Table S4. Concentration of 407 metabolites [µmol/L] in cats. Metabolites significant at α=0.05 in uncorrected analysis are highlighted in red

Metabolites	Median (interquartile range)	Range	Correlation with fPLI (R_s)	p-value without Bonferroni correction
AMINO ACIDS AND RELATED COMPOUNDS				
Proteinogenic amino acids				
Alanine	372 (302 – 466)	157 – 791	-0.201	0.167
Arginine	92.8 (75.5 – 124)	10.5 – 179	-0.288	0.045
Asparagine	44.9 (33.2 – 66.1)	15.4 – 101	-0.008	0.956
Aspartic Acid	25.6 (18 – 40.8)	6.27 – 104	0.261	0.070
Cysteine	27.6 (24.3 – 31.9)	17.2 – 88.5	-0.223	0.123
Glutamine	678 (565 – 835)	259 – 2262	-0.121	0.406
Glutamic Acid	128 (97.5 – 177)	28.3 – 1031	0.050	0.732
Glycine	322 (239 – 371)	122 – 940	-0.029	0.843
Histidine	113 (93.3 – 142)	64.5 – 571	-0.079	0.590
Isoleucine	94.7 (65.9 – 126)	36.3 – 390	0.142	0.331
Leucine	169 (113 – 211)	52.6 – 673	0.046	0.754
Lysine	140 (114 – 169)	55.8 – 267	0.159	0.275

Methionine	42.3 (30.6 – 65.1)	13.7 – 192	-0.103	0.483
Phenylalanine	78.5 (65.3 – 93.4)	44.5 – 183	0.081	0.579
Proline	156 (127 – 225)	69.8 – 491	-0.229	0.114
Serine	157 (115 – 200)	68.4 – 367	-0.140	0.338
Threonine	150 (117 – 179)	49.9 – 475	0.101	0.492
Tryptophan	52.4 (40.1 – 60.8)	12.6 – 92.5	-0.492	<0.001
Tyrosine	48.1 (37.3 – 54.9)	16.6 – 147	0.022	0.881
Valine	203 (151 – 262)	63.3 – 718	0.093	0.524
Non-proteinogenic amino acids				
beta-Alanine	2.5 (1.58 – 6.15)	0.881 – 29.6	0.039	0.790
Citrulline	12.7 (8.82 – 18.3)	3.03 – 28.4	0.165	0.257
Ornithine	19.5 (15.8 – 31.6)	9.51 – 125	0.343	0.016
Cystine	0.303 (0.169 – 0.69)	0.067 – 124	0.252	0.081
α-Amino-butyric acid	14.3 (9.53 – 20.2)	3.09 – 42.8	0.325	0.023
γ-Amino-butyric acid	0.477 (0.253 – 0.83)	0.07 – 2.52	-0.192	0.186
Homoarginine	0.751 (0.532 – 1.09)	0.072 – 4.54	-0.147	0.313
Homocysteine	5.96 (4.65 – 8.06)	2.60 – 21.1	-0.100	0.496

Taurine	155 (98.4 – 186)	28.0 – 314	-0.072	0.624
trans-4-Hydroxyproline	32.3 (19.9 – 53.2)	4.96 – 98.4	-0.060	0.682
Methionine sulfoxide	6.88 (4.05 – 9.89)	1.76 – 30.9	-0.122	0.402
Amino acid derivatives				
1-Methylhistidine	15.6 (9.42 – 29.1)	4.69 – 99.1	0.389	0.006
3-Methylhistidine	15.0 (9.07 – 28.1)	3.44 – 109	0.307	0.032
5-Aminovaleric acid	1.28 (0.606 – 2.49)	0.058 – 14.1	0.296	0.039
Asymmetric dimethylarginine (ADMA)	1.92 (1.8 – 2.59)	1.15 – 6.39	0.247	0.088
Symmetric dimethylarginine (SDMA)	0.516 (0.356 – 0.64)	0.235 – 2.99	0.379	0.007
α-Aminoadipic acid	2.42 (1.61 – 2.91)	1.13 – 12.4	0.360	0.011
Glycine betaine	171 (103 – 302)	35 – 1585	0.284	0.048
Proline betaine	0.535 (0.261 – 0.98)	0.091 – 5.30	0.378	0.007
Carnosine	34.8 (27.2 – 42.5)	2.01 – 110	0.080	0.586
L-Anserine	4.95 (3.48 – 7.52)	0.904 – 21.2	-0.011	0.941
Sarcosine	11.0 (5.79 – 21)	2.31 – 52.1	-0.236	0.102
Creatinine	104 (85.8 – 145)	42.9 – 909	0.344	0.016
Kynurenine	5.90 (4.70 – 8.98)	3.13 – 28.9	0.116	0.427

Phenylacetyl-glycine	3.61 (2.09 – 10.2)	0.666 – 39.5	0.367	0.010
Biogenic amines				
Putrescine	1.10 (0.879 – 1.72)	0.442 – 5.50	0.278	0.053
Serotonin	8.82 (0.745 – 16.0)	0.116 – 31.2	-0.074	0.616
Spermidine	0.456 (0.381 – 0.61)	0.263 – 1.14	-0.044	0.765
Indole derivatives				
Indoleacetic acid	1.45 (0.859 – 2.26)	0.209 – 21.4	0.175	0.228
Indoxyl sulfate	7.70 (3.36 – 16.8)	0.398 – 120	0.392	0.005
Cresol				
p-Cresol sulfate	29.6 (8.26 – 60.4)	0.042 – 140	0.321	0.025
CARBOHYDRATES				
Hexoses	5717 (4099 – 15516)	1035 – 28138	0.367	0.010
LIPIDS				
Acylcarnitines				
C0	31.0 (18.3 – 48.7)	7.45 – 314	0.130	0.374

C2	3.37 (1.83 – 7.16)	0.663 – 49.4	0.378	0.007
C4	0.084 (0.058 – 0.150)	0.036 – 0.760	0.454	0.001
C5	0.132 (0.095 – 0.210)	0.035 – 1.01	0.345	0.015
C18	0.193 (0.112 – 0.350)	0.056 – 1.11	0.424	0.002
C18:2	0.096 (0.052 – 0.140)	0.027 – 0.420	0.298	0.038
Fatty acids				
Arachidonic acid	15.2 (8.32 – 19.2)	1.46 – 37.6	0.056	0.703
Docosahexaenoic acid	14.8 (6.29 – 19.5)	1.82 – 59.6	0.275	0.056
Octadecenoic acid	188 (147 – 247)	71.6 – 499	0.134	0.360
Octadecadienoate	277 (184 – 355)	83.8 – 705	0.069	0.636
Eicosenoic acid	7.3 (4.24 – 14.5)	2.54 – 28.8	0.236	0.102
Eicosadienoic acid	4.5 (2.68 – 6.88)	1.64 – 19.8	0.171	0.241
Cholesterol esters				
CE(14:0)	3.31 (2.15 – 4.16)	0.875 – 9.74	-0.230	0.111
CE(16:0)	150 (120 – 193)	66.6 – 276	0.192	0.185
CE(16:1)	27.2 (21.6 – 35.7)	10.2 – 75.7	0.024	0.869
CE(17:0)	4.31 (3.47 – 6.16)	1.84 – 15.2	0.070	0.631

CE(17:1)	4.39 (3.21 – 5.26)	0.935 – 21.2	0.056	0.703
CE(18:0)	21.5 (18.9 – 31.9)	12.7 – 57.1	0.309	0.031
CE(18:1)	366 (285 – 543)	182 – 994	0.387	0.006
CE(18:2)	1732 (1366 – 2332)	711 – 3440	0.193	0.184
CE(18:3)	36.1 (28 – 57.4)	10.6 – 136	0.035	0.813
CE(20:3)	19.2 (15.6 – 26.9)	10.2 – 62.5	0.182	0.210
CE(20:4)	473 (281 – 628)	163 – 1419	0.184	0.206
CE(20:5)	97.2 (37.0 – 147)	8.43 – 587	-0.094	0.522
CE(22:2)	0.684 (0.488 – 1.22)	0.201 – 9.72	0.111	0.447
CE(22:5)	7.92 (4.25 – 10.8)	1.83 – 20.2	0.285	0.047
CE(22:6)	101 (52.4 – 202)	13.9 – 410	0.265	0.066
Bile acids				
TCA	1.50 (0.575 – 3.40)	0.035 – 127	0.218	0.132
Ceramides				
Cer(d16:1/18:0)	0.092 (0.065 – 0.120)	0.029 – 0.270	0.365	0.010
Cer(d16:1/20:0)	0.047 (0.037 – 0.060)	0.023 – 0.120	0.172	0.237
Cer(d16:1/22:0)	0.069 (0.051 – 0.090)	0.015 – 0.160	-0.038	0.797

Cer(d16:1/23:0)	0.051 (0.035 – 0.070)	0.006 – 0.19	-0.220	0.129
Cer(d18:1/16:0)	0.384 (0.281 – 0.550)	0.169 – 1.25	0.414	0.003
Cer(d18:1/18:0)	0.323 (0.241 – 0.570)	0.127 – 3.02	0.466	0.001
Cer(d18:1/20:0(OH))	0.895 (0.655 – 1.36)	0.338 – 3.77	0.410	0.003
Cer(d18:1/20:0)	0.139 (0.089 – 0.200)	0.047 – 0.750	0.290	0.043
Cer(d18:1/22:0)	0.386 (0.242 – 0.540)	0.123 – 1.68	0.277	0.054
Cer(d18:1/23:0)	0.62 (0.411 – 0.91)	0.196 – 1.80	0.257	0.074
Cer(d18:1/24:0)	0.824 (0.51 – 1.19)	0.294 – 1.55	0.281	0.050
Cer(d18:1/24:1)	0.686 (0.409 – 1.29)	0.284 – 2.92	0.443	0.001
Cer(d18:1/25:0)	0.326 (0.231 – 0.44)	0.089 – 1.03	0.249	0.084
Cer(d18:1/26:1)	0.035 (0.024 – 0.060)	0.012 – 0.130	0.374	0.008
Cer(d18:2/16:0)	0.036 (0.027 – 0.050)	0.017 – 0.070	0.213	0.142
Cer(d18:2/18:0)	0.051 (0.040 – 0.070)	0.020 – 0.120	0.352	0.013
Cer(d18:2/20:0)	0.034 (0.027 – 0.040)	0.014 – 0.060	0.196	0.177
Cer(d18:2/22:0)	0.044 (0.033 – 0.060)	0.014 – 0.100	0.061	0.675
Cer(d18:2/23:0)	0.031 (0.023 – 0.040)	0.010 – 0.070	-0.086	0.559
Cer(d18:2/24:0)	0.054 (0.047 – 0.070)	0.023 – 0.100	-0.114	0.435

Cer(d18:2/24:1)	0.063 (0.050 – 0.090)	0.026 – 0.160	0.341	0.017
Cerebrosides (monohexosylceramides)				
HexCer(d16:1/22:0)	0.032 (0.022 – 0.04)	0.010 – 0.060	0.000	0.999
HexCer(d16:1/24:0)	0.025 (0.021 – 0.03)	0.012 – 0.040	0.324	0.023
HexCer(d18:1/16:0)	0.998 (0.774 – 1.96)	0.372 – 4.60	0.510	<0.001
HexCer(d18:1/18:0)	0.428 (0.301 – 0.890)	0.150 – 2.49	0.526	<0.001
HexCer(d18:1/18:1)	0.095 (0.076 – 0.140)	0.045 – 0.400	0.422	0.003
HexCer(d18:1/20:0)	0.300 (0.254 – 0.510)	0.126 – 1.41	0.536	<0.001
HexCer(d18:1/22:0)	0.66 (0.495 – 1.05)	0.236 – 2.73	0.477	0.001
HexCer(d18:1/23:0)	0.47 (0.342 – 0.740)	0.174 – 1.73	0.496	<0.001
HexCer(d18:1/24:0)	0.428 (0.308 – 0.610)	0.192 – 1.28	0.556	<0.001
HexCer(d18:1/24:1)	1.21 (0.989 – 1.80)	0.593 – 5.31	0.580	<0.001
HexCer(d18:1/26:0)	0.115 (0.095 – 0.150)	0.050 – 0.330	0.389	0.006
HexCer(d18:1/26:1)	0.099 (0.081 – 0.120)	0.053 – 0.200	0.316	0.027
HexCer(d18:2/20:0)	0.066 (0.052 – 0.080)	0.024 – 0.130	0.237	0.101
HexCer(d18:2/22:0)	0.109 (0.074 – 0.160)	0.050 – 0.230	0.208	0.151
HexCer(d18:2/23:0)	0.091 (0.070 – 0.130)	0.034 – 0.240	0.339	0.017

HexCer(d18:2/24:0)	0.280 (0.206 – 0.330)	0.082 – 0.500	0.175	0.230
Dihexosylceramides				
Hex2Cer(d18:1/16:0)	0.412 (0.331 – 0.550)	0.169 – 1.04	0.482	<0.001
Hex2Cer(d18:1/18:0)	0.215 (0.164 – 0.250)	0.080 – 0.570	0.388	0.006
Hex2Cer(d18:1/20:0)	0.080 (0.064 – 0.090)	0.028 – 0.160	0.508	<0.001
Hex2Cer(d18:1/22:0)	0.062 (0.053 – 0.080)	0.023 – 0.350	0.398	0.005
Hex2Cer(d18:1/24:0)	0.043 (0.033 – 0.050)	0.020 – 0.090	0.250	0.083
Hex2Cer(d18:1/24:1)	0.068 (0.052 – 0.090)	0.034 – 0.160	0.520	<0.001
Trihexosylceramides				
Hex3Cer(d18:1/16:0)	0.642 (0.517 – 0.850)	0.289 – 1.27	0.369	0.009
Hex3Cer(d18:1/18:0)	0.129 (0.102 – 0.170)	0.047 – 0.300	0.307	0.032
Hex3Cer(d18:1/20:0)	0.103 (0.084 – 0.130)	0.039 – 0.190	0.288	0.045
Hex3Cer(d18:1/22:0)	0.125 (0.087 – 0.160)	0.048 – 0.250	0.244	0.091
Hex3Cer(d18:1/24:1)	0.120 (0.094 – 0.140)	0.058 – 0.440	0.455	0.001
Hex3Cer(d18:1/26:1)	0.330 (0.259 – 0.490)	0.167 – 1.21	0.307	0.032
Sphingomyelins				
SM (OH) C14:1	16.0 (12.5 – 19.3)	6.41 – 57.4	0.042	0.773

SM (OH) C16:1	5.91 (4.82 – 7.77)	3.50 – 18.1	0.344	0.016
SM (OH) C22:1	11.9 (9.99 – 15.9)	3.40 – 27.6	-0.066	0.651
SM (OH) C22:2	4.93 (4.25 – 5.75)	1.63 – 12.3	0.046	0.755
SM (OH) C24:1	1.18 (0.840 – 1.36)	0.257 – 2.32	-0.043	0.770
SM C16:0	146 (119 – 193)	78.4 – 264	0.285	0.047
SM C16:1	9.38 (7.04 – 10.5)	5.06 – 15.0	0.231	0.111
SM C18:0	34.7 (27.5 – 54.1)	15.1 – 96.6	0.554	<0.001
SM C18:1	7.11 (6.04 – 9.30)	3.61 – 12.5	0.401	0.004
SM C20:2	0.309 (0.271 – 0.41)	0.154 – 0.570	0.038	0.795
SM C22:3	0.724 (0.406 – 1.05)	0.204 – 4.48	-0.234	0.106
SM C24:0	14.5 (11.4 – 17.8)	6.09 – 25.0	0.098	0.502
SM C24:1	34.6 (28.1 – 48.1)	16.7 – 65.7	0.259	0.073
SM C26:0	0.205 (0.177 – 0.290)	0.062 – 0.990	-0.009	0.953
SM C26:1	0.422 (0.359 – 0.590)	0.184 – 1.09	0.105	0.473
Lyso-phosphatidylcholines (choline lyso-lecithins)				
lysoPC a C16:0	76.7 (59.3 – 83.8)	34.0 – 129	0.058	0.691
lysoPC a C16:1	2.10 (1.54 – 2.63)	0.891 – 4.59	-0.266	0.065

lysoPC a C17:0	1.81 (1.61 – 2.15)	0.878 – 5.00	-0.119	0.417
lysoPC a C18:0	85.6 (65.4 – 108)	36.8 – 172	0.050	0.733
lysoPC a C18:1	26.8 (21.6 – 32.8)	8.93 – 72.7	-0.103	0.479
lysoPC a C18:2	37.2 (25.5 – 56.5)	8.14 – 83.3	-0.267	0.064
lysoPC a C20:3	1.11 (0.858 – 1.55)	0.364 – 3.87	-0.261	0.071
lysoPC a C20:4	8.83 (6.90 – 12.5)	2.15 – 31.9	-0.180	0.216
lysoPC a C24:0	0.271 (0.197 – 0.400)	0.125 – 1.13	-0.114	0.434
lysoPC a C26:0	0.144 (0.126 – 0.250)	0.076 – 1.10	-0.067	0.647
lysoPC a C26:1	0.090 (0.074 – 0.150)	0.050 – 0.880	-0.013	0.930
lysoPC a C28:0	0.353 (0.292 – 0.490)	0.179 – 1.94	-0.047	0.747
lysoPC a C28:1	0.440 (0.343 – 0.510)	0.200 – 1.53	-0.202	0.164
Diacyl-phosphatidylcholines (choline lecithins)				
PC aa C24:0	0.128 (0.097 – 0.220)	0.050 – 1.26	-0.028	0.850
PC aa C28:1	2.15 (1.76 – 2.56)	0.905 – 4.92	-0.051	0.728
PC aa C30:0	4.64 (3.44 – 6.11)	2.31 – 8.60	0.202	0.164
PC aa C30:2	0.065 (0.05 – 0.07)	0.036 – 0.10	0.271	0.060
PC aa C32:0	11.5 (9.35 – 13.2)	5.68 – 21.9	0.058	0.692

PC aa C32:1	9.70 (8.37 – 14.2)	4.74 – 25.4	0.480	<0.001
PC aa C32:2	1.74 (1.54 – 2.26)	0.994 – 2.83	0.298	0.038
PC aa C32:3	0.325 (0.259 – 0.400)	0.149 – 0.740	0.057	0.699
PC aa C34:1	154 (123 – 223)	79 – 312	0.347	0.014
PC aa C34:2	331 (245 – 427)	158 – 607	0.140	0.338
PC aa C34:3	15.4 (11.4 – 19.9)	5.72 – 32.8	-0.106	0.469
PC aa C34:4	0.763 (0.591 – 1.00)	0.346 – 2.01	-0.137	0.348
PC aa C36:0	4.24 (3.29 – 5.67)	2.02 – 9.09	0.172	0.238
PC aa C36:1	122 (95 – 161)	61 – 229	0.179	0.219
PC aa C36:2	472 (410 – 574)	261 – 808	0.005	0.974
PC aa C36:3	113 (80.8 – 146)	48.9 – 249	0.024	0.871
PC aa C36:4	146 (114 – 178)	78.1 – 348	0.086	0.557
PC aa C36:5	15.9 (9.64 – 25.2)	4.51 – 106	-0.248	0.085
PC aa C36:6	0.874 (0.632 – 1.07)	0.365 – 3.01	-0.058	0.694
PC aa C38:0	2.18 (1.83 – 3.34)	1.02 – 5.07	-0.060	0.681
PC aa C38:1	0.665 (0.539 – 0.770)	0.328 – 1.03	0.024	0.869
PC aa C38:3	63.3 (51.3 – 79.7)	32.8 – 158	-0.077	0.597

PC aa C38:4	358 (264 – 464)	154 – 764	0.012	0.935
PC aa C38:5	87.9 (65.7 – 113)	41.8 – 275	-0.094	0.519
PC aa C38:6	101 (67.2 – 141)	22 – 301	0.176	0.227
PC aa C40:2	0.644 (0.516 – 0.93)	0.335 – 4.45	-0.004	0.979
PC aa C40:3	0.891 (0.757 – 1.19)	0.542 – 3.07	-0.046	0.754
PC aa C40:4	7.55 (5.98 – 10.6)	3.02 – 20.3	0.015	0.917
PC aa C40:5	27.6 (20.3 – 43.7)	11.5 – 65.8	0.145	0.319
PC aa C40:6	111 (69.5 – 171)	26.5 – 324	0.171	0.240
PC aa C42:0	0.228 (0.190 – 0.300)	0.113 – 1.58	0.061	0.675
PC aa C42:1	0.176 (0.150 – 0.210)	0.086 – 0.930	0.010	0.947
PC aa C42:2	0.254 (0.199 – 0.330)	0.113 – 0.830	-0.191	0.188
PC aa C42:4	0.308 (0.238 – 0.460)	0.131 – 2.33	-0.038	0.796
PC aa C42:5	0.401 (0.287 – 0.540)	0.203 – 1.02	-0.156	0.285
PC aa C42:6	0.652 (0.461 – 0.740)	0.338 – 1.41	-0.218	0.132
Acyl-alkyl-phosphatidylcholines (choline plasmalogens)				
PC ae C30:0	0.329 (0.279 – 0.400)	0.164 – 0.700	-0.166	0.254
PC ae C30:1	0.401 (0.325 – 0.480)	0.182 – 1.38	0.036	0.807

PC ae C30:2	0.136 (0.103 – 0.17)	0.056 – 0.46	-0.064	0.663
PC ae C32:1	2.54 (2.23 – 3.11)	1.60 – 6.22	0.232	0.108
PC ae C32:2	0.460 (0.384 – 0.530)	0.234 – 0.950	0.079	0.588
PC ae C34:0	1.53 (1.19 – 1.84)	0.718 – 10.1	0.059	0.689
PC ae C34:1	9.83 (7.96 – 11.5)	4.61 – 18.5	-0.069	0.640
PC ae C34:2	8.47 (6.76 – 10.0)	3.34 – 15.2	-0.247	0.087
PC ae C34:3	2.16 (1.78 – 2.73)	0.740 – 6.97	-0.136	0.352
PC ae C36:0	0.902 (0.660 – 1.17)	0.361 – 4.67	0.067	0.649
PC ae C36:1	9.33 (7.34 – 10.8)	4.04 – 22.6	0.080	0.587
PC ae C36:2	16.7 (13.8 – 19.5)	7.11 – 33.7	-0.118	0.418
PC ae C36:3	4.96 (4.04 – 5.67)	2.24 – 7.88	-0.154	0.291
PC ae C36:4	6.51 (4.82 – 8.25)	2.86 – 11.7	-0.030	0.837
PC ae C36:5	3.68 (2.49 – 4.56)	1.23 – 10.4	-0.010	0.948
PC ae C38:0	2.72 (2.17 – 3.72)	1.39 – 9.17	-0.202	0.165
PC ae C38:1	3.29 (2.40 – 3.95)	1.42 – 8.07	-0.055	0.706
PC ae C38:2	4.66 (3.67 – 5.97)	2.25 – 11.7	-0.233	0.108
PC ae C38:3	5.21 (4.20 – 6.07)	3.10 – 12.0	-0.053	0.715

PC ae C38:4	13.2 (11.1 – 16.6)	7.04 – 35.9	0.044	0.766
PC ae C38:5	11.1 (8.4 – 13.4)	4.97 – 20.5	-0.002	0.991
PC ae C38:6	4.97 (3.51 – 5.95)	1.88 – 9.09	-0.121	0.409
PC ae C40:1	1.61 (1.35 – 2.08)	0.819 – 3.28	0.031	0.833
PC ae C40:2	1.37 (1.15 – 1.81)	0.601 – 4.78	-0.083	0.571
PC ae C40:3	3.54 (2.08 – 5.66)	0.901 – 29.9	-0.071	0.628
PC ae C40:4	5.30 (4.25 – 7.80)	2.60 – 16.8	-0.101	0.491
PC ae C40:5	5.09 (4.06 – 6.77)	2.35 – 18.5	0.107	0.464
PC ae C40:6	4.19 (3.21 – 6.43)	1.92 – 7.83	0.154	0.291
PC ae C42:1	1.02 (0.761 – 1.16)	0.407 – 4.47	-0.135	0.354
PC ae C42:2	0.515 (0.412 – 0.640)	0.246 – 2.90	-0.093	0.526
PC ae C42:3	0.647 (0.557 – 1.07)	0.327 – 2.23	0.029	0.841
PC ae C42:4	0.603 (0.446 – 0.840)	0.227 – 4.25	-0.043	0.768
PC ae C44:3	0.193 (0.135 – 0.260)	0.089 – 1.15	-0.022	0.879
PC ae C44:5	0.157 (0.134 – 0.190)	0.101 – 0.32	-0.054	0.711
PC ae C44:6	0.204 (0.173 – 0.250)	0.118 – 0.54	-0.017	0.908
Diglycerides (diacyglycerols)				

DG(16:0_18:2)	1.41 (0.860 – 2.31)	0.444 – 7.93	0.395	0.005
DG(17:0_18:1)	0.655 (0.529 – 0.800)	0.295 – 1.89	0.069	0.635
DG(18:1_18:1)	1.18 (0.667 – 2.13)	0.227 – 9.71	0.298	0.038
DG(18:1_18:2)	4.30 (2.93 – 7.97)	1.40 – 27.2	0.301	0.035
DG(18:2_18:2)	4.41 (2.46 – 7.79)	0.878 – 26.3	0.284	0.048
Triglycerides (triacyglycerols)				
TG(14:0_34:2)	1.75 (0.683 – 4.07)	0.221 – 15.4	-0.084	0.565
TG(14:0_36:2)	3.39 (1.38 – 6.39)	0.613 – 53.7	-0.053	0.715
TG(14:0_36:3)	4.56 (1.83 – 7.69)	0.792 – 52.6	-0.104	0.477
TG(14:0_36:4)	1.75 (0.817 – 2.98)	0.243 – 16.8	-0.106	0.466
TG(14:0_38:5)	0.173 (0.11 – 0.27)	0.042 – 1.17	-0.072	0.625
TG(16:0_32:1)	3.93 (1.26 – 12.5)	0.140 – 72.0	-0.101	0.490
TG(16:0_32:2)	2.65 (0.934 – 5.61)	0.425 – 22.8	-0.065	0.657
TG(16:0_34:0)	6.60 (2.11 – 15.6)	0.544 – 103	0.059	0.688
TG(16:0_34:1)	38.4 (9.26 – 64.1)	3.15 – 419	0.060	0.681
TG(16:0_34:2)	34.4 (12.0 – 62.6)	4.41 – 330	0.034	0.817
TG(16:0_34:3)	7.75 (3.90 – 17.7)	0.751 – 74.3	-0.092	0.531

TG(16:0_34:4)	0.844 (0.436 – 1.82)	0.128 – 5.76	-0.165	0.258
TG(16:0_35:2)	1.61 (0.730 – 2.88)	0.254 – 16.8	0.046	0.754
TG(16:0_35:3)	0.788 (0.414 – 1.24)	0.167 – 7.32	0.008	0.954
TG(16:0_36:2)	78.5 (35.6 – 138)	11.2 – 995	0.136	0.352
TG(16:0_36:3)	109 (58.5 – 202)	15.6 – 1101	0.109	0.456
TG(16:0_36:4)	48.4 (27.0 – 87.6)	7.14 – 434	0.049	0.736
TG(16:0_36:5)	4.93 (2.60 – 10.1)	0.672 – 35.0	-0.095	0.516
TG(16:0_37:3)	0.641 (0.311 – 1.12)	0.165 – 3.86	0.055	0.708
TG(16:0_38:1)	0.651 (0.277 – 1.07)	0.122 – 6.12	-0.021	0.884
TG(16:0_38:2)	1.62 (0.789 – 2.41)	0.281 – 19.4	0.002	0.988
TG(16:0_38:3)	1.94 (1.11 – 3.17)	0.520 – 34.3	0.091	0.533
TG(16:0_38:4)	2.34 (1.33 – 3.77)	0.488 – 31.9	0.137	0.346
TG(16:0_38:5)	3.14 (1.96 – 6.53)	0.612 – 25.8	0.097	0.507
TG(16:0_38:6)	2.92 (2.06 – 6.29)	0.360 – 27.3	-0.006	0.970
TG(16:0_40:6)	2.05 (1.46 – 5.15)	0.461 – 30.3	0.088	0.549
TG(16:0_40:7)	2.49 (1.64 – 5.28)	0.206 – 44.0	0.149	0.306
TG(16:1_34:0)	1.79 (0.617 – 3.40)	0.334 – 23.2	-0.088	0.547

TG(16:1_34:1)	8.38 (3.37 – 15.3)	1.06 – 100	-0.119	0.417
TG(16:1_34:2)	6.94 (3.58 – 14.9)	0.909 – 87.9	-0.110	0.452
TG(16:1_34:3)	1.41 (0.671 – 2.97)	0.173 – 14.1	-0.232	0.109
TG(16:1_36:1)	3.65 (1.11 – 4.60)	0.425 – 66.5	-0.054	0.713
TG(16:1_36:2)	11.4 (4.81 – 16.3)	1.72 – 208	-0.114	0.435
TG(16:1_36:3)	12.7 (6.49 – 23.6)	2.93 – 212	-0.141	0.332
TG(16:1_36:4)	5.16 (2.81 – 11.5)	0.922 – 58.4	-0.183	0.209
TG(16:1_36:5)	0.678 (0.318 – 1.28)	0.091 – 5.42	-0.266	0.065
TG(16:1_38:3)	0.461 (0.259 – 0.780)	0.148 – 9.99	-0.084	0.566
TG(16:1_38:4)	0.577 (0.336 – 0.880)	0.143 – 9.33	-0.108	0.460
TG(16:1_38:5)	0.582 (0.433 – 0.780)	0.160 – 5.00	-0.114	0.436
TG(17:0_34:2)	1.16 (0.598 – 2.00)	0.231 – 11.3	0.071	0.629
TG(17:0_36:3)	2.74 (1.54 – 5.06)	0.496 – 36.1	0.092	0.528
TG(17:0_36:4)	1.25 (0.705 – 2.07)	0.285 – 12.0	0.045	0.758
TG(17:1_34:1)	0.886 (0.465 – 1.65)	0.232 – 10.6	0.028	0.846
TG(17:1_34:2)	0.768 (0.438 – 1.32)	0.126 – 8.22	-0.021	0.887
TG(17:1_36:3)	0.972 (0.570 – 1.83)	0.169 – 18.5	-0.024	0.871

TG(17:1_36:4)	0.449 (0.320 – 0.890)	0.084 – 5.70	-0.030	0.839
TG(17:1_38:5)	0.143 (0.096 – 0.210)	0.022 – 1.13	0.057	0.697
TG(17:1_38:6)	0.136 (0.084 – 0.200)	0.029 – 0.950	0.095	0.515
TG(17:2_34:2)	0.235 (0.116 – 0.310)	0.060 – 1.11	-0.107	0.465
TG(17:2_36:2)	0.278 (0.165 – 0.470)	0.078 – 3.37	0.008	0.958
TG(17:2_36:3)	0.244 (0.155 – 0.390)	0.047 – 2.33	0.000	0.999
TG(17:2_36:4)	0.191 (0.126 – 0.300)	0.065 – 1.88	0.106	0.467
TG(18:0_32:1)	1.49 (0.437 – 3.73)	0.118 – 22.0	-0.046	0.751
TG(18:0_32:2)	0.849 (0.308 – 1.59)	0.106 – 8.20	-0.049	0.736
TG(18:0_34:2)	11.9 (4.14 – 19.4)	1.39 – 166	0.062	0.670
TG(18:0_34:3)	2.29 (0.896 – 4.00)	0.453 – 39.9	-0.074	0.613
TG(18:0_36:3)	21.1 (11.3 – 41.6)	2.33 – 631	0.100	0.494
TG(18:0_36:4)	10.3 (5.59 – 22.0)	1.44 – 216	0.076	0.603
TG(18:0_36:5)	1.30 (0.584 – 2.29)	0.212 – 14.4	-0.043	0.769
TG(18:0_38:6)	1.52 (1.14 – 2.71)	0.182 – 16.3	0.069	0.636
TG(18:0_38:7)	0.505 (0.309 – 0.750)	0.074 – 2.58	-0.110	0.453
TG(18:1_30:0)	2.09 (0.798 – 6.49)	0.210 – 35.1	-0.083	0.569

TG(18:1_32:0)	18.5 (5.92 – 36.9)	1.45 – 246	0.052	0.725
TG(18:1_32:1)	12.4 (5.40 – 26.3)	1.57 – 171	-0.112	0.444
TG(18:1_32:2)	6.76 (2.26 – 11.0)	0.937 – 68.3	-0.122	0.404
TG(18:1_32:3)	0.902 (0.374 – 2.00)	0.140 – 7.36	-0.132	0.367
TG(18:1_33:0)	1.09 (0.488 – 2.41)	0.198 – 11.9	0.080	0.583
TG(18:1_33:1)	2.54 (1.30 – 5.10)	0.409 – 27.6	-0.003	0.983
TG(18:1_33:2)	1.49 (0.843 – 2.67)	0.449 – 14.9	-0.038	0.793
TG(18:1_33:3)	0.303 (0.150 – 0.510)	0.074 – 2.08	-0.079	0.589
TG(18:1_34:1)	135 (58.6 – 218)	16.2 – 1461	0.128	0.381
TG(18:1_34:2)	119 (54.5 – 202)	16.6 – 1221	0.092	0.528
TG(18:1_34:3)	15.7 (8.700 – 33.9)	3.10 – 241	-0.102	0.484
TG(18:1_34:4)	1.67 (0.740 – 3.42)	0.345 – 14.9	-0.157	0.28
TG(18:1_35:2)	3.67 (1.92 – 6.59)	0.575 – 62.2	0.065	0.656
TG(18:1_35:3)	1.15 (0.601 – 2.08)	0.234 – 20.3	-0.030	0.837
TG(18:1_36:1)	32.5 (12.8 – 51.9)	1.34 – 1023	0.135	0.355
TG(18:1_36:2)	80.1 (39.0 – 171)	9.24 – 1927	0.081	0.581
TG(18:1_36:3)	83.4 (39.7 – 203)	13.2 – 1838	0.066	0.653

TG(18:1_36:4)	34.0 (20.4 – 86.3)	5.28 – 768	0.020	0.892
TG(18:1_36:5)	5.20 (2.99 – 12.2)	0.755 – 62.0	-0.088	0.547
TG(18:1_36:6)	0.67 (0.366 – 1.44)	0.094 – 4.18	-0.180	0.216
TG(18:1_38:5)	5.96 (3.52 – 9.33)	1.10 – 78.3	0.153	0.293
TG(18:1_38:6)	4.85 (2.90 – 7.57)	0.477 – 48.0	0.117	0.425
TG(18:2_30:0)	1.94 (0.699 – 4.44)	0.334 – 17.6	-0.064	0.661
TG(18:2_30:1)	1.37 (0.51 – 3.28)	0.237 – 9.87	-0.134	0.359
TG(18:2_32:0)	12.5 (5.36 – 26.1)	1.42 – 136	0.044	0.765
TG(18:2_32:1)	10.2 (4.44 – 18.6)	1.23 – 100	-0.108	0.460
TG(18:2_32:2)	3.98 (1.63 – 6.89)	0.705 – 35.2	-0.137	0.347
TG(18:2_33:0)	1.02 (0.502 – 1.77)	0.155 – 9.14	0.053	0.717
TG(18:2_33:1)	1.89 (0.926 – 3.25)	0.404 – 17.3	-0.017	0.906
TG(18:2_33:2)	1.10 (0.674 – 2.25)	0.344 – 12.5	-0.072	0.623
TG(18:2_34:0)	19.2 (8.53 – 32.7)	3.00 – 216	0.086	0.555
TG(18:2_34:1)	104 (51.1 – 183)	14.0 – 1028	0.102	0.487
TG(18:2_34:2)	80.2 (44.1 – 154)	12.5 – 709	0.031	0.832
TG(18:2_34:3)	9.58 (5.68 – 23.9)	1.63 – 105	-0.135	0.354

TG(18:2_34:4)	1.18 (0.507 – 2.23)	0.148 – 7.37	-0.199	0.170
TG(18:2_35:1)	3.25 (1.69 – 5.92)	0.718 – 43.6	0.092	0.532
TG(18:2_35:2)	2.32 (1.34 – 3.92)	0.517 – 30.4	0.027	0.855
TG(18:2_35:3)	0.710 (0.446 – 1.42)	0.143 – 9.66	-0.062	0.674
TG(18:2_36:0)	3.77 (1.50 – 6.33)	0.288 – 93.1	0.089	0.542
TG(18:2_36:1)	23.3 (13.8 – 47.4)	3.20 – 704	0.083	0.570
TG(18:2_36:2)	54.1 (27 – 121)	8.79 – 1411	0.079	0.587
TG(18:2_36:3)	50.1 (27.3 – 132)	6.91 – 1131	0.037	0.800
TG(18:2_36:4)	19.4 (10.3 – 41.8)	2.24 – 321	0.005	0.974
TG(18:2_36:5)	3.72 (2.07 – 8.45)	0.349 – 41.6	-0.147	0.313
TG(18:2_38:4)	2.81 (1.94 – 5.15)	0.670 – 53.9	0.083	0.571
TG(18:2_38:5)	4.45 (2.81 – 8.17)	0.736 – 41.2	0.108	0.461
TG(18:2_38:6)	3.23 (2.24 – 5.82)	0.294 – 45.4	0.083	0.569
TG(18:3_34:0)	1.62 (0.612 – 2.49)	0.333 – 11.9	-0.060	0.681
TG(18:3_34:1)	8.59 (3.68 – 15.8)	1.27 – 61.5	-0.052	0.723
TG(18:3_34:2)	5.54 (3.04 – 11.8)	0.825 – 40.6	-0.133	0.364
TG(18:3_34:3)	1.00 (0.434 – 1.84)	0.099 – 7.13	-0.250	0.083

TG(18:3_35:2)	0.291 (0.153 – 0.450)	0.079 – 1.94	-0.134	0.360
TG(18:3_36:1)	1.92 (0.90 – 4.25)	0.319 – 37.4	-0.012	0.937
TG(18:3_36:2)	5.98 (3.11 – 12.6)	0.871 – 99.9	-0.055	0.708
TG(18:3_36:3)	4.92 (2.52 – 11.4)	0.672 – 60.1	-0.142	0.332
TG(18:3_36:4)	1.89 (1.01 – 4.89)	0.243 – 21.6	-0.167	0.250
TG(18:3_38:5)	0.527 (0.293 – 0.67)	0.101 – 2.15	-0.064	0.661
TG(18:3_38:6)	0.393 (0.262 – 0.55)	0.047 – 1.46	-0.205	0.157
TG(20:0_32:3)	0.297 (0.163 – 0.520)	0.061 – 3.11	0.091	0.533
TG(20:0_32:4)	0.434 (0.215 – 0.720)	0.076 – 3.55	0.110	0.450
TG(20:1_32:2)	0.390 (0.293 – 0.510)	0.082 – 1.54	0.052	0.721
TG(20:1_32:3)	0.118 (0.079 – 0.190)	0.037 – 0.890	-0.013	0.931
TG(20:1_34:1)	1.31 (0.650 – 2.32)	0.123 – 18.7	0.062	0.673
TG(20:1_34:2)	1.20 (0.639 – 1.99)	0.269 – 17.5	0.022	0.880
TG(20:1_34:3)	0.290 (0.177 – 0.520)	0.048 – 5.53	-0.063	0.669
TG(20:2_32:1)	0.304 (0.142 – 0.550)	0.074 – 3.57	-0.018	0.903
TG(20:2_34:1)	1.25 (0.606 – 1.93)	0.222 – 25.0	0.115	0.431
TG(20:2_34:2)	1.10 (0.684 – 2.02)	0.203 – 21.8	0.092	0.527

TG(20:2_34:3)	0.316 (0.197 – 0.680)	0.071 – 6.30	-0.081	0.579
TG(20:2_36:5)	0.119 (0.071 – 0.190)	0.032 – 1.23	0.000	0.998
TG(20:3_32:0)	0.331 (0.177 – 0.580)	0.058 – 2.61	0.073	0.618
TG(20:3_32:1)	0.303 (0.172 – 0.440)	0.071 – 1.91	-0.044	0.764
TG(20:3_34:1)	1.75 (1.01 – 3.16)	0.485 – 16.1	0.100	0.492
TG(20:3_34:2)	1.66 (0.996 – 2.77)	0.495 – 13.4	0.036	0.807
TG(20:3_34:3)	0.367 (0.213 – 0.600)	0.129 – 2.80	-0.132	0.364
TG(20:3_36:3)	2.14 (1.09 – 3.24)	0.434 – 29.4	0.120	0.410
TG(20:3_36:4)	0.994 (0.521 – 1.61)	0.227 – 9.64	0.046	0.756
TG(20:3_36:5)	0.182 (0.130 – 0.290)	0.042 – 0.770	-0.125	0.392
TG(20:4_32:1)	0.805 (0.554 – 1.29)	0.171 – 6.90	-0.021	0.886
TG(20:4_32:2)	0.398 (0.301 – 0.730)	0.123 – 3.32	-0.051	0.727
TG(20:4_33:2)	0.128 (0.086 – 0.220)	0.030 – 1.62	0.093	0.527
TG(20:4_34:0)	1.77 (0.976 – 3.66)	0.183 – 17.5	0.184	0.207
TG(20:4_34:1)	7.16 (4.52 – 16.4)	1.12 – 52.7	0.135	0.354
TG(20:4_34:2)	6.89 (4.62 – 13.2)	1.02 – 56.1	0.102	0.486
TG(20:4_34:3)	1.14 (0.847 – 1.93)	0.223 – 7.04	-0.087	0.552

TG(20:4_35:3)	0.130 (0.081 – 0.190)	0.030 – 0.790	0.074	0.611
TG(20:4_36:2)	10.1 (5.55 – 15.5)	1.15 – 98.7	0.182	0.211
TG(20:4_36:3)	11.1 (4.82 – 15.0)	1.11 – 80.8	0.140	0.338
TG(20:4_36:4)	3.87 (2.12 – 6.41)	0.378 – 34.4	0.088	0.546
TG(20:4_36:5)	0.798 (0.542 – 1.26)	0.105 – 3.75	-0.054	0.712
TG(20:5_34:0)	0.828 (0.407 – 1.38)	0.070 – 9.48	-0.175	0.229
TG(20:5_34:1)	2.96 (1.64 – 6.41)	0.251 – 29.1	-0.227	0.118
TG(20:5_34:2)	2.81 (1.93 – 7.04)	0.193 – 25.4	-0.251	0.082
TG(20:5_36:2)	3.47 (1.65 – 6.78)	0.188 – 29.5	-0.137	0.348
TG(20:5_36:3)	3.99 (2.12 – 7.63)	0.202 – 28.9	-0.180	0.216
TG(22:2_32:4)	0.127 (0.084 – 0.300)	0.027 – 1.99	0.036	0.805
TG(22:4_34:2)	0.918 (0.634 – 1.97)	0.215 – 13.4	0.098	0.503
TG(22:5_32:1)	0.358 (0.195 – 0.600)	0.099 – 3.43	-0.031	0.833
TG(22:5_34:1)	3.05 (2.12 – 6.77)	0.434 – 40.3	0.081	0.580
TG(22:5_34:2)	2.80 (1.95 – 6.23)	0.404 – 33.7	0.080	0.587
TG(22:5_34:3)	0.491 (0.289 – 0.740)	0.106 – 3.77	-0.097	0.508
TG(22:6_32:0)	1.07 (0.534 – 2.12)	0.094 – 31.4	0.164	0.260

TG(22:6_32:1)	0.654 (0.36 – 1.34)	0.078 – 7.34	0.038	0.795
TG(22:6_34:1)	6.09 (3.13 – 11.1)	0.310 – 141	0.217	0.134
TG(22:6_34:2)	6.47 (3.44 – 11.1)	0.236 – 157	0.185	0.203
TG(22:6_34:3)	0.784 (0.457 – 1.29)	0.073 – 9.89	-0.001	0.994
OTHERS				
Vitamins and cofactors				
Choline	14.0 (10.6 – 16.4)	5.48 – 40.6	0.004	0.981
Amine oxide				
Trimethylamine N-oxide	8.87 (3.55 – 20.2)	0.846 – 66.8	0.489	<0.001
Alkaloids				
Trigonelline	1.19 (0.626 – 1.91)	0.091 – 9.11	-0.009	0.953
Metabolites of purine nucleotide bases				
Hypoxanthine	8.94 (5.49 – 12.8)	0.963 – 31.5	-0.014	0.926
Carboxylic acids				
Aconitic acid	11.5 (7.72 – 15.2)	2.40 – 33.2	0.090	0.540
Lactic acid	4244 (3176 – 6792)	1505 – 15536	0.046	0.753