Electronic Supplementary Information (ESI) for *Analytical Methods*

Optimization of the sample preparation method for adherent cell metabolomics based on ultra-performance liquid chromatography coupled to mass spectrometry

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Fig. S1 Relative standard deviations of 17 metabolites among QC samples.

Fig. S2 Comparison of the extraction abundance between cold methanol and liquid nitrogen. Student's t tests (Unpaired) were performed between groups. Asterisk (*) denotes statistical significance: p-value (*) <0.05, (**) < 0.01. Fold-change values were calculated.

Fig. S3 Comparison of the extraction abundance between sonication and freezing/thawing. Student's t tests (Unpaired) were performed between groups. Asterisk (*) denotes statistical significance: p-value (*) <0.05, (**) < 0.01. Fold-change values were calculated.

Fig. S4 PCA score plot of cell samples collected by trypsinization and scraping.

Table S1 MRM conditions for metabolites for stability evaluation.

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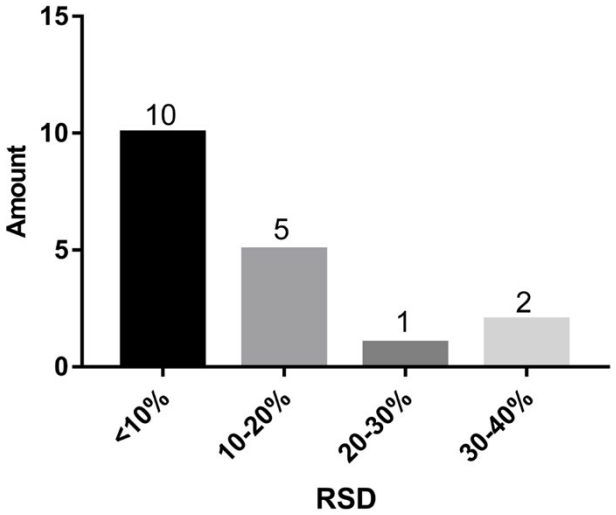

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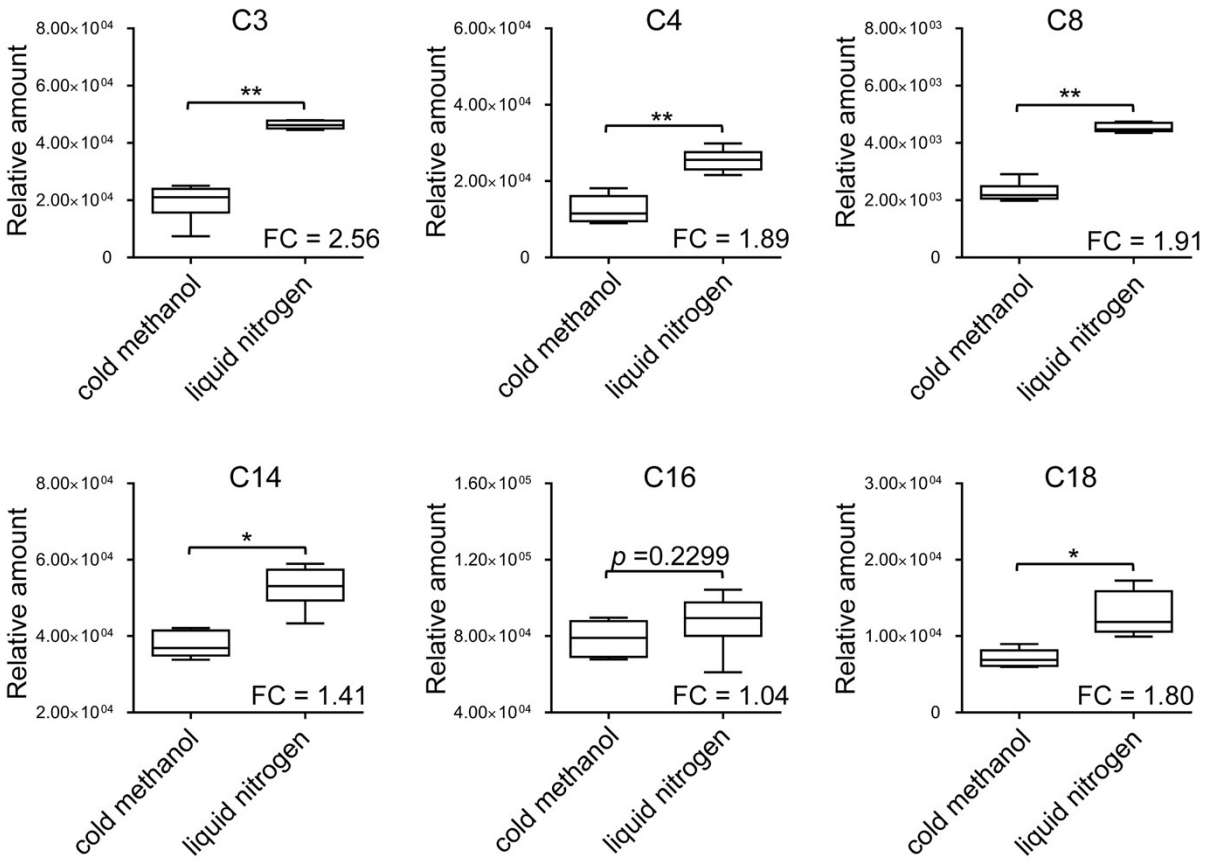

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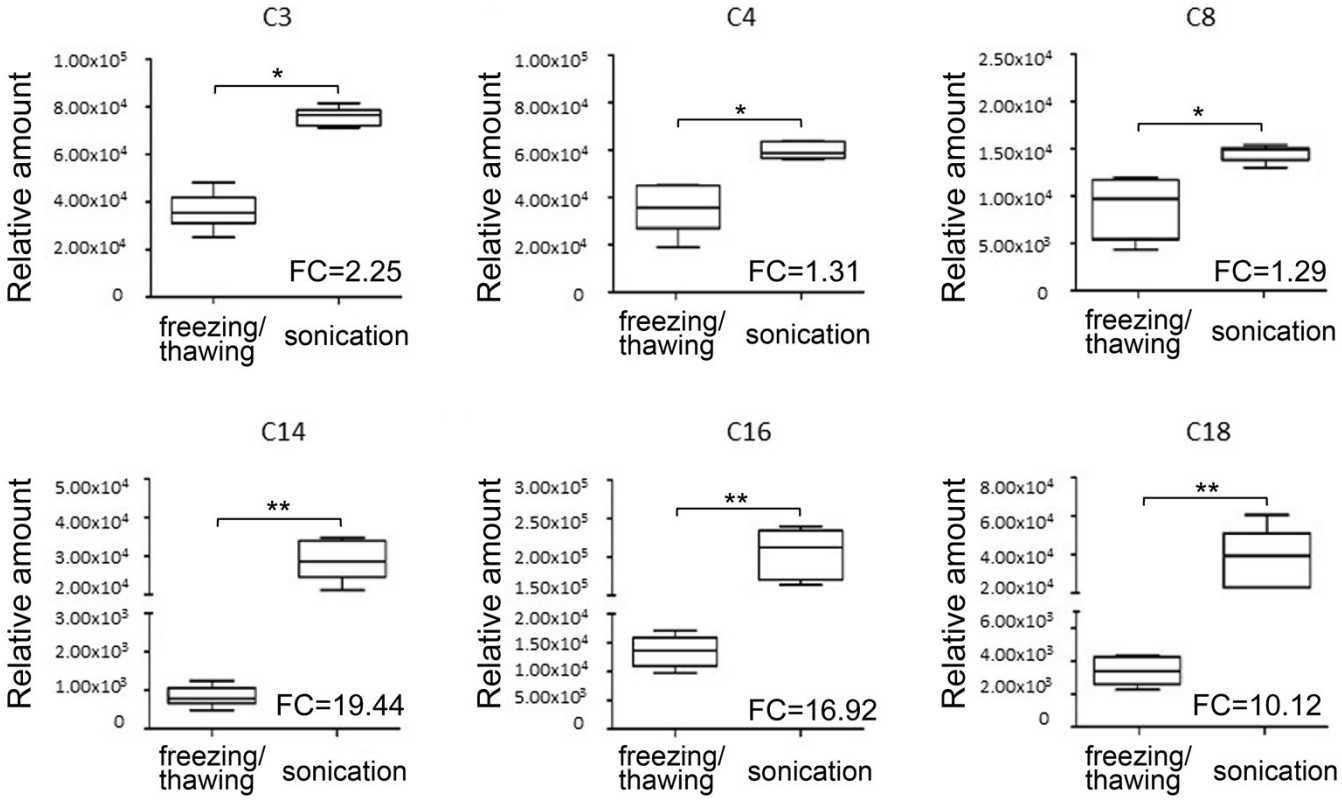

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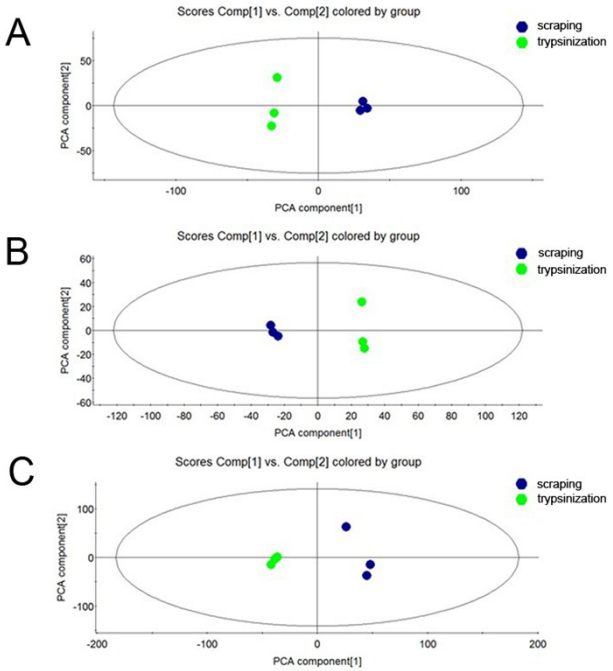

Fig. S4 PCA score plot of cell samples collected by trypsinization and scraping.

Table S1 MRM conditions for metabolites for stability evaluation.

Analyte	Precursor ion (*m/z*)	Product ion (*m/z*)	Dwell time (Secs)	Isolation width (Da)	CV (V)	CE (eV)
L-Serine	106	64	0.2	1	20	10
L-Lysine	147.1	84.1	0.2	1	20	10
L-Methionine	150.1	104	0.2	1	20	10
L-Tryptophan	205.1	188.1	0.2	1	20	10
Propionyl-L-carnitine	218.1	85.1	0.2	1	20	15
Butyryl-L-carnitine	232.1	85.1	0.2	1	20	15
Hexanoyl-L-carnitine	260.2	85.1	0.2	1	20	15
Tetradecanoyl-L-carnitine	372.3	85.1	0.2	1	20	15
Hexadecanoyl-L-carnitine	400.3	85.1	0.2	1	20	15
Octadecanoyl-L-carnitine	428.4	85.1	0.2	1	20	15
LysoPC(16:0)	496.3	184.1	0.2	1	20	20
LysoPC(O-16:0)	482.3	184.1	0.2	1	20	20
LysoPC(17:0)	510.4	184.1	0.2	1	20	20
LysoPC(18:0)	524.4	184.1	0.2	1	20	20
LysoPC(18:1)	522.4	184.1	0.2	1	20	20
LysoPC(18:2)	520.4	184.1	0.2	1	20	20
LysoPC(P-18:0)	508.4	184.1	0.2	1	20	20

Text S1 Experimental procedures for cell preparation with the candidate methods for each step.

Methods for cell quenching

The evaluation of quenching methods was conducted on eight duplicates of cells (four for each method) that the duplicates have the same number of cells. For quenching by liquid nitrogen, after the complete removal of the washing PBS, 500 ml liquid nitrogen was added into each dish for quenching. After liquid nitrogen was completely volatilized, the cells were further gently scraped with 300 μL of pre-cooled 75% methanol, which was then combined with another 100 μL of pre-cooled 75% methanol for washing the dishes. For quenching by cold methanol, after the complete removal of the washing PBS, 200 μL of pre-cooled methanol was added into each dish. The cells were gently gathered and combined with another 100 μL of pre-cooled 75% methanol for washing the dishes. And then add 100 μL pre-cooled deionized water.

For cell suspensions obtained by both methods, the following steps were exactly the same. Cell cracking was performed upon the cell suspensions by sonication for 2 min with 5 s/5 s intervals in an ice-water bath. Afterwards, the homogenates were transferred into new tubes and centrifuged at 12000 *g* for 15 min at 4°C, and 300 μL of the supernatant was dried by rotating-vacuum evaporation. The residuals were stored at in -80°C until analysis.

Methods for cell harvesting

For scraping, after the complete removal of the washing PBS, 500 μL of liquid nitrogen was added into each dish for quenching. The cells were further harvested via scraping with 120 μL of pre-cooled 75% methanol, which was then combined with another 120 μL of 75% methanol for washing the dishes, giving the cell suspension for further cracking. For trypsinization, after removing the washing PBS, 500 μL of pre-warmed trypsin was added to each dish, which was further discarded after being evenly coated. After incubation at 37°C for 2 min, the digestion was stopped by adding 500 μL of culture medium, and the cells were washed down and obtained via centrifugation at 800 *g* for 15 min. The medium was completely removed, and the cells were quenched by adding 500 μL of liquid nitrogen into the tubes. After the liquid nitrogen completely volatilized, 240 μL of pre-cooled 75% methanol was added into the frozen cells for further cracking.

For cell suspensions obtained by both methods, the following steps were exactly the same. Cell cracking was performed upon the cell suspension by sonication for 2 min with 5 s/5 s intervals in an ice-water bath. Two hundred microliters of the homogenates after sonication was transferred into new tubes and centrifuged at 12000 *g* for 15 min at 4°C. One hundred eighty microliters of the supernatants was isolated and dried by rotating-vacuum evaporation. The residues were stored at -80°C until analysis.

Methods for cell cracking

During the assessment of cracking methods, the cells were harvested by trypsinization as presented in the cell harvesting section. In detail, after the complete removal of the washing PBS, each dish of cells was digested by 500 μL of pre-warmed trypsin, which was further discarded after being evenly coated. After 2 min of incubation at 37°C, the digestion was stopped by adding 500 μL of culture medium, and the cells were washed down and collected by centrifugation at 800 x g for 15 min. The medium was completely removed, and the cells were quenched

by adding 500 μL of liquid nitrogen into the tubes.

For cracking by sonication, 240 μL of pre-cooled 75% methanol was added into the frozen cells after the liquid nitrogen completely volatilized. Then, the suspensions were kept in an ice-water bath and cracked with probe sonication for 2 min with 5 s/5 s intervals to give the cracked homogenates. For cracking with the alternative freezing/thawing method, 60 μL of pre-cooled deionized water was added into the cell residues, which were gently oscillated for 10 s. Then, the cell suspensions were further placed at -80°C and 37°C by alternating 2 min/2 min intervals five times to make the cells completely crack during the alternate freezing/thawing. Next, 180 μL of pre-cooled methanol was added into the suspension, followed by 10 s of vortexing, giving homogenates with theoretically the same composition and concentration of metabolites as those obtained by the sonication method.

Afterwards, the homogenates obtained by both methods were centrifuged at 12000 *g* for 15 min at 4°C, and 180 μL of the supernatant was dried by rotating-vacuum evaporation. The residuals were stored at in -80°C until analysis.

Methods for cell leveling

The cell duplicates for leveling were harvested by trypsinization and cracked by sonication, as presented above. In detail, after complete removal of the washing PBS, 500 μL of pre-warmed trypsin was added to each dish of cells for digestion, which was further discarded after being evenly coated. After 2 min of incubation at 37°C, the digestion was stopped by adding 500 μL of culture medium, and the cells were collected by centrifugation at 800 *g* for 15 min. Due to the very different operational principles, the work flows for leveling by cell counting and the other two methods (TP and GAPDH) were also different at mainly the working order among leveling, quenching and cracking.

For leveling by counting, after complete removal of the medium, 150 μL, 170 μL and 190 μL of PBS were added into three duplicates of cells to artificially obtain cells with presupposed densities. Next, 5 μL of the cell suspension was removed and diluted with 500 μL of PBS (100-fold dilution) for manual counting. The duplicates were further leveled based on the one with the smallest cell density. After leveling, the PBS was also completely removed by centrifugation at 800 *g* for 15 min. The cells were further quenched by adding 500 μL of liquid nitrogen. Next, 240 μL of pre-cooled PBS was added to the cell residues, and the cells were cracked by sonication in an ice-water bath for 2 min with 5 s/5 s intervals. Finally, 200 μL of the homogenates was isolated, and 600 μL of pre-cooled methanol was added for protein precipitation.

For cell leveling by TP and GAPDH, the cell duplicates after the removal of residual medium were first quenched via the addition of 500 μL of liquid nitrogen. Then, 150 μL, 170 μL and 190 μL of PBS was added to the cells to make the cell duplicates possess the same presupposed cell densities as those in the counting method. Next, for the TP method, the cell suspensions were cracked by sonication operated as described above. Then, 5 μL of the supernatant was taken out and diluted with 50 μL (10-fold) of PBS for the determination of the TP concentrations by using a BCA kit. The absorbance of each sample was obtained at 562 nm using a plate reader (Manufactory), and the TP concentrations were calculated based on the standard curve, which was obtained according to the guidelines of the manufacturer. For leveling with GAPDH, the cell suspensions were also cracked with sonication performed in the same conditions. Differently, 20 μL of the supernatant after cracking was taken out and 2.5-fold diluted with PBS to prepare for the measurement by using a Human GAPDH Elisa kit. After leveling by both methods, all of the leveled supernatants were diluted to 200 μL with pre-cooled PBS, followed by the addition of 600 μL of pre-cooled methanol for protein precipitation.

For protein precipitation, all of the homogenates obtained by the three methods were first mixed via vortex mixing for 1 min and placed in an ice-water bath for 10 min, followed by

centrifugation at 12000 *g* at 4°C for 15 min. Next, 750 μL of the supernatant was isolated and dried by rotating-vacuum evaporation. The residues were stored at in -80°C until analysis.

Methods for metabolite extraction

For extraction in which methanol was solely used, the cells were harvested via trypsinization and cracked by using sonication. In detail, after completely removing the washing PBS, each duplicate of cells was digested by 500 μL of pre-warmed trypsin, which was further discarded after being evenly coated. After 2 min of incubation at 37°C, the digestion reaction was ceased by adding 500 μL of culture medium, and the cells were washed down and collected by centrifugation at 800 *g* for 15 min. Then, the medium was completely removed, and the cells were quenched by adding 500 μL of liquid nitrogen into the tubes. Next, 240 μL of pre-cooled 75% methanol was added, and the cell suspensions were cracked with sonication in an ice-water bath for 2 min by 5 s/5 s intervals. Two hundred microliters of the homogenates was isolated and centrifuged at 12000 *g* and 4°C for 15 min. One hundred eighty microliters of the supernatant was taken out and dried by using rotating-vacuum evaporation, and the residues were stored at -80°C until analysis.

For the method with the additional use of chloroform, the procedures from cell culture to cracking were exactly the same as the method of using solely methanol. After cell cracking, 200 μL of the homogenates was isolated, and 500 μL of chloroform was added, followed by oscillation at 1000 rpm and 25°C for 30 min. Next, the mixtures were stratified by adding 125 μL of deionized water and oscillated at 1000 rpm and 25°C for 10 min. The mixtures were further centrifuged at 12000 *g* for 15 min at 4°C to separate the upper polar layer from the lower non-polar layer. Finally, 200 μL of the upper supernatant as well as 400 μL of the lower supernatant were transferred and dried by a rotating-vacuum. The residues were stored at -80°C until analysis.

For extraction with the addition of MTBE, the procedures were highly similar to those applied in chloroform extraction. The procedures from cell culture to cracking were also exactly the same as the method of using solely methanol. After cell cracking, 200 μL of the homogenates was isolated, and 500 μL of MTBE was added, followed by oscillation at 1000 rpm and 25°C for 30 min. Next, the mixtures were stratified by adding 125 μL of deionized water and oscillated at 1000 rpm and 25°C for 10 min. The mixtures were further centrifuged at 12000 *g* for 15 min at 4°C to separate the upper non-polar layer from the lower polar layer. Finally, 200 μL of the lower supernatant as well as 400 μL of the upper supernatant were transferred and dried by a rotating-vacuum. The residues were stored at -80°C until analysis.

Table S2 Summary of the polar metabolites identified in non-targeted metabolic profiles.

ID	HMDB ID	Category	Marker	Measured (*m/z*)	Retention time (*min*)	Formula	Ion mode
1	HMDB00143	Sac_1	D-galactose	179.0558	1.53	$C_6H_{12}O_6$	M–H
2	HMDB00929	AA_1	L-Tryptophan	205.0968	3.21	$C_{11}H_{12}N_2O_2$	M+H
3	HMDB00641	AA_2	L-Glutamine	145.0617	1.61	$C_5H_{10}N_2O_3$	M–H
4	HMDB00159	AA_3	L-Phenylalamine	164.0715	2.93	$C_9H_{11}NO_2$	M–H
5	HMDB00167	AA_4	L-Threonine	118.0507	1.54	$C_4H_9NO_3$	M–H
6	HMDB00182	AA_7	L-Lysine	147.1123	1.42	$C_6H_{14}N_2O_2$	M+H

7	HMDB00187	AA_8	L-Serine	104.0354	1.59	$C_3H_7NO_3$	M–H
8	HMDB00687	AA_9	L-Leucine	130.0869	2.66	$C_6H_{13}NO_2$	M–H
9	HMDB00517	AA_13	L-Arginine	173.103	1.51	$C_6H_{14}N_4O_2$	M–H
10	HMDB00148	AA_15	L-Glutamate	146.0458	1.59	$C_5H_9NO_4$	M–H
11	HMDB00123	AA	Glycine	74.0254	1.58	$C_2H_5NO_2$	M–H
12	HMDB00251	OA_3	Taurine	124.0073	1.54	$C_2H_7NO_3S$	M–H
13	HMDB00671	OA_5	3-Indolelactic acid	204.0659	4.03	$C_{10}H_9O$	M+FA–H
14	HMDB10382	LysoPC_1	LysoPC(16:0)	496.3391	8.33	$C_{24}H_{50}NO_7P$	M+H
15	HMDB10384	LysoPC_2	LysoPC(18:0)	524.3691	10.03	$C_{26}H_{54}NO_7P$	M+H
16	HMDB10385	LysoPC_3	LysoPC(18:1)	522.3551	8.75	$C_{26}H_{52}NO_7P$	M+H
17	HMDB10386	LysoPC_5	LysoPC(18:2)	564.3308	7.64	$C_{26}H_{50}NO_7P$	M+FA–H
18	HMDB10396	LysoPC_6	LysoPC(20:4)	588.3281	7.62	$C_{28}H_{50}NO_7P$	M+FA–H
19	HMDB10407	LysoPC_9	LysoPC(P-16:0)	524.3337	8.79	$C_{24}H_{50}NO_6P$	M+FA–H
20	HMDB11507	LysoPE_1	LysoPE(18:2)	478.2939	7.59	$C_{23}H_{44}NO_7P$	M+H
21	HMDB11130	LysoPE_2	LysoPE(18:0)	480.3104	10.16	$C_{23}H_{48}NO_7P$	M–H

22	HMDB10386	PC_1	1-Linoleoyl glycerophosphochline	520.3403	7.64	$C_{26}H_{50}NO_7P$	M+H
23	HMDB11151	PC_5	PC(O-16:0/2:0)	568.3614	10.01	$C_{26}H_{54}NO_7P$	M+FA–H
24	HMDB11337	PE_1	PE(P-16:0/0:0)	436.2832	8.76	$C_{21}H_{44}NO_6P$	M-H
25	HMDB11340	PE_2	PE(P-18:0/0:0)	464.3142	10.33	$C_{23}H_{48}NO_6P$	M–H
26	HMDB04667	FA_5	13(S)-HODE	295.2222	7.84	$C_{18}H_{32}O_3$	M–H
27	HMDB01043	FA_9	Arachidonic Acid	303.2324	10.75	$C_{20}H_{32}O_2$	M–H
28	HMDB10734	FA_11	(R)-3-Hydroxy-hexadecanoic acid	271.2276	7.52	$C_{16}H_{32}O_3$	M–H
29	HMDB00062	C0	L-Carnitine	162.1121	1.56	$C_7H_{15}NO_3$	M+H
30	HMDB00201	C2	Acetyl-L-carnitine	204.1228	1.59	$C_9H_{17}NO_4$	M+H
31	HMDB00824	C3	Propionyl-L-carnitine	218.138	2.74	$C_{10}H_{19}NO_4$	M+H
32	HMDB02013	C4	Butyryl-L-carnitine	232.1539	3.12	$C_{11}H_{21}NO_4$	M+H
33	HMDB13128	C5	Valeryl-L-carnitine	246.1697	3.45	$C_{12}H_{23}NO_4$	M+H
34	HMDB00756	C6	Hexanoyl-L-carnitine	260.1837	3.91	$C_{13}H_{25}NO_4$	M+H
35	HMDB00222	C16	Palmitoyl-L-carnitine	400.3435	8.38	$C_{23}H_{45}NO_4$	M+H

36	HMDB00848	C18	Stearoyl-L-carnitine	428.373	9.65	$C_{25}H_{49}NO_4$	M+H
37	HMDB02366	C5:1	Tiglyl-L-carnitine	244.1536	3.33	$C_{12}H_{21}NO_4$	M+H
38	HMDB13205	C10:1	Decenoyl-L-carnitine	314.2342	4.91	$C_{17}H_{31}NO_4$	M+H
39	HMDB05065	C18:1	Octadecenyl-L-carnitine	426.3563	8.68	$C_{25}H_{47}NO_4$	M+H
40	HMDB06469	C18:2	Octadecadienyl-L-carnitine	424.3414	7.75	$C_{25}H_{45}NO_4$	M+H
41	HMDB13340	C18:1OH	Hydroxyoctadecenoyl-L-carnitine	442.3521	7.3	$C_{25}H_{47}NO_5$	M+H

Table S3 Summary of the lipids in non-targeted metabolic profiles.

ID	HMDB ID	Category	Marker	Measured (*m/z*)	Retention time (*min*)	Formula	Ion mode
1	HMDB11694	SM(d16:1/18:1)	Sphingomyelin	701.5502	12.52	$C_{39}H_{77}N_2O_6P$	M+H
2	HMDB11694	SM(d16:1/25:0)	Sphingomyelin	801.6674	17.31	$C_{46}H_{93}N_2O_6P$	M+H
3	HMDB12097	SM(d18:1/14:0)	Sphingomyelin	675.5344	12.14	$C_{37}H_{75}N_2O_6P$	M+H

4	HMDB10169	SM(d18:1/17:0)	Sphingomyelin	717.5794	14.43	$C_{40}H_{81}N_2O_6P$	M+H
5	HMDB01348	SM(d18:1/18:0)	Sphingomyelin	731.5842	15.11	$C_{41}H_{83}N_2O_6P$	M+H
6	HMDB12102	SM(d18:1/20:0)	Sphingomyelin	759.6205	16.08	$C_{43}H_{87}N_2O_6P$	M+H
7	HMDB12103	SM(d18:1/22:0)	Sphingomyelin	787.6583	16.91	$C_{45}H_{91}N_2O_6P$	M+H
8	HMDB12106	SM(d18:1/24:0)	Sphingomyelin	815.6915	17.92	$C_{47}H_{95}N_2O_6P$	M+H
9	HMDB00252	Sphingosine	Sphingosine	300.2828	2.08	$C_{18}H_{37}NO_2$	M+H
10	HMDB11761	Cer(d18:0/18:0)	Ceramide	568.5578	15.03	$C_{36}H_{73}NO_3$	M+H
11	HMDB11764	Cer(d18:0/20:0)	Ceramide	596.5881	16.12	$C_{38}H_{77}NO_3$	M+H
12	HMDB11760	Cer(d18:1/16:0)	Ceramide	538.5108	15.56	$C_{34}H_{67}NO_3$	M+H
13	HMDB00674	PA(O-16:0/14:0)	Glycerophosphate	607.4603	17.1	$C_{33}H_{67}O_7P$	M+H
14	HMDB11145	PA(O-16:0/18:0)	Glycerophosphate	663.5448	18.47	$C_{37}H_{75}O_7P$	M+H
15	HMDB11517	PE(20:4/0:0)	Monoacylphosphatidyl	502.2836	1.94	$C_{25}H_{44}NO_7P$	M+H
16	HMDB11526	PE(22:6/0:0)	Monoacylphosphatidyl	526.2881	1.23	$C_{27}H_{44}NO_7P$	M+H
17	HMDB08847	PE(14:0/22:6)	Phosphatidylethanolamine	736.4834	12.23	$C_{41}H_{70}NO_8P$	M+H
18	HMDB08943	PE(16:0/22:4)	Phosphatidylethanolamine	768.5451	15.67	$C_{43}H_{78}NO_8P$	M+H

19	HMDB08944	PE(O-16:0/22:5)	Phosphatidylethanolamine	752.5506	16.1	$C_{43}H_{78}NO_7P$	M+H
20	HMDB09544	PE(P-18:1/22:6)	Phosphatidylethanolamine	774.5385	16.07	$C_{45}H_{76}NO_7P$	M+H
21	HMDB00564	PC(16:0/0:0)	Monoacylphosphatidylcholine	496.3308	2.35	$C_{24}H_{50}NO_7P$	M+H
22	HMDB08530	PC(17:0/0:0)	Monoacylphosphatidylcholine	510.3443	2.89	$C_{25}H_{52}NO_7P$	M+H
23	HMDB08036	PC(18:0/0:0)	Monoacylphosphatidylcholine	524.3627	3.62	$C_{26}H_{54}NO_7P$	M+H
24	HMDB07934	PC(15:0/15:0)	Phosphatidylcholine	706.5303	14.06	$C_{38}H_{76}NO_8P$	M+H
25	HMDB11188	PC(12:0/19:0)	Phosphatidylcholine	720.5441	14.62	$C_{39}H_{78}NO_8P$	M+H
26	HMDB08000	PC(16:0/15:1)	Phosphatidylcholine	718.5267	13.88	$C_{39}H_{76}NO_8P$	M+H
27	HMDB08328	PC(17:2/14:0)	Phosphatidylcholine	716.5387	14.81	$C_{39}H_{74}NO_8P$	M+H
28	HMDB08038	PC(18:1/12:0)	Phosphatidylcholine	704.5192	13.07	$C_{38}H_{74}NO_8P$	M+H
29	HMDB08307	PC(20:1/12:0)	Phosphatidylcholine	732.5454	14.31	$C_{40}H_{78}NO_8P$	M+H
30	HMDB07938	PC(15:1/18:0)	Phosphatidylcholine	746.5605	14.79	$C_{41}H_{80}NO_8P$	M+H
31	HMDB08793	PC(14:1/19:1)	Phosphatidylcholine	744.5442	13.93	$C_{41}H_{78}NO_8P$	M+H

32	HMDB08762	PC(14:1/19:1)	Phosphatidylcholine	744.5555	15.77	$C_{41}H_{78}NO_8P$	M+H
33	HMDB08556	PC(12:0/22:2)	Phosphatidylcholine	758.5609	14.5	$C_{42}H_{80}NO_8P$	M+H
34	HMDB07939	PC(17:1/17:2)	Phosphatidylcholine	756.546	13.71	$C_{42}H_{78}NO_8P$	M+H
35	HMDB07963	PC(17:1/17:2)	Phosphatidylcholine	756.5436	15.16	$C_{42}H_{78}NO_8P$	M+H
36	HMDB08037	PC(17:1/18:0)	Phosphatidylcholine	774.5943	17.17	$C_{43}H_{84}NO_8P$	M+H
37	HMDB08028	PC(16:1/19:1)	Phosphatidylcholine	772.5768	15.04	$C_{43}H_{82}NO_8P$	M+H
38	HMDB07946	PC(15:1/20:2)	Phosphatidylcholine	770.5605	14.11	$C_{43}H_{80}NO_8P$	M+H
39	HMDB08076	PC(17:0/19:1)	Phosphatidylcholine	788.6076	16.19	$C_{44}H_{86}NO_8P$	M+H
40	HMDB08170	PC(18:3/18:1)	Phosphatidylcholine	782.5601	13.79	$C_{44}H_{80}NO_8P$	M+H
41	HMDB08495	PC(20:5/16:0)	Phosphatidylcholine	780.5461	12.92	$C_{44}H_{78}NO_8P$	M+H
42	HMDB08170	PC(18:3/19:1)	Phosphatidylcholine	796.5663	14.83	$C_{45}H_{82}NO_8P$	M+H
43	HMDB08345	PC(20:4/17:2)	Phosphatidylcholine	792.5418	14.11	$C_{45}H_{78}NO_8P$	M+H
44	HMDB08506	PC(20:5/17:2)	Phosphatidylcholine	790.5311	13.24	$C_{45}H_{76}NO_8P$	M+H
45	HMDB08436	PC(20:4/18:3)	Phosphatidylcholine	804.556	16.15	$C_{46}H_{78}NO_8P$	M+H

46	HMDB10584	PG(16:0/22:6)	Phosphatidylglycerol	795.5098	12.94	$C_{44}H_{75}O_{10}P$	M+H
47	HMDB10599	PG(16:1/22:6)	Phosphatidylglycerol	793.4896	12.17	$C_{44}H_{73}O_{10}P$	M+H
48	HMDB10608	PG(18:3/20:5)	Phosphatidylglycerol	791.4749	11.29	$C_{44}H_{71}O_{10}P$	M+H
49	HMDB09901	PI(14:1/22:4)	Phosphatidylinositol	857.5048	12.71	$C_{45}H_{77}O_{13}P$	M+H
50	HMDB09793	PI(16:0/22:4)	Phosphatidylinositol	887.5525	13.33	$C_{47}H_{83}O_{13}P$	M+H
51	HMDB09912	PI(16:1/22:4)	Phosphatidylinositol	885.5371	13.4	$C_{47}H_{81}O_{13}P$	M+H
52	HMDB12442	PS(17:0/22:6)	Phosphatidylserine	822.5198	14.36	$C_{45}H_{76}NO_{10}P$	M+H
53	HMDB12449	PS(17:1/22:4)	Phosphatidylserine	824.5516	15.59	$C_{45}H_{78}NO_{10}P$	M+H
54	HMDB10167	PS(19:1/22:6)	Phosphatidylserine	848.5282	14.51	$C_{47}H_{78}NO_{10}P$	M+H
55	HMDB12439	PS(20:4/22:6)	Phosphatidylserine	856.5015	15.87	$C_{48}H_{74}NO_{10}P$	M+H
56	HMDB12340	PS(21:0/22:6)	Phosphatidylserine	878.5751	16.26	$C_{49}H_{84}NO_{10}P$	M+H
57	HMDB07015	DG(15:0/22:4/0:0)	Diacylglycerol	631.5182	17.51	$C_{40}H_{70}O_5$	M+H
58	HMDB47787	TG(12:0/14:0/22:5)	Triacylglycerol	797.6852	19.84	$C_{51}H_{88}O_6$	M+H
59	HMDB05361	TG(12:0/18:1/22:6)	Triacylglycerol	849.7189	19.87	$C_{48}H_{97}O_9P$	M+H

60	HMDB05362	TG(12:0/18:4/18:4)	Triacylglycerol	791.6134	16.19	$C_{51}H_{82}O_6$	M+H
61	HMDB05370	TG(12:0/22:3/22:6)	Triacylglycerol	901.7614	19.99	$C_{59}H_{96}O_6$	M+H
62	HMDB05396	TG(12:0/22:4/22:6)	Triacylglycerol	877.7576	20.14	$C_{59}H_{94}O_6$	M+H