

# Supplementary Materials: Wide-Targeted Metabolome Analysis Identifies Potential Biomarkers for Prognosis Prediction of Epithelial Ovarian Cancer

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**Table S1.** Significantly increased metabolites in the plasma of epithelial ovarian cancer patients.

Metabolite	Class	Cancer ( $\mu\text{M}$ , mean $\pm$ SD)	Cohort ( $\mu\text{M}$ , mean $\pm$ SD)	<i>p</i> -value	Fold change (Cancer/Cohort)
TG (16:0_40:6)	Triglycerides	2.72 $\pm$ 1.51	1.05 $\pm$ 0.45	$1.43 \times 10^{-16}$	2.58
Hypoxanthine	Nucleobases and related	9.43 $\pm$ 22.55	3.88 $\pm$ 2.17	$4.44 \times 10^{-2}$	2.43
Cortisol	Hormones and related	0.31 $\pm$ 0.10	0.16 $\pm$ 0.06	$4.35 \times 10^{-24}$	1.94
TG (18:1_36:2)	Triglycerides	64.19 $\pm$ 33.17	36.42 $\pm$ 22.01	$3.89 \times 10^{-9}$	1.76
TG (22:5_34:2)	Triglycerides	1.94 $\pm$ 0.85	1.11 $\pm$ 0.63	$1.40 \times 10^{-11}$	1.75
TG (18:2_36:2)	Triglycerides	29.32 $\pm$ 15.10	17.18 $\pm$ 11.01	$3.33 \times 10^{-8}$	1.71
TG (18:1_34:1)	Triglycerides	193.84 $\pm$ 98.13	114.61 $\pm$ 71.77	$3.04 \times 10^{-8}$	1.69
TG (18:1_36:3)	Triglycerides	52.68 $\pm$ 27.98	31.15 $\pm$ 20.70	$1.29 \times 10^{-7}$	1.69
TG (20:4_34:1)	Triglycerides	5.49 $\pm$ 2.33	3.31 $\pm$ 2.16	$3.19 \times 10^{-9}$	1.66
TG (16:0_36:2)	Triglycerides	99.75 $\pm$ 50.83	60.19 $\pm$ 38.32	$1.13 \times 10^{-7}$	1.66
TG (16:0_36:3)	Triglycerides	99.69 $\pm$ 48.48	60.21 $\pm$ 37.58	$4.34 \times 10^{-8}$	1.66
TG (18:2_34:1)	Triglycerides	99.06 $\pm$ 47.69	59.91 $\pm$ 36.66	$3.15 \times 10^{-8}$	1.65
GLCAS	Bile acids	0.27 $\pm$ 0.27	0.16 $\pm$ 0.14	$2.60 \times 10^{-3}$	1.65
TG (18:0_36:3)	Triglycerides	9.82 $\pm$ 4.43	5.98 $\pm$ 3.64	$9.19 \times 10^{-9}$	1.64
TG (18:1_34:2)	Triglycerides	110.15 $\pm$ 52.06	67.77 $\pm$ 40.23	$4.23 \times 10^{-8}$	1.63
TG (18:0_36:2)	Triglycerides	8.60 $\pm$ 3.94	5.30 $\pm$ 3.53	$4.79 \times 10^{-8}$	1.62
SM C26:1	Sphingomyelins	1.74 $\pm$ 0.81	1.08 $\pm$ 0.33	$1.78 \times 10^{-10}$	1.62
TG (18:2_36:1)	Triglycerides	10.62 $\pm$ 4.89	6.65 $\pm$ 4.10	$7.12 \times 10^{-8}$	1.60
TG (18:1_36:1)	Triglycerides	17.47 $\pm$ 8.41	10.97 $\pm$ 7.18	$3.18 \times 10^{-7}$	1.59
TG (18:2_35:1)	Triglycerides	1.64 $\pm$ 0.79	1.07 $\pm$ 0.50	$1.95 \times 10^{-8}$	1.53

TG (18:2_34:2)	Triglycerides	50.08 ± 25.05	32.81 ± 21.08	5.24 × 10 <sup>-6</sup>	1.53
TG (18:2_34:0)	Triglycerides	9.98 ± 4.60	6.65 ± 4.74	9.41 × 10 <sup>-6</sup>	1.50
TG (22:5_34:1)	Triglycerides	4.30 ± 2.00	2.88 ± 1.28	3.10 × 10 <sup>-9</sup>	1.49
TG (16:1_36:2)	Triglycerides	13.15 ± 6.87	8.83 ± 5.25	1.09 × 10 <sup>-5</sup>	1.49
TG (18:2_36:3)	Triglycerides	19.71 ± 11.82	13.29 ± 10.31	3.42 × 10 <sup>-4</sup>	1.48
TG (18:1_35:2)	Triglycerides	3.20 ± 1.57	2.21 ± 0.97	7.02 × 10 <sup>-7</sup>	1.45
TG (16:0_36:4)	Triglycerides	28.20 ± 14.55	19.99 ± 14.03	3.74 × 10 <sup>-4</sup>	1.41
TG (17:2_38:6)	Triglycerides	0.35 ± 0.17	0.25 ± 0.13	5.18 × 10 <sup>-5</sup>	1.39
TG (17:2_38:5)	Triglycerides	0.37 ± 0.16	0.26 ± 0.14	1.09 × 10 <sup>-4</sup>	1.39
TG (22:6_32:1)	Triglycerides	1.78 ± 1.06	1.32 ± 1.53	7.41 × 10 <sup>-3</sup>	1.35
Kynurenine	Amino acid related	2.04 ± 0.87	1.52 ± 0.57	1.25 × 10 <sup>-5</sup>	1.35
TG (18:1_33:1)	Triglycerides	3.74 ± 1.93	2.80 ± 1.35	1.23 × 10 <sup>-4</sup>	1.34
HCys	Amino acid related	27.69 ± 17.04	20.80 ± 12.81	4.37 × 10 <sup>-3</sup>	1.33
C18:1	Acylcarnitines	0.11 ± 0.05	0.09 ± 0.03	9.05 × 10 <sup>-3</sup>	1.32
TG (18:2_33:1)	Triglycerides	1.95 ± 0.82	1.47 ± 0.65	4.51 × 10 <sup>-6</sup>	1.32
TG (17:0_36:3)	Triglycerides	1.51 ± 0.69	1.15 ± 0.51	9.40 × 10 <sup>-5</sup>	1.32
TG (18:1_32:1)	Triglycerides	32.05 ± 16.03	24.39 ± 17.21	4.11 × 10 <sup>-3</sup>	1.31
TG (18:1_36:4)	Triglycerides	15.92 ± 9.03	12.18 ± 8.52	7.91 × 10 <sup>-3</sup>	1.31
TG (16:1_34:1)	Triglycerides	17.85 ± 8.15	13.70 ± 10.25	1.13 × 10 <sup>-2</sup>	1.30
TG (20:4_34:2)	Triglycerides	2.89 ± 1.12	2.22 ± 1.55	4.54 × 10 <sup>-4</sup>	1.30
TG (18:0_36:4)	Triglycerides	3.79 ± 1.68	2.91 ± 1.62	7.98 × 10 <sup>-4</sup>	1.30
TG (16:0_34:2)	Triglycerides	36.37 ± 17.48	28.27 ± 23.18	1.36 × 10 <sup>-2</sup>	1.29
TG (16:0_40:7)	Triglycerides	1.80 ± 1.47	1.40 ± 0.95	1.19 × 10 <sup>-2</sup>	1.29
t4-OH-Pro	Amino acid related	9.99 ± 4.72	7.77 ± 2.41	2.50 × 10 <sup>-4</sup>	1.29
Cer (d18:1/24:1)	Ceramides	2.13 ± 0.56	1.66 ± 0.34	1.11 × 10 <sup>-9</sup>	1.29
Hex2Cer (d18:1/24:1)	Dihexosylceramides	0.51 ± 0.17	0.40 ± 0.11	3.00 × 10 <sup>-5</sup>	1.28
TG (20:4_36:4)	Triglycerides	0.69 ± 0.27	0.54 ± 0.29	1.31 × 10 <sup>-3</sup>	1.28
TG (16:1_36:1)	Triglycerides	2.47 ± 1.03	1.94 ± 1.05	1.24 × 10 <sup>-4</sup>	1.28
TG (20:2_34:1)	Triglycerides	1.33 ± 0.54	1.05 ± 0.54	1.04 × 10 <sup>-4</sup>	1.27
DG (18:2_18:2)	Diglycerides	3.90 ± 1.78	3.06 ± 1.47	5.72 × 10 <sup>-4</sup>	1.27
TG (18:2_38:5)	Triglycerides	1.34 ± 0.53	1.06 ± 0.39	1.77 × 10 <sup>-4</sup>	1.27

TG (20:4_36:2)	Triglycerides	2.52 ± 0.98	1.99 ± 0.86	1.26 × 10 <sup>-4</sup>	1.26
TG (16:1_36:3)	Triglycerides	11.34 ± 5.51	9.01 ± 4.74	5.17 × 10 <sup>-4</sup>	1.26
beta-Ala	Biogenic amines	2.03 ± 1.13	1.63 ± 1.15	2.58 × 10 <sup>-2</sup>	1.25
TG (18:1_32:0)	Triglycerides	25.61 ± 12.88	20.53 ± 19.35	3.96 × 10 <sup>-2</sup>	1.25
TG (20:5_34:1)	Triglycerides	2.15 ± 1.01	1.72 ± 1.36	1.02 × 10 <sup>-2</sup>	1.25
TG (18:0_34:2)	Triglycerides	6.28 ± 2.57	5.06 ± 3.78	1.09 × 10 <sup>-2</sup>	1.24
TG (18:1_35:3)	Triglycerides	0.92 ± 0.49	0.74 ± 0.29	1.88 × 10 <sup>-3</sup>	1.24
TG (17:2_36:4)	Triglycerides	0.71 ± 0.35	0.58 ± 0.34	7.78 × 10 <sup>-3</sup>	1.24
Thr	Amino acids	138.81 ± 45.28	112.52 ± 24.63	1.02 × 10 <sup>-5</sup>	1.23
CE (22:5)	Cholesteryl esters	2.88 ± 1.79	2.34 ± 1.14	1.13 × 10 <sup>-2</sup>	1.23
TG (16:1_34:2)	Triglycerides	10.41 ± 4.35	8.49 ± 5.77	3.12 × 10 <sup>-2</sup>	1.23
TG (18:3_34:3)	Triglycerides	0.97 ± 0.52	0.80 ± 0.47	2.24 × 10 <sup>-2</sup>	1.22
TG (18:2_32:1)	Triglycerides	13.91 ± 6.42	11.54 ± 7.68	3.61 × 10 <sup>-2</sup>	1.20
TG (18:2_36:0)	Triglycerides	1.01 ± 0.43	0.86 ± 0.48	3.58 × 10 <sup>-3</sup>	1.17
SDMA	Amino acid related	0.54 ± 0.17	0.46 ± 0.08	2.86 × 10 <sup>-4</sup>	1.17
Asp	Amino acids	7.19 ± 4.39	6.15 ± 1.22	4.16 × 10 <sup>-2</sup>	1.17
ADMA	Amino acid related	0.52 ± 0.10	0.45 ± 0.13	1.67 × 10 <sup>-4</sup>	1.16
Ile	Amino acids	73.33 ± 20.92	64.53 ± 18.19	5.08 × 10 <sup>-3</sup>	1.14
SM C18:0	Sphingomyelins	41.84 ± 10.99	37.00 ± 8.32	2.01 × 10 <sup>-3</sup>	1.13
TG (18:3_34:0)	Triglycerides	1.11 ± 0.53	0.98 ± 0.62	2.02 × 10 <sup>-2</sup>	1.13
Gly	Amino acids	271.08 ± 82.02	240.34 ± 78.47	1.66 × 10 <sup>-2</sup>	1.13
C16:1	Acylcarnitines	0.04 ± 0.02	0.03 ± 0.01	2.41 × 10 <sup>-3</sup>	1.13
TG (16:0_38:2)	Triglycerides	1.35 ± 0.78	1.21 ± 0.81	3.87 × 10 <sup>-2</sup>	1.11
TG (20:4_32:0)	Triglycerides	0.92 ± 0.43	0.83 ± 0.63	3.22 × 10 <sup>-2</sup>	1.11
TG (16:0_38:3)	Triglycerides	1.55 ± 0.78	1.40 ± 0.83	4.42 × 10 <sup>-2</sup>	1.11
Hex2Cer(d18:1/16:0)	Dihexosylceramides	1.99 ± 0.56	1.80 ± 0.39	1.12 × 10 <sup>-2</sup>	1.11
Lys	Amino acids	186.06 ± 46.15	169.93 ± 47.05	3.01 × 10 <sup>-2</sup>	1.09
Cer(d18:1/25:0)	Ceramides	0.37 ± 0.09	0.34 ± 0.10	2.73 × 10 <sup>-2</sup>	1.09

**Table S2.** Significantly decreased metabolites in the plasma of epithelial ovarian cancer patients.

Metabolite	Class	Cancer ( $\mu\text{M}$ , mean $\pm$ SD)	Cohort ( $\mu\text{M}$ , mean $\pm$ SD)	<i>p</i> -value	Fold change (Cancer/Cohort)
PC ae C38:2	Phosphatidylcholines	2.39 $\pm$ 2.14	7.00 $\pm$ 1.29	$6.15 \times 10^{-37}$	0.34
Serotonin	Biogenic amines	0.12 $\pm$ 0.08	0.30 $\pm$ 0.20	$8.01 \times 10^{-12}$	0.40
CE (20:5)	Cholesteryl esters	61.64 $\pm$ 39.16	144.24 $\pm$ 106.50	$9.43 \times 10^{-10}$	0.43
DHA	Fatty acids	12.03 $\pm$ 16.07	26.67 $\pm$ 34.72	$7.86 \times 10^{-4}$	0.45
PC ae C38:3	Phosphatidylcholines	4.35 $\pm$ 1.93	9.54 $\pm$ 1.84	$1.80 \times 10^{-38}$	0.46
PC aa C40:2	Phosphatidylcholines	0.24 $\pm$ 0.16	0.50 $\pm$ 0.13	$4.76 \times 10^{-22}$	0.47
PC ae C40:3	Phosphatidylcholines	1.55 $\pm$ 0.75	3.07 $\pm$ 0.72	$8.18 \times 10^{-27}$	0.50
PC ae C38:1	Phosphatidylcholines	1.22 $\pm$ 1.19	2.34 $\pm$ 1.03	$1.52 \times 10^{-9}$	0.52
AA	Fatty acids	1.76 $\pm$ 1.20	3.29 $\pm$ 2.32	$1.10 \times 10^{-6}$	0.54
Cer(d18:2/23:0)	Ceramides	0.12 $\pm$ 0.06	0.21 $\pm$ 0.13	$1.96 \times 10^{-8}$	0.55
PC aa C42:4	Phosphatidylcholines	0.15 $\pm$ 0.05	0.26 $\pm$ 0.13	$8.63 \times 10^{-12}$	0.56
TG (22:6_34:3)	Triglycerides	0.82 $\pm$ 0.74	1.42 $\pm$ 0.95	$1.80 \times 10^{-3}$	0.58
PC aa C34:4	Phosphatidylcholines	0.50 $\pm$ 0.26	0.84 $\pm$ 0.24	$1.02 \times 10^{-14}$	0.60
CE (18:3)	Cholesteryl esters	37.41 $\pm$ 18.70	60.12 $\pm$ 22.13	$6.58 \times 10^{-11}$	0.62
PC ae C40:1	Phosphatidylcholines	0.68 $\pm$ 0.29	1.09 $\pm$ 0.26	$7.94 \times 10^{-17}$	0.62
PC aa C42:2	Phosphatidylcholines	0.23 $\pm$ 0.09	0.36 $\pm$ 0.10	$1.43 \times 10^{-16}$	0.62
C14:1	Acylcarnitines	0.04 $\pm$ 0.02	0.06 $\pm$ 0.02	$2.12 \times 10^{-11}$	0.64
PC aa C40:3	Phosphatidylcholines	0.59 $\pm$ 0.26	0.92 $\pm$ 0.25	$8.64 \times 10^{-14}$	0.64
PC ae C44:3	Phosphatidylcholines	0.08 $\pm$ 0.03	0.13 $\pm$ 0.04	$6.63 \times 10^{-15}$	0.65
TrpBetaine	Amino acid related	0.11 $\pm$ 0.14	0.17 $\pm$ 0.18	$2.60 \times 10^{-2}$	0.65
PC aa C36:0	Phosphatidylcholines	2.10 $\pm$ 1.02	3.22 $\pm$ 1.29	$6.90 \times 10^{-9}$	0.65
lysoPC a C20:3	Lysophosphatidylcholines	0.87 $\pm$ 0.32	1.31 $\pm$ 0.45	$1.64 \times 10^{-11}$	0.66
PC ae C40:4	Phosphatidylcholines	1.27 $\pm$ 0.43	1.93 $\pm$ 0.42	$4.96 \times 10^{-18}$	0.66
lysoPC a C24:0	Lysophosphatidylcholines	0.15 $\pm$ 0.04	0.22 $\pm$ 0.06	$7.78 \times 10^{-15}$	0.67
PC aa C36:6	Phosphatidylcholines	0.49 $\pm$ 0.27	0.74 $\pm$ 0.29	$1.37 \times 10^{-7}$	0.67
PC ae C42:1	Phosphatidylcholines	0.22 $\pm$ 0.06	0.32 $\pm$ 0.06	$3.61 \times 10^{-21}$	0.67
PC ae C30:2	Phosphatidylcholines	0.45 $\pm$ 0.20	0.67 $\pm$ 0.14	$7.98 \times 10^{-13}$	0.67

lysoPC a C18:2	Lysophosphatidylcholines	11.76 ± 5.74	17.49 ± 6.26	1.13 × 10 <sup>-8</sup>	0.67
p-Cresol-SO <sub>4</sub>	Cresols	14.18 ± 10.97	21.05 ± 17.34	3.44 × 10 <sup>-3</sup>	0.67
lysoPC a C18:0	Lysophosphatidylcholines	19.86 ± 8.02	29.47 ± 7.54	7.28 × 10 <sup>-13</sup>	0.67
PC ae C42:3	Phosphatidylcholines	0.61 ± 0.21	0.90 ± 0.19	1.25 × 10 <sup>-16</sup>	0.67
DHEAS	Hormones and related	1.57 ± 1.01	2.32 ± 1.34	8.55 × 10 <sup>-5</sup>	0.67
PC ae C42:4	Phosphatidylcholines	0.48 ± 0.23	0.71 ± 0.19	7.03 × 10 <sup>-11</sup>	0.68
PC aa C32:2	Phosphatidylcholines	3.38 ± 1.79	4.94 ± 0.95	1.28 × 10 <sup>-10</sup>	0.68
PC aa C42:5	Phosphatidylcholines	0.30 ± 0.12	0.44 ± 0.12	1.71 × 10 <sup>-11</sup>	0.69
Cer(d18:2/24:0)	Ceramides	0.42 ± 0.16	0.60 ± 0.18	1.53 × 10 <sup>-10</sup>	0.70
lysoPC a C16:1	Lysophosphatidylcholines	0.98 ± 0.40	1.40 ± 0.42	8.81 × 10 <sup>-10</sup>	0.70
PC ae C34:3	Phosphatidylcholines	4.08 ± 1.57	5.77 ± 1.55	1.55 × 10 <sup>-10</sup>	0.71
PC ae C42:2	Phosphatidylcholines	0.40 ± 0.15	0.56 ± 0.11	1.49 × 10 <sup>-11</sup>	0.72
Cit	Amino acid related	24.21 ± 8.32	33.46 ± 10.69	7.45 × 10 <sup>-9</sup>	0.72
lysoPC a C28:0	Lysophosphatidylcholines	0.15 ± 0.04	0.21 ± 0.08	2.09 × 10 <sup>-7</sup>	0.73
PC aa C40:4	Phosphatidylcholines	2.01 ± 0.56	2.76 ± 0.70	5.80 × 10 <sup>-12</sup>	0.73
PC ae C34:2	Phosphatidylcholines	6.19 ± 1.83	8.44 ± 2.05	1.25 × 10 <sup>-11</sup>	0.73
PC ae C36:1	Phosphatidylcholines	11.95 ± 3.27	16.28 ± 3.19	1.54 × 10 <sup>-14</sup>	0.73
lysoPC a C17:0	Lysophosphatidylcholines	1.06 ± 0.49	1.45 ± 0.38	9.64 × 10 <sup>-8</sup>	0.73
PC aa C42:1	Phosphatidylcholines	0.25 ± 0.09	0.34 ± 0.09	5.09 × 10 <sup>-9</sup>	0.74
PC ae C38:0	Phosphatidylcholines	1.17 ± 0.47	1.58 ± 0.43	2.98 × 10 <sup>-8</sup>	0.74
PC ae C40:5	Phosphatidylcholines	2.69 ± 0.77	3.64 ± 0.90	2.43 × 10 <sup>-11</sup>	0.74
TG (17:0_34:1)	Triglycerides	0.97 ± 0.33	1.31 ± 0.63	1.98 × 10 <sup>-4</sup>	0.74
PC ae C36:3	Phosphatidylcholines	3.75 ± 1.13	5.02 ± 1.11	2.63 × 10 <sup>-11</sup>	0.75
SM C24:0	Sphingomyelins	23.60 ± 5.43	31.41 ± 6.45	4.81 × 10 <sup>-14</sup>	0.75
PC aa C32:3	Phosphatidylcholines	0.74 ± 0.24	0.98 ± 0.20	1.94 × 10 <sup>-10</sup>	0.76
PC ae C38:6	Phosphatidylcholines	4.45 ± 1.56	5.87 ± 1.51	2.75 × 10 <sup>-8</sup>	0.76
lysoPC a C26:1	Lysophosphatidylcholines	0.09 ± 0.03	0.12 ± 0.04	9.38 × 10 <sup>-7</sup>	0.76
TG (20:3_36:4)	Triglycerides	0.28 ± 0.14	0.37 ± 0.22	1.36 × 10 <sup>-3</sup>	0.76
lysoPC a C18:1	Lysophosphatidylcholines	11.75 ± 4.55	15.37 ± 4.20	5.48 × 10 <sup>-7</sup>	0.76
SM C26:0	Sphingomyelins	0.56 ± 0.16	0.73 ± 0.19	3.13 × 10 <sup>-9</sup>	0.76
lysoPC a C16:0	Lysophosphatidylcholines	45.75 ± 16.73	59.39 ± 14.31	1.22 × 10 <sup>-7</sup>	0.77

Cer(d18:2/22:0)	Ceramides	0.32 ± 0.12	0.41 ± 0.15	2.26 × 10 <sup>-5</sup>	0.77
PC ae C36:5	Phosphatidylcholines	6.17 ± 2.05	7.97 ± 1.95	5.40 × 10 <sup>-8</sup>	0.77
PC aa C38:3	Phosphatidylcholines	36.30 ± 9.40	46.75 ± 9.53	7.56 × 10 <sup>-11</sup>	0.78
lysoPC a C28:1	Lysophosphatidylcholines	0.21 ± 0.07	0.26 ± 0.10	2.74 × 10 <sup>-5</sup>	0.78
PC ae C36:4	Phosphatidylcholines	7.97 ± 2.32	10.20 ± 2.42	1.74 × 10 <sup>-8</sup>	0.78
CE (22:6)	Cholesteryl esters	46.44 ± 23.63	59.33 ± 36.59	9.93 × 10 <sup>-3</sup>	0.78
His	Amino acids	64.02 ± 16.53	81.59 ± 11.26	5.61 × 10 <sup>-13</sup>	0.78
lysoPC a C26:0	Lysophosphatidylcholines	0.17 ± 0.05	0.22 ± 0.08	2.02 × 10 <sup>-5</sup>	0.79
PC aa C36:5	Phosphatidylcholines	20.93 ± 10.56	26.51 ± 12.79	3.08 × 10 <sup>-3</sup>	0.79
PC aa C38:5	Phosphatidylcholines	33.69 ± 9.66	42.66 ± 11.82	4.74 × 10 <sup>-7</sup>	0.79
PC aa C40:6	Phosphatidylcholines	34.44 ± 10.45	43.45 ± 13.17	3.77 × 10 <sup>-6</sup>	0.79
TG (18:1_38:7)	Triglycerides	0.28 ± 0.15	0.35 ± 0.11	7.29 × 10 <sup>-4</sup>	0.79
SM (OH) C22:2	Sphingomyelins	12.18 ± 2.95	15.30 ± 3.54	9.42 × 10 <sup>-9</sup>	0.80
C2	Acylcarnitines	5.67 ± 2.92	7.13 ± 2.72	1.76 × 10 <sup>-3</sup>	0.80
SM (OH) C24:1	Sphingomyelins	2.56 ± 0.72	3.21 ± 0.73	6.37 × 10 <sup>-8</sup>	0.80
lysoPC a C20:4	Lysophosphatidylcholines	2.80 ± 1.11	3.51 ± 0.84	1.14 × 10 <sup>-5</sup>	0.80
PC aa C34:3	Phosphatidylcholines	5.34 ± 2.09	6.69 ± 1.66	1.22 × 10 <sup>-5</sup>	0.80
PC aa C42:0	Phosphatidylcholines	0.54 ± 0.21	0.68 ± 0.18	3.22 × 10 <sup>-5</sup>	0.80
Taurine	Amino acid related	75.51 ± 34.51	94.00 ± 24.49	1.38 × 10 <sup>-4</sup>	0.80
Cer (d18:1/23:0)	Ceramides	0.82 ± 0.22	1.01 ± 0.26	6.28 × 10 <sup>-7</sup>	0.81
PC ae C40:2	Phosphatidylcholines	2.11 ± 0.66	2.62 ± 0.64	2.00 × 10 <sup>-6</sup>	0.81
PC ae C30:0	Phosphatidylcholines	0.22 ± 0.07	0.27 ± 0.08	1.59 × 10 <sup>-5</sup>	0.81
PC aa C36:1	Phosphatidylcholines	34.39 ± 8.83	42.49 ± 10.48	4.09 × 10 <sup>-7</sup>	0.81
PC aa C38:0	Phosphatidylcholines	3.02 ± 1.01	3.72 ± 1.05	3.28 × 10 <sup>-5</sup>	0.81
CE (18:0)	Cholesteryl esters	8.46 ± 4.19	10.40 ± 3.51	3.21 × 10 <sup>-3</sup>	0.81
PC aa C28:1	Phosphatidylcholines	2.60 ± 0.71	3.18 ± 0.69	4.20 × 10 <sup>-7</sup>	0.82
CE (20:3)	Cholesteryl esters	14.33 ± 4.25	17.52 ± 5.05	1.11 × 10 <sup>-4</sup>	0.82
PC aa C40:5	Phosphatidylcholines	6.78 ± 1.98	8.28 ± 2.41	3.06 × 10 <sup>-5</sup>	0.82
SM (OH) C22:1	Sphingomyelins	12.63 ± 3.10	15.37 ± 3.35	2.92 × 10 <sup>-7</sup>	0.82
CE (18:1)	Cholesteryl esters	208.33 ± 64.50	253.04 ± 65.21	2.34 × 10 <sup>-5</sup>	0.82
Val	Amino acids	166.82 ± 46.80	201.59 ± 40.01	1.20 × 10 <sup>-6</sup>	0.83

PC ae C40:6	Phosphatidylcholines	3.99 ± 1.30	4.80 ± 1.17	5.63 × 10 <sup>-5</sup>	0.83
PC aa C36:3	Phosphatidylcholines	67.87 ± 18.73	81.50 ± 18.98	9.72 × 10 <sup>-6</sup>	0.83
PC aa C38:6	Phosphatidylcholines	90.50 ± 27.54	108.56 ± 27.44	5.30 × 10 <sup>-5</sup>	0.83
Trp	Amino acids	43.51 ± 11.89	52.17 ± 9.22	7.85 × 10 <sup>-7</sup>	0.83
PC aa C30:0	Phosphatidylcholines	3.27 ± 1.11	3.92 ± 1.02	1.74 × 10 <sup>-4</sup>	0.83
PC ae C36:2	Phosphatidylcholines	8.86 ± 2.32	10.59 ± 2.31	4.82 × 10 <sup>-6</sup>	0.84
Cer (d18:1/24:0)	Ceramides	2.10 ± 0.58	2.50 ± 0.63	3.74 × 10 <sup>-5</sup>	0.84
PC aa C36:2	Phosphatidylcholines	168.44 ± 40.84	200.78 ± 40.91	1.49 × 10 <sup>-6</sup>	0.84
PC ae C36:0	Phosphatidylcholines	0.62 ± 0.18	0.74 ± 0.17	2.58 × 10 <sup>-5</sup>	0.84
DG (17:0_18:1)	Diglycerides	0.45 ± 0.16	0.53 ± 0.17	3.12 × 10 <sup>-3</sup>	0.84
HArg	Amino acid related	5.30 ± 2.91	6.26 ± 1.89	1.48 × 10 <sup>-2</sup>	0.85
PC aa C32:1	Phosphatidylcholines	9.44 ± 3.77	11.13 ± 3.96	6.42 × 10 <sup>-3</sup>	0.85
TG (18:0_36:5)	Triglycerides	0.73 ± 0.26	0.86 ± 0.39	2.48 × 10 <sup>-2</sup>	0.86
PC aa C38:4	Phosphatidylcholines	65.39 ± 16.86	75.51 ± 16.59	1.87 × 10 <sup>-4</sup>	0.87
PC ae C44:4	Phosphatidylcholines	0.26 ± 0.10	0.30 ± 0.06	3.00 × 10 <sup>-3</sup>	0.87
PC ae C38:4	Phosphatidylcholines	6.22 ± 1.71	7.19 ± 1.38	1.32 × 10 <sup>-4</sup>	0.87
PC ae C42:5	Phosphatidylcholines	1.55 ± 0.46	1.77 ± 0.38	1.81 × 10 <sup>-4</sup>	0.87
PC ae C32:1	Phosphatidylcholines	1.66 ± 0.44	1.88 ± 0.39	1.16 × 10 <sup>-3</sup>	0.88
CE (20:4)	Cholesteryl esters	139.76 ± 52.16	157.98 ± 51.80	2.80 × 10 <sup>-2</sup>	0.88
CE (16:0)	Cholesteryl esters	131.34 ± 37.06	148.25 ± 35.19	3.56 × 10 <sup>-3</sup>	0.89
PC ae C38:5	Phosphatidylcholines	9.23 ± 2.33	10.37 ± 2.00	1.12 × 10 <sup>-3</sup>	0.89
PC ae C32:2	Phosphatidylcholines	0.89 ± 0.24	0.99 ± 0.22	4.22 × 10 <sup>-3</sup>	0.89
Tyr	Amino acids	52.74 ± 14.27	58.63 ± 12.62	6.41 × 10 <sup>-3</sup>	0.90
PC ae C44:6	Phosphatidylcholines	0.88 ± 0.33	0.97 ± 0.23	3.17 × 10 <sup>-2</sup>	0.90
Gln	Amino acids	648.70 ± 124.61	689.46 ± 94.32	2.09 × 10 <sup>-2</sup>	0.94