6)	246605868 ± 4823285	223580365 ± 18516416
PE(16:0e/22:6)-H	748.5287	360.68	C ₄₃ H ₇₅ O ₇ NP	PE	(16:0e/22:6)	115638837 ± 4557845	98423945 ± 9333402
PE(18:0p/20:4)-H	750.5443	404.2	C ₄₃ H ₇₇ O ₇ NP	PE	(18:0p/20:4)	236589276 ± 4787893	230355851 ± 13192881
PE(18:0p/22:6)-H	774.5443	399.22	C ₄₅ H ₇₇ O ₇ NP	PE	(18:0p/22:6)	398871100 ± 4386945	375275344 ± 21898034
PE(18:0p/22:5)-H	776.56	427.14	C ₄₅ H ₇₉ O ₇ NP	PE	(18:0p/22:5)	17622931 ± 298452	15081144 ± 802522
PE(18:2/22:6)-H	786.5079	305.98	C ₄₅ H ₇₃ O ₈ NP	PE	(18:2/22:6)	6504750 ± 166953	7173665 ± 668375

PE(18:0/22:4)-H	794.5705	421.2	C ₄₅ H ₈₁ O ₈ NP	PE	(18:0/22:4)	94628112 ± 1727373	89680729 ± 5515864
PE(20:0p/22:6)-H	802.5756	441.24	C ₄₇ H ₈₁ O ₇ NP	PE	(20:0p/22:6)	6115589 ± 68271	6084246 ± 315391
PE(24:4/18:0)-H	822.6018	454.5	C ₄₇ H ₈₅ O ₈ NP	PE	(24:4/18:0)	5908148 ± 167841	5458527 ± 318142
Sphingomyelins							
SM(d18:1/16:0)+HCOO	747.5658	322.54	C ₄₀ H ₈₀ O ₈ N ₂ P	SM	(d18:1/16:0)	4065172 ± 148097	3640179 ± 359766
SM(d40:1)+HCOO	831.6597	459.7	C ₄₆ H ₉₂ O ₈ N ₂ P	SM	(d40:1)	7962239 ± 259331	6836804 ± 452914
SM(d22:1/20:1)+HCOO	857.6753	453.9	C ₄₈ H ₉₄ O ₈ N ₂ P	SM	(d22:1/20:1)	36205637 ± 1083919	30604632 ± 2069913
SM(d20:0/16:0)+HCOO	777.6127	387.04	C ₄₂ H ₈₆ O ₈ N ₂ P	SM	(d20:0/16:0)	4408764 ± 207855	3661766 ± 324815
Phosphatidylglycerol							
PG(16:0/18:1)-H	747.5182	338.68	C ₄₀ H ₇₆ O ₁₀ P	PG	(16:0/18:1)	14084177 ± 247181	12263540 ± 855537
PG(16:0/20:4)-H	769.5025	303.64	C ₄₂ H ₇₄ O ₁₀ P	PG	(16:0/20:4)	5698291 ± 183472	5835813 ± 496346
PG(18:0/20:4)-H	797.5338	342.54	C ₄₄ H ₇₈ O ₁₀ P	PG	(18:0/20:4)	5135325 ± 184218	5000016 ± 398882
PG(22:6/22:6)-H	865.5025	240	C ₅₀ H ₇₄ O ₁₀ P	PG	(22:6/22:6)	6903407 ± 189824	6730357 ± 587273
Phosphatidylserine							
PS(16:0/18:1)-H	760.5134	335.86	C ₄₀ H ₇₅ O ₁₀ NP	PS	(16:0/18:1)	15280841 ± 417463	13030588 ± 1218442
PS(18:1/18:1)-H	786.5291	339.52	C ₄₂ H ₇₇ O ₁₀ NP	PS	(18:1/18:1)	56504806 ± 1816231	48170540 ± 4657692

PS(18:0/18:1)-H	788.5447	378.52	C ₄₂ H ₇₉ O ₁₀ NP	PS	(18:0/18:1)	179935107 ± 4777208	146475633 ± 14424381
PS(16:0/22:6)-H	806.4978	289.64	C ₄₄ H ₇₃ O ₁₀ NP	PS	(16:0/22:6)	12223520 ± 1267910	11634111 ± 1510563
PS(18:0/20:4)-H	810.5291	341.86	C ₄₄ H ₇₇ O ₁₀ NP	PS	(18:0/20:4)	70437615 ± 1779938	61959944 ± 5499022
PS(18:0/20:1)-H	816.576	416.52	C ₄₄ H ₈₃ O ₁₀ NP	PS	(18:0/20:1)	20056213 ± 1772407	16461965 ± 1616123
PS(39:0)-H	832.6073	416.14	C ₄₅ H ₈₇ O ₁₀ NP	PS	(39:0)	390765053 ± 5688384	345313606 ± 24611362
PS(18:0/22:4)-H	838.5604	368.92	C ₄₆ H ₈₁ O ₁₀ NP	PS	(18:0/22:4)	56403819 ± 1940755	49839291 ± 4875249
PS(41:5)-H	850.5604	322.78	C ₄₇ H ₈₁ O ₁₀ NP	PS	(41:5)	114752816 ± 1422025	101645443 ± 9385382
PS(43:7)-H	874.5604	298.64	C ₄₉ H ₈₁ O ₁₀ NP	PS	(43:7)	4076522 ± 124030	4097940 ± 403580
PS(22:6/22:6)-H	878.4978	250.3	C ₅₀ H ₇₃ O ₁₀ NP	PS	(22:6/22:6)	8076274 ± 183712	7356860 ± 667546
PS(24:4/22:6)-H	910.5604	319.4	C ₅₂ H ₈₁ O ₁₀ NP	PS	(24:4/22:6)	5874390 ± 413455	4849389 ± 459667
Phosphatidylcholine							
PC(16:0p/16:0)+HCOO	762.5654	393.48	C ₄₁ H ₈₁ O ₉ NP	PC	(16:0p/16:0)	5187291 ± 223598	4226922 ± 331095
PC(16:0e/16:0)+HCOO	764.5811	399.68	C ₄₁ H ₈₃ O ₉ NP	PC	(16:0e/16:0)	6041154 ± 164798	5466009 ± 372591
PC(16:0e/18:1)+HCOO	790.5967	397.34	C ₄₃ H ₈₅ O ₉ NP	PC	(16:0e/18:1)	57151889 ± 1035177	48568590 ± 3669999
PC(16:0/18:2)+HCOO	802.5604	341.62	C ₄₃ H ₈₁ O ₁₀ NP	PC	(16:0/18:2)	39072481 ± 888473	41522110 ± 4006069
PC(16:0/18:1)+HCOO	804.576	375.38	C ₄₃ H ₈₃ O ₁₀ NP	PC	(16:0/18:1)	638646014 ± 10246996	575723044 ± 52073044

PC(17:0/18:1)+HCOO	818.5917	397.02	C ₄₄ H ₈₅ O ₁₀ NP	PC	(17:0/18:1)	8980789 ± 96651	8347490 ± 583352
PC(18:0e/18:1)+HCOO	818.628	446.74	C ₄₅ H ₈₉ O ₉ NP	PC	(18:0e/18:1)	14698371 ± 480618	11817529 ± 967529
PC(18:1/22:0)+HCOO	888.6699	503.1	C ₄₉ H ₉₅ O ₁₀ NP	PC	(18:1/22:0)	17114970 ± 574342	13970786 ± 884417
Phosphatidylinositol							
PI(18:1/18:1)-H	861.5499	328.02	C ₄₅ H ₈₂ O ₁₃ P	PI	(18:1/18:1)	4748030 ± 298152	3372502 ± 402950
PI(18:1/20:4)-H	883.5342	298.78	C ₄₇ H ₈₀ O ₁₃ P	PI	(18:1/20:4)	51384029 ± 1561335	48346716 ± 4255545
PI(18:0/20:4)-H	885.5499	327.28	C ₄₇ H ₈₂ O ₁₃ P	PI	(18:0/20:4)	540882579 ± 15367450	473655304 ± 53326862

m/z denotes mass-to-charge ratios of the features used for identification; RT denotes retention time in seconds.

Table S4. Lipid species that were significantly different in the brain of rats fed human milk or infant formula ($n = 12$) based on percentage contribution to respective class.

Lipid species	Human milk vs Infant formula	Lipid species	Human milk vs Infant formula
Positive ionization mode		Negative ionization mode	
CerG1(d18:0/24:0)+H	Human milk > Infant formula	PC(16:0p/16:0)+HCOO	Human milk > Infant formula
CerG1(d18:0/24:1)+H	Human milk > Infant formula	PC(18:0e/18:1)+HCOO	Human milk > Infant formula
CerG1(d18:1/22:1)+H	Human milk > Infant formula	PC(18:1/22:0)+HCOO	Human milk > Infant formula
CerG1(d18:1/24:2)+H	Human milk > Infant formula	PE(18:0/18:1)-H	Human milk > Infant formula
CerG1(d42:0+O)+H	Human milk > Infant formula	PE(18:0p/22:5)-H	Human milk > Infant formula
PC(34:1e)+H	Human milk > Infant formula	PG(16:0/18:1)-H	Human milk > Infant formula
PC(36:0)+H	Human milk > Infant formula	PI(18:1/18:1)-H	Human milk > Infant formula
PC(36:1)+H	Human milk > Infant formula	PS(18:0/18:1)-H	Human milk > Infant formula
PC(38:1)+H	Human milk > Infant formula	PC(16:0/18:2)+HCOO	Human milk < Infant formula
PC(40:1)+H	Human milk > Infant formula	PE(16:0/20:4)-H	Human milk < Infant formula
PC(40:2)+H	Human milk > Infant formula	PE(18:0p/20:4)-H	Human milk < Infant formula
PC(40:4)+H	Human milk > Infant formula	PE(18:1/18:2)-H	Human milk < Infant formula
PC(41:1)+H	Human milk > Infant formula	PE(18:2/22:6)-H	Human milk < Infant formula
PC(42:1)+H	Human milk > Infant formula	PG(16:0/20:4)-H	Human milk < Infant formula
PC(42:7)+H	Human milk > Infant formula	PS(43:7)-H	Human milk < Infant formula
PE(18:0/18:1)+H	Human milk > Infant formula		
PE(18:0/20:1)+H	Human milk > Infant formula		
PE(18:0e/18:1)+H	Human milk > Infant formula		
PE(18:0p/16:0)+H	Human milk > Infant formula		
PE(18:0p/18:1)+H	Human milk > Infant formula		
PE(18:1p/20:1)+H	Human milk > Infant formula		
SM(d40:2)+H	Human milk > Infant formula		
Cer(d18:2/18:0)+H	Human milk < Infant formula		
PC(34:2)+H	Human milk < Infant formula		
PC(36:3)+H	Human milk < Infant formula		
PE(16:0/20:4)+H	Human milk < Infant formula		

Significance tested by Fisher's LSD ($\alpha = 0.05$).

Table S5. Nutritional composition analysis of human milk and infant formula samples.

Test/Reference	Unit of measurement	Human milk	Infant formula
Total solids ISO 6731/IDF 21:2010	g/100g	11.2	12.9
Fat ISO 7208/IDF 22:2008	g/100g	1.88	3.67
Protein ISO 8968-2/IDF 20-2:2001	g/100g	1.10	1.46
Carbohydrate 1.2.8. FSANZ calculation	g/100g	8.10	7.40
Energy 1.2.8. FSANZ calculation	kJ/100g	225.00	287.00

Table S6. List of lipids identified by LipidSearch™ software.

Group	Lipid name
P-Choline	Lysophosphatidylcholine
	Platelet-activating factor
	Phosphatidylcholine
P-Ethanol Amine	Lysophosphatidylethanolamine
	Lysodimethylphosphatidylethanolamine
	Phosphatidylethanolamine
	Dimethylphosphatidylethanolamine
P-Serine	Lysophosphatidylserine
	Phosphatidylserine
P-Glycerol	Lysophosphatidylglycerol

	Phosphatidylglycerol
P-Inositol	Lysophosphatidylinositol
	Phosphatidylinositol
	Phosphatidylinositol
	Phosphatidylinositol
	Phosphatidylinositol
P-Ethanol	Lysophosphatidylethanol
	Phosphatidylethanol
P-Acid	Lysophosphatidic acid
	Phosphatidic acid
	Cyclic phosphatidic acid
P-Methanol	Lysophosphatidylmethanol
	Phosphatidylmethanol
Sphingolipids	Sphingomyelin
	Lysosphingomyelin
	Sphingomyelin(phytosphingosine)
Neutral glycerolipid	Monoglyceride
	Diglyceride
	Triglyceride
Fatty Acid	Fatty acid
	(O-acyl)-1-hydroxy fatty acid

Cardiolipin	Cardiolipin
Sphingoid base	Sphingosine
	Sphingosine phosphate
Neutral Glycosphingolipids	Glucosylsphingosine
	Simple glc series
	Simple glc series
	Simple glc series
	Simple glc series
	Simple glc series
	Simple glc series
Glycosphingolipids	Ceramides
	Ceramides phosphate
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides

	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
	Gangliosides
Steroid	Cholesteryl ester
	Zymosteryl ester
	Stigmasteryl ester
	Sitosteryl ester
	Deuterated cholesteryl ester
Coenzyme	Coenzyme
Glycoglycerolipid	Monogalactosylmonoacylglycerol
	Monogalactosyldiacylglycerol
	Digalactosylmonoacylglycerol
	Digalactosyldiacylglycerol
	Sulfoquinovosylmonoacylglycerol
	Sulfoquinovosyldiacylglycerol
Neutral glycerolipid (deuterated)	Deuterated diglyceride
	Deuterated triglyceride