

Supplementary Materials: Metabolomics and Lipidomics Study Reveals Metabolic Dysregulation in Epididymal Adipose Tissue of *db/db* Mice

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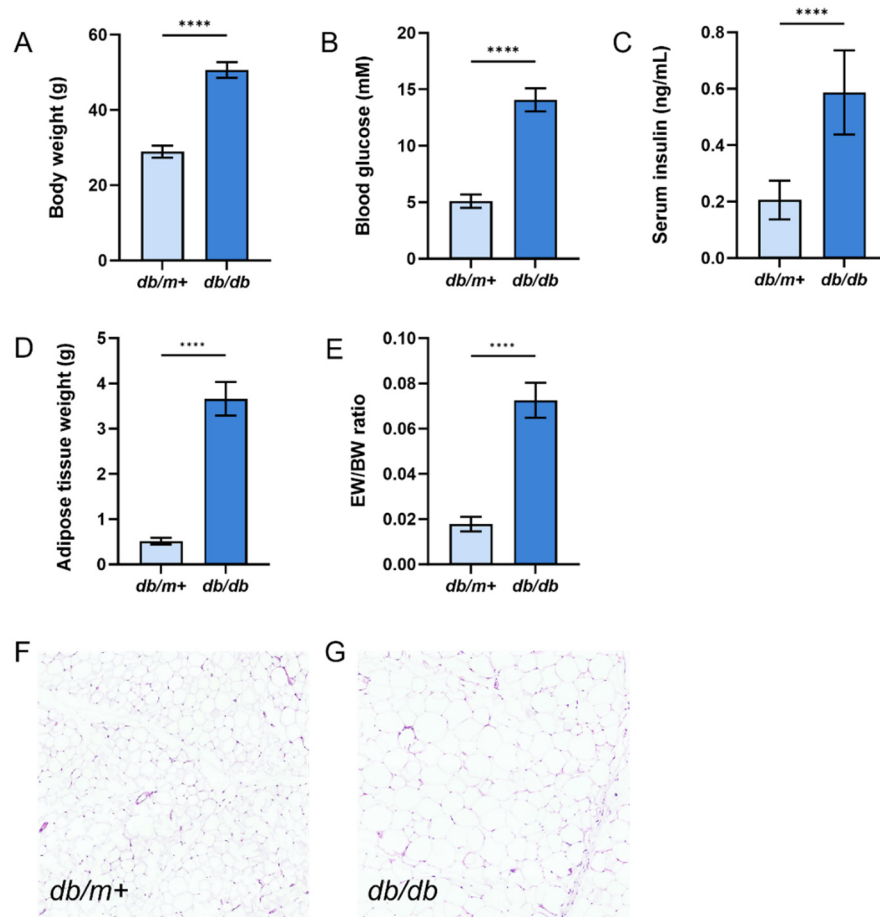


Figure S1. Phenotypic characteristics of *db/m+* and *db/db* mice. (A) Body weight; (B) Fasting blood glucose; (C) Serum insulin levels; (D) Weight of epididymal adipose tissues; (E) Ratio of epididymal adipose mass to body weight; (F,G) Representative histological images (20×) of epididymal adipose tissues from *db/m+* (F) and *db/db* (G) mice stained by H&E. The p value was calculated by t-student. **** $p < 0.001$.



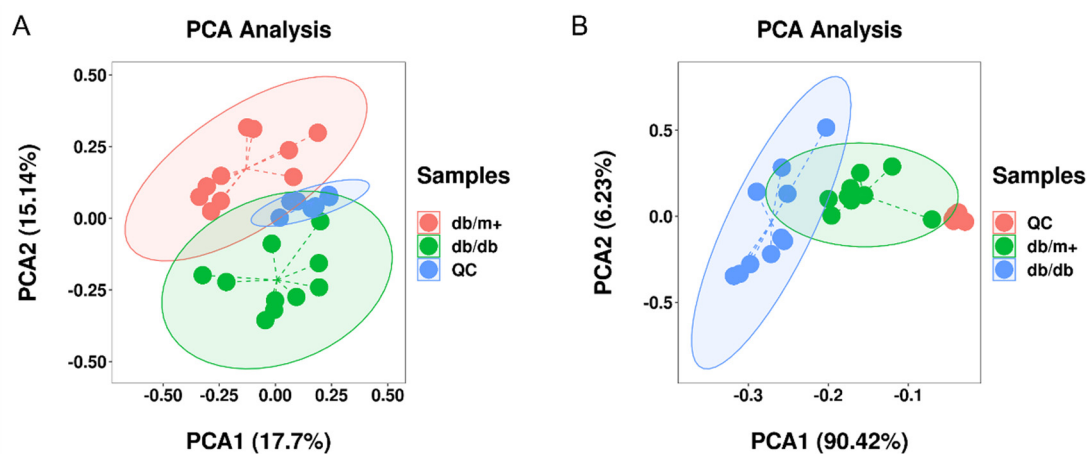


Figure S2. Overview of untargeted metabolomics and lipidomics results. (A) PCA score plot of detected metabolic features in both positive and negative ionization modes; (B) PCA score plot of detected lipids in both positive and negative ionization modes. Different colors represent different groups, and circles indicate the 95% confidence interval.

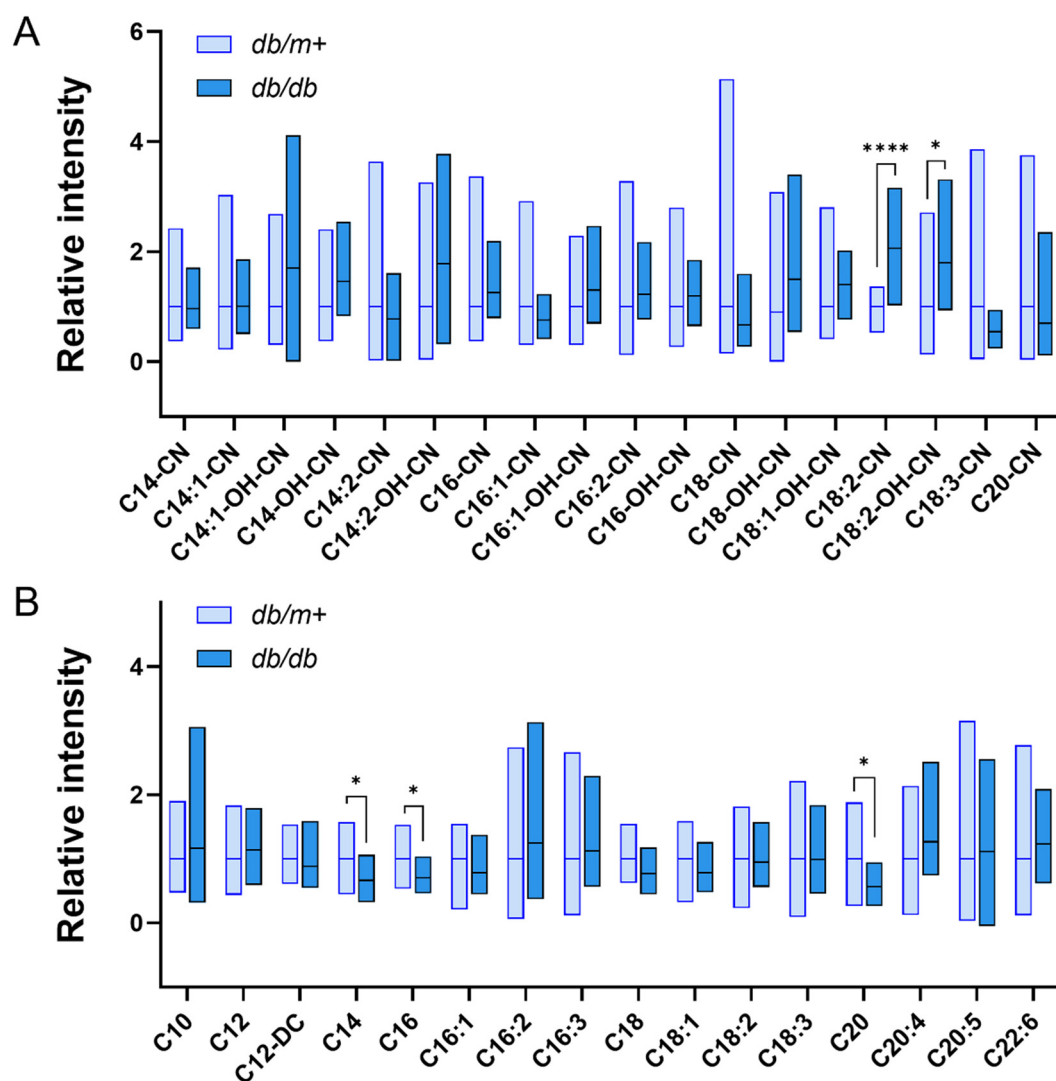


Figure S3. Targeted metabolomics analysis of metabolites in eWAT of *db/db* mice. (A) Long-chain acyl-carnitines; (B) Medium- and long-chain fatty acids. Data are presented as means $\pm$ SEM (n = 10). The *p* value was calculated by t-student. * *p* < 0.05, **** *p* < 0.001.

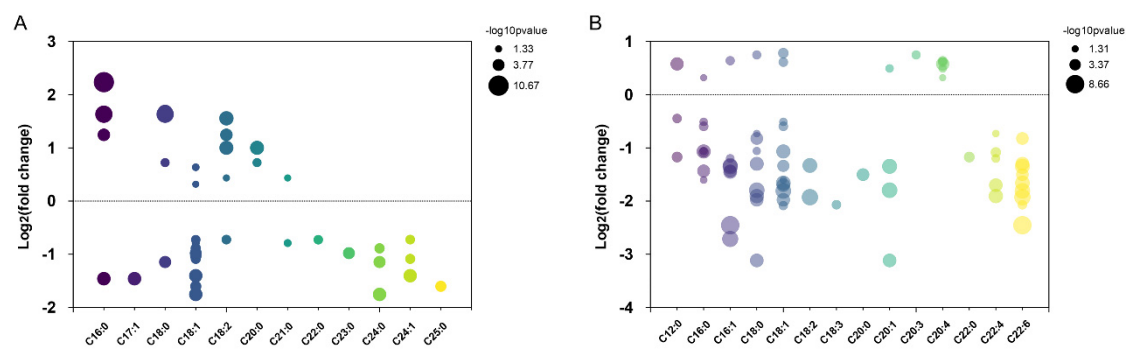


Figure S4. Bubble plot analysis of the relative intensity of fatty-acyl chains in eWAT of *db/db* mice. **(A)** Ceramides; **(B)** Phosphatidylethanolamines. Bubble size represents the fold change significance, and different colors denote various fatty-acyl chains.

Table S1. Instrumental method for the analysis of non-targeted metabolomics using UHPLC-QE Orbitrap MS.

Instrument	Thermo Scientific UHPLC coupled to a Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer	
Analytical Column	ACQUITY UPLC HSS T3 column (150 × 2.1 mm; 1.7 μm)	Acquity BEH amide column (150 × 2.1 mm; 1.7 μm)
Column Temperature (°C)	30	40
Mobile Phases	Phase A: 0.1% formic acid in water Phase B: 0.1% formic acid in acetonitrile	Phase A: 10 mM ammonium formate and 0.125% formic acid in water Phase B: 10 mM ammonium formate and 0.125% formic acid in 95% acetonitrile (acetonitrile/water, v/v = 95/5)
Gradient	0.0 min, 2% B; 1.0 min, 2% B; 19.0 min, 100% B; 21.0 min, 100% B; 21.1 min, 2% B; 25.0 min, 2% B;	0 min, 100% B; 2 min, 100% B; 7.7 min, 70% B; 9.5 min, 40% B; 10.3 min, 30% B; 12.3 min, 30% B; 14.8 min, 100% B; 20.0 min, 100% B;
Flow rate (mL/min)	0.30	
Injection volume	10 μL	5 μL
MS parameters	Full scan mode; Resolution = 35000; Scan range (<i>m/z</i>) = 60-1000; Spray voltage (kV) = 3.5 (positive ionization mode), 2.5 (negative ionization mode); Sheath gas flow rate (arbitrary units) = 45; Auxiliary gas flow rate (arbitrary units) = 10; Auxiliary gas heater temperature (°C) = 350; Capillary temperature (°C) = 320.	
MS/MS Parameters	Full scan and parallel reaction monitoring (PRM) mode; Collision energy (eV) = 10, 20, 40;	

Table S2. Instrumental method for the analysis of lipidomics samples using UHPLC-QE Orbitrap MS.

Instrument	Thermo Scientific UHPLC coupled to a Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer	
Analytical Column	CQUITY UPLC C18 column (1.7 µm particles, 2.1 mm × 100 mm, Waters, Milford, MA)	
Column Temperature (°C)	50	
Mobile Phases	Phase A: IPA/ACN (90:10, v/v) with 10 mM ammonium formate and 0.1% formic acid	
	Phase B: ACN/H ₂ O (60:40, v/v) with 10 mM ammonium formate and 0.1% formic acid	
Gradient	0.0 min, 30% A;	
	1.0 min, 30% A;	
	2.0 min, 45% A;	
	7.0 min, 70% A;	
	9.0 min, 85% A;	
	17.0 min, 100% A;	
	19.0 min, 100%A;	
	20.0 min, 30%A;	
	24.0 min, 30%A;	
Flow rate (mL/min)	0.26	
Injection volume (µL)	10	
MS parameters	Full scan mode	
	Resolution = 35000;	
	Scan range (<i>m/z</i>) = 60-1000;	
	Spray voltage (kV) = 3.5 (positive ionization mode), 2.5 (negative ionization mode);	
	Sheath gas flow rate (arbitrary units) = 45;	
	Auxiliary gas flow rate (arbitrary units) = 10;	
MS/MS Parameters	Auxiliary gas heater temperature (°C) = 350;	
	Capillary temperature (°C) = 320;	
	Full scan and ddMS2 mode;	
	Collision energy (eV) = 10, 20, 40;	

Table S3. Instrumental method for the analysis of acyl-carnitines using UHPLC-QE Orbitrap MS.

Instrument	Thermo Scientific UHPLC coupled to a Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer	
Analytical Column	Luna C18 (2.1 mm i.d. × 100 mm, 1.6 µm particle size, Phenomenex)	Synchronis HILIC column (2.1 mm id × 100 mm, 1.7 µm)
Column Temperature (°C)	30	30
Mobile Phases	Phase A: 10 mM ammonium acetate and 0.1% formic acid in water	
	Phase A: 0.1% formic acid in water Phase B: 0.1% formic acid in acetonitrile	Phase B: 10 mM ammonium acetate and 0.2% formic acid in 95% acetonitrile (acetonitrile/water, v/v = 95/5)
Gradient	0.0 min, 2% B;	0 min, 90% B;
	1.5 min, 2% B;	1.0 min, 90% B;
	14.5 min, 100% B;	9.0 min, 30% B;
	21.0 min, 100% B;	10.0 min, 30% B;
	21.1 min, 2% B;	10.1 min, 90% B;
	25.0 min, 2% B;	16.0 min, 90% B;
Flow rate (mL/min)	0.2	
Injection volume (µL)	10	10
MS parameters	Parallel reaction monitoring mode	
	Resolution = 30000;	
	Spray voltage (kV) = 3.6kV (positive ionization mode);	
	Maximum injection time: 100ms;	
	Automated gain control (AGC): 5 × 10 ⁴ ;	
	Sheath gas flow rate (arbitrary units) = 40;	
MS parameters	Auxiliary gas flow rate (arbitrary units) = 10;	
	Auxiliary gas heater temperature (°C) = 320;	
	Capillary temperature (°C) = 300;	

Table S4. Instrumental method for the analysis of fatty acids and TCA cycle metabolites using UHPLC-QqQ-MS.

Instrument	UltiMate 3000 liquid chromatography combined with triple quadrupole mass spectrometry (LC-QqQ-MS) (Thermo Fisher Scientific, MA, U.S.A.).
Analytical Column	Phenomenex polar C18 column (1.6 mm, 2.1 × 150 mm)
Column Temperature (°C)	30
Mobile Phases	Phase A: 0.01% formic acid in water Phase B: 0.01% formic acid in acetonitrile
Gradient	0.0 min, 30% B; 0.5 min, 30% B; 11.5 min, 100% B; 14.5 min, 100% B; 14.6 min, 30% B; 16.0 min, 30% B;
Flow rate (mL/min)	0.25
Injection volume (μL)	10
MS parameters	Selected reaction monitoring mode Spray voltage (kV) = 2.5 kV (positive ionization mode); Sheath gas flow rate (arbitrary units) = 40; Auxiliary gas flow rate (arbitrary units) = 10; Auxiliary gas heater temperature (°C) = 320; Capillary temperature (°C) = 300;

Table S5. Identification of significantly altered metabolites in eWAT of *db/db* mice.

No.	Compounds	Class	Column	<i>m/z</i>	RT (min)	FC	<i>p</i> value
1	MG (20:4_0:0_0:0)	Acylglycerides	T3	379.2841	18.40	3.61	2.54E-05
2	MG (16:0_0:0_0:0)	Acylglycerides	T3	331.2841	17.37	15.58	2.49E-07
3	MG (18:3_0:0_0:0)	Acylglycerides	T3	353.2690	17.43	15.50	7.43E-06
4	MG (22:5_0:0_0:0)	Acylglycerides	T3	405.3006	18.67	77.55	6.53E-06
5	L-Proline	Amino acids and derivatives	Amide	116.0706	10.44	1.95	2.78E-05
6	1-Methylhistamine	Amino acids and derivatives	Amide	126.1025	8.20	0.54	5.34E-04
7	L-Cyclo(alanylglycyl)	Amino acids and derivatives	Amide	129.0658	8.98	1.51	1.66E-02
8	L-Norleucine	Amino acids and derivatives	Amide	132.1019	7.84	3.93	4.03E-03
9	D-Aspartic acid	Amino acids and derivatives	Amide	134.0447	9.89	1.90	3.38E-05
10	D-Glutamic acid	Amino acids and derivatives	Amide	148.0603	9.45	2.74	3.20E-04
11	Ne,Ne dimethyllysine	Amino acids and derivatives	Amide	175.1441	9.88	2.03	7.00E-03
12	Carnosine	Amino acids and derivatives	Amide	227.1139	10.26	0.17	1.18E-02
13	Prolylhydroxyproline	Amino acids and derivatives	Amide	229.1180	9.42	2.21	1.89E-03
14	Anserine	Amino acids and derivatives	Amide	241.1291	10.23	0.15	1.28E-04
15	Glutamyllysine	Amino acids and derivatives	Amide	276.1552	10.52	2.49	2.10E-03
16	Tyrosyl-Lysine	Amino acids and derivatives	Amide	310.1751	8.66	5.23	2.42E-03
17	4-Hydroxynonenal glutathione	Amino acids and derivatives	Amide	464.2047	8.67	3.64	6.35E-03
18	Glutamylleucine	Amino acids and derivatives	T3	261.1445	5.71	3.48	1.56E-03
19	Tiglylcarnitine (C5:1-CN)	Fatty acids and derivatives	Amide	244.1540	6.77	6.11	4.97E-05
20	2-Methylbutyrylcarnitine (2-Me-C4-CN)	Fatty acids and derivatives	Amide	246.1699	6.53	3.58	8.45E-05
21	Malonylcarnitine	Fatty acids and derivatives	Amide	248.1125	9.28	2.94	5.12E-05
22	Hydroxybutyrylcarnitine (C4-OH-CN)	Fatty acids and derivatives	Amide	248.1490	8.28	8.56	8.28E-05
23	Hydroxyisovaleryl carnitine (isoC5-OH-CN)	Fatty acids and derivatives	Amide	262.1646	8.02	3.28	1.30E-07
24	Benzoylcarnitine	Fatty acids and derivatives	Amide	266.1388	6.76	2.39	1.85E-05
25	Phenethyl decanoate	Fatty acids and derivatives	Amide	277.2160	0.98	0.23	3.02E-03
26	Octadecanamide	Fatty acids and derivatives	Amide	284.2947	0.95	0.52	6.86E-03
27	12(13)-epoxy-6Z,9Z-octadecadienoic acid	Fatty acids and derivatives	Amide	295.2265	0.99	0.20	4.46E-03
28	2-Phenylpropyl isobutyrate	Fatty acids and derivatives	Amide	207.1384	1.01	2.55	1.29E-02
29	4-Oxododecanedioic acid	Fatty acids and derivatives	T3	243.1233	8.62	11.87	7.06E-03
30	(±)12,13-DiHOME (12,13-OH-C12)	Fatty acids and derivatives	T3	313.2381	13.98	0.31	9.36E-04
31	Pantothenic acid	Organic acids	Amide	220.1177	3.33	0.55	2.75E-03
32	4-Guanidinobutanoic acid	Organic acids	Amide	146.0923	8.24	2.73	4.87E-05
33	3,4,5,6-Tetrahydrohippuric acid	Organic acids	Amide	184.0965	3.34	0.54	5.41E-03
34	N1-Acetylspermidine	Organic acids	Amide	188.1754	9.57	2.09	1.36E-05

35	Piperidine	Others	T3	86.0964	2.35	2.66	2.48E-03
36	FAD	Others	T3	786.1634	5.70	0.57	6.47E-04
37	Thymine	Others	Amide	127.0500	8.69	2.02	1.73E-03
38	Glucosamine 6-phosphate	Others	Amide	260.0526	10.31	4.56	1.04E-06
39	3-Dehydrosphinganine	Others	Amide	300.2894	1.01	0.64	1.22E-02
40	LysoPE (18:0_0:0)	Phospholipids	T3	482.3241	17.22	1.37	1.52E-03
41	LysoPC (18:1_0:0)	Phospholipids	T3	522.3558	15.61	0.62	3.91E-03
42	LysoPE (20:4_0:0)	Phospholipids	T3	502.2928	14.51	0.74	2.74E-03
43	LysoPE (16:1_0:0)	Phospholipids	T3	452.2774	14.18	0.24	1.49E-08
44	LysoPC (20:3_0:0)	Phospholipids	T3	546.3558	15.23	0.40	3.41E-04
45	LysoPE (16:0_0:0)	Phospholipids	T3	454.2930	15.35	0.75	1.24E-04
46	LysoPI (20:4_0:0)	Phospholipids	T3	621.3039	14.50	0.59	8.56E-05
47	LysoPI (18:1_0:0)	Phospholipids	T3	597.3039	16.19	1.53	5.88E-03
48	LysoPS (16:0_0:0)	Phospholipids	T3	496.2677	15.41	1.72	6.85E-03
49	LysoPI (16:0_0:0)	Phospholipids	T3	571.2881	15.49	0.60	9.69E-03
50	LysoPE (22:6_0:0)	Phospholipids	T3	524.2773	14.81	0.46	4.43E-06
51	PE (16:1_18:2)	Phospholipids	Amide	714.5077	5.76	0.40	1.96E-02
52	PC (16:0_16:1)	Phospholipids	Amide	732.5532	5.07	0.73	7.43E-03
53	SM (d18:1_20:1)	Phospholipids	Amide	757.6212	6.50	0.44	3.59E-03
54	SM (d16:1_22:0)	Phospholipids	Amide	759.6378	6.50	0.34	4.00E-03
55	PE (20:3_18:3)	Phospholipids	Amide	764.5215	5.41	0.47	7.73E-03
56	PE (16:0_22:5)	Phospholipids	Amide	766.5396	5.07	0.59	1.80E-02
57	PS (18:2_18:0)	Phospholipids	Amide	788.5419	6.86	2.78	3.01E-03
58	Adenosine monophosphate	Purine nucleotides	T3	348.0705	5.70	0.59	3.58E-03
59	Xanthine	Purine nucleotides	T3	153.0408	1.94	0.40	3.44E-03
60	Uracil	Purine nucleotides	T3	113.0346	2.36	0.34	1.83E-03
61	ADP-glucose	Purine nucleotides	T3	588.0746	1.59	0.46	6.67E-04
62	Hypoxanthine	Purine nucleotides	Amide	137.0457	4.98	0.55	1.38E-02
63	Adenosine	Purine nucleotides	Amide	268.1037	4.98	0.33	1.87E-02
64	Inosine	Purine nucleotides	Amide	269.0876	7.22	0.38	9.42E-04
65	Progesterone	Steroids and derivatives	T3	315.2320	15.34	3.77	1.73E-06
66	Testosterone enanthate	Steroids and derivatives	T3	401.3053	19.98	1.94	1.48E-03
67	Testosterone Propionate	Steroids and derivatives	T3	345.2425	19.98	2.15	9.78E-04
68	Corticosterone	Steroids and derivatives	T3	347.2222	11.04	8.11	7.33E-04
69	Pregnanetriol	Steroids and derivatives	T3	337.2731	18.50	22.53	1.16E-06
70	Calcidiol	Steroids and derivatives	Amide	401.3422	0.96	2.11	2.90E-03

Notes: FC represents fold changes; *m/z* represents mass-to-charge ratio; RT represents retention time.

Table S6. Detailed information of acyl carnitines detected in eWAT of *db/db* mice.

NO.	Compounds	Abbreviations	R.T.	Parent/Product ions (<i>m/z</i>)
1	Carnitine	C0-CN	7.18/7.62	162.1/85.0
2	Acetyl-carnitine	C2-CN	6.17	204.1/85.0
3	Butyryl-carnitine	C4-CN	6.75	232.1/85.0
4	Crotonyl-carnitine	C4:1-CN	6.56	230.1/85.0
5	Valeryl-carnitine	C5-CN	8.48/8.56	246.2/85.0
6	2-Methylcrotonoyl-carnitine	2-Me-C4:1-CN	7.91	244.2/85.0
7	Hydroxyl valeryl-carnitine	C5-OH-CN	6.51	262.2/85.0
8	Hexanoyl-carnitine	C6-CN	9.64	260.2/85.0
9	Hydroxyl hexanoyl-carnitine	C6-OH-CN	7.87	276.2/85.0
10	Octenoyl-carnitine	C8:1-CN	11.26	286.2/85.0
11	Hydroxyl octanoyl-carnitine	C8-OH-CN	10.5	304.2/85.0
12	Decanoyl-carnitine	C10-CN	13.58	316.2/85.0
13	Decenoyl-carnitine	C10:1-CN	13.2	314.2/85.0
14	Dodecanoyl-carnitine	C12-CN	14.77	344.3/85.0
15	Dodecenoyl-carnitine	C12:1-CN	14.3	342.3/85.0
16	Tetradecanoyl-carnitine	C14-CN	15.47	372.3/85.0
17	Tetradecenoyl-carnitine	C14:1-CN	15.19	370.3/85.0
18	Hydroxyl tetradecenoyl-carnitine	C14:1-OH-CN	14.6	386.3/85.0
19	Hydroxyl tetradecanoyl-carnitine	C14-OH-CN	15.05	388.2/85.0
20	Tetradecandienoyl-carnitine	C14:2-CN	14.58	368.3/85.0
21	Hydroxyl tetradecandienoyl-carnitine	C14:2-OH-CN	14.15	384.3/85.0
22	Palmitoyl-carnitine	C16-CN	16.12	400.3/85.0
23	Hexadecenoyl-carnitine	C16:1-CN	15.68	398.3/85.0
24	Hydroxyl hexadecenoyl-carnitine	C16:1-OH-CN	15.23	414.3/85.0
25	Hexadecadienylcarnitine	C16:2-CN	15.33	396.3/85.0
26	Hydroxyl Hexadecanoyl-carnitine	C16-OH-CN	15.64	416.3/85.0

27	Octadecanoyl-carnitine	C18-CN	16.51	428.4/85.0
28	Hydroxyl stearoyl-carnitine	C18-OH-CN	16.13	444.4/85.0
29	Hydroxyl oleoyl-carnitine	C18:1-OH-CN	15.86	442.3/85.0
30	Linoleoyl-carnitine	C18:2-CN	15.93	424.3/85.0
31	Hydroxyl linoleoyl-carnitine	C18:2-OH-CN	11.8	495.3/85.0
32	Linoleyl carnitine	C18:3-CN	15.66	422.3/85.0
33	Arachidyl carnitine	C20-CN	16.85	456.2/85.0
34	Oleoyl-carnitine	C18:1	16.15	426.4/85.0
35	Octadecanoyl-carnitine	C18	16.51	428.4/85.0

Notes: R.T. represents retention time.

Table S7. Detailed information of fatty acids and TCA cycle metabolites detected in eWAT of *db/db* mice.

NO.	Compounds	Abbreviations	R.T.	Parent/Product ions (<i>m/z</i>)
1	Acetic acid	C2	3.22	193.9/136.8
2	Propanoic acid	C3	4.22	208.0/136.8
3	Malonic acid	C3_DC	5.72	373.0/177.8
4	3-hydroxypropionic acid	3_OH_C3	2.87	224.1/136.8
5	Butyric acid	C4	5.27	222.0/136.8
6	2-hydroxybutyric acid	2_OH_C4	3.47	238.1/136.8
7	3-hydroxyisobutyric acid	3_OH_isoC4	2.97	262.2/85.0
8	Valeric acid	C5	6.32	236.0/136.8
9	Isovaleric acid	iso_C5	6.45	236.0/136.8
10	5-hydroxyvaleric acid	5_OH_C5	3.64	252.1/136.8
11	Adipic acid	C6_DC	5.96	415.0/261.9
12	3-methylhexanoic acid	3_Me_C6	6.47	264.1/136.8
13	Decanoic acid	C10	9.94	306.12/136.8
14	Lauric acid	C12	11.08	334.2/136.8
15	Dodecanedioic acid	C12_DC	8.54	499.4/136.8
16	Myristic acid	C14	12.12	362.2/136.8
17	Palmitic acid	C16	13.08	390.3/136.8
18	Palmitelaidic acid	C16:1	12.37	388.2/136.8
19	Hexadecadienoic acid	C16:2	11.77	386.2/136.8
20	Hexadecatrienoic acid	C16:3	11.44	384.2/136.8
21	Stearic acid	C18	14.12	418.3/136.8
22	Oleic acid	C18:1	13.41	416.8/136.8
23	Linoleic acid	C18:2	12.63	414.8/136.8
24	Linolenic acid	C18:3	12.05	414.3/136.8
25	Arachidic acid	C20	14.89	446.3/136.8
26	Arachidonic acid	C20:4	12.52	438.2/136.8
27	Eicosapentaenoic acid	C20:5	12.01	436.2/136.8
28	Docosahexaenoic acid	C22:6	12.39	434.2/136.8
29	Malic acid	N.A.	5.13	405.1/153.8
30	Succinic acid	N.A.	5.55	387.1/233.9
31	Fumaric acid	N.A.	6.15	387.1/233.8
32	Isocitric acid	N.A.	6.58	596.1/233.9
33	Citric acid	N.A.	6.92	596.1/221.9
34	Oxaloacetic acid	N.A.	8.71	536.0/136.8
35	α -Ketoglutaric acid	N.A.	8.66	550.1/232.9

Notes: R.T. represents retention time.

Table S8. Identification of significantly changed lipids in eWAT of *db/db* mice.

No.	Lipids	Class	R.T.	<i>m/z</i>	FC	<i>p</i> value
1	AcCa (20:3)	AcCa	5.98	450.3578	1.87	6.40E-03
2	AEA (18:0)	AEA	5.49	328.3210	1.68	6.15E-03
3	AEA (18:2)	AEA	3.54	324.2897	1.53	2.74E-02
4	Cer (d17:1_16:0)	Cer	9.31	524.5037	0.36	1.63E-05
5	Cer (d18:1_19:0)	Cer	10.52	624.5572	1.25	4.65E-02
6	Cer (d18:1_21:0)	Cer	10.95	652.5885	0.58	2.17E-02
7	Cer (d18:1_22:0)	Cer	11.14	622.6133	0.60	4.11E-03
8	Cer (d18:1_22:1)	Cer	10.76	664.5885	1.55	2.75E-02
9	Cer (d18:1_23:0)	Cer	11.32	636.6289	0.51	1.70E-04
10	Cer (d18:1_24:0)	Cer	11.49	650.6446	0.30	1.81E-05
11	Cer (d18:1_24:1)	Cer	11.11	648.6289	0.47	2.07E-03
12	Cer (d18:1_25:0)	Cer	11.66	664.6602	0.33	5.36E-04
13	Cer (d18:2_16:0)	Cer	8.99	536.5037	2.37	7.89E-05
14	Cer (d18:2_18:0)	Cer	9.70	564.5350	2.94	4.27E-06
15	Cer (d18:2_20:0)	Cer	10.28	592.5663	2.00	6.95E-06
16	Cer (d18:2_21:0)	Cer	10.53	650.5729	1.35	4.46E-02
17	Cer (d18:2_24:1)	Cer	10.71	646.6133	0.61	3.46E-03
18	Cer (m18:0_16:0)	Cer	10.10	524.5401	3.10	1.43E-08
19	Cer (m18:0_18:0)	Cer	10.61	552.5714	3.18	7.85E-07
20	Cer (m18:0_20:0)	Cer	11.05	580.6027	1.65	6.78E-03
21	Cer(m18:0_24:0)	Cer	11.75	636.6653	0.45	1.35E-04
22	Cer (m18:1_16:0)	Cer	9.51	522.5245	4.71	2.12E-11
23	Cer (m18:1_20:4)	Cer	10.10	570.5245	0.49	3.21E-04
24	Cer (m18:1_24:0)	Cer	11.41	634.6497	0.54	1.62E-03
25	Cer (m18:1_24:1)	Cer	11.00	632.6340	0.38	1.96E-05
26	DG (12:0_18:2)	DG	8.85	554.4779	1.54	8.50E-04
27	DG (14:0_18:3)	DG	8.97	580.4936	0.70	9.46E-03
28	DG (16:0_12:0)	DG	9.44	530.4779	1.88	2.03E-04
29	DG (16:0_18:1)	DG	10.59	595.5296	1.87	4.32E-04
30	DG (16:1_18:2)	DG	9.63	608.5249	1.54	5.18E-03
31	DG (16:1_18:3)	DG	9.11	606.5092	1.50	1.91E-02
32	DG (18:1_12:0)	DG	9.47	556.4936	1.76	6.26E-04
33	DG (18:1_14:0)	DG	10.08	584.5249	1.51	1.28E-02
34	DG (18:1_18:1)	DG	10.59	638.5718	2.05	5.39E-03
35	DG (18:1_18:2)	DG	10.17	636.5562	2.07	1.91E-03
36	DG (18:1_20:3)	DG	10.27	662.5718	2.79	5.14E-04
37	DG (18:2_22:6)	DG	9.31	682.5405	3.75	9.62E-04
38	DG (20:3_18:2)	DG	10.03	660.5562	4.33	4.62E-05
39	Hex1Cer (d18:1_16:0)	Hex1Cer	9.13	700.5722	0.50	3.10E-03
40	Hex1Cer (d18:1_16:0+O)	Hex1Cer	8.97	716.5671	1.43	1.30E-02
41	Hex1Cer (d18:1_18:0)	Hex1Cer	9.80	728.6035	0.16	2.46E-06
42	Hex1Cer (d18:1_20:0+O)	Hex1Cer	10.23	772.6297	0.33	1.20E-03
43	Hex1Cer (d18:1_22:0)	Hex1Cer	10.79	784.6661	0.22	1.17E-05
44	Hex1Cer (d18:1_22:0+O)	Hex1Cer	10.69	800.6610	0.28	9.03E-05
45	Hex1Cer (d18:1_22:1)	Hex1Cer	10.69	782.6504	0.28	2.32E-04
46	Hex1Cer (d18:1_23:0)	Hex1Cer	10.98	842.6727	0.24	1.54E-04
47	Hex1Cer (d18:1_24:0)	Hex1Cer	11.16	812.6974	0.13	6.41E-05
48	Hex1Cer (d18:1_24:0+O)	Hex1Cer	11.08	828.6923	0.18	1.53E-05
49	Hex1Cer (d18:1_24:1)	Hex1Cer	10.74	810.6817	0.17	4.35E-05
50	Hex1Cer (d18:1_24:2)	Hex1Cer	10.32	808.6661	0.18	2.12E-05
51	Hex1Cer (d18:2_24:0+O)	Hex1Cer	10.64	826.6767	0.34	2.54E-04
52	Hex1Cer (d36:1)	Hex1Cer	9.81	772.5944	0.12	3.67E-04
53	Hex1Cer (d42:3)	Hex1Cer	10.33	852.6570	0.21	1.26E-03
54	Hex1Cer (t20:0_18:1)	Hex1Cer	10.23	816.6206	0.37	1.24E-02
55	Hex1Cer (t40:1)	Hex1Cer	10.69	844.6519	0.33	8.77E-03
56	Hex1Cer (t42:1)	Hex1Cer	11.08	872.6832	0.23	5.04E-03
57	Hex1Cer (t42:2)	Hex1Cer	10.64	870.6676	0.45	2.08E-02
58	LPC (16:0)	LPC	3.24	540.3307	0.63	1.40E-02
59	LPC (18:0)	LPC	4.54	524.3711	2.21	1.00E-02
60	LPC (20:3)	LPC	4.57	546.3554	2.25	6.46E-03

61	LPC (22:3)	LPC	5.73	574.3867	0.48	7.48E-06
62	LPC (24:0)	LPC	7.83	608.4650	0.58	1.93E-04
63	PC (14:0_22:4)	PC	8.50	782.5694	0.69	7.12E-03
64	PC (15:0_16:0)	PC	9.24	720.5538	0.31	1.55E-04
65	PC (16:0_14:0)	PC	8.87	750.5291	0.42	1.39E-05
66	PC (16:0_16:0)	PC	9.58	778.5604	0.54	8.84E-05
67	PC (16:0_16:1)	PC	8.94	776.5447	0.63	2.91E-04
68	PC (16:0_18:1)	PC	9.61	804.5760	0.79	3.52E-02
69	PC (16:0e_20:4)	PC	9.35	812.5811	0.47	7.37E-05
70	PC (16:1e_20:3)	PC	9.34	768.5902	0.68	4.89E-02
71	PC (18:0_16:0)	PC	10.15	806.5917	0.51	2.13E-02
72	PC (18:0_20:3)	PC	9.85	856.6073	1.71	1.43E-03
73	PC (18:0_20:4)	PC	9.59	854.5917	1.54	1.35E-04
74	PC (18:0_22:5)	PC	9.57	880.6073	1.28	5.97E-03
75	PC (18:0_22:6)	PC	9.39	878.5917	0.76	8.14E-03
76	PC (18:1_24:0)	PC	11.35	916.7012	0.19	2.98E-03
77	PC (18:1e_16:0)	PC	9.95	790.5967	0.45	2.00E-03
78	PC (18:1e_16:1)	PC	9.48	744.5902	0.47	6.64E-05
79	PC (18:2_22:6)	PC	8.13	874.5604	0.31	1.19E-06
80	PC (20:0_18:3)	PC	9.85	812.6164	2.86	1.90E-08
81	PC (20:1_14:1)	PC	9.05	758.5694	1.26	3.22E-02
82	PC (20:3_22:1)	PC	10.37	866.6633	0.49	3.72E-02
83	PC (21:0e)	PC	6.30	566.4180	1.34	1.36E-02
84	PC (22:5_18:2)	PC	8.52	832.5851	1.97	1.42E-04
85	PC (30:0)	PC	8.86	706.5381	0.49	1.48E-04
86	PC (30:0e)	PC	9.32	692.5589	0.30	4.88E-05
87	PC (30:1)	PC	8.15	704.5225	0.70	1.88E-02
88	PC (32:0)	PC	9.57	734.5694	0.66	1.22E-02
89	PC (32:0e)	PC	9.96	720.5902	0.32	4.32E-05
90	PC (32:1)	PC	8.95	732.5538	0.72	9.03E-03
91	PC (33:0)	PC	9.88	748.5851	0.33	1.42E-04
92	PC (34:0e)	PC	10.47	748.6215	0.23	6.38E-05
93	PC (34:1e)	PC	9.95	746.6058	0.57	7.95E-03
94	PC (34:3)	PC	8.36	756.5538	1.36	2.44E-02
95	PC (34:4)	PC	8.77	754.5381	0.38	5.37E-07
96	PC (36:2e)	PC	10.06	772.6215	0.27	1.91E-04
97	PC (36:3)	PC	9.09	784.5851	1.69	9.23E-06
98	PC (36:5)	PC	9.03	780.5538	1.41	4.61E-03
99	PC (36:5e)	PC	9.22	766.5745	1.36	1.81E-02
100	PC (36:6)	PC	7.91	778.5381	0.58	2.00E-02
101	PC (38:0)	PC	11.02	818.6633	1.85	1.15E-02
102	PC (38:1)	PC	10.62	816.6477	0.47	2.31E-03
103	PC (38:4)	PC	9.59	810.6007	2.40	3.99E-07
104	PC (38:5)	PC	8.95	808.5851	1.61	6.90E-05
105	PC (38:5e)	PC	9.85	794.6058	0.59	8.34E-03
106	PC (38:7)	PC	7.98	804.5538	0.69	1.51E-02
107	PC (38:7e)	PC	8.67	790.5745	1.64	3.03E-03
108	PC (40:1)	PC	11.01	844.6790	0.26	2.63E-03
109	PC (40:3)	PC	11.02	840.6477	3.13	1.22E-04
110	PC (40:6)	PC	9.38	834.6007	1.37	8.78E-03
111	PC (40:6e)	PC	9.34	820.6215	2.05	5.57E-03
112	PC (40:8)	PC	8.14	830.5694	0.61	5.82E-04
113	PC (42:1)	PC	11.35	872.7103	0.17	1.33E-03
114	PC (42:3)	PC	10.65	868.6790	0.25	1.65E-04
115	PC (44:11)	PC	7.95	880.5851	2.16	4.47E-04
116	PE (12:0_22:0)	PE	10.29	720.5538	0.44	1.05E-03
117	PE (14:0_20:4)	PE	8.46	712.4912	1.49	3.04E-05
118	PE (14:0p_20:4)	PE	8.72	696.4963	0.73	4.84E-03
119	PE (16:0_16:1)	PE	9.13	688.4923	0.37	5.06E-05
120	PE (16:0_18:1)	PE	9.78	716.5236	0.70	1.52E-02
121	PE (16:0p_16:1)	PE	9.47	674.5119	0.48	7.29E-06
122	PE (16:0p_18:1)	PE	10.06	702.5432	0.66	4.18E-03
123	PE (16:0p_20:4)	PE	9.43	724.5276	1.25	4.90E-02

124	PE (16:0p_22:4)	PE	9.86	752.5589	0.47	1.79E-03
125	PE (16:1_16:1)	PE	8.42	688.4912	0.15	2.24E-07
126	PE (16:1_18:2)	PE	8.56	712.4923	0.40	2.35E-06
127	PE (16:1_20:4)	PE	8.40	736.4923	0.37	1.22E-05
128	PE(16:1_22:6)	PE	8.17	760.4923	0.18	2.17E-09
129	PE (16:1e_16:1)	PE	9.48	672.4974	0.39	8.04E-07
130	PE (16:1e_22:4)	PE	9.91	750.5443	0.44	1.08E-02
131	PE (16:1p_20:4)	PE	8.75	722.5119	1.56	6.01E-03
132	PE (18:0_16:0)	PE	10.29	718.5392	0.48	1.78E-02
133	PE (18:0_20:1)	PE	10.72	772.5862	0.29	5.69E-07
134	PE (18:0_20:3)	PE	9.99	768.5549	1.68	7.09E-03
135	PE (18:0_22:4)	PE	10.13	794.5705	0.60	3.61E-02
136	PE (18:0_22:6)	PE	9.55	790.5392	0.57	7.51E-05
137	PE (18:0p_18:1)	PE	10.55	730.5745	0.25	2.22E-05
138	PE (18:0p_20:1)	PE	10.96	758.6058	0.12	1.59E-05
139	PE (18:0p_22:4)	PE	10.37	780.5902	0.27	5.48E-06
140	PE (18:0p_22:6)	PE	9.83	776.5589	0.41	1.07E-05
141	PE (18:1_18:1)	PE	9.88	744.5538	1.72	1.41E-03
142	PE (18:1_22:6)	PE	8.91	788.5236	0.29	5.04E-07
143	PE (18:1e_16:0)	PE	10.56	702.5443	0.33	3.25E-02
144	PE (18:1e_18:1)	PE	10.56	728.5600	0.24	6.00E-03
145	PE (18:1e_22:4)	PE	10.38	778.5756	0.31	1.71E-05
146	PE (18:1e_22:6)	PE	9.83	774.5443	0.32	2.87E-06
147	PE(18:1p_18:1)	PE	10.07	728.5589	0.40	1.64E-04
148	PE (18:1p_20:4)	PE	9.44	750.5432	1.53	4.25E-03
149	PE (18:2_22:6)	PE	8.31	786.5079	0.26	1.40E-07
150	PE (18:3e_22:6)	PE	8.73	770.5130	0.24	4.42E-03
151	PE (20:0p_22:6)	PE	10.34	804.5902	0.35	7.26E-05
152	PE (20:1_20:4)	PE	9.74	794.5694	1.41	1.37E-02
153	PE (20:1e_22:6)	PE	10.35	802.5756	0.39	1.77E-06
154	PE (20:4_20:4)	PE	8.31	788.5225	0.36	2.27E-05
155	PG (18:1_18:1)	PG	8.72	773.5338	2.26	2.48E-03
156	PG (18:1_18:2)	PG	8.15	790.5593	2.88	3.36E-06
157	PG (18:1_18:2)	PG	8.14	771.5182	2.07	4.78E-05
158	PG (18:1_20:4)	PG	8.00	795.5182	3.58	1.68E-03
159	PG (18:2_18:2)	PG	7.55	788.5436	2.36	1.77E-04
160	PG (18:2_18:2)	PG	7.54	769.5025	1.95	3.37E-03
161	PG (22:6_22:6)	PG	6.85	865.5025	0.59	5.12E-03
162	PG (28:3)	PG	7.95	659.3930	1.49	1.76E-02
163	PI (16:0_20:4)	PI	8.36	876.5597	3.11	1.84E-04
164	PI (18:0_20:4)	PI	9.11	887.5644	4.48	1.50E-05
165	PI (18:1_20:4)	PI	8.39	902.5753	4.98	1.08E-06
166	PI (18:1_20:4)	PI	8.39	883.5342	2.28	6.93E-03
167	PS (18:0_18:2)	PS	9.30	786.5291	2.06	3.94E-02
168	PS (18:0_20:4)	PS	9.18	810.5291	3.19	7.78E-04
169	SM (d17:0_23:3)	SM	9.66	783.6375	1.53	1.23E-03
170	SM (d18:1_21:0)	SM	10.46	773.6531	1.78	8.35E-04
171	SM (d18:1_23:0)	SM	10.88	801.6844	1.55	1.76E-02
172	SM (d18:1_24:3)	SM	10.68	809.6531	5.43	7.80E-10
173	SM (d32:1)	SM	8.06	675.5436	2.57	9.44E-05
174	SM (d33:1)	SM	8.50	689.5592	1.40	1.74E-02
175	SM (d34:0)	SM	9.20	705.5905	2.56	3.78E-07
176	SM (d34:1)	SM	8.89	703.5749	2.94	1.98E-05
177	SM (d34:2)	SM	8.16	701.5592	5.31	1.72E-11
178	SM (d36:0)	SM	9.87	733.6218	2.09	2.36E-05
179	SM (d36:1)	SM	9.64	731.6062	3.37	2.30E-09
180	SM (d36:2)	SM	8.98	729.5905	7.17	7.57E-13
181	SM (d36:3)	SM	8.35	727.5749	7.64	2.42E-08
182	SM (d36:4)	SM	8.86	725.5592	4.05	4.00E-05
183	SM (d36:5)	SM	8.16	723.5436	6.27	4.67E-09
184	SM (d37:1)	SM	9.94	789.6127	1.60	1.24E-02
185	SM (d38:1)	SM	10.22	759.6375	2.25	1.56E-06
186	SM (d38:2)	SM	9.66	757.6218	5.57	1.00E-09

187	SM (d40:1)	SM	10.68	787.6688	1.61	2.66E-03
188	SM(d40:2)	SM	10.23	785.6531	2.59	7.85E-06
189	SM (d41:1)	SM	10.89	845.6753	1.51	2.46E-02
190	SM (d41:2)	SM	10.47	799.6688	2.87	1.84E-04
191	SM (d42:4)	SM	9.67	809.6531	2.33	8.63E-07
192	SM (d43:1)	SM	11.25	829.7157	2.25	6.57E-05
193	SM (d43:2)	SM	10.83	827.7001	2.80	3.23E-04
194	SM (d43:4)	SM	10.88	823.6688	7.00	2.67E-04
195	SM (d44:5)	SM	10.63	835.6688	2.93	1.68E-06
196	SM (t18:0_16:1)	SM	8.66	719.5698	5.35	1.39E-07
197	SM (t18:0_24:3)	SM	10.00	827.6637	5.83	6.38E-08
198	SM (t42:2)	SM	10.47	829.6793	3.67	2.35E-06
199	TG (10:0_10:0_12:0)	TG	10.09	600.5198	4.95	1.64E-03
200	TG (10:0_12:0_12:0)	TG	10.59	628.5511	4.74	3.64E-03
201	TG (16:0_10:0_18:2)	TG	11.75	764.6763	3.23	1.97E-02
202	TG (16:0_12:0_14:0)	TG	12.06	740.6763	3.85	6.13E-04
203	TG (16:0_12:0_18:1)	TG	12.36	794.7232	2.24	3.37E-03
204	TG (16:0_12:0_18:2)	TG	12.06	792.7076	2.83	3.85E-03
205	TG (16:0_14:0_14:0)	TG	12.39	768.7076	1.98	5.58E-03
206	TG (16:0_14:0_18:2)	TG	12.35	820.7389	1.83	1.75E-02
207	TG (16:0_16:0_18:3)	TG	11.25	829.7280	1.63	1.62E-03
208	TG (16:1_16:1_16:1)	TG	12.05	818.7232	2.11	2.56E-02
209	TG (18:1_12:0_12:0)	TG	11.72	738.6606	2.53	2.71E-02
210	TG (18:1_12:0_14:0)	TG	12.04	766.6919	3.69	1.24E-03

Notes: FC represents fold changes; m/z represents mass-to-charge ratio; R.T. represents retention time.