

SUPPLEMENTARY INFORMATION

Retention behavior of lipids in reversed-phase ultrahigh-performance liquid chromatography – electrospray ionization mass spectrometry

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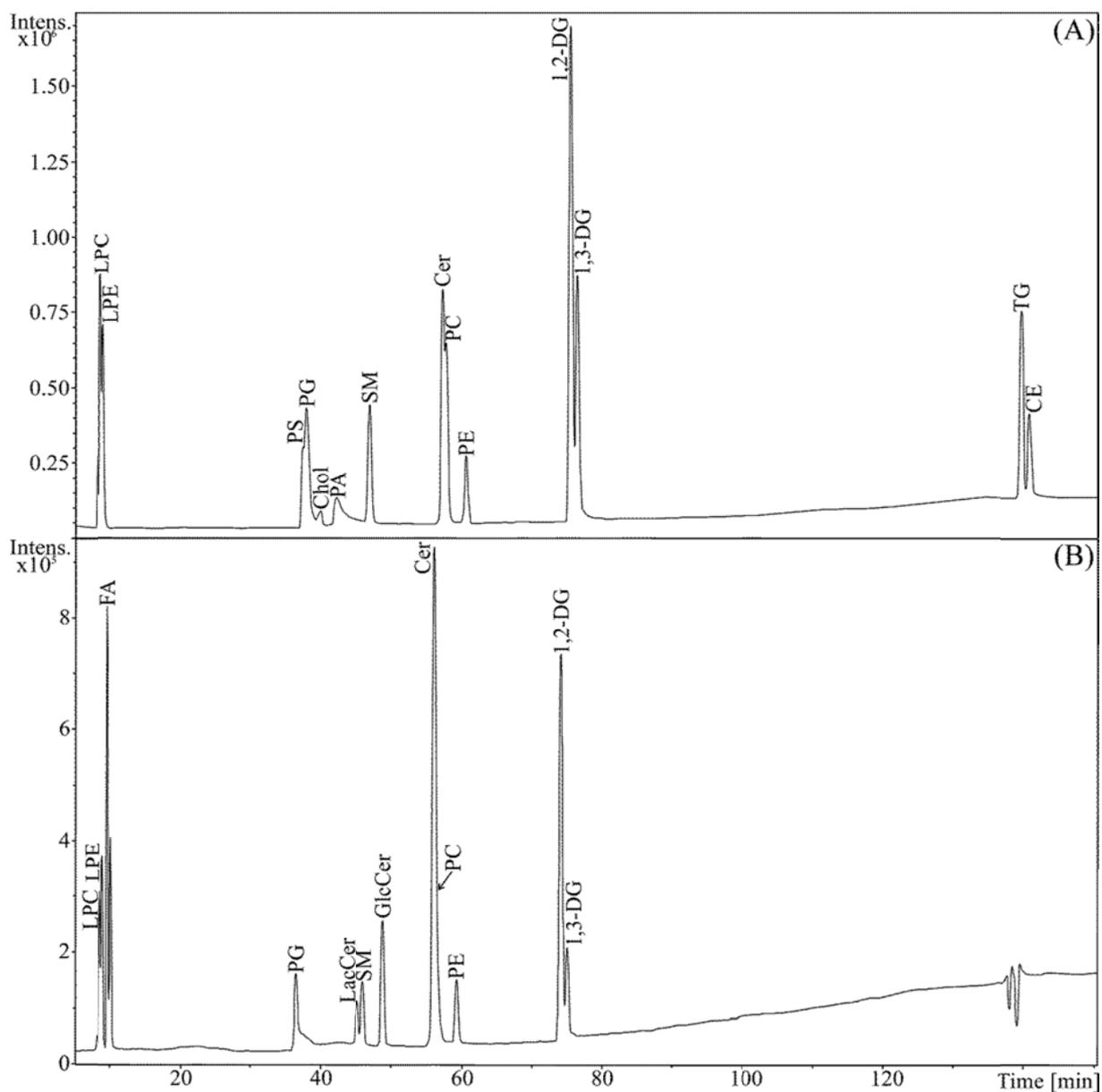


Fig. S1 RP-UHPLC/ESI-MS total ion current chromatograms of the lipid standard mixture containing 18:1 fatty acyls: **(A)** positive-ion and **(B)** negative-ion modes. Conditions are reported in Material and methods. Abbreviations: CE - cholesteryl ester, Cer - ceramide, Chol - cholesterol, DG - diacylglycerol, FA - fatty acid, GlcCer - glucosyl ceramide, LacCer - lactosyl ceramide, LPC - lysophosphatidylcholine, LPE - lysophosphatidylethanolamine, PA - phosphatidic acid, PC - phosphatidylcholine, PE - phosphatidylethanolamine, PG - phosphatidylglycerol, PS - phosphatidylserine, SM - sphingomyeline, and TG - triacylglycerol.

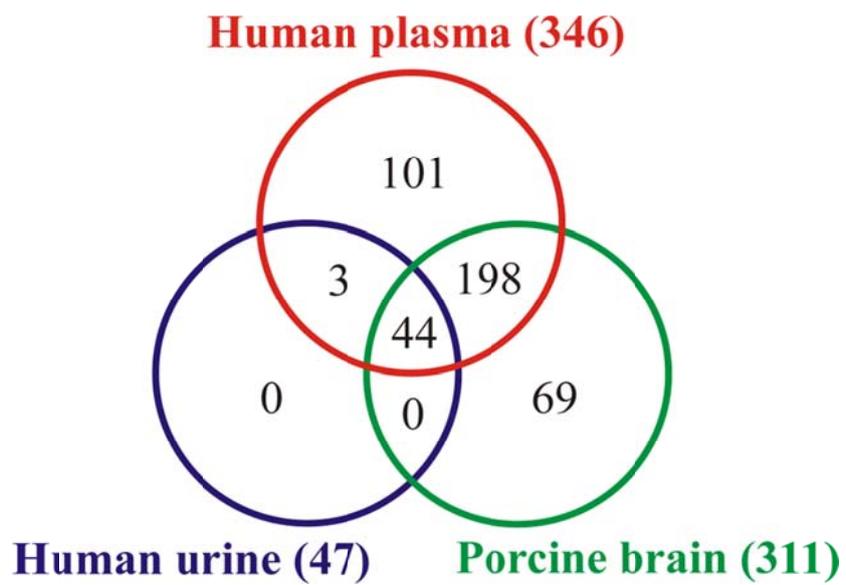


Fig. S2 Venn's diagram constructed based on the data from **Table 1**.

Table S1 List of lipids identified in total lipid extracts of human plasma, human erythrocytes, human urine and porcine brain.

t_R [min]	Lipid species level ^a	Fatty acyl/alkyl level ^a	ECN	m/z theoretical	Human plasma	Human urine	Porcine brain
FATTY ACIDS (FA) ^b							
5.7	FA 12:0		12	199.169	*	*	*
6.2	FA 20:5		10	301.216	*		*
6.5	FA 22:6		10	327.232	*	*	*
6.6	FA 18:3		12	277.216	*		*
7.1	FA 14:0		14	227.201	*	*	*
7.3	FA 20:4		12	303.232	*	*	*
7.4	FA 16:1		14	253.216	*	*	*
7.7	FA 22:5		12	329.248	*		*
7.8	FA 18:2		14	279.232	*	*	*
8.2	FA 15:0		15	241.216	*	*	*
8.3	FA 24:6		12	355.263			*
8.5	FA 20:3		14	305.248	*		*
8.6	FA 17:1		15	267.232	*		*
9	FA 20:3		14	305.248	*		*
9.2	FA 22:4		14	331.263	*		*
9.7	FA 16:0		16	255.232	*	*	*
9.8	FA 18:1		16	281.248	*	*	*
10.3	FA 20:2		16	307.263	*		*
10.4	FA 18:1		16	281.248	*	*	*

10.6	FA 17:0		17	269.248	*	*	*
10.8	FA 20:2		16	307.263	*		*
11.3	FA 17:0		17	269.248	*	*	*
11.8	FA 22:3		16	333.279			*
13.4	FA 18:0		18	283.263	*	*	*
13.6	FA 20:1		18	309.279	*		*
18.8	FA 22:1		20	337.31			*
19	FA 20:0		20	311.295	*		*
21.2	FA 21:0		21	325.31			*
22.8	FA 21:0		21	325.31			*
25.2	FA 22:0		22	339.326	*	*	*
26.4	FA 24:1		22	365.341	*	*	*
27	FA 22:0		22	339.326	*	*	*
29.8	FA 23:0		23	353.341	*	*	*
31.9	FA 23:0		23	353.341	*	*	*
36.7	FA 26:1		24	393.373			*
37.5	FA 24:0		24	367.357	*	*	*
43.8	FA 25:0		25	381.373			*
49.2	FA 28:1		26	421.404			*
50.3	FA 26:0		26	395.388	*	*	*
LYSOPHOSPHATIDYLCHOLINES (LPC) ^c							
6.2	LPC 22:6	PC 22:6_0:0	10	568.34	*		*
6.4	LPC 20:4	PC 20:4/0:0	12	544.34			*
6.5	LPC 16:1	PC 16:1/0:0	14	494.324	*		
6.6	LPC 20:4	PC 0:0/20:4	12	544.34	*		*

6.6	LPC 18:2	PC 18:2/0:0	14	520.34	*		
6.9	LPC 18:2	PC 0:0/18:2	14	520.34	*		
7.8	LPC 16:0	PC 16:0/0:0	16	496.34	*		*
8	LPC 18:1	PC 18:1/0:0	16	522.355	*		*
8.3	LPC 16:0	PC 0:0/16:0	16	496.34	*		*
10.5	LPC 18:0	PC 18:0/0:0	18	524.371	*		*
11.3	LPC 18:0	PC 0:0/18:0	18	524.371	*		*
LYSOPHOSPHATIDYLETHANOLAMINES (LPE) ^c							
6.4	LPE 22:6	PE 22:6_0:0	10	526.293	*		*
6.9	LPE 20:4	PE 20:4_0:0	12	502.293	*		*
8.3	LPE 18:2	PE 18:2_0:0	14	478.293	*		*
8.7	LPE 16:0	PE 16:0_0:0	16	454.293			*
9.3	LPE 18:1	PE 18:1_0:0	16	480.309	*		*
9.7	LPE 18:0	PE 18:0_0:0	18	482.324	*		*
SPHINGOMYELINES (SM) ^c							
23.9	SM 30:1		28	647.512	*		*
24.6	SM 32:2		28	673.528	*		
33.4	SM 32:1		30	675.544	*		*
34.2	SM 34:2		30	701.559	*		*
39.1	SM 33:1		31	689.559	*		
43	SM 34:1		32	703.575	*		
45.1	SM 34:1		32	703.575	*		*
45.8	SM 36:2		32	729.591	*		*
49.9	SM 34:0		34	705.591	*		*
58.2	SM 36:1		34	731.606	*	*	*

58.6	SM 38:2		34	757.622	*		
63.4	SM 36:0		36	733.622	*		*
69.2	SM 40:2		36	785.653	*		*
69.8	SM 42:3		36	811.669	*		
70.3	SM 42:3		36	811.669	*		*
71.2	SM 38:1		36	759.638	*		*
71.7	SM 38:1		36	759.638	*		*
71.7	SM 40:2		36	785.653	*		
71.9	SM 42:3		36	811.669	*		
75.9	SM 41:2		37	799.669	*		*
77.6	SM 39:1		37	773.653	*		
77.8	SM 41:2		37	799.669	*		*
80	SM 42:2		38	813.684	*		
80.2	SM 40:1		38	787.669	*		*
82.3	SM 42:2		38	813.684	*		*
84.5	SM 40:1		38	787.669	*		
84.4	SM 42:2		38	813.684	*		
88.2	SM 43:2		39	827.7	*		*
88.9	SM 40:0		40	789.684	*		*
90.5	SM 41:1		39	801.684	*		*
96.5	SM 42:1		40	815.7	*		*
99.1	SM 43:1		41	829.716	*		
101.7	SM 43:1		41	829.716	*		*
PHOSPHATIDYLINOSITOLS (PI)^b							
25.1	PI 38:6	PI 16:0/22:6	26	881.518	*		*

27.3	PI 32:1	PI 16:0/16:1	30	807.502	*		
27.4	PI 36:4	PI 16:0/20:4	28	857.518	*		*
27.6	PI 38:5	PI 18:1/20:4	28	883.533	*		*
28.8	PI 34:2	PI 16:0/18:2	30	833.518	*		
29.1	PI 36:3	PI 18:1/18:2	30	859.533	*		
31	PI 36:3	PI 16:0/20:3	30	859.533	*		
33.8	PI 40:6	PI 18:0/22:6	28	909.549	*		*
36.4	PI 34:1	PI 16:0/18:1	32	835.533	*		
36.6	PI 38:4	PI 18:0/20:4	30	885.549	*		*
38.4	PI 36:2	PI 18:0/18:2	32	861.549	*		
40.9	PI 38:3	PI 18:0/20:3	32	887.564	*		*
47.1	PI 36:1	PI 18:0/18:1	34	863.564	*		
PHOSPHATIDYLGLYCEROLS (PG) ^b							
28.4	PG 36:4		28	769.501			*
28.6	PG 38:5		28	795.517			*
37	PG 34:1	PG 16:0/18:1	32	747.517			*
37.3	PG 36:2		32	773.533	*		
37.8	PG 38:4		30	797.533			*
47.7	PG 36:1	PG 18:0/18:1	34	775.548			*
PHOSPHATIDYLETHANOLAMINES (PE) ^b							
32.8	PE 36:5		26	736.491	*		*
35.3	PE 40:7	PE 18:2/22:5	26	788.523	*		*
43.1	PE 38:6	PE 16:0/22:6	26	762.507	*	*	*
44.1	PE 38:5	PE 16:0/22:5	28	764.523	*	*	*
44.7	PE 40:6	PE 18:1/22:5	28	790.538	*		*

46.8	PE 36:4	PE 16:0/20:4	28	738.507	*	*	
48.3	PE P-38:6	PE P-16:0/22:6		746.512	*	*	*
49.2	PE 34:2	PE 16:0/18:2	30	714.507	*	*	*
49.3	PE 36:3	PE 18:1/18:2	30	740.523	*	*	*
52.3	PE P-36:4	PE P-16:0/20:4		722.512	*	*	*
52.4	PE P-38:5	PE P-18:1/20:4		748.528	*		*
55.2	PE P-34:2	PE P-16:0/18:2		698.512	*	*	
55.3	PE P-36:3	PE P-18:1/18:2		724.528	*		
56.8	PE 40:5	PE 18:0/22:5	30	792.554	*	*	*
57	PE 42:6		30	818.569	*	*	
59.1	PE 38:4	PE 18:0/20:4	30	766.538	*	*	*
59.6	PE 34:1	PE 16:0/18:1	32	716.623	*	*	*
60.6	PE P-40:6	PE P-18:0/22:6		774.543	*	*	*
61.8	PE 36:2	PE 18:0/18:2	32	742.538	*		*
63	PE P-40:5			776.559	*		*
64.6	PE 38:3	PE 18:0/20:3	32	768.554	*		*
65	PE P-38:4	PE P-18:0/20:4		750.543	*	*	*
65.9	PE P-34:1	PE P-16:0/18:1		700.528	*	*	*
67.8	PE 40:4		32	794.569	*		*
68	PE P-36:2	PE P-18:0/18:2		726.543	*		*
69.9	PE 42:5		32	820.585	*	*	*
72.5	PE 36:1	PE 18:0/18:1	34	744.554	*	*	*
73	PE 34:0	PE 16:0/18:0	34	718.538			*
77.4	PE P-40:4	PE P-18:0/22:4		778.575	*		
78.8	PE P-36:1	PE P-18:0/18:1		728.559	*	*	*

80.8	PE O-34:0			704.559	*		*
84.3	PE 40:2	PE 20:1/20:1	36	798.601			*
89.4	PE 40:1	PE 20:0/20:1	38	800.616			*
PHOSPHATIDYLCHOLINES (PC) ^c							
33.4	PC 36:5	PC 16:1/20:4	26	780.554	*		*
34.2	PC 36:5	PC 16:0/20:5	26	780.554	*		*
35	PC 32:2	PC 14:0/18:2	28	730.538	*		
35.2	PC 38:6	PC 18:2/20:4	26	806.569	*		
35.4	PC 34:3	PC 16:1/18:2	28	756.554	*		
36.4	PC 34:3	PC 14:0/20:3	28	756.554	*		
37.2	PC 36:4	PC 18:2/18:2	28	782.569	*		*
37.4	PC 34:3	PC 16:0/18:3	28	756.554	*		
38.2	PC 34:3	PC 16:0/18:3	28	756.554	*		
39.5	PC 38:6		26	806.569			*
39.8	PC 38:5	PC 18:2/20:3	28	808.585	*		
40	PC 40:7	PC 18:1/22:6	26	832.585			*
40	PC 34:3		28	756.554	*		
40.5	PC 33:2	PC 15:0/18:2	29	744.554	*		
40.5	PC 38:6	PC 16:0/22:6	26	806.569	*		*
40.6	PC 40:7	PC 18:1/22:6	26	832.585			*
41	PC 36:4	PC 16:0/20:4	28	782.569	*		
42	PC 36:4		28	782.569	*		*
43.6	PC 38:5	PC 18:1/20:4	28	808.585	*		*
44	PC 36:4	PC 16:0/20:4	28	782.569	*		*
44.1	PC 38:5	PC 16:0/22:5	28	808.585	*		*

44.3	PC 32:1	PC 14:0/18:1	30	732.554	*		*
44.3	PC 34:2	PC 16:1/18:1	30	758.569	*		*
45.4	PC 32:1	PC 14:0/18:1	30	732.554			*
45.6	PC 38:5	PC 18:1/20:4	28	808.585	*		
45.9	PC 36:3	PC 18:1/18:2	30	784.585	*		*
46.3	PC 34:2	PC 16:0/18:2	30	758.569	*		*
46.5	PC 32:1	PC 14:0/18:1	30	732.554			*
47.3	PC 40:6	PC 16:0/24:6	28	834.601	*		
47.7	PC 38:5	PC 18:0/20:5	28	808.585	*		*
48.5	PC 38:5	PC 16:0/22:5	28	808.585	*		*
49.1	PC 36:3	PC 16:0/20:3	30	784.585	*		*
50.2	PC 33:1		31	746.569	*		*
51.3	PC P-36:3	PC P-16:0/20:3		768.59	*		
52.1	PC 40:6	PC 18:0/22:6	28	834.601	*		
52.3	PC 38:4	PC 16:0/22:4	30	810.601	*		*
52.5	PC 35:2	PC 17:0/18:2	31	772.585	*		
53.3	PC 36:3	PC 16:0/20:3	30	784.585	*		*
55.3	PC 40:5	PC 20:1/20:4	30	836.616	*		
55	PC 36:2	PC 18:1/18:1	32	786.601			*
55.6	PC 34:1		32	760.585			*
55.7	PC 34:1	PC 16:0/18:1	32	760.585	*		*
56.1	PC 38:4	PC 18:0/20:4	30	810.601	*		*
56.4	PC 32:0	PC 16:0/16:0	32	734.569	*	*	*
56.5	PC 34:1	PC 16:0/18:1	32	760.585	*		*
56.5	PC O-34:1			760.585	*	*	*

57.4	PC 36:2	PC 16:0/20:2	32	786.601	*		*
58.7	PC 36:2	PC 18:0/18:2	32	786.601	*		*
60.7	PC 40:5	PC 18:0/22:5	30	836.616	*		*
61.6	PC 38:3		32	812.616	*		*
63.1	PC 38:3		32	812.616	*		
64.8	PC 40:4	PC 18:0/22:4	32	838.632	*		*
66	PC 38:3		32	812.616	*		*
68.6	PC 36:1	PC 16:0/20:1	34	788.616	*		*
69.4	PC 36:1	PC 18:0/18:1	34	788.616	*		*
69.5	PC 34:0	PC 18:0/16:0	34	762.601	*		*
71.3	PC 38:2	PC 18:0/20:2	34	814.632	*		*
SULFATIDES^b							
35.6	Sulfatide 36:1		34	806.545			*
46	Sulfatide 38:1		36	834.576			*
55.3	Sulfatide 42:2		38	888.623			*
61	Sulfatide 43:2		39	902.639			*
62.5	Sulfatide 41:1		39	876.623			*
66.6	Sulfatide 44:2		40	916.654			*
68	Sulfatide 42:1		40	890.639			*
CERAMIDES (Cer)^c							
56	Cer 34:1	Cer d18:1/16:0	32	538.519			*
56.7	Cer 36:2	Cer d18:2/18:0	32	564.535			*
58.5	Cer 36:1 (OH)		34	582.546			*
62.7	Cer 35:1		33	552.535			*
69.7	Cer 36:1	Cer d18:1/18:0	34	566.551			*

69.9	Cer 38:2		34	592.566			*
71.6	Cer 38:1 (OH)		36	610.577			*
76.3	Cer 37:1		35	580.566			*
82.7	Cer 38:1	Cer d18:1/20:0	36	594.582			*
84.2	Cer 40:1 (OH)		38	638.608			*
93	Cer 42:2	Cer d18:1/24:1	38	648.629			*
95	Cer 40:1	Cer d18:1/22:0	38	622.613			*
106.3	Cer 42:1	Cer d18:1/24:0	40	650.645			*
HEXOSYL CERAMIDES (HexCer)^c							
61.5	HexCer 36:1	HexCer d18:1/18:0	34	728.604			*
78.3	HexCer 36:0	HexCer d18:0/18:0	36	730.619			*
85.2	HexCer 42:2	HexCer d18:1/24:1	38	810.682			*
87.2	HexCer 40:1	HexCer d18:1/22:0	38	784.666			*
88.2	HexCer 44:1	HexCer d18:1/26:0	42	840.729			*
89.8	HexCer 42:1	HexCer d18:0/24:1	40	812.697			*
90.4	HexCer 42:0	HexCer d18:0/24:0	42	814.713			*
91.9	HexCer 40:0	HexCer d18:0/22:0	40	786.682			*
93.2	HexCer 41:1	HexCer d18:1/23:0	39	798.682			*
96.9	HexCer 44:2	HexCer d18:1/26:1	40	838.713			*
98.9	HexCer 42:1	HexCer d18:1/24:0	40	812.697			*
101.7	HexCer 44:0	HexCer d18:0/26:0	44	842.744			*
DIACYLGLYCEROLS (DG)^d							
63.6	1,2-DG 34:2		30	615.496	*		
63.7	1,2-DG 36:3		30	641.512	*		

64.5	1,3-DG 34:2		30	615.496	*		
64.5	1,3-DG 36:3		30	641.512	*		
72.6	1,2-DG 38:4		30	667.527			*
73.9	1,3-DG 38:4		30	667.527			*
74.4	1,2-DG 36:2		32	643.527	*		*
74.5	1,2-DG 34:1		32	617.512	*		*
74.7	1,2-DG 32:0		32	591.496	*		*
75.3	1,3-DG 36:2		32	643.527	*		*
75.3	1,3-DG 32:0		32	591.496	*		*
75.4	1,3-DG 34:1		32	617.512	*		*
87	1,2-DG 36:1		34	645.543	*		*
88	1,3-DG 36:1		34	645.543	*		*
88.1	DG 34:0		34	619.527			*
CHOLESTEROL (Chol)^e AND CHOLESTEROLESTERS (CE)^f							
39.4	Chol			369.352	*		*
118.6	CE 20:5		10	688.603	*		*
121.2	CE 22:6		10	714.618	*		*
121.9	CE 14:1		12	612.571	*		
123.7	CE 18:3		12	664.603	*		
124.1	CE 18:3		12	664.603	*		
126.1	CE 20:4		12	690.618	*		*
127.1	CE 20:4		12	690.618	*		
128.4	CE 22:5		12	716.634	*		
131	CE 16:1		14	640.603	*		
131.2	CE 18:2		14	666.618	*		*

131.4	CE 18:2		14	666.618	*		
131.7	CE 14:0		14	614.587	*		*
131.9	CE 20:3		14	692.634	*		
135.3	CE 17:1		15	654.618	*		
136.3	CE 15:0		15	628.603	*		
139.1	CE 18:1		16	668.634	*		
139.6	CE 18:1		16	668.634	*		*
140.6	CE 16:0		16	642.618	*		*
143.1	CE 17:0		17	656.634	*		
144.8	CE 17:0		17	656.634	*		
148.1	CE 18:0		18	670.65	*		*
TRIACYLGLYCEROLS (TG) ^{f, g}							
116.9	TG 46:2		42	792.708			*
116.8	TG 46:2		42	792.708			*
117	TG 50:4	TG 18:2/16:1/16:1	42	844.739	*		*
117.3	TG 48:3	TG 18:2/12:0/18:1	42	818.723	*		*
117.3	TG 44:1	TG 18:1/12:0/14:0	42	766.692	*		*
117.4	TG 52:5	TG 18:2/18:2/16:1	42	870.755	*		*
117.8	TG 48:3		42	818.723	*		
117.9	TG 50:4	TG 18:2/18:2/14:0	42	844.739	*		*
118	TG 54:6	TG 18:3/18:2/18:1	42	896.77	*		*
118.1	TG 46:2	TG 18:2/12:0/16:0	42	792.708			*
118.1	TG 42:0	TG 16:0/12:0/14:0	42	740.676	*		
118.3	TG 52:5	TG 18:3/18:2/16:0	42	870.755	*		*
118.6	TG 44:1	TG 16:1/14:0/14:0	42	766.692	*		*

119	TG 50:4	TG 18:3/16:1/16:0	42	844.739	*		*
119	TG 54:6	TG 20:4/18:1/16:1	42	896.77	*		*
119.2	TG 46:2		42	792.708			*
119.5	TG 52:5		42	870.755	*		*
119.7	TG 56:8	TG 22:6/18:2/16:0	40	920.77			*
119.8	TG 48:3	TG 18:3/14:0/16:0	42	818.723	*		
120.1	TG 54:6	TG 20:4/18:2/16:0	42	896.77	*		
120.2	TG 50:4	TG 18:3/16:1/16:0	42	844.739	*		
120.8	TG 52:5	TG 18:3/18:2/16:0	42	870.755	*		
121	TG 48:3	TG 18:3/14:0/16:0	42	818.723	*		
121.1	TG 50:4	TG 20:4/14:0/16:0	42	844.739	*		
121.6	TG 49:3	TG 18:2/16:1/15:0	43	832.739	*		
121.8	TG 54:6	TG 20:5/18:1/16:0	42	896.77	*		*
122.3	TG 56:7	TG 22:5/18:2/16:0	42	922.786			*
122.4	TG 52:5	TG 18:4/18:1/16:0	42	870.755	*		*
122.8	TG 54:6		42	896.77	*		*
123.1	TG 50:4		42	844.739	*		*
123.5	TG 56:7		42	922.786	*		
124.1	TG 54:6		42	896.77	*		
124.4	TG 50:3	TG 18:1/16:1/16:1	44	846.755	*		*
124.8	TG 52:4	TG 18:1/18:2/16:1	44	872.77	*		*
125	TG 48:2	TG 18:1/16:1/14:0	44	820.739	*		*
125.3	TG 54:5	TG 18:2/18:2/18:1	44	898.786	*		*
125.5	TG 48:2		44	820.739	*		
125.5	TG 50:3	TG 18:2/16:0/16:1	44	846.755	*		*

125.8	TG 46:1	TG 18:1/16:0/12:0	44	794.723	*		*
126	TG 52:4	TG 18:2/18:2/16:0	44	872.77	*		*
126.2	TG 54:5	TG 18:3/18:1/18:1	44	898.786	*		*
126.3	TG 56:7	TG 22:6/18:1/16:0	42	922.786			*
126.4	TG 50:3		44	846.755	*		
126.4	TG 48:2	TG 18:2/16:0/14:0	44	820.739	*		*
126.6	TG 44:0	TG 16:0/14:0/14:0	44	768.708	*		*
126.7	TG 46:1		44	794.723	*		
126.8	TG 52:4	TG 18:1/18:3/16:0	44	872.77	*		*
126.9	TG 54:5		44	898.786	*		
127.2	TG 46:1	TG 16:0/16:1/14:0	44	794.723	*		
127.2	TG 54:5		44	898.786	*		*
127.6	TG 48:2		44	820.739	*		*
127.7	TG 50:3		44	846.755	*		*
127.8	TG 54:5		44	898.786	*		*
128	TG 52:4	TG 16:0/20:4/16:0	44	872.77	*		
128.1	TG 56:6	TG 22:4/18:2/16:0	44	924.802	*		*
128.5	TG 49:2		45	834.755	*		
128.6	TG 56:6		44	924.802	*		*
128.8	TG 50:3		44	846.755	*		
128.9	TG 49:2		45	834.755	*		*
129.2	TG 56:6	TG 20:4/18:2/18:0	44	924.802	*		*
129.5	TG 54:5	TG 20:3/18:1/16:1	44	898.786	*		*
129.6	TG 51:3	TG 18:2/15:0/18:1	45	860.77	*		*
129.9	TG 50:3	TG 18:3/16:0/16:0	44	846.755	*		

130	TG 54:5	TG 20:4/18:1/16:0	44	898.786	*		*
130.1	TG 49:2		45	834.755	*		*
130.3	TG 56:6	TG 22:5/18:1/16:0	44	924.802	*		*
130.8	TG 52:4	TG 20:4/16:0/16:0	44	872.77	*		*
131.7	TG 54:4	TG 18:2/18:1/18:1	46	900.802	*		*
131.8	TG 52:3	TG 18:1/18:1/16:1	46	874.786	*		*
131.8	TG 56:6		44	924.802	*		
131.9	TG 48:1	TG 16:0/18:1/14:0	46	822.755	*		
132.1	TG 54:4		46	900.802	*		*
132.4	TG 52:3		46	874.786	*		*
132.5	TG 50:2	TG 18:1/16:1/16:0	46	848.77	*		*
132.9	TG 52:3	TG 18:1/18:2/16:0	46	874.786	*		*
133.2	TG 54:4	TG 18:2/18:2/18:0	46	900.802	*		*
133.4	TG 48:1		46	822.755	*		*
133.7	TG 50:2	TG 16:0/18:2/16:0	46	848.77	*		*
133.7	TG 54:4	TG 22:4/16:0/16:0	46	900.802	*		*
134	TG 52:3		46	874.786	*		
134.2	TG 48:1	TG 16:1/16:0/16:0	46	822.755	*	*	*
134.4	TG 46:0	TG 16:0/16:0/14:0	46	796.739	*		*
134.7	TG 48:1		46	822.755	*		*
134.7	TG 56:5	TG 22:4/16:0/18:1	46	926.817	*		*
134.5	TG 51:2	TG 16:0_17:0_18:2	47	862.786	*		
134.8	TG 53:3		47	888.802	*		
135.2	TG 56:5		46	926.817	*		
135.2	TG 53:3	TG 18:1/18:1/17:1	47	888.802	*		*

135.3	TG 49:1	TG 15:0_16:0_18:1	47	836.77	*		*
135.6	TG 51:2	TG 16:0_17:0_18:2	47	862.786	*		
135.6	TG 54:4	TG 20:4/16:0/18:0	46	900.802	*		*
135.8	TG 53:3		47	888.802	*		
136	TG 51:2		47	862.786	*		*
136	TG 54:4		46	900.802	*		*
136.3	TG 53:3	TG 18:1/18:2/17:0	47	888.802	*		*
136.4	TG 56:5	TG 20:4/18:1/18:0	46	926.817	*		*
136.8	TG 56:5		46	926.817	*		*
137	TG 49:1	TG 15:0_16:0_18:1	47	836.77	*		*
137.1	TG 51:2		47	862.786	*		*
137.6	TG 54:4		46	900.802	*		*
138	TG 52:2	TG 18:1/18:1/16:0	48	876.802	*		
138.1	TG 54:3	TG 18:1/18:1/18:1	48	902.817	*	*	*
138.5	TG 54:3		48	902.817	*		*
138.9	TG 50:1	TG 18:1/16:0/16:0	48	850.786	*		*
139	TG 52:2		48	876.802	*		*
139	TG 54:3		48	902.817	*		*
139.3	TG 52:2		48	876.802	*	*	*
139.6	TG 54:3	TG 18:1/18:2/18:0	48	902.817	*		*
139.8	TG 50:1		48	850.786	*		*
139.9	TG 52:2	TG 20:2/16:0/16:0	48	876.802	*		
140.2	TG 50:1		48	850.786	*		*
140.3	TG 52:2		48	876.802	*	*	*
140.7	TG 54:3		48	902.817	*		*

141	TG 50:1		48	850.786	*		*
141.1	TG 48:0	TG 18:0/16:0/14:0	48	824.77	*	*	*
141.1	TG 53:2	TG 18:1/18:1/17:0	49	890.817	*		
141.3	TG 52:2		48	876.802	*		*
141.4	TG 50:1	TG 18:1/16:0/16:0	48	850.786	*		*
141.9	TG 56:4		48	928.833			*
142	TG 51:1	TG 18:1_17:0_16:0	49	864.802	*		*
142.3	TG 50:1		48	850.786	*		*
142.5	TG 53:2	TG 18:0/18:2/17:0	49	890.817	*		*
143	TG 49:0	TG 17:0_16:0_16:0	49	838.786	*		
134.4	TG 51:1	TG 18:1_17:0_16:0	49	864.802	*		*
144.2	TG 56:3	TG 20:1/18:1/18:1	50	930.848	*		*
144.3	TG 49:0	TG 17:0_16:0_16:0	49	838.786	*		*
145	TG 54:2	TG 20:1/18:1/16:0	50	904.833	*		*
145.4	TG 54:2	TG 18:1/18:1/18:0	50	904.833	*		*
145.9	TG 52:1		50	878.817	*	*	*
146.4	TG 52:1	TG 18:0/18:1/16:0	50	878.817	*		*
147.3	TG 50:0	TG 18:0/16:0/16:0	50	852.802	*		*
148	TG 53:1	TG 18:1_18:0_17:0	51	892.833	*		*
148.8	TG 51:0	TG 18:0_17:0_16:0	51	866.817	*		
149.2	TG 53:1	TG 18:1_18:0_17:0	51	892.833	*		*
149.5	TG 58:3		52	958.88	*		
150.2	TG 51:0	TG 18:0_17:0_16:0	51	866.817	*		*
150.2	TG 58:3		52	958.88	*		
150.5	TG 56:2	TG 22:1/18:1/16:0	52	932.864	*		

151	TG 56:2		52	932.864	*		
151.4	TG 54:1	TG 18:0/20:1/16:0	52	906.848			*
151.7	TG 56:2	TG 22:0/18:2/16:0	52	932.864	*		
151.9	TG 54:1	TG 18:0/18:0/18:1	52	906.848	*		*
152.8	TG 58:3		52	958.88	*		
152.9	TG 52:0	TG 18:0/18:0/16:0	52	880.833	*		*
155.2	TG 58:2	TG 24:1/18:1/16:0	54	960.895	*		
155.9	TG 58:2		54	960.895	*		
156.6	TG 58:2	TG 24:0/16:0/18:2	54	960.895	*		
156.8	TG 56:1	TG 24:1/16:0/16:0	54	934.88	*		
157.7	TG 54:0		54	908.864			*

^a The lipid annotation follows the nomenclature recommended by Liebisch et al. [39], where the slash “/” denotes the prevailing *sn*-configuration in the detected lipid, while the underscore “_” is used in case, where the data does not provide the support for such identification.

^b Identified based on [M-H]⁻.

^c Identified based on [M+H]⁺.

^d Identified based on [M+Na]⁺.

^e Identified based on [M+H-H₂O]⁺.

^f Identified based on [M+NH₄]⁺.

^g Only prevailing *sn*-2 fatty acyl can be determined for TG, but the data does not give the information on *sn*-1 vs. *sn*-3 preference, for example TG 18:2/12:0/18:1 is the abbreviation for TG having 12:0 in *sn*-2 position, while 18:2 and 18:1 in *sn*-1 and *sn*-3 positions are not differentiated.

Table S2 Major observed ions for lipid standard mixture containing C18:1 fatty acyls.

Lipid standard (C18:1)	Positive-ion ESI-MS	Negative-ion ESI-MS
LPC	$[M+H]^+$, $[M+Na]^+$, m/z 184	$[M+CH_3COO]^-$
LPE	$[M+H]^+$, $[M+Na]^+$	$[M-H]^-$
FA	n.d. *	$[M-H]^-$
PS	$[M+H]^+$, $[M+Na]^+$	n.d. *
PG	$[M+H]^+$, $[M+Na]^+$	$[M+CH_3COO]^-$
Chol	m/z 369	n.d. *
PA	$[M+H]^+$, $[M+Na]^+$	n.d. *
LacCer	$[M+H]^+$	$[M-H]^-$, $[M+CH_3COO]^-$
SM	$[M+H]^+$, $[M+Na]^+$, m/z 184	$[M+CH_3COO]^-$
GlcCer	$[M+H]^+$	$[M-H]^-$, $[M+CH_3COO]^-$
Cer	$[M+H]^+$, $[M+Na]^+$	$[M-H]^-$, $[M+CH_3COO]^-$
PC	$[M+H]^+$, $[M+Na]^+$, m/z 184	$[M+CH_3COO]^-$
PE	$[M+H]^+$, $[M+Na]^+$	$[M+HCOO]^-$
DG	$[M+H]^+$, $[M+Na]^+$, $[M+H-H_2O]^+$	$[M+CH_3COO]^-$
TG	$[M+H-R_iCOOH]^+$, $[M+NH_4]^+$	n.d. *
CE	$[M+NH_4]^+$, $[M+Na]^+$, m/z 369	n.d. *

n.d. * – not detected.

Table S3 Comparison of predicted and experimental retention times for selected lipid standards.

Lipid standards	Logical series	Predicted t_R [min]	Experimental t_R [min]	Relative error [%]
FA d9 18:1	FA X:1	10.13	9.90	2.3
SM d18:1/12:0	SM X:1	22.68	23.80	4.9
Cer d18:1/12:0	Cer X:1	33.29	32.66	1.9
CE d7 16:0	CE X:0	144.09	141.54	1.8
TG 19:1/19:1/19:1	TG X:3	151.69	147.90	2.6

Table S4 Parameters of polynomial regressions $y=ax^2+bx+c$ of relative retention times of PC and TG series on the relative CN from previously published RP-HPLC data [48].

Lipid series	a	b	c	R ²	X
PC X:2	0.9450	0.2885	-0.2330	0.9999	32, 34, 36, 38
PC X:3	1.10^{-13}	2.1538	-1.1426	0.9873	32, 34, 36, 38, 40
PC X:4	-4.3478	10.4350	-5.0897	0.9980	34, 36, 38, 40
TG X:0	1.0430	-0.6484	0.5956	0.9927	34, 38, 40, 46, 48, 50, 52, 54, 56, 58
TG X:1	0.6289	0.0327	0.3185	0.9924	34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60
TG X:2	0.3376	0.5277	0.1086	0.9911	34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62
TG X:3	0.7752	-0.2554	0.4652	0.9945	40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62
TG X:4	-0.2549	1.3974	-0.1346	0.9946	42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62
TG X:5	-0.4895	1.8213	-0.3345	0.9934	42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62
TG X:6	0.7106	-0.2597	0.5481	0.9992	46, 48, 50, 52, 54, 56, 58, 60, 62
TG X:7	0.9812	-0.7266	0.7425	0.9986	48, 50, 52, 54, 56, 58, 60, 62
TG X:8	-0.4218	1.7801	-0.3609	0.9966	48, 50, 52, 54, 56, 58, 60
TG X:9	-1.6534	4.0295	-1.3724	0.9954	50, 52, 54, 56, 58, 60
TG X:10	-1.8987	4.4684	-1.5688	0.9966	54, 56, 58, 60
TG X:11	-0.9928	2.9271	-0.9337	0.9986	56, 58, 60, 62
TG X:12	-2.0360	5.0047	1.9669	0.9914	56, 58, 60, 62

Table S5 Parameters of polynomial regressions $y=ax^2+bx+c$ of relative retention times of PC and TG series on the relative DB number from previously published RP-HPLC data [48].

Lipid series	a	b	c	R ²	Y
PC 32:Y	0.0549	-0.3549	0.9976	0.9976	0, 1, 2, 3
PC 34:Y	0.0907	-0.4611	0.9944	0.9967	0, 1, 2, 3, 4
PC 36:Y	0.0952	-0.5755	1.0857	0.9887	1, 2, 3, 4, 5, 6
PC 38:Y	0.0558	-0.6502	1.1694	0.9895	2, 3, 4, 5, 6, 7, 8
PC 40:Y	-0.3634	-0.0677	1.0776	0.9875	3, 4, 5, 6, 7, 8
TG 40:Y	-4.10 ⁻¹⁵	-0.1322	1.0000	1.0000	0, 1, 2, 3
TG 42:Y	-0.06610	-0.1071	1.0105	0.9690	1, 2, 3, 4, 5
TG 44:Y	-0.0669	-0.0760	1.0368	0.9779	1, 2, 3, 4, 5
TG 46:Y	0.0450	-0.2276	0.9958	0.9946	0, 1, 2, 3, 4, 5, 6
TG 48:Y	0.0449	-0.2791	0.9934	0.9960	0, 1, 2, 3, 4, 5, 6, 7, 8
TG 50:Y	0.0669	-0.3482	0.9944	0.9976	0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
TG 52:Y	0.1072	-0.3624	0.9975	0.9987	0, 1, 2, 3, 4, 5, 6, 7, 8, 9
TG 54:Y	0.1580	-0.4367	0.9941	0.9988	0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
TG 56:Y	0.2169	-0.5379	0.9748	0.9873	0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
TG 58:Y	0.2658	-0.6154	0.9799	0.9907	0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13
TG 60:Y	0.3131	-0.6887	1.0355	0.9922	0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13
TG 62:Y	0.3421	-0.7601	1.0695	0.9751	2, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15

Table S6 Parameters of polynomial regressions $y=ax^2+bx+c$ of relative retention times of PC and TG series on the relative CN from previously published UHPSFC data [38].

Lipid series	a	b	c	R²	X
PC X:1	0.4381	-0.8532	1.4023	0.9954	32, 34, 35, 36, 37, 38, 40
PC X:2	0.0605	-0.1725	1.0992	0.9900	32, 34, 36, 38, 40
PC X:3	-0.3816	0.6307	0.7389	0.9053	32, 34, 36, 38
PC X:4	-0.2119	0.3284	0.8745	0.9020	34, 36, 38, 40
TG X:0	0.2266	0.0436	0.7292	0.9962	42, 44, 46, 48, 49, 50, 51, 52, 53, 54
TG X:1	0.1610	0.1425	0.6951	0.9948	42, 44, 46, 48, 49, 50, 51, 52, 53, 54, 55, 56
TG X:2	-0.2560	0.8328	0.4233	0.9942	42, 44, 46, 48, 49, 50, 51, 52, 53, 54, 55, 56, 58
TG X:3	-0.1888	0.7018	0.4872	0.9925	44, 48, 49, 50, 51, 52, 53, 54, 55, 56, 58
TG X:5	-0.0678	0.4691	0.5995	0.9550	51, 52, 53, 54, 55, 56, 58, 60

Table S7 Parameters of polynomial regressions $y=ax^2+bx+c$ of relative retention times of PC and TG series on the relative DB number from previously published UHPSFC data [38].

Lipid series	a	b	c	R²	Y
PC 34:Y	0.0000	0.0085	0.9915	1.0000	0, 1, 2, 3, 4
PC 36:Y	-0.0113	0.0294	0.9818	0.9975	1, 2, 3, 4, 5
PC 38:Y	0.0184	-0.0011	0.9830	0.9887	1, 2, 3, 4, 5, 6
PC 40:Y	-0.0004	0.0204	0.9817	0.9424	1, 2, 3, 4, 5, 6, 7, 8, 9
TG 44:Y	-7.10^{-15}	0.0294	0.9706	1.0000	0, 1, 2, 3
TG 48:Y	0.0000	0.0377	0.9623	1.0000	0, 1, 2, 3, 4
TG 49:Y	-4.10^{-15}	0.0283	0.9717	1.0000	0, 1, 2, 3
TG 50:Y	0.0000	0.0370	0.9630	1.0000	0, 1, 2, 3, 4
TG 51:Y	0.0205	0.0188	0.9617	0.9866	0, 1, 2, 3, 4, 5
TG 52:Y	0.0203	0.0187	0.9620	0.9866	0, 1, 2, 3, 4, 5
TG 53:Y	0.0201	0.0185	0.9624	0.9866	0, 1, 2, 3, 4, 5
TG 54:Y	0.0383	-2.10^{-14}	0.9632	0.9848	0, 1, 2, 3, 4, 5, 6
TG 56:Y	0.0282	0.0122	0.9605	0.9866	1, 2, 3, 4, 5, 6
TG 58:Y	-0.0304	0.0861	0.9431	0.9560	3, 4, 5, 6, 7
TG 60:Y	-0.0757	0.1643	0.9116	0.9655	5, 6, 7, 8, 9, 10