

SUPPORTING INFORMATION

A targeted metabolomic approach to assess the reproducibility of plasma metabolites over a four-month period in a free-living population

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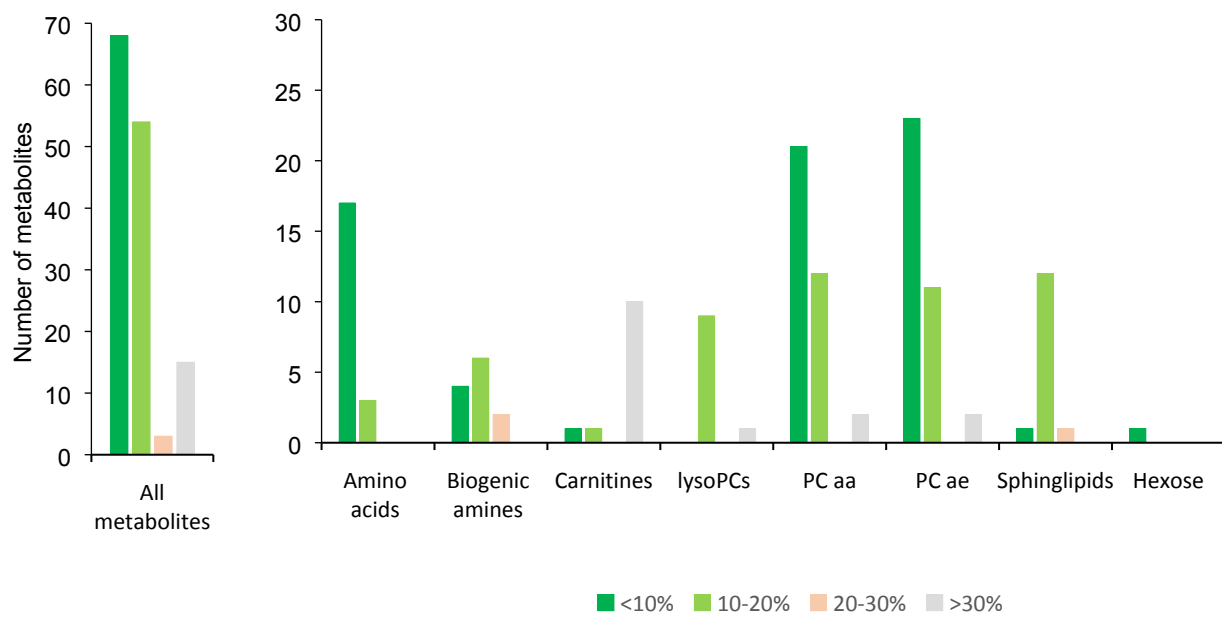


Figure S1. Distribution of % CV of metabolites quantified in pooled plasma QC sample. lysoPC: lysophosphatidylcholine; PC: phosphatidylcholine; aa: acyl-acyl; ae: acyl-alkyl.

Table S1 Concentrations (μM) of metabolites in each visit.

Metabolites	V1 (n=186)	V2 (n=166)	V3 (n=156)	V4 (n=151)
Amino acids				
Alanine	360.87 \pm 85.55	353.44 \pm 78.14	368.08 \pm 85.62	362.56 \pm 92.35
Arginine	101.43 \pm 20.18	99.4 \pm 19.41	103.27 \pm 20.03	100.39 \pm 19.64
Asparagine	48.43 \pm 8.66	49.96 \pm 28.89	48.13 \pm 10.32	47.46 \pm 8.02
Citrulline	31.93 \pm 7.34	31.95 \pm 7.21	32.33 \pm 7.01	32.3 \pm 7.28
Glutamine	716.37 \pm 90.98	722.25 \pm 91.01	720.34 \pm 83.2	705.59 \pm 92.48
Glutamate	30.86 \pm 18.72	31.9 \pm 18.27	35.17 \pm 19.00	35.33 \pm 18.65
Glycine	276.24 \pm 82.98	281.14 \pm 81.40	284.65 \pm 80.86	276.76 \pm 75.65
Histidine	105.13 \pm 12.17	105.11 \pm 12.96	105.53 \pm 12.24	103.32 \pm 12.02
Isoleucine	81.80 \pm 19.06	83.19 \pm 18.50	82.65 \pm 17.80	82.17 \pm 20.41
Leucine	174.28 \pm 37.64	176.63 \pm 36.63	174.93 \pm 34.75	172.97 \pm 39.05
Lysine	292.28 \pm 31.32	294.49 \pm 33.07	295.21 \pm 33.19	290.16 \pm 31.66
Methionine	28.74 \pm 5.58	28.84 \pm 5.30	29.09 \pm 5.32	28.64 \pm 5.36
Ornithine	75.69 \pm 15.42	75.36 \pm 16.21	77.01 \pm 15.68	75.41 \pm 16.30
Phenylalanine	102.46 \pm 11.89	102.93 \pm 11.86	103.11 \pm 10.98	101.61 \pm 12.06
Proline	180.99 \pm 56.94	185.92 \pm 56.77	184.03 \pm 53.30	184.28 \pm 67.34
Serine	126.04 \pm 27.63	127.68 \pm 26.07	128.52 \pm 24.26	125.96 \pm 25.56
Threonine	130.57 \pm 32.60	126.42 \pm 31.48	128.16 \pm 29.49	129.62 \pm 32.25
Tryptophan	85.83 \pm 12.83	85.76 \pm 13.10	86.04 \pm 12.56	84.76 \pm 12.75
Tyrosine	73.47 \pm 15.30	73.59 \pm 14.95	74.88 \pm 15.30	73.34 \pm 15.10
Valine	277.80 \pm 44.04	281.95 \pm 43.51	281.98 \pm 38.95	280.30 \pm 41.10
Biogenic amines				
Acetyloronithine	1.15 \pm 1.11	1.3 \pm 1.27	1.22 \pm 0.92	1.24 \pm 1.37
Asymmetric dimethylarginine	0.48 \pm 0.08	0.48 \pm 0.08	0.49 \pm 0.08	0.48 \pm 0.08
alpha-Aminoadipic acid	0.63 \pm 0.28	0.64 \pm 0.26	0.63 \pm 0.27	0.63 \pm 0.24
Creatinine	75.11 \pm 16.48	76.14 \pm 17.03	75.61 \pm 16.94	75.69 \pm 16.87
Kynurenine	2.38 \pm 0.52	2.39 \pm 0.53	2.39 \pm 0.52	2.39 \pm 0.54
Putrescine	0.13 \pm 0.03	0.13 \pm 0.04	0.12 \pm 0.03	0.13 \pm 0.03
Sarcosine	1.31 \pm 0.51	1.33 \pm 0.47	1.36 \pm 0.46	1.38 \pm 0.52
Symmetric dimethylarginine	0.47 \pm 0.08	0.47 \pm 0.08	0.47 \pm 0.08	0.46 \pm 0.08
Serotonin	0.17 \pm 0.13	0.14 \pm 0.09	0.14 \pm 0.11	0.13 \pm 0.08
<i>trans</i> -4-Hydroxyproline	9.26 \pm 4.95	9.57 \pm 6.19	9.7 \pm 4.74	9.34 \pm 4.75
Taurine	53.33 \pm 12.43	52.99 \pm 11.34	54.06 \pm 13.65	52.85 \pm 12.39
Acylcarnitines				
C0	30.18 \pm 7.42	30.82 \pm 7.45	31.04 \pm 7.55	30.69 \pm 7.17
C2	6.64 \pm 2.28	6.78 \pm 2.57	6.13 \pm 2.05	6.14 \pm 2.00
C3	0.29 \pm 0.09	0.3 \pm 0.09	0.3 \pm 0.10	0.3 \pm 0.10
C4	0.23 \pm 0.29	0.22 \pm 0.13	0.23 \pm 0.20	0.22 \pm 0.15
C6 (C4:1-DC)	0.10 \pm 0.08	0.10 \pm 0.10	0.10 \pm 0.10	0.10 \pm 0.10
C8	0.30 \pm 0.28	0.31 \pm 0.30	0.32 \pm 0.30	0.32 \pm 0.30
C10	0.41 \pm 0.34	0.42 \pm 0.35	0.42 \pm 0.34	0.41 \pm 0.34

C10:1	0.28±0.18	0.29±0.20	0.29±0.19	0.29±0.20
C14:1	0.17±0.17	0.19±0.20	0.19±0.20	0.19±0.21
C18:1	0.13±0.08	0.14±0.09	0.14±0.10	0.14±0.10
lysoPhosphatidylcholines				
lysoPC a C16:0	59.38±14.81	60.84±14.65	60.96±14.41	59.64±15
lysoPC a C16:1	17.58±124.97	1.85±0.62	1.83±0.63	1.79±0.62
lysoPC a C17:0	1.23±0.43	1.26±0.44	1.29±0.46	1.23±0.44
lysoPC a C18:0	18.00±5.61	18.17±5.46	18.67±5.62	18.09±5.82
lysoPC a C18:1	15.18±5.31	15.98±5.37	15.95±5.39	15.66±5.18
lysoPC a C18:2	25.76±11.11	26.95±10.52	27.42±10.18	27.27±10.17
lysoPC a C20:3	1.56±0.59	1.64±0.62	1.65±0.67	1.64±0.64
lysoPC a C20:4	4.49±1.68	4.69±1.74	4.64±1.74	4.56±1.74
lysoPC a C28:0	0.14±0.03	0.14±0.03	0.14±0.03	0.14±0.03
lysoPC a C28:1	0.33±0.15	0.33±0.15	0.33±0.15	0.33±0.15
Phosphatidylcholines				
PC aa C24:0	0.07±0.03	0.07±0.05	0.07±0.03	0.07±0.03
PC aa C28:1	2.59±0.77	2.56±0.75	2.53±0.71	2.48±0.66
PC aa C30:0	3.42±1.38	3.39±1.37	3.29±1.19	3.22±1.1
PC aa C32:0	11.14±2.46	11±2.22	10.76±2.35	10.47±2.09
PC aa C32:1	11.01±5.76	11.28±6.05	10.69±5.51	10.55±5.51
PC aa C32:2	3.57±1.80	3.52±1.68	3.55±1.74	3.44±1.45
PC aa C32:3	0.36±0.10	0.35±0.10	0.37±0.11	0.35±0.09
PC aa C34:1	172.45±42.23	176.58±43.99	173.15±39.91	170.31±41.23
PC aa C34:2	300.58±57.8	302.17±55.45	302.78±52.06	298.91±52.11
PC aa C34:3	13.58±4.49	13.87±4.88	14.10±4.72	13.76±4.48
PC aa C34:4	1.25±0.58	1.24±0.55	1.24±0.54	1.21±0.46
PC aa C36:0	2.45±1.15	2.35±1.04	2.39±1.02	2.24±0.99
PC aa C36:1	42.07±11.75	43.06±11.95	43.44±11.2	42.37±11.27
PC aa C36:2	204.8±47.86	206.17±44.59	210.31±41.25	205.98±41.9
PC aa C36:3	111.07±26.5	112.74±30.49	112.87±26.97	111.11±25.14
PC aa C36:4	147.11±38.09	146.6±37	142.81±32.11	141.17±32.59
PC aa C36:5	21.79±12.73	21.85±11.41	21.77±10.85	19.76±8.89
PC aa C36:6	0.90±0.45	0.90±0.43	0.91±0.43	0.84±0.35
PC aa C38:0	2.65±0.84	2.66±0.86	2.68±0.85	2.54±0.81
PC aa C38:1	0.88±0.54	0.89±0.61	0.96±0.60	0.86±0.58
PC aa C38:3	36.12±10.86	36.16±10.81	36.43±10.57	35.4±10.24
PC aa C38:4	81.47±21.91	80.55±22.45	80.11±19.31	77.93±19.47
PC aa C38:5	43.31±12.32	43.38±11.44	42.89±10.68	41.14±10.65
PC aa C38:6	65.31±23.25	65.18±22.69	63.98±21.2	60.05±18.68
PC aa C40:2	0.22±0.06	0.22±0.06	0.23±0.07	0.22±0.06
PC aa C40:3	0.42±0.10	0.42±0.10	0.43±0.10	0.41±0.09
PC aa C40:4	2.26±0.59	2.25±0.59	2.22±0.57	2.19±0.59
PC aa C40:5	7.3±2.34	7.2±2.16	7.23±2.20	7.05±2.25
PC aa C40:6	21.04±7.91	20.83±7.66	20.8±7.19	19.75±6.86

PC aa C42:0	0.48±0.11	0.48±0.12	0.48±0.11	0.45±0.10
PC aa C42:1	0.17±0.04	0.17±0.04	0.17±0.04	0.17±0.04
PC aa C42:2	0.18±0.04	0.18±0.05	0.18±0.04	0.18±0.05
PC aa C42:4	0.12±0.03	0.12±0.03	0.12±0.02	0.12±0.03
PC aa C42:5	0.26±0.08	0.25±0.07	0.26±0.07	0.24±0.06
PC aa C42:6	0.41±0.13	0.40±0.12	0.4±0.10	0.38±0.10
PC ae C30:0	0.31±0.09	0.31±0.10	0.31±0.09	0.30±0.09
PC ae C30:1	0.09±0.06	0.09±0.06	0.1±0.08	0.09±0.06
PC ae C30:2	0.09±0.02	0.09±0.02	0.09±0.02	0.08±0.02
PC ae C32:1	2.41±0.54	2.38±0.53	2.42±0.53	2.31±0.52
PC ae C32:2	0.62±0.15	0.62±0.16	0.63±0.16	0.60±0.15
PC ae C34:0	1.16±0.39	1.17±0.37	1.17±0.38	1.12±0.35
PC ae C34:1	8.09±1.77	8.13±1.89	8.12±1.74	7.81±1.70
PC ae C34:2	10.36±2.52	10.27±2.66	10.56±2.58	10.18±2.48
PC ae C34:3	7.72±2.30	7.45±2.12	7.64±2.20	7.38±2.14
PC ae C36:0	0.68±0.16	0.68±0.16	0.68±0.16	0.66±0.15
PC ae C36:1	5.8±1.54	5.87±1.57	5.87±1.51	5.62±1.45
PC ae C36:2	12.57±3.22	12.55±3.23	12.86±3.21	12.3±2.92
PC ae C36:3	6.84±1.56	6.82±1.65	7.01±1.62	6.78±1.56
PC ae C36:4	15.47±4.61	15.24±4.12	15.44±4.12	14.98±4.28
PC ae C36:5	10.08±4.02	9.74±2.87	9.93±3.06	9.53±3.15
PC ae C38:0	2.36±0.84	2.37±0.87	2.42±0.84	2.25±0.73
PC ae C38:1	0.33±0.15	0.33±0.15	0.370.14	0.33±0.15
PC ae C38:2	1.29±0.31	1.30±0.33	1.34±0.33	1.28±0.31
PC ae C38:3	2.64±0.69	2.66±0.69	2.69±0.70	2.57±0.63
PC ae C38:4	10.96±2.65	10.87±2.47	10.92±2.47	10.45±2.27
PC ae C38:5	14.04±3.48	13.88±2.93	14.03±2.96	13.49±3.03
PC ae C38:6	6.42±2.09	6.36±1.94	6.45±1.93	6.10±1.94
PC ae C40:1	1.12±0.29	1.11±0.28	1.14±0.28	1.09±0.26
PC ae C40:2	1.37±0.41	1.37±0.40	1.37±0.38	1.30±0.36
PC ae C40:3	0.64±0.12	0.65±0.13	0.65±0.13	0.63±0.11
PC ae C40:4	1.53±0.29	1.51±0.30	1.53±0.29	1.47±0.27
PC ae C40:5	2.36±0.50	2.35±0.45	2.35±0.46	2.25±0.43
PC ae C40:6	3.95±1.19	3.96±1.17	3.97±1.15	3.73±1.05
PC ae C42:1	0.28±0.05	0.28±0.05	0.28±0.05	0.28±0.05
PC ae C42:2	0.48±0.11	0.48±0.11	0.49±0.12	0.47±0.11
PC ae C42:3	0.65±0.13	0.65±0.15	0.65±0.15	0.63±0.13
PC ae C42:4	0.66±0.14	0.66±0.15	0.66±0.14	0.64±0.14
PC ae C42:5	1.55±0.31	1.54±0.32	1.54±0.29	1.49±0.28
PC ae C44:3	0.07±0.01	0.07±0.01	0.07±0.01	0.07±0.01
PC ae C44:4	0.31±0.07	0.31±0.07	0.31±0.06	0.30±0.07
PC ae C44:5	1.47±0.38	1.47±0.38	1.47±0.33	1.42±0.33
PC ae C44:6	1.05±0.26	1.05±0.25	1.05±0.24	1.00±0.23

Sphingomyelins

SM (OH) C14:1	6.57±2.08	6.55±2.00	6.49±1.85	6.29±1.77
SM (OH) C16:1	3.50±1.09	3.50±1.05	3.46±1.01	3.34±0.96
SM (OH) C22:1	12.67±3.39	12.62±3.23	12.46±2.93	12.07±2.73
SM (OH) C22:2	12.35±3.56	12.28±3.39	12.24±2.99	11.74±2.92
SM (OH) C24:1	1.24±0.35	1.24±0.32	1.23±0.31	1.19±0.30
SM C16:0	113.72±21.93	113.19±20.74	112.77±19.57	108.75±18.55
SM C16:1	15.77±3.37	15.66±3.29	15.59±3.08	15.18±3.03
SM C18:0	23.94±6.12	23.85±5.78	23.47±5.68	22.6±5.73
SM C18:1	11.41±3.09	11.45±3.05	11.29±2.8	10.94±2.74
SM C20:2	0.33±0.10	0.33±0.10	0.33±0.09	0.31±0.09
SM C24:0	20.32±4.44	20.24±4.54	19.87±3.96	19.46±3.91
SM C24:1	56.91±11.83	57.12±11.89	56.57±10.95	54.47±9.99
SM C26:0	0.11±0.03	0.11±0.04	0.11±0.03	0.11±0.03
SM C26:1	0.28±0.09	0.28±0.09	0.27±0.09	0.26±0.07
Hexose (H1)	4860.75±501.68	4907.77±565.99	4915.99±532.07	4855.54±494.15

Abbreviations are as follows. Cx:y: x=number of carbons in the fatty acid side chain, y=number of double bonds in the fatty acid side chain; DC: decarboxyl; OH: hydroxyl; lysoPC: lysophosphatidylcholine; PC: phosphatidylcholine; aa: acyl-acyl; ae: acyl-alkyl; SM: sphingomyelin.

Note: Amino acids and biogenic amines were quantified based on internal standards and calibration curves consisting of seven calibration standards, while acylcarnitines, LPCs, PCs, SMs and hexose were evaluated semi-quantitatively by using 13 internal standards for lipids and acylcarnitines and 1 for the hexose.

Table S2 Impact of sex and age groups on the metabolite levels.

Metabolites	P value (Sex) *	FDR adjusted (Sex) **	P value (Age) *	FDR adjusted (Age) **
Amino acids				
Alanine	0.7009	0.7677	0.9078	0.9211
Arginine	0.2033	0.2862	0.2031	0.2644
Asparagine	0.7205	0.7768	0.0007	0.0017
Citrulline	0.0322	0.0645	0.0387	0.0588
Glutamine	0.0129	0.0307	0.0014	0.0031
Glutamate	0.0004	0.0026	0.0000	7.0769E-06
Glycine	0.3734	0.4727	0.1145	0.1612
Histidine	0.5951	0.6844	0.8708	0.9070
Isoleucine	0.0000	1.4556E-09	0.5119	0.6143
Leucine	0.0000	8.2241E-12	0.8301	0.8853
Lysine	0.0859	0.1412	0.0015	0.0034
Methionine	0.0128	0.0307	0.3975	0.4898
Ornithine	0.0020	0.0093	0.0034	0.0066
Phenylalanine	0.0000	0.0004	0.5667	0.6410
Proline	0.0003	0.0021	0.6331	0.7046
Serine	0.1156	0.1772	0.1912	0.2513
Threonine	0.0440	0.0829	0.0099	0.0173
Tryptophan	0.0000	0.0001	0.2871	0.3668
Tyrosine	0.0038	0.0138	0.0554	0.0831
Valine	0.0000	0.0001	0.5448	0.6345
Biogenic amines				
Acetylorntithine	0.6156	0.6923	0.9015	0.9211
Asymmetric dimethylarginine	0.0636	0.1070	0.0000	1.0535E-06
alpha-Amino adipic acid	0.0000	3.9750E-07	0.0299	0.0479
Creatinine	0.0000	6.4671E-17	0.0868	0.1235
Kynurenine	0.0000	7.5845E-09	0.0100	0.0173
Putrescine	0.0127	0.0307	0.1787	0.2371
Sarcosine	0.0000	0.0001	0.8742	0.9070
Symmetric dimethylarginine	0.0000	0.0002	0.2053	0.2648
Serotonin	0.2611	0.3498	0.8209	0.8850
trans-4-Hydroxyproline	0.0481	0.0884	0.0706	0.1015
Taurine	0.9187	0.9391	0.0046	0.0086
Acylcarnitines				
C0	0.0000	2.1551E-06	0.0000	0.0001
C2	0.0532	0.0941	0.0338	0.0518
C3	0.0000	9.9427E-06	0.0005	0.0012
C4	0.0008	0.0040	0.6275	0.7040
C6 (C4:1-DC)	0.2194	0.3028	0.8039	0.8735
C8	0.1425	0.2161	0.5378	0.6343
C10	0.1845	0.2652	0.5208	0.6195
C10:1	0.0284	0.0594	0.6792	0.7442
C14:1	0.0117	0.0299	0.5563	0.6345

C18:1	0.0089	0.0236	0.1718	0.2302
lysoPhosphatidylcholines				
lysoPC a C16:0	0.0071	0.0201	0.0019	0.0040
lysoPC a C16:1	0.0071	0.0201	0.0001	0.0004
lysoPC a C17:0	0.0046	0.0151	0.0000	9.3259E-08
lysoPC a C18:0	0.0089	0.0236	0.0001	0.0004
lysoPC a C18:1	0.0100	0.0262	0.1497	0.2066
lysoPC a C18:2	0.0023	0.0101	0.5511	0.6345
lysoPC a C20:3	0.0000	1.7250E-05	0.0070	0.0128
lysoPC a C20:4	0.0000	0.0004	0.3857	0.4795
lysoPC a C28:0	0.3515	0.4534	0.0560	0.0831
lysoPC a C28:1	0.3611	0.4613	0.1569	0.2144
Phosphatidylcholines				
PC aa C24:0	0.8672	0.9066	0.0021	0.0044
PC aa C28:1	0.1873	0.2664	0.0000	6.3963E-10
PC aa C30:0	0.0004	0.0027	0.0006	0.0015
PC aa C32:0	0.0020	0.0093	0.0003	0.0008
PC aa C32:1	0.0127	0.0307	0.0013	0.0029
PC aa C32:2	0.0028	0.0114	0.0330	0.0512
PC aa C32:3	0.0058	0.0178	0.0000	3.6662E-06
PC aa C34:1	0.6171	0.6923	0.9046	0.9211
PC aa C34:2	0.7183	0.7768	0.4551	0.5525
PC aa C34:3	0.1534	0.2253	0.3159	0.3964
PC aa C34:4	0.0071	0.0201	0.0017	0.0036
PC aa C36:0	0.0876	0.1423	0.0012	0.0027
PC aa C36:1	0.9714	0.9785	0.0069	0.0128
PC aa C36:2	0.3005	0.3949	0.8340	0.8853
PC aa C36:3	0.0625	0.1065	0.0076	0.0139
PC aa C36:4	0.0295	0.0599	0.0678	0.0984
PC aa C36:5	0.2228	0.3044	0.0000	2.0378E-09
PC aa C36:6	0.0069	0.0201	0.0000	2.1361E-08
PC aa C38:0	0.0295	0.0599	0.0000	3.8333E-06
PC aa C38:1	0.3429	0.4465	0.0312	0.0496
PC aa C38:3	0.5456	0.6435	0.0010	0.0024
PC aa C38:4	0.5447	0.6435	0.0008	0.0019
PC aa C38:5	0.5372	0.6435	0.0000	6.3963E-10
PC aa C38:6	0.0057	0.0178	0.0000	4.9486E-07
PC aa C40:2	0.0211	0.0470	0.0041	0.0078
PC aa C40:3	0.0024	0.0102	0.0000	3.8333E-06
PC aa C40:4	0.7429	0.7886	0.0096	0.0170
PC aa C40:5	0.4073	0.5110	0.0000	2.5656E-08
PC aa C40:6	0.0968	0.1553	0.0000	6.3963E-10
PC aa C42:0	0.0032	0.0122	0.0015	0.0034
PC aa C42:1	0.0042	0.0145	0.0092	0.0165
PC aa C42:2	0.0223	0.0489	0.0330	0.0512
PC aa C42:4	0.0335	0.0660	0.1412	0.1968

PC aa C42:5	0.0515	0.0923	0.9858	0.9858
PC aa C42:6	0.0378	0.0724	0.0000	1.0350E-05
PC ae C30:0	0.0195	0.0441	0.0000	0.0001
PC ae C30:1	0.5584	0.6531	0.1653	0.2236
PC ae C30:2	0.1009	0.1601	0.0000	4.5905E-10
PC ae C32:1	0.0174	0.0401	0.0011	0.0026
PC ae C32:2	0.0002	0.0015	0.0000	2.1788E-06
PC ae C34:0	0.6100	0.6923	0.0000	1.2274E-06
PC ae C34:1	0.0023	0.0101	0.0000	7.0769E-06
PC ae C34:2	0.0006	0.0034	0.0130	0.0217
PC ae C34:3	0.0004	0.0026	0.5559	0.6345
PC ae C36:0	0.0002	0.0019	0.0010	0.0024
PC ae C36:1	0.1679	0.2439	0.0000	6.3963E-10
PC ae C36:2	0.0445	0.0829	0.0000	2.1253E-06
PC ae C36:3	0.0046	0.0151	0.0271	0.0445
PC ae C36:4	0.5031	0.6199	0.0297	0.0479
PC ae C36:5	0.8898	0.9164	0.0130	0.0217
PC ae C38:0	0.0077	0.0213	0.0000	5.6169E-11
PC ae C38:1	0.7940	0.8364	0.0019	0.0040
PC ae C38:2	0.0053	0.0171	0.0019	0.0040
PC ae C38:3	0.5855	0.6790	0.0000	6.3963E-10
PC ae C38:4	0.7370	0.7884	0.0004	0.0011
PC ae C38:5	0.8844	0.9164	0.0038	0.0074
PC ae C38:6	0.2554	0.3455	0.0000	2.4905E-06
PC ae C40:1	0.0662	0.1101	0.0000	5.1511E-07
PC ae C40:2	0.6717	0.7416	0.0000	2.7917E-08
PC ae C40:3	0.0041	0.0145	0.0000	6.1928E-07
PC ae C40:4	0.2097	0.2924	0.0127	0.0217
PC ae C40:5	0.5415	0.6435	0.0000	1.6829E-05
PC ae C40:6	0.1478	0.2193	0.0000	2.6195E-09
PC ae C42:1	0.6337	0.7052	0.8511	0.8966
PC ae C42:2	0.1154	0.1772	0.0000	4.3643E-09
PC ae C42:3	0.0014	0.0067	0.0000	0.0001
PC ae C42:4	0.0269	0.0571	0.9562	0.9631
PC ae C42:5	0.0492	0.0893	0.3049	0.3861
PC ae C44:3	0.9836	0.9836	0.0031	0.0063
PC ae C44:4	0.0257	0.0555	0.0646	0.0948
PC ae C44:5	0.1072	0.1681	0.6795	0.7442
PC ae C44:6	0.0153	0.0357	0.4564	0.5525
Sphingomyelins				
SM (OH) C14:1	0.2761	0.3663	0.0000	6.3963E-10
SM (OH) C16:1	0.4203	0.5225	0.0000	6.3963E-10
SM (OH) C22:1	0.0611	0.1054	0.0000	5.1371E-09
SM (OH) C22:2	0.0013	0.0067	0.0000	6.3963E-10
SM (OH) C24:1	0.9714	0.9785	0.0001	0.0002
SM C16:0	0.0005	0.0029	0.0000	2.6293E-06

SM C16:1	0.0000	4.6000E-05	0.0000	2.3341E-08
SM C18:0	0.0369	0.0718	0.0000	3.4305E-07
SM C18:1	0.0035	0.0132	0.0000	1.1223E-07
SM C20:2	0.0003	0.0019	0.0001	0.0002
SM C24:0	0.1470	0.2193	0.0000	2.3000E-05
SM C24:1	0.0001	0.0006	0.0000	1.8503E-06
SM C26:0	0.5321	0.6435	0.0000	3.8333E-06
SM C26:1	0.0611	0.1054	0.0000	1.3788E-06
Hexose (H1)	0.0030	0.0116	0.0000	7.0769E-06

* P values are from independent t-test.

**FDR-adjusted P values are adjusted for multiple comparisons using the Benjamini–Hochberg procedure.

Note: two age groups; group 1, age <45 years old; group 2, age >=45 years old.

Abbreviations are as follows. Cx:y: x=number of carbons in the fatty acid side chain, y=number of double bonds in the fatty acid side chain; DC: decarboxyl; OH: hydroxyl; lysoPC: lysophosphatidylcholine; PC: phosphatidylcholine; aa: acyl-acyl; ae: acyl-alkyl; SM: sphingomyelin.