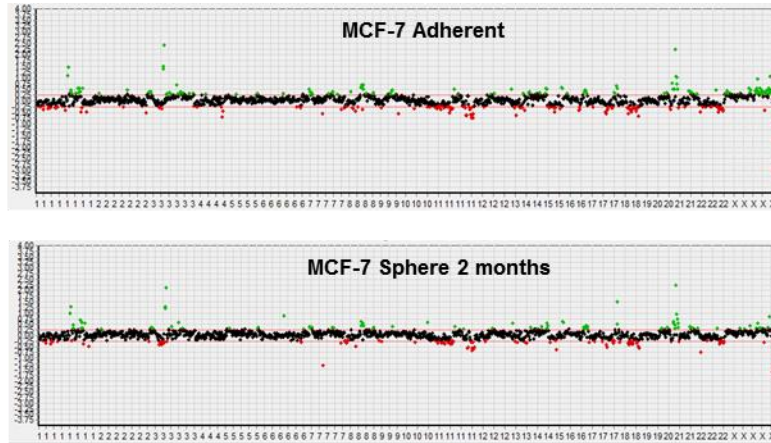


## *Supplementary Material*

### 1 Supplementary Figures and Tables

#### 1.1 Supplementary Figures

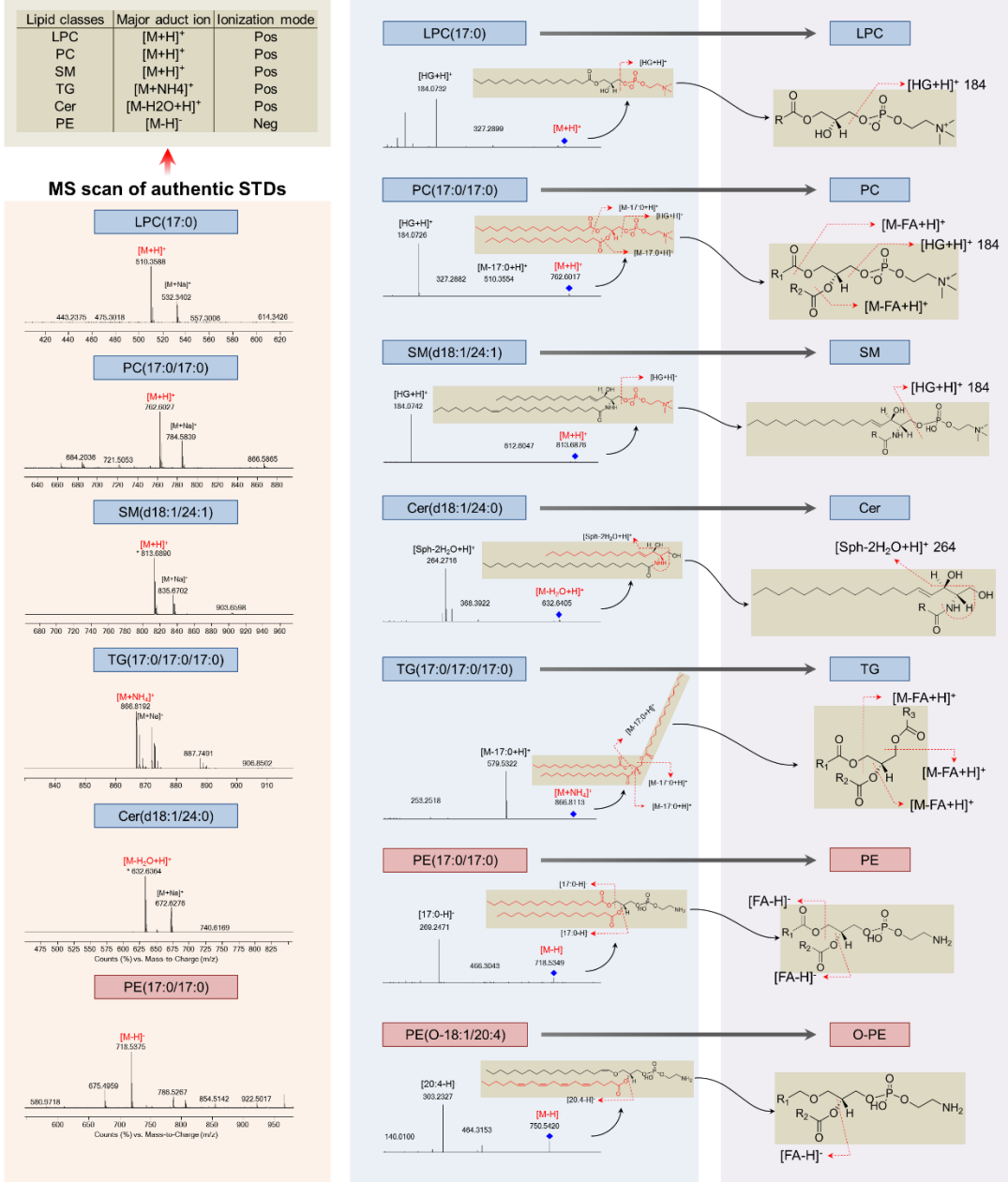


**Supplementary Figure 1.** Comparative genomic hybridization (CGH) analysis between Adherent and Sphere.

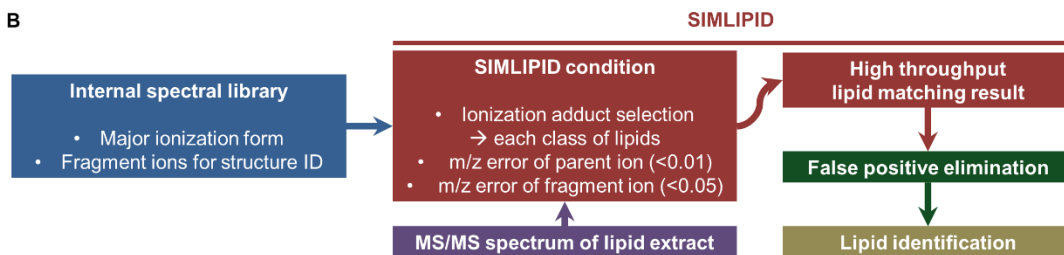
## Supplementary Figure 2. Internal spectral library and lipid identification process.

A

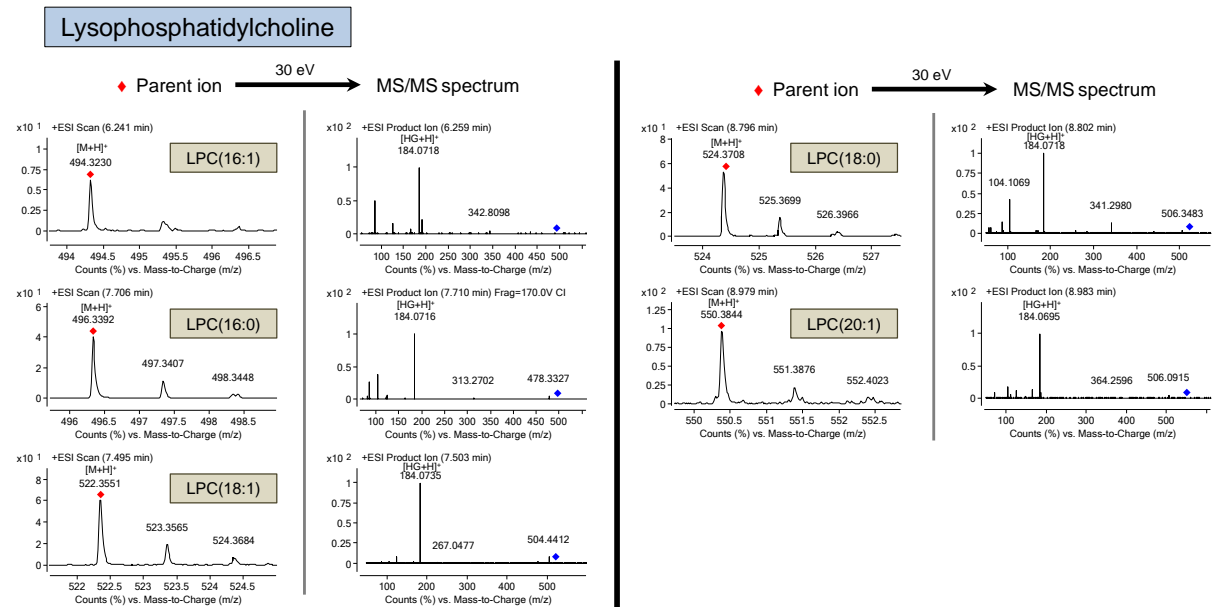
Major adduct ions of lipid classes → MS/MS spectrum of authentic STDs → Fragment ions for structure ID



B



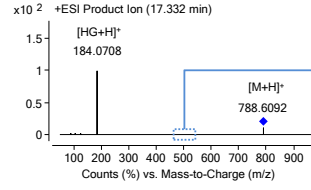
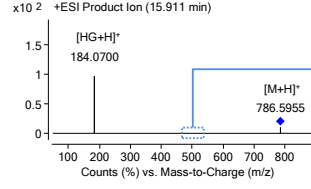
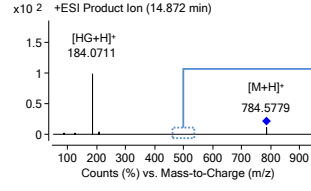
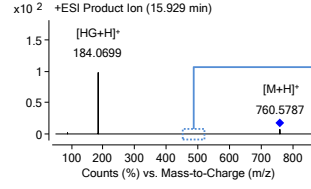
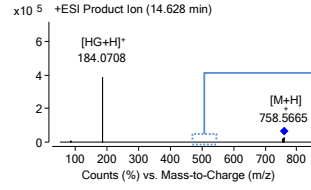
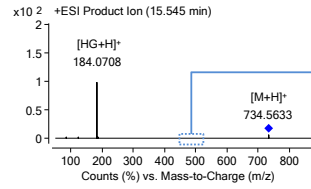
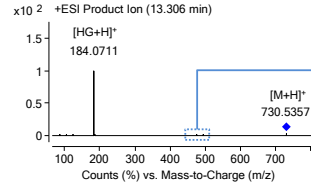
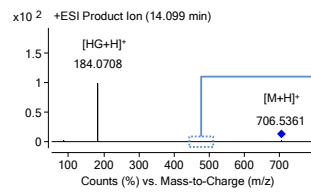
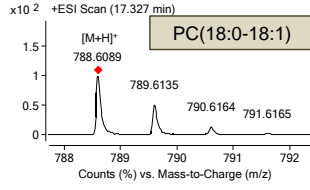
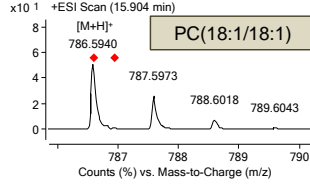
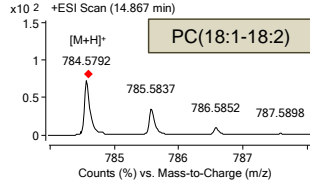
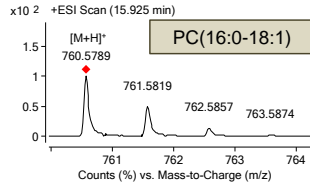
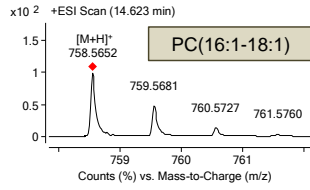
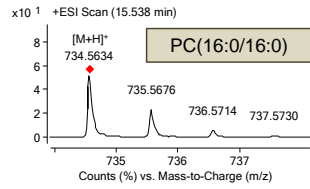
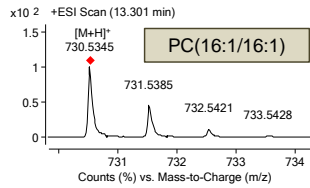
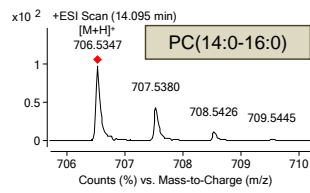
**Supplementary Figure 3. MS and MS/MS spectrum based identification of LPC, PC, O-PC, SM, TG, Cer, PE, and O-PE.**



Continued

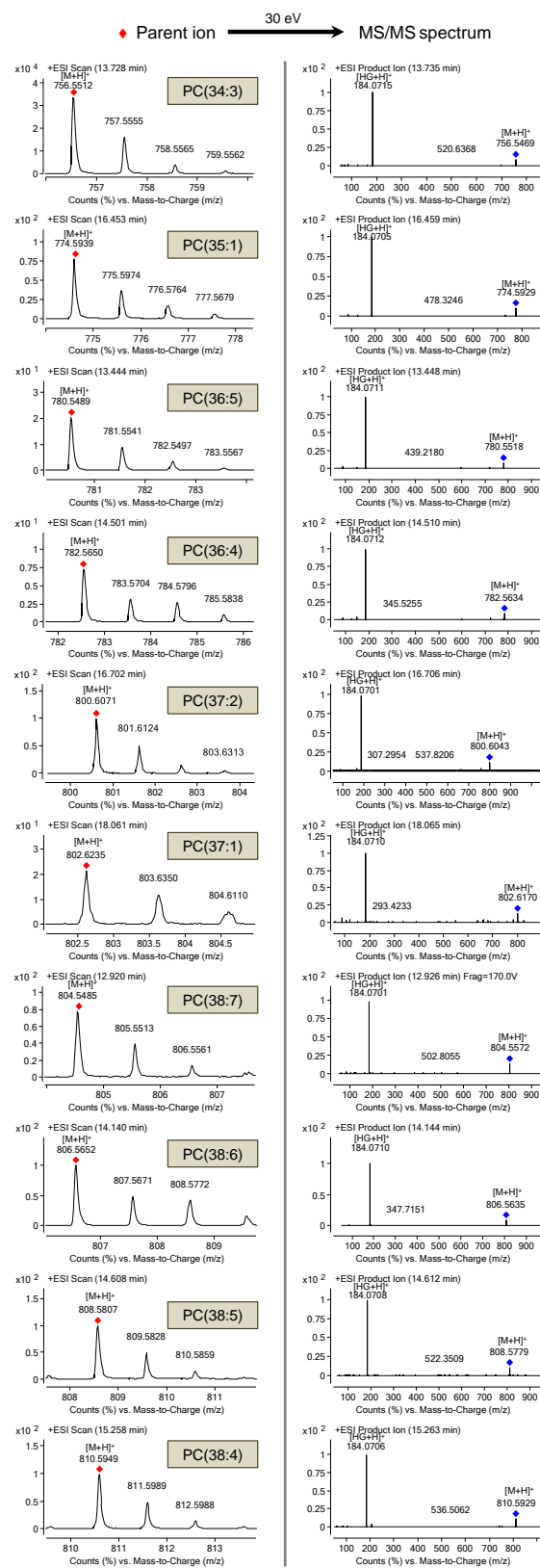
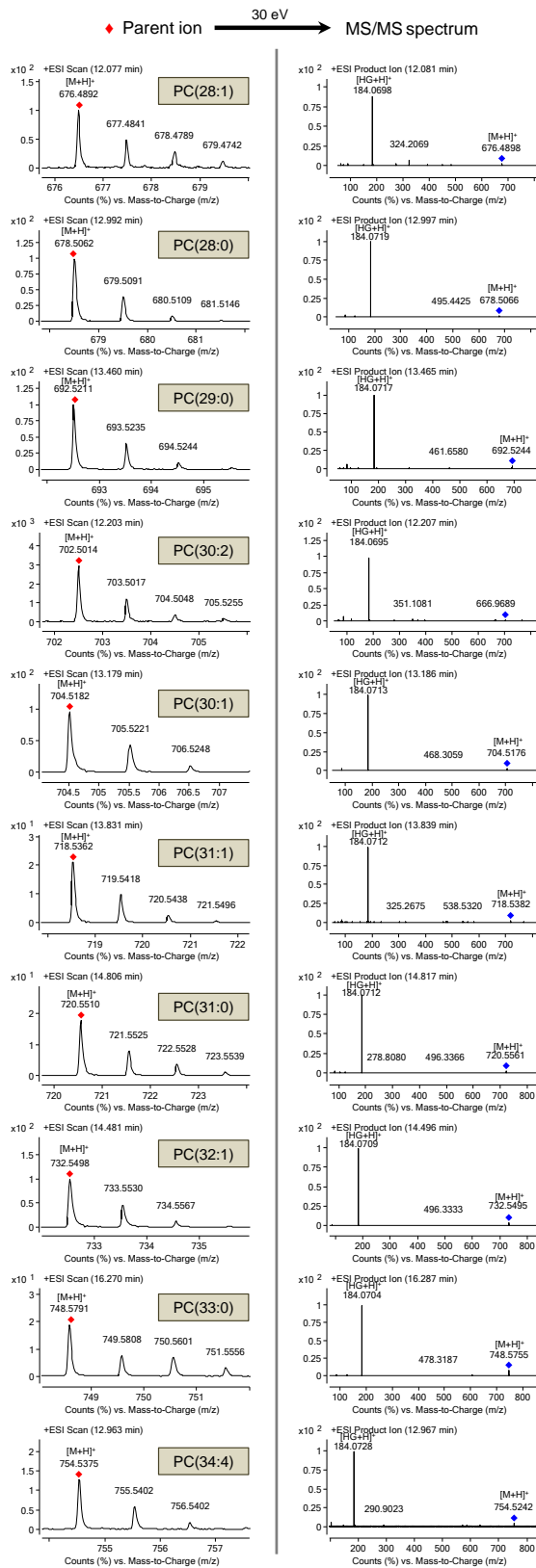
Phosphatidylcholine

♦ Parent ion  $\xrightarrow{30\text{ eV}}$  MS/MS spectrum



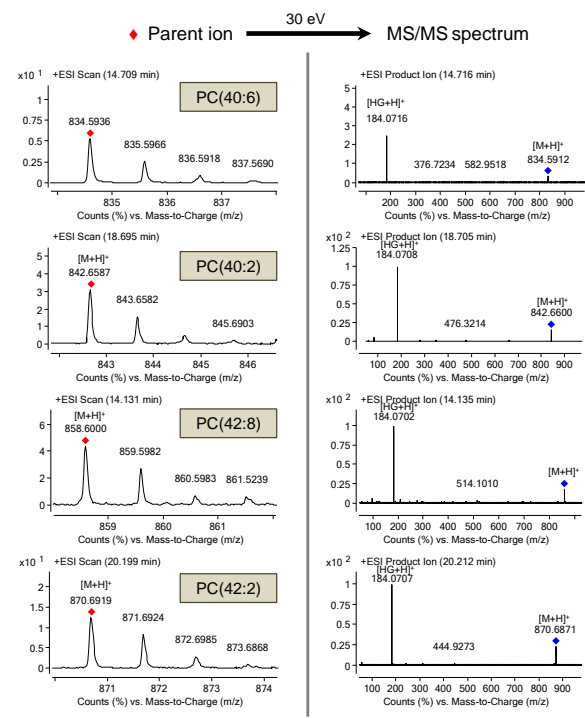
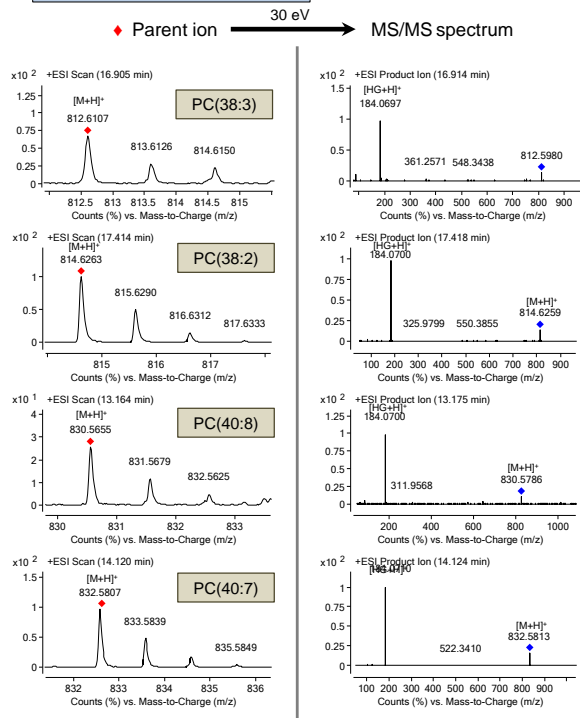
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## Phosphatidylcholine

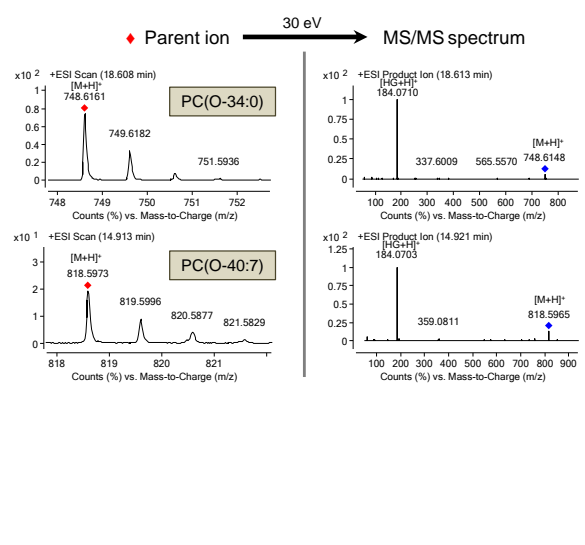
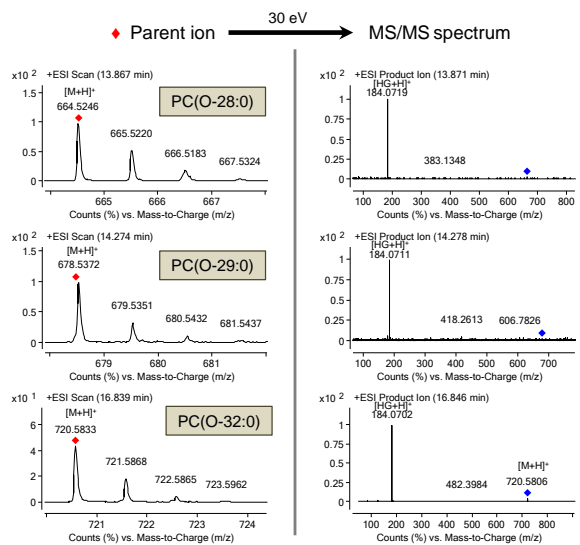


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Phosphatidylcholine

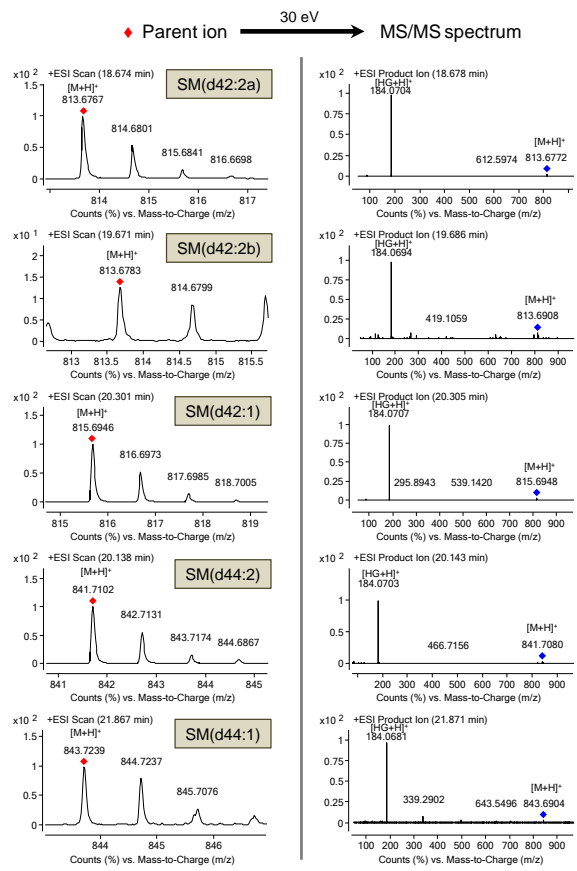
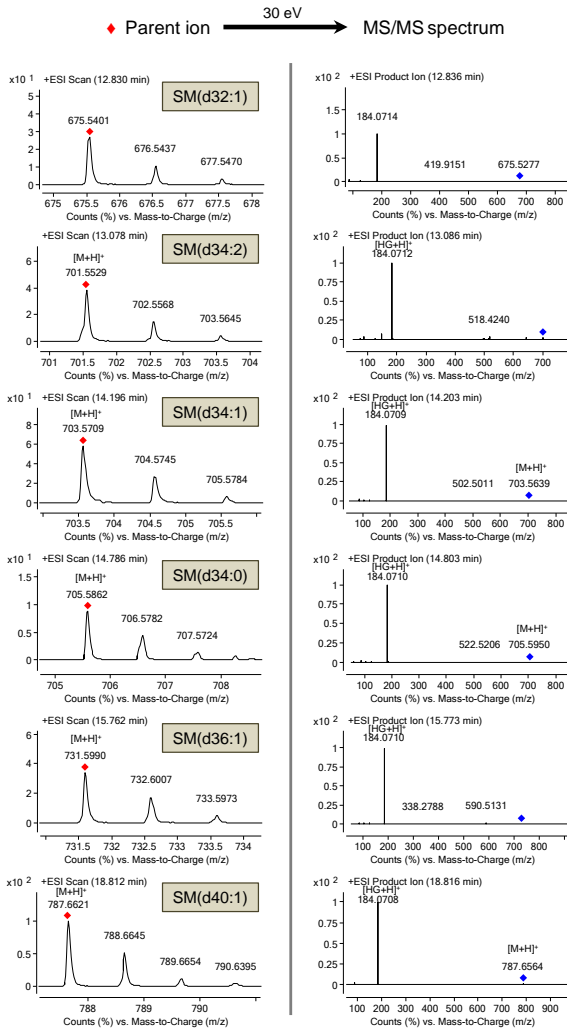


O-Phosphatidylcholine

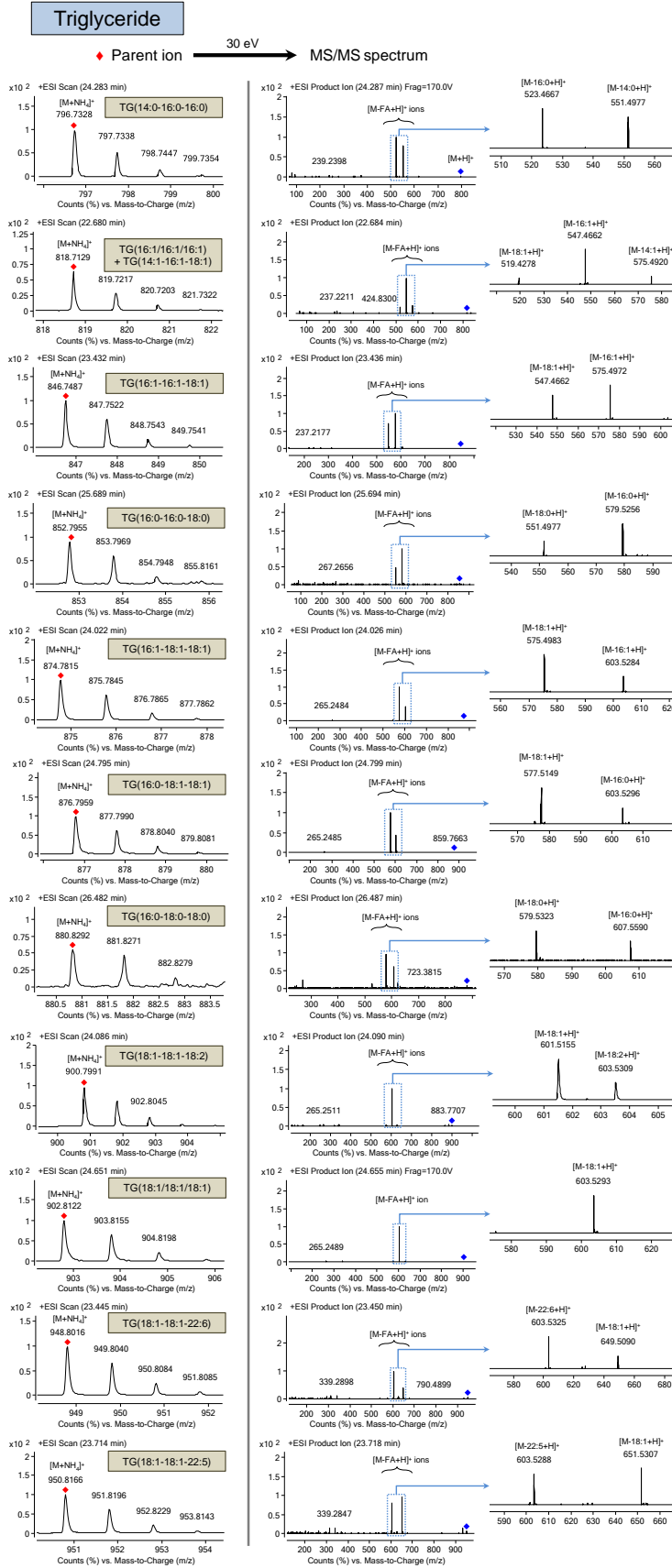


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Sphingomyelin



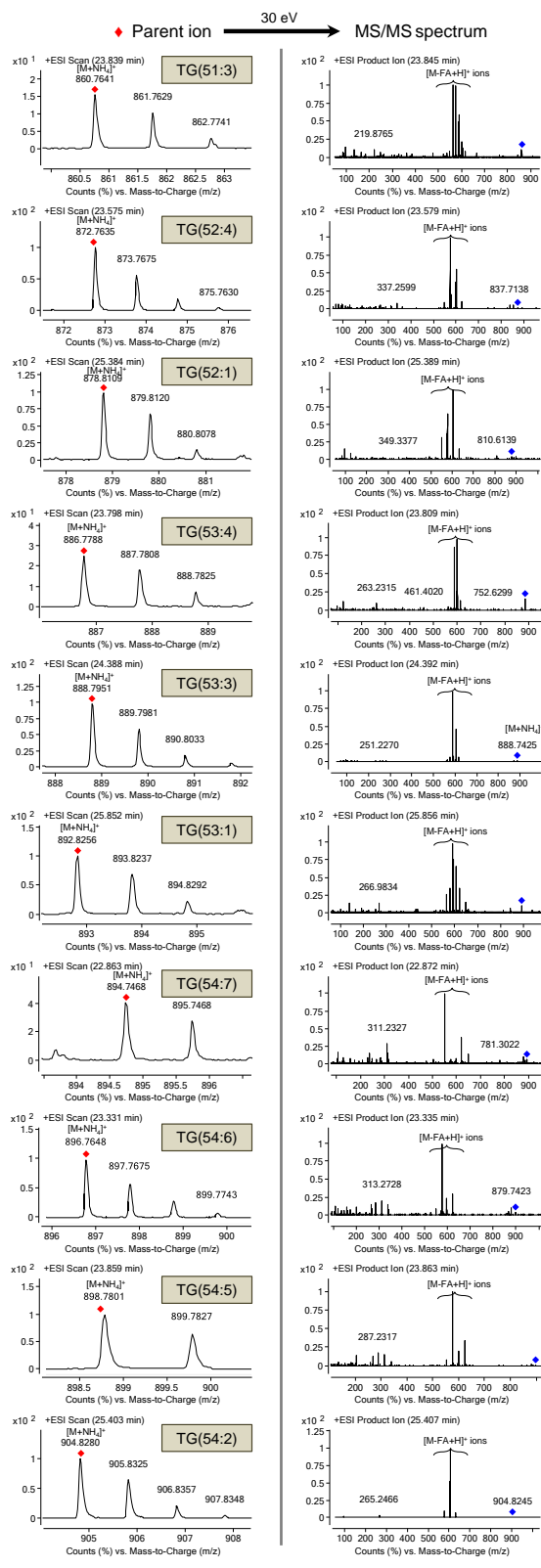
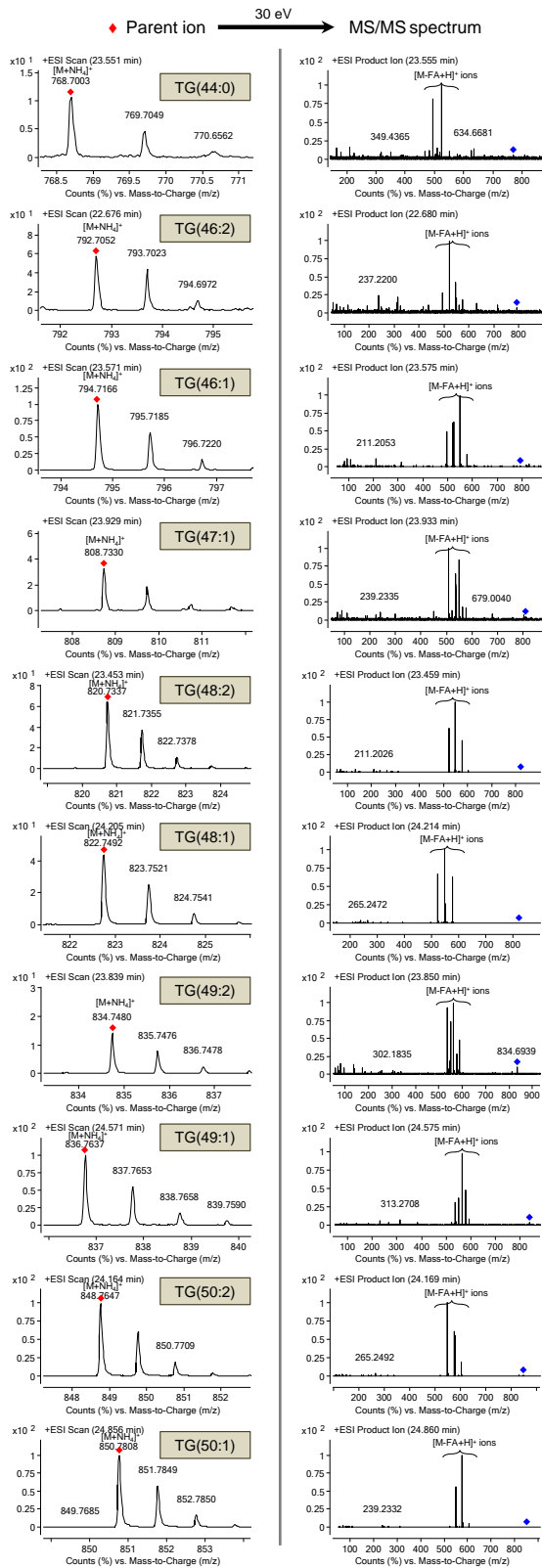
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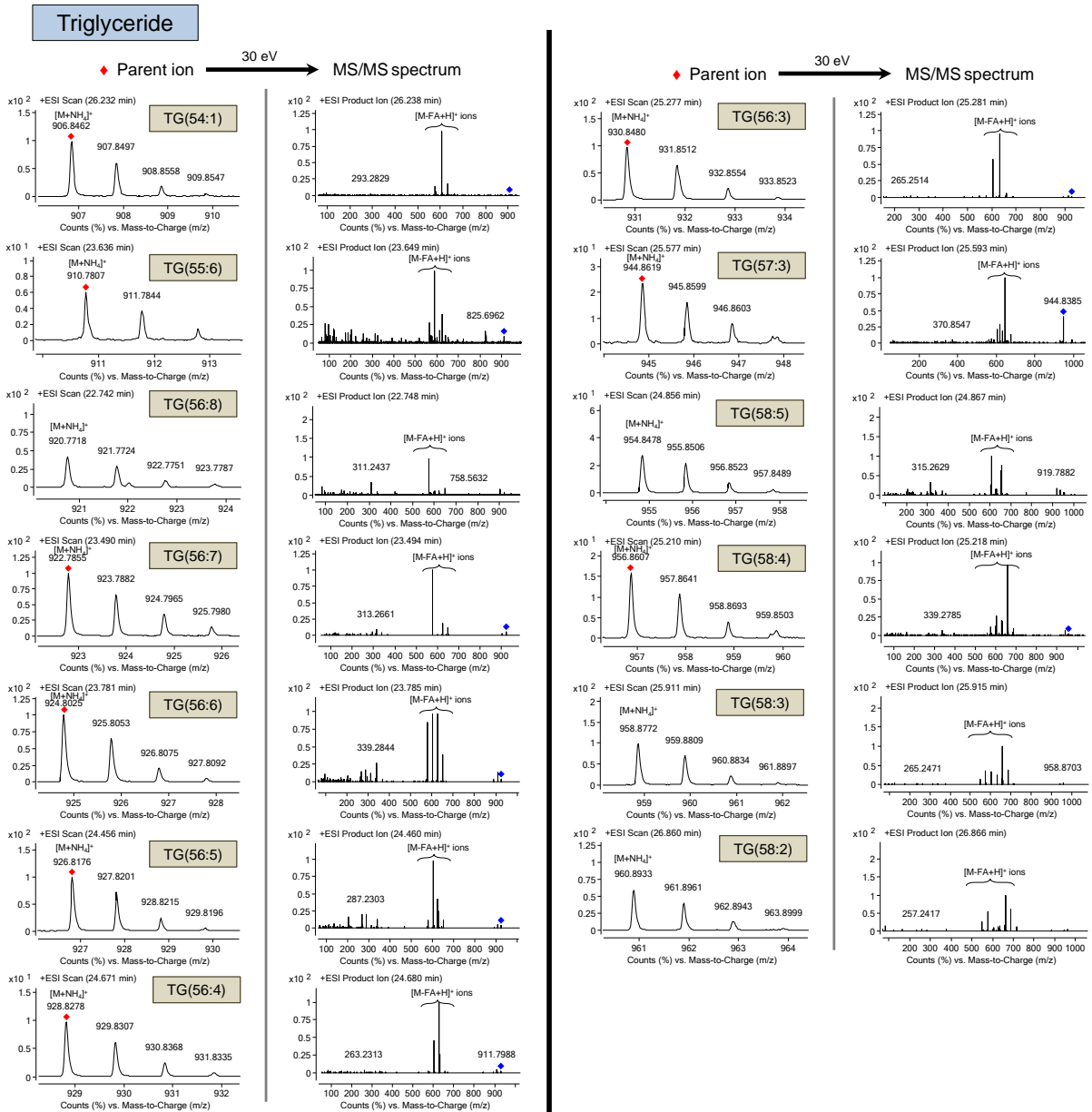
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### Triglyceride

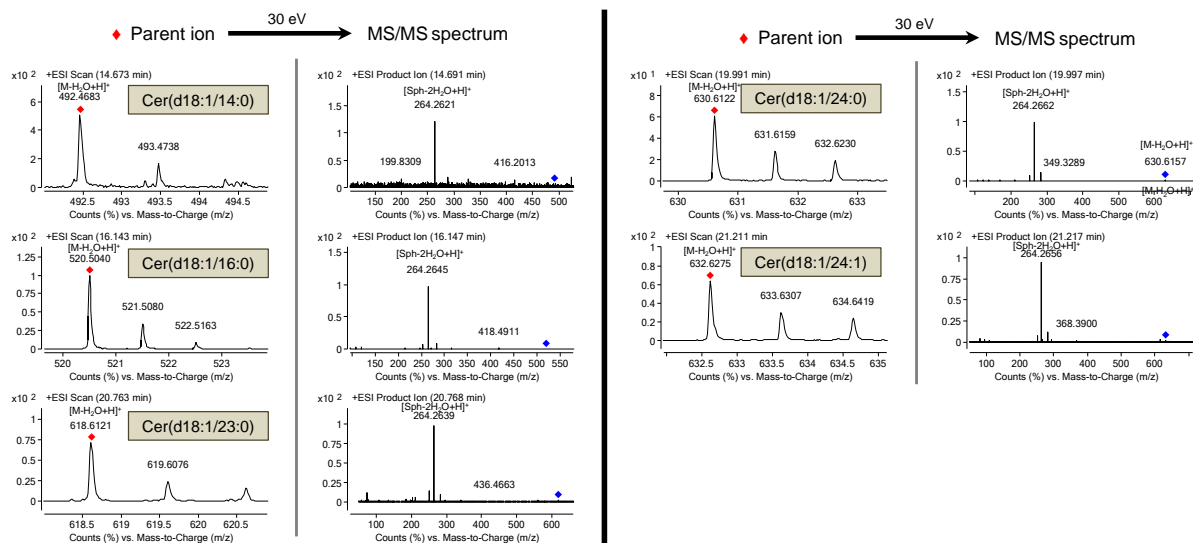


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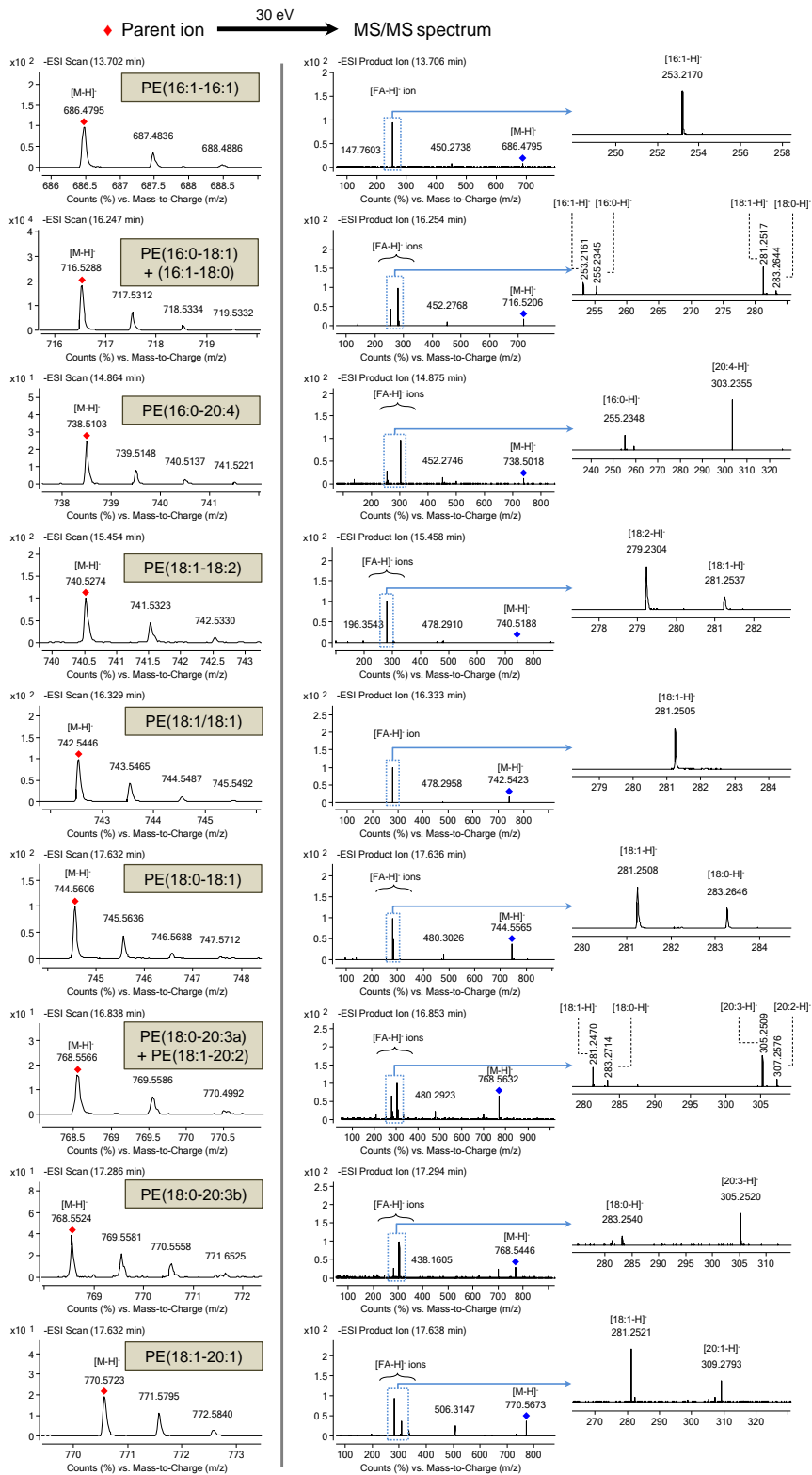
Continued

Ceramide



Continued

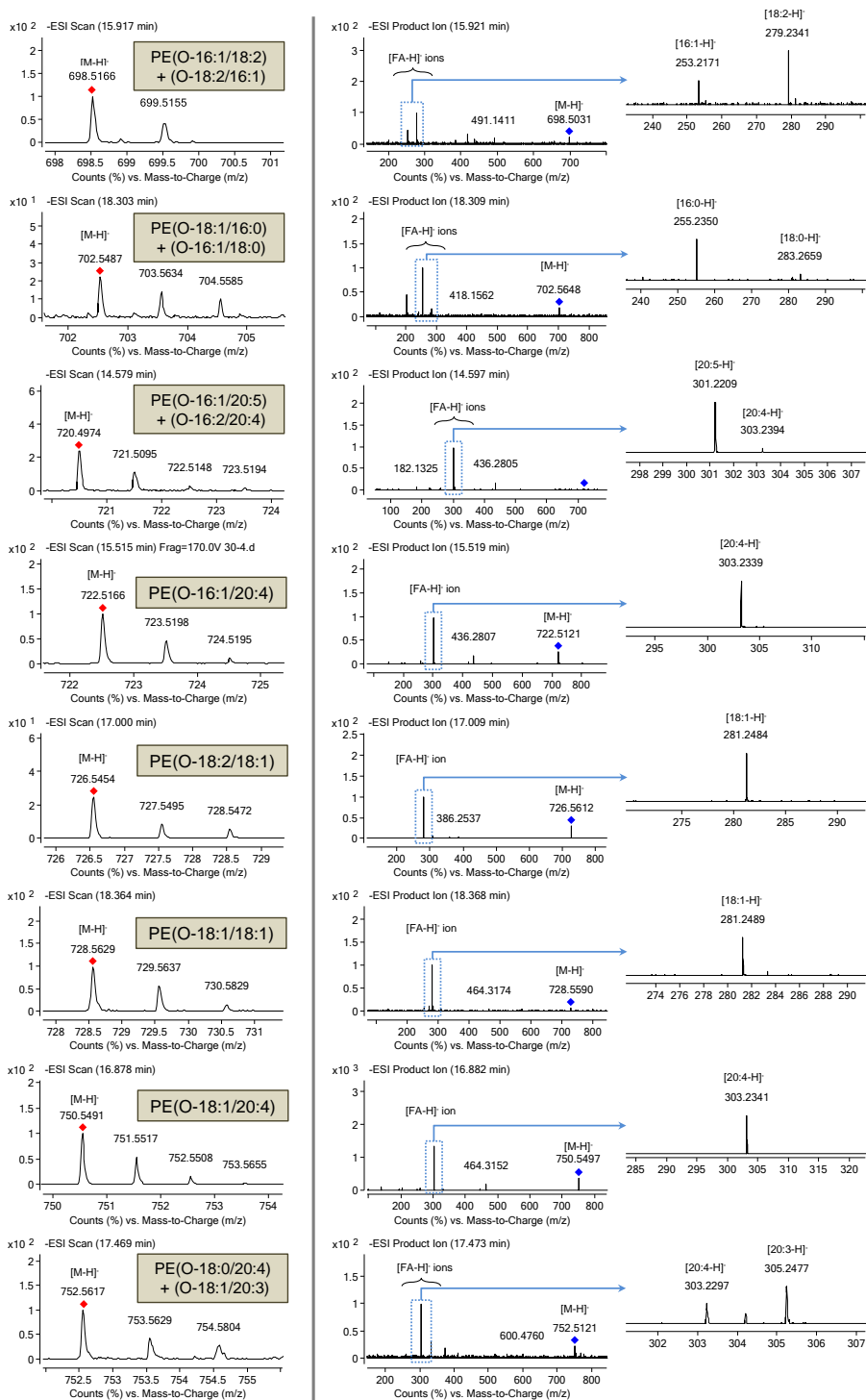
Phosphatidylethanolamine



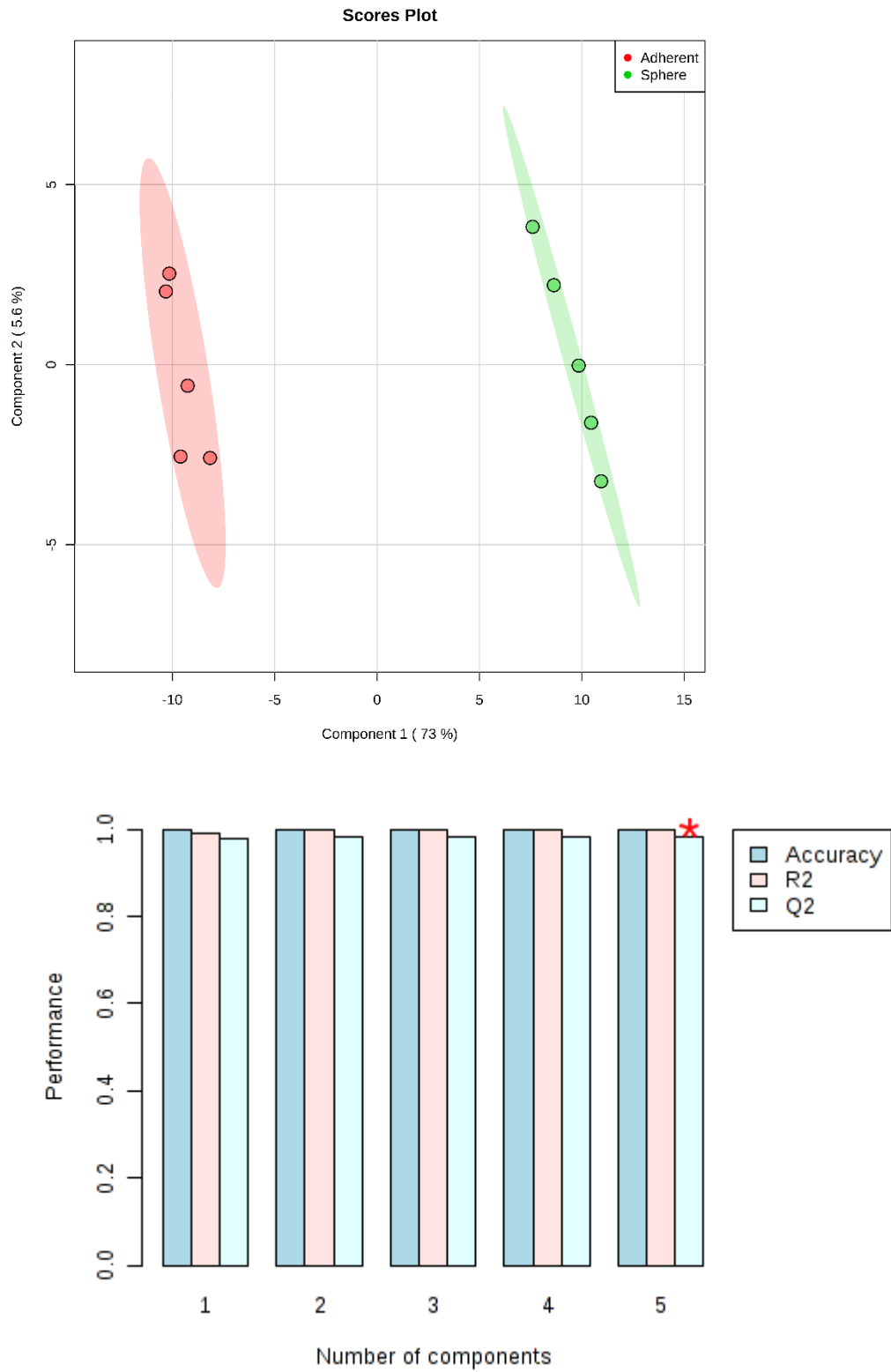
Continued

O-Phosphatidylethanolamine

Parent ion  $\xrightarrow{30\text{ eV}}$  MS/MS spectrum



Supplementary Figure 4. PLS-DA scores plot and cross-validation results.



## 1.2 Supplementary Table

**Supplementary Table 1.** Relative response factor (RRF) of 12 FAMES to internal standards.

<b>FAME</b>	<b>Target m/z</b>	<b>RRF (C17:0)</b>	<b>RRF (C23:0)</b>
C16:0	74	1.0	0.9
C16:1	55	0.3	0.3
C18:0	74	1.1	1.0
C18:1	55	0.4	0.4
C18:2	67	0.4	0.4
C20:0	74	1.1	1.0
C20:3n6	79	0.2	0.2
C20:4n6	79	0.3	0.3
C22:0	74	1.1	1.0
C22:5n3	79	0.5	0.4
C22:6n3	79	0.3	0.3
C24:0	74	1.1	1.0

**Supplementary Table 2.** Compositions of 123 lipid species and 8 lipid classes between adherent and sphere MCF-7 cells

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
14.61	[M-H <sub>2</sub> O+H] <sup>+</sup>	492.4743	492.4775	0.0032	Cer(d18:1/14:0)	0.00167	0.00194	0.00169	0.00114	0.00110	0.00339	0.00245	0.00591	0.00374	0.00517	0.001	0.003	1.5
16.19	[M-H <sub>2</sub> O+H] <sup>+</sup>	520.5038	520.5088	0.0050	Cer(d18:1/16:0)	0.00945	0.01131	0.00815	0.00129	0.00063	0.03684	0.00409	0.06244	0.02655	0.07032	0.032	0.060	2.7
20.90	[M-H <sub>2</sub> O+H] <sup>+</sup>	618.6132	618.6183	0.0051	Cer(d18:1/23:0)	0.00536	0.00581	0.00549	0.00285	0.00345	0.00272	0.00190	0.00425	0.00278	0.00400	0.097	0.159	-
21.45	[M-H <sub>2</sub> O+H] <sup>+</sup>	632.6293	632.6340	0.0047	Cer(d18:1/24:0)	0.05902	0.06273	0.05691	0.02865	0.03540	0.03919	0.02783	0.06531	0.04240	0.05759	0.855	0.899	-
20.19	[M-H <sub>2</sub> O+H] <sup>+</sup>	630.6133	630.6183	0.0050	Cer(d18:1/24:1)	0.16066	0.01247	0.16399	0.08106	0.09863	0.32302	0.22559	0.52945	0.34432	0.44763	0.014	0.032	1.9
7.45	[M+H] <sup>+</sup>	496.3407	496.3403	0.0004	LPC(16:0)	0.19220	0.20277	0.18155	0.10363	0.11453	0.10569	0.06916	0.67675	0.11160	0.14735	0.988	0.988	-
5.92	[M+H] <sup>+</sup>	494.3248	494.3241	0.0007	LPC(16:1)	0.02108	0.03124	0.02951	0.01686	0.01423	0.01730	0.01970	0.17548	0.02226	0.02827	0.385	0.493	-
8.92	[M+H] <sup>+</sup>	524.3723	524.3716	0.0007	LPC(18:0)	0.02687	0.02697	0.02832	0.01342	0.01633	0.01723	0.00787	0.07054	0.01157	0.01482	0.631	0.711	-
7.76	[M+H] <sup>+</sup>	522.3558	522.3559	0.0001	LPC(18:1)	0.10235	0.07614	0.12546	0.03804	0.04231	0.03356	0.05344	0.53650	0.08115	0.01906	0.986	0.988	-
9.07	[M+H] <sup>+</sup>	550.3875	550.3867	0.0008	LPC(20:1)	0.00557	0.00623	0.00688	0.00336	0.00367	0.00496	0.00372	0.03598	0.00556	0.00762	0.319	0.432	-
14.19	[M+H] <sup>+</sup>	706.5350	706.5387	0.0037	PC(14:0-16:0)	2.16198	2.17916	2.48730	1.28463	1.31154	1.15146	2.01159	1.87080	1.17333	1.74368	0.408	0.506	-
15.76	[M+H] <sup>+</sup>	734.5629	734.5700	0.0071	PC(16:0/16:0)	0.80140	0.05493	0.25559	0.13336	0.47603	0.03637	0.84165	0.03596	0.48875	0.05140	0.456	0.551	-
15.75	[M+H] <sup>+</sup>	760.5779	760.5856	0.0077	PC(16:0-18:1)	5.46140	5.46184	5.78045	3.24104	3.28987	3.34168	5.61236	5.28933	3.29846	4.86705	0.873	0.910	-
13.39	[M+H] <sup>+</sup>	730.5374	730.5387	0.0013	PC(16:1/16:1)	2.52199	2.53006	2.91783	1.40021	1.48999	3.07804	5.30833	5.15300	3.14254	4.70143	0.007	0.017	1.0
14.69	[M+H] <sup>+</sup>	758.5637	758.5700	0.0063	PC(16:1-18:1)	3.43603	3.44394	3.88446	2.07404	2.08145	3.52753	5.87264	5.59140	3.50381	5.23421	0.028	0.054	0.7
17.45	[M+H] <sup>+</sup>	788.6092	788.6169	0.0077	PC(18:0-18:1)	1.13062	1.14763	1.23598	0.61104	0.66149	0.71917	1.09575	1.01060	0.62620	0.83054	0.638	0.713	-
15.94	[M+H] <sup>+</sup>	786.5926	786.6013	0.0087	PC(18:1/18:1)	2.80195	2.79919	3.12470	1.68080	1.68865	2.42438	4.08792	3.90297	2.41918	3.61418	0.113	0.184	-

Continued

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
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14.90	[M+H] <sup>+</sup>	784.5795	784.5856	0.0061	PC(18:1-18:2)	0.36488	0.37788	0.29732	0.10491	0.22143	0.40334	0.66750	0.64102	0.39790	0.58482	0.021	0.043	1.0
13.01	[M+H] <sup>+</sup>	678.5082	678.5074	0.0008	PC(28:0)	1.12303	1.11086	1.28900	0.60543	0.66454	0.37878	0.66530	0.63385	0.38835	0.56964	0.018	0.037	-0.9
12.07	[M+H] <sup>+</sup>	676.4923	676.4917	0.0006	PC(28:1)	0.02278	0.02261	0.02416	0.01239	0.01331	0.01607	0.02862	0.02680	0.01743	0.02520	0.331	0.438	-
13.50	[M+H] <sup>+</sup>	692.5227	692.5230	0.0003	PC(29:0)	0.28121	0.28591	0.24798	0.15025	0.16512	0.04464	0.07605	0.07439	0.04324	0.06538	0.000	0.000	-1.9
13.09	[M+H] <sup>+</sup>	704.5225	704.5230	0.0005	PC(30:1)	3.07582	3.10765	3.59314	1.71382	1.83216	2.03719	1.70626	1.65806	0.95864	3.14094	0.172	0.262	-
12.33	[M+H] <sup>+</sup>	702.5068	702.5074	0.0006	PC(30:2)	0.01296	0.00826	0.01394	0.00461	0.00503	0.01377	0.02317	0.02314	0.01362	0.00761	0.080	0.134	-
14.50	[M+H] <sup>+</sup>	720.5482	720.5543	0.0061	PC(31:0)	0.07173	0.07094	0.08246	0.03931	0.04040	0.01333	0.02364	0.02146	0.01355	0.02070	0.000	0.001	-1.7
13.86	[M+H] <sup>+</sup>	718.5381	718.5387	0.0006	PC(31:1)	0.74423	0.74775	0.85697	0.40000	0.44169	0.18474	0.31441	0.31012	0.18032	0.27129	0.002	0.005	-1.3
14.42	[M+H] <sup>+</sup>	732.5495	732.5543	0.0048	PC(32:1)	6.63621	6.58136	4.37350	3.96673	3.97177	3.97459	6.89162	6.47826	4.08633	6.10506	0.657	0.721	-
16.28	[M+H] <sup>+</sup>	748.5767	748.5856	0.0089	PC(33:0)	0.12553	0.13291	0.14833	0.07419	0.07696	0.02570	0.04401	0.04164	0.02542	0.03844	0.000	0.001	-1.7
13.71	[M+H] <sup>+</sup>	756.5512	756.5543	0.0031	PC(34:3)	0.31215	0.31235	0.35567	0.17228	0.18433	0.41337	0.22502	0.68097	0.41422	0.61000	0.061	0.107	-
13.12	[M+H] <sup>+</sup>	754.5351	754.5387	0.0036	PC(34:4)	0.17122	0.16812	0.17926	0.00580	0.10284	0.06301	0.10947	0.10386	0.06656	0.09600	0.909	0.939	-
16.54	[M+H] <sup>+</sup>	774.5921	774.6013	0.0092	PC(35:1)	0.44207	0.01561	0.42758	0.24771	0.26100	0.11790	0.19884	0.00216	0.11540	0.16807	0.346	0.448	-
14.38	[M+H] <sup>+</sup>	782.5633	782.5700	0.0067	PC(36:4)	0.15409	0.18483	0.30790	0.10926	0.17849	0.05300	0.07499	0.07395	0.04720	0.06816	0.001	0.002	-1.6
13.48	[M+H] <sup>+</sup>	780.5510	780.5543	0.0033	PC(36:5)	0.22301	0.22138	0.23340	0.11779	0.13212	0.01235	0.02903	0.01329	0.00752	0.02524	0.000	0.000	-3.4
17.90	[M+H] <sup>+</sup>	802.6247	802.6326	0.0079	PC(37:1)	0.03246	0.00287	0.02888	0.01747	0.01939	0.01257	0.02087	0.02014	0.01187	0.01704	0.946	0.962	-
16.86	[M+H] <sup>+</sup>	800.6184	800.6169	0.0015	PC(37:2)	0.00884	0.00816	0.00839	0.00442	0.00478	0.00220	0.00338	0.00339	0.00198	0.00282	0.001	0.004	-1.3
17.44	[M+H] <sup>+</sup>	814.6244	814.6326	0.0082	PC(38:2)	0.48481	0.49892	0.55030	0.26667	0.28083	0.42130	0.72585	0.68260	0.41120	0.58720	0.135	0.213	-
17.26	[M+H] <sup>+</sup>	812.6188	812.6169	0.0019	PC(38:3)	0.00056	0.00008	0.00029	0.00112	0.00165	0.00024	0.00033	0.00055	0.00035	0.00038	0.643	0.713	-
15.26	[M+H] <sup>+</sup>	810.5932	810.6013	0.0081	PC(38:4)	0.07182	0.07407	0.08435	0.03965	0.04294	0.01549	0.02945	0.02134	0.01051	0.02490	0.001	0.004	-1.6

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RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
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14.51	[M+H] <sup>+</sup>	808.5786	808.5856	0.0070	PC(38:5)	0.27334	0.27605	0.14845	0.16256	0.17030	0.03184	0.03491	0.03318	0.02162	0.00482	0.000	0.002	-3.0
14.27	[M+H] <sup>+</sup>	806.5653	806.5700	0.0047	PC(38:6)	0.27442	0.28386	0.07520	0.16141	0.17299	0.04481	0.02427	0.02064	0.01416	0.01943	0.000	0.001	-3.0
12.93	[M+H] <sup>+</sup>	804.5537	804.5543	0.0006	PC(38:7)	0.05255	0.05141	0.05240	0.02748	0.03112	0.00075	0.00088	0.00084	0.00069	0.00089	0.000	0.000	-5.7
18.73	[M+H] <sup>+</sup>	842.6583	842.6639	0.0056	PC(40:2)	0.05588	0.05433	0.06286	0.02902	0.03206	0.03076	0.05786	0.04698	0.01701	0.04850	0.505	0.592	-
15.00	[M+H] <sup>+</sup>	834.5932	834.6007	0.0075	PC(40:6)	0.00817	0.06760	0.02489	0.03876	0.04180	0.00796	0.00603	0.00568	0.00358	0.00494	0.002	0.006	-2.7
14.16	[M+H] <sup>+</sup>	832.5781	832.5856	0.0075	PC(40:7)	0.19792	0.20078	0.21840	0.11735	0.12565	0.00442	0.00615	0.00600	0.00404	0.00546	0.000	0.000	-5.0
13.26	[M+H] <sup>+</sup>	830.5673	830.5700	0.0027	PC(40:8)	0.00833	0.00816	0.00853	0.00432	0.00504	0.00028	0.00025	0.00023	0.00016	0.00024	0.000	0.000	-4.9
20.15	[M+H] <sup>+</sup>	870.6890	870.6952	0.0062	PC(42:2)	0.04958	0.02368	0.05744	0.00557	0.01223	0.02040	0.03646	0.03566	0.02060	0.03100	0.583	0.670	-
14.10	[M+H] <sup>+</sup>	858.5955	858.6013	0.0058	PC(42:8)	0.00153	0.00166	0.00186	0.00098	0.00105	0.00004	0.00006	0.00004	0.00004	0.00004	0.000	0.000	-5.1
13.87	[M+H] <sup>+</sup>	664.5246	664.5281	0.0035	PC(O-28:0)	0.00294	0.00269	0.00296	0.00155	0.00165	0.00023	0.00018	0.00029	0.00018	0.00020	0.000	0.000	-3.4
14.32	[M+H] <sup>+</sup>	678.5391	678.5437	0.0046	PC(O-29:0)	0.00011	0.00005	0.00006	0.00008	0.00005	0.00001	0.00001	0.00001	0.00000	0.00001	0.000	0.000	-3.4
16.80	[M+H] <sup>+</sup>	720.5817	720.5907	0.0090	PC(O-32:0)	0.00368	0.00405	0.00417	0.00198	0.00187	0.00001	0.00001	0.00000	0.00000	0.00000	0.000	0.000	-9.2
18.96	[M+H] <sup>+</sup>	748.6139	748.6220	0.0081	PC(O-34:0)	0.00001	0.00004	0.00007	0.00004	0.00003	0.00000	0.00002	0.00000	0.00000	0.00000	0.002	0.006	-2.9
14.99	[M+H] <sup>+</sup>	818.5976	818.6063	0.0087	PC(O-40:7)	0.00001	0.00013	0.00001	0.00001	0.00000	0.00004	0.00007	0.00006	0.00001	0.00007	0.179	0.266	-
16.13	[M-H] <sup>-</sup>	716.5264	716.5236	0.0028	PE(16:0-18:1) + PE(16:1-18:0)	13.21690	14.10126	13.44505	16.44676	16.23264	13.41940	10.69481	10.58532	13.49184	11.13568	0.017	0.037	-0.3
14.72	[M-H] <sup>-</sup>	738.5118	738.5079	0.0039	PE(16:0-20:4)	3.09952	3.24912	3.22666	3.92056	4.88500	0.60325	0.54020	0.49326	0.64993	0.51478	0.000	0.000	-2.7
13.61	[M-H] <sup>-</sup>	686.4800	686.4766	0.0034	PE(16:1/16:1)	1.02441	1.08415	1.08109	1.31304	1.29848	3.98628	3.23333	3.22992	4.11097	3.58447	0.000	0.000	1.6
17.68	[M-H] <sup>-</sup>	744.5607	744.5549	0.0058	PE(18:0-18:1)	7.98581	8.55515	8.17684	10.23152	10.03026	5.86195	4.40386	4.75740	5.74619	4.95021	0.000	0.000	-0.8
16.72	[M-H] <sup>-</sup>	768.5532	768.5549	0.0017	PE(18:0-20:3a) + PE(18:1-20:2)	0.08436	0.11130	1.05899	1.31300	1.33355	0.81477	0.62209	0.64817	0.82844	0.68698	0.471	0.557	-

Continued

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
17.34	[M-H]-	768.5532	768.5549	0.0017	PE(18:0-20:3b)	0.06930	0.07698	0.07018	0.09708	0.09792	0.04389	0.03297	0.03105	0.06088	0.03023	0.001	0.004	-1.0
16.23	[M-H]-	742.5436	742.5392	0.0044	PE(18:1/18:1)	31.72315	33.26521	31.88965	39.58231	38.75855	43.99649	34.22331	34.20096	43.73264	35.94998	0.265	0.366	-
15.27	[M-H]-	740.5261	740.5236	0.0025	PE(18:1-18:2)	1.92500	2.04723	1.94159	2.48635	2.38994	4.02262	3.05577	3.19018	4.07979	3.33188	0.000	0.001	0.7
17.60	[M-H]-	770.5724	770.5705	0.0019	PE(18:1-20:1)	1.21455	1.24884	1.23018	1.56091	1.50480	1.66392	1.21500	1.35181	1.61687	1.41359	0.398	0.500	-
15.79	[M-H]-	698.5130	698.5130	0.0000	PE(O-16:1/18:2) + PE(O-18:2/16:1)	0.29855	0.32173	0.30084	0.35761	0.35229	0.00274	0.00103	0.00179	0.00210	0.00106	0.000	0.000	-7.5
15.42	[M-H]-	722.5090	722.5130	0.0040	PE(O-16:1/20:4)	0.29389	0.32051	0.32356	0.36104	0.36326	0.00123	0.00058	0.00000	0.00000	0.00000	0.000	0.001	-9.8
14.47	[M-H]-	720.4927	720.4974	0.0047	PE(O-16:1/20:5) + PE(O-16:2/20:4)	0.08567	0.09986	0.09263	0.11287	0.11259	0.00032	0.00045	0.00111	0.00105	0.00056	0.000	0.000	-7.2
17.41	[M-H]-	752.5647	752.5600	0.0047	PE(O-18:0/20:4) + PE(O-18:1/20:3)	0.01001	0.00893	0.00967	0.01282	0.01069	0.00000	0.00000	0.00000	0.00000	0.00000	0.000	0.000	-13.5
18.42	[M-H]-	702.5471	702.5443	0.0028	PE(O-18:1/16:0) + PE(O-16:1/18:0)	0.00342	0.00562	0.00666	0.00745	0.00782	0.00000	0.00000	0.00000	0.00000	0.00000	0.000	0.000	-12.8
18.36	[M-H]-	728.5645	728.5600	0.0045	PE(O-18:1/18:1)	0.17620	0.18249	0.17638	0.22111	0.21323	0.00000	0.00025	0.00000	0.00000	0.00000	0.000	0.000	-11.9
16.77	[M-H]-	750.5482	750.5443	0.0039	PE(O-18:1/20:4)	0.12248	0.13257	0.12698	0.15440	0.15093	0.01015	0.00906	0.00695	0.00922	0.00684	0.000	0.000	-4.0
17.05	[M-H]-	726.5482	726.5443	0.0039	PE(O-18:2/18:1)	0.15094	0.16083	0.15054	0.19008	0.18312	0.00000	0.00000	0.00000	0.00000	0.00000	0.000	0.000	-17.5
12.88	[M+H]+	675.5430	675.5422	0.0008	SM(d32:1)	0.05695	0.05742	0.06327	0.03211	0.03617	0.04267	0.07155	0.06822	0.04268	0.05997	0.395	0.500	-
14.90	[M+H]+	705.5843	705.5910	0.0067	SM(d34:0)	0.14815	0.13190	0.16216	0.08763	0.08717	0.08480	0.13759	0.12899	0.08128	0.11471	0.539	0.625	-
14.23	[M+H]+	703.5706	703.5754	0.0048	SM(d34:1)	1.52472	0.00729	0.06812	0.95107	0.00371	1.32378	2.30268	2.22549	1.39656	1.87768	0.034	0.062	1.8
13.08	[M+H]+	701.5537	701.5597	0.0060	SM(d34:2)	0.10222	0.10146	0.01772	0.05806	0.06443	0.02782	0.04372	0.04581	0.02695	0.03747	0.178	0.266	-
15.66	[M+H]+	731.6017	731.6067	0.0050	SM(d36:1)	0.00071	0.00053	0.00712	0.00275	0.00055	0.00049	0.00052	0.00057	0.00031	0.00045	0.080	0.134	-
18.89	[M+H]+	787.6612	787.6693	0.0081	SM(d40:1)	0.13361	0.13711	0.14789	0.06826	0.07705	0.05424	0.09095	0.08907	0.05460	0.04090	0.044	0.080	-0.8
20.29	[M+H]+	815.6939	815.7006	0.0067	SM(d42:1)	0.31877	0.32933	0.35327	0.16048	0.18182	0.07635	0.13333	0.13067	0.07738	0.09830	0.002	0.005	-1.4

Continued

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
18.69	[M+H] <sup>+</sup>	813.6772	813.6849	0.0077	SM(d42:2a)	1.04417	0.44401	1.17771	0.54382	0.60630	0.31388	1.47169	1.43009	0.86734	1.20765	0.457	0.551	-
19.78	[M+H] <sup>+</sup>	813.6790	813.6849	0.0059	SM(d42:2b)	0.01481	0.00568	0.01584	0.00748	0.00310	0.00937	0.01556	0.01520	0.00918	0.01261	0.230	0.330	-
21.81	[M+H] <sup>+</sup>	843.7227	843.7319	0.0092	SM(d44:1)	0.04404	0.04516	0.04557	0.01317	0.00931	0.00656	0.01101	0.01076	0.00662	0.00930	0.018	0.037	-1.8
20.16	[M+H] <sup>+</sup>	841.7089	841.7162	0.0073	SM(d44:2)	0.34294	0.34246	0.13121	0.16901	0.19248	0.10557	0.17726	0.17888	0.10525	0.10778	0.056	0.100	-
24.44	[M+NH4] <sup>+</sup>	796.7320	796.7394	0.0074	TG(14:0-16:0-16:0)	0.00273	0.00210	0.00195	0.00100	0.00112	0.00099	0.00071	0.00149	0.00125	0.00156	0.168	0.258	-
25.79	[M+NH4] <sup>+</sup>	852.7945	852.8020	0.0075	TG(16:0-16:0-18:0)	0.00140	0.00107	0.00094	0.00048	0.00049	0.00036	0.00024	0.00053	0.00041	0.00053	0.029	0.056	-1.1
26.63	[M+NH4] <sup>+</sup>	880.8262	880.8333	0.0071	TG(16:0-18:0-18:0)	0.00043	0.00033	0.00030	0.00016	0.00018	0.00013	0.00008	0.00021	0.00015	0.00023	0.070	0.121	-
24.86	[M+NH4] <sup>+</sup>	876.7915	876.8015	0.0100	TG(16:0-18:1-18:1)	0.11394	0.08614	0.08509	0.04249	0.04726	0.05157	0.03792	0.08039	0.06480	0.06850	0.469	0.557	-
22.89	[M+NH4] <sup>+</sup>	818.7166	818.7238	0.0072	TG(16:1/16:1/16:1) +TG(14:1-16:1-18:1)	0.00201	0.00156	0.00141	0.00071	0.00079	0.00737	0.00572	0.01168	0.00952	0.01037	0.000	0.000	2.8
23.59	[M+NH4] <sup>+</sup>	846.7481	846.7551	0.0070	TG(16:1-16:1-18:1)	0.02047	0.01579	0.01566	0.00734	0.00831	0.02912	0.02216	0.04599	0.03765	0.04084	0.003	0.008	1.4
24.22	[M+NH4] <sup>+</sup>	874.7792	874.7864	0.0072	TG(16:1-18:1-18:1)	0.06755	0.05120	0.05100	0.02568	0.02818	0.04983	0.03760	0.07949	0.06399	0.06849	0.192	0.278	-
24.80	[M+NH4] <sup>+</sup>	902.8091	902.8177	0.0086	TG(18:1/18:1/18:1)	0.08735	0.06767	0.06617	0.03336	0.03631	0.04284	0.03224	0.06838	0.05357	0.05858	0.694	0.755	-
24.21	[M+NH4] <sup>+</sup>	900.7945	900.8015	0.0070	TG(18:1-18:1-18:2)	0.00867	0.00630	0.00642	0.00242	0.00231	0.00594	0.00447	0.00936	0.00671	0.00818	0.235	0.332	-
23.83	[M+NH4] <sup>+</sup>	950.8079	950.8177	0.0098	TG(18:1-18:1-22:5)	0.00522	0.00409	0.00398	0.00180	0.00214	0.00008	0.00007	0.00013	0.00012	0.00012	0.000	0.000	-5.0
23.55	[M+NH4] <sup>+</sup>	948.7928	948.8020	0.0092	TG(18:1-18:1-22:6)	0.00396	0.00306	0.00305	0.00139	0.00163	0.00004	0.00002	0.00007	0.00004	0.00005	0.000	0.000	-5.8
23.76	[M+NH4] <sup>+</sup>	768.7026	768.7081	0.0055	TG(44:0)	0.00096	0.00070	0.00070	0.00031	0.00040	0.00037	0.00028	0.00058	0.00049	0.00055	0.329	0.438	-
23.67	[M+NH4] <sup>+</sup>	794.7172	794.7238	0.0066	TG(46:1)	0.00745	0.00581	0.00548	0.00253	0.00298	0.00423	0.00316	0.00642	0.00543	0.00576	0.747	0.792	-
22.91	[M+NH4] <sup>+</sup>	792.7018	792.7081	0.0063	TG(46:2)	0.00201	0.00160	0.00156	0.00050	0.00080	0.00427	0.00325	0.00647	0.00547	0.00577	0.001	0.003	2.0
24.02	[M+NH4] <sup>+</sup>	808.7324	808.7389	0.0065	TG(47:1)	0.00193	0.00155	0.00145	0.00069	0.00080	0.00043	0.00031	0.00063	0.00055	0.00071	0.009	0.020	-1.3

Continued

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
24.35	[M+NH4] <sup>+</sup>	822.7481	822.7551	0.0070	TG(48:1)	0.02432	0.01804	0.01745	0.00869	0.00971	0.01040	0.00778	0.01575	0.01301	0.01420	0.412	0.507	-
23.64	[M+NH4] <sup>+</sup>	820.7331	820.7394	0.0063	TG(48:2)	0.02251	0.01732	0.01704	0.00806	0.00919	0.01927	0.01472	0.02993	0.02492	0.02661	0.073	0.124	-
24.64	[M+NH4] <sup>+</sup>	836.7628	836.7707	0.0079	TG(49:1)	0.00403	0.00165	0.00294	0.00140	0.00161	0.00071	0.00052	0.00108	0.00088	0.00109	0.005	0.012	-1.4
23.96	[M+NH4] <sup>+</sup>	834.7477	834.7551	0.0074	TG(49:2)	0.00312	0.00252	0.00237	0.00107	0.00128	0.00067	0.00030	0.00103	0.00043	0.00101	0.008	0.018	-1.6
24.99	[M+NH4] <sup>+</sup>	850.7788	850.7864	0.0076	TG(50:1)	0.03185	0.02456	0.02312	0.01148	0.01289	0.01215	0.00895	0.01883	0.01497	0.01627	0.191	0.278	-
24.26	[M+NH4] <sup>+</sup>	848.7610	848.7707	0.0097	TG(50:2)	0.07637	0.05939	0.05706	0.02983	0.03227	0.04206	0.03213	0.06474	0.05345	0.05815	0.939	0.962	-
23.93	[M+NH4] <sup>+</sup>	860.7627	860.7707	0.0080	TG(51:3)	0.00202	0.00040	0.00155	0.00068	0.00083	0.00047	0.00034	0.00074	0.00056	0.00067	0.124	0.199	-
25.65	[M+NH4] <sup>+</sup>	878.8099	878.8177	0.0078	TG(52:1)	0.01259	0.00989	0.00881	0.00059	0.00475	0.00289	0.00207	0.00436	0.00337	0.00088	0.269	0.368	-
23.61	[M+NH4] <sup>+</sup>	872.7636	872.7707	0.0071	TG(52:4)	0.00395	0.00310	0.00304	0.00143	0.00162	0.00485	0.00367	0.00756	0.00624	0.00666	0.008	0.018	1.1
25.96	[M+NH4] <sup>+</sup>	892.8244	892.8333	0.0089	TG(53:1)	0.00088	0.00074	0.00068	0.00031	0.00038	0.00013	0.00010	0.00022	0.00016	0.00021	0.001	0.003	-1.9
24.52	[M+NH4] <sup>+</sup>	888.7934	888.8020	0.0086	TG(53:3)	0.00501	0.00395	0.00367	0.00171	0.00198	0.00078	0.00058	0.00106	0.00093	0.00097	0.001	0.002	-1.9
23.97	[M+NH4] <sup>+</sup>	886.7779	886.7864	0.0085	TG(53:4)	0.00059	0.00047	0.00045	0.00022	0.00026	0.00013	0.00008	0.00019	0.00015	0.00018	0.004	0.010	-1.4
26.41	[M+NH4] <sup>+</sup>	906.8408	906.8490	0.0082	TG(54:1)	0.00184	0.00140	0.00132	0.00064	0.00071	0.00046	0.00033	0.00072	0.00060	0.00063	0.019	0.040	-1.1
25.53	[M+NH4] <sup>+</sup>	904.8257	904.8333	0.0076	TG(54:2)	0.03542	0.02782	0.02541	0.01190	0.01347	0.00981	0.00720	0.01502	0.01165	0.01262	0.030	0.057	-1.0
23.72	[M+NH4] <sup>+</sup>	898.7780	898.7864	0.0084	TG(54:5)	0.00224	0.00178	0.00184	0.00083	0.00095	0.00096	0.00074	0.00148	0.00123	0.00138	0.344	0.448	-
23.32	[M+NH4] <sup>+</sup>	896.7615	896.7707	0.0092	TG(54:6)	0.00248	0.00194	0.00188	0.00086	0.00105	0.00011	0.00009	0.00016	0.00014	0.00017	0.000	0.000	-3.6
22.86	[M+NH4] <sup>+</sup>	894.7477	894.7551	0.0074	TG(54:7)	0.00142	0.00109	0.00088	0.00049	0.00060	0.00005	0.00004	0.00008	0.00005	0.00007	0.000	0.000	-3.9
23.60	[M+NH4] <sup>+</sup>	910.7780	910.7864	0.0084	TG(55:6)	0.00047	0.00037	0.00036	0.00017	0.00020	0.00001	0.00001	0.00002	0.00002	0.00002	0.000	0.000	-4.4
25.40	[M+NH4] <sup>+</sup>	930.8405	930.8490	0.0085	TG(56:3)	0.01601	0.01693	0.01607	0.00746	0.00840	0.00980	0.00745	0.01554	0.01175	0.01347	0.714	0.770	-

Continued

RT (min)	Adduct ion	row m/z	theo m/z	delta m/z	Lipids	Adherent_1	Adherent_2	Adherent_3	Adherent_4	Adherent_5	Sphere_1	Sphere_2	Sphere_3	Sphere_4	Sphere_5	p.value	FDR	log2(Fc)
24.78	[M+NH4] <sup>+</sup>	928.8242	928.8333	0.0091	TG(56:4)	0.00115	0.00205	0.00095	0.00042	0.00077	0.00105	0.00091	0.00234	0.00184	0.00130	0.238	0.332	-
24.45	[M+NH4] <sup>+</sup>	926.8090	926.8177	0.0087	TG(56:5)	0.00067	0.00088	0.00079	0.00050	0.00025	0.00008	0.00004	0.00004	0.00002	0.00004	0.000	0.000	-3.8
23.87	[M+NH4] <sup>+</sup>	924.7947	924.8020	0.0073	TG(56:6)	0.00567	0.00449	0.00427	0.00186	0.00227	0.00013	0.00010	0.00020	0.00014	0.00018	0.000	0.000	-4.6
23.44	[M+NH4] <sup>+</sup>	922.7785	922.7864	0.0079	TG(56:7)	0.00190	0.00128	0.00151	0.00065	0.00081	0.00004	0.00003	0.00006	0.00006	0.00007	0.000	0.000	-4.6
22.89	[M+NH4] <sup>+</sup>	920.7627	920.7702	0.0075	TG(56:8)	0.00111	0.00089	0.00089	0.00037	0.00046	0.00004	0.00002	0.00005	0.00004	0.00004	0.000	0.000	-4.3
25.69	[M+NH4] <sup>+</sup>	944.8554	944.8646	0.0092	TG(57:3)	0.00097	0.00080	0.00052	0.00032	0.00037	0.00024	0.00017	0.00037	0.00026	0.00034	0.021	0.043	-1.1
27.07	[M+NH4] <sup>+</sup>	960.8876	960.8954	0.0078	TG(58:2)	0.00429	0.00326	0.00325	0.00147	0.00172	0.00159	0.00113	0.00247	0.00185	0.00215	0.166	0.258	-
26.09	[M+NH4] <sup>+</sup>	958.8723	958.8797	0.0074	TG(58:3)	0.00584	0.00672	0.00319	0.00189	0.00355	0.00237	0.00196	0.00384	0.00386	0.00701	0.737	0.788	-
25.38	[M+NH4] <sup>+</sup>	956.8549	956.8646	0.0097	TG(58:4)	0.00211	0.00162	0.00159	0.00073	0.00083	0.00101	0.00077	0.00130	0.00125	0.00141	0.623	0.709	-
24.94	[M+NH4] <sup>+</sup>	954.8396	954.8484	0.0088	TG(58:5)	0.00034	0.00016	0.00021	0.00005	0.00010	0.00001	0.00003	0.00008	0.00004	0.00007	0.020	0.040	-1.9

**Supplementary Table 3.** Features with VIP scores of 1 or higher.

<b>Compound</b>	<b>VIP score</b>
PEO-18:2/18:1	2.7079
PEO-18:1/18:1	2.5836
PEO-16:1/20:4	2.4774
PEO-18:0/20:4 or PEO-18:1/20:3	2.2061
PEO-16:1/18:2 or PEO-18:2/16:1	2.0295
PEO-18:1/16:0 or PEO-16:1/18:0	2.0063
PEO-16:1/20:5 or PEO-16:2/20:4	1.858
PCO-40:7	1.6907
PCO-32:0	1.6645
TG16:1/16:1/16:1 or TG14:1-16:1-18:1	1.6344
PC38:7	1.576
PC40:7	1.5621
Cerd18:1/16:0	1.5064
TG46:2	1.4789
SMd34:1	1.4429
PCO-34:0	1.3865
PE16:0-20:4	1.3607
PEO-18:1/20:4	1.3074
PC40:8	1.2865
Cerd18:1/14:0	1.2788
TG16:1-16:1-18:1	1.2752
TG52:4	1.2535
TG16:0-18:0-18:0	1.2346
TG56:4	1.2043
PC36:5	1.1816
Cerd18:1/24:1	1.1571
TG18:1-18:1-22:6	1.1522
TG58:5	1.1468
TG18:1-18:1-22:5	1.1226
PCO-29:0	1.1206
TG44:0	1.1157
TG16:1-18:1-18:1	1.0977
PC3:02	1.0806
TG56:6	1.0746
TG48:2	1.0578
PE16:1/16:1	1.0553
TG53:4	1.0529
TG58:4	1.0286
TG18:1-18:1-18:2	1.0019

**Supplementary Table 4.** Altered genes involved in unsaturated fatty acid biosynthesis between adherent and sphere MCF-7 cells.

<b>Genes</b>	<b>Fold change</b>
<i>PTPLB</i>	-1.22
<i>PECR</i>	-0.96
<i>ELOVL2</i>	-0.63
<i>ACOT4</i>	-0.46
<i>ACOX1</i>	-0.24
<i>ACOT7</i>	-0.22
<i>ELOVL6</i>	0.2
<i>HADHA</i>	0.47
<i>FADS1</i>	0.8
<i>ACOX3</i>	0.84
<i>SCD</i>	1.88