SUPPORTING INFORMATION

High-Throughput and Comprehensive Lipidomic Analysis Using Ultrahigh-Performance Supercritical Fluid Chromatography - Mass Spectrometry

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Figures: 8

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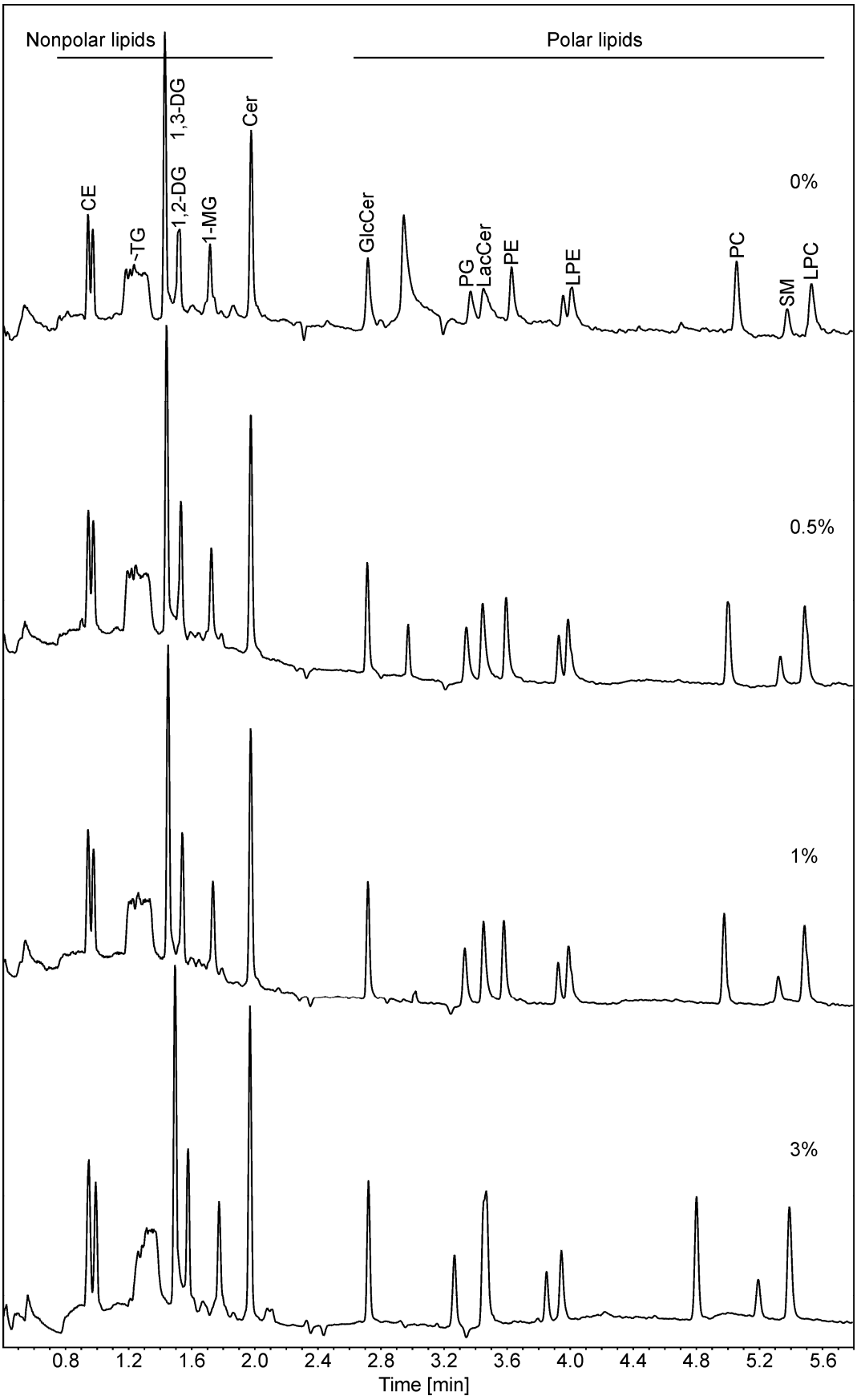

Figure S-1. Effect of water concentration in the modifier on the UHPSFC analysis of lipid class standards. UHPSFC conditions: Acquity BEH UPC^2 column (100 × 3 mm, 1.7 µm, Waters), the flow rate 1.9 mL/min, the column temperature 60°C, the ABPR pressure 1500 psi and the gradient of methanol – water mixture containing 30 mM of ammonium acetate as the modifier: 0 min – 1 %, 5 min – 51%, 6 min – 51%.

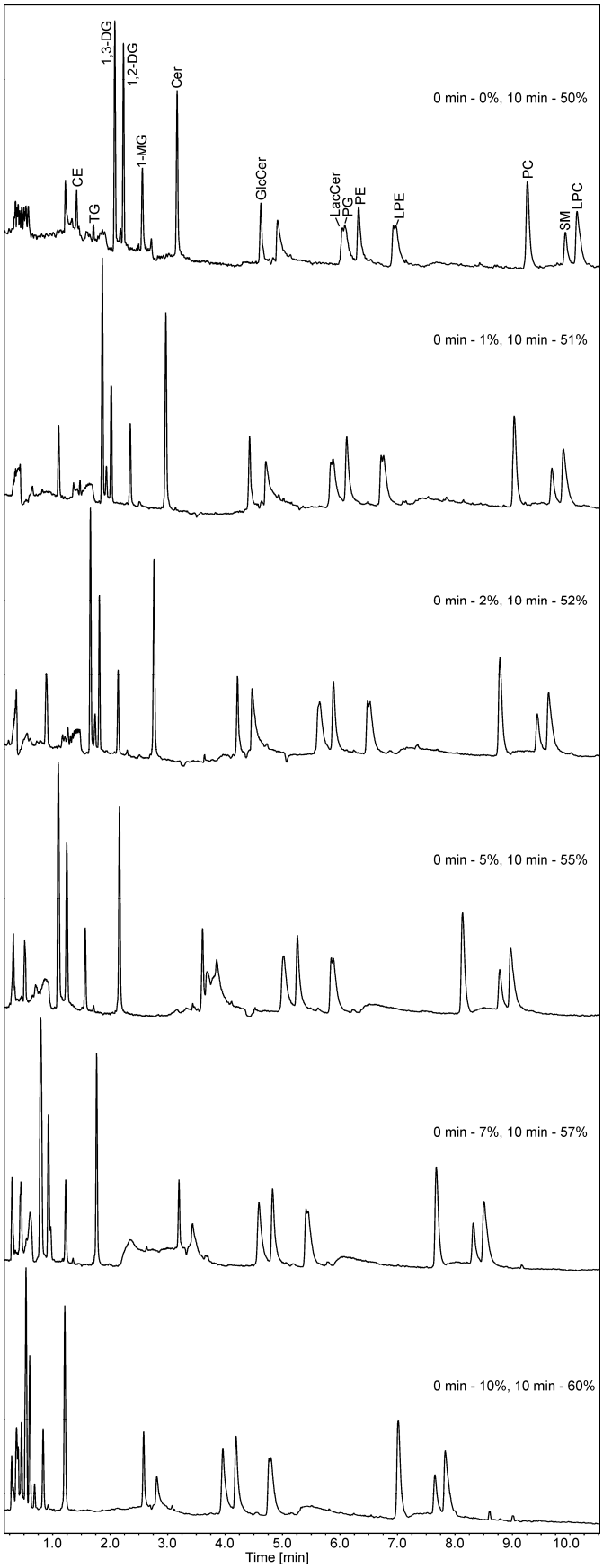

Figure S-2. Effect of the modifier initial concentration on the UHPSFC analysis of lipid class standards. UHPSFC conditions: Acquity BEH UPC^2 column (100 × 3 mm, 1.7 µm, Waters), the flow rate 1.9 mL/min, the column temperature 60°C, the ABPR pressure 1500 psi and methanol with 10 mM of ammonium acetate as the modifier.

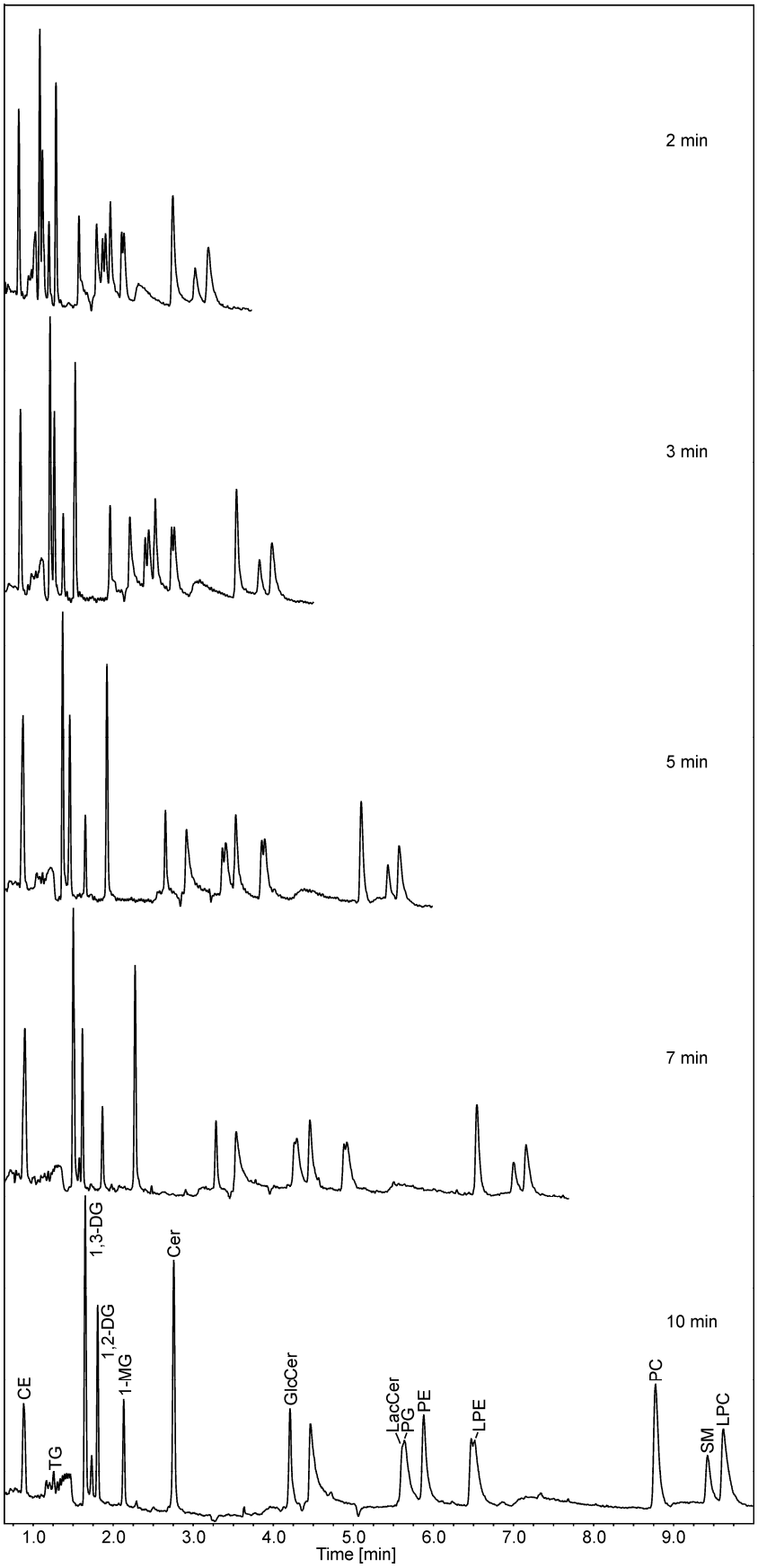

Figure S-3. Effect of modifier gradient steepness on the UHPSFC analysis of lipid class standards. Modifier gradient from 2% to 52% within 2, 3, 5, 7 and 10 min. UHPSFC conditions: Acquity BEH UPC2 column (100 × 3 mm, 1.7 µm, Waters), the flow rate 1.9 mL/min, the column temperature 60°C, the ABPR pressure 1500 psi and methanol with 10 mM of ammonium acetate as the modifier.

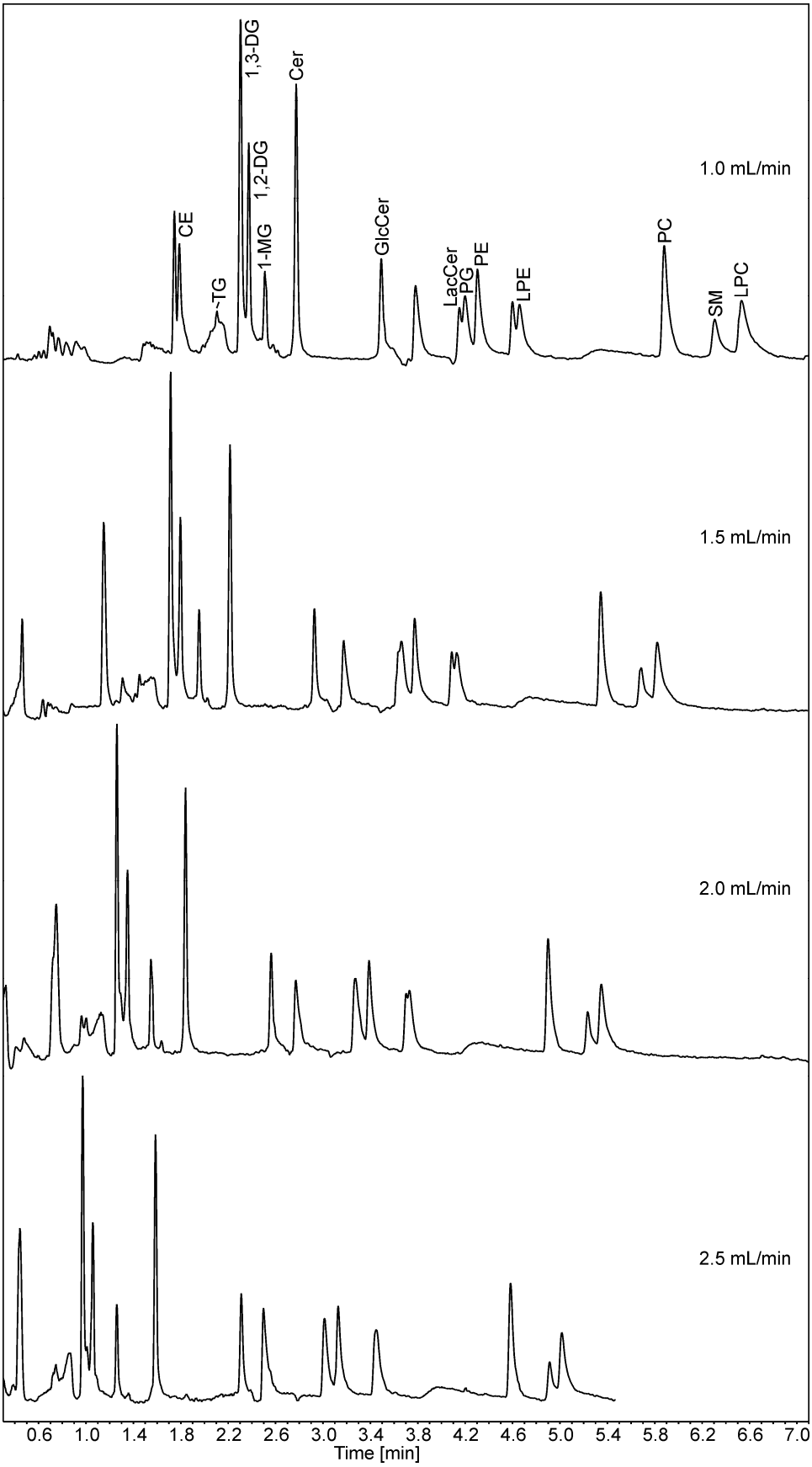

Figure S-4. Effect of flow rate on the UHPSFC analysis of lipid class standards. UHPSFC conditions: Acquity BEH UPC^2 column (100 × 3 mm, 1.7 µm, Waters), the column temperature 60°C, the ABPR pressure 1500 psi and the gradient of methanol with 10 mM of ammonium acetate as the modifier: 0 min – 2 %, 5 min – 52%, 6 min – 52%.

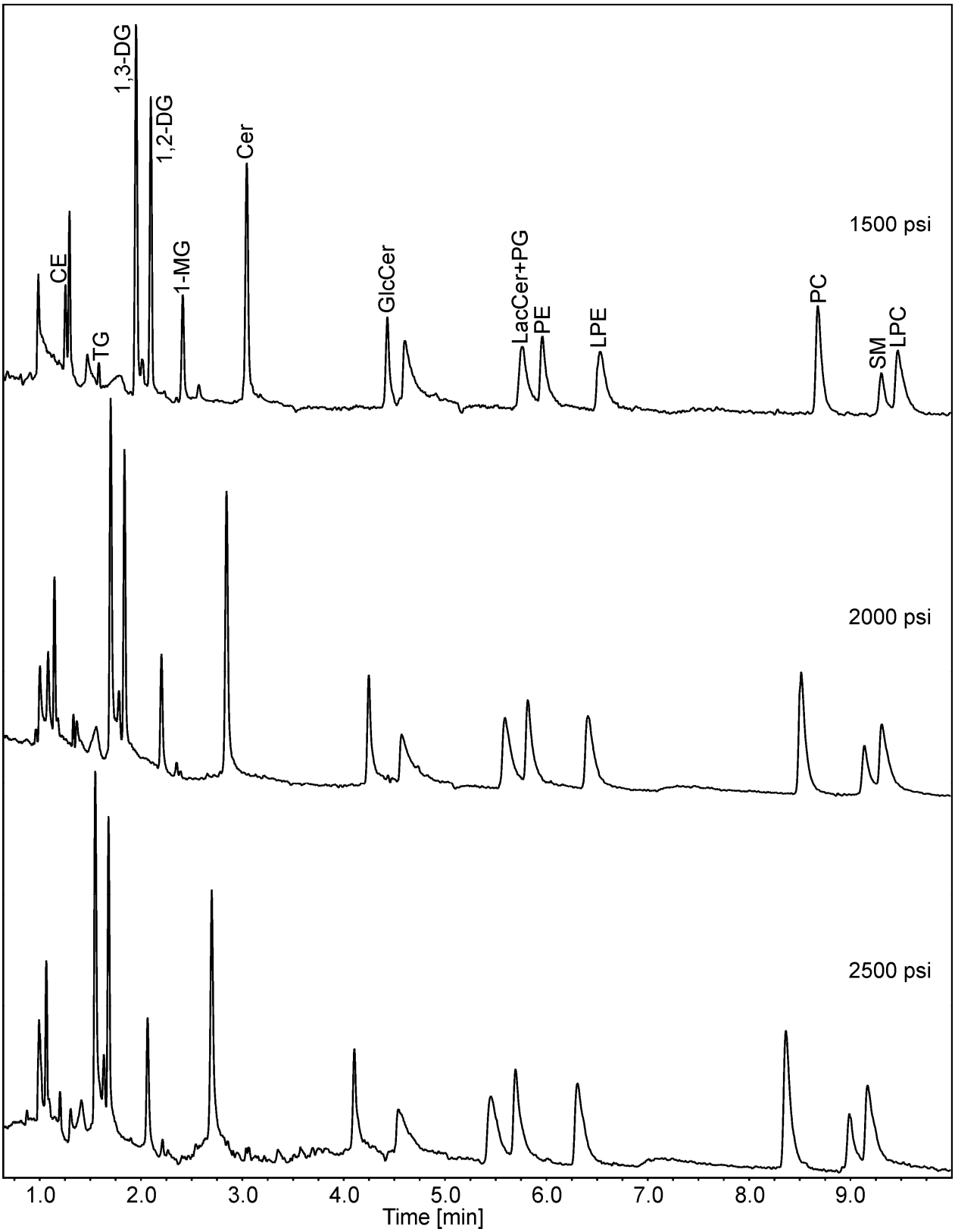

Figure S-5. Effect of ABPR pressure on the UHPSFC analysis of lipid class standards. UHPSFC conditions: Acquity BEH UPC^2 column (100 × 3 mm, 1.7 µm, Waters), the flow rate 1.9 mL/min, the column temperature 60°C and the gradient of methanol with 10 mM of ammonium acetate as modifier: 0 min – 0 %, 10 min – 50%, 11 min – 50%.

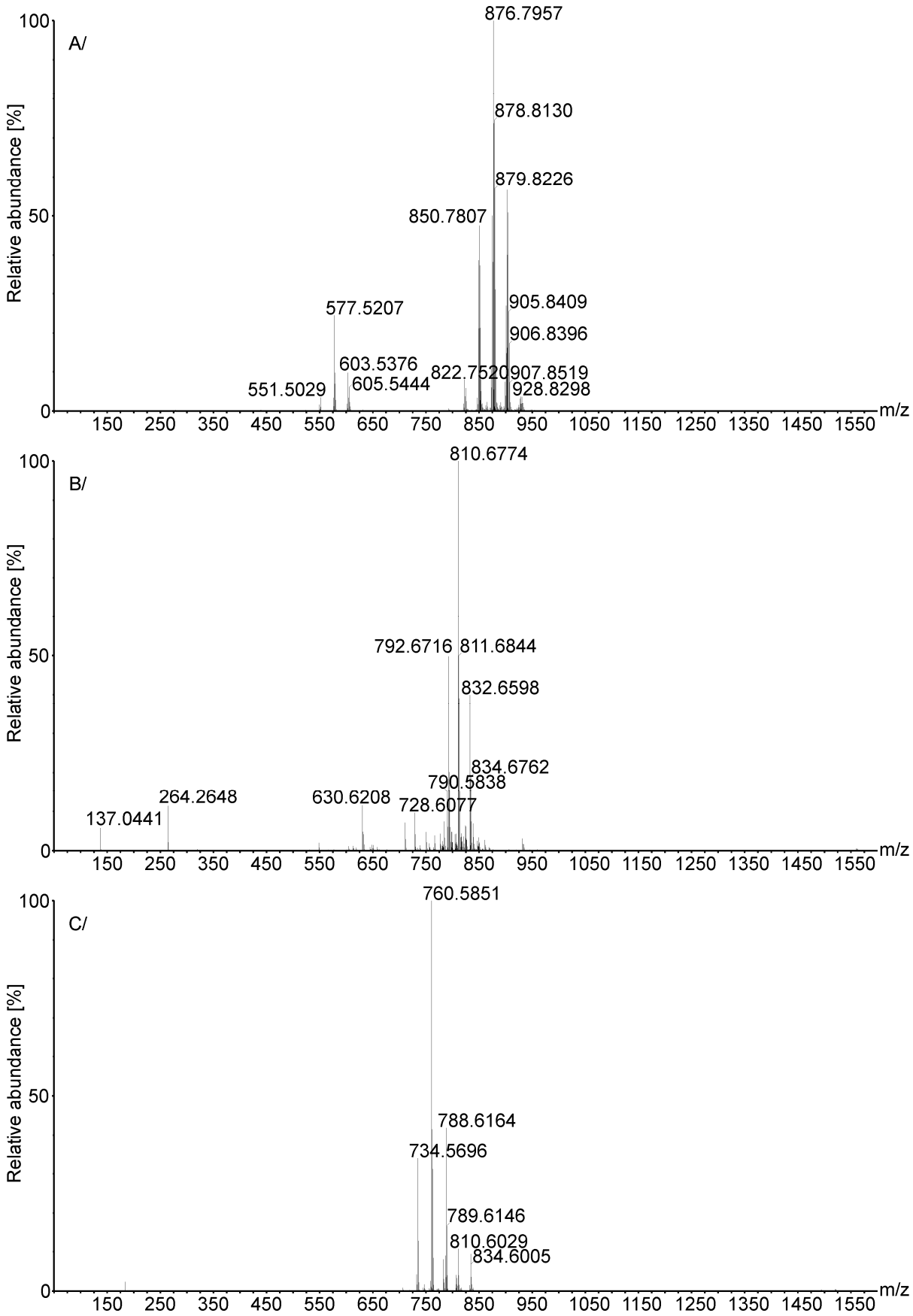

Figure S-6. Examples of ESI mass spectra of lipid classes from UHPSFC/ESI-MS analysis of porcine brain extract: A/ triacylglycerols, B/ hexosylceramides and C/ phosphatidylcholines.

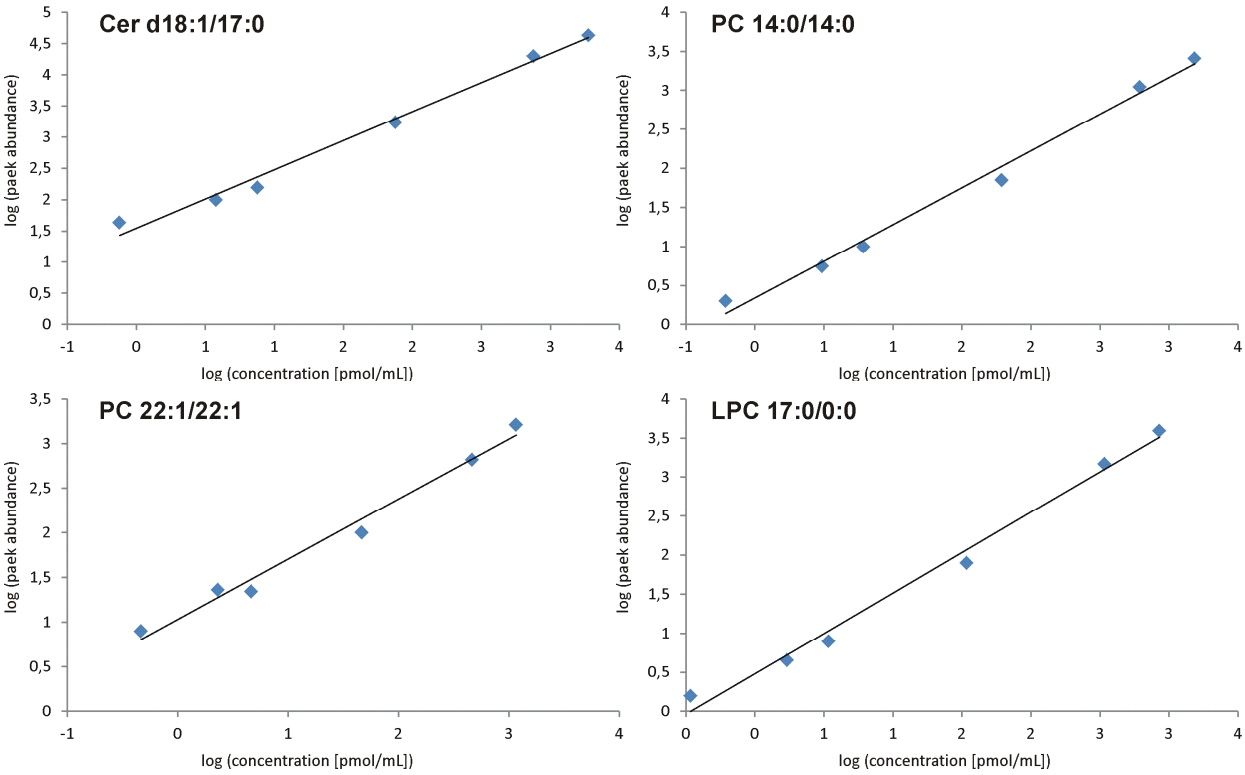

Figure S-7. Examples of calibration curves of selected internal standards spiked into the porcine brain matrix from validation of UHPSFC/ESI-MS method.

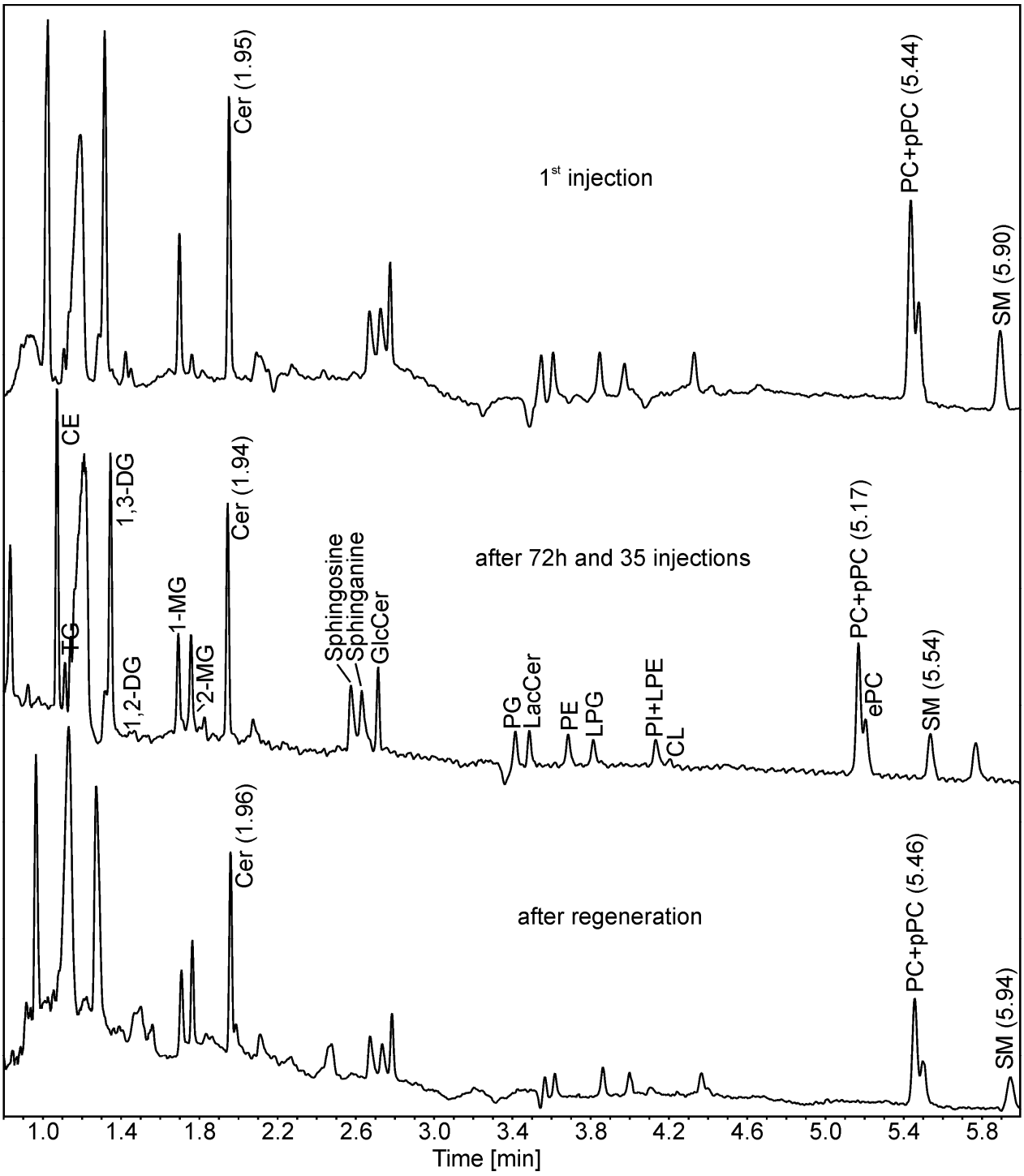

Figure S-8. Effect of column regeneration by 5 consecutive injections of 10 µL of water and acetonitrile into 100% CO_2 at 0.5 mL/min flow rate on the UHPSFC/ESI-MS analysis of lipid class standards. UHPSFC conditions: Acquity BEH UPC^2 column (100 × 3 mm, 1.7 µm, Waters), the flow rate 1.9 mL/min, the column temperature 60°C, the ABPR pressure 1800 psi and the gradient of methanol – water mixture (99:1, v/v) containing 30 mM of ammonium acetate as the modifier: 0 min – 1 %, 5 min – 51%, 6 min – 51%.

Table S-1 Effect of ammonium acetate concentration in the modifier on the peak areas of lipid class standards using UHPSFC/ESI-MS.

Lipids	Concentration of ammonium acetate [mM]					
	0	**5**	**10**	**20**	**30**	**50**
CE	23801	46699	51496	52902	60826	61489
TG	6047	3084	3619	3480	3149	2846
1,3-DG	61210	72691	77782	71427	71601	70630
1-MG	57411	24484	25864	24034	26835	23893
Cer	90954	70497	65481	67225	64274	65083
GlcCer	76252	31069	41681	34572	31970	27184
LacCer	61065	25856	23335	26375	17037	10739
PE	- [a]	26220	29073	27018	26176	21553
LPE	- [a]	10514	12074	12383	9458	8960
PC	- [a]	62893	67915	64427	65359	58108
SM	- [a]	15864	16802	16041	16717	14678
LPC	- [a]	55125	63494	57427	54900	54903

[a] Peak areas cannot be integrated due to peak tailing.

Table S-2 Lipid species identified in porcine brain extract using UHPSFC/ESI-MS method.

Retention time [min]	Lipids	*m/z* experimental	*m/z* theoretical	Concentration [pmol/mg]
Cholesteryl esters (CE) [a]				
0.82	CE 16:0	647.5692	647.5743	< LOQ
0.84	CE 16:1	645.5603	645.5586	413
0.86	CE 18:0	675.6010	675.6056	< LOQ
0.86	CE 18:1	673.5944	673.5900	905
0.88	CE 18:2	671.5794	671.5743	3700
0.90	CE 18:3	669.5562	669.5586	319
0.90	CE 20:2	699.6011	699.6056	330
0.93	CE 20:4	695.5777	695.5743	2572
0.95	CE 20:5	693.5531	693.5586	68
0.95	CE 22:4	723.6091	723.6056	< LOQ
0.97	CE 22:6	719.5757	719.5743	< LOQ
Triacylglycerols (TG) [b]				
0.97	TG 42:0	740.6746	740.6763	8
0.98	TG 42:1	738.6566	738.6606	5
0.99	TG 42:2	736.6413	736.6450	9
0.99	TG 44:0	768.7076	768.7076	19
1.00	TG 44:1	766.6883	766.6919	23
1.01	TG 44:2	764.6713	764.6763	12
1.01	TG 46:0	796.7444	796.7389	40
1.01	TG 46:1	794.7251	794.7232	57
1.02	TG 44:3	762.6570	762.6606	< LOQ
1.02	TG 46:2	792.7084	792.7076	38
1.02	TG 48:0	824.7689	824.7702	157
1.03	TG 48:1	822.7520	822.7545	173
1.03	TG 49:0	838.7805	838.7858	13
1.04	TG 48:2	820.7375	820.7389	85
1.04	TG 49:1	836.7708	836.7702	22
1.04	TG 50:0	852.8062	852.8015	482
1.05	TG 48:3	818.7256	818.7232	16
1.05	TG 49:2	834.7518	834.7545	16
1.05	TG 50:1	850.7807	850.7858	1124
1.05	TG 51:0	866.8206	866.8171	13
1.05	TG 51:1	864.8043	864.8015	69
1.06	TG 48:4	816.7036	816.7076	8
1.06	TG 49:3	832.7354	832.7389	7
1.06	TG 50:2	848.7704	848.7702	775
1.06	TG 51:2	862.7902	862.7858	48
1.06	TG 52:0	880.8327	880.8328	545

1.06	TG 52:1	878.8130	878.8171	1587
1.07	TG 50:3	846.7497	846.7545	109
1.07	TG 51:3	860.7657	860.7702	21
1.07	TG 52:2	876.7957	876.8015	1874
1.07	TG 53:0	894.8527	894.8484	< LOQ
1.07	TG 53:1	892.8300	892.8328	19
1.08	TG 50:4	844.7441	844.7389	24
1.08	TG 51:4	858.7563	858.7545	15
1.08	TG 52:3	874.7806	874.7858	1232
1.08	TG 53:2	890.8226	890.8171	62
1.08	TG 54:0	908.8649	908.8641	< LOQ
1.08	TG 54:1	906.8527	906.8484	298
1.08	TG 54:2	904.8297	904.8328	1013
1.09	TG 51:5	856.7366	856.7389	< LOQ
1.09	TG 52:4	872.7678	872.7702	313
1.09	TG 53:3	888.8046	888.8015	48
1.09	TG 54:3	902.8220	902.8171	1357
1.09	TG 55:1	920.8655	920.8641	< LOQ
1.09	TG 55:2	918.8431	918.8484	9
1.10	TG 52:5	870.7574	870.7545	47
1.10	TG 53:4	886.7887	886.7858	22
1.10	TG 54:4	900.8034	900.8015	779
1.10	TG 55:3	916.8301	916.8328	15
1.10	TG 56:1	934.8790	934.8797	9
1.10	TG 56:2	932.8649	932.8641	56
1.11	TG 53:5	884.7752	884.7702	30
1.11	TG 54:5	898.7871	898.7858	299
1.11	TG 55:4	914.8224	914.8171	10
1.11	TG 55:5	912.8036	912.8015	11
1.11	TG 56:3	930.8529	930.8484	130
1.11	TG 58:2	960.8947	960.8954	6
1.12	TG 54:6	896.7731	896.7702	77
1.12	TG 56:4	928.8298	928.8328	142
1.12	TG 58:3	958.8798	958.8797	7
1.13	TG 56:5	926.8223	926.8171	155
1.13	TG 58:4	956.8670	956.8641	13
1.14	TG 56:6	924.8036	924.8015	114
1.14	TG 58:5	954.8428	954.8484	25
1.14	TG 58:6	952.8342	952.8328	39
1.15	TG 58:7	950.8143	950.8171	37
1.15	TG 60:5	982.8838	982.8797	3
1.16	TG 60:6	980.8596	980.8641	5
1.17	TG 60:7	978.8511	978.8484	4

1.17	TG 60:8	976.8311	976.8328	6
1.18	TG 60:9	974.8134	974.8171	< LOQ
1.18	TG 60:10	972.7972	972.8015	12
Fatty acids (FA) [c]				
1.14	FA 14:0	227.1998	227.2017	< LOQ
1.15	FA 15:0	241.2192	241.2173	< LOQ
1.17	FA 16:0	255.2324	255.2330	3085
1.18	FA 16:1	253.2192	253.2173	444
1.18	FA 17:0	269.2468	269.2486	241
1.19	FA 18:0	283.2605	283.2643	5184
1.20	FA 18:1	281.2494	281.2486	4959
1.20	FA 19:0	297.2756	297.2799	3647
1.21	FA 20:0	311.2899	311.2956	130
1.22	FA 18:2	279.2307	279.2330	603
1.22	FA 20:1	309.2813	309.2799	183
1.22	FA 21:0	325.3116	325.3112	83
1.22	FA 22:0	339.3283	339.3269	181
1.23	FA 20:2	307.2638	307.2643	92
1.23	FA 23:0	353.3449	353.3425	117
1.24	FA 18:3	277.2194	277.2173	45
1.24	FA 24:0	367.3604	367.3582	277
1.24	FA 22:1	337.3113	337.3112	48
1.25	FA 20:3	305.2454	305.2486	190
1.25	FA 22:2	335.2923	335.2956	16
1.26	FA 25:0	381.3755	381.3738	128
1.26	FA 24:1	365.3451	365.3425	41
1.26	FA 22:3	333.2793	333.2799	38
1.26	FA 26:0	395.3922	395.3895	127
1.27	FA 20:4	303.2336	303.2330	5835
1.28	FA 26:1	393.3706	393.3738	45
1.29	FA 22:4	331.2644	331.2643	447
1.29	FA 28:1	421.3996	421.4051	< LOQ
1.29	FA 20:5	301.2132	301.2173	111
1.31	FA 22:5	329.2477	329.2486	383
1.33	FA 20:6	299.1996	299.2017	92
1.34	FA 22:6	327.2293	327.2330	2371
1.30 [d]	Coenzyme Q10	863.6879	863.6912	- [g]
1,3-Diacylglycerols (DG) [b]				
1.31	DG 34:0	614.5679	614.5718	- [g]
1.32	DG 34:1	612.5569	612.5561	- [g]
1.33	DG 34:2	610.5385	610.5405	- [g]
1.33	DG 35:0	628.5837	628.5874	- [g]
1.33	DG 36:0	642.6027	642.6031	- [g]

1.33	DG 36:1	640.5905	640.5874	- [g]
1.34	DG 36:2	638.5704	638.5718	- [g]
1.35	DG 36:3	636.5536	636.5561	- [g]
1.36	DG 36:4	634.5399	634.5404	- [g]
1.38	DG 38:4	662.5721	662.5718	- [g]
1.43	DG 40:6	686.5704	686.5718	- [g]
1.43	DG 40:7	684.5590	684.5561	- [g]
1,2-Diacylglycerols (DG) [b]				
1.38	DG 30:0	558.5147	558.5092	15 [h]
1.40	DG 32:0	586.5450	586.5405	51 [h]
1.41	DG 32:1	584.5277	584.5248	48 [h]
1.42	DG 34:0	614.5679	614.5718	58 [h]
1.42	DG 34:1	612.5569	612.5561	786 [h]
1.43	DG 34:2	610.5385	610.5405	132 [h]
1.43	DG 35:0	628.5837	628.5874	< LOQ [h]
1.43	DG 35:1	626.5718	626.5718	< LOQ [h]
1.44	DG 35:2	624.5522	624.5561	49 [h]
1.44	DG 36:0	642.6027	642.6031	7 [h]
1.44	DG 36:1	640.5905	640.5874	476 [h]
1.45	DG 35:3	622.5457	622.5405	< LOQ [h]
1.45	DG 36:2	638.5704	638.5718	358 [h]
1.46	DG 36:3	636.5536	636.5561	1024 [h]
1.46	DG 36:4	634.5399	634.5404	252 [h]
1.46	DG 38:1	668.6191	668.6187	46 [h]
1.46	DG 38:2	666.6004	666.6031	44 [h]
1.47	DG 38:3	664.5847	664.5874	127 [h]
1.47	DG 38:4	662.5721	662.5718	1412 [h]
1.49	DG 38:5	660.5513	660.5561	207 [h]
1.50	DG 38:6	658.5351	658.5405	165 [h]
1.50	DG 40:4	690.6021	690.6031	99 [h]
1.51	DG 40:5	688.5848	688.5874	62 [h]
1.51	DG 40:6	686.5704	686.5718	213 [h]
1.52	DG 40:7	684.5590	684.5561	50 [h]
1.43 [e]	Cholesterol	369.3549	369.3521	70760
1-Monoacylglycerols (MG) [a]				
1.64	MG 16:0	353.2686	353.2668	79 [h]
1.65	MG 18:0	381.2944	381.2981	63 [h]
1.67	MG 18:1	379.2856	379.2824	224 [h]
1.71	MG 20:4	401.2629	401.2668	23 [h]
1.75	MG 22:6	425.2712	425.2668	12 [h]
2-Monoacylglycerols (MG) [a]				
1.72	MG 16:0	353.2686	353.2668	- [g]
1.78	MG 20:4	401.2629	401.2668	- [g]

1.82	MG 22:6	425.2712	425.2668	- [g]
Fatty amides [d]				
1.67	14:0	228.2339	228.2327	- [g]
1.67	15:0	242.2507	242.2484	- [g]
1.68	16:0	256.2658	256.2640	- [g]
1.69	16:1	254.2504	254.2484	- [g]
1.69	17:0	270.2802	270.2797	- [g]
1.69	18:0	284.2921	284.2953	- [g]
1.70	17:1	268.2604	268.2640	- [g]
1.70	17:2	266.2520	266.2484	- [g]
1.70	18:1	282.2792	282.2797	- [g]
1.71	19:1	296.2944	296.2953	- [g]
1.71	20:0	310.3107	310.3110	- [g]
1.72	18:2	280.2662	280.2640	- [g]
1.73	20:1	308.2995	308.2953	- [g]
1.73	22:0	338.3428	338.3423	- [g]
1.74	18:3	278.2454	278.2484	- [g]
1.74	22:1	336.3227	336.3266	- [g]
1.76	22:2	334.3165	334.3110	- [g]
Ceramides (Cer) [e]				
1.84	Cer 34:1	520.5131	520.5088	24
1.84	Cer 35:1	534.5278	534.5245	< LOQ
1.85	Cer 36:1	548.5445	548.5401	455
1.85	Cer 37:1	562.5563	562.5558	4
1.85	Cer 38:1	576.5666	576.5714	83
1.86	Cer 36:2	546.5222	546.5245	71
1.86	Cer 38:2	574.5560	574.5558	< LOQ
1.86	Cer 40:1	604.5996	604.6027	9
1.86	Cer 42:1	632.6282	632.6340	9
1.87	Cer 42:2	630.6208	630.6184	33
2.46 [e]	Sphingosine	282.2792	282.2791	- [g]
2.52 [d]	Sphinganine	302.3051	302.3054	- [g]
Hexosyl ceramides (HexCer) [d]				
2.51	HexCer 44:0	842.7409	842.7449	< LOQ
2.51	HexCer 43:0	828.7348	828.7292	< LOQ
2.51	HexCer 42:0	814.7090	814.7130	743
2.51	HexCer 41:0	800.6928	800.6979	< LOQ
2.51	HexCer 40:0	786.6859	786.6817	169
2.52	HexCer 38:0	758.6483	758.6504	43
2.52	HexCer 36:0	730.6238	730.6191	68
2.53	HexCer 44:1	840.7274	840.7287	< LOQ
2.54	HexCer 43:1	826.7130	826.7130	< LOQ
2.54	HexCer 42:1	812.6920	812.6974	1397

2.54	HexCer 41:1	798.6798	798.6817	326
2.54	HexCer 40:1	784.6672	784.6661	308
2.55	HexCer 38:1	756.6299	756.6348	135
2.55	HexCer 36:1	728.6077	728.6035	374
2.56	HexCer 44:2	838.7164	838.7130	421
2.56	HexCer 43:2	824.6937	824.6974	559
2.56	HexCer 42:2	810.6774	810.6817	4215
2.56	HexCer 40:2	782.6512	782.6504	877
2.57	HexCer 36:2	726.5826	726.5878	160
2.58	HexCer 42:3	808.6654	808.6661	1709
2.68	HexCer 46:0 (OH)	886.7647	886.7706	< LOQ
2.68	HexCer 44:0 (OH)	858.7338	858.7393	< LOQ
2.68	HexCer 43:0 (OH)	844.7188	844.7236	70
2.68	HexCer 42:0 (OH)	830.7087	830.7080	648
2.68	HexCer 41:0 (OH)	816.6911	816.6923	198
2.68	HexCer 40:0 (OH)	802.6815	802.6767	457
2.68	HexCer 46:1 (OH)	884.7492	884.7549	< LOQ
2.68	HexCer 44:1 (OH)	856.7238	856.7236	156
2.68	HexCer 43:1 (OH)	842.7029	842.7080	213
2.68	HexCer 42:1 (OH)	828.6971	828.6923	1584
2.68	HexCer 41:1 (OH)	814.6716	814.6767	< LOQ
2.68	HexCer 40:1 (OH)	800.6661	800.6610	566
2.69	HexCer 38:0 (OH)	774.6492	774.6454	36
2.69	HexCer 36:0 (OH)	746.6128	746.6141	< LOQ
2.69	HexCer 38:1 (OH)	772.6339	772.6297	72
2.69	HexCer 36:1 (OH)	744.5999	744.5984	78
2.70	HexCer 44:2 (OH)	854.7065	854.7080	332
2.70	HexCer 43:2 (OH)	840.6895	840.6923	< LOQ
2.70	HexCer 42:2 (OH)	826.6754	826.6767	1306
2.70	HexCer 40:2 (OH)	798.6428	798.6454	< LOQ
Phosphatidylglycerols (PG) [c]				
3.15	PG 36:1	775.5477	775.5495	22
3.16	PG 34:1	747.5174	747.5182	7
3.16	PG 36:2	773.5293	773.5338	8
3.17	PG 34:2	745.5001	745.5025	2
3.17	PG 38:4	797.5288	797.5338	4
3.18	PG 36:3	771.5135	771.5182	7
3.18	PG 36:4	769.5004	769.5025	< LOQ
3.18	PG 38:5	795.5190	795.5182	2
Sulfatides [c]				
3.17	42:0	892.6581	892.6548	260
3.17	41:0	878.6422	878.6391	< LOQ
3.18	40:0	864.6214	864.6235	352

3.18	38:0	836.5896	836.5922	20
3.19	36:0	808.5601	808.5609	19
3.21	42:1	890.6360	890.6391	937
3.21	41:1	876.6230	876.6235	98
3.21	40:1	862.6057	862.6078	165
3.22	38:1	834.5816	834.5765	52
3.22	44:2	916.6526	916.6548	155
3.22	43:2	902.6335	902.6391	136
3.22	42:2	888.6292	888.6235	1646
3.23	36:1	806.5487	806.5452	206
3.23	41:2	874.6030	874.6078	44
3.23	40:2	860.5922	860.5922	57
3.24	44:0 (OH)	936.6816	936.6810	6
3.24	43:0 (OH)	922.6678	922.6653	7
3.24	42:0 (OH)	908.6542	908.6497	45
3.24	44:1 (OH)	934.6636	934.6653	28
3.25	41:0 (OH)	894.6303	894.6340	46
3.25	40:0 (OH)	880.6137	880.6184	56
3.25	43:1 (OH)	920.6517	920.6497	24
3.25	42:1 (OH)	906.6394	906.6340	179
3.25	41:1 (OH)	892.6190	892.6184	< LOQ
3.26	38:0 (OH)	852.5876	852.5871	2
3.26	40:1 (OH)	878.6033	878.6033	101
3.26	38:1 (OH)	850.5732	850.5720	245
3.26	44:2 (OH)	932.6474	932.6497	46
3.26	43:2 (OH)	918.6379	918.6340	89
3.26	42:2 (OH)	904.6156	904.6148	229
3.26	41:2 (OH)	890.5969	890.6027	937
3.27	36:1 (OH)	822.5464	822.5407	14
3.27	40:2 (OH)	876.5842	876.5871	91
3.27	44:3 (OH)	930.6342	930.6340	12
3.28	42:3 (OH)	902.6063	902.6027	136
Phosphatidylethanolamines (PE) [d]				
3.38	PE 36:1	746.5664	746.5694	489
3.38	PE 35:1	732.5481	732.5538	< LOQ
3.38	PE O-40:2; PE P-40:1	786.6370	786.6377	67
3.38	PE O-38:2; PE P-38:1	758.6002	758.6058	170
3.38	PE O-36:2; PE P-36:1	730.5766	730.5745	998
3.39	PE O-34:2; PE P-34:1	702.5481	702.5432	1319
3.39	PE 34:0	720.5479	720.5538	27
3.39	PE O-40:3; PE P-40:2	784.6183	784.6215	180
3.39	PE O-38:3; PE P-38:2	756.5939	756.5902	394
3.39	PE 38:3	770.5727	770.5694	109

3.40	PE 34:1	718.5340	718.5381	346
3.40	PE O-40:4; PE P-40:3	782.6023	782.6058	108
3.40	PE O-40:5; PE P-40:4	780.5889	780.5902	475
3.40	PE O-38:4; PE P-38:3	754.5782	754.5745	199
3.40	PE O-38:5; PE P-38:4	752.5533	752.5589	2046
3.40	PE O-36:3; PE P-36:2	728.5605	728.5589	2613
3.41	PE O-34:3; PE P-34:2	700.5250	700.5276	148
3.41	PE O-36:4; PE P-36:3	726.5474	726.5432	127
3.41	PE 36:2	744.5522	744.5538	624
3.41	PE 40:4	796.5842	796.5851	351
3.41	PE 38:4	768.5506	768.5538	2417
3.42	PE 36:3	742.5408	742.5381	74
3.42	PE O-36:5; PE P-36:4	724.5251	724.5276	543
3.42	PE O-40:6; PE P-40:5	778.5781	778.5745	673
3.42	PE O-38:6; PE P-38:5	750.5430	750.5432	1177
3.43	PE 36:4	740.5203	740.5225	233
3.43	PE 40:5	794.5651	794.5694	393
3.43	PE 38:5	766.5433	766.5381	422
3.43	PE O-40:7; PE P-40:6	776.5576	776.5589	2286
3.44	PE O-38:7; PE P-38:6	748.5236	748.5276	450
3.44	PE O-40:8; PE P-40:7	774.5399	774.5432	370
3.44	PE 40:6	792.5486	792.5538	3417
3.45	PE 38:6	764.5265	764.5225	644
3.45	PE 40:7	790.5347	790.5381	464
Phosphatidylinositols (PI) [d]				
3.74	PI 38:4	887.5688	887.5644	22
3.74	PI 40:6	911.5645	911.5644	3
3.75	PI 40:7	909.5493	909.5488	12
3.76	PI 38:5	885.5543	885.5488	7
3.76	PI 36:4	859.5368	859.5331	5
Lysophosphatidylethanolamines (LPE) [c]				
3.75	LPE O-18:1; LPE P-18:0	464.3143	464.3147	13
3.76	LPE O-16:1; LPE P-16:0	436.2821	436.2834	4
3.78	LPE 18:0	480.3128	480.3096	20
Cardiolipins (CL) [f]				
3.85	CL 72:4	727.5136	727.5090	- [g]
3.86	CL 70:3	714.5037	714.5012	- [g]
3.86	CL 70:4	713.4880	713.4934	- [g]
3.86	CL 72:5	726.5005	726.5012	- [g]
3.86	CL 74:6	739.5118	739.5090	- [g]
3.86	CL 72:6	725.4882	725.4934	- [g]
3.86	CL 74:7	738.5023	738.5012	- [g]
3.87	CL 68:2	701.4954	701.4934	- [g]

3.87	CL 68:3	700.4805	700.4856	- [g]
3.87	CL 68:4	699.4728	699.4777	- [g]
3.87	CL 70:5	712.4847	712.4856	- [g]
3.87	CL 68:5	698.4669	698.4699	- [g]
3.87	CL 70:6	711.4822	711.4777	- [g]
3.87	CL 72:7	724.4883	724.4856	- [g]
3.87	CL 76:8	751.5124	751.5090	- [g]
3.87	CL 74:8	737.4935	737.4934	- [g]
3.87	CL 72:8	723.4773	723.4777	- [g]
3.87	CL 76:9	750.5067	750.5012	- [g]
3.88	CL 70:7	710.4687	710.4699	- [g]
3.88	CL 74:9	736.4853	736.4856	- [g]
3.88	CL 78:10	763.5039	763.5090	- [g]
3.88	CL 76:10	749.4896	749.4934	- [g]
3.88	CL 74:10	735.4778	735.4777	- [g]
3.89	CL 78:11	762.4992	762.5012	- [g]
3.89	CL 76:11	748.4853	748.4856	- [g]
3.89	CL 78:12	761.4982	761.4934	- [g]
3.89	CL 76:12	747.4816	747.4777	- [g]
3.90	CL 80:13	774.5016	774.5012	- [g]
3.90	CL 78:13	760.4858	760.4856	- [g]
3.90	CL 80:14	773.4928	773.4934	- [g]
3.90	CL 78:14	759.4831	759.4777	- [g]
3.90	CL 80:15	772.4846	772.4856	- [g]
Lysophosphatidylinositols (LPI) [c]				
4.13	LPI 18:0	599.3222	599.3202	- [g]
4.15	LPI 16:0	571.2928	571.2889	- [g]
4.16	LPI 18:1	597.3024	597.3045	- [g]
4.17	LPI 20:4	619.2943	619.2889	- [g]
Phosphatidylcholines (PC) [d]				
4.66	PC O-34:0	748.6191	748.6220	47
4.66	PC 40:1	844.6807	844.6790	17
4.66	PC 40:2	842.6649	842.6634	2
4.66	PC 38:1	816.6422	816.6477	129
4.66	PC 37:1	802.6320	802.6321	26
4.67	PC O-38:2; PC P-38:1	800.6547	800.6528	19
4.67	PC O-40:3; PC P-40:2	826.6628	826.6684	8
4.67	PC 36:1	788.6214	788.6164	3148
4.67	PC 38:2	814.6342	814.6321	68
4.67	PC 38:3	812.6173	812.6164	41
4.68	PC O-34:1; PC P-34:0	746.6022	746.6058	268
4.68	PC O-36:2; PC P-36:1	772.6217	772.6215	85
4.68	PC 34:0	762.5967	762.6008	1910

4.68	PC 35:1	774.6006	774.6008	119
4.68	PC 40:4	838.6279	838.6321	72
4.69	PC O-32:0	720.5947	720.5907	43
4.69	PC O-38:3; PC P-38:2	798.6305	798.6377	10
4.69	PC 34:1	760.5851	760.5851	6403
4.69	PC 36:2	786.6002	786.6008	917
4.69	PC 38:4	810.6029	810.6008	1060
4.69	PC 40:5	836.6193	836.6164	119
4.70	PC O-38:4; PC P-38:3	796.6212	796.6220	18
4.70	PC 32:0	734.5696	734.5695	2865
4.70	PC 34:2	758.5641	758.5695	394
4.71	PC O-30:0	692.5419	692.5438	8
4.71	PC O-32:1; PC P-32:0	718.5691	718.5745	53
4.71	PC O-34:2; PC P-34:1	744.5880	744.5902	130
4.71	PC O-36:3; PC P-36:2	770.6091	770.6058	92
4.71	PC O-38:5; PC P-38:4	794.6021	794.6058	31
4.71	PC 36:3	784.5817	784.5851	147
4.71	PC 34:3	756.5579	756.5538	72
4.71	PC 40:6	834.6005	834.6008	1218
4.71	PC 42:7	860.6121	860.6164	34
4.72	PC 30:0	706.5335	706.5382	160
4.72	PC 32:1	732.5579	732.5538	644
4.72	PC 32:2	730.5412	730.5382	26
4.72	PC 36:4	782.5657	782.5695	964
4.72	PC 34:4	754.5423	754.5382	18
4.72	PC 38:5	808.5909	808.5851	463
4.72	PC 42:9	856.5833	856.5851	40
4.73	PC 32:3	728.5252	728.5225	6
4.73	PC 36:5	780.5523	780.5538	40
4.73	PC 40:7	832.5842	832.5851	402
4.73	PC 40:8	830.5703	830.5695	27
4.73	PC 40:9	828.5589	828.5538	30
4.74	PC 38:6	806.5692	806.5695	1113
Phosphatidylserines (PS) [d]				
4.94	PS 38:1	818.5882	818.5906	- [h]
4.94	PS 36:1	790.5593	790.5593	- [h]
4.94	PS 36:2	788.5386	788.5436	- [h]
4.94	PS 34:1	762.5244	762.5280	- [h]
4.95	PS 40:3	842.5889	842.5906	- [h]
4.95	PS 40:4	840.5756	840.5749	- [h]
4.95	PS 38:2	816.5703	816.5749	- [h]
4.95	PS 38:3	814.5595	814.5593	- [h]
4.95	PS 38:4	812.5427	812.5436	- [h]

4.96	PS 40:5	838.5540	838.5593	- [h]
4.96	PS 40:6	836.5436	836.5436	- [h]
4.97	PS 42:9	858.5262	858.5280	- [h]
Sphingomyelins (SM) [d]				
4.87	SM 40:0	789.6882	789.6844	46
4.89	SM 38:0	761.6568	761.6531	25
4.93	SM 36:0	733.6235	733.6218	37
4.95	SM 34:0	705.5941	705.5905	< LOQ
4.99	SM 42:1	815.7050	815.7000	234
5.00	SM 41:1	801.6801	801.6844	53
5.00	SM 44:2	841.7148	841.7157	37
5.01	SM 40:1	787.6656	787.6687	202
5.01	SM 43:2	827.7048	827.7000	43
5.02	SM 42:2	813.6877	813.6844	1168
5.03	SM 41:2	799.6669	799.6687	47
5.05	SM 38:1	759.6344	759.6374	636
5.05	SM 40:2	785.6579	785.6531	104
5.05	SM 42:3	811.6719	811.6687	39
5.07	SM 37:1	745.6245	745.6218	< LOQ
5.07	SM 38:2	757.6268	757.6218	25
5.08	SM 36:1	731.6033	731.6061	4125
5.08	SM 38:3	755.6007	755.6061	29
5.10	SM 35:1	717.5866	717.5905	< LOQ
5.11	SM 34:1	703.5781	703.5748	239
5.11	SM 36:2	729.5859	729.5905	146
Lysophosphatidylcholines (LPC) [d]				
5.09	LPC 18:0	524.3741	524.3711	82
5.15	LPC 18:1	522.3571	522.3554	103
5.16	LPC 16:0	496.3432	496.3398	179
5.20	LPC 16:1	494.3226	494.3241	9
5.24	LPC 20:4	544.3408	544.3398	23

Experimental and theoretical *m/z* values correspond to: [a] $[M+Na]^+$, [b] $[M+NH_4]^+$, [c] $[M-H]^-$, [d] $[M+H]^+$, [e] $[M+H-H_2O]^+$ and [f] $[M-2H]^{2-}$ ions in ESI-MS spectra.

[g] Not quantified due to lack of IS.

[h] Concentration corresponds to the sum of isomers.