Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Exposure of nano-polystyrene induces metabolic alteration on lipid homeostasis in Caco-2

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Fig. S1. The principal component analysis (PCA) score plots and hierarchical clustering dendrograms for an evaluation of suspension buffer toxicity by untargeted metabolic profiling in positive and negative ionization modes.

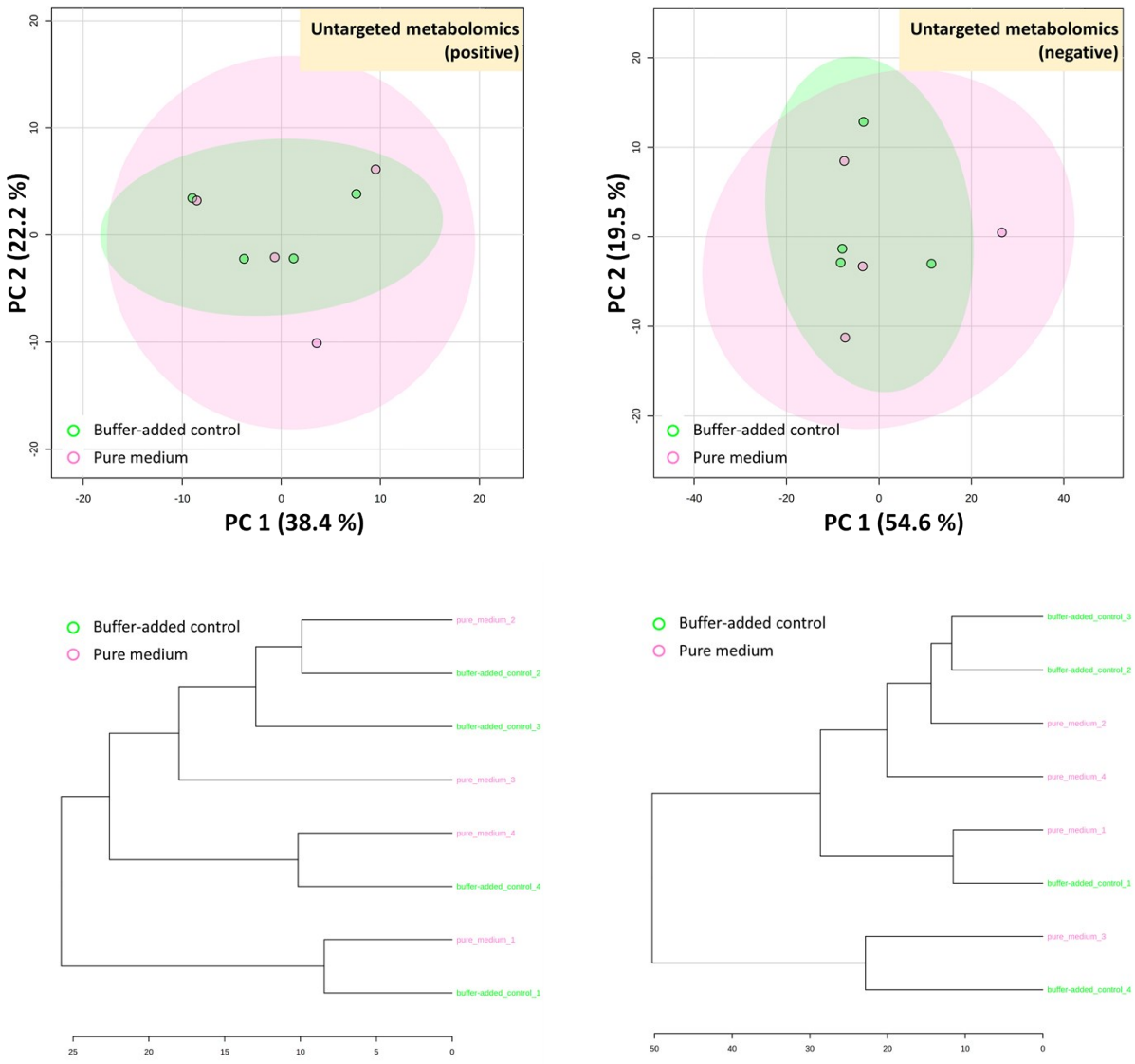

Fig. S2. The PCA score plots for the acute exposure model. (A) PCA plots of a three-group comparison from the lipidomics data. **(B)** A PCA plot of a three-group comparison from the large-scale targeted metabolomics data.

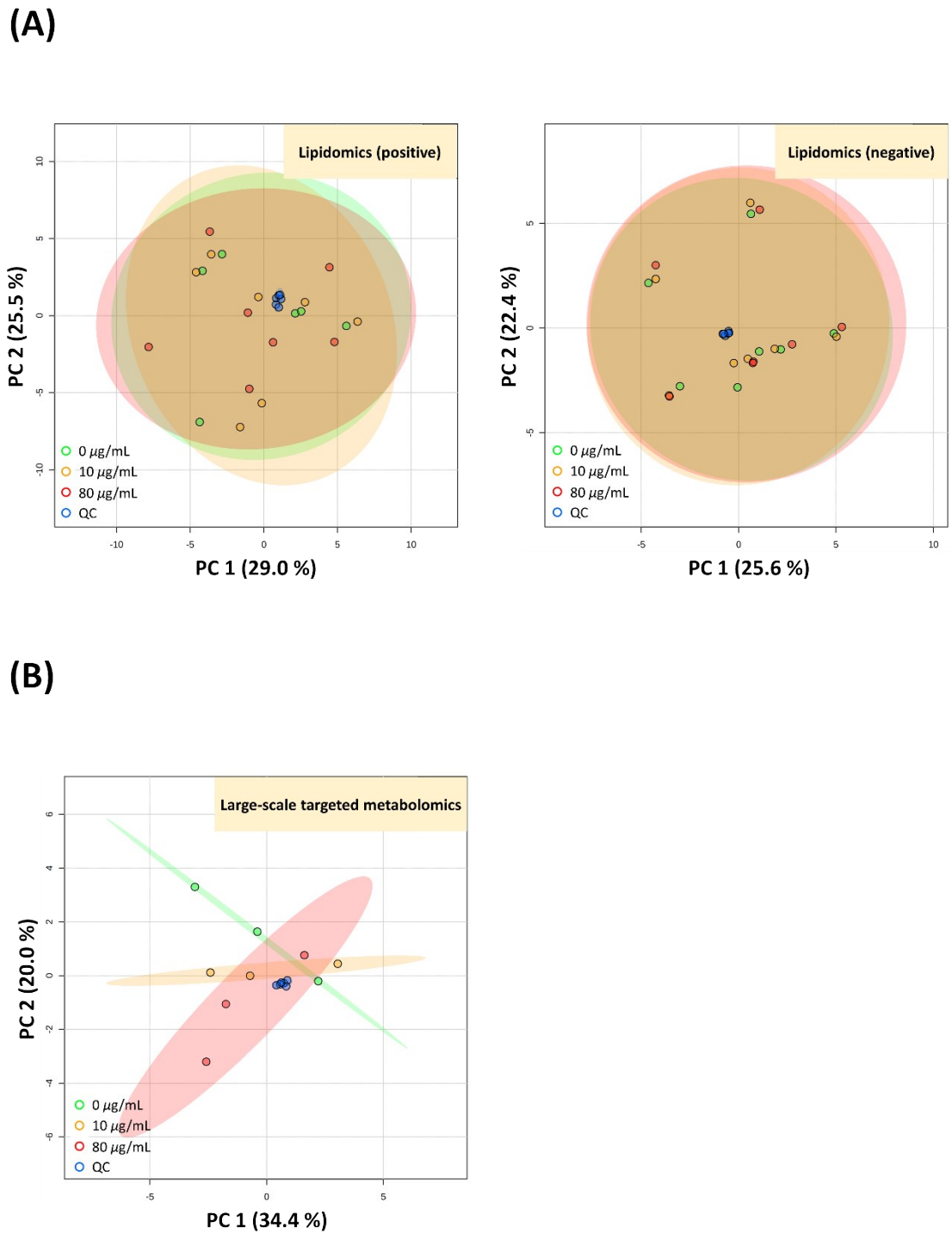

Fig. S3. Pairwise partial least squares-discriminant analysis and cross-validation for the acute exposure model. R^2: coefficient of determination; Q^2: coefficient of prediction.

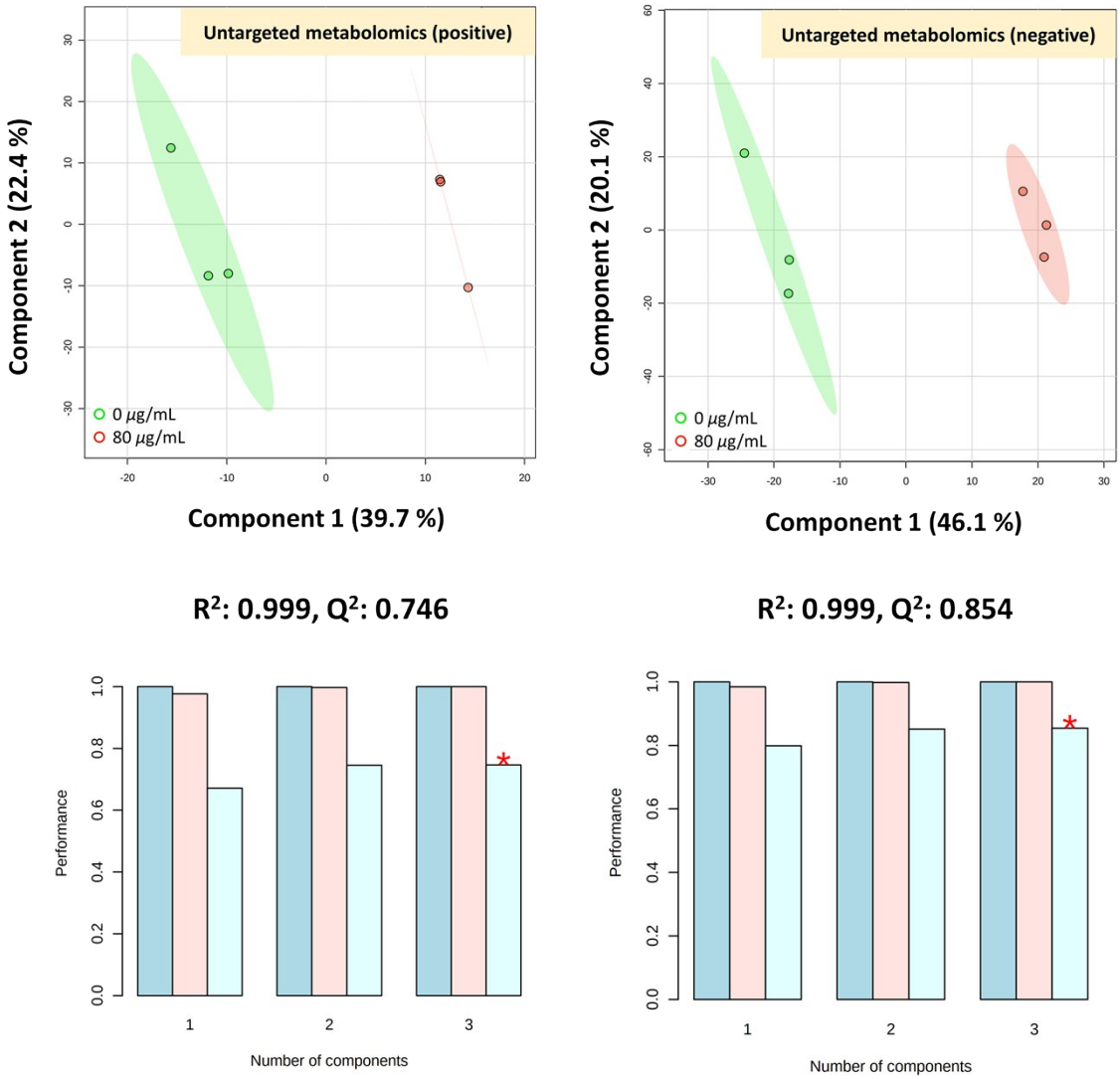

Table S1. MS parameters for untargeted lipidomics, large-scale targeted metabolomics, and untargeted metabolomics.

Thermo Scientific Q Exactive Plus		**Agilent 6460 Triple Quadrupole Mass Spectrometer**		**Agilent 6530 hybrid quadrupole Time of Flight Mass Spectrometer**	
Untargeted lipidomics		**Large-scale targeted metabolomics**		**Untargeted metabolomics**	
MS1		ESI polarity	Positive/negative ion-switching	ESI polarity	Positive, negative
ESI polarity	Positive, negative	Polarity switching time	30 ms	MS resolution	4 Ghz
Sheath gas pressure	60 arbitrary units	Dwell time	3 ms	Capillary voltage	3.5 kV
Aux gas flow	15 arbitrary units	Capillary voltage	3.5 kV	MS1 range	60-1000 m/z
Sweep gas flow	3 arbitrary units	Drying gas	8 L/min	Nozzle voltage	1000 V
Spray voltage	3.6 kV	Nebulizer gas	35 psi	Fragmentor voltage	135 V
Capillary temperature	275℃	Sheath gas temperature	350℃	Gas temperature	325℃
S-lens rf level	55	Sheath gas flow	11 L/min	Drying gas	8 L/min
Aux gas heater temperature	450℃			Nebulizer gas	35 psi
Ms1 mass range	120-1200 m/z			Sheath gas temperature	350℃
Microscans	1			Sheath gas flow	11 L/min
Resolution	70,000 FWHM (m/z 200)			MS1 acquisition speed	2 spectra/s
Agc target	1e6				
Maximum it	100 ms				
Number of scans	1 spectra/s				
Spectrum data type	Profile				
MS/MS (ddMS2)					
Microscans	1				
Resolution	17,500 FWHM (m/z 200)				
Agc target	1e5				
Maximum it	50 ms				
Loop count	4				
Msx count	1				
TopN	4				
Isolation window	1.0 m/z				

Isolation offset	0.0 m/z
Normalized collision energy	20
Spectrum data type	Profile

Table S2. The 212 targeted metabolites and their transitions for large-scale targeted metabolomics: a modified list from the method by Yuan et al. (*Nature Protocols*, 2012, **7**, 872-881).

Number	Metabolite list	ESI	Precursor	Product	Number	Metabolite list	ESI	Precursor	Product
1	1-Methyladenosine	+	281.8	150	107	GMP	+	364	152
2	1-Methyl-Histidine	+	170.1	124	108	GTP	-	522	424
3	2,3-Dihydroxybenzoic acid	-	153	109	109	Guanidoacetic acid	-	116.001	74.3
4	2,3-Diphosphoglyceric acid	-	265.1	167.1	110	guanine	+	152.2	110
5	2-Aminooctanoic acid	+	160	55.3	111	guanosine	+	284.1	135
6	2-Dehydro-D-gluconate	-	193	103	112	hexose-phosphate	-	259	79
7	2-Hydroxy-2-methylbutanedioic acid	-	147.001	85.1	113	histidine	+	156.1	110.1
8	2-Isopropylmalic acid	-	175.002	115	114	histidinol	+	142.1	95
9	2-Ketohaxanoic acid	-	129.005	101.3	115	homocysteine	+	136.12	90.1
10	2-Keto-isovalerate	-	115.05	71.05	116	homoserine	+	120.15	44.2
11	2-Oxobutanoate	-	101	57.2	117	Hydroxyisocaproic acid	-	131.006	85.1
12	3-Methylphenylacetic acid	-	149.002	105	118	Hydroxyphenylacetic acid	-	151.004	107
13	3-Phosphoglycerate	-	185	97	119	hydroxyphenylpyruvate	-	179.05	107
14	3-Phosphoserine	+	186	88	120	hydroxyproline	+	132	68.2
15	3-S-methylthiopropionate	-	119.02	47	121	hypoxanthine	-	135	92
16	4-Aminobutyrate	+	104.01	69	122	IDP	-	427	159
17	4-Pyridoxic acid	-	182.003	138	123	Imidazoleacetic acid	+	127.002	81
18	5-Methyl-THF	+	460.1	313.1	124	IMP	+	349	137
19	6-Phospho-D-gluconate	-	275	97	125	indole	+	118	91
20	7-Methylguanosine	+	298.002	166	126	Indole-3-carboxylic acid	-	160.002	116
21	acetoacetate	-	101.05	57.2	127	inosine	-	267	135
22	Acetylcarnitine DL	+	204	85	128	isocitrate	-	191.02	117
23	acetyl-CoA	+	810	303	129	isoleucine	+	132.1	86
24	aconitate	-	173.05	85	130	Kynurenic acid	-	188	144
25	adenine	+	136	119	131	Kynurenine	+	209	146
26	adenosine	+	268.15	136.1	132	lactate	-	89	43.2
27	adenosine 5-phosphosulfate	-	426	346	133	leucine	+	132.1	86
28	ADP	-	426.1	159	134	lipoate	-	205	171
29	alpha-ketoglutarate	-	145	101	135	lysine	+	147	67

30	alanine	+	90.1	44.2	136	malate	-	133	115
31	allantoate	-	175	132	137	Maleic acid	-	115.03	71.03
32	allantoin	-	157.05	114	138	methionine	+	150.1	133
33	Aminoadipic acid	-	160.001	116	139	Methionine sulfoxide	+	166	74
34	AMP	+	348.15	136	140	Methylcysteine	+	136.02	119.02
35	arginine	+	175.02	60	141	Methylmalonic acid	-	117.002	73.1
36	Ascorbic acid	-	175.001	87	142	methylnicotinamide	+	137.001	94
37	asparagine	+	133.1	74	143	myo-inositol	-	179	161
38	aspartate	+	134	74	144	N-acetyl-glucosamine-1-phosphate	-	300	79
39	betaine	+	118.02	58	145	N-Acetyl-L-alanine	-	130	88
40	betaine aldehyde	+	102	58	146	N-acetyl-L-ornithine	+	175	115.1
41	biotin	+	245.1	227	147	N-Acetylputrescine	+	131	114
42	Carbamoyl phosphate	-	140	79	148	NAD+	+	664.1	428
43	carnitine	+	162.1	103	149	NADH	+	666.1	514
44	CDP	-	402	384	150	NADP+	+	744.2	136
45	CDP-choline	-	487	428	151	NADPH	-	744	408
46	CDP-ethanolamine	-	445	273	152	N-carbamoyl-L-aspartate	-	175.03	132
47	cholesteryl sulfate	-	465.2	97	153	Ng,NG-dimethyl-L-arginine	+	203	70
48	Cholic acid	-	407.2	345.2	154	nicotinamide	+	123.1	80
49	choline	+	104	60	155	Nicotinamide ribotide	+	335	123
50	Citraconic acid	-	129.003	85.1	156	nicotinate	-	122	78
51	citrate	-	191.05	87	157	O-acetyl-L-serine	+	148	106
52	CMP	+	324	112	158	octulose-monophosphate (O8P-O1P)	-	319	97
53	coenzyme A	-	766	408	159	ornithine	+	133	70
54	creatine	+	132.003	90	160	orotate	-	155	111
55	Creatinine	+	114	44.2	161	orotidine-5-phosphate	-	367	323
56	CTP	-	482	384	162	oxaloacetate	-	131	87
57	cyclic-AMP	-	328	134.05	163	p-aminobenzoate	-	136.05	92
58	cystathionine	+	223	134	164	pantothenate	-	218	146
59	cysteine	+	122.1	59.1	165	phenylalanine	+	166.1	103
60	cytidine	+	244.1	112	166	Phenyllactic acid	-	165.006	103.1
61	cytosine	+	112.1	95	167	phosphoenolpyruvate	-	167	79

62	dAMP	+	332.1	136	168	Phosphorylcholine	+	184.001	125
63	dATP	-	490	159	169	p-hydroxybenzoate	-	137	93
64	dCDP	-	386	159	170	proline	+	116.1	70.1
65	dCMP	+	308	112	171	purine	+	121	94
66	dCTP	-	466	159	172	pyridoxine	+	170	134
67	deoxyadenosine	+	252	136	173	Pyroglutamic acid	-	128	82.1
68	Deoxycholic acid	-	391.202	345.2	174	Pyrophosphate	-	176.8	158.8
69	deoxyribose-phosphate	-	213	79	175	pyruvate	-	87	43
70	dephospho-CoA	+	688	348	176	quinolinate	-	166	122
71	D-erythrose-4-phosphate	-	199	97	177	riboflavin	+	377	243
72	D-glucarate	-	209	85	178	ribose-phosphate	-	229	79
73	D-gluconate	-	195	129	179	S-adenosyl-L-homocysteine	+	385.1	136
74	D-glyceraldehdye-3-phosphate	-	169.05	97	180	S-adenosyl-L-methionine	+	399.1	250
75	dGMP	+	348.1	135	181	serine	+	106	60
76	dGTP	-	506.12	159	182	shikimate	-	173	93
77	dihydroorotate	-	157	113	183	shikimate-3-phosphate	-	253.1	97
78	dihydroxy-acetone-phosphate	-	169	79	184	sn-glycerol-3-phosphate	-	171	79
79	dimethylglycine	+	104.02	58	185	spermidine	+	146	112
80	DL-Pipecolic acid	+	130	84	186	spermine	+	203.1	129.1
81	D-sedoheptulose-1-7-phosphate	-	289	97	187	succinate	-	117	73
82	dTDP	-	401	159	188	taurine	-	124	80
83	dTMP	+	323	81	189	Taurodeoxycholic acid	-	498.2	124
84	dTTP	-	481	159	190	thiamine	+	265	122
85	dUMP	-	307	195	191	Thiamine pyrophosphate	-	423.1	302
86	dUTP	-	467	159	192	thiamine-phosphate	+	345.2	122
87	ethanolamine	+	62.1	44.2	193	threonine	+	120	74
88	FAD	+	786	348	194	thymidine	-	241	125
89	FMN	-	455	213	195	thymine	+	127.1	110
90	folate	+	442	295	196	trans, trans-farnesyl diphosphate	-	381	79
91	fructose-1,6-bisphosphate	-	339	97	197	trehalose-6-Phosphate	-	421	79
92	fumarate	-	115	71	198	tryptophan	+	205	146
93	GDP	-	442	159	199	tyrosine	+	182.1	77

94	Geranyl-PP	-	313	79	200	UDP	-	403	159
95	glucono-D-lactone	-	177	129	201	UDP-D-glucose	-	565	323
96	glucosamine	+	180	162	202	UDP-D-glucuronate	-	579	403
97	glucose-6-phosphate	-	259.02	199	203	UDP-N-acetyl-glucosamine	-	606	385
98	glutamate	+	148.1	84.1	204	UMP	+	325	97
99	glutamine	+	147.1	84.1	205	uracil	-	111.05	42.1
100	glutathione	+	308.1	162	206	Urea	+	61.1	44.2
101	glutathione disulfide	+	613	231	207	Uric acid	-	167.001	124
102	glycerate	-	105	75	208	uridine	-	243	200
103	Glycerophosphocholine	+	258.1	104	209	valine	+	118.1	55.2
104	Glycine	+	169	134	210	xanthine	-	151	108
105	glycolate	-	75	45.2	211	xanthosine	-	283	151
106	glyoxylate	-	73	45	212	Xanthurenic acid	-	204.001	160

Table S3. Data processing parameters for untargeted lipidomics (MSDIAL) and untargeted metabolomics (XCMS).

Untargeted lipidomics (MS-DIAL)	
Data collection	
MS1 tolerance	0.001 Da
MS2 tolerance	0.05 Da
Retention time begin	0 min
Retention time end	16 min
Mass range begin	120 Da
Mass range end	1200 Da
Maximum charged number	2
Peak detection	
Minimum peak height	10000 amplitude
Mass slice width	0.1 Da
Smoothing method	Linear weighted moving average
Smoothing level	3 scan
Minimum peak width	5 scan
MS2 Dec	
Sigma window value	0.1
MS/MS abundance cut off	0 amplitude
Exclude after precursor ion	checked
Keep the isotopic ions until	0.5 Da
Identification	
Retention time tolerance	100 min
Accurate mass tolerance (MS1)	0.01 Da
Accurate mass tolerance (MS2)	0.05 Da
Identification score cut off	80%
Adduct	
Positive: [M+H]+, [M+NH4]+, [M+Na]+, [M+ACN+H]+, [M+H-H2O]+, [M+H-2H2O]+, [2M+H]+, [2M+NH4]+, [2M+Na]+	
Negative: [M-H]-, [M-H2O-H]-, [M+Cl]-, [M+Hac-H]-, [M+CH3COONa-H]-, [2M-H]-	
Alignment	
Reference file	one of QC sample file
Retention time tolerance	0.05 min
MS1 tolerance	0.015 Da

Blank filter: sample max / blank average	3 fold change

Untargeted metabolomics (XCMS)

	Positive ESI	Negative ESI
Method	centWave	centWave
m/z tolerance (ppm)	20	20
minimum peak width	7.75	7.3
maximum peak width	33.75	15
mzdiff	-0.001	-0.001
signal-to-noise threshold	6	6
noise filter	0	0
prefilter peaks	3	3
prefilter intensity	100	100
Integration method	1	1

Table S4. Lists of annotated lipids in positive and negative ESI lipidomics analysis: bond type level and/or fatty acyl/alkyl level.

Positive ESI

Number	Metabolite name	Adduct type	Number	Metabolite name	Adduct type	Number	Metabolite name	Adduct type
1	Cer 18:1;2O/16:0	[M+H]+	142	PC O-44:4_1	[M+H]+	283	TG 14:0_16:0_16:1_1	[M+NH4]+
2	Cer 18:2;2O/16:0	[M+H-H2O]+	143	PC O-44:4_2	[M+H]+	284	TG 14:0_16:0_16:1_2	[M+NH4]+
3	Cer 18:1;2O/18:0	[M+H]+	144	PC O-44:5	[M+H]+	285	TG 14:0_16:0_17:0_1	[M+NH4]+
4	Cer 18:1;2O/20:0	[M+H]+	145	PC O-44:6	[M+H]+	286	TG 14:0_16:0_17:0_2	[M+NH4]+
5	Cer 18:1;2O/22:0	[M+H]+	146	PC O-46:6_1	[M+H]+	287	TG 14:0_16:0_18:1_1	[M+NH4]+
6	Cer 18:1;2O/22:1	[M+H-H2O]+	147	PC O-46:6_2	[M+H]+	288	TG 14:0_16:0_18:1_2	[M+NH4]+
7	Cer 18:1;2O/23:0	[M+H]+	148	PC O-48:6	[M+H]+	289	TG 14:0_16:0_22:5	[M+NH4]+
8	Cer 18:1;2O/24:0	[M+H]+	149	PE 14:0_16:1	[M+H]+	290	TG 14:0_16:0_22:6	[M+NH4]+
9	Cer 18:1;2O/24:1	[M+H]+	150	PE 16:0_16:0	[M+H]+	291	TG 14:0_16:0_24:0	[M+NH4]+
10	Cer 18:2;2O/24:1	[M+H]+	151	PE 16:0_16:1	[M+H]+	292	TG 14:0_16:0_26:0	[M+NH4]+
11	Cer 18:1;2O/26:1	[M+H]+	152	PE 16:1_16:1	[M+H]+	293	TG 14:0_16:1_18:1_1	[M+NH4]+
12	DG 16:0_16:0	[M+NH4]+	153	PE 16:0_17:1	[M+H]+	294	TG 14:0_16:1_18:1_2	[M+NH4]+
13	DG 14:0_18:1	[M+NH4]+	154	PE 16:1_17:1	[M+H]+	295	TG 14:0_16:1_18:1_3	[M+NH4]+
14	DG 16:0_18:1	[M+NH4]+	155	PE 16:0_18:0	[M+H]+	296	TG 14:0_16:1_22:5	[M+NH4]+
15	DG 16:1_18:1	[M+NH4]+	156	PE 16:0_18:1	[M+H]+	297	TG 14:0_18:0_20:0	[M+NH4]+
16	DG 16:0_20:1	[M+NH4]+	157	PE 16:1_18:1	[M+H]+	298	TG 14:0_25:0_16:1	[M+NH4]+
17	DG 18:1_18:1	[M+NH4]+	158	PE 16:1_18:2_1	[M+H]+	299	TG 14:1_14:1_14:1	[M+NH4]+
18	DG 18:0_18:2	[M+NH4]+	159	PE 16:1_18:2_2	[M+H]+	300	TG 14:1_14:1_16:1	[M+NH4]+
19	DG 18:1_18:2	[M+NH4]+	160	PE 17:0_18:1_1	[M+H]+	301	TG 14:1_16:1_16:1	[M+NH4]+
20	DG 16:0_20:3	[M+NH4]+	161	PE 17:0_18:1_2	[M+H]+	302	TG 14:1_16:1_18:1	[M+NH4]+
21	DG 16:0_20:4	[M+NH4]+	162	PE 17:1_18:1	[M+H]+	303	TG 14:1_17:1_18:1	[M+NH4]+
22	DG 18:0_20:1	[M+NH4]+	163	PE 18:0_18:1	[M+H]+	304	TG 15:0_14:1_16:1	[M+NH4]+
23	DG 18:1_20:1	[M+NH4]+	164	PE 18:1_18:1_1	[M+H]+	305	TG 15:0_15:1_17:1_1	[M+NH4]+
24	DG 18:0_20:2	[M+NH4]+	165	PE 18:1_18:1_2	[M+H]+	306	TG 15:0_15:1_17:1_2	[M+NH4]+
25	DG 18:1_20:2	[M+NH4]+	166	PE 18:2_18:2	[M+H]+	307	TG 15:0_16:0_16:1_1	[M+NH4]+
26	DG 18:0_20:3	[M+NH4]+	167	PE 16:0_20:4	[M+H]+	308	TG 15:0_16:0_17:0	[M+NH4]+
27	DG 16:0_22:5	[M+NH4]+	168	PE 16:1_20:4	[M+H]+	309	TG 15:0_16:0_18:0_1	[M+NH4]+
28	DG 16:0_24:1	[M+NH4]+	169	PE 16:0_20:5	[M+H]+	310	TG 15:0_16:0_18:0_2	[M+NH4]+
29	DG 18:0_22:4	[M+NH4]+	170	PE 16:1_20:5	[M+H]+	311	TG 15:0_16:0_18:1_1	[M+NH4]+
30	DG 18:0_22:5	[M+NH4]+	171	PE 18:0_19:1	[M+H]+	312	TG 15:0_16:0_18:1_2	[M+NH4]+

31	DG 18:1_22:5	[M+NH4]+	172	PE 18:1_19:1	[M+H]+	313	TG 15:0_16:0_24:0	[M+NH4]+
32	DG 18:1_24:1	[M+NH4]+	173	PE 18:0_20:1	[M+H]+	314	TG 15:0_16:1_18:1	[M+NH4]+
33	HexCer 18:1;2O/16:0	[M+H]+	174	PE 18:1_20:1	[M+H]+	315	TG 15:0_17:1_17:1	[M+NH4]+
34	HexCer 18:1;2O/22:0;O	[M+H]+	175	PE 18:0_20:3	[M+H]+	316	TG 16:0_14:1_16:1_1	[M+NH4]+
35	HexCer 18:1;2O/24:0;O	[M+H]+	176	PE 18:1_20:3	[M+H]+	317	TG 16:0_14:1_16:1_2	[M+NH4]+
36	HexCer 18:1;2O/24:1;O_1	[M+H]+	177	PE 18:0_20:4	[M+H]+	318	TG 16:0_16:0_16:0	[M+NH4]+
37	HexCer 18:1;2O/24:1;O_2	[M+H]+	178	PE 16:0_22:4	[M+H]+	319	TG 16:0_16:0_18:0_1	[M+NH4]+
38	LPC 14:0	[M+H]+	179	PE 18:1_20:4	[M+H]+	320	TG 16:0_16:0_18:0_2	[M+NH4]+
39	LPC 16:0	[M+H]+	180	PE 18:0_20:5	[M+H]+	321	TG 16:0_16:0_18:1	[M+NH4]+
40	LPC 16:1	[M+H]+	181	PE 16:1_22:6	[M+H]+	322	TG 16:0_16:1_17:1	[M+NH4]+
41	LPC 18:1/0:0	[M+H]+	182	PE 22:0_18:1	[M+H]+	323	TG 16:0_16:1_18:1_1	[M+NH4]+
42	LPC 20:0/0:0	[M+H]+	183	PE 18:1_22:1	[M+H]+	324	TG 16:0_16:1_18:1_2	[M+NH4]+
43	LPC 20:1	[M+H]+	184	PE 18:0_22:4	[M+H]+	325	TG 16:0_16:1_20:5	[M+NH4]+
44	LPC 20:1/0:0	[M+H]+	185	PE 18:0_22:5_1	[M+H]+	326	TG 16:0_16:1_22:6	[M+NH4]+
45	LPC 22:0/0:0	[M+H]+	186	PE 18:0_22:5_2	[M+H]+	327	TG 16:0_17:0_18:0	[M+NH4]+
46	LPC 22:1/0:0	[M+H]+	187	PE 18:0_22:6	[M+H]+	328	TG 16:0_17:0_18:1_1	[M+NH4]+
47	LPC 24:0/0:0	[M+H]+	188	PE 18:1_22:6	[M+H]+	329	TG 16:0_17:0_18:1_2	[M+NH4]+
48	LPC 24:1/0:0	[M+H]+	189	PE 22:1_20:4	[M+H]+	330	TG 16:0_18:0_18:_1	[M+NH4]+
49	LPC 26:1/0:0	[M+H]+	190	PE 20:1_22:6	[M+H]+	331	TG 16:0_18:0_18:1_2	[M+NH4]+
50	LPE 18:0	[M+H]+	191	PE 18:1_26:1	[M+H]+	332	TG 16:0_18:0_20:4	[M+NH4]+
51	LPE 18:1	[M+H]+	192	PE P-16:0_14:0	[M+H]+	333	TG 16:0_18:1_18:1	[M+NH4]+
52	LPE 24:0	[M+H]+	193	PE P-14:0_16:1	[M+H]+	334	TG 16:0_18:1_18:2_1	[M+NH4]+
53	LPE O-16:1	[M+H]+	194	PE P-16:0_16:1	[M+H]+	335	TG 16:0_18:1_18:2_2	[M+NH4]+
54	LPE O-18:1	[M+H]+	195	PE P-18:1_14:1	[M+H]+	336	TG 16:0_18:1_20:1_1	[M+NH4]+
55	LPE O-18:2	[M+H]+	196	PE P-17:0_16:1	[M+H]+	337	TG 16:0_18:1_20:1_2	[M+NH4]+
56	LPE O-20:1	[M+H]+	197	PE P-16:0_17:1	[M+H]+	338	TG 16:0_18:1_22:1	[M+NH4]+
57	LPE O-22:1	[M+H]+	198	PE P-18:0_16:0	[M+H]+	339	TG 16:0_18:1_22:4_1	[M+NH4]+
58	LPE O-24:2	[M+H]+	199	PE P-16:0_18:1	[M+H]+	340	TG 16:0_18:1_22:4_2	[M+NH4]+
59	PC 14:0_14:0	[M+H]+	200	PE P-18:1_16:1	[M+H]+	341	TG 16:0_18:1_22:5	[M+NH4]+

60	PC 14:0_16:1	[M+H]+	201	PE P-16:0_18:2	[M+H]+	342	TG 16:0_18:1_22:6	[M+NH4]+
61	PC 16:0_16:1	[M+H]+	202	PE P-16:0_18:3	[M+H]+	343	TG 16:0_18:1_24:1	[M+NH4]+
62	PC 16:1_16:1	[M+H]+	203	PE P-14:0_20:4	[M+H]+	344	TG 16:0_18:1_26:1	[M+NH4]+
63	PC 16:0_17:1	[M+H]+	204	PE P-18:1_17:0	[M+H]+	345	TG 16:0_19:1_20:1	[M+NH4]+
64	PC 16:0_18:0	[M+H]+	205	PE P-17:0_18:1	[M+H]+	346	TG 16:0_20:0_18:1	[M+NH4]+
65	PC 16:0_18:1	[M+H]+	206	PE P-18:1_17:1	[M+H]+	347	TG 16:0_22:5_22:6	[M+NH4]+
66	PC 16:1_18:1	[M+H]+	207	PE P-18:0_18:1	[M+H]+	348	TG 16:0_23:0_18:1	[M+NH4]+
67	PC 16:1_18:2_1	[M+H]+	208	PE P-18:1_18:1	[M+H]+	349	TG 16:0_24:0_16:1	[M+NH4]+
68	PC 16:1_18:2_2	[M+H]+	209	PE P-18:0_18:2	[M+H]+	350	TG 16:0_24:0_18:1	[M+NH4]+
69	PC 17:0_18:1	[M+H]+	210	PE P-16:0_20:3_2	[M+H]+	351	TG 16:0_24:1_26:1	[M+NH4]+
70	PC 17:1_18:1	[M+H]+	211	PE P-16:0_20:4	[M+H]+	352	TG 16:0_26:0_18:1	[M+NH4]+
71	PC 16:0_20:1	[M+H]+	212	PE P-16:0_20:5	[M+H]+	353	TG 16:1_16:1_18:1	[M+NH4]+
72	PC 18:1_18:1	[M+H]+	213	PE P-22:1_16:0	[M+H]+	354	TG 16:1_16:1_18:2	[M+NH4]+
73	PC 18:1_18:2_1	[M+H]+	214	PE P-16:0_22:2	[M+H]+	355	TG 16:1_17:1_18:1_2	[M+NH4]+
74	PC 18:1_18:2_2	[M+H]+	215	PE P-20:1_18:2	[M+H]+	356	TG 16:1_17:1_18:2	[M+NH4]+
75	PC 16:1_20:3	[M+H]+	216	PE P-18:0_20:3_1	[M+H]+	357	TG 16:1_18:1_18:2	[M+NH4]+
76	PC 16:0_20:4	[M+H]+	217	PE P-18:0_20:3_2	[M+H]+	358	TG 16:1_18:1_18:3	[M+NH4]+
77	PC 14:0_22:6	[M+H]+	218	PE P-18:1_20:3	[M+H]+	359	TG 16:1_18:1_20:1	[M+NH4]+
78	PC 18:1_19:1	[M+H]+	219	PE P-18:0_20:4	[M+H]+	360	TG 16:1_18:1_20:4	[M+NH4]+
79	PC 18:1_20:1	[M+H]+	220	PE P-16:0_22:4	[M+H]+	361	TG 16:1_18:1_22:5	[M+NH4]+
80	PC 18:1_20:2_1	[M+H]+	221	PE P-18:1_20:4	[M+H]+	362	TG 16:1_18:1_26:1	[M+NH4]+
81	PC 18:1_20:2_2	[M+H]+	222	PE P-16:0_22:5	[M+H]+	363	TG 16:1_19:1_24:1	[M+NH4]+
82	PC 18:1_20:3	[M+H]+	223	PE P-18:1_20:5	[M+H]+	364	TG 17:0_16:1_18:1	[M+NH4]+
83	PC 18:0_20:4	[M+H]+	224	PE P-21:0_18:1	[M+H]+	365	TG 17:0_18:0_18:1_1	[M+NH4]+
84	PC 16:0_22:4	[M+H]+	225	PE P-24:1_16:0	[M+H]+	366	TG 17:0_18:0_18:1_2	[M+NH4]+
85	PC 18:1_20:4	[M+H]+	226	PE P-24:0_16:1	[M+H]+	367	TG 17:0_18:1_18:1	[M+NH4]+
86	PC 16:0_22:5	[M+H]+	227	PE P-22:1_18:1	[M+H]+	368	TG 17:0_18:1_20:4	[M+NH4]+
87	PC 18:1_20:5	[M+H]+	228	PE P-22:1_18:2	[M+H]+	369	TG 17:0_18:1_22:5	[M+NH4]+
88	PC 16:0_22:6	[M+H]+	229	PE P-20:1_20:3	[M+H]+	370	TG 17:1_18:1_18:1	[M+NH4]+
89	PC 24:0_16:1	[M+H]+	230	PE P-20:0_20:4	[M+H]+	371	TG 17:1_18:1_18:2	[M+NH4]+
90	PC 16:0_24:1	[M+H]+	231	PE P-18:0_22:4	[M+H]+	372	TG 17:1_18:1_22:5	[M+NH4]+
91	PC 20:1_20:3	[M+H]+	232	PE P-18:0_22:5_1	[M+H]+	373	TG 17:1_18:1_26:1	[M+NH4]+
92	PC 18:1_22:5_1	[M+H]+	233	PE P-18:0_22:5_2	[M+H]+	374	TG 18:0_18:1_20:3	[M+NH4]+
93	PC 18:1_22:5_2	[M+H]+	234	PE P-18:0_22:6_2	[M+H]+	375	TG 18:0_18:1_22:3	[M+NH4]+

94	PC 18:0_22:6	[M+H]+	235	PE P-18:1_22:6	[M+H]+	376	TG 18:0_18:1_22:4	[M+NH4]+
95	PC 18:1_22:6	[M+H]+	236	PE P-24:1_17:1	[M+H]+	377	TG 18:0_18:1_22:5	[M+NH4]+
96	PC 26:0_16:1	[M+H]+	237	PE P-24:1_18:1	[M+H]+	378	TG 18:0_18:1_22:6	[M+NH4]+
97	PC 42:2	[M+H]+	238	PE P-22:1_20:4	[M+H]+	379	TG 18:0_20:1_20:4	[M+NH4]+
98	PC 18:1_26:1	[M+H]+	239	PE P-22:1_20:5	[M+H]+	380	TG 18:0_20:1_22:4	[M+NH4]+
99	PC O-29:0	[M+H]+	240	PE P-20:1_22:5	[M+H]+	381	TG 18:0_20:1_22:5	[M+NH4]+
100	PC O-30:0	[M+H]+	241	PE P-20:0_22:6	[M+H]+	382	TG 18:0_21:1_26:1	[M+NH4]+
101	PC O-30:1	[M+H]+	242	PE P-24:1_20:4	[M+H]+	383	TG 18:1_18:1_18:1_1	[M+NH4]+
102	PC O-32:0	[M+H]+	243	PE P-24:1_20:5	[M+H]+	384	TG 18:1_18:1_18:1_2	[M+NH4]+
103	PC O-32:1	[M+H]+	244	PE P-22:1_22:5	[M+H]+	385	TG 18:1_18:1_18:1_3	[M+NH4]+
104	PC O-33:1	[M+H]+	245	PE P-22:1_22:6	[M+H]+	386	TG 18:1_18:1_18:2	[M+NH4]+
105	PC O-33:2	[M+H]+	246	PE P-24:1_22:5	[M+H]+	387	TG 18:1_18:1_19:1_1	[M+NH4]+
106	PC O-36:0	[M+H]+	247	PE P-24:1_22:6	[M+H]+	388	TG 18:1_18:1_19:1_2	[M+NH4]+
107	PC O-36:1	[M+H]+	248	PI 32:2	[M+NH4]+	389	TG 18:1_18:1_20:1	[M+NH4]+
108	PC O-36:2	[M+H]+	249	PI 34:2_1	[M+NH4]+	390	TG 18:1_18:1_20:3	[M+NH4]+
109	PC O-36:4	[M+H]+	250	PI 38:2_1	[M+NH4]+	391	TG 18:1_18:1_21:3	[M+NH4]+
110	PC O-37:10	[M+H]+	251	PI 38:6_1	[M+NH4]+	392	TG 18:1_18:1_22:4	[M+NH4]+
111	PC O-38:1	[M+H]+	252	PI 38:6_2	[M+NH4]+	393	TG 18:1_18:1_22:5_1	[M+NH4]+
112	PC O-38:4_1	[M+H]+	253	PS 18:0_16:1	[M+H]+	394	TG 18:1_18:1_22:5_2	[M+NH4]+
113	PC O-38:4_2	[M+H]+	254	PS 18:0_18:1	[M+H]+	395	TG 18:1_18:1_22:6	[M+NH4]+
114	PC O-38:5	[M+H]+	255	PS 18:1_18:1	[M+H]+	396	TG 18:1_18:1_24:6	[M+NH4]+
115	PC O-38:6_1	[M+H]+	256	SM 18:0;2O/21:0	[M+H]+	397	TG 18:1_18:1_26:1	[M+NH4]+
116	PC O-38:6_2	[M+H]+	257	SM 18:1;2O/18:0_1	[M+H]+	398	TG 18:1_18:2_22:6	[M+NH4]+
117	PC O-39:10_1	[M+H]+	258	SM 18:1;2O/18:0_2	[M+H]+	399	TG 18:1_19:1_20:1	[M+NH4]+
118	PC O-39:10_2	[M+H]+	259	SM 18:1;2O/20:1	[M+H]+	400	TG 18:1_19:1_26:1	[M+NH4]+
119	PC O-40:1_1	[M+H]+	260	SM 18:1;2O/26:0	[M+H]+	401	TG 18:1_20:1_20:1	[M+NH4]+
120	PC O-40:1_2	[M+H]+	261	SM 18:2;2O/25:0	[M+H]+	402	TG 18:1_20:1_22:4	[M+NH4]+
121	PC O-40:2	[M+H]+	262	TG 12:0_12:0_14:0	[M+NH4]+	403	TG 18:1_20:1_22:6	[M+NH4]+
122	PC O-40:3_1	[M+H]+	263	TG 12:0_14:0_14:0_1	[M+NH4]+	404	TG 18:1_20:1_26:1	[M+NH4]+
123	PC O-40:3_2	[M+H]+	264	TG 12:0_14:0_14:0_2	[M+NH4]+	405	TG 18:1_21:1_26:1	[M+NH4]+
124	PC O-40:4	[M+H]+	265	TG 12:0_14:0_14:1	[M+NH4]+	406	TG 18:1_22:1_22:5	[M+NH4]+
125	PC O-40:5_1	[M+H]+	266	TG 12:0_14:0_16:0	[M+NH4]+	407	TG 18:1_22:1_26:1	[M+NH4]+
126	PC O-40:5_2	[M+H]+	267	TG 12:0_14:0_16:1	[M+NH4]+	408	TG 18:1_24:1_20:4	[M+NH4]+
127	PC O-40:6_1	[M+H]+	268	TG 12:0_14:1_16:1	[M+NH4]+	409	TG 18:1_24:1_22:5_2	[M+NH4]+

128	PC O-40:6_2	[M+H]+	269	TG 12:0_15:0_16:0	[M+NH4]+	410	TG 18:1_24:1_24:2	[M+NH4]+
129	PC O-40:7_1	[M+H]+	270	TG 13:0_14:0_16:0	[M+NH4]+	411	TG 18:1_26:1_20:4	[M+NH4]+
130	PC O-40:7_2	[M+H]+	271	TG 13:0_16:1_18:1	[M+NH4]+	412	TG 18:1_26:1_22:4	[M+NH4]+
131	PC O-40:7_3	[M+H]+	272	TG 14:0_14:0_16:0	[M+NH4]+	413	TG 18:1_26:1_22:5	[M+NH4]+
132	PC O-41:11_2	[M+H]+	273	TG 14:0_14:1_16:1	[M+NH4]+	414	TG 18:1_26:1_24:2	[M+NH4]+
133	PC O-42:1_1	[M+H]+	274	TG 14:0_15:0_16:0_1	[M+NH4]+	415	TG 18:1_26:1_26:1	[M+NH4]+
134	PC O-42:1_2	[M+H]+	275	TG 14:0_15:0_16:0_2	[M+NH4]+	416	TG 18:2_18:2_18:3	[M+NH4]+
135	PC O-42:2	[M+H]+	276	TG 14:0_15:0_16:1_1	[M+NH4]+	417	TG 23:0_16:1_26:1	[M+NH4]+
136	PC O-42:3	[M+H]+	277	TG 14:0_15:0_16:1_2	[M+NH4]+	418	TG 26:0_18:1_18:1	[M+NH4]+
137	PC O-42:5	[M+H]+	278	TG 14:0_16:0_14:1_1	[M+NH4]+	419	TG 26:0_18:1_20:1	[M+NH4]+
138	PC O-42:6_1	[M+H]+	279	TG 14:0_16:0_14:1_2	[M+NH4]+	420	TG 26:0_18:1_24:1	[M+NH4]+
139	PC O-42:6_2	[M+H]+	280	TG 14:0_16:0_14:1_3	[M+NH4]+	421	TG 26:0_18:1_26:1	[M+NH4]+
140	PC O-43:11	[M+H]+	281	TG 14:0_16:0_14:1_4	[M+NH4]+	422	TG 27:0_18:1_18:1	[M+NH4]+
141	PC O-44:2	[M+H]+	282	TG 14:0_16:0_16:0	[M+NH4]+			

Negative ESI

Number	Metabolite name	Adduct type	Number	Metabolite name	Adduct type	Number	Metabolite name	Adduct type
1	Cer 18:0;2O/14:0	[M-H]-	121	PE O-16:0_18:1	[M-H]-	241	PE O-18:1_26:1	[M-H]-
2	Cer 18:1;2O/14:0	[M-H]-	122	PE O-18:1_16:0	[M-H]-	242	PE O-24:2_20:1	[M-H]-
3	Cer 18:0;2O/16:0	[M-H]-	123	PE 16:1_18:1	[M-H]-	243	PE O-24:2_20:2	[M-H]-
4	Cer 18:1;2O/16:0_1	[M-H]-	124	PE O-16:1_18:1	[M-H]-	244	PE O-26:3_18:1_1	[M-H]-
5	Cer 18:2;2O/16:0	[M-H]-	125	PE 16:1_18:2_1	[M-H]-	245	PE O-26:3_18:1_2	[M-H]-
6	Cer 18:0;2O/18:0	[M-H]-	126	PE 16:1_18:2_2	[M-H]-	246	PE O-24:1_20:4_1	[M-H]-
7	Cer 18:1;2O/18:0	[M-H]-	127	PE O-16:1_18:2_1	[M-H]-	247	PE O-24:1_20:4_2	[M-H]-
8	Cer 18:1;2O/20:0	[M-H]-	128	PE O-16:1_18:2_2	[M-H]-	248	PE O-24:2_20:3_1	[M-H]-
9	Cer 18:0;2O/22:0	[M-H]-	129	PE O-18:2_16:1	[M-H]-	249	PE O-24:2_20:3_2	[M-H]-
10	Cer 18:1;2O/22:0	[M-H]-	130	PE O-14:0_20:4	[M-H]-	250	PE O-22:2_22:4	[M-H]-
11	Cer 18:1;2O/22:1	[M-H]-	131	PE O-16:1_18:3	[M-H]-	251	PE O-24:2_20:4	[M-H]-
12	Cer 18:0;2O/23:0	[M-H]-	132	PE O-18:3_16:1_1	[M-H]-	252	PE O-22:1_22:6	[M-H]-
13	Cer 18:1;2O/23:0	[M-H]-	133	PE O-18:3_16:1_2	[M-H]-	253	PE O-22:2_22:5	[M-H]-
14	Cer 17:1;2O/24:1	[M-H]-	134	PE O-14:1_20:4_1	[M-H]-	254	PE O-24:2_20:5	[M-H]-
15	Cer 18:0;2O/24:0	[M-H]-	135	PE O-14:1_20:4_2	[M-H]-	255	PE O-22:2_22:6	[M-H]-
16	Cer 18:0;2O/24:1	[M-H]-	136	PE O-14:1_20:5	[M-H]-	256	PE O-26:2_20:1	[M-H]-
17	Cer 18:1;2O/24:0	[M-H]-	137	PE 17:0_18:1_1	[M-H]-	257	PE O-24:2_22:4	[M-H]-
18	Cer 18:1;2O/24:1	[M-H]-	138	PE 17:0_18:1_2	[M-H]-	258	PE O-26:2_20:4	[M-H]-
19	Cer 18:2;2O/24:1	[M-H]-	139	PE 17:1_18:1	[M-H]-	259	PE O-24:2_22:5	[M-H]-
20	Cer 18:1;2O/25:0	[M-H]-	140	PE O-17:1_18:1	[M-H]-	260	PE O-24:2_22:6	[M-H]-
21	Cer 18:0;2O/26:1	[M-H]-	141	PE O-18:2_17:0	[M-H]-	261	PE O-26:2_22:6	[M-H]-
22	Cer 18:1;2O/26:0	[M-H]-	142	PE O-16:1_19:2	[M-H]-	262	PG 16:0_16:0	[M-H]-
23	Cer 18:1;2O/26:1	[M-H]-	143	PE O-18:2_17:1	[M-H]-	263	PG 14:0_18:1	[M-H]-
24	CL 14:1_16:1_16:1_18:1	[M-2H]2-	144	PE 15:0_20:4	[M-H]-	264	PG 16:1_16:1	[M-H]-
25	CL 14:0_16:1_18:1_18:1	[M-2H]2-	145	PE O-16:1_19:3	[M-H]-	265	PG 16:0_18:1	[M-H]-
26	CL 16:1_16:1_16:1_18:1	[M-2H]2-	146	PE 18:0_18:1	[M-H]-	266	PG 18:0_18:1	[M-H]-
27	CL 16:1_16:1_16:1_18:2	[M-2H]2-	147	PE O-18:0_18:1_2	[M-H]-	267	PG 18:1_18:1	[M-H]-
28	CL	[M-2H]2-	148	PE O-18:0_18:1_4	[M-H]-	268	PG 18:1_18:2	[M-H]-

	16:0_16:0_18:1_18:1							
29	CL 16:0_16:1_18:1_18:1	[M-2H]2-	149	PE O-20:1_16:0	[M-H]-	269	PG 18:1_20:1	[M-H]-
30	CL 16:1_16:1_18:1_18:1	[M-2H]2-	150	PE 18:1_18:1	[M-H]-	270	PG 18:1_20:2	[M-H]-
31	CL 16:1_16:1_18:1_18:2	[M-2H]2-	151	PE O-18:1_18:1	[M-H]-	271	PI 14:1_16:1	[M-H]-
32	CL 16:1_18:1_18:1_18:1	[M-2H]2-	152	PE 16:0_20:3	[M-H]-	272	PI 16:0_16:0	[M-H]-
33	CL 16:1_18:1_18:1_18:2	[M-2H]2-	153	PE 18:1_18:2_2	[M-H]-	273	PI 16:0_16:1	[M-H]-
34	CL 18:1_18:1_18:2_18:2	[M-2H]2-	154	PE O-18:1_18:2	[M-H]-	274	PI O-16:0_16:1	[M-H]-
35	DMPE 14:0_14:0	[M-H]-	155	PE O-18:2_18:1	[M-H]-	275	PI 16:1_16:1	[M-H]-
36	DMPE 14:0_16:0	[M-H]-	156	PE 16:0_20:4	[M-H]-	276	PI 16:0_18:1	[M-H]-
37	DMPE 14:0_16:1	[M-H]-	157	PE 16:1_20:3	[M-H]-	277	PI 16:0_18:2	[M-H]-
38	DMPE 16:1_16:1	[M-H]-	158	PE O-16:0_20:4	[M-H]-	278	PI 16:1_18:1	[M-H]-
39	Hex2Cer 34:1;2O	[M+CH3COO]-	159	PE O-16:1_20:3_1	[M-H]-	279	PI 18:0_18:1_1	[M-H]-
40	Hex2Cer 40:1;2O	[M+CH3COO]-	160	PE O-16:1_20:3_2	[M-H]-	280	PI 18:0_18:1_2	[M-H]-
41	Hex2Cer 42:1;2O	[M+CH3COO]-	161	PE 16:0_20:5	[M-H]-	281	PI O-16:0_20:1	[M-H]-
42	Hex2Cer 42:2;2O	[M+CH3COO]-	162	PE O-16:1_20:4_1	[M-H]-	282	PI 18:0_18:2_1	[M-H]-
43	Hex2Cer 44:2;2O	[M+CH3COO]-	163	PE O-16:1_20:4_2	[M-H]-	283	PI 18:0_18:2_2	[M-H]-
44	Hex3Cer 34:1;2O	[M+CH3COO]-	164	PE O-14:1_22:5	[M-H]-	284	PI 18:1_18:1	[M-H]-
45	Hex3Cer 42:1;2O	[M+CH3COO]-	165	PE O-16:1_20:5	[M-H]-	285	PI O-18:1_18:1	[M-H]-
46	Hex3Cer 42:2;2O	[M+CH3COO]-	166	PE 18:1_19:1	[M-H]-	286	PI 16:0_20:3	[M-H]-
47	LPC 14:0	[M+CH3COO]-	167	PE O-17:1_20:1	[M-H]-	287	PI 18:1_18:2	[M-H]-
48	LPC 16:0	[M+CH3COO]-	168	PE O-19:1_18:1	[M-H]-	288	PI 16:0_20:4	[M-H]-
49	LPC 16:1	[M+CH3COO]-	169	PE O-16:1_21:2	[M-H]-	289	PI O-16:0_20:4	[M-H]-
50	LPC 18:0	[M+CH3COO]-	170	PE O-18:1_19:2	[M-H]-	290	PI 16:0_20:5	[M-H]-
51	LPC 18:1	[M+CH3COO]-	171	PE O-17:1_20:3	[M-H]-	291	PI 16:1_20:4	[M-H]-
52	LPC 20:0	[M+CH3COO]-	172	PE O-18:1_19:3	[M-H]-	292	PI 18:1_19:1	[M-H]-
53	LPC 20:1	[M+CH3COO]-	173	PE O-17:1_20:4_1	[M-H]-	293	PI 18:0_20:2_1	[M-H]-
54	LPC 22:1	[M+CH3COO]-	174	PE O-17:1_20:4_2	[M-H]-	294	PI 18:0_20:2_2	[M-H]-
55	LPC 24:1	[M+CH3COO]-	175	PE O-17:1_20:5	[M-H]-	295	PI 18:1_20:1	[M-H]-

56	LPE 16:0	[M-H]-	176	PE 18:0_20:1	[M-H]-	296	PI 18:0_20:3_1	[M-H]-
57	LPE 16:1	[M-H]-	177	PE O-22:1_16:0	[M-H]-	297	PI 18:0_20:3_2	[M-H]-
58	LPE 17:1	[M-H]-	178	PE 18:0_20:2	[M-H]-	298	PI 18:1_20:2	[M-H]-
59	LPE 18:0	[M-H]-	179	PE 18:1_20:1	[M-H]-	299	PI 16:0_22:4	[M-H]-
60	LPE 18:1	[M-H]-	180	PE 18:0_20:3_1	[M-H]-	300	PI 18:0_20:4	[M-H]-
61	LPE 18:2	[M-H]-	181	PE 18:0_20:3_2	[M-H]-	301	PI 18:1_20:3	[M-H]-
62	LPE 20:1	[M-H]-	182	PE O-18:1_20:2	[M-H]-	302	PI O-18:0_20:4	[M-H]-
63	LPE 20:3	[M-H]-	183	PE 16:0_22:4	[M-H]-	303	PI 16:0_22:5	[M-H]-
64	LPE 20:4	[M-H]-	184	PE 18:0_20:4	[M-H]-	304	PI 18:1_20:4	[M-H]-
65	LPE 22:0	[M-H]-	185	PE 18:1_20:3	[M-H]-	305	PI O-16:0_22:5	[M-H]-
66	LPE 22:5	[M-H]-	186	PE O-18:0_20:4_1	[M-H]-	306	PI 16:0_22:6	[M-H]-
67	LPE 22:6	[M-H]-	187	PE O-18:0_20:4_2	[M-H]-	307	PI 18:2_20:4	[M-H]-
68	LPE 24:0	[M-H]-	188	PE O-18:1_20:3_1	[M-H]-	308	PI O-16:0_22:6	[M-H]-
69	LPE 24:1	[M-H]-	189	PE O-18:1_20:3_2	[M-H]-	309	PI 19:0_20:4	[M-H]-
70	LPE 26:0	[M-H]-	190	PE 18:0_20:5	[M-H]-	310	PI 18:0_22:2	[M-H]-
71	LPE 26:1	[M-H]-	191	PE 18:1_20:4	[M-H]-	311	PI 18:1_22:2	[M-H]-
72	LPG 18:1	[M-H]-	192	PE O-16:1_22:4	[M-H]-	312	PI 18:0_22:5_1	[M-H]-
73	LPG 22:6	[M-H]-	193	PE O-18:1_20:4	[M-H]-	313	PI 18:0_22:5_2	[M-H]-
74	LPG O-17:1	[M-H]-	194	PE 16:0_22:6	[M-H]-	314	PI O-18:0_22:5	[M-H]-
75	LPI 18:0	[M-H]-	195	PE O-18:1_20:5	[M-H]-	315	PI 18:0_22:6	[M-H]-
76	LPI 18:1	[M-H]-	196	PE O-18:2_20:4	[M-H]-	316	PI 18:1_22:5_1	[M-H]-
77	LPI 20:4	[M-H]-	197	PE O-16:1_22:6	[M-H]-	317	PI 18:1_22:5_2	[M-H]-
78	LPS 16:1	[M-H]-	198	PE O-18:2_20:5	[M-H]-	318	PI O-18:0_22:6	[M-H]-
79	LPS 18:1	[M-H]-	199	PE O-17:1_22:4	[M-H]-	319	PI O-18:1_22:5	[M-H]-
80	MMPE 16:0_16:1	[M-H]-	200	PE O-19:1_20:4	[M-H]-	320	PI 18:1_22:6	[M-H]-
81	PA 18:0_16:1	[M-H]-	201	PE O-17:1_22:5	[M-H]-	321	PI O-18:1_22:6	[M-H]-
82	PC O-16:0_14:0	[M+CH3COO]-	202	PE O-24:1_16:0	[M-H]-	322	PMeOH 14:0_16:1	[M-H]-
83	PC O-16:0_16:0	[M+CH3COO]-	203	PE O-24:2_16:0	[M-H]-	323	PMeOH 16:0_16:1	[M-H]-
84	PC O-18:1_16:0	[M+CH3COO]-	204	PE O-22:2_18:1	[M-H]-	324	PMeOH 16:1_16:1	[M-H]-
85	PC O-18:1_16:1	[M+CH3COO]-	205	PE 18:0_22:4	[M-H]-	325	PMeOH 16:1_18:1	[M-H]-
86	PC O-18:1_18:1	[M+CH3COO]-	206	PE 20:0_20:4	[M-H]-	326	PS 16:0_16:1_2	[M-H]-
87	PC O-18:2_18:1	[M+CH3COO]-	207	PE O-20:1_20:3_1	[M-H]-	327	PS 17:0_16:1	[M-H]-
88	PC O-16:0_20:4	[M+CH3COO]-	208	PE O-20:1_20:3_2	[M-H]-	328	PS 16:0_18:1	[M-H]-
89	PC O-16:1_20:4	[M+CH3COO]-	209	PE 18:0_22:5	[M-H]-	329	PS 18:0_16:1_1	[M-H]-

90	PC O-16:0_22:6	[M+CH3COO]-	210	PE O-18:0_22:5	[M-H]-	330	PS 18:0_16:1_2	[M-H]-
91	PC O-18:2_20:4	[M+CH3COO]-	211	PE O-18:1_22:4_1	[M-H]-	331	PS 16:1_18:1_1	[M-H]-
92	PC O-24:0_16:0	[M+CH3COO]-	212	PE O-18:1_22:4_2	[M-H]-	332	PS 16:1_18:1_3	[M-H]-
93	PC O-24:1_16:0	[M+CH3COO]-	213	PE O-20:1_20:4	[M-H]-	333	PS 17:0_18:1_1	[M-H]-
94	PC O-24:1_16:1	[M+CH3COO]-	214	PE 18:0_22:6	[M-H]-	334	PS 18:0_18:1_1	[M-H]-
95	PC O-24:0_18:1	[M+CH3COO]-	215	PE O-20:1_20:5	[M-H]-	335	PS 18:0_18:1_3	[M-H]-
96	PC O-24:1_18:1	[M+CH3COO]-	216	PE 18:1_22:6	[M-H]-	336	PS 18:1_18:1_1	[M-H]-
97	PC O-24:1_18:2	[M+CH3COO]-	217	PE O-18:1_22:6	[M-H]-	337	PS 18:1_18:1_2	[M-H]-
98	PC O-26:1_18:1	[M+CH3COO]-	218	PE O-18:2_22:5_1	[M-H]-	338	PS 18:1_18:1_3	[M-H]-
99	PE 14:0_14:0	[M-H]-	219	PE O-18:2_22:5_2	[M-H]-	339	PS 18:1_18:2_1	[M-H]-
100	PE 14:0_16:0	[M-H]-	220	PE O-18:3_22:6	[M-H]-	340	PS 18:1_18:2_2	[M-H]-
101	PE 14:0_16:1	[M-H]-	221	PE O-21:1_20:1	[M-H]-	341	PS 18:0_20:3_1	[M-H]-
102	PE O-16:0_14:1	[M-H]-	222	PE O-24:0_18:1	[M-H]-	342	PS 18:0_20:3_2	[M-H]-
103	PE O-16:1_14:0	[M-H]-	223	PE 18:1_24:1	[M-H]-	343	PS 18:0_20:4_1	[M-H]-
104	PE O-16:1_14:1	[M-H]-	224	PE O-24:1_18:1_1	[M-H]-	344	PS 18:0_20:4_2	[M-H]-
105	PE O-16:0_16:0	[M-H]-	225	PE O-24:1_18:1_2	[M-H]-	345	PS 18:1_20:4	[M-H]-
106	PE 16:0_16:1	[M-H]-	226	PE O-26:2_16:0	[M-H]-	346	PS 22:0_18:1_1	[M-H]-
107	PE O-16:0_16:1	[M-H]-	227	PE O-24:2_18:1	[M-H]-	347	PS 22:0_18:1_2	[M-H]-
108	PE O-16:1_16:0	[M-H]-	228	PE 22:0_20:4	[M-H]-	348	PS 22:0_18:1_3	[M-H]-
109	PE 16:1_16:1	[M-H]-	229	PE O-24:2_18:2	[M-H]-	349	PS 18:1_22:1_1	[M-H]-
110	PE O-16:1_16:1	[M-H]-	230	PE O-22:1_20:4	[M-H]-	350	PS 18:1_22:1_2	[M-H]-
111	PE O-14:1_18:2	[M-H]-	231	PE O-22:2_20:3_1	[M-H]-	351	PS 18:0_22:4	[M-H]-
112	PE O-18:2_14:1	[M-H]-	232	PE O-22:2_20:3_2	[M-H]-	352	PS 18:0_22:5_1	[M-H]-
113	PE 16:0_17:1	[M-H]-	233	PE O-18:2_24:4	[M-H]-	353	PS 18:0_22:5_2	[M-H]-
114	PE O-16:1_17:0	[M-H]-	234	PE O-22:2_20:4	[M-H]-	354	PS 18:0_22:5_3	[M-H]-
115	PE 16:1_17:1	[M-H]-	235	PE 20:1_22:6	[M-H]-	355	PS 18:0_22:6_1	[M-H]-
116	PE O-16:1_17:1	[M-H]-	236	PE O-20:1_22:6	[M-H]-	356	PS 18:0_22:6_2	[M-H]-
117	PE O-18:2_15:0	[M-H]-	237	PE O-20:2_22:5	[M-H]-	357	PS 18:1_22:6	[M-H]-
118	PE O-13:1_20:4	[M-H]-	238	PE O-22:2_20:5	[M-H]-	358	PS 18:1_24:1_1	[M-H]-
119	PE 16:0_18:0	[M-H]-	239	PE O-20:2_22:6	[M-H]-	359	PS 18:1_24:1_2	[M-H]-
120	PE 16:0_18:1	[M-H]-	240	PE 18:1_26:1	[M-H]-			

Table S5. Mass peaks to pathways analysis of positive untargeted metabolomics data in acute model (0 versus 80 μg/mL): top 16 pathways.

Name of pathway	Total features	Hits	Significant hits	P-value (combined)
Porphyrin and chlorophyll metabolism	27	18	7	0.012
Biosynthesis of unsaturated fatty acids	34	6	3	0.029
Mannose type O-glycan biosynthesis	16	6	2	0.070
Terpenoid backbone biosynthesis	15	7	3	0.076
Arachidonic acid metabolism	35	26	6	0.090
Glycosylphosphatidylinositol (GPI)-anchor biosynthesis	11	5	1	0.097
Sphingolipid metabolism	9	8	3	0.100
Amino sugar and nucleotide sugar metabolism	35	29	7	0.114
Steroid hormone biosynthesis	85	64	14	0.149
Primary bile acid biosynthesis	46	37	9	0.176
Propanoate metabolism	19	7	3	0.182
Thiamine metabolism	5	2	1	0.219
N-Glycan biosynthesis	38	8	2	0.225
Glycosphingolipid biosynthesis - globo and isoglobo series	15	9	4	0.247
Folate biosynthesis	24	17	5	0.248
Fatty acid biosynthesis	10	6	1	0.260

Table S6. Mass peaks to pathways analysis of positive untargeted metabolomics data in acute model (0 versus 80 μg/mL) with selected *m/z* features through the Jonckheere-Terpstra test: top 16 pathways and excluded pathways from Table S1.

Name of pathway	Total features	Hits	Significant hits	P-value (combined)
Porphyrin and chlorophyll metabolism	27	6	6	0.052
Arachidonic acid metabolism	35	12	5	0.152
Steroid hormone biosynthesis	85	15	9	0.162
Riboflavin metabolism	4	2	2	0.209
Sphingolipid metabolism	9	4	3	0.276
Terpenoid backbone biosynthesis	15	3	3	0.295
Biosynthesis of unsaturated fatty acids	34	2	2	0.303
Galactose metabolism	27	3	1	0.327
Pyruvate metabolism	19	1	1	0.368
Thiamine metabolism	5	1	1	0.368
Fatty acid biosynthesis	10	1	1	0.398
Starch and sucrose metabolism	13	1	1	0.398
Glycosylphosphatidylinositol (GPI)-anchor biosynthesis	11	1	1	0.398
Tryptophan metabolism	41	3	3	0.436
Purine metabolism	65	7	4	0.438
Valine, leucine and isoleucine degradation	35	6	3	0.448
Amino sugar and nucleotide sugar metabolism	35	3	1	0.490
Folate biosynthesis	24	4	3	0.499
Mannose type O-glycan biosynthesis	16	4	2	0.572
Propanoate metabolism	19	3	3	0.761
Primary bile acid biosynthesis	46	12	7	0.803
N-Glycan biosynthesis	38	1	1	0.864
Glycosphingolipid biosynthesis - globo and isoglobo series	15	3	2	0.928

Table S7. Matched metabolite list from two major pathways: ‘steroid hormone biosynthesis’ and 'arachidonic acid metabolism'.

Detected MS	Detected RT	Adduct	MS difference	Name
Steroid hormone biosynthesis				
309.1528244	1.66	M+Na-2H[-]	0.0055327	Estriol; 2-Hydroxyestradiol
323.1682221	1.65	M+Na-2H[-]	0.005280336	11beta-Hydroxyandrost-4-ene-3,17-dione; 2-Methoxy-17beta-estradiol; 19-Hydroxyandrostenedione; 19-Oxotestosterone; 16alpha-Hydroxyandrost-4-ene-3,17-dione
325.1837363	1.61	M+Na-2H[-]	0.005144472	16alpha-Hydroxydehydroepiandrosterone; 19-Hydroxytestosterone; 11-Dehydrocorticosterone; 11beta-Hydroxytestosterone; 7alpha-Hydroxydehydroepiandrosterone
327.184569	1.61	M+Cl37[-]	0.005911204	Androstenediol; Etiocholanolone; Androsterone; Dihydrotestosterone; 5beta-Dihydrotestosterone
341.1793854	1.12	M-H2O-H[-]	0.003587861	Aldosterone; Cortisone
342.2007354	1.60	M+ACN-H[-]	0.006727831	11beta-Hydroxyandrost-4-ene-3,17-dione; 2-Methoxy-17beta-estradiol; 19-Hydroxyandrostenedione; 19-Oxotestosterone; 16alpha-Hydroxyandrost-4-ene-3,17-dione
351.1987698	1.62	M+Na-2H[-]	0.004527908	11-Deoxycorticosterone; 17alpha-Hydroxyprogesterone
353.2157519	1.58	M+Na-2H[-]	0.005859944	21-Hydroxypregnenolone; 17alpha-Hydroxypregnenolone; 5alpha-Dihydrodeoxycorticosterone; 7alpha-Hydroxypregnenolone; 17alpha,20alpha-Dihydroxypregn-4-en-3-one
369.209161	1.10	M+Na-2H[-]	0.004354422	17alpha,21-Dihydroxypregnenolone; 11beta,21-Dihydroxy-5beta-pregnane-3,20-dione; 3alpha,21-Dihydroxy-5beta-pregnane-11,20-dione
370.2316755	1.55	M+ACN-H[-]	0.007087859	11-Deoxycorticosterone; 17alpha-Hydroxyprogesterone
371.0915447	5.47	M+Na-2H[-]	0.00199687	Estrone 3-sulfate;
381.1751086	1.09	M+Na-2H[-]	0.006687528	Aldosterone; Cortisone
381.1898467	5.31	M+Cl[-]	0.006537252	Corticosterone; 21-Hydroxy-5beta-pregnane-3,11,20-trione; 11-Deoxycortisol; 21-Deoxycortisol
381.2323024	1.39	M-H+O[-]	0.004044669	Tetrahydrocortisol;
390.2678775	2.88	M+ACN-H[-]	0.002899391	Tetrahydrocorticosterone;
459.2051908	1.59	M-H2O-H[-]	0.002784581	2-Methoxy-estradiol-17beta 3-glucuronide;
465.3032775	1.39	M-H[-]	0.001126683	Cholesterol sulfate;
481.2993456	1.57	M-H+O[-]	3.14E-05	Cholesterol sulfate;

Arachidonic acid metabolism				
303.2321205	1.09	M-H[-]	0.000833301	Arachidonic acid
381.2323024	1.39	M+HCOO[-]	0.004597888	15-Hydroxy-11,12-epoxyeicosatrienoic acid; 11-Hydroxy-14,15-epoxyeicosatrienoic acid; 15-Hydroperoxyeicosatetraenoic acid; 5(S)-Hydroperoxy-6-trans-8,11,14-cis-eicosatetraenoic acid; Leukotriene B4; (5Z,9E,11Z,14Z)-(8S)-8-Hydroperoxyeicosa-5,9,11,14-tetraenoic acid; (5Z,8Z,10E,14Z)-(12R)-12-Hydroperoxyeicosa-5,8,10,14-tetraenoic acid; (5Z,8Z,10E,14Z)-(12S)-12-Hydroperoxyicosa-5,8,10,14-tetraenoic acid
339.1999486	1.59	M+Na-2H[-]	0.005706708	Leukotriene A4
369.2314619	1.56	M-H+O[-]	0.003204169	11,12,15-Trihydroxyicosatrienoic acid; 11,14,15-Trihydroxyicosatrienoic acid; 11-epi-Prostaglandin F2alpha; Prostaglandin F2alpha