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Supplementary Information for

Locust density shapes energy metabolism and oxidative stress
resulting in divergence of flight traits

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Supplementary text
Figures S1 to S8
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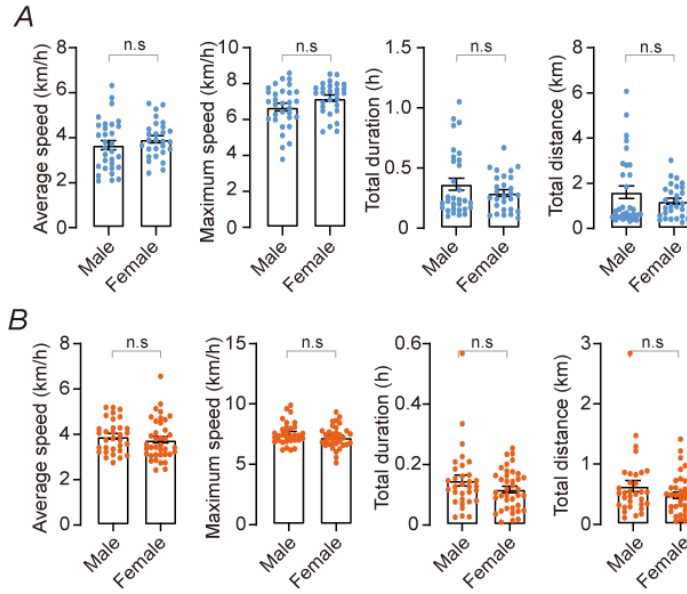
42 **Supplementary Information Text**

43 **Metabolomic Profiling, Data Processing, and Statistics.** About 20 ± 0.5 mg of flight muscle
44 tissue was weighed, transferred into a homogenizer tube, and mixed with 600 μ L prechilled
45 methanol water mixture (8/2, v/v) for metabolism quenching. After mixing with 300 μ L of tissue
46 homogenate, 900 μ L of methyl tert-butyl ether and 250 μ L ddH₂O, samples were centrifuged for 15
47 min. After centrifugation, 300 μ L of the top layer containing lipid and 250 μ L of the bottom layer
48 containing polar metabolites were transferred out and freeze dried, respectively. Polar metabolites
49 extracts were reconstituted with 150 μ L methanol water mixture (8/2, v/v) and then split into three
50 fractions for three different analytical methods as described below. Furthermore, lipid extracts were
51 redissolved with 250 μ L of acetonitrile and isopropanol mixture solution (5/5, v/v; containing 20%
52 hexane) for untargeted lipidomic analyses.

53 Muscle extract samples were submitted to the meta-Phenotyper™ high-definition metabolomic
54 platform developed by iPhenome Biotechnology (Dalian, China), in which five complementary
55 analytical methods based on UPLC-HRMS were used. Untargeted metabolomic analyses were
56 conducted on an Ultimate™ 3000 UHPLC system coupled to a Q Exactive™ quadrupole Orbitrap
57 mass spectrometer (Thermo Scientific, San Jose, CA, USA). In a typical procedure, the first fraction
58 of polar extracts was separated using an ACE Excel PFP-C18 column (Advanced Chromatography
59 Technologies Ltd., Aberdeen, Scotland, 2.1×100 mm²) and eluted with 0.1% formate/water and
60 0.1% formate/acetonitrile through linear gradient ramping from 2% organic mobile phase to 98% in
61 12 min. Detection was performed under positive electrospray mode. The second fraction
62 comprising water and ammonium acetonitrile/methanol both containing 5 mM ammonium
63 bicarbonate buffer salt was used to elute metabolites separated on an Acquity HSS C18 column
64 (Waters Corporation, Milford, USA; 1.7μ m, 2.1×100 mm²), and finally detected under negative
65 electrospray mode. The third polar fraction was analyzed by hydrophilic interaction chromatography
66 on an Acquity BEH Amide column (Waters Corporation, Milford, USA; 1.7μ m, 2.1×100 mm²) and
67 detected under negative electrospray ionization mode, in which 10% acetonitrile as weak eluent
68 and 50% acetonitrile as strong eluent were mixed with 10 mM ammonium acetate as buffer salt to
69 improve separation. Untargeted lipidomic analyses were performed under the same
70 chromatographic separation conditions operated under positive and negative ionization detection
71 modes, respectively. An Accucore C30 core-shell column (Thermo Scientific, Bellefonte, USA; 2.6
72 μ m, 2.1×100 mm²) was utilized for lipid molecule separation. A binary mobile phase comprising
73 60% acetonitrile in water and 10% acetonitrile in isopropanol both containing 10 mM ammonium
74 formate and 0.1% formate was used to elute lipid molecules. In all profiling methods, full-scan
75 mass-spectral data under 70 000 FWHM resolution and the top 10 full-scan data-dependent
76 MS/MS spectra data were acquired with XCalibur software (Thermo Scientific, San Jose, CA, USA).

77 The peaks were further processed with Compound Discoverer software (Thermo Scientific,
78 San Jose, CA, USA) for metabolic component extraction. The polar metabolites were structurally
79 annotated by searching against a local HMDB metabolite database and a local proprietary MS/MS
80 spectrum library (Small Molecule Orbitrap-based Library) created using authentic standards and
81 the online mzCloud library (www.mzcloud.org). Multiple chemical information including exact mass
82 of precursor, isotopic pattern fit score, MS/MS spectra similarity, and retention time was obtained
83 for metabolites structure annotation. Moreover, untargeted lipidomics data were processed with
84 LipidSearch software including peak picking and lipid identification. The acquired MS² spectra were
85 searched against in silico predicted spectra of diverse endogenous lipid classes. Lipid identification
86 was strictly manually checked and investigated one by one to eliminate false positives chiefly
87 basing on peak shake, adduct ions behavior, fragmentation pattern, and chromatographic behavior.
88 Finally, the resultant quantitative information from all measurements was merged and those
89 detected with multiple methods were excluded to guarantee the uniqueness of metabolite and lipid
90 for final statistical analysis. Principal component analysis and orthogonal partial-least-square-
91 discriminant analysis were performed with SIMCA-P software (Sartorius Umetrics, Germany).
92 Metabolic pathway enrichment analysis was conducted on the MetaboAnalyst website.

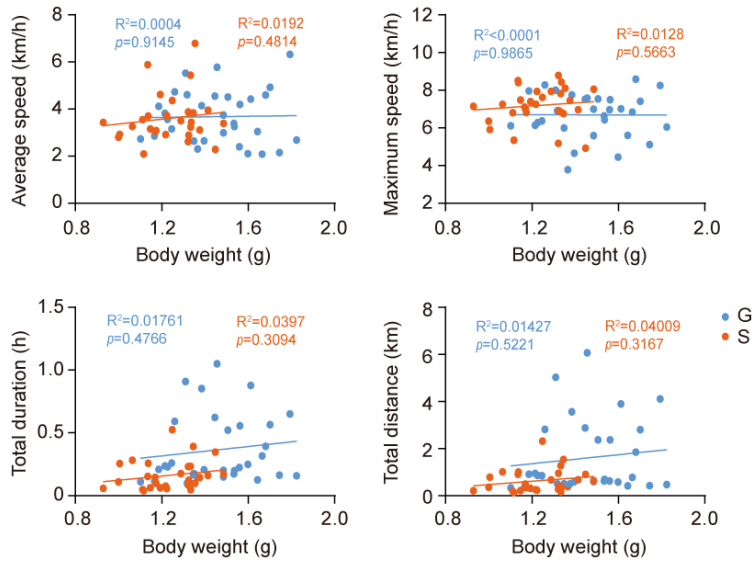
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97 **Fig. S1.** Comparison of flight traits between male and female locusts. Flight trait divergence
 98 between male and female in (A) gregarious and (B) solitary locusts. Blue point represents the
 99 gregarious individual and red point represents the solitary individual. All data are presented as the
 100 mean \pm SEM, n.s, not significant.

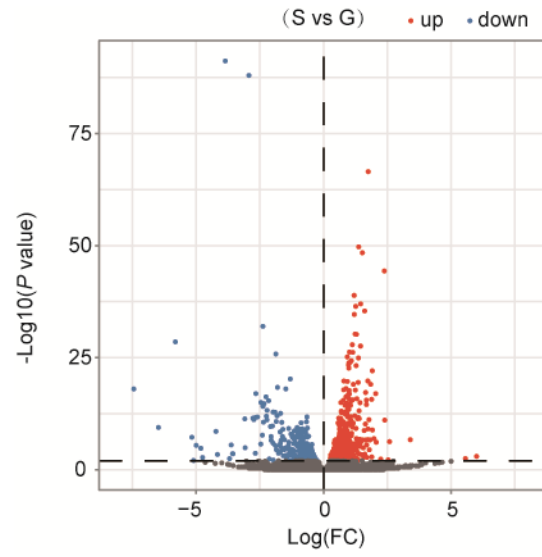
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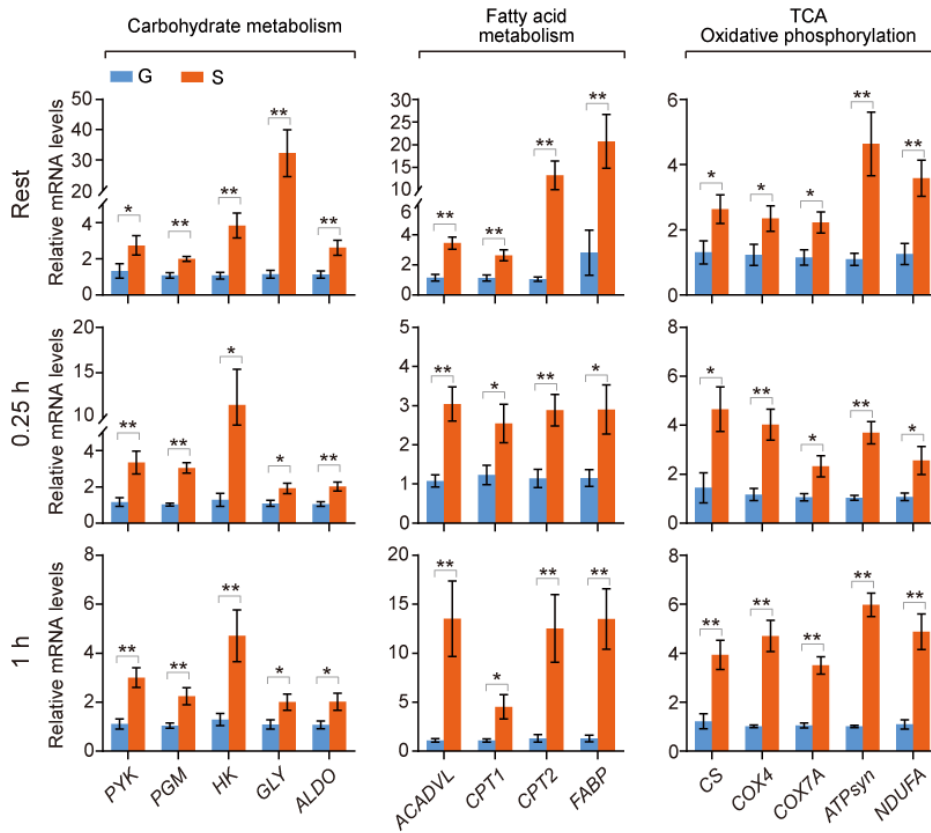
103 **Fig. S2.** Linear regression analysis of flight traits and body weight in gregarious and solitary locusts.
 104 Blue point represents the gregarious individual (G) and red point represents the solitary individual
 105 (S). Pearson correlation coefficients (R^2) and p values are presented. All data are presented as the
 106 mean \pm SEM.

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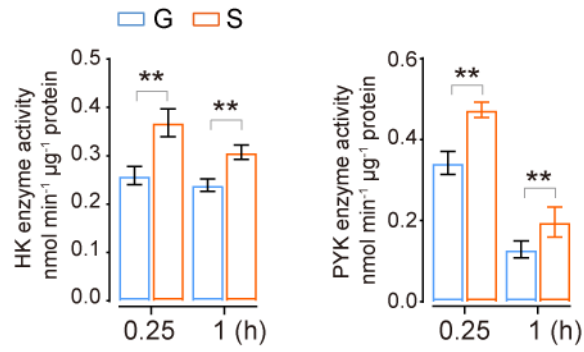
109 **Fig. S3.** Volcano plot of differential expression genes (DEGs) in flight muscles. DEGs with $p < 0.01$
110 were selected in solitary locusts (red point) and gregarious locusts (blue point). G and S represent
111 gregarious and solitary locusts, respectively.
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114 **Fig. S4.** qPCR verification of energy metabolism genes. Error bars represent the SEM. Significant
 115 differences are denoted by * $p < 0.05$, ** $p < 0.01$ ($n = 8$, Student's t test). Abbreviations: S, solitary;
 116 G, gregarious; PYK, pyruvate kinase; PGM; phosphoglucomutase; HK, hexokinase; GLY, glycogen
 117 phosphorylase; ALDO, fructose-bisphosphate aldolase; ACADVL, very long-chain specific acyl-
 118 CoA dehydrogenase; CPT, carnitine O-palmitoyl transferase; FABP, fatty acid binding protein; CS,
 119 citrate synthase; COX, cytochrome c oxidase subunit; ATPsyn, ATP synthase; NDUFA, NADH
 120 dehydrogenase subcomplex subunit. All data are presented as the mean \pm SEM, * $p < 0.05$, ** $p <$
 121 0.01.

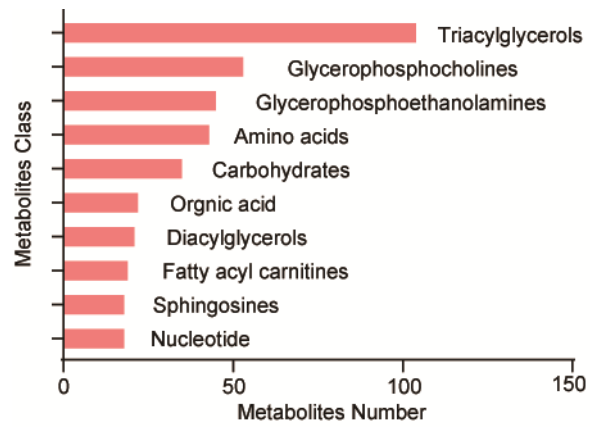
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124 **Fig. S5.** Comparison of enzyme activities of hexokinase and pyruvate kinase during the flight
 125 process between gregarious and solitary locusts (n = 8 replicates, 3 locusts/replicate, Student's t
 126 test). G and S represent gregarious and solitary locusts, respectively. All data are presented as the
 127 mean ± SEM, **p* < 0.05, ***p* < 0.01.

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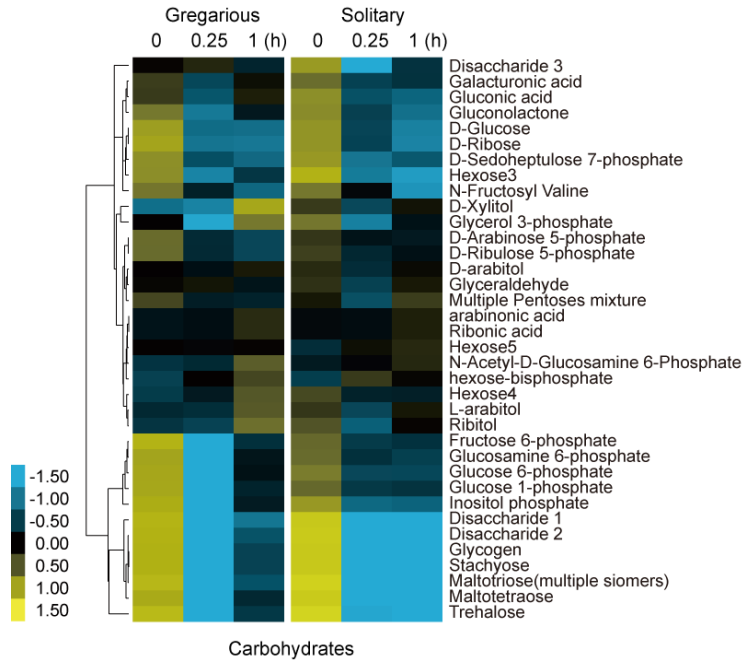


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130 **Fig. S6.** Metabolite class analysis of all differential metabolites after flight treatment. Metabolites
 131 with a *p* value of less than 0.05 are included.

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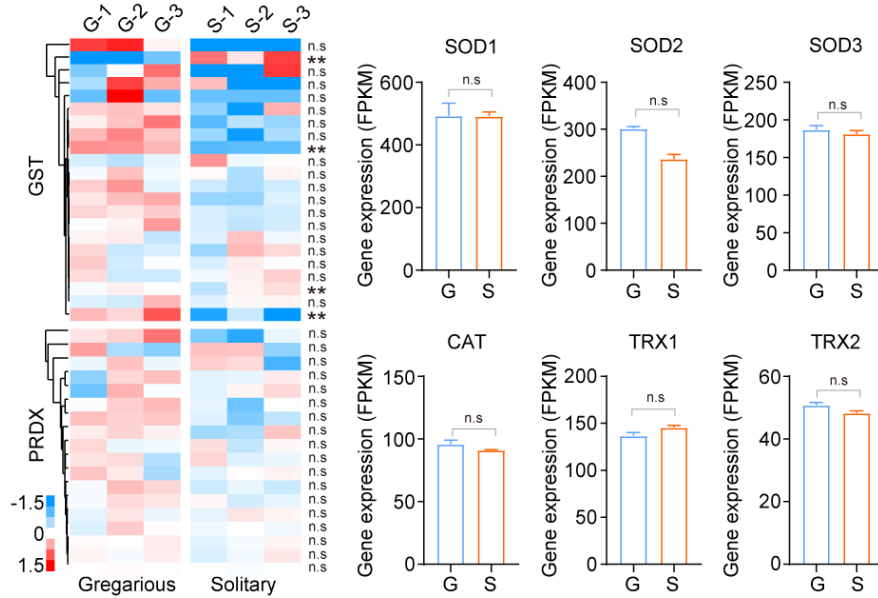
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135 **Fig. S7.** The variation of carbohydrates after flight treatment between gregarious and solitary
136 locusts. Yellow and blue signals represent higher and lower levels, respectively. The dendrograms
137 generated by the hierarchical clustering of metabolites are also provided. Heat-map signal indicates
138 \log_2 fold-change value relative to the median expression level within the gregarious and solitary
139 groups, respectively.

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Fig.S8. Comparison of antioxidant genes expression between gregarious and solitary locusts. Red signal represents higher expression, whereas blue represents lower expression. GST, Glutathione S-transferase; PRDX, Peroxiredoxin; SOD, Superoxide dismutase; CAT, Catalase; TRX, Thioredoxin reductase; G, gregarious locusts; S, solitary locusts. (n = 3 replicates, 6 locusts/replicate). Student's *t* test. Mean \pm SEM. Significant differences are denoted by * $p < 0.05$, ** $p < 0.01$, and n.s, not significant.

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Table S1. The list of metabolites that have different abundance after 0.25 or 1 h flight treatment in flight muscle. G and S represent gregarious and solitary locusts, respectively. 0/0.25 h, 0/1 h represent different time flight treatments compared to the rest condition samples. Five biological replicates for each flight treatment time point, and each replicate contains six locusts.

Metabolite	Class	G: 0/0.25 h (p value)	G: 0/1 h (p value)	S: 0/0.25 h (p value)	S: 0/1 h (p value)
WE(23:4)_WE(23:4)	Wax monoesters	0.0430	0.0084	0.0259	0.0023
Pantothenic acid	Vitamin	0.0235	0.1434	0.4497	0.4717
Riboflavin	Vitamin	0.6567	0.2964	0.0014	0.1010
Trigonelline	Vitamin	0.4828	0.2025	0.1582	0.0264
Coenzyme Q10	Ubiquinones	0.8542	0.0082	0.0473	0.0883
Coenzyme Q9	Ubiquinones	0.6794	0.0773	0.0661	0.0450
TG(42:0)_TG(16:0/12:0/14:0)	Triacylglycerols	0.8021	0.0269	0.0439	0.3545
TG(42:1)_TG(14:0/14:1/14:0)	Triacylglycerols	0.7233	0.4192	0.0216	0.7047
TG(44:0)_TG(16:0/14:0/14:0)	Triacylglycerols	0.3806	0.0305	0.0220	0.0520
TG(44:3)_TG(16:0/10:0/18:3)	Triacylglycerols	0.2189	0.0479	0.1125	0.7380
TG(45:0)_TG(15:0/14:0/16:0)	Triacylglycerols	0.3460	0.0334	0.4641	0.5279
TG(45:2)_TG(15:0/16:1/14:1)	Triacylglycerols	0.3677	0.2293	0.0002	0.0004
TG(45:3)_TG(15:1/15:1/15:1)	Triacylglycerols	0.2480	0.0511	0.0107	0.0125
TG(46:1)_TG(14:0/18:1/14:0)	Triacylglycerols	0.1910	0.0223	0.0352	0.0547
TG(46:1)_TG(16:0/12:0/18:1)	Triacylglycerols	0.1910	0.0223	0.0352	0.0547
TG(46:1)_TG(16:0/14:0/16:1)	Triacylglycerols	0.1910	0.0223	0.0352	0.0547
TG(46:2)_TG(10:0/18:1/18:1)	Triacylglycerols	0.2938	0.1007	0.0048	0.0122
TG(46:3)_TG(10:0/18:1/18:2)	Triacylglycerols	0.5917	0.3280	0.0317	0.1185
TG(46:3)_TG(16:0/12:0/18:3)	Triacylglycerols	0.2902	0.0366	0.1357	0.1834
TG(47:2)_TG(14:0/15:0/18:2)	Triacylglycerols	0.9449	0.2158	0.0117	0.1907
TG(47:3)_TG(12:0/17:1/18:2)	Triacylglycerols	0.1346	0.6200	0.0066	0.0365
TG(47:4)_TG(12:0/17:1/18:3)	Triacylglycerols	0.3706	0.0468	0.2764	0.1655
TG(48:1)_TG(16:0/14:0/18:1)	Triacylglycerols	0.1557	0.0405	0.0325	0.0122
TG(48:2)_TG(12:0/18:1/18:1)	Triacylglycerols	0.3230	0.1079	0.0022	0.0067
TG(48:2)_TG(16:0/14:0/18:2)	Triacylglycerols	0.3230	0.1079	0.0022	0.0067
TG(48:2)_TG(16:1/14:0/18:1)	Triacylglycerols	0.3388	0.0377	0.0658	0.0421
TG(48:3)_TG(14:0/18:3/16:0)	Triacylglycerols	0.2965	0.0148	0.1104	0.1245
TG(48:3)_TG(18:1/12:0/18:2)	Triacylglycerols	0.2496	0.1222	0.3382	0.0422
TG(48:5)_TG(12:0/18:2/18:3)	Triacylglycerols	0.2922	0.0348	0.2514	0.2036
TG(48:6)_TG(12:0/18:3/18:3)	Triacylglycerols	0.2311	0.0224	0.0523	0.2290
TG(49:0)_TG(16:0/16:0/17:0)	Triacylglycerols	0.6819	0.1358	0.0020	0.0088
TG(49:1)_TG(49:1)	Triacylglycerols	0.3361	0.1340	0.0335	0.0460
TG(49:2)_TG(15:0/16:0/18:2)	Triacylglycerols	0.1264	0.0282	0.0021	0.0038
TG(49:2)_TG(15:0/16:1/18:1)	Triacylglycerols	0.1490	0.0482	0.0023	0.0049
TG(49:3)_TG(15:0/16:0/18:3)	Triacylglycerols	0.1670	0.0293	0.1573	0.1037
TG(49:4)_TG(14:0/20:4/15:0)	Triacylglycerols	0.4407	0.0404	0.3330	0.3702
TG(50:1)_TG(16:0/16:0/18:1)	Triacylglycerols	0.1130	0.0258	0.2949	0.0404
TG(50:2)_TG(16:0/16:0/18:2)	Triacylglycerols	0.3324	0.2126	0.0047	0.0158
TG(50:3)_TG(16:0/16:0/18:3)	Triacylglycerols	0.0965	0.0223	0.4540	0.3332
TG(50:3)_TG(16:1/16:1/18:1)	Triacylglycerols	0.3104	0.1397	0.0050	0.0082
TG(50:5)_TG(14:0/18:2/18:3)	Triacylglycerols	0.2826	0.0494	0.1686	0.1970
TG(50:6)_TG(14:0/14:0/22:6)	Triacylglycerols	0.4222	0.0139	0.0154	0.0350
TG(50:6)_TG(14:0/18:3/18:3)	Triacylglycerols	0.4479	0.0123	0.0331	0.0713
TG(51:0)_TG(18:0/16:0/17:0)	Triacylglycerols	0.8372	0.0848	0.0001	0.0004
TG(51:1)_TG(15:0/20:0/16:1)	Triacylglycerols	0.3433	0.3455	0.0326	0.0034
TG(51:1)_TG(16:0/17:0/18:1)	Triacylglycerols	0.4212	0.0829	0.0005	0.0010
TG(51:2)_TG(16:0/17:0/18:2)	Triacylglycerols	0.3874	0.1063	0.0003	0.0011
TG(51:2)_TG(16:0/17:1/18:1)	Triacylglycerols	0.3549	0.0270	0.4340	0.4500
TG(51:3)_TG(15:0/18:1/18:2)	Triacylglycerols	0.3404	0.0088	0.8739	0.4009
TG(51:4)_TG(16:0/17:1/18:3)	Triacylglycerols	0.7647	0.0106	0.0120	0.0407
TG(51:5)_TG(15:0/18:2/18:3)	Triacylglycerols	0.3124	0.0645	0.0369	0.0052
TG(52:0)_TG(18:0/16:0/18:0)	Triacylglycerols	0.4414	0.0375	0.0028	0.0088
TG(52:1)_TG(18:0/16:0/18:1)	Triacylglycerols	0.2456	0.0687	0.0170	0.0286
TG(52:2)_TG(18:0/16:0/18:2)	Triacylglycerols	0.4035	0.1723	0.0254	0.0354
TG(52:2p)_TG(52:2p)	Triacylglycerols	0.7370	0.8133	0.0767	0.0172
TG(52:3)_TG(16:0/18:1/18:2)	Triacylglycerols	0.6303	0.0620	0.0156	0.0568
TG(52:3)_TG(16:1/18:1/18:1)	Triacylglycerols	0.3668	0.2427	0.0034	0.0087
TG(52:3)_TG(18:0/16:0/18:3)	Triacylglycerols	0.6303	0.0620	0.0156	0.0568
TG(52:4)_TG(16:0/18:1/18:3)	Triacylglycerols	0.3783	0.1425	0.2076	0.0032
TG(52:5)_TG(16:0/18:2/18:3)	Triacylglycerols	0.3321	0.1055	0.0497	0.0487
TG(52:8)_TG(14:0/18:3/20:5)	Triacylglycerols	0.4384	0.0733	0.0126	0.8178
TG(52:9)_TG(12:0/18:3/22:6)	Triacylglycerols	0.4850	0.0560	0.0016	0.0255
TG(53:0)_TG(17:0/18:0/18:0)	Triacylglycerols	0.6612	0.3015	0.0009	0.0030
TG(53:1)_TG(15:0/22:0/16:1)	Triacylglycerols	0.3236	0.1590	0.0023	0.0034
TG(53:1)_TG(17:0/18:0/18:1)	Triacylglycerols	0.4778	0.0540	0.0001	0.0003
TG(53:2)_TG(17:0/18:1/18:1)	Triacylglycerols	0.3836	0.0903	0.0005	0.0013
TG(53:3)_TG(17:0/18:1/18:2)	Triacylglycerols	0.4120	0.1232	0.0002	0.0008
TG(53:3)_TG(17:1/18:1/18:1)	Triacylglycerols	0.9483	0.6142	0.3509	0.0245
TG(53:4)_TG(17:1/18:1/18:2)	Triacylglycerols	0.3882	0.1502	0.0005	0.0026
TG(53:5)_TG(17:0/18:2/18:3)	Triacylglycerols	0.1873	0.0601	0.0093	0.0185
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TG(53:6)_TG(15:0/16:1/22:5)	Triacylglycerols	0.1935	0.0763	0.0161	0.0542

TG(53:6)_TG(17:0/18:3/18:3)	Triacylglycerols	0.3636	0.1306	0.0003	0.0024
TG(53:7)_TG(17:1/18:3/18:3)	Triacylglycerols	0.2817	0.3360	0.0030	0.0107
TG(54:0)_TG(18:0/18:0/18:0)	Triacylglycerols	0.5360	0.2934	0.0062	0.0125
TG(54:1)_TG(18:0/18:0/18:1)	Triacylglycerols	0.4329	0.0707	0.0193	0.0286
TG(54:2)_TG(18:0/18:0/18:2)	Triacylglycerols	0.4551	0.1150	0.0008	0.0022
TG(54:2)_TG(18:0/18:1/18:1)	Triacylglycerols	0.2572	0.0890	0.0173	0.0330
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TG(54:3)_TG(18:1/18:1/18:1)	Triacylglycerols	0.2674	0.1159	0.0290	0.0568
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TG(54:4)_TG(18:1/18:1/18:2)	Triacylglycerols	0.4008	0.2931	0.0813	0.0547
TG(54:5)_TG(16:0/18:1/20:4)	Triacylglycerols	0.3779	0.0781	0.0022	0.0025
TG(54:6)_TG(16:0/18:1/20:5)	Triacylglycerols	0.4988	0.0375	0.2688	0.9878
TG(54:6)_TG(18:1/18:2/18:3)	Triacylglycerols	0.9395	0.5060	0.9956	0.0002
TG(54:7)_TG(16:1/18:2/20:4)	Triacylglycerols	0.4386	0.1620	0.0410	0.0016
TG(54:7)_TG(18:1/18:3/18:3)	Triacylglycerols	0.2024	0.0556	0.3480	0.5015
TG(54:9)_TG(18:3/18:3/18:3)	Triacylglycerols	0.5583	0.0279	0.0064	0.0144
TG(55:3)_TG(18:0/18:1/18:2)	Triacylglycerols	0.3231	0.1068	0.0001	0.0020
TG(55:3)_TG(19:1/18:1/18:1)	Triacylglycerols	0.3549	0.0939	0.0013	0.0119
TG(55:4)_TG(19:1/18:1/18:2)	Triacylglycerols	0.2969	0.0669	0.0025	0.0154
TG(55:6)_TG(19:1/18:2/18:3)	Triacylglycerols	0.2203	0.0715	0.0054	0.0261
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TG(58:1)_TG(16:0/18:1/24:0)	Triacylglycerols	0.6348	0.5465	0.0014	0.0085
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TG(58:4)_TG(22:0/18:2/18:2)	Triacylglycerols	0.2732	0.1642	0.0009	0.2457
TG(58:5)_TG(18:0/18:1/22:4)	Triacylglycerols	0.9674	0.7993	0.0107	0.0997
TG(58:5)_TG(18:1/18:1/22:3)	Triacylglycerols	0.2463	0.1329	0.0107	0.0997
TG(58:6)_TG(18:1/18:1/22:4)	Triacylglycerols	0.1815	0.0376	0.0990	0.9571
TG(59:1)_TG(15:0/22:1/22:0)	Triacylglycerols	0.3861	0.0738	0.0016	0.0094
Cer(d32:1)_Cer(d18:1/14:0)	Sphingosines	0.1425	0.0792	0.3754	0.0493
Cer(d34:1)_Cer(d14:1/20:0)	Sphingosines	0.3461	0.0249	0.2615	0.0437
Cer(d34:1)_Cer(d16:1/18:0)	Sphingosines	0.0271	0.0272	0.2471	0.0521
Cer(d35:1)_Cer(d18:1/17:0)	Sphingosines	0.8037	0.0116	0.0097	0.4967
Cer(d36:1)_Cer(d16:1/20:0)	Sphingosines	0.3403	0.0128	0.5389	0.1220
Cer(d38:1)_Cer(d16:1/22:0)	Sphingosines	0.4131	0.0334	0.6445	0.3633
Cer(d38:1)_Cer(d18:1/20:0)	Sphingosines	0.4131	0.0334	0.6445	0.3633
Cer(d40:1)_Cer(d16:1/24:0)	Sphingosines	0.3832	0.0163	0.7859	0.0649
Phytosphingosine	Sphingosines	0.8900	0.0403	0.8013	0.9347
SM(d32:2)_SM(d32:2)	Sphingosines	0.3123	0.7868	0.0350	0.1940
SM(d34:1+PO)_SM(d34:1(OH))	Sphingosines	0.5004	0.6913	0.0515	0.0040
SM(d34:2)_SM(d34:2)	Sphingosines	0.0888	0.0301	0.3142	0.2514
SM(d35:1)_SM(d35:1)	Sphingosines	0.4313	0.5069	0.0142	0.0106
SM(d35:2)_SM(d35:2)	Sphingosines	0.1665	0.0130	0.3389	0.2896
SM(d36:0)_SM(d36:0)	Sphingosines	0.7672	0.5019	0.4288	0.0447
SM(d36:1)_SM(d36:1)	Sphingosines	0.5784	0.0281	0.2563	0.0027
SM(d37:1)_SM(d37:1)	Sphingosines	0.8284	0.3843	0.0020	0.0051
SM(d38:2)_SM(d38:2)	Sphingosines	0.0368	0.2335	0.0935	0.4995
SM(d39:1)_SM(d39:1)	Sphingosines	0.9228	0.6200	0.1255	0.0007
Glycerophosphoric acid	Phosphates	0.1171	0.2170	0.0015	0.0886
Ala-Ala[alanyl-alanine]	Peptides	0.1431	0.4521	0.9602	0.0136
Ala-Gly[alanyl-glycine]	Peptides	0.0901	0.0131	0.0394	0.0283
gamma-Glu-Ile[gamma-Glutamylisoleucine]	Peptides	0.4887	0.0794	0.9540	0.0221
Glu-ala[gamma-Glutamylalanine]	Peptides	0.0286	0.0214	0.0059	0.0055
Glu-Met[gamma-Glutamyl-methionine]	Peptides	0.5489	0.4201	0.0536	0.0073
Gly-Gly[Gly-glycine]	Peptides	0.0209	0.0367	0.4749	0.6940
Homo-L-arg[Homo-L-arginine]	Peptides	0.2659	0.5684	0.0422	0.0305
N,N,N-Trimethyl-L-alanyl-L-proline betaine	Peptides	0.7680	0.6988	0.0013	0.0022
Ophthalmic acid(analogue glutathione)	Peptides	0.2434	0.1983	0.0452	0.0444
Val-Asp	Peptides	0.4080	0.2003	0.0233	0.2412
Val-Lys	Peptides	0.3311	0.4475	0.0404	0.0828
Val-Val	Peptides	0.0002	0.0015	0.0001	0.0084
(R)-3-Hydroxyisobutyric acid	Organic acid	0.0395	0.3895	0.2396	0.3768
(R)-b-aminoisobutyric acid	Organic acid	0.0191	0.7769	0.1854	0.5240
(R)-beta-Hydroxybutyric acid	Organic acid	0.0012	0.0009	0.0450	0.0004
(S)-3,4-Dihydroxybutyric acid	Organic acid	0.0001	0.0001	0.0003	0.0000

(S)-3-Hydroxyisobutyric acid	Orgnic acid	0.0441	0.0012	0.1501	0.0016
2-Hydroxyglutarate	Orgnic acid	0.4197	0.0212	0.0114	0.0252
3-Oxoglutaric acid	Orgnic acid	0.1064	0.1310	0.0026	0.0099
acetyl citrate	Orgnic acid	0.1043	0.1290	0.0028	0.0108
Aconitic acid	Orgnic acid	0.6918	0.2601	0.0011	0.5353
Adipic acid	Orgnic acid	0.0000	0.0000	0.0000	0.0002
beta-Hydroxybutyric acid	Orgnic acid	0.8284	0.2168	0.0013	0.1274
cis-aconitic acid	Orgnic acid	0.0676	0.9664	0.0278	0.4627
Citraconic acid	Orgnic acid	0.5956	0.2857	0.0009	0.2220
Citric acid	Orgnic acid	0.1272	0.4862	0.0368	0.1565
Fumaric acid	Orgnic acid	0.0013	0.2212	0.9817	0.0509
Glutaconic acid	Orgnic acid	0.6253	0.2790	0.0009	0.2257
Glutaric acid	Orgnic acid	0.2211	0.9101	0.0071	0.0197
Hydroxypropionic acid	Orgnic acid	0.0017	0.0041	0.0033	0.0001
L-Malic acid	Orgnic acid	0.0001	0.6339	0.7194	0.1074
Methylglutaric acid	Orgnic acid	0.5864	0.9234	0.0033	0.0055
Pyruvic acid	Orgnic acid	0.1230	0.1368	0.0020	0.0065
Succinic acid	Orgnic acid	0.0087	0.1297	0.0001	0.3385
Succinic acid semialdehyde	Orgnic acid	0.0000	0.0001	0.0005	0.0000
5'-Methylthioadenosine	Nucleotide	0.1604	0.2896	0.0034	0.1754
5-Methyluridine(Ribothymidine)	Nucleotide	0.2122	0.0150	0.7140	0.4639
Adenosine	Nucleotide	0.0186	0.1223	0.6915	0.4259
Adenosine monophosphate	Nucleotide	0.0671	0.0755	0.0959	0.2837
Adenosine triphosphate	Nucleotide	0.4204	0.0421	0.6241	0.8344
ADP	Nucleotide	0.7442	0.3405	0.2047	0.7702
Allantoin	Nucleotide	0.3432	0.3535	0.0141	0.0991
Citicoline	Nucleotide	0.8714	0.1923	0.0489	0.0593
Cytidine	Nucleotide	0.8011	0.0133	0.3255	0.1019
Guanosine	Nucleotide	0.3927	0.5861	0.0047	0.0385
Guanosine diphosphate	Nucleotide	0.0404	0.0965	0.0208	0.0528
Hypoxanthine	Nucleotide	0.7097	0.1303	0.0272	0.0950
Inosine	Nucleotide	0.0180	0.2234	0.0439	0.0254
Inosinic acid	Nucleotide	0.1945	0.8113	0.0015	0.0239
Pseudouridine	Nucleotide	0.0277	0.3746	0.7621	0.3627
Succinyladenosine	Nucleotide	0.6616	0.0038	0.0082	0.0170
Uracil	Nucleotide	0.2218	0.2874	0.2419	0.0219
Uric acid	Nucleotide	0.4380	0.1599	0.0388	0.0091
Uridine	Nucleotide	0.0006	0.7071	0.0003	0.1979
Uridine diphosphate-	Nucleotide	0.1245	0.0150	0.0042	0.2973
N-acetylglucosamine	Nucleotide	0.5631	0.0496	0.0041	0.0105
Xanthine	Nucleotide	0.0024	0.0425	0.1142	0.9005
LysoPS(18:0)	Glycerophosphoserines	0.1342	0.0449	0.4432	0.1701
PS(36:2)_PS(18:0/18:2)	Glycerophosphoserines	0.1845	0.0102	0.8028	0.0883
PS(36:2)_PS(18:1/18:1)	Glycerophosphoserines	0.1637	0.1453	0.0234	0.1018
PS(40:6)_PS(18:0/22:6)	Glycerophosphoserines	0.4419	0.1090	0.0075	0.1610
LysoPI(0:0/18:0)	Glycerophosphoinositols	0.0360	0.1119	0.3911	0.7594
LysoPI(18:0/0:0)	Glycerophosphoinositols	0.2429	0.4809	0.0383	0.0837
LysoPI(18:2)	Glycerophosphoinositols	0.0035	0.3015	0.6203	0.1827
PI(32:0)_PI(16:0/16:0)	Glycerophosphoinositols	0.2846	0.0909	0.0012	0.0064
PI(32:1)_PI(16:0/16:1)	Glycerophosphoinositols	0.7319	0.7857	0.0322	0.5516
PI(34:1)_PI(16:0/18:1)	Glycerophosphoinositols	0.1758	0.1061	0.0102	0.2080
PI(34:2)_PI(16:0/18:2)	Glycerophosphoinositols	0.4911	0.2465	0.0029	0.0185
PI(36:2)_PI(18:1/18:1)	Glycerophosphoinositols	0.2378	0.3246	0.3405	0.0306
PI(36:3)_PI(18:1/18:2)	Glycerophosphoinositols	0.0161	0.1386	0.9312	0.1589
PI(38:3)_PI(18:0/20:3)	Glycerophosphoinositols	0.5363	0.7524	0.0019	0.8372
PG(34:1)_PG(16:0/18:1)	Glycerophosphoglycerols	0.0653	0.3558	0.0016	0.2819
PG(34:2)_PG(16:0/18:2)	Glycerophosphoglycerols	0.0653	0.3558	0.0016	0.2819
PG(34:2)_PG(16:1/18:1)	Glycerophosphoglycerols	0.4852	0.9056	0.0471	0.9816
PG(36:1)_PG(36:1)	Glycerophosphoglycerols	0.4456	0.3424	0.0009	0.0512
PG(36:2)_PG(18:1/18:1)	Glycerophosphoglycerols	0.1576	0.5889	0.0226	0.2398
PG(36:3)_PG(18:1/18:2)	Glycerophosphoglycerols	0.0783	0.0866	0.0509	0.0201
PG(36:5)_PG(18:3/18:2)	Glycerophosphoglycerols	0.1798	0.4282	0.1595	0.0281
LysoPE(0:0/16:0)	Glycerophosphoethanolamines	0.6095	0.7689	0.0220	0.1324
LysoPE(0:0/18:2)	Glycerophosphoethanolamines	0.2182	0.3881	0.1016	0.0443
LysoPE(16:0/0:0)	Glycerophosphoethanolamines	0.3211	0.2904	0.5554	0.0396
LysoPE(17:0/0:0)	Glycerophosphoethanolamines	0.7532	0.8015	0.0314	0.1937
LysoPE(18:2/0:0)	Glycerophosphoethanolamines	0.0075	0.6795	0.7755	0.1640
PE(30:0)_PE(16:0/14:0)	Glycerophosphoethanolamines	0.0008	0.0598	0.1995	0.6024
PE(32:1)_PE(16:0/16:1)	Glycerophosphoethanolamines	0.1778	0.0619	0.0390	0.0047
PE(32:1p)_PE(16:0p/16:1)	Glycerophosphoethanolamines	0.0001	0.2208	0.0734	0.0138
PE(33:1)_PE(17:1/16:0)	Glycerophosphoethanolamines				

PE(33:3)_PE(33:3)	Glycerophosphoethanola mines	0.0415	0.2062	0.2731	0.9260
PE(34:0)_PE(18:0/16:0)	Glycerophosphoethanola mines	0.0151	0.0044	0.3554	0.3395
PE(34:1)_PE(16:0/18:1)	Glycerophosphoethanola mines	0.0109	0.1225	0.0246	0.1433
PE(34:1p)_PE(34:1p)	Glycerophosphoethanola mines	0.0095	0.4494	0.0488	0.9320
PE(34:2)_PE(16:0/18:2)	Glycerophosphoethanola mines	0.0120	0.5027	0.0292	0.5920
PE(34:2)_PE(16:1/18:1)	Glycerophosphoethanola mines	0.0120	0.5027	0.0292	0.5920
PE(34:2p)_PE(34:2p)	Glycerophosphoethanola mines	0.0657	0.9401	0.0306	0.2225
PE(35:2)_PE(17:1/18:1)	Glycerophosphoethanola mines	0.1370	0.9868	0.0002	0.0008
PE(35:2p)_PE(18:1p/17:1)	Glycerophosphoethanola mines	0.4078	0.7598	0.0211	0.0101
PE(35:3)_PE(17:1/18:2)	Glycerophosphoethanola mines	0.0009	0.1555	0.0449	0.1628
PE(35:4)_PE(17:1/18:3)	Glycerophosphoethanola mines	0.0335	0.0843	0.4091	0.4986
PE(36:1)_PE(18:0/18:1)	Glycerophosphoethanola mines	0.2036	0.9895	0.0468	0.2070
PE(36:1p)_PE(36:1p)	Glycerophosphoethanola mines	0.8955	0.0664	0.1494	0.0098
PE(36:2)_PE(18:0/18:2)	Glycerophosphoethanola mines	0.1846	0.0171	0.0014	0.0299
PE(36:2)_PE(18:1/18:1)	Glycerophosphoethanola mines	0.0545	0.6526	0.0261	0.2481
PE(36:2p)_PE(18:0p/18:2)	Glycerophosphoethanola mines	0.9615	0.0469	0.0131	0.0362
PE(36:3)_PE(18:1/18:2)	Glycerophosphoethanola mines	0.0005	0.0780	0.0402	0.1861
PE(36:3p)_PE(P-16:0/20:3n6)	Glycerophosphoethanola mines	0.3412	0.0489	0.0233	0.4673
PE(36:3p)_PE(P-16:0/20:3n9)	Glycerophosphoethanola mines	0.3412	0.0489	0.0233	0.4673
PE(36:3p)_PE(P-18:1/18:2)	Glycerophosphoethanola mines	0.3418	0.0491	0.0233	0.4674
PE(36:6)_PE(18:3/18:3)	Glycerophosphoethanola mines	0.1351	0.1914	0.0042	0.1378
PE(37:2)_PE(19:0/18:2)	Glycerophosphoethanola mines	0.5844	0.4549	0.0001	0.0008
PE(37:2)_PE(19:1/18:1)	Glycerophosphoethanola mines	0.9693	0.2733	0.0035	0.0069
PE(37:3)_PE(19:0/18:3)	Glycerophosphoethanola mines	0.0947	0.5583	0.0026	0.0383
PE(38:1)_PE(20:0/18:1)	Glycerophosphoethanola mines	0.1312	0.5571	0.0028	0.0194
PE(38:1)_PE(38:1)	Glycerophosphoethanola mines	0.1730	0.9551	0.0065	0.0004
PE(38:1p)_PE(18:0p/20:1)	Glycerophosphoethanola mines	0.0605	0.0261	0.3050	0.0071
PE(38:2)_PE(20:0/18:2)	Glycerophosphoethanola mines	0.4122	0.0579	0.0468	0.1052
PE(38:2p)_PE(38:2p)	Glycerophosphoethanola mines	0.2431	0.0408	0.0137	0.0325
PE(38:3p)_PE(18:0p/20:3)	Glycerophosphoethanola mines	0.7985	0.0718	0.0426	0.0263
PE(38:3p)_PE(18:0p/20:3)isomer	Glycerophosphoethanola mines	0.8809	0.0324	0.3511	0.6809
PE(38:4)_PE(20:1/18:3)	Glycerophosphoethanola mines	0.3810	0.4449	0.0242	0.1881
PE(38:4)_PE(20:2/18:2)	Glycerophosphoethanola mines	0.0615	0.0082	0.7288	0.5773
PE(38:5)_PE(18:0/20:5)	Glycerophosphoethanola mines	0.0370	0.1724	0.4914	0.6832
PE(40:2)_PE(18:1/22:1)	Glycerophosphoethanola mines	0.3309	0.0650	0.0031	0.0015
PE(40:5)_PE(18:1/22:4)	Glycerophosphoethanola mines	0.0745	0.8285	0.0061	0.0014
PE(42:4)_PE(22:0/20:4)	Glycerophosphoethanola mines	0.9172	0.5782	0.2425	0.0100
LysoPC(0:0/14:0)	Glycerophosphocholines	0.3211	0.2904	0.5554	0.0396
LysoPC(0:0/15:0)	Glycerophosphocholines	0.0280	0.1403	0.4780	0.2908
LysoPC(0:0/18:1)	Glycerophosphocholines	0.3146	0.6806	0.0069	0.9693
LysoPC(0:0/18:2)	Glycerophosphocholines	0.9331	0.8712	0.0008	0.0985
LysoPC(0:0/18:3)	Glycerophosphocholines	0.5406	0.2741	0.0205	0.2795
LysoPC(14:0/0:0)	Glycerophosphocholines	0.3211	0.2904	0.5554	0.0396
LysoPC(15:0/0:0)	Glycerophosphocholines	0.0280	0.1403	0.4780	0.2908

LysoPC(17:0/0:0)	Glycerophosphocholines	0.0420	0.1976	0.1331	0.3641
LysoPC(18:0e)	Glycerophosphocholines	0.0000	0.0318	0.1084	0.6030
LysoPC(18:0p)	Glycerophosphocholines	0.0015	0.0608	0.6145	0.4820
LysoPC(18:1/0:0)	Glycerophosphocholines	0.2365	0.4916	0.0057	0.9742
LysoPC(18:2/0:0)	Glycerophosphocholines	0.6404	0.6510	0.0010	0.0584
LysoPC(18:3/0:0)	Glycerophosphocholines	0.5148	0.3545	0.0149	0.3184
PC(30:0)_PC(30:0)	Glycerophosphocholines	0.0034	0.0062	0.5870	0.7681
PC(30:0e)_PC(30:0e)	Glycerophosphocholines	0.0423	0.3564	0.2932	0.8603
PC(30:1)_PC(16:1/14:0)	Glycerophosphocholines	0.4640	0.3951	0.0462	0.2209
PC(31:1)_PC(17:1/14:0)	Glycerophosphocholines	0.0029	0.0357	0.0757	0.7265
PC(31:1)_PC(31:1)	Glycerophosphocholines	0.0751	0.0058	0.9649	0.7436
PC(32:0)_PC(16:0/16:0)	Glycerophosphocholines	0.0117	0.0341	0.9467	0.6563
PC(32:1)_PC(16:0/16:1)	Glycerophosphocholines	0.0009	0.1749	0.0208	0.5720
PC(32:1e)_PC(32:1e)	Glycerophosphocholines	0.1200	0.7088	0.9349	0.0137
PC(32:2)_PC(14:0/18:2)	Glycerophosphocholines	0.2406	0.0678	0.0030	0.8484
PC(32:4)_PC(32:4)	Glycerophosphocholines	0.0335	0.0843	0.4091	0.4986
PC(33:1)_PC(17:1/16:0)	Glycerophosphocholines	0.0033	0.0050	0.0605	0.0215
PC(33:2)_PC(33:2)	Glycerophosphocholines	0.0059	0.1353	0.0772	0.0763
PC(33:3)_PC(15:0/18:3)	Glycerophosphocholines	0.0245	0.0869	0.4129	0.3729
PC(34:1)_PC(16:0/18:1)	Glycerophosphocholines	0.0147	0.0309	0.0128	0.0673
PC(34:2)_PC(16:0/18:2)	Glycerophosphocholines	0.0005	0.5162	0.0014	0.0119
PC(35:2)_PC(17:0/18:2)	Glycerophosphocholines	0.5398	0.2659	0.0006	0.0053
PC(35:2)_PC(35:2)	Glycerophosphocholines	0.0456	0.1753	0.0189	0.0053
PC(35:4)_PC(17:1/18:3)	Glycerophosphocholines	0.0250	0.1164	0.1350	0.9515
PC(36:1)_PC(18:0/18:1)	Glycerophosphocholines	0.7220	0.7775	0.0973	0.0192
PC(36:1e)_PC(36:1e)	Glycerophosphocholines	0.8350	0.7072	0.0174	0.5462
PC(36:1p)_PC(18:0p/18:1)	Glycerophosphocholines	0.2230	0.0452	0.0018	0.1475
PC(36:2)_PC(18:0/18:2)	Glycerophosphocholines	0.3175	0.0297	0.0003	0.0005
PC(36:2e)_PC(36:2e)	Glycerophosphocholines	0.4915	0.1649	0.0276	0.1221
PC(36:3)_PC(16:0/20:3)	Glycerophosphocholines	0.6184	0.1909	0.0003	0.0147
PC(36:3)_PC(18:0/18:3)	Glycerophosphocholines	0.0012	0.0865	0.1290	0.1576
PC(36:3)_PC(18:1/18:2)	Glycerophosphocholines	0.0012	0.0865	0.1290	0.1576
PC(36:4e)_PC(36:4e)	Glycerophosphocholines	0.0386	0.0216	0.7419	0.9970
PC(36:6)_PC(18:3/18:3)	Glycerophosphocholines	0.5827	0.0549	0.0074	0.1657
PC(37:1)_PC(19:1/18:0)	Glycerophosphocholines	0.8396	0.9350	0.1076	0.0020
PC(37:2)_PC(37:2)mixture	Glycerophosphocholines	0.4625	0.7661	0.0463	0.6456
PC(38:1)_PC(22:0/16:1)	Glycerophosphocholines	0.3095	0.0916	0.3937	0.0361
PC(38:2)_PC(18:0/20:2)	Glycerophosphocholines	0.3427	0.9625	0.0337	0.5346
PC(38:2)_PC(38:2)	Glycerophosphocholines	0.8076	0.0112	0.0243	0.0035
PC(38:3)_PC(18:0/20:3)	Glycerophosphocholines	0.1424	0.9631	0.0018	0.1477
PC(38:3)_PC(18:1/20:2)	Glycerophosphocholines	0.5127	0.0017	0.7260	0.4916
PC(38:3e)_PC(38:3e)	Glycerophosphocholines	0.0225	0.0011	0.8901	0.5258
PC(38:4)_PC(18:0/20:4)	Glycerophosphocholines	0.6961	0.5107	0.0840	0.0115
PC(38:4)_PC(18:1/20:3)	Glycerophosphocholines	0.0139	0.0469	0.0250	0.0012
PC(38:4e)_PC(38:4e)	Glycerophosphocholines	0.1086	0.0040	0.7113	0.7184
PC(38:4p)_PC(38:4p)	Glycerophosphocholines	0.6136	0.3295	0.0086	0.0299
PC(38:6p)_PC(38:6p)	Glycerophosphocholines	0.8031	0.0686	0.0470	0.2048
2-trans,4-cis-Decadienoylcarnitine(acCa(10:2)9,12-	Fatty acyl carnitines	0.0027	0.2436	0.0374	0.3057
Hexadecadienoylcarnitine(acCa(16:2)6:2)	Fatty acyl carnitines	0.0005	0.1446	0.7891	0.1575
arachidonoylcarnitineacCa(20:4)	Fatty acyl carnitines	0.3769	0.9944	0.4417	0.0113
arachidylcarnitineacCa(20:0)	Fatty acyl carnitines	0.0900	0.0312	0.8674	0.0110
Butyrylcarnitine(acCa(4:0)cis-5-	Fatty acyl carnitines	0.0063	0.0543	0.0458	0.0004
Tetradecenoylcarnitine(acCa(14:1)	Fatty acyl carnitines	0.0068	0.3714	0.5372	0.3866
EicosenoylcarnitineacCa(20:1)	Fatty acyl carnitines	0.6747	0.6389	0.9761	0.0287
Hexanoylcarnitine(acCa(6:0)	Fatty acyl carnitines	0.2843	0.2070	0.3559	0.0033
Hydroxyhexadecanoylcarnitine(acCa(16:0-OH)	Fatty acyl carnitines	0.0163	0.0647	0.6519	0.5201
L-acetylcarnitine	Fatty acyl carnitines	0.7330	0.0573	0.0115	0.3555
Linolenyl carnitineacCa(18:3)	Fatty acyl carnitines	0.0047	0.0060	0.1238	0.0083
Linoleyl carnitine	Fatty acyl carnitines	0.0026	0.0079	0.8389	0.0224
L-Palmitoylcarnitine(AcCa(16:0)	Fatty acyl carnitines	0.0360	0.0909	0.8622	0.1675
Malonylcarnitine	Fatty acyl carnitines	0.1171	0.0099	0.0409	0.0875
Oleoylcarnitine(acCa(18:1)	Fatty acyl carnitines	0.0176	0.1357	0.8641	0.6290
Propionylcarnitine(acCa(3:0)	Fatty acyl carnitines	0.0007	0.3107	0.0152	0.0352
Succinylcarnitine	Fatty acyl carnitines	0.0106	0.0136	0.0005	0.0004
Tetradecadienecarnitine(AcCa14:2)	Fatty acyl carnitines	0.0020	0.3939	0.4462	0.2522
Tetradecanoylcarnitine(acCa(14:0)	Fatty acyl carnitines	0.0420	0.5687	0.7654	0.4241
Tetradecenoylcarnitine(acCa(14:1)	Fatty acyl carnitines	0.4267	0.6104	0.4790	0.0345
13S-hydroxyoctadecadienoic acid	Fatty acid	0.7481	0.6893	0.0235	0.0697
7Z,10Z-Hexadecadienoic acid(FFA(16:2)	Fatty acid	0.0685	0.1917	0.8583	0.0081
9,10,13-TriHOME	Fatty acid	0.6953	0.9400	0.0207	0.1538
9,12,13-TriHOME	Fatty acid	0.6840	0.9270	0.0202	0.1070
alpha-Linolenic acid	Fatty acid	0.0492	0.5171	0.8177	0.7572
Dodecanoic acid(FFA(12:0)	Fatty acid	0.8479	0.5543	0.1773	0.0184
Gamma-Linolenic acid	Fatty acid	0.0492	0.5171	0.8177	0.7572
Palmitoleic acid(FFA(16:1)	Fatty acid	0.1475	0.0211	0.6999	0.0602

Pentadecanoic acid(FFA(15:0)	Fatty acid	0.5248	0.0096	0.5694	0.4453
Diisobutyl phthalate	Exogenous	0.0275	0.9129	0.7554	0.4402
DG(32:1)_DG(18:1/14:0)	Diacylglycerols	0.0597	0.0717	0.3454	0.0184
DG(32:2)_DG(14:0/18:2)	Diacylglycerols	0.0368	0.0389	0.2982	0.0047
DG(32:3)_DG(14:0/18:3)	Diacylglycerols	0.0116	0.0165	0.3358	0.0043
DG(34:0)_DG(18:0/16:0)	Diacylglycerols	0.0679	0.0743	0.0574	0.0126
DG(34:1)_DG(16:0/18:1)	Diacylglycerols	0.1966	0.1086	0.1584	0.0488
DG(34:2)_DG(16:0/18:2)	Diacylglycerols	0.0588	0.0597	0.1573	0.0125
DG(34:2)_DG(16:1/18:1)	Diacylglycerols	0.0588	0.0597	0.1573	0.0125
DG(34:3)_DG(16:1/18:2)	Diacylglycerols	0.1082	0.0377	0.7328	0.0101
DG(35:2)_DG(17:0/18:2)	Diacylglycerols	0.0657	0.3337	0.0260	0.0371
DG(35:3)_DG(17:0/18:3)	Diacylglycerols	0.4477	0.5959	0.5103	0.0139
DG(35:3)_DG(17:1/18:2)	Diacylglycerols	0.1176	0.0280	0.2582	0.0048
DG(36:2)_DG(18:0/18:2)	Diacylglycerols	0.0371	0.0600	0.0641	0.0085
DG(36:3)_DG(18:0/18:3)	Diacylglycerols	0.0581	0.0598	0.1355	0.0308
DG(36:3)_DG(18:1/18:2)	Diacylglycerols	0.0103	0.0169	0.5596	0.0045
DG(36:4)_DG(18:2/18:2)	Diacylglycerols	0.2685	0.0581	0.0135	0.0418
DG(36:6)_DG(18:3/18:3)	Diacylglycerols	0.2876	0.2195	0.0455	0.0045
DG(37:4)_DG(19:1/18:3)	Diacylglycerols	0.3257	0.9378	0.8205	0.0014
DG(38:3)_DG(18:0/20:3)1	Diacylglycerols	0.0928	0.0717	0.0831	0.0011
DG(38:3)_DG(18:0/20:3)2	Diacylglycerols	0.8133	0.0182	0.8305	0.0011
DG(38:4)_DG(18:1/20:3)	Diacylglycerols	0.1430	0.0381	0.4836	0.0010
DG(38:5)_DG(18:2/18:3)	Diacylglycerols	0.2872	0.1263	0.3738	0.0105
DG(38:5)_DG(18:3/20:2)	Diacylglycerols	0.2872	0.1263	0.3738	0.0105
Glycerophosphocholine	Cholines	0.0002	0.0011	0.0031	0.0000
Phosphorylcholine	Cholines	0.3406	0.0432	0.0886	0.0272
CL(68:5)_CL(18:2/16:1/16:1/18:1)	Cardiolipins	0.7645	0.0832	0.0074	0.0004
CL(68:6)_CL(18:3/16:0/16:0/18:3)	Cardiolipins	0.7688	0.7834	0.0065	0.0024
CL(70:5)_CL(18:2/18:1/16:1/18:1)	Cardiolipins	0.9136	0.1682	0.1534	0.0326
CL(70:8)_CL(18:3/18:2/16:0/18:3)	Cardiolipins	0.1773	0.3146	0.0090	0.2722
CL(70:9)_CL(18:3/16:0/18:3/18:3)	Cardiolipins	0.3894	0.1137	0.0003	0.0117
CL(72:10)_CL(18:3/18:2/18:3/18:2)	Cardiolipins	0.4136	0.3314	0.0232	0.0060
CL(72:11)_CL(18:3/18:2/18:3/18:3)	Cardiolipins	0.1087	0.1458	0.1386	0.0236
CL(72:8)_CL(18:3/18:1/18:2/18:2)	Cardiolipins	0.5108	0.1073	0.0419	0.0047
arabinonic acid	Carbohydrates	0.8643	0.1290	0.8810	0.0359
D-Arabinose 5-phosphate	Carbohydrates	0.1221	0.0221	0.2254	0.1627
D-arabitol	Carbohydrates	0.7719	0.6688	0.0025	0.3313
D-Glucose	Carbohydrates	0.0001	0.0002	0.0004	0.0000
Disaccharide 1	Carbohydrates	0.0020	0.0059	0.0006	0.0010
Disaccharide 2	Carbohydrates	0.0000	0.0009	0.0001	0.0002
Disaccharide 3	Carbohydrates	0.6586	0.3713	0.0021	0.0161
D-Ribose	Carbohydrates	0.0001	0.0002	0.0005	0.0000
D-Ribulose 5-phosphate	Carbohydrates	0.1234	0.0216	0.1555	0.1710
D-Sedoheptulose 7-phosphate	Carbohydrates	0.0605	0.0545	0.0022	0.0019
D-Xylitol	Carbohydrates	0.7423	0.0000	0.0751	0.5553
Fructose 6-phosphate	Carbohydrates	0.0040	0.0472	0.0158	0.0353
Galacturonic acid	Carbohydrates	0.0625	0.5184	0.0003	0.0004
Gluconic acid	Carbohydrates	0.0410	0.6708	0.1431	0.1239
Gluconolactone	Carbohydrates	0.0003	0.0458	0.0004	0.0000
Glucosamine 6-phosphate	Carbohydrates	0.0039	0.1003	0.0331	0.0230
Glucose 1-phosphate	Carbohydrates	0.0010	0.0360	0.0075	0.0173
Glucose 6-phosphate	Carbohydrates	0.0026	0.1152	0.0083	0.0141
Glyceraldehyde	Carbohydrates	0.6355	0.1583	0.0120	0.4676
Glycerol 3-phosphate	Carbohydrates	0.0766	0.2586	0.0037	0.1668
Glycogen	Carbohydrates	0.0001	0.0049	0.0016	0.0026
Hexose3	Carbohydrates	0.0018	0.0083	0.0043	0.0022
Hexose4	Carbohydrates	0.6104	0.3293	0.0477	0.0420
Hexose5	Carbohydrates	0.7126	0.9989	0.0376	0.0124
hexose-bisphosphate	Carbohydrates	0.3685	0.0289	0.0078	0.1508
Inositol phosphate	Carbohydrates	0.0024	0.1063	0.0068	0.0114
L-arabitol	Carbohydrates	0.8716	0.0023	0.0551	0.5768
Maltotetraose	Carbohydrates	0.0000	0.0142	0.0088	0.0076
Maltotriose(multiple siomers)	Carbohydrates	0.0000	0.0015	0.0001	0.0001
Multiple Pentoses mixture	Carbohydrates	0.2737	0.3696	0.0013	0.5725
N-Acetyl-D-Glucosamine 6-Phosphate	Carbohydrates	0.6514	0.0021	0.2025	0.0206
N-Fructosyl Valine	Carbohydrates	0.0004	0.0001	0.0295	0.0002
Ribitol	Carbohydrates	0.6688	0.0002	0.0781	0.3877
Ribonic acid	Carbohydrates	0.8643	0.1290	0.8810	0.0359
Stachyose	Carbohydrates	0.0001	0.0049	0.0016	0.0026
Trehalose	Carbohydrates	0.0009	0.0112	0.0062	0.0029
(R)-2,3-Dihydroxy-3-methylvalerate	Amino acids	0.9946	0.2901	0.0018	0.0069
2-Hydroxyethanesulfonate	Amino acids	0.2596	0.8713	0.0115	0.1094
2-Oxoarginine	Amino acids	0.0009	0.0359	0.1395	0.4580
3-Sulfinoalanine	Amino acids	0.0512	0.0447	0.0632	0.1956
Agmatine	Amino acids	0.9869	0.1897	0.0130	0.1036
allysine	Amino acids	0.0036	0.0037	0.0006	0.0021
aspartylglycosamine	Amino acids	0.0000	0.0008	0.0017	0.0000
beta-alanine	Amino acids	0.8654	0.6800	0.0132	0.0014
Dopaquinone	Amino acids	0.6240	0.0028	0.7788	0.0241

Glutathione	Amino acids	0.8581	0.3440	0.0135	0.4578
Glutathione	Amino acids	0.8581	0.3440	0.0135	0.4578
Indoleacetaldehyde	Amino acids	0.0285	0.0361	0.8334	0.1046
L-alanine	Amino acids	0.5690	0.0851	0.0338	0.0011
L-arginine	Amino acids	0.4532	0.4423	0.8378	0.0134
L-Glutamic acid	Amino acids	0.0016	0.2997	0.0015	0.2958
L-Glutamine	Amino acids	0.4155	0.9355	0.7319	0.0018
L-Histidine	Amino acids	0.0606	0.0406	0.0072	0.0044
L-Isoleucine	Amino acids	0.1411	0.1419	0.6863	0.0036
L-Methionine	Amino acids	0.9820	0.0102	0.0172	0.0126
L-Proline	Amino acids	0.0000	0.0000	0.0005	0.0000
L-Threonine	Amino acids	0.0115	0.7483	0.2317	0.8801
L-Tryptophan	Amino acids	0.8780	0.0458	0.3207	0.0260
L-Tyrosine	Amino acids	0.2369	0.0032	0.5250	0.0054
N6,N6,N6-Trimethyl-L-lysine	Amino acids	0.8995	0.0089	0.1663	0.0008
N-acetylaspartylglutamic acid	Amino acids	0.0006	0.7290	0.0004	0.1228
N-acetyldopamine	Amino acids	0.9077	0.0405	0.0318	0.0894
N-acetylglutamine	Amino acids	0.0077	0.0011	0.7219	0.0030
N-acetylhistidine	Amino acids	0.1782	0.0044	0.0784	0.6494
N-acetylisoleucine	Amino acids	0.4569	0.6223	0.0469	0.3329
N-acetyl-L-alanine	Amino acids	0.0132	0.1160	0.2464	0.7585
N-acetyltaurine	Amino acids	0.1449	0.0011	0.8310	0.0002
N-acetyltyramine	Amino acids	0.0356	0.0059	0.1744	0.7592
N-acetylvaline	Amino acids	0.0502	0.0027	0.0561	0.0062
N-Methylalanine	Amino acids	0.3541	0.0168	0.1387	0.1876
N-oleoyltaurine	Amino acids	0.0056	0.0043	0.0578	0.0001
N-oleoyltaurine	Amino acids	0.0065	0.0046	0.0639	0.0000
O-acetylserine	Amino acids	0.0585	0.2374	0.0469	0.1971
O-acetyltyramine	Amino acids	0.7453	0.0403	0.5955	0.7283
Oxidized glutathione	Amino acids	0.7852	0.8135	0.0413	0.7997
Palmitoylglycine	Amino acids	0.9647	0.3870	0.0331	0.1121
Phosphoserine	Amino acids	0.6821	0.3200	0.0274	0.7364
Pyroglutamic acid	Amino acids	0.6927	0.5109	0.1306	0.0385
Sarcosine	Amino acids	0.9078	0.3517	0.0281	0.2255
Spermidine	Amino acids	0.5068	0.1181	0.2092	0.0498
Suberylglycine	Amino acids	0.0027	0.0017	0.0846	0.1540

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Table S2. Primers used in this study

Primer name	Sequence,5'-3'	Description
<i>CS-T7F</i>	TAATACGACTCACTATAGGGTGCGAAACTTCTGTGCTGG	CS-dsRNA
<i>CS-T7R</i>	TAATACGACTCACTATAGGCACCGATGCCCTTTGACTCT	
<i>CS-rtF</i>	GTACAGCGAGGGTGTCAACA	qPCR
<i>CS-rtR</i>	CACCGATGCCCTTTGACTCT	
<i>PYK-rtF</i>	TGTGCCCTCGACATTGACTC	
<i>PYK-rtR</i>	TTATCGTTTTCTGCGTGGTAT	
<i>PGM-rtF</i>	ACAACAAAACAGTCGCCTGC	
<i>PGM-rtR</i>	TGCAGCCAACTGTGCAAATC	
<i>HK-rtF</i>	CGCGAACAATGCAAAGAGCT	
<i>HK-rtR</i>	TTCTCCCAAGTCAAGTGCC	
<i>GLY-rtF</i>	CCGTTCCCTCCAGAACACAA	
<i>GLY-rtR</i>	GGCCTCCATTACCCAAACCA	
<i>ALDO-rtF</i>	GTTCCATTGTTTCGGCTCTGA	
<i>ALDO-rtR</i>	TAGCGTGCCAGAACATTAGC	
<i>ACADVL-rtF</i>	GAGCCGAGCTGTACTGTCTC	
<i>ACADVL-rtR</i>	TGACTGGCGTCTGAGCAAAT	
<i>CPT1-rtF</i>	AGGCAGTGAACGGTCATG	
<i>CPT1-rtR</i>	CATCTGGCACCAAGGGAG	
<i>CPT2-rtF</i>	GGACAGGGATTTGACAGAC	
<i>CPT2-rtR</i>	GCACCAGCCAGAACTACAT	
<i>FABP-rtF</i>	GCCGCAAGGTCAAGTCTATC	
<i>FABP-rtR</i>	TATTCTCGTCGCCACCAAGT	
<i>COX4-rtF</i>	GACCGAACGGACTTTCCCAT	
<i>COX4-rtR</i>	AGGTGCCTGGATTTCTGCAA	
<i>COX7A-rtF</i>	GGGTTGCACCACCAGTTAGA	
<i>COX7A-rtR</i>	GAACCGGAACACCATCTCGT	
<i>ATPsyn-rtF</i>	GCGAATCCAGAAAATCCGCC	
<i>ATPsyn-rtR</i>	GTGTGACGTTGTCAGGTGGA	
<i>NDUF-rtF</i>	ACAGAGCAGAAGCACGGAAA	
<i>NDUF-rtR</i>	TTTAGCCCTGCATTGCGGTA	

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