

Table S7. List of all lipid molecular species identified from human skin tissue using capillary UPLC-MS and the HSS T3 material. The chain length denotes the total number of acyl carbons followed by total double bonds.

Molecular Species	Formula	Formula Mass (isotopic)	Expected m/z	Observed m/z	Ion Type	Mass Error (ppm)	Retention Time (min)	Ion Intensity
16:1 Cholesteryl ester	C ₄₃ H ₇₄ O ₂	622.5689	640.6032	640.6015	[M+NH ₄] ⁺	-2.64	67.54	7.74E+04
Cer(d36:3)	C ₃₆ H ₆₇ NO ₃	561.5121	562.5199	562.5169	[M+NH ₄] ⁺	-5.36	47.85	1.12E+05
Cer(d40:1)	C ₄₀ H ₇₉ NO ₃	621.6060	622.6138	622.6118	[M+NH ₄] ⁺	-3.16	52.18	3.53E+05
Cer(d40:2)	C ₄₀ H ₇₇ NO ₃	619.5903	620.5981	620.5951	[M+NH ₄] ⁺	-4.84	50.39	1.89E+05
Cer(d42:0)	C ₄₂ H ₈₅ NO ₃	651.6529	652.6607	652.6596	[M+NH ₄] ⁺	-1.79	56.10	2.39E+05
Cer(d42:1)	C ₄₂ H ₈₃ NO ₃	649.6373	650.6451	650.6446	[M+NH ₄] ⁺	-0.76	58.14	7.49E+05
Cer(d42:2)	C ₄₂ H ₈₁ NO ₃	647.6216	648.6294	648.6269	[M+NH ₄] ⁺	-3.87	50.73	5.17E+05
Cer(d44:1)	C ₄₄ H ₈₇ NO ₃	677.6686	678.6764	678.6745	[M+NH ₄] ⁺	-2.79	58.37	2.06E+06
Cer(d44:2)	C ₄₄ H ₈₅ NO ₃	675.6529	676.6607	676.6597	[M+NH ₄] ⁺	-1.59	57.14	8.45E+05
Cer(t42:0)	C ₄₂ H ₈₅ NO ₄	667.6478	668.6557	668.6541	[M+NH ₄] ⁺	-2.36	55.46	2.50E+05
DG(32:0)	C ₃₅ H ₆₈ O ₅	568.5066	586.5410	586.5380	[M+NH ₄] ⁺	-5.11	48.61	1.42E+05
DG(34:0)	C ₃₇ H ₇₂ O ₅	596.5379	614.5723	614.5710	[M+NH ₄] ⁺	-2.08	53.34	8.21E+04
DG(34:1)	C ₃₇ H ₇₀ O ₅	594.5223	612.5567	612.5537	[M+NH ₄] ⁺	-4.79	49.02	2.31E+05
DG(36:0)	C ₃₉ H ₇₆ O ₅	624.5692	642.6036	642.6024	[M+NH ₄] ⁺	-1.84	54.68	2.55E+05
DG(36:1)	C ₃₉ H ₇₄ O ₅	622.5536	640.5880	640.5841	[M+NH ₄] ⁺	-5.96	50.35	1.01E+05
DG(36:2)	C ₃₉ H ₇₂ O ₅	620.5379	638.5723	638.5694	[M+NH ₄] ⁺	-4.54	48.85	4.10E+05
DG(36:3)	C ₃₉ H ₇₀ O ₅	618.5223	636.5567	636.5536	[M+NH ₄] ⁺	-4.77	44.69	1.19E+05
DG(36:4)	C ₃₉ H ₆₈ O ₅	616.5066	634.5410	634.5398	[M+NH ₄] ⁺	-1.97	43.69	8.38E+04
DG(37:2)	C ₄₀ H ₇₄ O ₅	634.5536	652.5880	652.5927	[M+NH ₄] ⁺	7.31	55.08	1.75E+04
DG(38:0)	C ₄₁ H ₈₀ O ₅	652.6005	670.6349	670.6393	[M+NH ₄] ⁺	6.48	69.26	8.30E+04
DG(38:1)	C ₄₁ H ₇₈ O ₅	650.5849	668.6193	668.6175	[M+NH ₄] ⁺	-2.70	56.50	3.54E+04
DG(38:2)	C ₄₁ H ₇₆ O ₅	648.5692	666.6036	666.6028	[M+NH ₄] ⁺	-1.28	51.54	3.72E+04
DG(38:4)	C ₄₁ H ₇₂ O ₅	644.5379	662.5723	662.5695	[M+NH ₄] ⁺	-4.22	48.54	2.92E+05
DG(40:1)	C ₄₃ H ₈₂ O ₅	678.6162	696.6506	696.6487	[M+NH ₄] ⁺	-2.68	57.95	6.84E+04

DG(42:1)	C ₄₅ H ₈₆ O ₅	706.6475	724.6819	724.6804	[M+NH ₄] ⁺	-2.00	59.19	6.55E+04
FA(14:0)	C ₁₄ H ₂₈ O ₂	228.2089	227.2011	227.2018	[M-H] ⁻	3.07	18.95	7.56E+05
FA(16:0)	C ₁₆ H ₃₂ O ₂	256.2402	255.2324	255.2330	[M-H] ⁻	2.34	22.46	1.46E+07
FA(16:1)	C ₁₆ H ₃₀ O ₂	254.2246	253.2167	253.2175	[M-H] ⁻	2.95	18.60	7.78E+04
FA(17:0)	C ₁₇ H ₃₄ O ₂	270.2559	269.2480	269.2494	[M-H] ⁻	4.92	23.94	1.89E+06
FA(17:1)	C ₁₇ H ₃₂ O ₂	268.2402	267.2324	267.2324	[M-H] ⁻	0.07	22.24	6.67E+04
FA(18:0)	C ₁₈ H ₃₆ O ₂	284.2715	283.2637	283.2641	[M-H] ⁻	1.44	26.26	1.45E+07
FA(18:1)	C ₁₈ H ₃₄ O ₂	282.2559	281.2480	281.2487	[M-H] ⁻	2.34	22.85	1.61E+06
FA(18:2)	C ₁₈ H ₃₂ O ₂	280.2402	279.2324	279.2337	[M-H] ⁻	4.78	17.92	5.38E+04
FA(18:3)	C ₁₈ H ₃₀ O ₂	278.2246	277.2167	277.2182	[M-H] ⁻	5.07	17.91	8.69E+04
FA(19:0)	C ₁₉ H ₃₈ O ₂	298.2872	297.2793	297.2805	[M-H] ⁻	3.99	27.98	3.85E+05
FA(20:0)	C ₂₀ H ₄₀ O ₂	312.3028	311.2950	311.2963	[M-H] ⁻	4.35	29.41	3.82E+05
FA(20:1)	C ₂₀ H ₃₈ O ₂	310.2872	309.2794	309.2796	[M-H] ⁻	0.87	25.61	3.23E+05
FA(20:2)	C ₂₀ H ₃₆ O ₂	308.2715	307.2637	307.2644	[M-H] ⁻	2.21	22.99	5.74E+04
FA(20:3)	C ₂₀ H ₃₄ O ₂	306.2559	305.2481	305.2492	[M-H] ⁻	3.59	21.50	6.02E+04
FA(20:4)	C ₂₀ H ₃₂ O ₂	304.2402	303.2324	303.2334	[M-H] ⁻	3.22	19.92	1.48E+05
FA(20:5)	C ₂₀ H ₃₀ O ₂	302.2246	301.2167	301.2178	[M-H] ⁻	3.37	19.94	1.39E+05
FA(21:0)	C ₂₁ H ₄₂ O ₂	326.3185	325.3106	325.3112	[M-H] ⁻	1.87	26.01	2.51E+04
FA(22:0)	C ₂₂ H ₄₄ O ₂	340.3341	339.3263	339.3276	[M-H] ⁻	4.00	35.24	1.68E+05
FA(22:1)	C ₂₂ H ₄₂ O ₂	338.3185	337.3106	337.3123	[M-H] ⁻	4.94	30.16	1.45E+05
FA(22:3)	C ₂₂ H ₃₈ O ₂	334.2872	333.2793	333.2804	[M-H] ⁻	3.14	24.64	5.68E+04
FA(22:4)	C ₂₂ H ₃₆ O ₂	332.2715	331.2637	331.2641	[M-H] ⁻	1.11	21.91	3.65E+04
FA(22:5)	C ₂₂ H ₃₄ O ₂	330.2559	329.2481	329.2492	[M-H] ⁻	3.42	19.97	4.92E+04
FA(22:6)	C ₂₂ H ₃₂ O ₂	328.2402	327.2324	327.2331	[M-H] ⁻	2.16	18.39	6.99E+04
FA(24:0)	C ₂₄ H ₄₈ O ₂	368.3654	367.3576	367.3588	[M-H] ⁻	3.42	41.57	6.34E+05
FA(24:1)	C ₂₄ H ₄₆ O ₂	366.3497	365.3419	365.3431	[M-H] ⁻	3.41	34.11	9.50E+05
FA(25:0)	C ₂₅ H ₅₀ O ₂	382.3811	381.3732	381.3745	[M-H] ⁻	3.24	44.46	3.95E+04
FA(26:0)	C ₂₆ H ₅₂ O ₂	396.3967	395.3889	395.3900	[M-H] ⁻	2.77	47.94	6.89E+05
FA(26:1)	C ₂₆ H ₅₀ O ₂	394.3811	393.3732	393.3745	[M-H] ⁻	3.17	39.37	3.58E+05
LPA(14:0)	C ₁₇ H ₃₅ O ₇ P	382.2120	381.2042	381.2055	[M-H] ⁻	3.32	10.29	1.79E+04

LPA(17:0)	C ₂₀ H ₄₁ O ₇ P	424.2590	423.2512	423.2524	[M-H] ⁻	2.99	12.72	3.38E+04
LPA(18:2)	C ₂₁ H ₃₉ O ₇ P	434.2433	433.2355	433.2368	[M-H] ⁻	3.09	12.12	2.61E+04
LPA(20:4)	C ₂₃ H ₃₉ O ₇ P	458.2433	457.2355	457.2374	[M-H] ⁻	4.10	11.16	3.79E+04
LPC(14:0) or PC(O-14:0)	C ₂₂ H ₄₆ NO ₇ P	467.3012	468.3090	468.3090	[M+H] ⁺	0.11	13.30	5.39E+05
LPC(16:0)	C ₂₄ H ₅₀ NO ₇ P	495.3325	496.3403	496.3399	[M+H] ⁺	-0.75	16.22	1.66E+07
LPC(16:1)	C ₂₄ H ₄₈ NO ₇ P	493.3168	494.3246	494.3239	[M+H] ⁺	-1.51	13.73	1.93E+06
LPC(17:0) or PC(O-17:0)	C ₂₅ H ₅₂ NO ₇ P	509.3481	510.3559	510.3555	[M+H] ⁺	-0.97	18.07	1.44E+05
LPC(17:1)	C ₂₅ H ₅₀ NO ₇ P	507.3325	508.3403	508.3397	[M+H] ⁺	-1.09	15.24	7.79E+04
LPC(18:0)	C ₂₆ H ₅₄ NO ₇ P	523.3638	524.3716	524.3695	[M+H] ⁺	-3.96	19.26	2.33E+06
LPC(18:1) or PC(O-18:1) or PC(P-18:0)	C ₂₆ H ₅₂ NO ₇ P	521.3481	522.3559	522.3556	[M+H] ⁺	-0.62	16.09	2.39E+06
LPC(18:2)	C ₂₆ H ₅₀ NO ₇ P	519.3325	520.3403	520.3398	[M+H] ⁺	-0.92	14.91	5.37E+05
LPC(18:3)	C ₂₆ H ₄₈ NO ₇ P	517.3168	518.3246	518.3226	[M+H] ⁺	-3.96	13.70	1.38E+05
LPC(20:1) or PC(O-20:1) or PC(P-20:0)	C ₂₈ H ₅₆ NO ₇ P	549.3794	550.3872	550.3864	[M+H] ⁺	-1.55	19.58	2.98E+05
LPC(20:2)	C ₂₈ H ₅₄ NO ₇ P	547.3638	548.3716	548.3700	[M+H] ⁺	-2.82	17.69	6.03E+04
LPC(20:3)	C ₂₈ H ₅₂ NO ₇ P	545.3481	546.3559	546.3520	[M+H] ⁺	-7.24	16.96	2.97E+05
LPC(20:4)	C ₂₈ H ₅₀ NO ₇ P	543.3325	544.3403	544.3395	[M+H] ⁺	-1.47	14.36	2.05E+06
LPC(22:6)	C ₃₀ H ₅₀ NO ₇ P	567.3325	568.3403	568.3395	[M+H] ⁺	-1.38	12.97	2.56E+05
LPC(O-17:0) or PC(O-16:0/O-1:0)	C ₂₅ H ₅₄ NO ₆ P	495.3689	496.3767	496.3757	[M+H] ⁺	-1.94	12.80	4.14E+04
LPC(O-18:1) or LPC(P-18:0)	C ₂₆ H ₅₄ NO ₆ P	507.3689	508.3767	508.3758	[M+H] ⁺	-1.70	17.96	1.00E+05
LPC(P-18:1)	C ₂₆ H ₅₂ NO ₆ P	505.3532	506.3610	506.3593	[M+H] ⁺	-3.36	17.71	1.21E+05
LPE(16:0)	C ₂₁ H ₄₄ NO ₇ P	453.2855	454.2933	454.2930	[M+H] ⁺	-0.79	16.69	5.97E+05
LPE(16:1)	C ₂₁ H ₄₂ NO ₇ P	451.2699	452.2777	452.2768	[M+H] ⁺	-2.09	14.11	8.88E+04
LPE(18:0)	C ₂₃ H ₄₈ NO ₇ P	481.3168	482.3246	482.3239	[M+H] ⁺	-1.61	19.27	6.05E+05
LPE(18:1)	C ₂₃ H ₄₆ NO ₇ P	479.3012	480.3090	480.3069	[M+H] ⁺	-4.46	17.47	4.08E+05
LPE(18:2)	C ₂₃ H ₄₄ NO ₇ P	477.2855	478.2933	478.2923	[M+H] ⁺	-2.27	14.75	7.78E+04
LPE(20:1)	C ₂₅ H ₅₀ NO ₇ P	507.3325	508.3403	508.3404	[M+H] ⁺	0.25	19.93	6.70E+04
LPE(20:3)	C ₂₅ H ₄₆ NO ₇ P	503.3012	504.3090	504.3084	[M+H] ⁺	-1.12	15.74	4.68E+04
LPE(22:6)	C ₂₇ H ₄₄ NO ₇ P	525.2855	526.2933	526.2929	[M+H] ⁺	-0.76	14.00	1.12E+05
LPG(18:1)	C ₂₄ H ₄₇ O ₉ P	510.2958	509.2879	509.2900	[M-H] ⁻	4.15	14.16	2.53E+04
LPG(20:4)	C ₂₆ H ₄₅ O ₉ P	532.2801	531.2723	531.2741	[M-H] ⁻	3.42	12.56	1.89E+04

LPI(18:0)	C ₂₇ H ₅₃ O ₁₂ P	600.3275	599.3196	599.3218	[M-H] ⁻	3.70	15.76	3.61E+04
LPI(20:3)	C ₂₉ H ₅₁ O ₁₂ P	622.3118	621.3040	621.3063	[M-H] ⁻	3.66	13.64	1.23E+04
LPI(20:4)	C ₂₉ H ₄₉ O ₁₂ P	620.2962	619.2883	619.2901	[M-H] ⁻	2.92	11.66	2.92E+04
LPS(18:0)	C ₂₄ H ₄₈ NO ₉ P	525.3067	526.3145	526.3143	[M+H] ⁺	-0.24	15.32	7.86E+04
LPS(20:3)	C ₂₆ H ₄₆ NO ₉ P	547.2910	548.2988	548.2989	[M+H] ⁺	0.12	13.39	1.90E+04
LPS(20:4)	C ₂₆ H ₄₄ NO ₉ P	545.2754	546.2832	546.2829	[M+H] ⁺	-0.55	12.43	1.14E+05
PC(28:0)	C ₃₆ H ₇₂ NO ₈ P	677.4995	678.5074	678.5052	[M+H] ⁺	-3.12	29.15	4.77E+06
PC(29:0)	C ₃₇ H ₇₄ NO ₈ P	691.5152	692.5230	692.5216	[M+H] ⁺	-2.10	30.58	1.13E+06
PC(29:1)	C ₃₇ H ₇₂ NO ₈ P	689.4995	690.5074	690.5064	[M+H] ⁺	-1.37	30.52	3.88E+04
PC(30:0)	C ₃₈ H ₇₆ NO ₈ P	705.5308	706.5387	706.5356	[M+H] ⁺	-4.26	32.85	2.38E+07
PC(30:1)	C ₃₈ H ₇₄ NO ₈ P	703.5152	704.5230	704.5218	[M+H] ⁺	-1.68	27.67	1.23E+06
PC(31:0)	C ₃₉ H ₇₈ NO ₈ P	719.5465	720.5543	720.5526	[M+H] ⁺	-2.32	33.64	2.76E+06
PC(31:2)	C ₃₉ H ₇₄ NO ₈ P	715.5152	716.5230	716.5212	[M+H] ⁺	-2.56	33.23	2.23E+05
PC(32:0)	C ₄₀ H ₈₀ NO ₈ P	733.5621	734.5700	734.5677	[M+H] ⁺	-3.10	38.57	3.08E+07
PC(32:1)	C ₄₀ H ₇₈ NO ₈ P	731.5465	732.5543	732.5521	[M+H] ⁺	-2.99	33.34	4.64E+07
PC(32:2)	C ₄₀ H ₇₆ NO ₈ P	729.5308	730.5387	730.5366	[M+H] ⁺	-2.85	30.89	7.72E+06
PC(32:3)	C ₄₀ H ₇₄ NO ₈ P	727.5152	728.5230	728.5199	[M+H] ⁺	-4.20	28.83	1.18E+06
PC(33:0)	C ₄₁ H ₈₂ NO ₈ P	747.5778	748.5856	748.5824	[M+H] ⁺	-4.27	39.23	3.99E+05
PC(33:3)	C ₄₁ H ₇₆ NO ₈ P	741.5308	742.5387	742.5374	[M+H] ⁺	-1.69	34.54	2.51E+05
PC(33:4)	C ₄₁ H ₇₄ NO ₈ P	739.5152	740.5230	740.5197	[M+H] ⁺	-4.40	34.50	1.49E+06
PC(33:5)	C ₄₁ H ₇₂ NO ₈ P	737.4995	738.5074	738.5042	[M+H] ⁺	-4.27	31.03	2.09E+05
PC(34:0)	C ₄₂ H ₈₄ NO ₈ P	761.5934	762.6012	762.5988	[M+H] ⁺	-3.24	45.55	6.05E+06
PC(34:1)	C ₄₂ H ₈₂ NO ₈ P	759.5778	760.5856	760.5814	[M+H] ⁺	-5.52	32.84	5.38E+07
PC(34:2)	C ₄₂ H ₈₀ NO ₈ P	757.5621	758.5700	758.5673	[M+H] ⁺	-3.52	33.35	4.44E+07
PC(34:3)	C ₄₂ H ₇₈ NO ₈ P	755.5465	756.5543	756.5518	[M+H] ⁺	-3.32	29.57	1.68E+06
PC(34:4)	C ₄₂ H ₇₆ NO ₈ P	753.5308	754.5387	754.5367	[M+H] ⁺	-2.62	30.02	1.47E+06
PC(35:1)	C ₄₃ H ₈₄ NO ₈ P	773.5934	774.6012	774.5980	[M+H] ⁺	-4.23	40.66	1.12E+06
PC(35:2)	C ₄₃ H ₈₂ NO ₈ P	771.5778	772.5856	772.5823	[M+H] ⁺	-4.30	32.14	8.35E+05
PC(35:3)	C ₄₃ H ₈₀ NO ₈ P	769.5621	770.5700	770.5667	[M+H] ⁺	-4.18	34.73	3.07E+05
PC(35:4)	C ₄₃ H ₇₈ NO ₈ P	767.5465	768.5543	768.5508	[M+H] ⁺	-4.58	37.51	9.32E+05

PC(35:5)	C43H76NO8P	765.5308	766.5387	766.5350	[M+H] ⁺	-4.83	35.08	1.53E+06
PC(35:6)	C43H74NO8P	763.5152	764.5230	764.5202	[M+H] ⁺	-3.67	31.55	1.71E+05
PC(36:0)	C44H88NO8P	789.6247	790.6325	790.6382	[M+H] ⁺	7.17	46.85	3.58E+04
PC(36:1)	C44H86NO8P	787.6091	788.6169	788.6134	[M+H] ⁺	-4.42	46.09	1.99E+07
PC(36:2)	C44H84NO8P	785.5934	786.6012	786.5970	[M+H] ⁺	-5.44	38.21	4.19E+07
PC(36:3)	C44H82NO8P	783.5778	784.5856	784.5801	[M+H] ⁺	-7.05	34.39	2.39E+07
PC(36:4)	C44H80NO8P	781.5621	782.5700	782.5670	[M+H] ⁺	-3.77	33.63	5.56E+07
PC(36:5)	C44H78NO8P	779.5465	780.5543	780.5512	[M+H] ⁺	-3.99	30.18	3.20E+06
PC(36:6)	C44H76NO8P	777.5308	778.5387	778.5367	[M+H] ⁺	-2.50	28.46	2.87E+05
PC(37:1)	C45H88NO8P	801.6247	802.6325	802.6297	[M+H] ⁺	-3.53	47.65	1.76E+05
PC(37:2)	C45H86NO8P	799.6091	800.6169	800.6137	[M+H] ⁺	-3.99	40.42	1.63E+05
PC(37:3)	C45H84NO8P	797.5934	798.6012	798.5968	[M+H] ⁺	-5.54	38.23	2.43E+05
PC(37:4)	C45H82NO8P	795.5778	796.5856	796.5835	[M+H] ⁺	-2.63	43.72	9.37E+05
PC(37:5)	C45H80NO8P	793.5621	794.5700	794.5666	[M+H] ⁺	-4.22	32.81	2.25E+05
PC(38:1)	C46H90NO8P	815.6404	816.6482	816.6443	[M+H] ⁺	-4.78	50.42	1.78E+05
PC(38:2)	C46H88NO8P	813.6247	814.6325	814.6294	[M+H] ⁺	-3.91	38.91	1.39E+06
PC(38:3)	C46H86NO8P	811.6091	812.6169	812.6146	[M+H] ⁺	-2.81	36.03	3.37E+06
PC(38:4)	C46H84NO8P	809.5934	810.6012	810.5977	[M+H] ⁺	-4.36	36.02	2.08E+07
PC(38:5)	C46H82NO8P	807.5778	808.5856	808.5814	[M+H] ⁺	-5.14	34.30	2.75E+07
PC(38:6)	C46H80NO8P	805.5621	806.5700	806.5671	[M+H] ⁺	-3.55	31.06	3.02E+06
PC(40:2)	C48H92NO8P	841.6560	842.6638	842.6614	[M+H] ⁺	-2.94	47.33	2.54E+05
PC(40:3)	C48H90NO8P	839.6404	840.6482	840.6467	[M+H] ⁺	-1.76	41.60	3.31E+05
PC(40:4)	C48H88NO8P	837.6247	838.6325	838.6287	[M+H] ⁺	-4.60	36.91	1.87E+06
PC(40:5)	C48H86NO8P	835.6091	836.6169	836.6124	[M+H] ⁺	-5.36	37.27	2.84E+06
PC(40:6)	C48H84NO8P	833.5934	834.6012	834.5967	[M+H] ⁺	-5.48	34.68	3.44E+06
PC(40:7)	C48H82NO8P	831.5778	832.5856	832.5815	[M+H] ⁺	-4.95	33.49	8.23E+05
PC(40:8)	C48H80NO8P	829.5621	830.5700	830.5668	[M+H] ⁺	-3.82	29.98	1.71E+05
PC(41:3)	C49H92NO8P	853.6560	854.6638	854.6609	[M+H] ⁺	-3.50	23.96	2.20E+05
PC(42:10)	C50H80NO8P	853.5621	854.5700	854.5635	[M+H] ⁺	-7.54	27.18	7.95E+04
PC(42:11)	C50H78NO8P	851.5465	852.5543	852.5595	[M+H] ⁺	6.15	27.26	4.20E+05

PC(42:2)	C ₅₀ H ₉₆ NO ₈ P	869.6873	870.6951	870.6936	[M+H] ⁺	-1.76	52.95	1.21E+05
PC(42:3)	C ₅₀ H ₉₄ NO ₈ P	867.6717	868.6795	868.6778	[M+H] ⁺	-1.96	47.26	6.31E+04
PC(42:4)	C ₅₀ H ₉₂ NO ₈ P	865.6560	866.6638	866.6608	[M+H] ⁺	-3.53	48.15	2.00E+05
PC(42:5)	C ₅₀ H ₉₀ NO ₈ P	863.6404	864.6482	864.6444	[M+H] ⁺	-4.37	38.64	2.00E+05
PC(42:6)	C ₅₀ H ₈₈ NO ₈ P	861.6247	862.6325	862.6284	[M+H] ⁺	-4.80	38.69	3.30E+05
PC(42:7)	C ₅₀ H ₈₆ NO ₈ P	859.6091	860.6169	860.6126	[M+H] ⁺	-4.93	36.40	4.16E+05
PC(42:8)	C ₅₀ H ₈₄ NO ₈ P	857.5934	858.6012	858.5971	[M+H] ⁺	-4.88	33.74	4.81E+05
PC(44:12)	C ₅₂ H ₈₀ NO ₈ P	877.5621	878.5700	878.5743	[M+H] ⁺	4.92	28.05	2.07E+05
PC(44:8)	C ₅₂ H ₈₈ NO ₈ P	885.6247	886.6325	886.6289	[M+H] ⁺	-4.14	36.60	3.80E+05
PC(O-16:0)	C ₂₄ H ₅₀ NO ₇ P	495.3325	496.3403	496.3395	[M+H] ⁺	-1.62	13.78	1.47E+06
PC(O-18:0)	C ₂₆ H ₅₄ NO ₇ P	523.3638	524.3716	524.3695	[M+H] ⁺	-3.96	17.11	2.33E+06
PC(O-30:0)	C ₃₈ H ₇₈ NO ₇ P	691.5516	692.5594	692.5572	[M+H] ⁺	-3.11	36.61	4.00E+05
PC(O-30:1) or PC(P-30:0)	C ₃₈ H ₇₆ NO ₇ P	689.5359	690.5437	690.5400	[M+H] ⁺	-5.40	35.50	4.17E+05
PC(O-32:1) or PC(P-32:0)	C ₄₀ H ₈₀ NO ₇ P	717.5672	718.5750	718.5736	[M+H] ⁺	-2.05	42.06	2.14E+06
PC(O-32:2) or PC(P-32:1)	C ₄₀ H ₇₈ NO ₇ P	715.5516	716.5594	716.5571	[M+H] ⁺	-3.15	36.81	4.84E+05
PC(O-34:2) or PC(P-34:1)	C ₄₂ H ₈₂ NO ₇ P	743.5829	744.5907	744.5875	[M+H] ⁺	-4.29	39.47	7.41E+05
PC(O-36:2) or PC(P-36:1)	C ₄₄ H ₈₆ NO ₇ P	771.6142	772.6220	772.6194	[M+H] ⁺	-3.29	41.13	2.71E+05
PC(O-36:4) or PC(P-36:3)	C ₄₄ H ₈₂ NO ₇ P	767.5829	768.5907	768.5892	[M+H] ⁺	-1.93	34.41	9.47E+05
PC(O-36:5) or PC(P-36:4)	C ₄₄ H ₈₀ NO ₇ P	765.5672	766.5750	766.5721	[M+H] ⁺	-3.82	43.38	9.66E+04
PC(O-38:5) or PC(P-38:4)	C ₄₆ H ₈₄ NO ₇ P	793.5985	794.6063	794.6026	[M+H] ⁺	-4.70	36.96	2.88E+06
PC(O-38:6) or PC(P-38:5)	C ₄₆ H ₈₂ NO ₇ P	791.5829	792.5907	792.5872	[M+H] ⁺	-4.45	36.46	8.65E+06
PC(O-40:5) or PC(P-40:4)	C ₄₈ H ₈₈ NO ₇ P	821.6298	822.6376	822.6338	[M+H] ⁺	-4.68	41.88	2.23E+05
PC(O-40:6) or PC(P-40:5)	C ₄₈ H ₈₆ NO ₇ P	819.6142	820.6220	820.6183	[M+H] ⁺	-4.49	40.24	2.89E+05
PC(P-34:4)	C ₄₂ H ₇₆ NO ₇ P	737.5359	738.5437	738.5406	[M+H] ⁺	-4.27	40.41	2.51E+05
PC(P-35:2)	C ₄₃ H ₈₂ NO ₇ P	755.5829	756.5907	756.5885	[M+H] ⁺	-2.91	47.35	1.63E+05
PC(P-40:6)	C ₄₈ H ₈₄ NO ₇ P	817.5985	818.6063	818.6032	[M+H] ⁺	-3.86	35.80	2.32E+05
PE(34:0)	C ₃₉ H ₇₈ NO ₈ P	719.5465	720.5543	720.5538	[M+H] ⁺	-0.66	39.88	2.63E+05
PE(34:1)	C ₃₉ H ₇₆ NO ₈ P	717.5308	718.5387	718.5364	[M+H] ⁺	-3.09	40.03	3.32E+05
PE(34:2)	C ₃₉ H ₇₄ NO ₈ P	715.5152	716.5230	716.5212	[M+H] ⁺	-2.56	33.23	2.23E+05
PE(35:0)	C ₄₀ H ₈₀ NO ₈ P	733.5621	734.5700	734.5671	[M+H] ⁺	-3.85	49.26	4.39E+05
PE(35:1)	C ₄₀ H ₇₈ NO ₈ P	731.5465	732.5543	732.5517	[M+H] ⁺	-3.55	41.09	4.97E+05
PE(36:0)	C ₄₁ H ₈₂ NO ₈ P	747.5778	748.5856	748.5824	[M+H] ⁺	-4.27	39.23	3.99E+05

PE(36:1)	C41H80NO8P	745.5621	746.5700	746.5675	[M+H] ⁺	-3.29	33.49	1.29E+06
PE(36:2)	C41H78NO8P	743.5465	744.5543	744.5518	[M+H] ⁺	-3.43	40.51	7.94E+05
PE(36:3)	C41H76NO8P	741.5308	742.5387	742.5374	[M+H] ⁺	-1.69	34.54	2.51E+05
PE(36:4)	C41H74NO8P	739.5152	740.5230	740.5197	[M+H] ⁺	-4.40	34.50	1.49E+06
PE(36:5)	C41H72NO8P	737.4995	738.5074	738.5042	[M+H] ⁺	-4.27	31.03	2.09E+05
PE(37:1)	C42H82NO8P	759.5778	760.5856	760.5828	[M+H] ⁺	-3.68	42.25	3.91E+06
PE(37:3)	C42H78NO8P	755.5465	756.5543	756.5552	[M+H] ⁺	1.24	27.58	6.83E+04
PE(38:1)	C43H84NO8P	773.5934	774.6012	774.5980	[M+H] ⁺	-4.23	40.66	1.12E+06
PE(38:3)	C43H80NO8P	769.5621	770.5700	770.5667	[M+H] ⁺	-4.18	34.73	3.07E+05
PE(38:4)	C43H78NO8P	767.5465	768.5543	768.5508	[M+H] ⁺	-4.58	37.51	9.32E+05
PE(38:5)	C43H76NO8P	765.5308	766.5387	766.5350	[M+H] ⁺	-4.83	35.08	1.53E+06
PE(38:6)	C43H74NO8P	763.5152	764.5230	764.5202	[M+H] ⁺	-3.67	31.55	1.71E+05
PE(39:1)	C44H86NO8P	787.6091	788.6169	788.6172	[M+H] ⁺	0.43	53.15	1.83E+05
PE(39:2)	C44H84NO8P	785.5934	786.6012	786.5980	[M+H] ⁺	-4.09	41.38	4.49E+06
PE(39:3)	C44H82NO8P	783.5778	784.5856	784.5829	[M+H] ⁺	-3.45	39.38	4.98E+05
PE(39:4)	C44H80NO8P	781.5621	782.5700	782.5646	[M+H] ⁺	-6.90	38.37	9.01E+05
PE(40:1)	C45H88NO8P	801.6247	802.6325	802.6297	[M+H] ⁺	-3.53	47.65	1.76E+05
PE(40:2)	C45H86NO8P	799.6091	800.6169	800.6137	[M+H] ⁺	-3.99	40.42	1.63E+05
PE(40:3)	C45H84NO8P	797.5934	798.6012	798.5968	[M+H] ⁺	-5.54	38.23	2.43E+05
PE(40:4)	C45H82NO8P	795.5778	796.5856	796.5835	[M+H] ⁺	-2.63	43.72	9.37E+05
PE(41:3)	C46H86NO8P	811.6091	812.6169	812.6154	[M+H] ⁺	-1.89	49.38	7.31E+04
PE(41:4)	C46H84NO8P	809.5934	810.6012	810.5998	[M+H] ⁺	-1.79	25.64	2.19E+05
PG(32:1)	C38H73O10P	720.4941	719.4863	719.4898	[M-H] ⁻	4.82	27.20	1.86E+04
PG(34:1)	C40H77O10P	748.5254	747.5176	747.5212	[M-H] ⁻	4.84	29.42	7.41E+04
PG(34:2)	C40H75O10P	746.5098	745.5019	745.5037	[M-H] ⁻	2.30	25.56	2.07E+04
PG(36:2)	C42H79O10P	774.5411	773.5332	773.5347	[M-H] ⁻	1.87	28.97	2.85E+05
PG(36:3)	C42H77O10P	772.5254	771.5176	771.5190	[M-H] ⁻	1.88	26.42	4.01E+04
PG(36:4)	C42H75O10P	770.5098	769.5019	769.5043	[M-H] ⁻	3.02	24.79	3.32E+04
PG(38:3)	C44H81O10P	800.5567	799.5489	799.5512	[M-H] ⁻	2.85	29.17	4.87E+04
PG(38:4)	C44H79O10P	798.5411	797.5332	797.5357	[M-H] ⁻	3.13	28.35	5.30E+04

PG(38:5)	C44H77O10P	796.5254	795.5176	795.5187	[M-H] ⁻	1.36	26.28	1.05E+05
PG(38:6)	C44H75O10P	794.5098	793.5019	793.5042	[M-H] ⁻	2.87	24.46	2.27E+04
PG(40:6)	C46H79O10P	822.5411	821.5332	821.5353	[M-H] ⁻	2.50	27.34	1.89E+05
PG(40:7)	C46H77O10P	820.5254	819.5176	819.5218	[M-H] ⁻	5.12	24.66	2.00E+04
PG(40:8)	C46H75O10P	818.5098	817.5019	817.5037	[M-H] ⁻	2.11	24.87	3.84E+05
PG(42:10)	C48H75O10P	842.5098	841.5019	841.5039	[M-H] ⁻	2.28	24.21	4.92E+04
PG(42:7)	C48H81O10P	848.5567	847.5489	847.5524	[M-H] ⁻	4.16	27.70	3.72E+04
PG(42:8)	C48H79O10P	846.5411	845.5332	845.5339	[M-H] ⁻	0.74	26.13	8.24E+04
PG(42:9)	C48H77O10P	844.5254	843.5176	843.5186	[M-H] ⁻	1.17	25.40	8.54E+04
PG(44:10)	C50H79O10P	870.5411	869.5332	869.5340	[M-H] ⁻	0.93	26.31	6.22E+04
PI(32:1)	C41H77O13P	808.5102	807.5023	807.5039	[M-H] ⁻	1.94	26.49	6.01E+04
PI(34:2)	C43H79O13P	834.5258	833.5180	833.5205	[M-H] ⁻	3.00	27.23	5.75E+05
PI(36:1)	C45H85O13P	864.5728	863.5649	863.5733	[M-H] ⁻	9.69	29.12	2.40E+04
PI(36:2)	C45H83O13P	862.5571	861.5493	861.5524	[M-H] ⁻	3.65	30.25	1.68E+05
PI(36:3)	C45H81O13P	860.5415	859.5336	859.5363	[M-H] ⁻	3.08	27.64	3.16E+05
PI(36:4)	C45H79O13P	858.5258	857.5180	857.5196	[M-H] ⁻	1.93	27.34	1.02E+06
PI(38:2)	C47H87O13P	890.5884	889.5806	889.5886	[M-H] ⁻	8.99	32.07	2.60E+04
PI(38:3)	C47H85O13P	888.5728	887.5649	887.5716	[M-H] ⁻	7.48	30.41	4.77E+05
PI(38:4)	C47H83O13P	886.5571	885.5493	885.5502	[M-H] ⁻	1.09	29.72	5.33E+06
PI(38:5)	C47H81O13P	884.5415	883.5336	883.5352	[M-H] ⁻	1.80	27.53	2.49E+06
PI(38:6)	C47H79O13P	882.5258	881.5180	881.5183	[M-H] ⁻	0.33	25.58	1.89E+04
PI(40:4)	C49H87O13P	914.5884	913.5806	913.5820	[M-H] ⁻	1.59	31.27	2.84E+04
PI(40:5)	C49H85O13P	912.5728	911.5649	911.5664	[M-H] ⁻	1.65	29.53	6.99E+04
PI(40:6)	C49H83O13P	910.5571	909.5493	909.5507	[M-H] ⁻	1.59	27.45	5.97E+04
PI(40:7)	C49H81O13P	908.5415	907.5336	907.5355	[M-H] ⁻	2.07	27.05	3.79E+04
PS(27:0)	C33H64NO10P	665.4268	666.4346	666.4346	[M+H] ⁺	-0.05	15.65	6.29E+04
PS(28:1)	C34H64NO10P	677.4268	678.4346	678.4343	[M+H] ⁺	-0.39	18.37	2.05E+04
PS(34:1)	C40H76NO10P	761.5207	762.5285	762.5261	[M+H] ⁺	-3.11	30.76	5.86E+05
PS(34:2)	C40H74NO10P	759.5050	760.5128	760.5108	[M+H] ⁺	-2.71	28.64	1.97E+05
PS(36:1)	C42H80NO10P	789.5520	790.5598	790.5578	[M+H] ⁺	-2.54	31.00	9.24E+05

PS(36:2)	C42H78NO10P	787.5363	788.5441	788.5410	[M+H] ⁺	-4.00	30.82	1.17E+06
PS(38:2)	C44H82NO10P	815.5676	816.5754	816.5725	[M+H] ⁺	-3.63	35.05	1.73E+05
PS(38:3)	C44H80NO10P	813.5520	814.5598	814.5554	[M+H] ⁺	-5.42	33.71	3.12E+05
PS(38:4)	C44H78NO10P	811.5363	812.5441	812.5403	[M+H] ⁺	-4.71	31.93	2.22E+06
PS(40:2)	C46H86NO10P	843.5989	844.6067	844.6052	[M+H] ⁺	-1.76	52.31	1.96E+04
PS(40:3)	C46H84NO10P	841.5833	842.5911	842.5894	[M+H] ⁺	-1.96	28.67	1.21E+05
PS(40:5)	C46H80NO10P	837.5520	838.5598	838.5587	[M+H] ⁺	-1.34	25.94	4.20E+05
PS(40:6)	C46H78NO10P	835.5363	836.5441	836.5417	[M+H] ⁺	-2.86	24.68	2.98E+05
PS(42:7)	C48H80NO10P	861.5520	862.5598	862.5584	[M+H] ⁺	-1.66	24.93	1.41E+05
PS(44:10)	C50H78NO10P	883.5363	884.5441	884.5419	[M+H] ⁺	-2.51	24.02	1.39E+05
PS(44:8)	C50H82NO10P	887.5676	888.5754	888.5747	[M+H] ⁺	-0.84	25.97	1.76E+05
SM(d30:1)	C35H71N2O6P	646.5050	647.5128	647.5125	[M+H] ⁺	-0.35	25.33	9.56E+04
SM(d32:0)	C37H77N2O6P	676.5519	677.5597	677.5582	[M+H] ⁺	-2.31	30.19	4.12E+05
SM(d32:1)	C37H75N2O6P	674.5363	675.5441	675.5426	[M+H] ⁺	-2.23	29.90	9.71E+05
SM(d32:2)	C37H73N2O6P	672.5206	673.5284	673.5276	[M+H] ⁺	-1.17	25.69	1.98E+05
SM(d33:1)	C38H77N2O6P	688.5519	689.5597	689.5581	[M+H] ⁺	-2.31	29.34	7.80E+05
SM(d34:0)	C39H81N2O6P	704.5832	705.5910	705.5878	[M+H] ⁺	-4.51	35.50	5.69E+05
SM(d34:1)	C39H79N2O6P	702.5675	703.5754	703.5731	[M+H] ⁺	-3.19	33.43	3.15E+07
SM(d34:2)	C39H77N2O6P	700.5519	701.5597	701.5585	[M+H] ⁺	-1.68	27.81	6.00E+05
SM(d36:1)	C41H83N2O6P	730.5988	731.6067	731.6049	[M+H] ⁺	-2.42	38.33	1.60E+06
SM(d36:2)	C41H81N2O6P	728.5832	729.5910	729.5885	[M+H] ⁺	-3.50	33.74	5.88E+05
SM(d40:1)	C45H91N2O6P	786.6614	787.6693	787.6663	[M+H] ⁺	-3.80	51.02	1.71E+06
SM(d41:1)	C46H93N2O6P	800.6771	801.6849	801.6836	[M+H] ⁺	-1.66	47.66	4.59E+05
SM(d41:2)	C46H91N2O6P	798.6614	799.6693	799.6656	[M+H] ⁺	-4.60	47.03	1.78E+06
SM(d42:1)	C47H95N2O6P	814.6927	815.7006	815.6982	[M+H] ⁺	-2.93	51.61	4.50E+06
SM(d42:2)	C47H93N2O6P	812.6771	813.6849	813.6813	[M+H] ⁺	-4.48	50.37	1.62E+07
SM(d42:3)	C47H91N2O6P	810.6614	811.6693	811.6653	[M+H] ⁺	-4.93	44.77	3.60E+06
SM(d43:2)	C48H95N2O6P	826.6927	827.7006	827.6968	[M+H] ⁺	-4.51	47.18	2.60E+05
SM(d44:1)	C49H99N2O6P	842.7240	843.7319	843.7306	[M+H] ⁺	-1.52	56.81	1.22E+05
SM(d44:2)	C49H97N2O6P	840.7084	841.7162	841.7122	[M+H] ⁺	-4.83	50.19	1.11E+06

TG(46:0)	C ₄₉ H ₉₄ O ₆	778.7050	796.7394	796.7362	[M+NH ₄] ⁺	-3.94	64.75	3.43E+05
TG(48:0)	C ₅₁ H ₉₈ O ₆	806.7363	824.7707	824.7687	[M+NH ₄] ⁺	-2.43	66.55	2.37E+06
TG(48:1)	C ₅₁ H ₉₆ O ₆	804.7207	822.7550	822.7520	[M+NH ₄] ⁺	-3.65	64.85	2.21E+06
TG(48:3)	C ₅₁ H ₉₂ O ₆	800.6894	818.7237	818.7203	[M+NH ₄] ⁺	-4.15	61.96	5.92E+05
TG(49:0)	C ₅₂ H ₁₀₀ O ₆	820.7520	838.7863	838.7801	[M+NH ₄] ⁺	-7.38	65.61	1.73E+05
TG(49:1)	C ₅₂ H ₉₈ O ₆	818.7363	836.7707	836.7679	[M+NH ₄] ⁺	-3.32	66.23	4.96E+05
TG(49:2)	C ₅₂ H ₉₆ O ₆	816.7207	834.7550	834.7532	[M+NH ₄] ⁺	-2.13	64.61	1.57E+05
TG(50:0)	C ₅₃ H ₁₀₂ O ₆	834.7676	852.8020	852.7995	[M+NH ₄] ⁺	-2.94	69.11	4.62E+05
TG(50:1)	C ₅₃ H ₁₀₀ O ₆	832.7520	850.7863	850.7835	[M+NH ₄] ⁺	-3.29	66.21	9.27E+06
TG(50:2)	C ₅₃ H ₉₈ O ₆	830.7363	848.7707	848.7680	[M+NH ₄] ⁺	-3.19	64.80	1.10E+07
TG(50:3)	C ₅₃ H ₉₆ O ₆	828.7207	846.7550	846.7518	[M+NH ₄] ⁺	-3.85	63.14	3.99E+06
TG(50:4)	C ₅₃ H ₉₄ O ₆	826.7050	844.7394	844.7376	[M+NH ₄] ⁺	-2.09	62.17	5.50E+05
TG(50:5)	C ₅₃ H ₉₂ O ₆	824.6894	842.7237	842.7227	[M+NH ₄] ⁺	-1.23	61.01	1.65E+05
TG(51:0)	C ₅₄ H ₁₀₄ O ₆	848.7832	866.8176	866.8166	[M+NH ₄] ⁺	-1.18	69.35	1.23E+05
TG(51:1)	C ₅₄ H ₁₀₂ O ₆	846.7676	864.8020	864.8000	[M+NH ₄] ⁺	-2.32	67.84	1.88E+05
TG(51:2)	C ₅₄ H ₁₀₀ O ₆	844.7520	862.7863	862.7836	[M+NH ₄] ⁺	-3.15	66.24	4.18E+05
TG(51:3)	C ₅₄ H ₉₈ O ₆	842.7363	860.7707	860.7681	[M+NH ₄] ⁺	-2.97	64.71	3.80E+05
TG(52:0)	C ₅₅ H ₁₀₆ O ₆	862.7989	880.8333	880.8322	[M+NH ₄] ⁺	-1.26	70.55	5.75E+05
TG(52:1)	C ₅₅ H ₁₀₄ O ₆	860.7832	878.8176	878.8160	[M+NH ₄] ⁺	-1.89	69.17	6.49E+04
TG(52:2)	C ₅₅ H ₁₀₂ O ₆	858.7676	876.8020	876.8000	[M+NH ₄] ⁺	-2.23	66.16	1.06E+07
TG(52:3)	C ₅₅ H ₁₀₀ O ₆	856.7520	874.7863	874.7873	[M+NH ₄] ⁺	1.15	62.92	5.82E+04
TG(52:4)	C ₅₅ H ₉₈ O ₆	854.7363	872.7707	872.7676	[M+NH ₄] ⁺	-3.53	64.84	4.57E+06
TG(52:5)	C ₅₅ H ₉₆ O ₆	852.7207	870.7550	870.7533	[M+NH ₄] ⁺	-1.99	62.45	1.61E+06
TG(52:6)	C ₅₅ H ₉₄ O ₆	850.7050	868.7394	868.7360	[M+NH ₄] ⁺	-3.86	61.96	6.52E+05
TG(52:7)	C ₅₅ H ₉₂ O ₆	848.6894	866.7237	866.7217	[M+NH ₄] ⁺	-2.33	61.03	1.14E+05
TG(53:1)	C ₅₆ H ₁₀₆ O ₆	874.7989	892.8333	892.8315	[M+NH ₄] ⁺	-1.95	68.40	8.70E+04
TG(53:2)	C ₅₆ H ₁₀₄ O ₆	872.7832	890.8176	890.8150	[M+NH ₄] ⁺	-2.96	66.63	1.75E+05

TG(53:3)	C ₅₆ H ₁₀₂ O ₆	870.7676	888.8020	888.7995	[M+NH ₄] ⁺	-2.77	65.22	1.58E+05
TG(53:5)	C ₅₆ H ₉₈ O ₆	866.7363	884.7707	884.7692	[M+NH ₄] ⁺	-1.69	64.28	1.56E+05
TG(53:6)	C ₅₆ H ₉₆ O ₆	864.7207	882.7550	882.7543	[M+NH ₄] ⁺	-0.85	62.53	8.90E+04
TG(54:0)	C ₅₇ H ₁₁₀ O ₆	890.8302	908.8646	908.8635	[M+NH ₄] ⁺	-1.21	72.21	5.39E+04
TG(54:1)	C ₅₇ H ₁₀₈ O ₆	888.8145	906.8489	906.8490	[M+NH ₄] ⁺	0.14	69.53	5.21E+05
TG(54:2)	C ₅₇ H ₁₀₆ O ₆	886.7989	904.8333	904.8321	[M+NH ₄] ⁺	-1.29	68.75	2.09E+05
TG(54:3)	C ₅₇ H ₁₀₄ O ₆	884.7832	902.8176	902.8170	[M+NH ₄] ⁺	-0.72	68.63	7.79E+04
TG(54:4)	C ₅₇ H ₁₀₂ O ₆	882.7676	900.8020	900.7968	[M+NH ₄] ⁺	-5.71	65.16	8.61E+06
TG(54:5)	C ₅₇ H ₁₀₀ O ₆	880.7520	898.7863	898.7826	[M+NH ₄] ⁺	-4.11	63.90	9.13E+06
TG(54:6)	C ₅₇ H ₉₈ O ₆	878.7363	896.7707	896.7677	[M+NH ₄] ⁺	-3.30	62.78	2.94E+06
TG(54:7)	C ₅₇ H ₉₆ O ₆	876.7207	894.7550	894.7535	[M+NH ₄] ⁺	-1.72	61.69	5.13E+05
TG(54:8)	C ₅₇ H ₉₄ O ₆	874.7050	892.7394	892.7377	[M+NH ₄] ⁺	-1.83	60.68	1.46E+05
TG(54:9)	C ₅₇ H ₉₂ O ₆	872.6894	890.7237	890.7214	[M+NH ₄] ⁺	-2.60	59.10	2.06E+04
TG(55:1)	C ₅₈ H ₁₁₀ O ₆	902.8302	920.8646	920.8657	[M+NH ₄] ⁺	1.24	69.82	3.04E+04
TG(55:2)	C ₅₈ H ₁₀₈ O ₆	900.8145	918.8489	918.8470	[M+NH ₄] ⁺	-2.13	68.21	8.47E+04
TG(55:3)	C ₅₈ H ₁₀₆ O ₆	898.7989	916.8333	916.8303	[M+NH ₄] ⁺	-3.21	66.71	1.53E+05
TG(55:4)	C ₅₈ H ₁₀₄ O ₆	896.7832	914.8176	914.8142	[M+NH ₄] ⁺	-3.75	66.65	1.91E+05
TG(55:5)	C ₅₈ H ₁₀₂ O ₆	894.7676	912.8020	912.7977	[M+NH ₄] ⁺	-4.69	64.86	1.74E+05
TG(55:6)	C ₅₈ H ₁₀₀ O ₆	892.7520	910.7863	910.7841	[M+NH ₄] ⁺	-2.46	63.70	1.04E+05
TG(56:0)	C ₅₉ H ₁₁₄ O ₆	918.8615	936.8959	936.8992	[M+NH ₄] ⁺	3.57	73.37	2.41E+04
TG(56:1)	C ₅₉ H ₁₁₂ O ₆	916.8458	934.8802	934.8802	[M+NH ₄] ⁺	0.00	70.03	4.95E+04
TG(56:2)	C ₅₉ H ₁₁₀ O ₆	914.8302	932.8646	932.8619	[M+NH ₄] ⁺	-2.82	69.22	8.53E+05
TG(56:3)	C ₅₉ H ₁₀₈ O ₆	912.8145	930.8489	930.8453	[M+NH ₄] ⁺	-3.91	68.13	1.03E+06
TG(56:4)	C ₅₉ H ₁₀₆ O ₆	910.7989	928.8333	928.8292	[M+NH ₄] ⁺	-4.37	66.98	3.70E+06
TG(56:5)	C ₅₉ H ₁₀₄ O ₆	908.7832	926.8176	926.8141	[M+NH ₄] ⁺	-3.79	65.70	7.93E+06
TG(56:6)	C ₅₉ H ₁₀₂ O ₆	906.7676	924.8020	924.7980	[M+NH ₄] ⁺	-4.33	65.11	4.15E+06
TG(56:7)	C ₅₉ H ₁₀₀ O ₆	904.7520	922.7863	922.7809	[M+NH ₄] ⁺	-5.86	62.96	3.89E+06

TG(56:8)	C ₅₉ H ₉₈ O ₆	902.7363	920.7707	920.7678	[M+NH ₄] ⁺	-3.08	63.19	1.94E+06
TG(56:9)	C ₅₉ H ₉₆ O ₆	900.7207	918.7550	918.7542	[M+NH ₄] ⁺	-0.86	60.87	1.11E+05
TG(57:1)	C ₆₀ H ₁₁₄ O ₆	930.8615	948.8959	948.8965	[M+NH ₄] ⁺	0.71	70.82	5.04E+04
TG(58:0)	C ₆₁ H ₁₁₈ O ₆	946.8928	964.9272	964.9264	[M+NH ₄] ⁺	-0.82	75.07	1.48E+04
TG(58:1)	C ₆₁ H ₁₁₆ O ₆	944.8771	962.9115	962.9104	[M+NH ₄] ⁺	-1.16	71.21	8.81E+04
TG(58:10)	C ₆₁ H ₉₈ O ₆	926.7363	944.7707	944.7686	[M+NH ₄] ⁺	-2.19	62.18	4.18E+05
TG(58:2)	C ₆₁ H ₁₁₄ O ₆	942.8615	960.8959	960.8947	[M+NH ₄] ⁺	-1.23	70.56	3.85E+05
TG(58:3)	C ₆₁ H ₁₁₂ O ₆	940.8458	958.8802	958.8766	[M+NH ₄] ⁺	-3.80	68.57	4.51E+05
TG(58:4)	C ₆₁ H ₁₁₀ O ₆	938.8302	956.8646	956.8589	[M+NH ₄] ⁺	-5.89	67.64	6.58E+05
TG(58:5)	C ₆₁ H ₁₀₈ O ₆	936.8145	954.8489	954.8468	[M+NH ₄] ⁺	-2.23	67.37	1.77E+06
TG(58:6)	C ₆₁ H ₁₀₆ O ₆	934.7989	952.8333	952.8294	[M+NH ₄] ⁺	-4.10	66.17	1.54E+06
TG(58:7)	C ₆₁ H ₁₀₄ O ₆	932.7832	950.8176	950.8119	[M+NH ₄] ⁺	-6.02	64.56	2.70E+06
TG(58:8)	C ₆₁ H ₁₀₂ O ₆	930.7676	948.8020	948.7985	[M+NH ₄] ⁺	-3.61	64.04	6.08E+06
TG(58:9)	C ₆₁ H ₁₀₀ O ₆	928.7520	946.7863	946.7830	[M+NH ₄] ⁺	-3.51	63.20	1.28E+06
TG(59:2)	C ₆₂ H ₁₁₆ O ₆	956.8771	974.9115	974.9104	[M+NH ₄] ⁺	-1.10	70.68	5.99E+04
TG(59:4)	C ₆₂ H ₁₁₂ O ₆	952.8458	970.8802	970.8774	[M+NH ₄] ⁺	-2.91	68.87	1.75E+04
TG(60:0)	C ₆₃ H ₁₂₂ O ₆	974.9241	992.9585	992.9589	[M+NH ₄] ⁺	0.41	76.33	1.01E+04
TG(60:1)	C ₆₃ H ₁₂₀ O ₆	972.9084	990.9428	990.9411	[M+NH ₄] ⁺	-1.77	72.41	3.87E+04
TG(60:10)	C ₆₃ H ₁₀₂ O ₆	954.7676	972.8020	972.7977	[M+NH ₄] ⁺	-4.36	63.15	1.25E+06
TG(60:11)	C ₆₃ H ₁₀₀ O ₆	952.7520	970.7863	970.7841	[M+NH ₄] ⁺	-2.27	62.46	4.47E+05
TG(60:12)	C ₆₃ H ₉₈ O ₆	950.7363	968.7707	968.7700	[M+NH ₄] ⁺	-0.67	60.88	1.05E+05
TG(60:2)	C ₆₃ H ₁₁₈ O ₆	970.8928	988.9272	988.9266	[M+NH ₄] ⁺	-0.54	70.80	1.12E+05
TG(60:3)	C ₆₃ H ₁₁₆ O ₆	968.8771	986.9115	986.9094	[M+NH ₄] ⁺	-2.15	69.92	6.34E+05
TG(60:4)	C ₆₃ H ₁₁₄ O ₆	966.8615	984.8959	984.8931	[M+NH ₄] ⁺	-2.78	69.00	4.09E+05
TG(60:5)	C ₆₃ H ₁₁₂ O ₆	964.8458	982.8802	982.8775	[M+NH ₄] ⁺	-2.80	67.90	2.87E+05
TG(60:6)	C ₆₃ H ₁₁₀ O ₆	962.8302	980.8646	980.8629	[M+NH ₄] ⁺	-1.73	67.69	3.22E+05
TG(60:7)	C ₆₃ H ₁₀₈ O ₆	960.8145	978.8489	978.8453	[M+NH ₄] ⁺	-3.69	65.96	3.31E+05

TG(60:8)	C ₆₃ H ₁₀₆ O ₆	958.7989	976.8333	976.8295	[M+NH ₄] ⁺	-3.86	65.71	1.72E+06
TG(60:9)	C ₆₃ H ₁₀₄ O ₆	956.7832	974.8176	974.8144	[M+NH ₄] ⁺	-3.33	64.58	9.64E+05
TG(61:3)	C ₆₄ H ₁₁₈ O ₆	982.8928	1000.9272	1000.9264	[M+NH ₄] ⁺	-0.78	70.23	1.09E+04
TG(62:0)	C ₆₅ H ₁₂₆ O ₆	1002.9554	1020.9898	1020.9912	[M+NH ₄] ⁺	1.36	78.27	1.58E+04
TG(62:1)	C ₆₅ H ₁₂₄ O ₆	1000.9397	1018.9741	1018.9724	[M+NH ₄] ⁺	-1.67	73.69	1.06E+04
TG(62:10)	C ₆₅ H ₁₀₆ O ₆	982.7989	1000.8333	1000.8298	[M+NH ₄] ⁺	-3.48	64.23	3.92E+05
TG(62:12)	C ₆₅ H ₁₀₂ O ₆	978.7676	996.8020	996.7994	[M+NH ₄] ⁺	-2.56	62.04	1.48E+05
TG(62:2)	C ₆₅ H ₁₂₂ O ₆	998.9241	1016.9585	1016.9593	[M+NH ₄] ⁺	0.81	71.96	5.54E+04
TG(62:3)	C ₆₅ H ₁₂₀ O ₆	996.9084	1014.9428	1014.9406	[M+NH ₄] ⁺	-2.18	70.61	3.53E+04
TG(62:5)	C ₆₅ H ₁₁₆ O ₆	992.8771	1010.9115	1010.9098	[M+NH ₄] ⁺	-1.67	69.32	2.33E+05
TG(62:6)	C ₆₅ H ₁₁₄ O ₆	990.8615	1008.8959	1008.8927	[M+NH ₄] ⁺	-3.11	68.81	2.24E+05
TG(62:7)	C ₆₅ H ₁₁₂ O ₆	988.8458	1006.8802	1006.8784	[M+NH ₄] ⁺	-1.77	67.76	9.34E+04
TG(62:9)	C ₆₅ H ₁₀₈ O ₆	984.8145	1002.8489	1002.8458	[M+NH ₄] ⁺	-3.11	65.34	1.98E+05
TG(64:12)	C ₆₇ H ₁₀₆ O ₆	1006.7989	1024.8333	1024.8300	[M+NH ₄] ⁺	-3.18	63.49	8.02E+04
TG(64:2)	C ₆₇ H ₁₂₆ O ₆	1026.9554	1044.9898	1044.9884	[M+NH ₄] ⁺	-1.29	73.08	4.02E+04
TG(64:3)	C ₆₇ H ₁₂₄ O ₆	1024.9397	1042.9741	1042.9736	[M+NH ₄] ⁺	-0.51	71.66	1.99E+04
TG(64:4)	C ₆₇ H ₁₂₂ O ₆	1022.9241	1040.9585	1040.9532	[M+NH ₄] ⁺	-5.09	70.87	2.95E+04
TG(64:5)	C ₆₇ H ₁₂₀ O ₆	1020.9084	1038.9428	1038.9406	[M+NH ₄] ⁺	-2.15	71.28	5.30E+04
TG(64:6)	C ₆₇ H ₁₁₈ O ₆	1018.8928	1036.9272	1036.9244	[M+NH ₄] ⁺	-2.64	69.29	6.94E+04
TG(64:7)	C ₆₇ H ₁₁₆ O ₆	1016.8771	1034.9115	1034.9099	[M+NH ₄] ⁺	-1.60	68.41	6.11E+04
TG(64:9)	C ₆₇ H ₁₁₂ O ₆	1012.8458	1030.8802	1030.8772	[M+NH ₄] ⁺	-2.92	66.96	1.35E+05
TG(66:2)	C ₆₉ H ₁₃₀ O ₆	1054.9867	1073.0211	1073.0204	[M+NH ₄] ⁺	-0.65	74.08	3.28E+04
TG(66:3)	C ₆₉ H ₁₂₈ O ₆	1052.9710	1071.0054	1071.0037	[M+NH ₄] ⁺	-1.57	72.74	3.98E+04