

Supplementary Table 1

Antibody	Source	Catalog Number	Note
Anti-IR-pY1150/1151 (19H6)	Cell Signaling	#3024	labeled as pY 1152/1153 IR
anti-AKT (40D4)	Cell Signaling	#2920	
anti-pS473 AKT (D9E)	Cell Signaling	#4060	
anti-ERK1/2 (L34F12)	Cell Signaling	#4696	
anti-pERK1/2 (197G2)	Cell Signaling	#4377	
anti-HSL	Cell Signaling	#4107	
anti-pS563 HSL	Cell Signaling	#4139	
anti-IR-pY960	Millipore	#07-838	labeled as pY962
anti-IR (CT-3)	Millipore	MABS65	
anti-CEACAM1	Invitrogen	#MA5-29684	
anti-ACTIN (C4)	Santa Cruz	Sc-47778	
anti-PKC ϵ	BD Biosciences	#610086	
anti-Na-K ATPase	Abcam	#ab7671	
anti-GAPDH	Cell Signaling	#5174	
anti-rabbit immunoglobulin G (IgG) (H + L)	Cell Signaling	#5151	
anti-mouse IgG (H + L)	Cell Signaling	#5470	

Supplementary Table 2

Srebp1 FW: 5'-GGAGCCATGGATTGCACATT-3',
RV: 5'-GGCCCCGGAAGTCACTGT-3'

Scd1 FW: 5'-TTCTTGCGATACTCTGGTGC-3',
RV: 5'-CGGGATTGAATGTTCTTGTCTG-3'

Acc1 FW: 5'-GATGAACCATCTCCGTTGGC-3',
RV: 5'-GACCCAATTATGAATCGGGAGTG-3'

Fasn FW: 5'-TCGTGATGAACGTGTACCGG-3',
RV: 5'-CGGGTGAGGACGTTTACAAAG-3'

Agpat3 FW: 5'-CTGCTTGCCTACCTGAAGACC-3',
RV: 5'-GATACGGCGGTATAGGTGCTT-3'

Dgat1 FW: 5'-TCCGTCCAGGGTGGTAGTG-3',
RV: 5'-TGAACAAAGAATCTTGCAGACGA-3'

Dgat2 FW: 5'-GCGCTACTTCCGAGACTACTT-3',
RV: 5'-GGGCCTTATGCCAGGAACT-3'

Cd36 FW: 5'-ATGGGCTGTGATCGGAACTG-3',
RV: 5'-GTCTTCCCAATAAGCATGTCTCC-3'

Slc27a2 FW: 5'-TCCTCCAAGATGTGCGGTACT-3',
RV: 5'-TAGGTGAGCGTCTCGTCTCG-3'

Fabp4 FW: 5'-ATCAGCGTAAATGGGGATTGG-3',
RV: 5'-GTCTGCGGTGATTCATCGAA-3'

G6pc FW: 5'-CGACTCGCTATCTCCAAGTGA-3',
RV: 5'-GGGCGTTGTCCAAACAGAAT-3'

Pepck FW: 5'-CCACAGCTGCTGCAGAACA-3',
RV: 5'-GAAGGGTCGCATGGCAAA-3'

Gck FW: 5'-CTGTTAGCAGGATGGCAGCTT-3',
RV: 5'-TTTCCTGGAGAGATGCTGTGG-3'

Cpt1a FW: 5'-CTCCGCCTGAGCCATGAAG-3',
RV: 5'-CACCAGTGATGATGCCATTCT-3'

Pparg FW: 5'-GGAAGACCACTCGCATTCTT-3',
RV: 5'-GTAATCAGCAACCATTGGGTCA-3'

Lpl FW: 5'-TTGCCCTAAGGACCCCTGAA-3',
RV: 5'-TTGAAGTGGCAGTTAGACACAG-3'

Lipe FW: 5'-GATTTACGCACGATGACACAGT-3',

RV: 5'-ACCTGCAAAGACATTAGACAGC-3'

Abhd5 FW: 5'-TGGTGTCCCACATCTACATCA-3',

RV: 5'-CAGCGTCCATATTCTGTTTCCA-3'

Plin1 FW: 5'-CTGTGTGCAATGCCTATGAGA-3',

RV: 5'-CTGGAGGGTATTGAAGAGCCG-3'

Glut4 FW: 5'-GTGACTGGAACACTGGTCCTA-3',

RV: 5'-CCAGCCACGTTGCATTGTAG-3'

Pcx FW: 5'-CTGAAGTTCCAAACAGTTCGAGG-3',

RV: 5'-CGCACGAAACACTCGGATG-3'

Gapdh FW: 5'-CCTGCTTCACCACCTTCTTGAT-3',

RV: 5'-TGTGTCCGTCGTGGATCTGA-3'

Hibch FW: 5'-GTGGAGGCGTCATAACGCTC-3',

RV: 5'-AGGAATGTGTCAGGGTCTTGT-3'

Lvd FW: 5'-GGACGGCGAGTTTCCAGTT-3',

RV: 5'-CTCCTCGTTTAGCCCGTTGA-3'

Acadm FW: 5'-AGGGTTTAGTTTTGAGTTGACGG-3',

RV: 5'-CCCCGCTTTTGTTCATATTCCG-3'

Dbt FW: 5'-AGACTGACCTGTGTTTCGCTAT-3',

RV: 5'-GAGTGACGTGGCTGACTGTA-3'

Supplementary Table 3. VIP list-biorep-TIC normalization with HMDB

	HMDB	Comp. 1
calcitroic acid	HMDB0006472	1.981
ALANINE	HMDB0000161	1.8231
TYROSINE	HMDB00158	1.819
Docosapentaenoic acid	HMDB0006528	1.8118
L-CARNITINE	HMDB0000062	1.8053
GLUTAMINE	HMDB00641	1.7961
Docosatetraenoic acid	HMDB0002226	1.7927
L-Pyroglutamic acid	HMDB0000267	1.7924
(5beta)-Chola-7,9(11)-dien-24-oic acid	0	1.7847
DOCOSAHEXAENOIC ACID	HMDB0002183	1.773
Docosatrienoic acid	HMDB0002823	1.7649
Gluconate	HMDB00625	1.7099
1-linoleoyl-sn-glycero-3-phosphoethanolamine	HMDB0011507	1.6891
(9E)-11-Methoxy-11-(3-pentyl-2-oxiranyl)-9-undecenoic acid	0	1.6712
Arachidonic acid	HMDB0001043	1.6656
?-Hydroxyisobutyric acid	HMDB0000729	1.6599
Eicosatrienoic acid	HMDB0002925	1.6512
(15R,21S)-18,21,22-Trihydroxy-3-methyl-18-oxido-12-oxo-13,17,19-trioxa-18lambda~5~-phosphadocosan-15-yl 22-methyltricosanoate	#N/A	1.6448
lentiginosine	0	1.6321
5212188 (1,2-di-[(9Z,12Z)-octadecadienoyl]-sn-glycero-3-phosphocholine, Mouse metabolite)	HMDB0008138	1.631
para-Cresol Sulfate	HMDB0011635	1.624
MFCD00133435 (1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine)	HMDB0002815	1.603
Eicosadienoic acid	HMDB0005060	1.6019
Creatine	HMDB0000064	1.5721
N6-METHYLLYSINE	HMDB0002038	1.567
INDOLE	HMDB0000738	1.5637
Taurine	HMDB00251	1.5594
ELAIDIC ACID	HMDB0000573	1.5414
1-[(9Z)-hexadecenoyl]-sn-glycero-3-phosphocholine	HMDB0010383	1.5246
Glutamic acid	HMDB00148	1.5055
MFCD12546417 (3,4-Dihydroxybenzenesulfonic acid)	0	1.5041
Diisopropylphosphate	HMDB0251359	1.4954
Itaconic acid	HMDB0002092	1.4885
12-HAS (12-hydroxy stearic acid)	HMDB0061706	1.4828
Palmitoyl sphingomyelin	HMDB0010169	1.4456
Palmitic acid	HMDB00220	1.4451
O-ACETYLCARNITINE	HMDB0000201	1.403
docosaheptaenoic acid	HMDB0039133	1.3959
L-alpha-lysophosphatidylcholine	HMDB0010382	1.3881
1-stearoyl-2-arachidonoyl-sn-glycero-3-phospho-1D-myo-inositol	0	1.3708
TRANS-ACONITATE	HMDB0000958	1.3675
1810343 (Glycerol triundecanoate)	HMDB0031089	1.3657
Methionine Sulfoxide	HMDB0002005	1.3541
1-hexadecanoyl-2-[(7Z,10Z,13Z,16Z,19Z)-docosapentaenoyl]-sn-glycero-3-phosphocholine	HMDB0007990	1.3523
Pentacosanoic acid	HMDB0002361	1.3489
TRYPTOPHAN	HMDB00929	1.3429
Aspartate	HMDB0000191	1.3426
MFCD00273074 (1-Heptadecanoyl-rac-glycerol)	0	1.3382
Deoxycarnitine	HMDB0001161	1.3233
Proline Betaine (Stachydrine)	HMDB0004827	1.3059
Eicosapentaenoic acid	HMDB01999	1.2617
Methionine	HMDB00696	1.2384
3-oxopalmitic acid	HMDB0010733	1.2317

Hippurate	HMDB00714	1.2305
N-Benzylformamide	HMDB0304423	1.1943
3-Methyl-3-buten-1-yl stearate	0	1.1928
Phosphoric acid	HMDB0002142	1.1846
Cystine	HMDB0000192	1.1752
Tridecanoic acid	HMDB0000910	1.1611
(2S)-2,3-Dihydroxypropyl pentadecanoate	0	1.1608
(8E)-8-Heptadecenedioic acid	0	1.1487
L-Pipecolic acid	HMDB0000716	1.1395
9a,11b-Dimethyl-9-[5-(2-methylcyclopropyl)-2-hexanyl]hexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-3-ol	0	1.1369
1788230 [Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester]	HMDB0072869	1.1327
Methyl (9Z,12Z,16E)-15-hydroperoxy-9,12,16-octadecatrienoate	0	1.1302
L-Lysine	HMDB0000182	1.1234
Creatinine	HMDB0000562	1.1166
Androsterone sulfate	HMDB0002759	1.115
2-Hydroxyhippuric acid	HMDB0000840	1.1105
1-(4Z,7Z,10Z,13Z,16Z,19Z-docosaheptaenoyl)-sn-glycero-3-phosphocholine	HMDB0062307	1.0625
Isophthalic acid	HMDB0002107	1.0545
(5E,9E)-5,9-Tetracosadienoic acid	HMDB0062248	1.0445
Nervonic acid	HMDB0002368	1.0435
D-Malic acid	HMDB0031518	1.0386
L-Arginine	HMDB0000517	1.0338
13Z,16Z-Docosadienoic Acid	HMDB0061714	1.0326
13(S)-HOTrE (13S-hydroxy-9Z,11E,15Z-octadecatrienoic acid, 15-lipoxygenase product of linolenic acid)	#N/A	1.0121
cIMP	0	0.99697
Betaine	HMDB0000043	0.99057
(2E)-decenoic acid	HMDB0010726	0.98389
DL-Leucine	HMDB0000687	0.98025
(3R,4S,9R,11R)-27-(4-Hydroxyphenyl)-4-methyl-3,9,11-heptacosanetriol	0	0.97575
(3i,5i,22i,25S)-Spirosolan-3-yl 4-O-i-D-glucopyranosyl-i-D-galactopyranoside	#N/A	0.94889
3-Methylhexadecanedioic acid	0	0.94142
Erucamide	HMDB0244507	0.93517
PALMITOLEIC ACID	HMDB03229	0.92822
PHOSPHORYLCHOLINE	HMDB0001565	0.92383
2908 (Piperidine)	HMDB0034301	0.91159
Valproic acid	HMDB0001877	0.91103
D-Sedoheptulose	HMDB0003219	0.89912
Proline	HMDB00162	0.86504
11(12)-EET (11,12-epoxyeicosatrienoic acid)	#N/A	0.86468
11-deoxy Prostaglandin F1	#N/A	0.85485
Pentadecanoic acid	HMDB0000826	0.83846
2-chloro Stearic Acid	HMDB0245076	0.82593
(1R,9S,12S,13R,14S,17R,18Z,21S,23S,24S,25S,27R)-17-Allyl-1,14,25-trihydroxy-12-(1E)-1-[(1R,3R,4R)-4-hydroxy-3-methoxycyclohexyl]-1-propen-2-yl-23-methoxy-13,19,21,27-tetramethyl-11,28-dioxo-4-azatri cyclo[22.3.1.0-4,9-]octacos-18-ene-2,3,10,16-tetrone	#N/A	0.8074
2-Aminobutnoic acid	HMDB0000452	0.80182
Sphingosine	HMDB00252	0.78367
4-Hydroxybenzaldehyde	HMDB0011718	0.77884
4-Methyleneglutamine	0	0.76792
cis-cis 9-12 octadecadienoyl L-Carnitine	HMDB0006469	0.76347
soyasapogenol A	HMDB0034505	0.7568
Prolinamide	0	0.7563
lysoPC a C28:0	HMDB0029206	0.74397
SEROTONIN	HMDB00259	0.73903
Prostaglandin F1± Alcohol	#N/A	0.7362
Stearic acid	HMDB00827	0.72866

Adenosine 5'-monophosphate	HMDB0000045	0.72402
(5Z,7E)-9,10-Secocholesta-5,7,10-triene	0	0.72034
Glucose	HMDB00122	0.71997
L-Kynurenine	HMDB0000684	0.70294
Histamine	HMDB0000870	0.68822
ALPHA-KETOGLUTARIC ACID	HMDB0000208	0.67936
O-ureido-D-serine	0	0.66971
PC	HMDB0000564	0.6414
PG(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0010595	0.64089
L-Cysteinylglycine disulfide	HMDB0000709	0.63368
235BBF3K97 (Anhydroretinol)	HMDB0062447	0.6113
cis-4-Decenoyl carnitine	HMDB0240585	0.61078
N-[(2S,3R)-1-(beta-D-Glucopyranosyloxy)-3-hydroxy-2-octadecanyl]tetradecanamide	0	0.58954
2-Ketohexanoic acid	HMDB0001864	0.58897
LAURIC ACID (Dodecanoic acid, Plasma)	HMDB00638	0.58754
N,N-DIMETHYLARGININE	HMDB0001539	0.58733
INDOXYL SULFATE	HMDB0000682	0.58545
PHENYLALANINE	HMDB00159	0.57911
(2S)-1-Hydroxy-3-(pentadecanoyloxy)-2-propanyl (6Z,9Z,12Z,15Z)-6,9,12,15-octadecatetraenoate	0	0.56583
ODYA (17-octadecynoic acid)	0	0.56464
Labdanolic acid	0	0.54496
Docosanoic acid	HMDB0000944	0.53767
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	0	0.53619
Tetraneurin E	0	0.53496
Acetyl-methylcholine	#N/A	0.52927
Heneicosylic acid	HMDB0002345	0.47898
Myristic Acid Alkyne	0	0.47426
Nicotinamide	HMDB0001406	0.46846
ricinelaiddic acid	0	0.46487
Valine	HMDB0000883	0.45398
Bilirubin	HMDB0000054	0.45102
(20Z)-6-Hydroxy-6-oxido-12-oxo-5,7,11-trioxa-2-aza-6lambda-5-phosphapentacos-20-en-9-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate	#N/A	0.44577
CITRULLINE	HMDB0000904	0.42988
Methyl (9E)-9-octadecenoate	0	0.41841
MFCD22416941 (Oleoyle-L-carnitine)	HMDB0005065	0.41768
Octadecadienoic acid	0	0.41135
Propionylcarnitine	HMDB00824	0.40205
trans-2-Tetradecenoyl-L-carnitine	HMDB0013329	0.39472
LEUCINE	HMDB00687	0.392
Palmitoyl-DL-carnitine	HMDB00222	0.38369
Choline	HMDB0000097	0.37055
hydroxycitric acid	HMDB0031159	0.35567
Erucic acid	HMDB0002068	0.35381
L-alpha-Glycerolphosphorylcholine	HMDB0000086	0.35268
MYRISTIC ACID	HMDB00806	0.35139
1-Octen-3-ol	#N/A	0.35073
Linolenic acid	HMDB0001388	0.31176
Methyl stearate	HMDB0034154	0.31162
Eicosenoic acid	HMDB0002231	0.29769
Asparagine	HMDB0000168	0.29517
4-Phenolsulfonic acid	0	0.27595
(9Z,11R,12Z,15Z)-11-(Stearoyloxy)-9,12,15-octadecatrienoic acid	HMDB0031934	0.26266
4-Indolecarbaldehyde	0	0.26137
Cyclopentadecanolide	HMDB0034455	0.261
Dehydroepiandrosterone sulfate	HMDB0001032	0.25694
Methyl palmitate	HMDB0061709	0.25678

2-Hexadecynoic acid	0	0.25165
N-{15-Methyl-3-[(15-methylhexadecanoyl)oxy]hexadecanoyl}-L-serine	0	0.24808
Ornithine	HMDB03374	0.23397
N-Acetylglycine	HMDB00532	0.22728
D-Tryptophan	HMDB0013609	0.22443
L-Threonic acid	HMDB0000943	0.21869
N,N-Diisopropylethylamine (DIPEA)	0	0.21594
trans-3-Indoleacrylic acid	HMDB0000734	0.19978
a-Linolenic acid	HMDB0001388	0.17891
6-Methylquinoline	HMDB0033115	0.17782
Lysolecithin	0	0.17284
Decanoylcarnitine	HMDB0000651	0.14199
Arachidic acid	HMDB0002212	0.13319
Histidine	HMDB0000177	0.13191
(5Z,13E,15S,17Z)-15-Hydroxy-11-oxoprostano-5,9,13,17-tetraen-1-oic acid	HMDB0002664	0.12375
2-hydroxyvaleric acid	HMDB0001863	0.12185
cis,cis-tetradeca-5,8-dienoyl-CoA	HMDB0002288	0.11859
2-Amino-4-methylpyrimidine	HMDB0247327	0.10911
Diginatigenin	0	0.10847
(7R)-4-Hydroxy-N,N,N-trimethyl-10-oxo-7-(palmitoyloxy)-3,5,9-trioxo-4-phosphapentacosan-1-aminium 4-oxide	0	0.10456
ANTHRANILIC ACID	HMDB0001123	0.095831
Myristoleic acid	HMDB0002000	0.089469
Uric acid	HMDB00289	0.079525
(6Z,18R,24S)-21,24,25-Trihydroxy-21-oxido-15-oxo-16,20,22-trioxa-21lambda-5-phosphapentacos-6-en-18-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosaehexaenoate	#N/A	0.07798
Typhasterol	FDB031232	0.068446
1-Palmitoyl-2-docosaehexaenoyl-sn-glycero-3-phosphocholine	HMDB0007991	0.058815
L-(+) Lactic acid	HMDB0000190	0.047189
trans-10-Heptadecenoic acid	HMDB0244268	0.040652
4-Oxoproline	HMDB0304793	0.026734
Glycol distearate	HMDB0032260	0.023565
(2R)-3-[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-2-[(1Z)-1-octadecen-1-yloxy]propyl (5Z,8Z,11Z,14Z,17Z)-5,8,11,14,17-icosapentaenoate	#N/A	0.022778
16-Heptadecynoic acid	HMDB0002259	0.020995
18:0 Lyso PC	HMDB0010384	0.017657

Supplementary Table 4.

Name	Median Area															
Name	4A-1	4A-2	4A-3	4A-4	4A-5	4A-6	4A-7	4A-8	WT-1	WT-2	WT-3	WT-4	WT-5	WT-6	WT-7	
1-Octen-3-ol	5.4 0E-06	5.7 8E-06	5.4 8E-06	6.2 6E-06	6.2 0E-06	6.0 0E-06	6.3 7E-06	5.2 4E-06	5.8 6E-06	5.8 5E-06	5.8 2E-06	6.5 2E-06	5.8 3E-06	5.9 4E-06	5.2 2E-06	
11(12)-EET (11,12-epoxyicosatrienoic acid)	5.1 4E-05	4.0 1E-05	0.0 002 916 9	0.0 001 252 7	1.2 6E-05	8.7 7E-06	1.5 8E-05	9.8 9E-06	6.4 8E-06	8.2 4E-06	6.6 6E-06	9.7 4E-06	1.3 5E-05	1.7 3E-05	9.1 8E-05	
(15R,21S)-18,21,22-Trihydroxy-3-methyl-18-oxido-12-oxo-13,17,19-trioxa-18lambda-5-phosphadocosan-15-yl 22-methyltricosanoate	0.0 001 568 2	0.0 001 380 7	0.0 001 518 8	0.0 001 648 5	0.0 001 581	0.0 001 869 1	0.0 001 784 8	0.0 001 597 6	9.9 3E-05	0.0 001 543 4	0.0 001 130 8	0.0 001 112 4	0.0 001 374 2	0.0 001 276 9	0.0 001 308 2	
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	8.9 7E-06	1.1 7E-05	1.3 4E-05	1.3 6E-05	1.2 6E-05	1.0 7E-05	1.1 3E-05	1.0 6E-05	8.4 8E-06	1.1 3E-05	1.0 8E-05	1.1 3E-05	1.1 1E-05	1.0 6E-05	1.0 8E-05	
(1R,9S,12S,13R,14S,17R,18Z,21S,23S,24S,25S,27R)-17-Allyl-1,14,25-trihydroxy-12-(1E)-1-[(1R,3R,4R)-4-hydroxy-3-methoxycyclohexyl]-1-propen-2-yl-23-methoxy-13,19,21,27-tetramethyl-11,28-dioxa-4-azatri-cyclo[22.3.1.0-4,9]-octacos-18-ene-2,3,10,16-tetrone	6.1 8E-05	4.6 7E-05	4.9 0E-05	4.1 7E-05	6.7 1E-05	6.1 1E-05	4.5 1E-05	5.9 1E-05	7.3 9E-05	7.0 2E-05	8.1 4E-05	7.1 2E-05	6.1 6E-05	5.7 9E-05	3.5 4E-05	
(20Z)-6-Hydroxy-6-oxido-12-oxo-5,7,11-trioxa-2-aza-6lambda-5-phosphapentacos-20-en-9-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate	4.3 3E-05	4.7 8E-05	4.2 3E-05	4.2 9E-05	4.6 5E-05	5.0 1E-05	3.9 2E-05	4.1 1E-05	3.2 0E-05	3.9 5E-05	4.3 0E-05	4.3 5E-05	4.6 7E-05	4.5 3E-05	3.9 6E-05	
(2E)-decanoic acid	5.7 2E-05	6.7 6E-05	5.0 4E-05	6.4 0E-05	6.6 5E-05	3.8 0E-05	5.7 6E-05	4.7 7E-05	3.9 9E-05	3.0 3E-05	3.3 1E-05	3.5 4E-05	4.0 6E-05	6.1 8E-05	7.5 2E-05	
(2R)-3-[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy]-2-[(1Z)-1-octadecen-1-yloxy]propyl (5Z,8Z,11Z,14Z,17Z)-5,8,11,14,17-icosapentaenoate	0.0 001 045	0.0 001 355	0.0 001 327	0.0 001 203	0.0 001 035	0.0 001 105	0.0 001 007	0.0 001 213	0.0 001 063	7.3 2E-05	0.0 001 103	9.1 9E-05	0.0 001 196	0.0 001 213	0.0 002 075	
(2S)-1-Hydroxy-3-(pentadecanoyloxy)-2-propanyl (6Z,9Z,12Z,15Z)-6,9,12,15-octadecatetraenoate	4.9 7E-05	5.6 7E-05	5.8 2E-05	4.7 1E-05	4.0 0E-05	4.6 1E-05	4.7 2E-05	5.4 5E-05	4.5 5E-05	4.8 9E-05	4.3 3E-05	3.8 8E-05	4.6 3E-05	4.5 5E-05	5.6 2E-05	
(2S)-2,3-Dihydroxypropyl pentadecanoate	0.0 003 978 6	0.0 004 257 1	0.0 006 275 5	0.0 006 796 9	0.0 006 383	0.0 005 671	0.0 006 831	0.0 004 849	0.0 003 881	0.0 005 125	0.0 004 134	0.0 004 502	0.0 004 383	0.0 004 279	0.0 004 803	
(3i,5i,22i,25S)-Spirosolan-3-yl 4-O-i-D-glucopyranosyl-i-D-galactopyranoside	4.4 8E-05	4.5 8E-05	4.6 7E-05	4.6 7E-05	5.2 4E-05	5.7 7E-05	4.4 0E-05	4.5 8E-05	3.7 4E-05	4.6 3E-05	4.6 0E-05	4.4 3E-05	4.5 2E-05	3.7 9E-05	3.5 4E-05	
(3R,4S,9R,11R)-27-(4-Hydroxyphenyl)-4-methyl-3,9,11-heptacosanetriol	0.0 004 996 5	0.0 003 445 4	0.0 003 436 1	0.0 003 769 7	0.0 002 789	0.0 002 142	0.0 003 694	0.0 004 383	0.0 002 633	0.0 002 482	0.0 001 976	0.0 001 974	0.0 002 638	0.0 002 164	0.0 005 758	
(5beta)-Chola-7,9(11)-dien-24-oic acid	0.0 001 920 8	0.0 001 616 3	0.0 002 160 8	0.0 002 614 3	0.0 003 393	0.0 002 034	0.0 003 229	0.0 001 865	0.0 001 213	0.0 001 369	0.0 001 349	0.0 001 159	9.9 4E-05	9.0 001 465	0.0 001 490	
(5E,9E)-5,9-Tetracosadienoic acid	4.3 6E-05	5.3 3E-05	4.4 6E-05	4.7 2E-05	5.6 4E-05	4.5 8E-05	7.2 8E-05	4.5 4E-05	3.2 8E-06	4.0 3E-05	4.1 6E-05	5.0 4E-05	4.6 5E-05	4.1 7E-05	4.1 8E-05	
(5Z,13E,15S,17Z)-15-Hydroxy-11-oxoprostano-5,9,13,17-tetraen-1-oic acid	7.9 4E-06	9.7 0E-06	9.3 4E-06	9.6 0E-06	9.1 5E-06	9.7 4E-06	9.0 3E-06	8.5 8E-06	8.6 0E-06	8.8 1E-06	8.8 2E-06	9.9 2E-06	8.5 6E-06	8.7 6E-06	8.3 0E-06	
(5Z,7E)-9,10-Secocholesta-5,7,10-triene	0.0 016 848 4	0.0 018 692 9	0.0 010 603 4	0.0 010 812 3	0.0 011 919	0.0 005 262	0.0 007 536	0.0 014 097	0.0 010 515	0.0 008 221	0.0 008 525	0.0 011 540	0.0 015 855	0.0 016 990	0.0 023 152	
(6Z,18R,24S)-21,24,25-Trihydroxy-21-oxido-15-oxo-16,20,22-trioxa-21lambda-5-phosphapentacos-6-en-18-yl (4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoate	2.3 5E-05	2.3 1E-05	3.1 3E-05	2.5 4E-05	3.0 1E-05	3.4 0E-05	2.7 4E-05	2.5 1E-05	2.3 2E-05	2.9 1E-05	3.3 5E-05	2.8 6E-05	2.9 6E-05	2.6 8E-05	1.9 9E-05	
(7R)-4-Hydroxy-N,N,N-trimethyl-10-oxo-7-(palmitoyloxy)-3,5,9-trioxa-4-phosphapentacosan-1-aminium 4-oxide	0.0 005 296	0.0 007 357	0.0 005 642	0.0 006 179	0.0 005 050	0.0 006 913	0.0 005 412	0.0 005 881	0.0 005 629	0.0 005 178	0.0 005 593	0.0 006 680	0.0 005 817	0.0 005 548	0.0 006 589	
(8E)-8-Heptadecenedioic acid	5.1 8E-05	4.3 4E-05	3.9 1E-05	3.7 7E-05	3.3 4E-05	2.4 7E-05	5.1 1E-05	4.3 6E-05	2.6 7E-05	1.5 5E-05	1.6 6E-05	1.9 2E-05	2.8 0E-05	3.1 4E-05	6.7 7E-05	
(9E)-11-Methoxy-11-(3-pentyl-2-oxiranyl)-9-undecenoic acid	0.0 043 045 8	0.0 046 451 2	0.0 046 533 2	0.0 044 492 1	0.0 041 422 1	0.0 039 975 4	0.0 045 640 8	0.0 050 024 9	0.0 029 013 4	0.0 028 041 5	0.0 030 916 1	0.0 027 768 1	0.0 032 613 9	0.0 037 908 9	0.0 050 884 9	
(9Z,11R,12Z,15Z)-11-(Stearoyloxy)-9,12,15-octadecatatrienoic acid	0.0 045 471 5	0.0 036 962 7	0.0 031 209 4	0.0 032 571 4	0.0 027 113	0.0 019 595	0.0 034 751	0.0 030 633	0.0 033 393	0.0 022 204	0.0 023 721	0.0 023 508	0.0 026 995	0.0 032 790	0.0 053 432	
1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine	0.0 022 23	0.0 033 274 1	0.0 041 656 1	0.0 038 593 8	0.0 035 425 4	0.0 041 780 2	0.0 029 706 3	0.0 030 171 5	0.0 022 448 4	0.0 027 890 6	0.0 026 899 6	0.0 030 164 6	0.0 026 696 5	0.0 031 783 5	0.0 031 843 39	
1-[(9Z)-hexadecenoyl]-sn-glycero-3-phosphocholine	0.0 006 276 9	0.0 006 992 1	0.0 006 381 9	0.0 006 462 3	0.0 007 627 4	0.0 007 322 8	0.0 007 055 2	0.0 004 837 9	0.0 004 605 4	0.0 005 180 4	0.0 005 341 9	0.0 006 516 9	0.0 005 539 4	0.0 005 219 6	0.0 005 843 2	
1-hexadecanoyl-2-[(7Z,10Z,13Z,16Z,19Z)-docosapentaenoyl]-sn-glycero-3-phosphocholine	0.0 031 729 8	0.0 029 470 4	0.0 029 691 1	0.0 036 506	0.0 037 226 9	0.0 034 481 6	0.0 036 717 3	0.0 026 531 1	0.0 022 547 2	0.0 027 940 1	0.0 027 673 9	0.0 027 990 1	0.0 026 990 1	0.0 030 742 2	0.0 026 795 9	

1-linoleoyl-sn-glycero-3-phosphoethanolamine	0.00032386	0.00032529	0.00042709	0.00045313	0.00038404	0.00051998	0.00056735	0.00030896	0.00025506	0.00022807	0.00020021	0.00027238	0.00026798	0.00018847	0.00031448
1-Palmitoyl-2-docosaheaxenoyl-sn-glycero-3-phosphocholine	0.00724023	0.01056475	0.01262582	0.00991131	0.00849337	0.01097331	0.00781055	0.01052584	0.00823587	0.00880287	0.00903078	0.01061671	0.0089076	0.0097630	0.010097100
1-stearoyl-2-arachidonoyl-sn-glycero-3-phospho-1D-myo-inositol	0.00125006	0.00137494	0.00152524	0.00169087	0.00211275	0.00193934	0.00216255	0.00188852	0.00086355	0.00143816	0.00128304	0.00114953	0.0013988	0.0014870	0.00125921
11-deoxy Prostaglandin F1	0.003031031	0.00303073	0.00300118	0.002002906	0.002002582	0.003003487	0.003003168	0.003003172	0.002002770	0.002002511	0.002002455	0.002002459	0.002002519	0.002002519	0.003003498
12-hydroxy stearic acid	0.0010759	9.61E-05	0.0010209	0.00102459	0.00104115	9.37E-05	0.00102434	0.0010001	6.52E-05	7.30E-05	6.31E-05	7.14E-05	0.0010065	9.00105	0.0011784
13(S)-HOTrE (13S-hydroxy-9Z,11E,15Z-octadecatrienoic acid, 15-lipoxygenase product of linolenic acid)	3.30E-05	2.54E-05	1.89E-05	2.29E-05	2.54E-05	1.18E-05	2.38E-05	1.44E-05	1.23E-05	1.58E-05	1.03E-05	1.39E-05	1.54E-05	1.84E-05	2.57E-05
13Z,16Z-Docosadienoic Acid	5.07E-05	5.93E-05	4.73E-05	6.47E-05	6.33E-05	5.03E-05	7.11E-05	5.20E-05	4.26E-05	4.08E-05	4.76E-05	4.55E-05	4.25E-05	4.24E-05	7.25E-05
16-Heptadecynoic acid	0.0019632	0.001001894	0.001001717	0.001001578	0.001001285	0.001001184	0.001001687	0.001001001	0.001001620	0.001001343	0.001001346	0.001001186	0.001001524	0.001001877	0.00200247
1788230 [Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester]	0.0033509	0.00020742	0.00020023	0.0002002104	0.0002002353	0.001003498	0.001003054	0.002002735	0.001001523	0.001001595	0.001001499	0.001001340	0.001001876	0.002002139	0.003003012
18:0 Lyso PC	0.00718201	0.01002036	0.01281301	0.01279434	0.01091247	0.01148064	0.01211980	0.0109122	0.0105109	0.0105133	0.0105136	0.0105145	0.0105145	0.0105145	0.0105145
1810343 (Glycerol triundecanoate)	1.41E-05	1.45E-05	1.39E-05	1.54E-05	1.47E-05	1.18E-05	1.53E-05	1.39E-05	1.48E-05	1.36E-05	1.45E-05	1.62E-05	1.64E-05	1.72E-05	1.61E-05
2-Amino-4-methylpyrimidine	0.00687859	0.0043973	0.00452439	0.00540354	0.00672186	0.00494476	0.00421769	0.0030030	0.0048048	0.0051051	0.0064833	0.0049707	0.0049584	0.0046765	0.00417463
2-Aminobutnoic acid	0.0031357	0.002002279	0.002002332	0.003003431	0.003003699	0.003003755	0.003003181	0.002002975	0.002002410	0.002002958	0.003003235	0.002002812	0.002002294	0.002002449	0.004004145
2-chloro Stearic Acid	7.90E-05	6.26E-05	5.31E-05	5.89E-05	5.04E-05	4.21E-05	4.80E-05	5.00E-05	6.54E-05	6.65E-05	5.30E-05	4.72E-05	5.57E-05	6.10E-05	7.56E-05
2-Hexadecynoic acid	0.0015427	0.001013452	0.001011643	0.001010489	0.001009071	0.001007013	0.001015292	0.001012063	0.001012012	0.001007393	0.001007407	0.001007270	0.001010062	0.001012427	0.002002387
2-Hydroxyhippuric acid	5.28E-06	6.27E-06	6.19E-06	6.10E-06	6.21E-06	6.28E-06	6.81E-06	6.52E-06	4.80E-06	5.54E-06	5.72E-06	6.10E-06	5.65E-06	5.28E-06	5.36E-06
2-hydroxyvaleric acid	0.0036137	0.0040404	0.004004829	0.005005097	0.003003964	0.005005606	0.003003272	0.002002979	0.003003595	0.004004263	0.003003946	0.005005337	0.004004378	0.003003913	0.003003399
2-Ketohexanoic acid	0.0051388	0.005005335	0.004004105	0.007007667	0.004004894	0.005005809	0.006006407	0.00700711	0.003003939	0.004004809	0.004004546	0.004004505	0.004004398	0.004004324	0.009009598
235BBF3K97 (Anhydroretinol)	0.0036579	0.0075906	0.00300394	0.003003169	0.002002952	0.002002879	0.003003393	0.005005695	0.002002365	0.005005744	0.002002889	0.002002928	0.006006388	0.007007380	0.008008312
2908 (Piperidine)	0.00509842	0.00590074	0.00932615	0.00785785	0.00634177	0.00681919	0.0068166225	0.0087087	0.0081081	0.0083083	0.0092092	0.0081081	0.0083083	0.0075075	0.0089089
3-Methyl-3-buten-1-yl stearate	1.52E-05	1.67E-05	1.12E-05	1.64E-05	1.50E-05	1.66E-05	2.51E-05	1.18E-05	5.44E-05	1.14E-05	7.64E-06	6.99E-06	1.98E-05	1.30E-05	1.27E-05
3-Methylhexadecanedioic acid	0.00120319	0.000909748	0.001000862	0.001010687	0.0008008497	0.001007902	0.001012545	0.001008748	0.001006866	0.001007779	0.001008614	0.001008112	0.001009493	0.001008447	0.003003372
3-oxopalmitic acid	6.75E-05	4.46E-05	3.67E-05	4.83E-05	4.97E-05	2.65E-05	5.11E-05	5.24E-05	1.84E-05	2.46E-05	2.25E-05	2.61E-05	3.22E-05	3.12E-05	7.21E-05
4-Hydroxybenzaldehyde	6.74E-05	3.02E-05	6.93E-05	7.90E-05	5.58E-05	7.55E-05	9.62E-05	7.19E-05	5.48E-05	6.31E-05	5.67E-05	5.81E-05	3.95E-05	5.95E-05	3.48E-05
4-Indolecarbaldehyde	0.004406	0.005007852	0.006006433	0.006006984	0.006006673	0.008008042	0.006006286	0.007007413	0.005005440	0.007007913	0.008008574	0.008008549	0.007007249	0.005005813	0.005005135
4-Methyleneglutamine	0.0041731	0.0028923	0.0025324	0.0027604	0.002703394	0.0032033575	0.0027027066	0.002002021	0.0036036	0.0034034	0.0028028	0.0027027	0.0037037	0.0035035	0.0028028
4-Oxoproline	0.0012019	0.001001557	0.001001711	0.001001452	0.001001137	9.70E-05	0.001001372	0.001001450	0.001001242	0.001001161	0.001001119	0.001001240	0.001001733	0.001001309	0.001001454

4-Phenolsulfonic acid	0.0 007 942 3	0.0 012 810 5	0.0 006 007 8	0.0 016 927 7	0.0 017 982 2	0.0 031 242 1	0.0 021 218 6	0.0 016 373 7	0.0 006 743 4	0.0 017 419 1	0.0 009 289 2	0.0 013 921 4	0.0 008 356 4	0.0 021 423 5	0.0 019 077 4
5212188 (1,2-di-[(9Z,12Z)-octadecadienoyl]-sn-glycero-3-phosphocholine, Mouse metabolite))	0.0 076 808 5	0.0 085 318 2	0.0 077 208 9	0.0 084 277 8	0.0 087 816 7	0.0 089 067 2	0.0 086 608 9	0.0 075 049 9	0.0 060 589 8	0.0 068 722 8	0.0 059 872 8	0.0 066 481 2	0.0 070 491 1	0.0 078 890 7	0.0 072 498 0
6-Methylquinoline	0.0 006 724 2	0.0 008 027 3	0.0 008 263 5	0.0 008 684 7	0.0 009 143 5	0.0 008 717 5	0.0 008 540 6	0.0 008 671 6	0.0 006 921 7	0.0 009 584 9	0.0 011 964 5	0.0 009 317 5	0.0 008 077 1	0.0 007 156 7	0.0 006 986 2
9a,11b-Dimethyl-9-[5-(2-methylcyclopropyl)-2-hexanyl]hexadecahydrocyclopenta[1,2]phenanthro[8a,9-b]oxiren-3-ol	0.0 001 133	0.0 001 168 3	0.0 001 186 1	0.0 001 337 9	0.0 35- 0E- 05	0.0 4E- 05	0.0 8.7 1E- 05	0.0 001 106 6	0.0 6.7 4E- 05	0.0 8.0 8E- 05	0.0 6.9 2E- 05	0.0 7.7 2E- 05	0.0 7.7 6E- 05	0.0 9.0 7E- 05	0.0 7.3 5E- 05
a-Linolenic acid	0.0 174 070 7	0.0 166 457 1	0.0 152 936 5	0.0 137 3 3	0.0 101 693 1	0.0 106 340 7	0.0 139 438 2	0.0 149 148 2	0.0 124 776 6	0.0 118 182 4	0.0 102 344 3	0.0 097 353 9	0.0 129 704 8	0.0 158 486 2	0.0 221 787 9
Acetyl-methylcholine	0.0 062 673 6	0.0 055 274 5	0.0 011 650 4	0.0 010 649 8	0.0 015 798 8	0.0 015 821 9	0.0 060 138 9	0.0 061 295 8	0.0 028 980 6	0.0 025 622 9	0.0 024 003 1	0.0 020 014 6	0.0 075 858 9	0.0 077 269 9	0.0 050 531 3
Adenosine 5'-monophosphate	0.0 001 351 6	0.0 007 342 6	0.0 010 976 6	0.0 006 914 6	0.0 2.2 0E- 05	0.0 3.5 7E- 05	0.0 6.4 5E- 05	0.0 001 011 3	0.0 3.7 2E- 05	0.0 5.9 7E- 05	0.0 9.6 2E- 06	0.0 0.02 424 9	0.0 4.7 9E- 05	0.0 6E- 05	0.0 004 218 2
ALANINE	0.0 017 92	0.0 010 565 4	0.0 013 060 3	0.0 015 827 2	0.0 017 582 6	0.0 015 681 9	0.0 017 841 6	0.0 009 608 9	0.0 013 103 1	0.0 010 632 5	0.0 009 193 6	0.0 010 124 2	0.0 009 521 2	0.0 010 113 4	0.0 011 475 0
ALPHA-KETOGLUTARIC ACID	0.0 018 237 5	0.0 011 240 5	0.0 003 771 4	0.0 007 043 7	0.0 014 599 2	0.0 008 597 8	0.0 008 499 8	0.0 007 778 5	0.0 002 861 5	0.0 010 201 6	0.0 007 172 2	0.0 008 020 3	0.0 008 006 4	0.0 007 840 8	0.0 005 970 9
Androsterone sulfate	5.8 9E- 06	6.9 8E- 06	6.9 1E- 06	6.7 1E- 06	7.0 0E- 06	7.0 1E- 06	7.5 9E- 06	5.3 0E- 06	6.1 3E- 06	6.2 7E- 06	6.8 4E- 06	6.8 0E- 06	6.2 4E- 06	5.8 9E- 06	5.9 7E- 06
ANTHRANILIC ACID	8.4 9E- 05	8.0 1E- 05	0.0 001 152 3	0.0 001 077 6	7.1 5E- 05	9.4 4E- 05	6.4 3E- 05	9.9 8E- 05	6.9 0E- 05	0.0 001 587 3	0.0 0.0 161 3	7.0 9E- 05	7.7 2E- 05	6.9 9E- 05	8.3 9E- 05
Arachidic acid	0.0 003 464 7	0.0 003 823 2	0.0 003 098 8	0.0 003 555 3	0.0 003 154 1	0.0 003 328 7	0.0 002 951 4	0.0 004 057 8	0.0 002 081 8	0.0 003 934 6	0.0 003 008 5	0.0 002 735 5	0.0 004 118 7	0.0 003 827 1	0.0 003 722 8
Arachidonic acid	0.0 080 557 1	0.0 089 966 7	0.0 100 801 9	0.0 096 048 9	0.0 078 838 5	0.0 077 893 9	0.0 097 412 9	0.0 076 802 6	0.0 052 459 5	0.0 068 430 2	0.0 053 389 7	0.0 057 279 4	0.0 068 027 1	0.0 072 286 1	0.0 088 808 0
Asparagine	0.0 048 930 9	0.0 017 352 9	0.0 017 709 7	0.0 022 833 1	0.0 030 777 4	0.0 020 735 5	0.0 025 636 9	0.0 015 893 7	0.0 020 055 1	0.0 024 356 1	0.0 022 389 7	0.0 021 602 6	0.0 023 466 9	0.0 023 140 6	0.0 016 132 7
Aspartate	0.0 004 615 6	0.0 006 164 2	0.0 006 381 9	0.0 006 587 4	0.0 003 676 7	0.0 006 966 5	0.0 007 171 9	0.0 003 185 1	0.0 002 004 6	0.0 004 218 8	0.0 004 824 9	0.0 005 076 8	0.0 004 544 5	0.0 005 036 5	0.0 001 041 0
Betaine	0.0 089 944 2	0.0 043 721 1	0.0 061 413 9	0.0 068 776 8	0.0 068 963 1	0.0 098 295 4	0.0 059 453 3	0.0 064 977 6	0.0 061 094 6	0.0 059 764 9	0.0 054 430 4	0.0 049 704 1	0.0 059 457 9	0.0 050 331 9	0.0 041 0
Bilirubin	0.0 010 267 2	0.0 003 954 4	0.0 002 632 7	0.0 010 109 5	0.0 002 785 9	0.0 002 239 5	0.0 004 628 5	0.0 003 236 1	0.0 002 872 1	0.0 003 024 7	0.0 002 575 3	0.0 004 762 5	0.0 002 514 1	0.0 004 243 4	0.0 003 804 4
calcitroic acid	0.0 002 193 1	0.0 002 424 6	0.0 003 024 6	0.0 003 461 9	0.0 002 030 6	0.0 002 614 6	0.0 003 795 1	0.0 001 065 8	0.0 001 222 1	0.0 001 172 8	0.0 001 269 1	0.0 001 061 2	0.0 001 608 5	0.0 001 487 2	0.0 002 214 6
Choline	0.0 090 960 8	0.0 071 364 5	0.0 103 365 4	0.0 084 719 8	0.0 085 801 6	0.0 086 980 6	0.0 116 008 3	0.0 114 936 4	0.0 128 656 8	0.0 112 444 4	0.0 087 718 7	0.0 126 329 5	0.0 085 476 5	0.0 080 287 6	0.0 074 870 8
cIMP	0.0 075 291 4	0.0 060 747 7	0.0 063 835 4	0.0 061 466 7	0.0 078 934 8	0.0 077 857 3	0.0 062 135 2	0.0 080 785 8	0.0 101 840 2	0.0 089 385 6	0.0 095 826 5	0.0 097 377 8	0.0 079 895 8	0.0 078 232 7	0.0 051 659 1
cis-4-Decenoyl carnitine	0.0 002 348 9	0.0 001 300 3	0.0 7E- 05	0.0 001 301 7	0.0 001 358 2	0.0 8E- 05	0.0 001 196 9	0.0 5E- 05	0.0 8.5 0E- 05	0.0 7.2 9E- 05	0.0 8.5 0E- 05	0.0 7.2 1E- 05	0.0 9.9 0E- 05	0.0 0.01 218 9	0.0 0.01 542 3
cis-cis_9-12_octadecadienoyl_L-Carnitine	0.0 016 423 4	0.0 011 580 8	0.0 007 317 6	0.0 012 054 6	0.0 011 951 6	0.0 011 004 8	0.0 011 200 6	0.0 009 755 9	0.0 006 266 4	0.0 008 957 7	0.0 010 266 9	0.0 009 220 4	0.0 008 460 4	0.0 009 545 6	0.0 014 109 2
cis,cis-tetradeca-5,8-dienoyl-CoA	3.6 5E- 05	2.7 4E- 05	3.5 0E- 05	2.8 3E- 05	3.3 4E- 05	4.3 1E- 05	3.0 6E- 05	3.5 0E- 05	3.0 3E- 05	3.5 6E- 05	3.7 2E- 05	3.6 6E- 05	3.7 7E- 05	2.4 5E- 05	2.4 5E- 05
CITRULLINE	0.0 081 908 6	0.0 054 189 8	0.0 051 378 5	0.0 053 796 7	0.0 063 696 2	0.0 062 546 5	0.0 051 437 4	0.0 037 852 5	0.0 054 132 6	0.0 067 132 4	0.0 055 010 7	0.0 051 951 8	0.0 071 302 8	0.0 065 743 8	0.0 047 631 7
Creatine	0.0 082 625 1	0.0 078 929 3	0.0 085 397 7	0.0 082 334 4	0.0 076 178 5	0.0 103 551 5	0.0 081 304 3	0.0 072 217 9	0.0 050 134 7	0.0 079 140 9	0.0 054 428 9	0.0 058 782 4	0.0 072 6 6	0.0 058 071 0	0.0 071 768 0
Creatinine	0.0 028	0.0 023	0.0 025	0.0 024	0.0 022	0.0 026	0.0 030	0.0 026	0.0 020	0.0 024	0.0 020	0.0 025	0.0 024	0.0 018	0.0 020

	363 2	600 1	328 9	373 7	103 6	307 2	065 4	067 9	270 1	787 4	784 6	828 2	037 4	577 9	634 4
Cyclopentadecanolide	0.0 002 495 9	0.0 001 987 5	0.0 001 496 2	0.0 001 499 4	0.0 001 3 3	0.0 001 323 9	0.0 002 107 9	0.0 001 570 5	0.0 001 425 9	0.0 001 221 9	0.0 001 106 9	0.0 001 077 1	0.0 001 696 4	0.0 001 880 7	0.0 002 694 9
Cystine	0.0 006 918 5	0.0 013 834 7	0.0 011 623 2	0.0 007 298 6	0.0 006 860 6	0.0 014 484 8	0.0 006 090 6	0.0 012 626 2	0.0 014 408 3	0.0 012 647 2	0.0 012 920 5	0.0 013 388 7	0.0 014 874 3	0.0 016 297 6	0.0 009 101 1
D-Malic acid	0.0 025 938 3	0.0 018 219 4	0.0 009 594 7	0.0 013 664 4	0.0 021 862 6	0.0 014 278 6	0.0 021 292 7	0.0 018 893 6	0.0 005 251 8	0.0 015 855 6	0.0 006 073 2	0.0 014 590 5	0.0 015 172 5	0.0 017 104 7	0.0 012 567 4
D-Sedoheptulose	4.9 2E- 05	0.0 001 023 2	8.1 4E- 05	6.6 0E- 05	5.1 8E- 05	8.8 2E- 05	5.9 6E- 05	0.0 001 065 2	0.0 001 036 1	9.5 1E- 05	9.2 1E- 05	7.9 5E- 05	8.1 3E- 05	9.4 1E- 05	7.0 5E- 05
D-Tryptophan	0.0 045 701 7	0.0 072 325 6	0.0 056 995 9	0.0 061 245 6	0.0 058 410 6	0.0 070 011 8	0.0 055 233 9	0.0 064 304 3	0.0 048 153 9	0.0 069 608 9	0.0 093 361 5	0.0 072 451 5	0.0 060 077 3	0.0 052 026 8	0.0 045 109 2
Decanoylcarnitine	8.7 3E- 05	6.6 7E- 05	4.9 9E- 05	8.1 5E- 05	7.2 5E- 05	4.4 0E- 05	5.7 2E- 05	4.8 8E- 05	3.3 2E- 05	6.7 1E- 05	5.6 3E- 05	4.6 1E- 05	6.1 2E- 05	7.9 2E- 05	0.0 001 337 7
Dehydroepiandrosterone sulfate	5.7 6E- 06	6.7 2E- 06	7.5 3E- 06	6.7 3E- 06	7.4 3E- 06	6.8 4E- 06	8.5 7E- 06	8.9 3E- 06	6.7 1E- 06	7.2 6E- 06	6.9 3E- 06	6.8 1E- 06	6.3 0E- 06	7.2 0E- 06	6.9 7E- 06
Deoxycarnitine	0.0 002 946 2	0.0 002 253 3	0.0 002 468 6	0.0 002 581 3	0.0 003 731 8	0.0 002 306 9	0.0 003 431 5	0.0 002 068 3	7.4 4E- 05	0.0 002 239 8	0.0 002 181 9	0.0 001 359 9	0.0 002 204 9	0.0 002 054 1	0.0 001 857 4
Diginatigenin	0.0 002 355 5	0.0 002 577 2	7.9 5E- 05	0.0 002 109 4	0.0 002 190 7	0.0 002 933 7	1.2 6E- 05	0.0 001 720 5	3.5 9E- 05	0.0 002 359 6	0.0 002 389 2	0.0 002 005 2	0.0 001 360 2	0.0 001 749 2	8.6 3E- 05
Diisopropylphosphate	0.0 876 2	0.0 547 4	0.0 002 670 3	0.0 002 523 6	0.0 002 200 1	0.0 002 427 5	0.0 002 448 8	0.0 001 427 6	0.0 001 718 9	0.0 001 792 9	0.0 001 995 7	0.0 002 083 7	0.0 001 909 2	0.0 002 035 9	0.0 002 178 9
DL-Leucine	0.0 221 275 6	0.0 263 194 9	0.0 399 177 9	0.0 343 623 7	0.0 272 898 1	0.0 427 775 4	0.0 293 985 1	0.0 377 597 7	0.0 351 597 5	0.0 362 939 8	0.0 408 534 5	0.0 361 395 5	0.0 370 155 1	0.0 333 815 3	0.0 383 950 3
docosaheptaenoic acid	6.3 4E- 05	6.2 8E- 05	8.0 4E- 05	7.6 2E- 05	7.6 4E- 05	4.8 2E- 05	0.0 001 078 9	5.5 4E- 05	5.0 7E- 05	4.5 6E- 05	4.4 7E- 05	3.6 8E- 05	4.4 7E- 05	5.0 3E- 05	7.8 4E- 05
DOCOSAHEXAENOIC ACID	0.0 174 708 3	0.0 167 368 1	0.0 211 654 6	0.0 211 712 3	0.0 206 984 9	0.0 156 317 3	0.0 256 056 4	0.0 183 338 9	0.0 124 571 8	0.0 123 781 6	0.0 100 479 6	0.0 099 479 5	0.0 138 602 6	0.0 141 338 3	0.0 181 196 1
Docosanoic acid	5.8 7E- 05	4.7 5E- 05	4.1 9E- 05	5.0 0E- 05	5.0 6E- 05	5.9 3E- 05	5.4 0E- 05	4.7 5E- 05	3.2 6E- 05	4.4 5E- 05	4.5 3E- 05	3.2 9E- 05	8.2 1E- 05	4.8 6E- 05	4.3 1E- 05
Docosapentaenoic acid	0.0 027 470 4	0.0 026 342 9	0.0 035 950 9	0.0 035 171 2	0.0 037 516 7	0.0 032 269 1	0.0 036 693 7	0.0 030 704 5	0.0 018 693 2	0.0 021 337 6	0.0 017 075 2	0.0 018 075 7	0.0 018 967 5	0.0 022 217 1	0.0 032 917 6
Docosatetraenoic acid	0.0 008 219 9	0.0 006 698 2	0.0 006 297 9	0.0 007 611 3	0.0 009 139 4	0.0 007 117 5	0.0 009 245 8	0.0 005 362 1	0.0 004 947 4	0.0 004 903 5	0.0 003 012 4	0.0 004 012 7	0.0 004 327 9	0.0 005 005 5	0.0 006 928 5
Docosatrenoic acid	5.1 5E- 05	4.5 8E- 05	4.6 7E- 05	4.8 8E- 05	5.9 7E- 05	4.4 5E- 05	5.9 2E- 05	4.0 4E- 05	3.1 6E- 05	3.2 9E- 05	3.3 2E- 05	3.0 4E- 05	3.4 1E- 05	4.1 6E- 05	4.5 9E- 05
Eicosadienoic acid	0.0 011 867 7	0.0 011 08 2	0.0 011 032 2	0.0 011 460 2	0.0 011 894 4	0.0 008 808 6	0.0 013 526 6	0.0 010 148 3	0.0 008 484 9	0.0 007 780 4	0.0 007 828 4	0.0 006 075 6	0.0 007 543 6	0.0 009 400 2	0.0 012 126 2
Eicosapentaenoic acid	0.0 028 906 6	0.0 043 538 7	0.0 044 155 9	0.0 040 025 3	0.0 031 710 9	0.0 032 538 9	0.0 035 763 8	0.0 041 594 1	0.0 020 081 4	0.0 022 887 6	0.0 021 653 9	0.0 021 653 3	0.0 029 759 1	0.0 033 795 6	0.0 048 734 2
Eicosatrienoic acid	0.0 020 411 7	0.0 019 180 6	0.0 017 575 9	0.0 018 265 6	0.0 018 009 6	0.0 014 892 3	0.0 025 252 1	0.0 016 64 1	0.0 012 015 4	0.0 012 213 5	0.0 011 603 7	0.0 009 594 7	0.0 012 949 4	0.0 016 380 7	0.0 018 392 4
Eicosenoic acid	0.0 026 681 1	0.0 025 563 5	0.0 020 181 4	0.0 025 087 2	0.0 020 126 9	0.0 020 018 9	0.0 026 266 3	0.0 026 732 6	0.0 022 076 1	0.0 016 606 2	0.0 017 294 8	0.0 015 979 7	0.0 023 74 7	0.0 028 877 7	0.0 035 328 5
ELAIDIC ACID	0.0 648 163 2	0.0 583 941 1	0.0 564 511 8	0.0 554 759 8	0.0 522 8 2	0.0 488 084 2	0.0 614 957 3	0.0 573 491 1	0.0 494 449 3	0.0 444 300 7	0.0 451 810 2	0.0 415 276 7	0.0 454 384 7	0.0 466 681 7	0.0 589 305 1
Erucamide	7.0 4E- 05	0.0 001 265 1	0.0 001 312 7	9.2 4E- 05	8.4 9E- 05	0.0 001 286 7	0.0 001 084 9	0.0 0.0 327 9	5.9 5E- 05	0.0 001 161 3	0.0 0.0 152 4	9.0 0E- 05	7.4 3E- 05	6.6 6E- 05	7.7 6E- 05
Erucic acid	0.0 001 629 3	0.0 002 115 9	0.0 001 866 2	0.0 002 109 2	0.0 001 639 9	0.0 002 663 9	0.0 001 240 3	0.0 001 930 5	0.0 001 227 5	0.0 001 77 7	0.0 001 574 2	0.0 001 354 4	0.0 002 127 2	0.0 002 728 4	0.0 002 517 7
Gluconate	0.0 003 613 9	0.0 004 821 5	0.0 004 921 6	0.0 003 937 7	0.0 003 737 9	0.0 004 677 9	0.0 004 037 5	0.0 005 602 2	0.0 005 757 2	0.0 005 538 7	0.0 004 013 12	0.0 006 013 8	0.0 006 006 8	0.0 006 596 7	0.0 008 400 5

Glucose	0.0 008 781 6	0.0 013 150 3	0.0 011 396 5	0.0 012 959	0.0 012 660 1	0.0 013 160 1	0.0 009 732 3	0.0 018 040 1	0.0 008 198 5	0.0 013 762 9	0.0 011 782 2	0.0 012 804 2	0.0 008 491 6	0.0 010 538 3	0.0 007 109 6
Glutamic acid	0.0 003 347 3	0.0 002 694 9	0.0 003 925 2	0.0 002 776 4	0.0 002 935 4	0.0 001 827 1	0.0 004 878 8	0.0 002 253 1	0.0 008 172 8	0.0 003 940 8	0.0 006 938 1	0.0 006 395 3	0.0 006 741 5	0.0 004 172 3	0.0 002 921 3
GLUTAMINE	0.0 430 496 3	0.0 393 625 9	0.0 329 525 2	0.0 331 525 9	0.0 369 580 2	0.0 373 580 5	0.0 321 278 1	0.0 310 948 2	0.0 525 441 2	0.0 545 986 2	0.0 479 907 8	0.0 389 907 7	0.0 554 822 1	0.0 546 429 3	0.0 413 662 8
Glycol distearate	5.0 6E- 05	4.1 8E- 05	2.0 7E- 05	3.6 2E- 05	2.8 2E- 05	2.1 3E- 05	3.8 1E- 05	4.0 2E- 05	3.0 5E- 05	2.9 6E- 05	1.9 5E- 05	1.5 1E- 05	4.5 3E- 05	5.3 5E- 05	6.0 8E- 05
Heneicosylic acid	1.5 9E- 05	2.4 7E- 05	1.7 9E- 05	2.4 3E- 05	1.6 3E- 05	3.2 1E- 05	2.2 8E- 05	1.8 7E- 05	9.6 1E- 06	2.1 3E- 05	1.6 1E- 05	7.8 0E- 06	2.6 8E- 05	2.9 5E- 05	2.5 1E- 05
Hippurate	3.8 8E- 05	3.4 7E- 05	5.7 7E- 05	4.4 5E- 05	4.0 7E- 05	2.4 7E- 05	2.9 8E- 05	2.1 9E- 05	4.8 7E- 06	5.6 2E- 06	5.7 9E- 06	6.2 4E- 06	4.4 0E- 05	4.6 0E- 05	3.8 5E- 05
Histamine	0.0 001 319 3	0.0 001 724 05	0.0 7E- 05	0.0 001 708 9	0.0 001 885 8	0.0 001 524 05	3.0 0E- 05	7.5 6E- 05	0.0 002 747 3	0.0 001 658 9	0.0 002 001 2	0.0 001 517 8	0.0 001 503 6	0.0 001 3E- 05	7.0 05
Histidine	0.0 225 560 2	0.0 150 520 6	0.0 148 509 4	0.0 179 895 1	0.0 217 997 1	0.0 163 214 4	0.0 138 182 3	0.0 103 126 8	0.0 163 646 4	0.0 169 372 3	0.0 214 334 9	0.0 124 973 9	0.0 160 713 9	0.0 168 364 4	0.0 142 364 4
hydroxycitric acid	0.0 002 476 9	0.0 005 585 3	0.0 005 070 9	0.0 004 236 8	0.0 002 166 2	0.0 004 166 5	0.0 003 346 7	0.0 005 345 2	0.0 002 690 2	0.0 004 349 7	0.0 002 976 6	0.0 004 258 9	0.0 003 468 2	0.0 004 062 5	0.0 003 735 8
INDOLE	0.0 002 030 2	0.0 001 746 9	0.0 002 327 1	0.0 001 778 9	0.0 001 551 6	0.0 001 760 1	0.0 002 343 5	0.0 001 328 2	0.0 001 180 6	0.0 001 210 6	0.0 001 518 4	0.0 001 178 9	0.0 001 267 9	0.0 001 295 7	0.0 001 776 6
INDOXYL SULFATE	0.0 005 251 6	0.0 007 101 2	0.0 012 307 4	0.0 012 075 1	0.0 007 342 7	0.0 015 805 9	0.0 006 101 8	0.0 007 426 1	0.0 005 616 8	0.0 009 018 2	0.0 003 363 3	0.0 003 882 9	0.0 012 697 7	0.0 006 708 9	0.0 010 794 7
Isophthalic acid	1.0 6E- 05	1.2 6E- 05	1.3 3E- 05	1.2 3E- 05	1.2 3E- 05	1.2 7E- 05	1.3 6E- 05	1.3 4E- 05	1.0 4E- 05	1.1 5E- 05	1.1 5E- 05	1.2 6E- 05	1.1 3E- 05	1.0 6E- 05	1.0 8E- 05
Itaconic acid	0.0 003 272 5	0.0 003 296 9	0.0 003 208 4	0.0 002 368 4	0.0 003 059 6	0.0 003 683 9	0.0 003 731 8	0.0 003 578 8	0.0 003 317 8	0.0 003 545 8	0.0 003 826 8	0.0 004 055 8	0.0 004 910 8	0.0 003 953 7	0.0 004 506 5
L-(+) Lactic acid	0.0 127 544 5	0.0 092 109 1	0.0 112 845 6	0.0 125 362 7	0.0 105 910 3	0.0 188 098 1	0.0 181 696 9	0.0 110 294 2	0.0 121 966 1	0.0 093 834 2	0.0 122 670 8	0.0 161 404 8	0.0 131 099 7	0.0 030 047 7	0.0 138 196 1
L-alpha-Glycerolphosphorylcholine	0.0 007 438	0.0 013 875 7	0.0 014 829 7	0.0 012 297 9	0.0 008 962 6	0.0 011 070 6	0.0 013 153 7	0.0 010 260 8	0.0 005 523 8	0.0 015 393 2	0.0 016 128 3	0.0 011 814 6	0.0 014 527 9	0.0 014 694 9	0.0 011 271 3
L-alpha-lysophosphatidylcholine	0.0 001 226 6	9.1 3E- 05	0.0 001 338 8	0.0 001 437 4	0.0 001 499 5	0.0 001 422 7	0.0 002 011 193 6	8.0 4E- 05	9.8 9E- 05	0.0 001 011 168	0.0 001 011 168	9.7 0E- 05	0.0 001 073 7	9.8 3E- 05	0.0 001 073 7
L-Arginine	0.0 106 298 4	0.0 081 832 5	0.0 073 754 9	0.0 084 381 8	0.0 117 710 4	0.0 089 540 1	0.0 070 706 1	0.0 066 142 6	0.0 107 467 1	0.0 147 893 7	0.0 108 297 9	0.0 087 226 6	0.0 108 178 9	0.0 067 970 9	0.0 067 970 9
L-CARNITINE	0.0 001 075	0.0 001 100 7	0.0 001 001 5	0.0 001 001 4	0.0 001 001 5	0.0 002 001 3	0.0 002 001 2	0.0 001 001 4	7.8 4E- 05	0.0 001 175 3	6.5 8E- 05	8.1 0E- 05	8.8 2E- 05	8.6 5E- 05	6.9 5E- 05
L-Cysteinyglycine disulfide	6.0 0E- 05	9.0 8E- 05	8.5 2E- 05	8.3 6E- 05	7.3 3E- 05	8.3 1E- 05	0.0 001 149	0.0 001 018 3	8.6 4E- 05	6.3 8E- 05	6.2 3E- 05	8.8 9E- 05	7.9 0E- 05	6.1 7E- 05	8.8 4E- 05
L-Kynurenine	8.6 8E- 05	0.0 001 025 5	7.8 1E- 05	6.7 0E- 05	8.1 5E- 05	9.6 2E- 05	8.0 0E- 05	8.2 5E- 05	4.2 4E- 05	8.8 8E- 05	8.1 0E- 05	8.6 9E- 05	7.7 9E- 05	8.0 5E- 05	5.4 0E- 05
L-Lysine	0.0 095 369 2	0.0 058 517 3	0.0 058 456	0.0 059 821 2	0.0 001 517 7	0.0 077 210 9	0.0 048 048 6	0.0 049 093 4	0.0 131 485 9	0.0 104 712 3	0.0 097 208 3	0.0 097 366	0.0 070 130 9	0.0 092 460 6	0.0 053 235 1
L-Pipecolic acid	0.0 035 282 1	0.0 022 002 7	0.0 021 775 3	0.0 022 236 2	0.0 038 114 6	0.0 028 289 2	0.0 018 119 8	0.0 018 222 3	0.0 049 393 9	0.0 051 988 7	0.0 037 102 7	0.0 026 864 3	0.0 035 250 4	0.0 019 338 9	0.0 019 338 9
L-Pyroglutamic acid	0.0 255 234 4	0.0 230 384 2	0.0 189 486 1	0.0 196 993 6	0.0 217 051 8	0.0 182 217 2	0.0 848 512 1	0.0 178 177 1	0.0 317 512 5	0.0 339 752 2	0.0 290 163 8	0.0 232 507 3	0.0 331 553 3	0.0 037 553 8	0.0 242 701 8
L-Threonine acid	0.0 007 289 1	0.0 013 940 6	0.0 014 061 1	0.0 011 512 6	0.0 008 246 7	0.0 011 169 6	0.0 010 246 3	0.0 013 710 5	0.0 007 750 7	0.0 011 905 6	0.0 008 582 6	0.0 012 654 2	0.0 010 510 6	0.0 010 880 8	0.0 010 880 8
Labdanolic acid	8.6 7E- 06	4.8 4E- 06	6.2 5E- 06	5.6 0E- 06	7.5 2E- 06	5.6 4E- 06	1.1 3E- 05	5.3 1E- 06	6.6 4E- 06	5.1 7E- 06	2.0 6E- 06	6.6 9E- 06	5.3 4E- 06	5.4 2E- 06	6.7 5E- 06
LAURIC ACID (Dodecanoic acid, Plasma)	0.0 004 552 5	0.0 002 961 9	0.0 002 766 4	0.0 003 128 8	0.0 002 960 9	0.0 001 999 1	0.0 004 005 5	0.0 003 489 9	0.0 002 527 3	0.0 000 180 3	0.0 000 371 1	0.0 000 750 8	0.0 002 913 5	0.0 000 172 7	0.0 004 883 9

lentiginosine	0.0 003 653 9	0.0 001 363 8	0.0 001 858 9	0.0 002 290 1	0.0 002 870 1	0.0 002 521 7	0.0 003 625 5	0.0 001 221 4	9.8 1E- 05	0.0 001 353 3	0.0 001 080 5	6.9 1E- 05	0.0 001 549 3	0.0 001 261 2	9.5 3E- 05
LEUCINE	0.0 009 048 3	0.0 012 228 6	0.0 020 892 4	0.0 015 247 2	0.0 011 646 1	0.0 017 546 6	0.0 013 770 8	0.0 017 303 5	0.0 011 584 5	0.0 012 392 4	0.0 013 127 7	0.0 011 538 7	0.0 013 177 5	0.0 012 592 8	0.0 017 130 8
Linolenic acid	0.0 002 854 2	0.0 001 325 4	9.7 0E- 05	0.0 001 305 8	0.0 001 347 7	6.1 4E- 05	0.0 001 464 8	9.2 4E- 05	0.0 001 139 1	9.3 1E- 05	9.4 0E- 05	0.0 001 148 4	9.6 1E- 05	0.0 001 054 7	0.0 001 733 9
Lysolecithin	0.0 202 708 8	0.0 264 86 1	0.0 280 157 5	0.0 270 233 3	0.0 233 275 7	0.0 275 027 3	0.0 253 711 6	0.0 286 869 4	0.0 235 379 3	0.0 230 784 1	0.0 267 218 6	0.0 315 328 4	0.0 233 753 1	0.0 235 931 0	0.0 212 665 9
lysoPC a C28:0	0.0 001 645 6	0.0 001 126 6	0.0 001 277 6	0.0 001 106 3	0.0 001 726 2	0.0 001 695 3	0.0 001 365 5	0.0 001 657 4	0.0 001 977 7	0.0 002 035 1	0.0 002 058 5	0.0 002 073 6	0.0 001 464 3	0.0 001 678 0	8.9 2E- 05
Methionine	0.0 002 675 1	0.0 001 883 2	0.0 002 739 3	0.0 002 673 5	0.0 003 621 7	0.0 003 330 2	0.0 003 511 7	0.0 002 79 5	0.0 001 474 5	0.0 002 513 5	0.0 002 539 5	0.0 002 465 5	0.0 001 760 1	0.0 002 342 8	0.0 001 550 9
Methionine Sulfoxide	0.0 001 368 6	0.0 001 442 3	0.0 001 142 9	0.0 001 321 8	0.0 001 142 4	0.0 001 292 9	9.9 1E- 05	8.8 6E- 05	0.0 001 564 3	0.0 002 759 2	0.0 001 049 1	0.0 002 751 2	0.0 001 961 6	0.0 001 666 9	9.3 5E- 05
Methyl (9E)-9-octadecenoate	0.0 006 367 2	0.0 004 732 6	0.0 002 982 2	0.0 003 719 8	0.0 003 293 8	0.0 003 077 3	0.0 003 743 6	0.0 003 477 3	0.0 003 337 6	0.0 002 671 9	0.0 003 144 1	0.0 002 523 5	0.0 004 360 1	0.0 004 417 3	0.0 004 868 7
Methyl (9Z,12Z,16E)-15-hydroperoxy-9,12,16-octadecatrienoate	0.0 005 638 9	0.0 005 542 2	0.0 005 238 2	0.0 004 881 9	0.0 003 676 3	0.0 003 725 5	0.0 005 115 3	0.0 005 005 6	0.0 002 859 4	0.0 002 860 9	0.0 002 827 4	0.0 002 877 9	0.0 003 839 9	0.0 004 062 7	0.0 007 336 4
Methyl palmitate	0.0 019 410 5	0.0 017 931 1	0.0 012 483 9	0.0 014 095 4	0.0 012 574 5	0.0 011 886 3	0.0 014 574 6	0.0 013 182 5	0.0 012 053 2	0.0 011 743 2	0.0 010 010 2	0.0 009 361 9	0.0 019 171 3	0.0 015 072 5	0.0 017 468 5
Methyl stearate	0.0 002 515 3	0.0 003 487 2	0.0 002 218 2	0.0 002 639 1	0.0 002 137 5	0.0 002 175 7	0.0 002 461 1	0.0 002 270 5	0.0 001 706 4	0.0 002 180 5	0.0 001 600 2	0.0 001 726 6	0.0 003 390 6	0.0 002 800 5	0.0 003 120 5
MFCD00133435 (1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine)	0.0 071 820 1	0.0 049 838 4	0.0 051 142 7	0.0 053 858 2	0.0 061 239 6	0.0 062 945 6	0.0 053 744 1	0.0 051 868 3	0.0 039 290 4	0.0 041 199 4	0.0 045 630 1	0.0 050 057 7	0.0 042 808 3	0.0 044 361 5	0.0 038 076 4
MFCD00273074 (1-Heptadecanoyl-rac-glycerol)	0.0 001 379 5	0.0 001 723 4	0.0 001 514 6	0.0 001 745 6	0.0 001 651 8	0.0 001 389 8	0.0 001 646 3	0.0 001 697 2	0.0 001 214 5	0.0 001 369 2	0.0 001 199 5	0.0 001 235 6	0.0 001 51 5	0.0 001 513 1	0.0 001 556 7
MFCD12546417 (3,4-Dihydroxybenzenesulfonic acid)	0.0 001 336 3	0.0 001 174 3	0.0 002 255 5	0.0 001 296 5	8.1 5E- 05	0.0 001 154 4	9.2 2E- 05	8.4 4E- 05	2.7 0E- 05	5.4 7E- 05	7.1 9E- 05	2.3 8E- 05	9.9 6E- 05	6.0 6E- 05	9.1 2E- 05
MFCD22416941 (Oleoyl-L-carnitine)	0.0 020 535 7	0.0 014 560 6	0.0 009 048 1	0.0 013 598 9	0.0 013 706 3	0.0 014 682 4	0.0 016 455 6	0.0 011 819 9	0.0 010 999 6	0.0 011 526 2	0.0 014 463 2	0.0 012 956 2	0.0 012 140 3	0.0 010 264 9	0.0 015 441 4
MYRISTIC ACID	0.0 093 192 7	0.0 057 330 7	0.0 056 529 1	0.0 059 294 2	0.0 066 919 7	0.0 039 723 5	0.0 071 821 2	0.0 063 519 4	0.0 066 383 1	0.0 060 623 1	0.0 051 451 1	0.0 050 630 1	0.0 062 071 7	0.0 096 682 6	0.0 015 441 4
Myristic Acid Alkyne	0.0 008 444 4	0.0 007 160 3	0.0 005 162 8	0.0 006 855 6	0.0 006 616 9	0.0 003 667 5	0.0 007 641 7	0.0 005 332 1	0.0 004 043 3	0.0 004 095 3	0.0 003 330 7	0.0 004 482 6	0.0 005 507 9	0.0 007 132 1	0.0 011 132 1
Myristoleic acid	0.0 015 760 2	0.0 009 648 7	0.0 008 554 7	0.0 010 892 6	0.0 008 117 1	0.0 006 795 3	0.0 011 973 3	0.0 010 007 6	0.0 007 321 6	0.0 008 185 3	0.0 007 288 3	0.0 010 012 3	0.0 011 067 1	0.0 018 991 6	0.0 018 991 6
N-[(2S,3R)-1-(beta-D-Glucopyranosyloxy)-3-hydroxy-2-octadecanyl]tetradecanamide	8.4 2E- 05	6.5 5E- 05	7.7 8E- 05	6.1 3E- 05	8.4 8E- 05	8.2 2E- 05	6.9 2E- 05	8.4 0E- 05	9.4 5E- 05	9.8 5E- 05	9.9 001 020 1	9.9 2E- 05	7.7 8E- 05	8.3 1E- 05	4.6 5E- 05
N-{15-Methyl-3-[(15-methylhexadecanoyl)oxy]hexadecanoyl}-L-serine	7.0 1E- 05	7.3 9E- 05	6.6 6E- 05	5.9 7E- 05	8.2 4E- 05	8.2 6E- 05	5.8 6E- 05	6.8 7E- 05	6.1 0E- 05	6.5 3E- 05	6.2 6E- 05	7.3 1E- 05	7.0 0E- 05	7.4 3E- 05	5.9 0E- 05
N-Acetyl glycine	0.0 001 528 1	0.0 002 611 1	0.0 002 884 7	0.0 002 308 5	0.0 001 546 4	0.0 003 938 5	0.0 002 382 4	0.0 003 103 9	0.0 002 895 3	0.0 001 580 2	0.0 002 181 7	0.0 002 364 7	0.0 002 538 8	0.0 001 977 2	0.0 002 405 4
N-Benzylformamide	9.9 0E- 05	3.6 5E- 05	8.8 4E- 05	9.4 9E- 05	0.0 001 375 6	0.0 001 083 6	0.0 001 440 2	0.0 001 4E- 05	4.7 2E- 05	7.5 2E- 05	7.1 9E- 05	7.3 0E- 05	4.0 3E- 05	6.3 6E- 05	3.6 1E- 05
N,N-Diisopropylethylamine (DIPEA)	7.7 1E- 05	0.0 001 190 7	8.2 8E- 05	7.6 9E- 05	5.6 9E- 05	7.9 8E- 05	0.0 001 062 8	6.2 1E- 05	8.3 0E- 05	8.9 3E- 05	7.0 1E- 05	8.4 0E- 05	0.0 001 403 2	5.9 1E- 05	7.0 1E- 05
N,N-DIMETHYLARGININE	0.0 003 150 2	0.0 001 429 2	0.0 001 805 3	0.0 002 583 6	0.0 002 858 1	0.0 002 264 1	0.0 002 112 2	0.0 003 977 2	0.0 003 451 9	0.0 004 122 8	0.0 003 137 6	0.0 001 852 6	0.0 002 830 7	0.0 002 479 2	0.0 001 342 4
N6-METHYLLYSINE	0.0 004 288 6	0.0 003 651 7	0.0 002 361 9	0.0 002 535 3	0.0 002 517 3	0.0 002 932 5	0.0 003 764 4	0.0 002 265 6	0.0 008 922 1	0.0 007 548 7	0.0 005 977 5	0.0 005 73 42	0.0 004 005 8	0.0 005 724 8	0.0 002 574 9

Nervonic acid	0.0 001 135 1	0.0 001 436 2	0.0 001 021 5	0.0 001 495 6	0.0 001 344 6	0.0 001 323 6	0.0 001 759 4	0.0 001 192 5	6.9 4E- 05	0.0 001 094 7	0.0 001 099 2	9.3 4E- 05	0.0 001 423 1	0.0 001 244 1	0.0 001 128 6
Nicotinamide	0.0 009 464 4	0.0 016 259 4	0.0 024 865 4	0.0 018 6 5	0.0 017 787 7	0.0 017 209 5	0.0 014 462 6	0.0 019 357 9	0.0 010 217 5	0.0 013 015 6	0.0 014 216 6	0.0 012 411 5	0.0 015 524 3	0.0 015 850 8	0.0 018 447 8
O-ACETYLCARNITINE	0.0 032 581 5	0.0 044 815 2	0.0 062 084 2	0.0 043 973 1	0.0 030 973 4	0.0 065 191 2	0.0 036 977 3	0.0 031 298 5	0.0 020 174 5	0.0 030 759 5	0.0 026 174 5	0.0 027 174 5	0.0 033 975 1	0.0 028 682 1	0.0 030 862 2
O-ureido-D-serine	0.0 059 697 6	0.0 051 549 8	0.0 066 433 5	0.0 056 043 3	0.0 077 644 7	0.0 060 644 8	0.0 044 655 1	0.0 035 781 8	0.0 095 501 8	0.0 072 569 8	0.0 063 811 5	0.0 079 921 1	0.0 074 279 1	0.0 040 904 3	0.0 042 695 3
Octadecadienoic acid	0.1 017 353 7	0.0 998 377 6	0.0 947 509 3	0.0 949 830 8	0.0 843 251 8	0.0 776 001 8	0.0 965 265 2	0.0 937 082 2	0.0 896 666 4	0.0 759 009 4	0.0 776 448 9	0.0 802 753 3	0.0 866 454 3	0.0 890 054 3	0.1 193 328 9
ODYA (17-octadecynoic acid)	0.0 007 580 2	0.0 007 466 1	0.0 007 431 3	0.0 005 891 9	0.0 004 590 9	0.0 003 985 9	0.0 006 450 6	0.0 005 819 9	0.0 003 685 2	0.0 003 815 2	0.0 002 718 2	0.0 003 368 2	0.0 005 306 5	0.0 007 156 1	0.0 013 358 6
Ornithine	0.0 013 564 6	0.0 006 960 8	0.0 009 367 3	0.0 008 583 6	0.0 020 492 2	0.0 020 683 5	0.0 012 690 2	0.0 008 547 4	0.0 013 064 2	0.0 013 029 8	0.0 020 207 4	0.0 012 973 7	0.0 009 195 2	0.0 013 676 9	0.0 007 676 8
Palmitic acid	0.0 500 569 4	0.0 561 692 1	0.0 582 572 3	0.0 616 282 2	0.0 530 787 1	0.0 498 806 4	0.0 549 951 1	0.0 582 246 2	0.0 397 853 1	0.0 490 216 1	0.0 409 339 2	0.0 419 544 1	0.0 490 050 9	0.0 449 697 7	0.0 620 545 7
PALMITOLEIC ACID	0.0 293 618 9	0.0 223 086 3	0.0 223 373 4	0.0 214 544 9	0.0 188 646 4	0.0 169 977 1	0.0 244 672 3	0.0 229 235 8	0.0 233 428 5	0.0 234 915 3	0.0 213 587 0	0.0 222 587 2	0.0 237 241 2	0.0 228 358 1	0.0 328 680 1
Palmitoyl sphingomyelin	0.0 001 626 3	0.0 002 184 4	0.0 002 257 4	0.0 002 306 8	0.0 001 002 5	0.0 002 243 5	0.0 002 521 3	0.0 000 107 9	0.0 001 001 8	0.0 001 842 3	0.0 001 001 9	0.0 001 564 3	0.0 001 631 6	0.0 001 262 7	0.0 002 254 8
Palmitoyl-DL-carnitine	0.0 019 112 9	0.0 014 833 7	0.0 011 477 5	0.0 013 822 1	0.0 014 356 4	0.0 013 200 8	0.0 016 941 8	0.0 010 985 6	0.0 010 472 4	0.0 011 444 6	0.0 013 580 6	0.0 012 140 3	0.0 013 511 4	0.0 017 911 2	0.0 017 911 1
para-Cresol Sulfate	0.0 004 954 9	0.0 017 145 8	0.0 016 379 9	0.0 015 174 4	0.0 006 506 9	0.0 013 575 2	0.0 008 276 7	0.0 008 134 4	0.0 001 706 1	0.0 004 297 4	0.0 001 386 2	0.0 002 851 5	0.0 005 663 8	0.0 007 936 3	0.0 003 985 3
PC	0.0 168 554 9	0.0 240 050 2	0.0 212 658 2	0.0 201 577 8	0.0 201 813 4	0.0 222 156 8	0.0 191 873 5	0.0 219 094 5	0.0 201 671 8	0.0 202 702 9	0.0 010 864 8	0.0 255 873 8	0.0 201 989 5	0.0 220 55 5	0.0 214 500 4
Pentacosanoic acid	4.0 5E- 06	4.5 8E- 06	4.2 9E- 06	4.5 2E- 06	4.6 0E- 06	4.5 3E- 06	4.6 7E- 06	4.1 0E- 06	5.3 7E- 06	5.2 1E- 06	5.7 3E- 06	6.9 8E- 06	5.1 2E- 06	4.9 6E- 06	4.1 6E- 06
Pentadecanoic acid	0.0 009 402 8	0.0 010 886 9	0.0 007 921 7	0.0 008 104 2	0.0 008 443 1	0.0 006 593 1	0.0 009 593 2	0.0 007 885 1	0.0 007 692 2	0.0 006 692 2	0.0 006 327 4	0.0 006 378 3	0.0 010 378 9	0.0 007 109 4	0.0 008 237 4
PG(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))	2.2 2E- 05	1.4 2E- 05	1.4 5E- 05	1.1 5E- 05	2.5 2E- 05	2.3 1E- 05	2.0 6E- 05	2.4 2E- 05	2.9 4E- 05	2.9 3E- 05	2.7 1E- 05	2.8 1E- 05	1.9 4E- 05	2.1 6E- 05	1.0 4E- 05
PHENYLALANINE	0.0 102 001 5	0.0 112 130 7	0.0 140 944 7	0.0 134 240 7	0.0 128 148 6	0.0 146 534 6	0.0 151 434 1	0.0 130 592 9	0.0 112 434 9	0.0 124 465 2	0.0 129 123 6	0.0 113 760 7	0.0 110 447 7	0.0 121 060 7	0.0 017 203 4
Phosphoric acid	0.0 011 692 7	0.0 012 381 8	0.0 019 975 5	0.0 019 702 7	0.0 019 017 6	0.0 016 594 9	0.0 017 218 9	0.0 011 427 9	0.0 010 940 4	0.0 009 415 9	0.0 010 159 6	0.0 012 437 2	0.0 014 985 1	0.0 011 985 9	0.0 015 096 7
PHOSPHORYLCHOLINE	0.0 006 152 9	0.0 006 855 5	0.0 007 33 3	0.0 007 381 2	0.0 006 380 3	0.0 008 506 7	0.0 007 209 3	0.0 007 267 6	0.0 005 291 3	0.0 007 020 3	0.0 006 291 5	0.0 006 722 5	0.0 006 184 6	0.0 006 540 6	0.0 006 498 7
Prolinamide	0.0 002 575 3	7.9 6E- 05	0.0 001 696 1	0.0 001 169 3	0.0 003 408 3	0.0 002 230 2	0.0 002 040 9	8.4 5E- 05	0.0 002 404 6	0.0 003 090 1	0.0 003 162 1	0.0 003 518 6	0.0 001 684 6	0.0 001 554 6	0.0 001 337 8
Proline	0.0 039 677 2	0.0 021 306 1	0.0 023 999 2	0.0 025 296 5	0.0 036 968 6	0.0 028 751 1	0.0 031 036 9	0.0 025 904 6	0.0 019 437 2	0.0 028 755 3	0.0 023 961 9	0.0 023 574 3	0.0 023 132 7	0.0 025 499 7	0.0 017 203 4
Proline Betaine (Stachydrine)	0.0 008 371 2	0.0 003 559 9	0.0 004 623 9	0.0 004 901 7	0.0 005 354 3	0.0 005 023 3	0.0 006 264 4	0.0 003 157 3	0.0 001 72 4	0.0 006 26 8	0.0 002 587 1	0.0 001 717 1	0.0 003 957 7	0.0 003 518 4	0.0 002 842 1
Propionylcarnitine	0.0 002 592 6	0.0 001 185 4	0.0 001 636 6	0.0 001 771 2	0.0 003 492 3	0.0 001 373 3	0.0 002 216 9	0.0 001 486 5	0.0 002 332 3	0.0 001 762 3	0.0 001 001 5	0.0 001 782 5	0.0 001 150 2	0.0 001 854 1	0.0 001 393 8
Prostaglandin F1E± Alcohol	0.0 003 175 8	0.0 002 014 9	0.0 003 189 9	0.0 003 053 3	0.0 002 749 9	0.0 002 388 6	0.0 003 047 6	0.0 003 925 9	0.0 002 558 6	0.0 002 558 1	0.0 003 405 5	0.0 002 001 9	0.0 001 986 6	0.0 002 434 5	0.0 002 942 5
ricinelaidic acid	3.8 7E- 05	2.9 3E- 05	1.6 0E- 05	2.7 0E- 05	3.0 0E- 05	1.2 4E- 05	3.2 1E- 05	1.9 6E- 05	1.9 1E- 05	1.9 8E- 05	1.3 2E- 05	1.3 2E- 05	2.6 3E- 05	2.9 7E- 05	3.4 2E- 05
SEROTONIN	1.3 6E- 05	0.0 005 012	0.0 004 012	0.0 004 012	1.5 0E- 05	1.7 1E- 05	1.5 7E- 05	1.6 0E- 05	1.4 0E- 05	1.6 2E- 05	1.3 8E- 05	1.7 1E- 05	1.4 3E- 05	1.4 4E- 05	0.0 002

		557 5	733 7	177 4												093 8
soyasapogenol A	3.1 1E- 05	2.1 6E- 05	2.4 4E- 05	2.2 9E- 05	2.0 3E- 05	2.1 4E- 05	2.2 0E- 05	2.5 1E- 05	1.8 6E- 05	1.9 4E- 05	1.8 3E- 05	2.2 8E- 05	1.9 8E- 05	1.9 8E- 05	2.9 6E- 05	
Sphingosine	4.0 6E- 05	3.0 8E- 05	3.3 0E- 05	3.7 2E- 05	3.7 2E- 05	2.3 8E- 05	3.8 5E- 05	2.7 6E- 05	2.4 4E- 05	2.8 1E- 05	2.6 1E- 05	3.0 0E- 05	2.9 1E- 05	3.5 2E- 05	3.2 5E- 05	
Stearic acid	0.0 160 701 7	0.0 187 206	0.0 164 759 2	0.0 206 529 2	0.0 170 227 6	0.0 173 213 8	0.0 179 882 6	0.0 199 811 6	0.0 141 234 8	0.0 150 974 8	0.0 141 707 9	0.0 149 319 4	0.0 196 355 1	0.0 180 546 9	0.0 198 222 3	
Taurine	0.0 014 428 5	0.0 015 107	0.0 020 853 6	0.0 019 234 2	0.0 013 053 6	0.0 014 340 6	0.0 021 285 1	0.0 015 467 1	0.0 004 767 2	0.0 008 464 7	0.0 009 791 1	0.0 008 215 1	0.0 013 531 5	0.0 009 887 4	0.0 016 669 6	
Tetraneurin E	7.9 1E- 06	9.8 3E- 06	9.9 1E- 06	1.0 6E- 05	9.7 7E- 06	9.7 0E- 06	1.1 3E- 05	1.1 7E- 05	8.8 3E- 06	1.0 2E- 05	9.1 9E- 06	9.4 4E- 06	8.9 2E- 06	9.5 8E- 06	9.1 7E- 06	
trans-10-Heptadecenoic acid	0.0 015 463 8	0.0 012 803 5	0.0 009 659 2	0.0 009 668 9	0.0 008 194 2	0.0 008 426 8	0.0 010 842 8	0.0 009 990 8	0.0 009 332 4	0.0 008 894 4	0.0 009 593 9	0.0 008 311 5	0.0 011 220 2	0.0 011 261 2	0.0 013 940 4	
trans-2-Tetradecenoyl-L-carnitine	0.0 006 471 4	0.0 003 975 1	0.0 002 655 8	0.0 004 693 2	0.0 004 696 2	0.0 003 533 3	0.0 004 258 3	0.0 003 448 6	0.0 002 137 5	0.0 003 655 5	0.0 003 598 6	0.0 003 746 9	0.0 003 843 4	0.0 006 523 7	0.0 006 523 7	
trans-3-Indoleacrylic acid	0.0 056 109 1	0.0 086 273 4	0.0 069 566	0.0 073 946	0.0 070 297	0.0 083 535 9	0.0 068 275 9	0.0 077 279 5	0.0 058 956 6	0.0 082 550 9	0.0 111 933 6	0.0 087 801 1	0.0 072 580 2	0.0 062 649 4	0.0 053 746 3	
TRANS-ACONITATE	0.0 003 182 7	0.0 002 937 8	0.0 002 202 7	0.0 001 923 5	0.0 001 175 3	0.0 001 771 8	0.0 002 332 7	0.0 001 889 5	0.0 003 167 1	0.0 003 323 6	0.0 002 564 8	0.0 003 908 1	0.0 003 089 5	0.0 002 780 8	0.0 002 294 6	
Tridecanoic acid	0.0 001 978 2	0.0 001 717 8	0.0 001 228	0.0 001 901 8	0.0 001 236 1	0.0 001 135 5	0.0 001 862 4	0.0 001 447 3	9.1 5E- 05	0.0 001 359 6	8.4 7E- 05	0.0 001 038 5	0.0 001 048 2	0.0 001 511 1	0.0 002 056 3	
TRYPTOPHAN	0.0 005 869 6	0.0 009 310 5	0.0 008 048 7	0.0 007 940 1	0.0 007 666 9	0.0 008 216 1	0.0 008 448 5	0.0 008 166 1	0.0 004 201 5	0.0 006 345 8	0.0 008 156 8	0.0 006 778 8	0.0 005 953 4	0.0 005 135 6	0.0 005 583 7	
Typhasterol	7.0 2E- 05	7.4 3E- 05	7.0 6E- 05	6.9 9E- 05	6.1 9E- 05	5.8 8E- 05	7.3 0E- 05	6.8 4E- 05	6.4 9E- 05	6.6 4E- 05	5.9 0E- 05	6.8 9E- 05	6.8 5E- 05	6.6 3E- 05	7.4 5E- 05	
TYROSINE	0.0 003 167 1	0.0 002 879 7	0.0 002 918	0.0 003 261 4	0.0 003 978 4	0.0 003 321 1	0.0 004 401	0.0 002 607	0.0 001 316	0.0 002 046 4	0.0 001 970 1	0.0 001 877 5	0.0 001 985 6	0.0 002 314 2	0.0 002 593 8	
Uric acid	0.0 007 860 5	0.0 005 791 9	0.0 008 424 7	0.0 007 186 2	0.0 006 923 2	0.0 004 013	0.0 006 390 9	0.0 005 724 5	0.0 007 162 3	0.0 007 134 6	0.0 005 160 5	0.0 006 503 3	0.0 005 208 3	0.0 005 852 3	0.0 007 729 1	
Valine	0.0 009	0.0 007 527 7	0.0 009 76	0.0 009 501 7	0.0 012 334 8	0.0 014 295 6	0.0 009 771	0.0 011 099 8	0.0 009 913 6	0.0 011 237 6	0.0 014 967 5	0.0 009 967 3	0.0 011 065 8	0.0 010 181 5	0.0 009 212 5	
Valproic acid	2.2 3E- 05	4.3 7E- 05	1.6 5E- 05	1.7 6E- 05	1.0 8E- 05	1.2 7E- 05	1.2 1E- 05	1.0 7E- 05	1.8 9E- 05	1.7 1E- 05	2.3 3E- 05	1.9 4E- 05	2.6 3E- 05	1.5 6E- 05	5.7 4E- 05	
Hydroxyisobutyric acid	0.0 017 133 2	0.0 023 234 8	0.0 018 086 7	0.0 024 048	0.0 016 009 8	0.0 029 999	0.0 014 457 1	0.0 023 603 2	0.0 024 250 8	0.0 035 585	0.0 025 790 1	0.0 037 082 8	0.0 033 132 9	0.0 034 167 9	0.0 032 638 4	