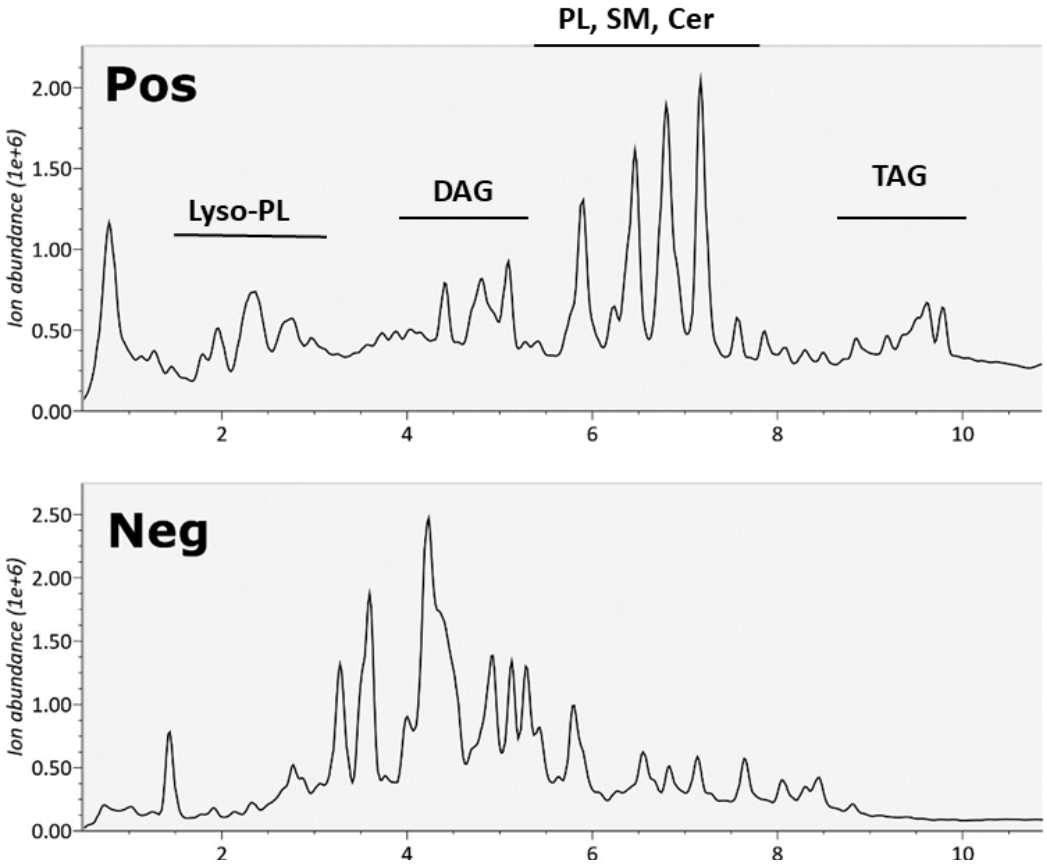
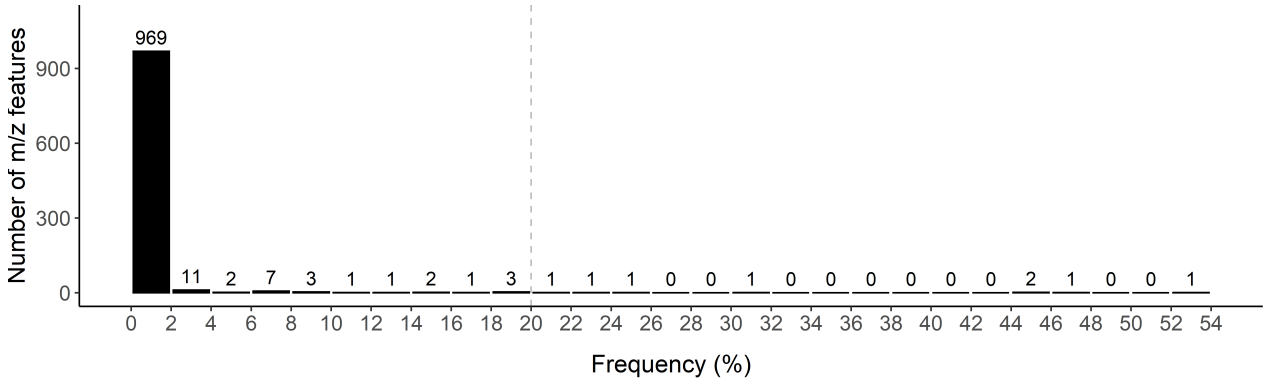
Supplementary Material

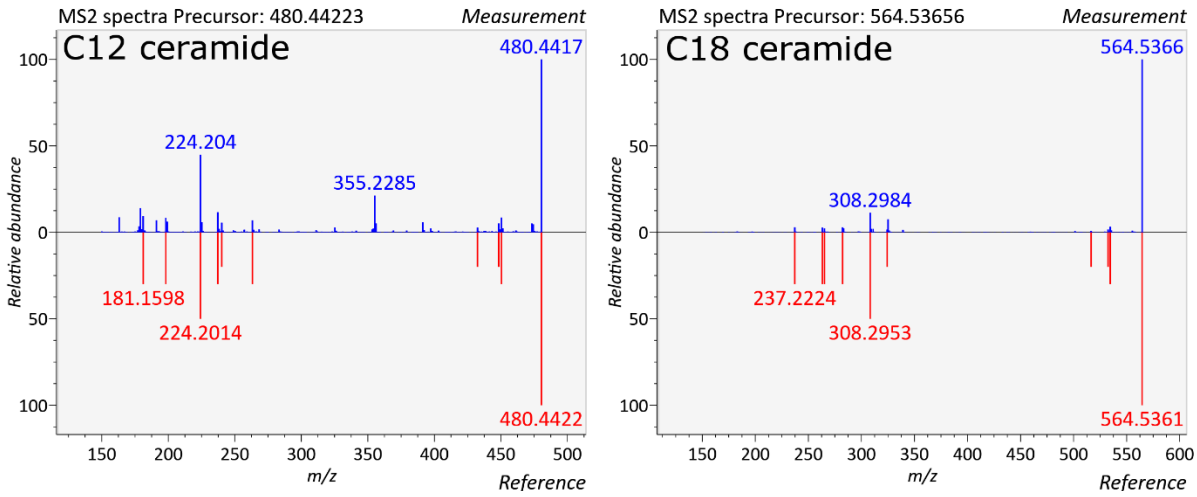
Cerebrospinal Fluid C18 Ceramide Associates with Markers of Alzheimer's Disease and Inflammation at the Pre- and Early Stages of Dementia



Supplementary Figure 1. Total ion chromatographs from CSF extracts, both in negative and positive mode. Labels show roughly the distribution of major lipid classes according to retention time. PL, phospholipids; SM, sphingomyelins; Cer, ceramides; DAG, diacylglycerols; TAG, triacylglycerols; Lyso-PL, lysophospholipids.



Supplementary Figure 2. Distribution of m/z features significantly distinguishing between CSF profiles (AD and non-AD), in both discovery and validation sets, after 1000 bootstrap replications. Vast majority (969 of 1008 features) did only distinguish between the profiles in 0-2% of the replications (870 in less than 1% and 99 in between 1-2%). Of the remaining features, 31 distinguished between the profiles in 2-20% of the replications and 8 in 20% of the replications or higher. The vertical dotted line presents the cut-off point for selection of features.



Supplementary Figure 3. Negative mode MS/MS (MS2) spectra of C12 and C18 ceramide standards as measured (Blue) compared to a spectral reference provided by LipidBlast library (Red). C12 ceramide was added to all samples as an internal standard, C18 ceramide was run separately.

Supplementary Table 1a. LipidBlast annotations of all measured m/z features in positive ionization mode

Average RT (min)	Feature/peak (m/z)	Annotated lipid species
4.12	330.2805	ACar 11:0; [M]+
3.39	328.2675	ACar 11:1; [M]+
1.72	356.2661	ACar 13:1; [M]+
4.33	384.3145	ACar 15:1; [M]+
1.91	382.3138	ACar 15:2; [M]+
8.51	412.3458	ACar 17:1; [M]+
5.46	410.3392	ACar 17:2; [M]+
3.73	408.3291	ACar 17:3; [M]+
6.81	454.3737	ACar 20:1; [M]+
5.53	444.2991	ACar 20:6; [M]+
6.56	470.422	ACar 21:0; [M]+
4.46	462.3705	ACar 21:4; [M]+
3.49	482.4069	ACar 22:1; [M]+
3.16	472.3647	ACar 22:6; [M]+
3.81	496.4225	ACar 23:1; [M]+
2.43	488.3601	ACar 23:5; [M]+
2.88	502.3761	ACar 24:5; [M]+
3.17	500.3621	ACar 24:6; [M]+
3.1	516.3904	ACar 25:5; [M]+
3.86	538.4984	ACar 26:1; [M]+
6.7	532.4372	ACar 26:4; [M]+
2.63	300.2366	ACar 9:1; [M]+
5.68	670.4631	BMP 27:0; BMP 5:0-22:0; [M+NH4]+
2.21	708.4869	BMP 30:2; BMP 14:1-16:1; [M+NH4]+
2.88	736.5172	BMP 32:2; BMP 13:1-19:1; [M+NH4]+
7.69	886.6542	BMP 43:4; BMP 23:0-20:4; [M+NH4]+
2.25	664.613	CE 18:3; [M+NH4]+
6.01	468.4431	Cer-NDS d29:1; Cer-NDS d15:0/14:1; [M+H]+
7.82	594.5826	Cer-NDS d38:1; Cer-NDS d22:0/16:1; [M+H]+
4.6	606.5599	Cer-NDS d39:2; Cer-NDS d19:0/20:2; [M+H]+
2.73	634.6001	Cer-NDS d41:2; Cer-NDS d21:0/20:2; [M+H]+
4.05	424.3601	Cer-NS d26:2; Cer-NS d14:1/12:1; [M+H]+
6.01	482.4583	Cer-NS d30:1; Cer-NS d18:1/12:0; [M+H]+
4.65	476.3901	Cer-NS d30:4; Cer-NS d14:3/16:1; [M+H]+
5.03	492.4216	Cer-NS d31:3; Cer-NS d15:1/16:2; [M+H]+
8.19	506.4733	Cer-NS d32:3; Cer-NS d14:3/18:0; [M+H]+
3.87	506.4607	Cer-NS d32:3; Cer-NS d17:3/15:0; [M+H]+
5.93	504.4403	Cer-NS d32:4; Cer-NS d17:3/15:1; [M+H]+
5.41	544.4728	Cer-NS d35:5; Cer-NS d15:3/20:2; [M+H]+
7.47	566.5524	Cer-NS d36:1; Cer-NS d20:1/16:0; [M+H]+
2.33	576.5523	Cer-NS d37:3; Cer-NS d21:1/16:2; [M+H]+
5.96	572.5032	Cer-NS d37:5; Cer-NS d15:3/22:2; [M+H]+
2.77	590.5693	Cer-NS d38:3; Cer-NS d25:3/13:0; [M+H]+
2.29	620.5825	Cer-NS d40:2; Cer-NS d21:1/19:1; [M+H]+
7.82	616.5629	Cer-NS d40:4; Cer-NS d20:3/20:1; [M+H]+
8.56	650.6429	Cer-NS d42:1; Cer-NS d19:1/23:0; [M+H]+
6.83	760.7443	Cer-NS d50:2; Cer-NS d15:2/35:0; [M+H]+
3.58	292.2317	DAG 11:0; DAG 5:0-6:0; [M+NH4]+
2.07	334.2782	DAG 14:0; DAG 6:0-8:0; [M+NH4]+
2.14	348.2934	DAG 15:0; DAG 5:0-10:0; [M+NH4]+
1.61	362.2707	DAG 16:0; DAG 6:0-10:0; [M+NH4]+
2.69	376.3246	DAG 17:0; DAG 7:0-10:0; [M+NH4]+
1.93	376.2858	DAG 17:0; DAG 8:0-9:0; [M+NH4]+

4.69	400.2915	DAG 19:2; DAG 2:0-17:2; [M+NH4]+
1.91	400.3239	DAG 19:2; DAG 3:0-16:2; [M+NH4]+
1.62	396.2929	DAG 19:4; DAG 3:0-16:4; [M+NH4]+
1.89	418.3344	DAG 20:0; DAG 5:0-15:0; [M+NH4]+
3.28	416.3544	DAG 20:1; DAG 6:0-14:1; [M+NH4]+
2.75	412.2878	DAG 20:3; DAG 2:0-18:3; [M+NH4]+
2.19	432.3497	DAG 21:0; DAG 9:0-12:0; [M+NH4]+
5.31	428.3221	DAG 21:2; DAG 5:0-16:2; [M+NH4]+
1.65	424.324	DAG 21:4; DAG 5:0-16:4; [M+NH4]+
4.96	452.3371	DAG 23:4; DAG 7:0-16:4; [M+NH4]+
3.06	468.3869	DAG 24:3; DAG 6:0-18:3; [M+NH4]+
2.84	464.3538	DAG 24:5; DAG 4:0-20:5; [M+NH4]+
4.15	484.416	DAG 25:2; DAG 9:0-16:2; [M+NH4]+
2.14	476.3177	DAG 25:6; DAG 3:0-22:6; [M+NH4]+
3.1	512.416	DAG 27:2; DAG 11:0-16:2; [M+NH4]+
4.11	510.438	DAG 27:3; DAG 7:0-20:3; [M+NH4]+
3.44	526.4323	DAG 28:2; DAG 14:1-14:1; [M+NH4]+
3.76	540.4475	DAG 29:2; DAG 13:0-16:2; [M+NH4]+
5.01	538.4621	DAG 29:3; DAG 7:0-22:3; [M+NH4]+
2.12	536.4103	DAG 29:4; DAG 13:1-16:3; [M+NH4]+
5.54	536.4109	DAG 29:4; DAG 5:0-24:4; [M+NH4]+
3.8	532.4153	DAG 29:6; DAG 7:0-22:6; [M+NH4]+
4.06	554.4628	DAG 30:2; DAG 14:1-16:1; [M+NH4]+
3.86	554.4572	DAG 30:2; DAG 6:0-24:2; [M+NH4]+
5.03	552.4813	DAG 30:3; DAG 8:0-22:3; [M+NH4]+
2.82	546.4022	DAG 30:6; DAG 8:0-22:6; [M+NH4]+
4.36	568.4781	DAG 31:2; DAG 15:1-16:1; [M+NH4]+
4.62	566.463	DAG 31:3; DAG 9:0-22:3; [M+NH4]+
3.06	560.4155	DAG 31:6; DAG 13:1-18:5; [M+NH4]+
4.98	596.5092	DAG 33:2; DAG 11:0-22:2; [M+NH4]+
6.06	612.5336	DAG 34:1; DAG 13:0-21:1; [M+NH4]+
6.31	604.5151	DAG 34:5; DAG 12:0-22:5; [M+NH4]+
4.53	600.4768	DAG 34:7; DAG 16:2-18:5; [M+NH4]+
5.63	620.5088	DAG 35:4; DAG 15:1-20:3; [M+NH4]+
3.66	628.4977	DAG 36:7; DAG 18:2-18:5; [M+NH4]+
6.15	648.5393	DAG 37:4; DAG 19:1-18:3; [M+NH4]+
4.25	656.5286	DAG 38:7; DAG 16:1-22:6; [M+NH4]+
5.22	656.5074	DAG 38:7; DAG 22:3-16:4; [M+NH4]+
4.5	654.5128	DAG 38:8; DAG 16:2-22:6; [M+NH4]+
5.31	668.5377	DAG 39:8; DAG 17:2-22:6; [M+NH4]+
4.85	684.5598	DAG 40:7; DAG 22:2-18:5; [M+NH4]+
4.34	682.5427	DAG 40:8; DAG 20:3-20:5; [M+NH4]+
6.6	696.5535	DAG 41:8; DAG 19:2-22:6; [M+NH4]+
2.64	722.6609	DAG 42:2; DAG 18:0-24:2; [M+NH4]+
5.34	708.5588	DAG 42:9; DAG 22:4-20:5; [M+NH4]+
7.29	724.6053	DAG 43:8; DAG 21:2-22:6; [M+NH4]+
6.39	732.5512	DAG 44:11; DAG 22:5-22:6; [M+NH4]+
6.02	736.5986	DAG 44:9; DAG 24:4-20:5; [M+NH4]+
7.19	762.5958	DAG 46:10; DAG 24:4-22:6; [M+NH4]+
7.91	792.6667	DAG 48:9; DAG 26:4-22:5; [M+NH4]+
4.84	413.2693	Dioctyl phthalate (also known as the production of plastic)
6.31	744.6244	HexCer-NDS d37:0; HexCer-NDS d21:0/16:0; [M+H]+
3.35	614.4825	HexCer-NS d28:2; HexCer-NS d16:1/12:1; [M+H]+
6.74	644.5001	HexCer-NS d30:1; HexCer-NS d16:1/14:0; [M+H]+
3.96	642.5135	HexCer-NS d30:2; HexCer-NS d18:1/12:1; [M+H]+
2.25	664.4615	HexCer-NS d32:5; HexCer-NS d14:3/18:2; [M+H]+

2.68	678.478	HexCer-NS d33:5; HexCer-NS d15:3/18:2; [M+H]+
8.57	754.631	HexCer-NS d38:2; HexCer-NS d14:1/24:1; [M+H]+
8.66	1084.9532	HexCer-NS d62:5; HexCer-NS d26:3/36:2; [M+H]+
1.72	434.2415	LPC 10:0; [M+Na]+
3.41	426.2667	LPC 11:0(SN2); [M+H]+
4.61	440.2678	LPC 12:0(SN2); [M+H]+
4.16	482.3297	LPC 15:0(SN2); [M+H]+
4.93	480.2951	LPC 15:1(SN2); [M+H]+
3.26	496.3411	LPC 16:0(SN2); [M+H]+
1.67	494.3277	LPC 16:1(SN2); [M+H]+
4.69	510.3595	LPC 17:0(SN2); [M+H]+
4.28	508.3435	LPC 17:1(SN2); [M+H]+
3.88	506.3289	LPC 17:2(SN2); [M+H]+
3.64	524.3748	LPC 18:0(SN2); [M+H]+
4.43	529.408	LPC 18:1(d7); [M+H]+
3.21	534.3411	LPC 19:2(SN2); [M+H]+
3.04	588.4109	LPC 21:0; [M+Na]+
3.53	578.4047	LPC 22:1(SN2); [M+H]+
2.33	576.4109	LPC 22:2(SN2); [M+H]+
3	604.4413	LPC 24:2(SN2); [M+H]+
3.07	600.4105	LPC 24:4(SN2); [M+H]+
4.99	420.2201	LPC 9:0; [M+Na]+
2.75	356.2258	LPE 10:0e; [M+H]+
2.45	384.2568	LPE 12:0e; [M+H]+
2.76	398.2721	LPE 13:0e; [M+H]+
1.91	440.3159	LPE 16:0e; [M+H]+
4.35	450.2462	LPE 16:2; [M+H]+
2.75	434.2691	LPE 16:3e; [M+H]+
3.16	468.3092	LPE 17:0; [M+H]+
3.3	468.3336	LPE 18:0e; [M+H]+
3.49	487.3626	LPE 18:1(d7); [M+H]+
4.99	476.2818	LPE 18:3; [M+H]+
5.75	482.365	LPE 19:0e; [M+H]+
5.64	494.364	LPE 20:1e; [M+H]+
3.3	490.3154	LPE 20:3e; [M+H]+
3.4	538.3901	LPE 22:0; [M+H]+
4.71	532.3436	LPE 22:3; [M+H]+
3.88	528.3094	LPE 22:5; [M+H]+
6.75	550.4262	LPE 24:1e; [M+H]+
3.13	544.3851	LPE 24:4e; [M+H]+
3.88	580.4359	LPE 25:0; [M+H]+
6.71	566.4569	LPE 25:0e; [M+H]+
7.22	594.4876	LPE 27:0e; [M+H]+
2.41	306.2837	MAG 13:0; [M+NH4]+
4.71	320.2964	MAG 14:0; [M+NH4]+
4.51	334.3143	MAG 15:0; [M+NH4]+
4.54	332.2967	MAG 15:1; [M+NH4]+
3.14	348.291	MAG 16:0; [M+NH4]+
2.41	346.2756	MAG 16:1; [M+NH4]+
4.21	342.2504	MAG 16:3; [M+NH4]+
2.6	340.2676	MAG 16:4; [M+NH4]+
3.08	362.3088	MAG 17:0; [M+NH4]+
4.26	358.3139	MAG 17:2; [M+NH4]+
5.57	376.3585	MAG 18:0; [M+NH4]+
4.26	381.3511	MAG 18:1(d7); [M+NH4]+
4.85	370.2812	MAG 18:3; [M+NH4]+

6.4	390.3738	MAG 19:0; [M+NH4]+
6.95	418.4045	MAG 21:0; [M+NH4]+
5.61	422.345	MAG 22:5; [M+NH4]+
5.92	446.4379	MAG 23:0; [M+NH4]+
2.75	180.107	MAG 4:0; [M+NH4]+
1.89	236.1694	MAG 8:0; [M+NH4]+
3.16	462.2151	PC 11:0; PC 4:0-7:0; [M+Na]+
3.46	476.2308	PC 12:0; PC 5:0-7:0; [M+Na]+
4.15	538.3902	PC 19:0e; PC 14:0e/5:0; [M+H]+
4.87	548.3204	PC 19:2; PC 3:0-16:2; [M+H]+
4.06	564.3719	PC 20:1; PC 2:0-18:1; [M+H]+
3.61	564.373	PC 20:1; PC 5:0-15:1; [M+H]+
5.69	590.3658	PC 22:2; PC 2:0-20:2; [M+H]+
4.36	592.4362	PC 23:1e; PC 14:1e/9:0; [M+H]+
3.44	622.4301	PC 24:0; PC 11:0-13:0; [M+H]+
2.29	620.4363	PC 24:1; PC 11:0-13:1; [M+H]+
2.73	634.4525	PC 25:1; PC 10:0-15:1; [M+H]+
2.98	632.4365	PC 25:2; PC 6:0-19:2; [M+H]+
6.25	632.43	PC 25:2; PC 8:0-17:2; [M+H]+
2.96	648.4661	PC 26:1; PC 12:0-14:1; [M+H]+
5.18	660.4972	PC 28:2e; PC 16:2e/12:0; [M+H]+
6.28	706.5356	PC 30:0; PC 15:0-15:0; [M+H]+
3.27	702.5328	PC 31:2e; PC 14:1e/17:1; [M+H]+
3.28	710.4811	PC 31:5; PC 15:1-16:4; [M+H]+
7.21	708.5081	PC 32:6e; PC 14:1e/18:5; [M+H]+
6.65	784.5828	PC 34:0; PC 12:0-22:0; [M+Na]+
6.48	782.5665	PC 34:1; PC 18:0-16:1; [M+Na]+
7.09	746.6017	PC 34:1e; PC 14:0e/20:1; [M+H]+
6.52	758.5668	PC 34:2; PC 10:0-24:2; [M+H]+
7.06	744.5869	PC 34:2e; PC 14:0e/20:2; [M+H]+
4.16	744.5804	PC 34:2e; PC 14:1e/20:1; [M+H]+
6.76	756.5488	PC 34:3; PC 18:0-16:3; [M+H]+
6.41	754.5337	PC 34:4; PC 17:2-17:2; [M+H]+
2.17	752.5128	PC 34:5; PC 16:0-18:5; [M+H]+
4.26	770.5947	PC 35:3; PC 15:1-20:2; [M+H]+
2.61	766.5291	PC 35:5; PC 17:1-18:4; [M+H]+
3.54	752.5598	PC 35:5e; PC 18:3e/17:2; [M+H]+
7.09	812.6159	PC 36:0; PC 12:0-24:0; [M+Na]+
4.12	788.6062	PC 36:1; PC 10:0-26:1; [M+H]+
6.91	810.5982	PC 36:1; PC 10:0-26:1; [M+Na]+
4.75	772.6116	PC 36:2e; PC 14:1e/22:1; [M+H]+
6.84	782.5642	PC 36:4; PC 18:2-18:2; [M+H]+
6.77	768.5869	PC 36:4e; PC 14:0e/22:4; [M+H]+
6.18	780.5516	PC 36:5; PC 18:0-18:5; [M+H]+
6.44	780.5506	PC 36:5; PC 20:2-16:3; [M+H]+
6.71	766.5721	PC 36:5e; PC 18:0e/18:5; [M+H]+
6.62	804.6611	PC 37:0; PC 16:0-21:0; [M+H]+
7.22	776.5559	PC 37:7e; PC 18:5e/19:2; [M+H]+
4.7	816.6381	PC 38:1; PC 17:0-21:1; [M+H]+
3.7	810.6019	PC 38:4; PC 18:1-20:3; [M+H]+
7.16	810.5968	PC 38:4; PC 19:2-19:2; [M+H]+
6.45	796.6216	PC 38:4e; PC 14:0e/24:4; [M+H]+
6.8	794.6022	PC 38:5e; PC 16:0e/22:5; [M+H]+
6.4	806.5672	PC 38:6; PC 16:2-22:4; [M+H]+
6.6	806.566	PC 38:6; PC 18:3-20:3; [M+H]+
6.76	792.5862	PC 38:6e; PC 16:0e/22:6; [M+H]+

6.5	804.5497	PC 38:7; PC 18:2-20:5; [M+H]+
7.75	832.6656	PC 39:0; PC 15:0-24:0; [M+H]+
3.08	842.5604	PC 39:6; PC 17:1-22:5; [M+Na]+
2.57	810.5549	PC 40:11e; PC 18:5e/22:6; [M+H]+
6.84	834.5987	PC 40:6; PC 20:3-20:3; [M+H]+
6.95	832.5811	PC 40:7; PC 16:3-24:4; [M+H]+
6.5	832.5827	PC 40:7; PC 18:2-22:5; [M+H]+
6.43	828.5494	PC 40:9; PC 18:3-22:6; [M+H]+
4.08	832.6329	PC 41:7e; PC 20:5e/21:2; [M+H]+
2.54	854.5814	PC 42:10; PC 20:5-22:5; [M+H]+
7.03	864.6849	PC 43:5e; PC 18:5e/25:0; [M+H]+
4.04	876.6595	PC 43:6; PC 21:1-22:5; [M+H]+
4.65	860.6649	PC 43:7e; PC 22:5e/21:2; [M+H]+
3.8	890.6583	PC 44:6; PC 20:2-24:4; [M+H]+
9.66	902.8162	PC 45:0e; PC 18:0e/27:0; [M+H]+
4.61	904.6923	PC 45:6; PC 23:0-22:6; [M+H]+
7.53	932.7495	PC 48:6e; PC 22:4e/26:2; [M+H]+
3.98	926.6876	PC 48:9e; PC 22:5e/26:4; [M+H]+
4.12	984.7329	PC 49:5; PC 27:0-22:5; [M+Na]+
5.07	548.3201	PE 22:2; PE 3:0-19:2; [M+H]+
3.24	592.3992	PE 25:1; PE 12:0-13:1; [M+H]+
2.77	590.4275	PE 26:2e; PE 18:2e/8:0; [M+H]+
5.49	664.5337	PE 31:0e; PE 14:0e/17:0; [M+H]+
3.36	666.4554	PE 32:6e; PE 14:1e/18:5; [M+H]+
6	692.5635	PE 33:0e; PE 14:0e/19:0; [M+H]+
6.76	734.567	PE 35:0; PE 17:0-18:0; [M+H]+
3.98	708.496	PE 35:6e; PE 18:4e/17:2; [M+H]+
6.61	746.5673	PE 36:1; PE 23:0-13:1; [M+H]+
5.84	728.559	PE 36:3e; PE 22:3e/14:0; [M+H]+
6.83	760.5833	PE 37:1; PE 18:0-19:1; [M+H]+
7.04	774.5973	PE 38:1; PE 21:0-17:1; [M+H]+
7.27	788.6135	PE 39:1; PE 19:0-20:1; [M+H]+
6.98	786.5978	PE 39:2; PE 18:0-21:2; [M+H]+
6.86	786.5983	PE 39:2; PE 20:0-19:2; [M+H]+
6.92	808.5805	PE 41:5; PE 19:0-22:5; [M+H]+
6.52	808.5828	PE 41:5; PE 23:0-18:5; [M+H]+
2.14	796.5389	PE 42:11e; PE 22:6e/20:5; [M+H]+
8.08	816.6984	PE 42:1e; PE 16:0e/26:1; [M+H]+
7	812.6591	PE 42:3e; PE 18:1e/24:2; [M+H]+
3.59	446.2206	PG 11:0; PG 5:0-6:0; [M+NH4]+
6.83	850.5532	PG 41:8; PG 19:2-22:6; [M+NH4]+
2.59	276.2368	Phytophingosine 15:0; [M+H]+
1.83	304.3065	Phytophingosine 17:0; [M+H]+
2.69	332.336	Phytophingosine 19:0; [M+H]+
3.39	360.366	Phytophingosine 21:0; [M+H]+
5.47	388.3611	Phytophingosine 23:0; [M+H]+
1.98	402.3765	Phytophingosine 24:0; [M+H]+
6.03	416.3914	Phytophingosine 25:0; [M+H]+
6.61	444.4223	Phytophingosine 27:0; [M+H]+
5.54	668.375	PS 28:6; PS 6:0-22:6; [M+H]+
2.64	722.5031	PS 31:0; PS 10:0-21:0; [M+H]+
3.14	798.5334	PS 37:4; PS 21:1-16:3; [M+H]+
3.21	754.5072	SHexCer d32:0; SHexCer d18:0/14:0; [M+H]+
4.34	832.5496	SHexCer d38:3; SHexCer d20:1/18:2; [M+H]+
3	587.4152	SM d26:3; SM d14:3/12:0; [M+H]+
7.56	605.4787	SM d27:1; SM d14:0/13:1; [M+H]+

5.51	599.4279	SM d27:4; SM d14:3/13:1; [M+H]+
5.03	641.4554	SM d30:4; SM d14:2/16:2; [M+H]+
8.05	659.5166	SM d31:2; SM d14:2/17:0; [M+H]+
5.72	675.5406	SM d32:1; SM d14:1/18:0; [M+H]+
8.95	671.535	SM d32:3; SM d14:1/18:2; [M+H]+
4.28	681.4922	SM d33:5; SM d17:3/16:2; [M+H]+
6.25	703.5724	SM d34:1; SM d14:1/20:0; [M+H]+
8.44	703.5994	SM d34:1; SM d21:0/13:1; [M+H]+
5.85	701.5561	SM d34:2; SM d21:2/13:0; [M+H]+
9.2	699.566	SM d34:3; SM d14:1/20:2; [M+H]+
7.25	697.5207	SM d34:4; SM d14:2/20:2; [M+H]+
8.75	695.5353	SM d34:5; SM d14:3/20:2; [M+H]+
8.13	715.56	SM d35:2; SM d14:1/21:1; [M+H]+
8.52	713.574	SM d35:3; SM d16:2/19:1; [M+H]+
7.51	711.5306	SM d35:4; SM d15:2/20:2; [M+H]+
6.75	731.6035	SM d36:1; SM d14:1/22:0; [M+H]+
6.37	729.5886	SM d36:2; SM d14:1/22:1; [M+H]+
6.27	727.5991	SM d36:3; SM d16:1/20:2; [M+H]+
6.25	725.5546	SM d36:4; SM d16:2/20:2; [M+H]+
7.33	723.5354	SM d36:5; SM d14:3/22:2; [M+H]+
6.51	739.5695	SM d37:4; SM d17:2/20:2; [M+H]+
6.75	753.5848	SM d38:4; SM d14:2/24:2; [M+H]+
7.97	753.582	SM d38:4; SM d14:3/24:1; [M+H]+
6.88	795.6607	SM d41:4; SM d15:2/26:2; [M+H]+
7.6	813.6812	SM d42:2; SM d21:1/21:1; [M+H]+
7.29	811.6606	SM d42:3; SM d14:1/28:2; [M+H]+
9.1	821.6562	SM d43:5; SM d15:3/28:2; [M+H]+
9.66	883.7721	SM d47:2; SM d14:1/33:1; [M+H]+
8.67	881.7552	SM d47:3; SM d15:1/32:2; [M+H]+
8.49	879.7394	SM d47:4; SM d15:2/32:2; [M+H]+
9.66	907.7718	SM d49:4; SM d21:2/28:2; [M+H]+
9.51	905.7562	SM d49:5; SM d15:3/34:2; [M+H]+
3.89	300.2941	Sphingosine 18:1; [M+H]+
4.56	328.3252	Sphingosine 20:1; [M+H]+
3.63	342.3194	Sphingosine 21:1; [M+H]+
7	652.5474	TAG 36:2; TAG 12:0-12:0-12:2; [M+NH4]+
7.23	650.549	TAG 36:3; TAG 12:0-12:0-12:3; [M+NH4]+
6.46	646.5173	TAG 36:5; TAG 12:0-12:2-12:3; [M+NH4]+
8.95	666.58	TAG 37:2; TAG 12:0-12:2-13:0; [M+NH4]+
3.3	658.508	TAG 37:6; TAG 12:3-12:3-13:0; [M+NH4]+
6.98	680.5734	TAG 38:2; TAG 12:2-13:0-13:0; [M+NH4]+
7.58	678.5791	TAG 38:3; TAG 12:3-13:0-13:0; [M+NH4]+
6.63	676.5695	TAG 38:4; TAG 12:1-12:3-14:0; [M+NH4]+
7.19	672.53	TAG 38:6; TAG 12:2-12:3-14:1; [M+NH4]+
3.62	672.5263	TAG 38:6; TAG 12:3-12:3-14:0; [M+NH4]+
9.2	694.6113	TAG 39:2; TAG 12:0-13:0-14:2; [M+NH4]+
8.96	692.5953	TAG 39:3; TAG 12:1-12:2-15:0; [M+NH4]+
8.74	690.5798	TAG 39:4; TAG 12:1-12:2-15:1; [M+NH4]+
5.38	690.5788	TAG 39:4; TAG 12:2-13:1-14:1; [M+NH4]+
3.91	686.5381	TAG 39:6; TAG 12:2-12:3-15:1; [M+NH4]+
2.92	692.4913	TAG 40:10; TAG 12:2-12:3-16:5; [M+NH4]+
4.2	700.5544	TAG 40:6; TAG 12:0-12:1-16:5; [M+NH4]+
9.42	722.642	TAG 41:2; TAG 12:0-14:0-15:2; [M+NH4]+
4.8	728.5857	TAG 42:6; TAG 12:0-14:1-16:5; [M+NH4]+
4.3	726.5685	TAG 42:7; TAG 14:2-14:2-14:3; [M+NH4]+
7.59	748.6354	TAG 43:3; TAG 12:1-13:0-18:2; [M+NH4]+

6.7	740.6002	TAG 43:7; TAG 12:3-14:1-17:3; [M+NH4]+
7.15	736.5405	TAG 43:9; TAG 12:3-13:1-18:5; [M+NH4]+
2.6	766.6912	TAG 44:1; TAG 12:0-14:1-18:0; [M+NH4]+
6.1	758.6394	TAG 44:5; TAG 12:2-14:0-18:3; [M+NH4]+
7.14	768.6309	TAG 45:7; TAG 14:2-14:3-17:2; [M+NH4]+
9.44	796.7357	TAG 46:0; TAG 14:0-16:0-16:0; [M+NH4]+
9.25	794.7197	TAG 46:1; TAG 14:0-16:0-16:1; [M+NH4]+
9.51	810.7521	TAG 47:0; TAG 15:0-16:0-16:0; [M+NH4]+
9.11	798.6728	TAG 47:6; TAG 12:0-13:0-22:6; [M+NH4]+
9.62	824.767	TAG 48:0; TAG 16:0-16:0-16:0; [M+NH4]+
9.46	822.7516	TAG 48:1; TAG 14:0-16:0-18:1; [M+NH4]+
9.29	820.7357	TAG 48:2; TAG 14:0-16:1-18:1; [M+NH4]+
9.18	812.6887	TAG 48:6; TAG 12:2-14:3-22:1; [M+NH4]+
9.78	852.7989	TAG 50:0; TAG 16:0-16:0-18:0; [M+NH4]+
9.63	850.7829	TAG 50:1; TAG 16:0-16:0-18:1; [M+NH4]+
9.48	848.7679	TAG 50:2; TAG 16:0-16:1-18:1; [M+NH4]+
9.31	846.7516	TAG 50:3; TAG 16:0-16:1-18:2; [M+NH4]+
7.65	842.6277	TAG 51:12; TAG 12:3-17:3-22:6; [M+NH4]+
9.92	880.8313	TAG 52:0; TAG 16:0-18:0-18:0; [M+NH4]+
7.26	878.8082	TAG 52:1; TAG 12:0-18:0-22:1; [M+NH4]+
9.81	878.8157	TAG 52:1; TAG 16:0-18:0-18:1; [M+NH4]+
7.92	856.6433	TAG 52:12; TAG 12:3-20:4-20:5; [M+NH4]+
9.65	876.7997	TAG 52:2; TAG 16:0-16:0-20:2; [M+NH4]+
9.5	874.7842	TAG 52:3; TAG 16:0-18:1-18:2; [M+NH4]+
9.36	872.768	TAG 52:4; TAG 16:0-16:1-20:3; [M+NH4]+
7.94	870.6589	TAG 53:12; TAG 12:3-19:3-22:6; [M+NH4]+
7.62	868.6436	TAG 53:13; TAG 12:3-19:5-22:5; [M+NH4]+
3.85	868.6453	TAG 53:13; TAG 14:3-19:5-20:5; [M+NH4]+
7.35	866.6274	TAG 53:14; TAG 12:3-19:5-22:6; [M+NH4]+
8.08	884.6762	TAG 54:12; TAG 12:3-20:5-22:4; [M+NH4]+
9.82	904.8318	TAG 54:2; TAG 16:0-18:1-20:1; [M+NH4]+
9.53	900.8006	TAG 54:4; TAG 18:1-18:1-18:2; [M+NH4]+
9.37	898.7849	TAG 54:5; TAG 18:1-18:2-18:2; [M+NH4]+
9.19	896.7692	TAG 54:6; TAG 18:1-18:2-18:3; [M+NH4]+
8.29	898.6913	TAG 55:12; TAG 14:3-19:3-22:6; [M+NH4]+
8.34	938.7243	TAG 58:13; TAG 16:4-20:3-22:6; [M+NH4]+
4.57	948.7203	TAG 59:15; TAG 16:4-21:4-22:7; [M+NH4]+
8.6	966.7564	TAG 60:13; TAG 17:1-21:5-22:7; [M+NH4]+
7.97	1000.8161	TAG 62:10; TAG 20:1-20:2-22:7; [M+NH4]+
4.52	992.7492	TAG 62:14; TAG 20:5-20:6-22:3; [M+NH4]+
8.7	1006.7911	TAG 63:14; TAG 21:4-21:5-21:5; [M+NH4]+
4.25	1042.7799	TAG 66:17; TAG 22:5-22:5-22:7; [M+NH4]+
5.12	313.1418	w/o MS2:Benzyl butyl phthalate (also known as chemical regent)
4.61	622.5173	w/o MS2:LPC 26:0e; [M+H]+
5.32	440.4484	w/o MS2:Sphingosine 28:1; [M+H]+

Supplementary Table 1b. LipidBlast annotations of all measured m/z features in negative ionization mode

Average RT (min)	Feature/peak (m/z)	Annotated lipid species
4	319.2303	12-HETE
7.85	869.6244	AcylGlcADG 40:0; AcylGlcADG 12:0-12:0-16:0; [M-H]-
7.71	867.6087	AcylGlcADG 40:1; AcylGlcADG 12:0-14:0-14:1; [M-H]-
7.43	865.595	AcylGlcADG 40:2; AcylGlcADG 12:0-12:0-16:2; [M-H]-
6.02	863.6027	AcylGlcADG 40:3; AcylGlcADG 12:0-12:0-16:3; [M-H]-
7.87	897.6705	AcylGlcADG 42:0; AcylGlcADG 12:0-12:0-18:0; [M-H]-
8.18	897.6548	AcylGlcADG 42:0; AcylGlcADG 14:0-14:0-14:0; [M-H]-
8.08	895.6412	AcylGlcADG 42:1; AcylGlcADG 12:0-14:1-16:0; [M-H]-
8.48	925.6866	AcylGlcADG 44:0; AcylGlcADG 12:0-16:0-16:0; [M-H]-
8.04	981.7627	AcylGlcADG 48:0; AcylGlcADG 14:0-16:0-18:0; [M-H]-
7.87	979.7463	AcylGlcADG 48:1; AcylGlcADG 14:0-14:1-20:0; [M-H]-
8.62	1033.7963	AcylGlcADG 52:2; AcylGlcADG 16:0-16:1-20:1; [M-H]-
6.89	564.4536	Cer-AP t34:3; Cer-AP t14:2/20:1; [M-H]-
7.15	636.4813	Cer-AP t36:4; Cer-AP t18:2/18:2; [M+FA-H]-
7.59	664.511	Cer-AP t38:4; Cer-AP t22:2/16:2; [M+FA-H]-
6.78	678.5439	Cer-AP t39:4; Cer-AP t23:2/16:2; [M+FA-H]-
6.7	566.5142	Cer-AS d35:1; Cer-AS d16:1/19:0; [M-H]-
8.44	664.6243	Cer-AS d42:1; Cer-AS d18:1/24:0; [M-H]-
6.84	646.5189	Cer-BS d38:5; Cer-BS d14:3/24:2; [M+FA-H]-
7.64	676.5648	Cer-BS d40:4; Cer-BS d14:3/26:1; [M+FA-H]-
8.03	704.5949	Cer-BS d42:4; Cer-BS d15:3/27:1; [M+FA-H]-
7.47	610.5344	Cer-NS d36:1; Cer-NS d18:1/18:0; [M+FA-H]-
7.47	564.5366	Cer-NS d36:1; Cer-NS d18:1/18:0; [M-H]-
1.74	265.1504	Dodecyl sulfate
5.14	325.191	Dodecylbenzenesulfonic acid
4.69	255.2359	FA 16:0; [M-H]-
6.76	253.2196	FA 16:1; [M-H]-
1.62	245.1573	FA 16:5; [M-H]-
7.19	269.2523	FA 17:0; [M-H]-
5.39	283.2668	FA 18:0; [M-H]-
4.81	281.251	FA 18:1; [M-H]-
4.34	279.2356	FA 18:2; [M-H]-
3.89	277.2204	FA 18:3; [M-H]-
5.22	297.2839	FA 19:0; [M-H]-
5.55	311.298	FA 20:0; [M-H]-
5.35	309.282	FA 20:1; [M-H]-
4.69	305.2505	FA 20:3; [M-H]-
4.51	303.2357	FA 20:4; [M-H]-
4.07	301.2196	FA 20:5; [M-H]-
3.6	299.2061	FA 20:6; [M-H]-
3.98	325.3206	FA 21:0; [M-H]-
6.7	339.3284	FA 22:0; [M-H]-
4.93	333.2827	FA 22:3; [M-H]-
2.94	327.2339	FA 22:6; [M-H]-
2.97	325.2134	FA 22:7; [M-H]-
2.1	325.2374	FAHFA 19:1; FAHFA 4:0/15:1; [M-H]-
1.94	337.2393	FAHFA 20:2; FAHFA 4:0/16:2; [M-H]-
2.05	335.2249	FAHFA 20:3; FAHFA 4:0/16:3; [M-H]-
2.83	331.1933	FAHFA 20:5; FAHFA 18:5/2:0; [M-H]-
3.88	349.2413	FAHFA 21:3; FAHFA 18:3/3:0; [M-H]-
3.16	359.2233	FAHFA 22:5; FAHFA 18:5/4:0; [M-H]-
4.46	377.2747	FAHFA 23:3; FAHFA 3:0/20:3; [M-H]-
3.02	385.2401	FAHFA 24:6; FAHFA 22:6/2:0; [M-H]-

2.9	399.256	FAHFA 25:6; FAHFA 22:6/3:0; [M-H]-
3.99	433.3326	FAHFA 27:3; FAHFA 11:0/16:3; [M-H]-
4.55	433.3336	FAHFA 27:3; FAHFA 18:3/9:0; [M-H]-
3.47	427.2863	FAHFA 27:6; FAHFA 22:6/5:0; [M-H]-
2.76	453.3875	FAHFA 28:0; FAHFA 18:0/10:0; [M-H]-
4.4	461.3631	FAHFA 29:3; FAHFA 20:3/9:0; [M-H]-
3.93	507.4396	FAHFA 32:1; FAHFA 12:0/20:1; [M-H]-
3.46	495.3436	FAHFA 32:7; FAHFA 16:4/16:3; [M-H]-
5.52	525.3958	FAHFA 34:6; FAHFA 16:3/18:3; [M-H]-
5.4	523.3845	FAHFA 34:7; FAHFA 18:5/16:2; [M-H]-
5.96	521.3665	FAHFA 34:8; FAHFA 18:5/16:3; [M-H]-
5.78	539.4122	FAHFA 35:6; FAHFA 18:5/17:1; [M-H]-
5.3	537.394	FAHFA 35:7; FAHFA 22:6/13:1; [M-H]-
4.12	563.497	FAHFA 36:1; FAHFA 14:1/22:0; [M-H]-
6.11	553.4328	FAHFA 36:6; FAHFA 16:4/20:2; [M-H]-
5.53	551.4111	FAHFA 36:7; FAHFA 22:6/14:1; [M-H]-
6.48	549.4042	FAHFA 36:8; FAHFA 18:5/18:3; [M-H]-
6.22	565.4265	FAHFA 37:7; FAHFA 20:5/17:2; [M-H]-
5.78	565.4263	FAHFA 37:7; FAHFA 22:6/15:1; [M-H]-
6.63	581.4538	FAHFA 38:6; FAHFA 22:6/16:0; [M-H]-
7.24	579.4412	FAHFA 38:7; FAHFA 18:4/20:3; [M-H]-
6.06	579.4413	FAHFA 38:7; FAHFA 18:5/20:2; [M-H]-
6.84	595.4725	FAHFA 39:6; FAHFA 22:5/17:1; [M-H]-
6.63	593.459	FAHFA 39:7; FAHFA 22:6/17:1; [M-H]-
7.21	591.4449	FAHFA 39:8; FAHFA 22:6/17:2; [M-H]-
6.12	601.4247	FAHFA 40:10; FAHFA 18:5/22:5; [M-H]-
7.11	609.4901	FAHFA 40:6; FAHFA 18:1/22:5; [M-H]-
7.74	607.472	FAHFA 40:7; FAHFA 18:5/22:2; [M-H]-
6.9	607.473	FAHFA 40:7; FAHFA 20:4/20:3; [M-H]-
6.57	607.4756	FAHFA 40:7; FAHFA 22:5/18:2; [M-H]-
7.34	605.4567	FAHFA 40:8; FAHFA 18:5/22:3; [M-H]-
5.99	605.457	FAHFA 40:8; FAHFA 20:4/20:4; [M-H]-
7.02	603.4427	FAHFA 40:9; FAHFA 18:5/22:4; [M-H]-
7.34	623.4977	FAHFA 41:6; FAHFA 24:4/17:2; [M-H]-
6.43	619.4747	FAHFA 41:8; FAHFA 22:6/19:2; [M-H]-
4.75	629.4535	FAHFA 42:10; FAHFA 20:5/22:5; [M-H]-
7.55	637.5183	FAHFA 42:6; FAHFA 24:4/18:2; [M-H]-
8.07	635.5027	FAHFA 42:7; FAHFA 20:3/22:4; [M-H]-
7.56	633.4908	FAHFA 42:8; FAHFA 20:4/22:4; [M-H]-
8.45	663.532	FAHFA 44:7; FAHFA 22:3/22:4; [M-H]-
6.87	715.5743	FAHFA 48:9; FAHFA 26:4/22:5; [M-H]-
4.02	631.3989	GlcADG 24:0; GlcADG 12:0-12:0; [M-H]-
4	659.4298	GlcADG 26:0; GlcADG 12:0-14:0; [M-H]-
4.29	657.4215	GlcADG 26:1; GlcADG 12:0-14:1; [M-H]-
4.51	673.4442	GlcADG 27:0; GlcADG 12:0-15:0; [M-H]-
6.46	669.4136	GlcADG 27:2; GlcADG 13:1-14:1; [M-H]-
6.87	701.4918	GlcADG 29:0; GlcADG 14:0-15:0; [M-H]-
4.5	697.4395	GlcADG 29:2; GlcADG 12:0-17:2; [M-H]-
4.08	693.4136	GlcADG 29:4; GlcADG 13:0-16:4; [M-H]-
5.52	707.4457	GlcADG 30:4; GlcADG 14:0-16:4; [M-H]-
4.49	707.4302	GlcADG 30:4; GlcADG 14:1-16:3; [M-H]-
4.59	705.4153	GlcADG 30:5; GlcADG 12:0-18:5; [M-H]-
4.55	729.5056	GlcADG 31:0; GlcADG 15:0-16:0; [M-H]-
4.68	727.4928	GlcADG 31:1; GlcADG 15:0-16:1; [M-H]-
5.08	725.4856	GlcADG 31:2; GlcADG 15:0-16:2; [M-H]-
4.17	723.4688	GlcADG 31:3; GlcADG 14:1-17:2; [M-H]-

4.93	721.4446	GlcADG 31:4; GlcADG 15:0-16:4; [M-H]-
4.51	743.5303	GlcADG 32:0; GlcADG 16:0-16:0; [M-H]-
6.78	739.4828	GlcADG 32:2; GlcADG 15:1-17:1; [M-H]-
5	735.4609	GlcADG 32:4; GlcADG 16:1-16:3; [M-H]-
5.47	733.457	GlcADG 32:5; GlcADG 14:0-18:5; [M-H]-
4.64	727.4023	GlcADG 32:8; GlcADG 16:4-16:4; [M-H]-
7.27	755.5382	GlcADG 33:1; GlcADG 16:0-17:1; [M-H]-
5.04	761.4749	GlcADG 34:5; GlcADG 16:0-18:5; [M-H]-
5.13	759.4586	GlcADG 34:6; GlcADG 12:0-22:6; [M-H]-
4.49	757.4513	GlcADG 34:7; GlcADG 18:3-16:4; [M-H]-
5.31	773.4754	GlcADG 35:6; GlcADG 13:0-22:6; [M-H]-
5.23	797.5666	GlcADG 36:1; GlcADG 14:0-22:1; [M-H]-
5.36	795.5563	GlcADG 36:2; GlcADG 15:1-21:1; [M-H]-
4.69	791.5179	GlcADG 36:4; GlcADG 18:1-18:3; [M-H]-
7.7	809.5734	GlcADG 37:2; GlcADG 15:0-22:2; [M-H]-
7.66	823.5833	GlcADG 38:2; GlcADG 20:0-18:2; [M-H]-
5.47	817.5394	GlcADG 38:5; GlcADG 22:1-16:4; [M-H]-
5.33	815.5218	GlcADG 38:6; GlcADG 16:1-22:5; [M-H]-
7.88	839.6127	GlcADG 39:1; GlcADG 18:0-21:1; [M-H]-
7.94	837.599	GlcADG 39:2; GlcADG 17:0-22:2; [M-H]-
5.67	831.5523	GlcADG 39:5; GlcADG 17:1-22:4; [M-H]-
5.88	829.5375	GlcADG 39:6; GlcADG 21:1-18:5; [M-H]-
8	851.6138	GlcADG 40:2; GlcADG 20:0-20:2; [M-H]-
7.96	849.5994	GlcADG 40:3; GlcADG 22:0-18:3; [M-H]-
7.69	849.5986	GlcADG 40:3; GlcADG 24:0-16:3; [M-H]-
6	847.6072	GlcADG 40:4; GlcADG 19:2-21:2; [M-H]-
7.41	847.5842	GlcADG 40:4; GlcADG 24:0-16:4; [M-H]-
3.96	843.5658	GlcADG 40:6; GlcADG 18:3-22:3; [M-H]-
5.95	865.6301	GlcADG 41:2; GlcADG 19:1-22:1; [M-H]-
8.12	865.6304	GlcADG 41:2; GlcADG 20:0-21:2; [M-H]-
6.35	861.6121	GlcADG 41:4; GlcADG 21:0-20:4; [M-H]-
7.08	853.5469	GlcADG 41:8; GlcADG 19:2-22:6; [M-H]-
5.8	879.6522	GlcADG 42:2; GlcADG 22:0-20:2; [M-H]-
8.3	879.6455	GlcADG 42:2; GlcADG 25:0-17:2; [M-H]-
5.8	869.5674	GlcADG 42:7; GlcADG 22:2-20:5; [M-H]-
8.07	891.645	GlcADG 43:3; GlcADG 22:1-21:2; [M-H]-
7.4	883.6053	GlcADG 43:7; GlcADG 21:1-22:6; [M-H]-
8.6	907.6776	GlcADG 44:2; GlcADG 20:1-24:1; [M-H]-
8.35	919.6759	GlcADG 45:3; GlcADG 24:1-21:2; [M-H]-
8.15	917.6619	GlcADG 45:4; GlcADG 19:0-26:4; [M-H]-
7.85	915.6487	GlcADG 45:5; GlcADG 21:1-24:4; [M-H]-
6.58	933.6898	GlcADG 46:3; GlcADG 26:0-20:3; [M-H]-
6.28	923.6148	GlcADG 46:8; GlcADG 24:2-22:6; [M-H]-
8.62	947.7083	GlcADG 47:3; GlcADG 26:1-21:2; [M-H]-
8.49	959.7078	GlcADG 48:4; GlcADG 24:2-24:2; [M-H]-
8.72	987.7383	GlcADG 50:4; GlcADG 26:0-24:4; [M-H]-
8.48	985.722	GlcADG 50:5; GlcADG 26:1-24:4; [M-H]-
8.27	983.7084	GlcADG 50:6; GlcADG 26:2-24:4; [M-H]-
6.84	618.4316	HexCer-AP t26:1; HexCer-AP t14:0/12:1; [M-H]-
7.56	674.4922	HexCer-AP t30:1; HexCer-AP t17:0/13:1; [M-H]-
8.13	730.5532	HexCer-AP t34:1; HexCer-AP t22:1/12:0; [M-H]-
6.89	906.6996	HexCer-AP t47:4; HexCer-AP t23:2/24:2; [M-H]-
2.94	602.4553	HexCer-NDS d27:0; HexCer-NDS d15:0/12:0; [M-H]-
6.5	644.5029	HexCer-NDS d30:0; HexCer-NDS d14:0/16:0; [M-H]-
3.58	670.5217	HexCer-NDS d32:1; HexCer-NDS d18:0/14:1; [M-H]-
5.5	652.4893	HexCer-NS d31:3; HexCer-NS d14:3/17:0; [M-H]-

7.67	760.565	HexCer-NS d39:5; HexCer-NS d23:3/16:2; [M-H]-
2.14	367.1934	LPA 13:0; [M-H]-
3.35	395.2249	LPA 15:0; [M-H]-
2.42	409.2394	LPA 16:0; [M-H]-
4.74	403.1958	LPA 16:3; [M-H]-
2.67	401.1734	LPA 16:4; [M-H]-
2.89	423.256	LPA 17:0; [M-H]-
2.37	421.2267	LPA 17:1; [M-H]-
2.58	437.2712	LPA 18:0; [M-H]-
2.67	435.255	LPA 18:1; [M-H]-
3.59	433.2422	LPA 18:2; [M-H]-
2.97	451.2809	LPA 19:0; [M-H]-
3.32	449.2709	LPA 19:1; [M-H]-
3.09	465.2983	LPA 20:0; [M-H]-
3.6	463.2841	LPA 20:1; [M-H]-
3.61	461.2696	LPA 20:2; [M-H]-
5.13	459.2461	LPA 20:3; [M-H]-
3.66	457.2402	LPA 20:4; [M-H]-
5.05	479.3191	LPA 21:0; [M-H]-
3.73	477.3026	LPA 21:1; [M-H]-
3.05	475.2884	LPA 21:2; [M-H]-
3.72	493.3321	LPA 22:0; [M-H]-
3.48	491.3165	LPA 22:1; [M-H]-
4.09	489.3014	LPA 22:2; [M-H]-
4.79	507.3499	LPA 23:0; [M-H]-
4.72	519.3471	LPA 24:1; [M-H]-
4.03	517.3295	LPA 24:2; [M-H]-
6.15	535.3806	LPA 25:0; [M-H]-
4.7	545.3575	LPA 26:2; [M-H]-
6.66	563.416	LPA 27:0; [M-H]-
3.39	496.3093	LPC 14:1e; [M+FA-H]-
2.45	524.3001	LPC 15:1; [M+FA-H]-
2.72	538.3502	LPC 17:1e; [M+FA-H]-
3.73	573.3939	LPC 18:1(d7); [M+FA-H]-
2.77	552.3687	LPC 18:1e; [M+FA-H]-
2.94	566.3846	LPC 19:1e; [M+FA-H]-
3.6	582.4146	LPC 20:0e; [M+FA-H]-
2.79	592.4003	LPC 21:2e; [M+FA-H]-
4.76	604.4003	LPC 22:3e; [M+FA-H]-
4.97	624.4628	LPC 23:0e; [M+FA-H]-
6.11	680.5259	LPC 27:0e; [M+FA-H]-
2.45	344.1549	LPC 3:0e; [M+FA-H]-
2.64	400.1777	LPC 6:0; [M+FA-H]-
2.39	386.1991	LPC 6:0e; [M+FA-H]-
3.09	400.2152	LPC 7:0e; [M+FA-H]-
3.54	428.2295	LPC 9:0e; [M+FA-H]-
3.36	368.189	LPE 10:0; [M-H]-
2.83	354.1955	LPE 10:0e; [M-H]-
2.21	368.219	LPE 11:0e; [M-H]-
2.44	396.2236	LPE 12:0; [M-H]-
2.44	382.2419	LPE 12:0e; [M-H]-
1.72	410.2344	LPE 13:0; [M-H]-
2.71	396.256	LPE 13:0e; [M-H]-
2.54	424.2506	LPE 14:0; [M-H]-
2.7	410.2715	LPE 14:0e; [M-H]-
2.45	408.2546	LPE 14:1e; [M-H]-

2.98	438.2685	LPE 15:0; [M-H]-
2.89	424.2849	LPE 15:0e; [M-H]-
2.48	452.283	LPE 16:0; [M-H]-
2.4	450.2657	LPE 16:1; [M-H]-
3.11	448.2501	LPE 16:2; [M-H]-
3.44	432.2563	LPE 16:3e; [M-H]-
3.56	444.2044	LPE 16:4; [M-H]-
2.59	466.2966	LPE 17:0; [M-H]-
1.8	452.318	LPE 17:0e; [M-H]-
3.94	472.2365	LPE 18:4; [M-H]-
1.64	492.3125	LPE 19:1; [M-H]-
5.54	476.3221	LPE 19:2e; [M-H]-
3.21	498.2688	LPE 20:5; [M-H]-
3.12	522.3567	LPE 21:0; [M-H]-
3.37	536.3737	LPE 22:0; [M-H]-
3.35	534.3591	LPE 22:1; [M-H]-
4.11	520.38	LPE 22:1e; [M-H]-
6.55	532.3448	LPE 22:2; [M-H]-
4.76	530.3297	LPE 22:3; [M-H]-
2.04	516.3512	LPE 22:3e; [M-H]-
4.53	514.3322	LPE 22:4e; [M-H]-
3.57	550.3901	LPE 23:0; [M-H]-
3.75	564.405	LPE 24:0; [M-H]-
3.85	578.4206	LPE 25:0; [M-H]-
5.6	564.4438	LPE 25:0e; [M-H]-
6.29	592.4727	LPE 27:0e; [M-H]-
2.34	326.1831	LPE 8:0e; [M-H]-
2.31	469.2599	LPG 15:0; [M-H]-
1.94	467.2462	LPG 15:1; [M-H]-
2.57	525.3226	LPG 19:0; [M-H]-
2.67	523.3064	LPG 19:1; [M-H]-
3.15	521.2985	LPG 19:2; [M-H]-
2.73	539.3308	LPG 20:0; [M-H]-
2.68	537.3215	LPG 20:1; [M-H]-
2.59	535.3069	LPG 20:2; [M-H]-
3.65	567.3704	LPG 22:0; [M-H]-
3.18	565.3563	LPG 22:1; [M-H]-
6.43	563.3282	LPG 22:2; [M-H]-
4.49	561.3216	LPG 22:3; [M-H]-
4.05	595.4016	LPG 24:0; [M-H]-
3.23	593.3836	LPG 24:1; [M-H]-
3.58	591.3652	LPG 24:2; [M-H]-
3.44	587.3403	LPG 24:4; [M-H]-
3.64	615.3688	LPG 26:4; [M-H]-
5.75	709.4324	LPI 26:1; [M-H]-
4.48	501.3157	Medicagenic acid
3.43	565.3229	MGDG 17:0; MGDG 7:0-10:0; [M+FA-H]-
6.63	579.3444	MGDG 18:0; MGDG 9:0-9:0; [M+FA-H]-
2.43	573.2901	MGDG 18:3; MGDG 2:0-16:3; [M+FA-H]-
5.56	593.3677	MGDG 19:0; MGDG 3:0-16:0; [M+FA-H]-
6.83	593.3596	MGDG 19:0; MGDG 9:0-10:0; [M+FA-H]-
6	607.3752	MGDG 20:0; MGDG 10:0-10:0; [M+FA-H]-
3.17	607.3704	MGDG 20:0; MGDG 9:0-11:0; [M+FA-H]-
6.33	597.2894	MGDG 20:5; MGDG 2:0-18:5; [M+FA-H]-
3.6	621.3913	MGDG 21:0; MGDG 10:0-11:0; [M+FA-H]-
5.5	621.3939	MGDG 21:0; MGDG 9:0-12:0; [M+FA-H]-

6.5	611.3046	MGDG 21:5; MGDG 3:0-18:5; [M+FA-H]-
5.02	635.4092	MGDG 22:0; MGDG 10:0-12:0; [M+FA-H]-
5.74	635.4092	MGDG 22:0; MGDG 9:0-13:0; [M+FA-H]-
3.6	631.3694	MGDG 22:2; MGDG 4:0-18:2; [M+FA-H]-
6.67	625.3224	MGDG 22:5; MGDG 2:0-20:5; [M+FA-H]-
5.98	649.4228	MGDG 23:0; MGDG 11:0-12:0; [M+FA-H]-
6.15	663.4405	MGDG 24:0; MGDG 10:0-14:0; [M+FA-H]-
6.23	663.4398	MGDG 24:0; MGDG 12:0-12:0; [M+FA-H]-
5.85	677.4552	MGDG 25:0; MGDG 10:0-15:0; [M+FA-H]-
6.32	677.4551	MGDG 25:0; MGDG 11:0-14:0; [M+FA-H]-
5.81	677.4564	MGDG 25:0; MGDG 12:0-13:0; [M+FA-H]-
3.98	675.444	MGDG 25:1; MGDG 11:0-14:1; [M+FA-H]-
5.59	675.4399	MGDG 25:1; MGDG 12:0-13:1; [M+FA-H]-
6.04	691.4697	MGDG 26:0; MGDG 11:0-15:0; [M+FA-H]-
6.72	689.455	MGDG 26:1; MGDG 12:0-14:1; [M+FA-H]-
4.67	685.4199	MGDG 26:3; MGDG 6:0-20:3; [M+FA-H]-
6.93	703.4695	MGDG 27:1; MGDG 9:0-18:1; [M+FA-H]-
6.55	733.5151	MGDG 29:0; MGDG 11:0-18:0; [M+FA-H]-
6.75	733.5183	MGDG 29:0; MGDG 14:0-15:0; [M+FA-H]-
7.27	747.5253	MGDG 30:0; MGDG 12:0-18:0; [M+FA-H]-
7.88	747.5317	MGDG 30:0; MGDG 7:0-23:0; [M+FA-H]-
6.35	747.5275	MGDG 30:0; MGDG 9:0-21:0; [M+FA-H]-
5.86	743.5011	MGDG 30:2; MGDG 12:0-18:2; [M+FA-H]-
6.84	761.5477	MGDG 31:0; MGDG 15:0-16:0; [M+FA-H]-
6.39	775.563	MGDG 32:0; MGDG 13:0-19:0; [M+FA-H]-
6.44	771.5242	MGDG 32:2; MGDG 16:1-16:1; [M+FA-H]-
7.4	829.6093	MGDG 36:1; MGDG 20:0-16:1; [M+FA-H]-
7.1	845.6404	MGDG 37:0; MGDG 13:0-24:0; [M+FA-H]-
6.98	843.6244	MGDG 37:1; MGDG 20:0-17:1; [M+FA-H]-
6.94	913.7015	MGDG 42:1; MGDG 22:0-20:1; [M+FA-H]-
7.6	913.7023	MGDG 42:1; MGDG 23:0-19:1; [M+FA-H]-
7.5	911.6871	MGDG 42:2; MGDG 24:0-18:2; [M+FA-H]-
6.59	983.6745	MGDG 48:8; MGDG 24:4-24:4; [M+FA-H]-
8.4	1049.8262	MGDG 52:3; MGDG 26:1-26:2; [M+FA-H]-
8.31	1047.8103	MGDG 52:4; MGDG 26:2-26:2; [M+FA-H]-
1.64	453.1941	MGDG 9:0; MGDG 3:0-6:0; [M+FA-H]-
2.99	339.2028	Norethisterone acetate
6.56	868.569	OxPC 38:5+1O; OxPC 18:1-20:4+1O; [M+FA-H]-
5.13	804.5173	OxPE 40:7+1O; OxPE 18:1-22:6+1O ; [M-H]-
6.41	781.5237	OxPG 34:0+2O; OxPG 16:0-18:0+2O; [M-H]-
6.09	813.5334	OxPG 38:4+1O; OxPG 18:0-20:4+1O; [M-H]-
5.93	800.5051	OxPS 36:3+1O; OxPS 18:0-18:3+1O; [M-H]-
3.43	381.1715	PA 13:0; PA 4:0-9:0; [M-H]-
2.33	421.193	PA 16:1; PA 3:0-13:1; [M-H]-
2.77	437.241	PA 17:0; PA 2:0-15:0; [M-H]-
2.99	451.2503	PA 18:0; PA 2:0-16:0; [M-H]-
2.47	449.235	PA 18:1; PA 4:0-14:1; [M-H]-
3.22	465.2658	PA 19:0; PA 2:0-17:0; [M-H]-
2.57	477.2688	PA 20:1; PA 7:0-13:1; [M-H]-
2.77	475.2475	PA 20:2; PA 2:0-18:2; [M-H]-
2.8	493.2953	PA 21:0; PA 10:0-11:0; [M-H]-
3.19	493.2956	PA 21:0; PA 2:0-19:0; [M-H]-
2.95	493.2946	PA 21:0; PA 5:0-16:0; [M-H]-
3.76	493.2962	PA 21:0; PA 7:0-14:0; [M-H]-
3.96	507.3121	PA 22:0; PA 10:0-12:0; [M-H]-
2.83	507.312	PA 22:0; PA 7:0-15:0; [M-H]-

2.79	505.2991	PA 22:1; PA 7:0-15:1; [M-H]-
3.15	503.2806	PA 22:2; PA 2:0-20:2; [M-H]-
4.32	521.3281	PA 23:0; PA 11:0-12:0; [M-H]-
3.86	521.3255	PA 23:0; PA 6:0-17:0; [M-H]-
3.28	521.3232	PA 23:0; PA 7:0-16:0; [M-H]-
3.46	521.3283	PA 23:0; PA 9:0-14:0; [M-H]-
3.13	519.3093	PA 23:1; PA 2:0-21:1; [M-H]-
3.66	519.3137	PA 23:1; PA 5:0-18:1; [M-H]-
2.85	519.3101	PA 23:1; PA 9:0-14:1; [M-H]-
4.48	517.3016	PA 23:2; PA 3:0-20:2; [M-H]-
3.08	535.3412	PA 24:0; PA 12:0-12:0; [M-H]-
3.82	535.3423	PA 24:0; PA 9:0-15:0; [M-H]-
3.1	533.3215	PA 24:1; PA 5:0-19:1; [M-H]-
3.81	549.3577	PA 25:0; PA 12:0-13:0; [M-H]-
5.25	547.3424	PA 25:1; PA 10:0-15:1; [M-H]-
3.9	547.3425	PA 25:1; PA 9:0-16:1; [M-H]-
3.12	545.3246	PA 25:2; PA 6:0-19:2; [M-H]-
4.51	545.3276	PA 25:2; PA 9:0-16:2; [M-H]-
3.4	543.3105	PA 25:3; PA 9:0-16:3; [M-H]-
4.09	563.3644	PA 26:0; PA 12:0-14:0; [M-H]-
4.05	561.3606	PA 26:1; PA 13:0-13:1; [M-H]-
3.48	561.3579	PA 26:1; PA 7:0-19:1; [M-H]-
2.86	561.3481	PA 26:1; PA 8:0-18:1; [M-H]-
4.81	559.3411	PA 26:2; PA 10:0-16:2; [M-H]-
5.04	557.3309	PA 26:3; PA 6:0-20:3; [M-H]-
4.47	577.399	PA 27:0; PA 11:0-16:0; [M-H]-
3.58	575.3725	PA 27:1; PA 9:0-18:1; [M-H]-
3.44	573.3579	PA 27:2; PA 13:1-14:1; [M-H]-
3.83	571.342	PA 27:3; PA 9:0-18:3; [M-H]-
4.12	589.3894	PA 28:1; PA 14:0-14:1; [M-H]-
4.29	587.3737	PA 28:2; PA 10:0-18:2; [M-H]-
3.63	587.3728	PA 28:2; PA 14:1-14:1; [M-H]-
3.87	585.3573	PA 28:3; PA 10:0-18:3; [M-H]-
3.78	583.344	PA 28:4; PA 2:0-26:4; [M-H]-
4.74	603.4064	PA 29:1; PA 15:0-14:1; [M-H]-
4.43	601.3889	PA 29:2; PA 9:0-20:2; [M-H]-
4.05	599.3728	PA 29:3; PA 9:0-20:3; [M-H]-
3.85	597.3582	PA 29:4; PA 13:1-16:3; [M-H]-
4.71	615.4027	PA 30:2; PA 11:0-19:2; [M-H]-
4.73	615.4028	PA 30:2; PA 13:0-17:2; [M-H]-
3.83	613.3889	PA 30:3; PA 14:1-16:2; [M-H]-
4.07	611.3722	PA 30:4; PA 14:1-16:3; [M-H]-
4.42	633.4504	PA 31:0; PA 14:0-17:0; [M-H]-
4.44	629.4177	PA 31:2; PA 12:0-19:2; [M-H]-
4.69	627.4034	PA 31:3; PA 13:0-18:3; [M-H]-
3.78	627.4028	PA 31:3; PA 13:1-18:2; [M-H]-
5.33	645.4501	PA 32:1; PA 12:0-20:1; [M-H]-
4.85	641.4207	PA 32:3; PA 16:1-16:2; [M-H]-
4.48	639.4043	PA 32:4; PA 12:0-20:4; [M-H]-
4.36	655.4343	PA 33:3; PA 15:1-18:2; [M-H]-
4.59	653.4193	PA 33:4; PA 17:1-16:3; [M-H]-
4.46	651.4039	PA 33:5; PA 13:0-20:5; [M-H]-
7.59	675.4974	PA 34:0; PA 16:0-18:0; [M-H]-
5.32	669.4573	PA 34:3; PA 17:1-17:2; [M-H]-
4.95	667.4335	PA 34:4; PA 18:1-16:3; [M-H]-
5.35	687.4963	PA 35:1; PA 19:0-16:1; [M-H]-

4.48	681.4496	PA 35:4; PA 13:1-22:3; [M-H]-
5.69	679.4341	PA 35:5; PA 17:0-18:5; [M-H]-
4.78	679.4353	PA 35:5; PA 19:1-16:4; [M-H]-
5.29	677.4186	PA 35:6; PA 13:0-22:6; [M-H]-
5.13	701.5115	PA 36:1; PA 22:0-14:1; [M-H]-
3.61	683.3616	PA 36:10; PA 18:5-18:5; [M-H]-
4.74	697.4778	PA 36:3; PA 18:1-18:2; [M-H]-
4.43	695.4655	PA 36:4; PA 18:2-18:2; [M-H]-
5.65	693.4503	PA 36:5; PA 16:1-20:4; [M-H]-
3.98	691.4354	PA 36:6; PA 16:1-20:5; [M-H]-
5.27	691.4343	PA 36:6; PA 18:1-18:5; [M-H]-
4.89	689.4174	PA 36:7; PA 20:3-16:4; [M-H]-
6.26	685.3851	PA 36:9; PA 16:4-20:5; [M-H]-
6.06	713.5107	PA 37:2; PA 18:0-19:2; [M-H]-
4.99	711.4964	PA 37:3; PA 15:0-22:3; [M-H]-
6.46	711.4925	PA 37:3; PA 17:0-20:3; [M-H]-
5.2	707.4641	PA 37:5; PA 17:0-20:5; [M-H]-
6.1	707.4658	PA 37:5; PA 19:0-18:5; [M-H]-
5.24	705.4504	PA 37:6; PA 19:1-18:5; [M-H]-
4.7	725.5107	PA 38:3; PA 18:1-20:2; [M-H]-
5.48	725.5109	PA 38:3; PA 20:1-18:2; [M-H]-
5.4	721.4776	PA 38:5; PA 18:1-20:4; [M-H]-
5.36	719.465	PA 38:6; PA 22:2-16:4; [M-H]-
5.18	717.4515	PA 38:7; PA 18:3-20:4; [M-H]-
5.28	739.5264	PA 39:3; PA 19:0-20:3; [M-H]-
5.45	733.4752	PA 39:6; PA 17:2-22:4; [M-H]-
6.33	731.4639	PA 39:7; PA 17:1-22:6; [M-H]-
6.06	755.5585	PA 40:2; PA 22:0-18:2; [M-H]-
6.33	741.4474	PA 40:9; PA 20:4-20:5; [M-H]-
5.87	769.5728	PA 41:2; PA 19:0-22:2; [M-H]-
6.48	783.5858	PA 42:2; PA 18:0-24:2; [M-H]-
5.7	779.5589	PA 42:4; PA 21:2-21:2; [M-H]-
5.37	793.573	PA 43:4; PA 23:0-20:4; [M-H]-
7.08	795.4931	PA 44:10; PA 22:4-22:6; [M-H]-
6.89	805.5759	PA 44:5; PA 20:1-24:4; [M-H]-
6.36	797.5306	PA 44:9; PA 22:3-22:6; [M-H]-
6.09	797.5125	PA 44:9; PA 26:4-18:5; [M-H]-
6.71	823.6207	PA 45:3; PA 27:0-18:3; [M-H]-
5.61	817.5704	PA 45:6; PA 19:2-26:4; [M-H]-
7.96	817.5668	PA 45:6; PA 23:0-22:6; [M-H]-
6.51	837.6357	PA 46:3; PA 26:0-20:3; [M-H]-
6.36	847.6218	PA 47:5; PA 25:0-22:5; [M-H]-
8.44	845.6101	PA 47:6; PA 25:0-22:6; [M-H]-
5.97	861.6332	PA 48:5; PA 22:1-26:4; [M-H]-
6.31	859.6201	PA 48:6; PA 26:1-22:5; [M-H]-
6.5	875.6539	PA 49:5; PA 27:0-22:5; [M-H]-
7.27	891.681	PA 50:4; PA 24:2-26:2; [M-H]-
7.1	905.696	PA 51:4; PA 25:0-26:4; [M-H]-
8.76	905.6967	PA 51:4; PA 27:0-24:4; [M-H]-
6.62	915.6813	PA 52:6; PA 26:2-26:4; [M-H]-
7.1	911.6505	PA 52:8; PA 26:4-26:4; [M-H]-
2.57	538.318	PC 16:1e; PC 14:1e/2:0; [M+FA-H]-
5.82	710.4338	PC 29:6e; PC 22:6e/7:0; [M+FA-H]-
6.87	804.572	PC 34:1; PC 16:0-18:1; [M+FA-H]-
6.53	802.5593	PC 34:2; PC 16:0-18:2; [M+FA-H]-
7.36	832.5991	PC 36:1; PC 17:0-19:1; [M+FA-H]-

6.82	830.5889	PC 36:2; PC 18:0-18:2; [M+FA-H]-
6.51	828.569	PC 36:3; PC 16:0-20:3; [M+FA-H]-
6.57	826.5565	PC 36:4; PC 16:0-20:4; [M+FA-H]-
7.22	824.5411	PC 36:5; PC 14:0-22:5; [M+FA-H]-
4.76	802.501	PC 36:9e; PC 20:5e/16:4; [M+FA-H]-
7.21	848.6301	PC 37:0; PC 13:0-24:0; [M+FA-H]-
6.99	854.5801	PC 38:4; PC 18:0-20:4; [M+FA-H]-
4.37	830.5316	PC 38:9e; PC 20:4e/18:5; [M+FA-H]-
4.76	930.6204	PC 44:8; PC 22:4-22:4; [M+FA-H]-
2.9	452.2789	PE 16:0e; PE 14:0e/2:0; [M-H]-
2.67	464.2816	PE 17:1e; PE 14:1e/3:0; [M-H]-
2.97	480.3084	PE 18:0e; PE 16:0e/2:0; [M-H]-
3.93	490.2469	PE 18:2; PE 2:0-16:2; [M-H]-
2.91	522.3219	PE 20:0; PE 5:0-15:0; [M-H]-
3	520.3073	PE 20:1; PE 6:0-14:1; [M-H]-
3.87	536.3392	PE 21:0; PE 7:0-14:0; [M-H]-
4.52	532.2897	PE 21:2; PE 3:0-18:2; [M-H]-
4.72	518.3334	PE 21:2e; PE 16:2e/5:0; [M-H]-
4.51	516.3115	PE 21:3e; PE 18:3e/3:0; [M-H]-
2.92	528.2775	PE 21:4; PE 5:0-16:4; [M-H]-
4.8	546.319	PE 22:2; PE 2:0-20:2; [M-H]-
5.09	546.3052	PE 22:2; PE 6:0-16:2; [M-H]-
1.83	532.3453	PE 22:2e; PE 18:2e/4:0; [M-H]-
4.08	564.3707	PE 23:0; PE 8:0-15:0; [M-H]-
3.93	568.2957	PE 24:5; PE 4:0-20:5; [M-H]-
3.2	590.3836	PE 25:1; PE 10:0-15:1; [M-H]-
3.62	576.4034	PE 25:1e; PE 16:1e/9:0; [M-H]-
4.36	574.3979	PE 25:2e; PE 18:2e/7:0; [M-H]-
4.14	582.314	PE 25:5; PE 3:0-22:5; [M-H]-
2.04	586.3917	PE 26:3e; PE 22:3e/4:0; [M-H]-
3.86	596.3252	PE 26:5; PE 4:0-22:5; [M-H]-
2.57	600.4056	PE 27:3e; PE 22:3e/5:0; [M-H]-
2.43	616.4374	PE 28:2e; PE 14:1e/14:1; [M-H]-
5.23	648.4593	PE 29:0; PE 14:0-15:0; [M-H]-
5.94	634.4779	PE 29:0e; PE 14:0e/15:0; [M-H]-
5.13	642.4591	PE 30:3e; PE 18:3e/12:0; [M-H]-
6.89	642.4546	PE 30:3e; PE 22:3e/8:0; [M-H]-
5.77	676.4924	PE 31:0; PE 6:0-25:0; [M-H]-
6.43	662.5117	PE 31:0e; PE 16:0e/15:0; [M-H]-
5.43	672.4601	PE 31:2; PE 13:0-18:2; [M-H]-
6.21	664.4426	PE 32:6e; PE 16:2e/16:4; [M-H]-
6.03	678.4559	PE 33:6e; PE 22:6e/11:0; [M-H]-
4.02	694.4747	PE 34:5e; PE 14:0e/20:5; [M-H]-
4.04	692.4662	PE 34:6e; PE 14:1e/20:5; [M-H]-
4.7	692.4653	PE 34:6e; PE 22:6e/12:0; [M-H]-
5.87	712.529	PE 35:3e; PE 18:1e/17:2; [M-H]-
5.81	710.5197	PE 35:4e; PE 20:4e/15:0; [M-H]-
3.82	722.4736	PE 35:5; PE 13:1-22:4; [M-H]-
4.83	720.4617	PE 35:6; PE 13:0-22:6; [M-H]-
5.39	720.4681	PE 35:6; PE 15:1-20:5; [M-H]-
3.97	706.4811	PE 35:6e; PE 22:6e/13:0; [M-H]-
6.9	744.5522	PE 36:1; PE 18:0-18:1; [M-H]-
3.92	736.4902	PE 36:5; PE 16:1-20:4; [M-H]-
5.57	762.5154	PE 38:6; PE 18:1-20:5; [M-H]-
7.64	768.5824	PE 39:3e; PE 18:3e/21:0; [M-H]-
5.37	794.5742	PE 40:4; PE 16:0-24:4; [M-H]-

6.56	780.5847	PE 40:4e; PE 22:3e/18:1; [M-H]-
6.44	778.5813	PE 40:5e; PE 18:0e/22:5; [M-H]-
5.39	784.4921	PE 40:9; PE 20:4-20:5; [M-H]-
6.7	808.5805	PE 41:4; PE 15:0-26:4; [M-H]-
6.28	820.5244	PE 44:12e; PE 22:6e/22:6; [M-H]-
6.38	848.6224	PE 44:5; PE 18:1-26:4; [M-H]-
6.63	930.7006	PE 50:6; PE 26:2-24:4; [M-H]-
3.2	563.3635	PEtOH 24:0; PEtOH 12:0-12:0; [M-H]-
3.87	603.4037	PEtOH 27:1; PEtOH 14:0-13:1; [M-H]-
4.59	619.4352	PEtOH 28:0; PEtOH 14:0-14:0; [M-H]-
4.02	643.4348	PEtOH 30:2; PEtOH 14:1-16:1; [M-H]-
4.28	643.4358	PEtOH 30:2; PEtOH 15:1-15:1; [M-H]-
4.08	641.4208	PEtOH 30:3; PEtOH 14:1-16:2; [M-H]-
4.7	657.4499	PEtOH 31:2; PEtOH 13:1-18:1; [M-H]-
4.06	657.4498	PEtOH 31:2; PEtOH 14:1-17:1; [M-H]-
3.82	655.4362	PEtOH 31:3; PEtOH 15:1-16:2; [M-H]-
4.57	671.465	PEtOH 32:2; PEtOH 16:1-16:1; [M-H]-
5.61	761.5099	PEtOH 39:6; PEtOH 19:2-20:4; [M-H]-
6.78	781.5732	PEtOH 40:3; PEtOH 24:1-16:2; [M-H]-
5.9	775.526	PEtOH 40:6; PEtOH 20:3-20:3; [M-H]-
5.89	807.5874	PEtOH 42:4; PEtOH 21:2-21:2; [M-H]-
6.58	817.5784	PEtOH 43:6; PEtOH 19:2-24:4; [M-H]-
6.38	815.5577	PEtOH 43:7; PEtOH 21:2-22:5; [M-H]-
6.24	829.5742	PEtOH 44:7; PEtOH 24:2-20:5; [M-H]-
8.62	891.6869	PEtOH 48:4; PEtOH 26:1-22:3; [M-H]-
6.94	915.6832	PEtOH 50:6; PEtOH 24:2-26:4; [M-H]-
2.59	539.3056	PG 19:0; PG 9:0-10:0; [M-H]-
2.44	553.3187	PG 20:0; PG 9:0-11:0; [M-H]-
5.52	593.3417	PG 23:1; PG 3:0-20:1; [M-H]-
6.04	593.3389	PG 23:1; PG 5:0-18:1; [M-H]-
5.73	591.3242	PG 23:2; PG 2:0-21:2; [M-H]-
3.37	603.3292	PG 24:3; PG 2:0-22:3; [M-H]-
6.02	677.4284	PG 29:1; PG 11:0-18:1; [M-H]-
3.83	675.4288	PG 29:2; PG 13:1-16:1; [M-H]-
4.05	671.3913	PG 29:4; PG 5:0-24:4; [M-H]-
6.19	691.4426	PG 30:1; PG 14:0-16:1; [M-H]-
4.33	689.4402	PG 30:2; PG 10:0-20:2; [M-H]-
5.83	709.4075	PG 32:6; PG 16:3-16:3; [M-H]-
4.72	725.444	PG 33:5; PG 15:1-18:4; [M-H]-
4	723.4182	PG 33:6; PG 11:0-22:6; [M-H]-
3.67	723.4218	PG 33:6; PG 17:2-16:4; [M-H]-
4.6	743.4999	PG 34:3; PG 14:0-20:3; [M-H]-
6.72	763.5539	PG 35:0; PG 9:0-26:0; [M-H]-
4.94	757.4999	PG 35:3; PG 13:1-22:2; [M-H]-
4.54	751.4551	PG 35:6; PG 13:0-22:6; [M-H]-
5.73	777.5786	PG 36:0; PG 17:0-19:0; [M-H]-
6.73	833.6393	PG 40:0; PG 20:0-20:0; [M-H]-
5.84	825.5623	PG 40:4; PG 16:0-24:4; [M-H]-
6.4	845.6381	PG 41:1; PG 27:0-14:1; [M-H]-
7.36	839.5782	PG 41:4; PG 25:0-16:4; [M-H]-
7.76	853.5942	PG 42:4; PG 16:2-26:2; [M-H]-
7.79	851.5789	PG 42:5; PG 16:1-26:4; [M-H]-
8.01	881.624	PG 44:4; PG 20:0-24:4; [M-H]-
8.1	879.6109	PG 44:5; PG 26:1-18:4; [M-H]-
8.34	965.7302	PG 50:4; PG 24:2-26:2; [M-H]-
6.29	599.2897	PI 17:0; PI 5:0-12:0; [M-H]-

6.5	613.3027	PI 18:0; PI 9:0-9:0; [M-H]-
6.65	627.3179	PI 19:0; PI 8:0-11:0; [M-H]-
5.86	641.3214	PI 20:0; PI 10:0-10:0; [M-H]-
6.61	631.2513	PI 20:5; PI 2:0-18:5; [M-H]-
6.34	683.3839	PI 23:0; PI 9:0-14:0; [M-H]-
7.34	809.5236	PI 32:0; PI 16:0-16:0; [M-H]-
6.07	807.4951	PI 32:1; PI 12:0-20:1; [M-H]-
7.44	823.5392	PI 33:0; PI 9:0-24:0; [M-H]-
7.55	837.5554	PI 34:0; PI 17:0-17:0; [M-H]-
5.16	865.579	PI 36:0; PI 10:0-26:0; [M-H]-
6.65	893.6118	PI 38:0; PI 18:0-20:0; [M-H]-
6.26	885.5521	PI 38:4; PI 19:2-19:2; [M-H]-
8.44	949.6769	PI 42:0; PI 17:0-25:0; [M-H]-
8.07	1047.7783	PI 49:0; PI 24:0-25:0; [M-H]-
4.24	575.3961	PMeOH 26:1; PMeOH 12:0-14:1; [M-H]-
3.77	601.3855	PMeOH 28:2; PMeOH 14:1-14:1; [M-H]-
4.11	629.4202	PMeOH 30:2; PMeOH 14:1-16:1; [M-H]-
5.11	703.437	PMeOH 36:7; PMeOH 16:3-20:4; [M-H]-
4.49	701.4249	PMeOH 36:8; PMeOH 18:4-18:4; [M-H]-
4.8	725.4235	PMeOH 38:10; PMeOH 18:5-20:5; [M-H]-
5.51	759.4957	PMeOH 40:7; PMeOH 22:2-18:5; [M-H]-
5.73	791.5576	PMeOH 42:5; PMeOH 20:1-22:4; [M-H]-
6.65	783.4962	PMeOH 42:9; PMeOH 20:3-22:6; [M-H]-
6.62	815.5591	PMeOH 44:7; PMeOH 22:1-22:6; [M-H]-
6.77	813.5434	PMeOH 44:8; PMeOH 22:4-22:4; [M-H]-
6.4	811.5266	PMeOH 44:9; PMeOH 24:4-20:5; [M-H]-
7.22	847.6261	PMeOH 46:5; PMeOH 24:0-22:5; [M-H]-
6.53	843.5895	PMeOH 46:7; PMeOH 20:3-26:4; [M-H]-
6.66	867.585	PMeOH 48:9; PMeOH 26:4-22:5; [M-H]-
6.6	929.6949	PMeOH 52:6; PMeOH 26:2-26:4; [M-H]-
4.6	630.3476	PS 25:3; PS 5:0-20:3; [M-H]-
6.09	678.4382	PS 28:0; PS 13:0-15:0; [M-H]-
4.36	710.4035	PS 31:5; PS 9:0-22:5; [M-H]-
4.69	708.3926	PS 31:6; PS 9:0-22:6; [M-H]-
4.61	724.4221	PS 32:5; PS 10:0-22:5; [M-H]-
7.07	742.4598	PS 33:3; PS 13:0-20:3; [M-H]-
7.88	854.5961	PS 41:3; PS 19:1-22:2; [M-H]-
3.99	297.2453	Ricinoleic acid
4.58	664.3855	SHexCer d26:2; [M-H]-
5.43	694.4133	SHexCer d28:1; [M-H]-
5.4	720.4339	SHexCer d30:2; [M-H]-
5.49	736.4553	SHexCer d31:1; [M-H]-
5.26	732.4462	SHexCer d31:3; [M-H]-
5.52	818.5316	SHexCer d37:2; [M-H]-
8.42	920.6796	SHexCer d44:0; [M-H]-
6.39	635.4495	SM d26:1; SM d14:0/12:1; [M+FA-H]-
3.71	633.4202	SM d26:2; SM d14:2/12:0; [M+FA-H]-
6.93	651.4777	SM d27:0; SM d14:0/13:0; [M+FA-H]-
4.08	649.4461	SM d27:1; SM d14:1/13:0; [M+FA-H]-
6.36	647.4469	SM d27:2; SM d14:1/13:1; [M+FA-H]-
3.92	661.4447	SM d28:2; SM d16:2/12:0; [M+FA-H]-
6.79	691.5032	SM d30:1; SM d16:0/14:1; [M+FA-H]-
6.92	689.4907	SM d30:2; SM d14:0/16:2; [M+FA-H]-
7.3	705.5204	SM d31:1; SM d19:0/12:1; [M+FA-H]-
4.02	701.483	SM d31:3; SM d15:1/16:2; [M+FA-H]-
4.78	717.5062	SM d32:2; SM d20:2/12:0; [M+FA-H]-

7.23	749.5853	SM d34:0; SM d17:0/17:0; [M+FA-H]-
8.54	749.5832	SM d34:0; SM d21:0/13:0; [M+FA-H]-
6.6	761.5782	SM d35:1; SM d19:1/16:0; [M+FA-H]-
7.93	759.5673	SM d35:2; SM d22:1/13:1; [M+FA-H]-
6.87	775.5937	SM d36:1; SM d19:1/17:0; [M+FA-H]-
7.62	817.6441	SM d39:1; SM d20:1/19:0; [M+FA-H]-
9.92	873.7043	SM d43:1; SM d22:1/21:0; [M+FA-H]-
8.6	931.7809	SM d47:0; SM d17:0/30:0; [M+FA-H]-
3.82	721.4098	SQDG 27:1; SQDG 12:0-15:1; [M-H]-
5.93	741.3986	SQDG 29:5; SQDG 13:1-16:4; [M-H]-
4.14	755.3959	SQDG 30:5; SQDG 12:0-18:5; [M-H]-
4.67	775.4549	SQDG 31:2; SQDG 15:1-16:1; [M-H]-
5.29	821.5532	SQDG 34:0; SQDG 12:0-22:0; [M-H]-
7.51	849.5674	SQDG 36:0; SQDG 17:0-19:0; [M-H]-
7.22	847.559	SQDG 36:1; SQDG 14:0-22:1; [M-H]-
7.56	841.4991	SQDG 36:4; SQDG 18:2-18:2; [M-H]-
7.12	863.5823	SQDG 37:0; SQDG 13:0-24:0; [M-H]-