

Table S1. All untargeted biochemicals which had a p<0.1 when concentration on test food was compared to control in any genotype.

Biochemical Name	GG TEST	AA TEST	AG TEST	GG TEST	AA TEST	AG TEST			
	GG CTRL	AA CTRL	AG CTRL	GG CTRL	AA CTRL	AG CTRL			
				p-value	q-value	p-value	q-value	p-value	q-value
glycine	0.92	0.97	1.03	0.029960.135060.660720.504790.840400.576400069 2123 6337 4224 0425 7059					
sarcosine	1.64	1.39	1.76	0.000810.036730.002960.075160.000240.041087492 4416 6577 4263 5183 8109					
dimethylglycine	1.14	1.09	1.27	0.254060.407220.620210.492940.036080.162462933 9788 8065 256 7896 7472					
betaine	2.28	2.06	2.6	2.072E-3.9852E1.556140.000240.000120.0315208 -06 E-06 971 5404 2945					
N-acetylserine	0.93	0.9	1.17	0.022170.120570.096830.257850.007350.127938431 0985 9527 7023 7053 2774					
N-acetylthreonine	0.85	0.85	1.08	0.003000.047610.042590.204300.165220.243588041 4135 0858 6918 7541 9669					
allo-threonine	1.11	0.54	0.91	0.665590.625980.008650.122470.854860.579804632 8494 0362 9891 0249 4408					
N-methylalanine	2.51	1.18	1.58	0.001000.036730.459420.431670.144000.22628785 4416 0935 8512 4028 0918					
N,N-dimethylalanine	0.45	0.51	0.48	0.026820.127361.3344E0.001280.115170.210559143 1579 -05 4769 405 6643					
aspartate	0.89	0.91	1.17	0.107950.252450.093770.256480.274480.313621669 0363 1429 8137 7383 9361					
asparagine	0.92	0.95	1.06	0.026460.127360.078660.245910.277790.315047446 1579 808 6263 0611 8798					
N-acetylaspargine	0.81	0.85	1.02	0.066490.196750.002230.066390.850840.579611851 8971 8858 0469 0387 3827					
hydroxyasparagine	0.81	0.85	0.96	0.001170.036730.007190.115490.148930.229671973 4416 7362 4559 0524 4679					
glutamate	0.91	0.93	1.22	0.051060.171320.161240.318000.077800.190808426 6585 8381 8092 0464 3079					
glutamine	0.95	0.95	1.05	0.013730.097570.167340.323580.258420.304982544 7835 3068 1916 8132 4095					
alpha-ketoglutamamate	1.26	1.2	1.67	0.002550.047610.070740.235120.006610.127931594 4135 2044 1437 8531 2774					
pyroglutamine	1.28	1.3	1.83	0.006070.068150.001830.066390.009640.134699745 556 1886 0469 4319 0715					
N-acetyl-aspartyl-glutamate (NAAG)	0.9	0.89	1.42	0.046460.164480.004670.094440.047530.182664832 9242 2102 7584 503 1208					
2-pyrrolidinone	0.83	0.92	1.24	0.033340.138620.182840.332910.288890.321717496 355 5047 3203 5191 7856					
histidine	1.01	0.99	1.15	0.705120.632540.724470.519110.005690.127933226 422 4833 7628 9254 2774					
3-methylhistidine	0.97	0.96	1.06	0.676910.625980.423680.425810.071850.188740739 8494 5625 1742 584 5601					
N-acetylhistidine	0.92	0.85	0.81	0.697640.630600.407450.420350.045590.182665821 4564 8987 1028 8932 1208					
imidazole propionate	1.29	1.21	1.88	0.004500.061660.068090.235120.003620.110355775 0247 6221 1437 6925 0299					
formiminoglutamate	1.11	0.97	1.47	0.240340.396280.775520.533090.014090.147707511 6516 359 6551 2635 0418					

carnosine	0.91	0.94	1.2	0.025250.127360.104620.265070.000740.06744 1276 1579 7845 6514 2393 0674
N-acetylcarnosine	0.9	0.91	1.2	0.106810.252450.014340.153810.001520.08544 301 0363 2031 5112 9669 7992
anserine	0.78	0.87	1.51	0.127870.273010.124120.280270.029000.15852 6409 9429 2865 9855 8873 2177
histamine	0.96	1.14	1.65	0.949200.690690.460900.431670.204890.26756 8365 9436 788 8512 7736 1383
1-methyl-5-imidazoleacetate	1.01	1.11	1.47	0.844650.667630.570830.477930.023450.15765 8453 0561 8732 7813 5001 4649
1-ribosyl-imidazoleacetate	1.11	0.89	1.35	0.415200.521360.038570.204300.051850.18506 5689 3947 8467 6918 1087 7015
4-imidazoleacetate	1.43	1.2	1.85	0.018000.110020.203160.343620.050570.18506 4197 535 7304 1116 3966 7015
lysine	1	1.02	1.1	0.780760.658570.583520.481010.171080.24358 9641 4968 7271 4012 2479 9669
N6-acetyllysine	0.95	0.96	1.32	0.379340.499140.682990.510470.021770.15765 374 771 0199 8406 3323 4649
N6-methyllysine	0.95	0.99	0.99	0.065580.195080.348130.402680.993620.61306 7108 2128 6766 1864 639 8922
N6,N6-dimethyllysine	0.94	0.95	1.15	0.006140.068150.282100.368900.006590.12793 1916 556 927 9448 4369 2774
N6,N6,N6-trimethyllysine	0.91	0.95	1.13	0.004700.061660.502780.446570.093070.20282 1725 0247 6117 3973 3198 035
hydroxy-N6,N6,N6-trimethyllysine	0.7	0.79	1.29	0.001200.036730.139390.295600.235140.28833 9556 4416 0015 7347 118 1332
5-(galactosylhydroxy)-L-lysine	0.73	0.88	1.7	0.001050.036730.334490.396610.181360.24824 1721 4416 2492 5568 0472 2476
2-oxoadipate	1.03	0.78	0.91	0.983320.699720.043170.204300.522370.43953 2618 4318 1484 6918 9539 2946
glutaryl carnitine (C5-DC)	0.71	0.83	1.15	0.000930.036730.109520.267640.349460.36092 035 4416 7578 9647 6829 854
6-oxopiperidine-2-carboxylate	0.87	0.85	1.23	0.015240.101110.043240.204300.044030.18145 5115 4206 9665 6918 2607 1923
5-aminovalerate	1.28	1	1.22	0.029590.134460.830250.546760.348040.36092 4687 5465 328 7435 2746 854
N,N,N-trimethyl-5-aminovalerate	0.9	1	1.37	0.227770.389530.676120.506990.035160.16246 1571 2061 2308 0305 4008 7472
phenylalanine	0.95	0.95	1.09	0.029570.134460.056330.223880.129380.22050 7313 5465 0593 2146 6944 3478
N-acetylphenylalanine	0.87	0.83	1.14	0.175340.333910.005620.102360.385650.37942 1135 9604 0234 2942 5129 4363
phenyllactate (PLA)	0.99	0.88	1.09	0.965560.695680.085060.249170.593730.46997 9561 4408 9734 401 9191 7996
2-hydroxyphenylacetate	1.09	0.96	1.08	0.086480.226840.456640.431610.202980.26732 8483 872 6516 4187 4348 4439
tyrosine	0.98	0.92	1.15	0.375440.497270.247470.355730.085820.19882 7209 6584 4319 5911 0341 7981
N-acetyltyrosine	0.81	0.85	1.22	0.017380.109060.082630.247200.174550.24426 9436 8265 3391 3017 9076 7837
m-tyramine sulfate	1.01	0.81	1.07	0.740070.643140.040840.204300.478520.42355 9089 7796 3454 6918 7312 0693
3-(4-hydroxyphenyl)lactate	0.97	0.91	1.15	0.229600.390130.131150.283120.068140.18874 0969 8436 2652 0417 7978 5601

dopamine 3-O-sulfate	0.91	0.87	1.36	0.139110.288760.671450.505820.016580.14770 7876 1225 9025 8125 6722 0418
3-hydroxyphenylacetate sulfate	3.03	1.58	3.01	0.239170.396280.053260.217280.473260.42117 4495 6516 0376 5946 8021 6529
C-glycosyltryptophan	0.89	0.84	1.24	0.006690.070190.037430.204300.045310.18266 0699 5544 3714 6918 646 1208
kynurenine	0.99	0.93	1.2	0.731970.639310.199800.343250.055120.18785 9849 6219 9726 149 7762 1722
anthranilate	1.73	0.79	0.92	0.063540.192180.329690.391890.625000.48283 534 4883 673 4378 2286 6437
5-hydroxyindoleacetate	1.03	0.85	1.55	0.531340.560520.422640.425810.015560.14770 9985 3826 692 1742 3332 0418
indolelactate	0.96	0.9	1.14	0.416260.521360.042910.204300.291010.32253 7497 3947 2584 6918 2708 1196
indoleacetyl glycine	0.75	0.84	1.17	0.087380.227120.142200.297640.328170.34588 0067 2484 6471 661 3115 4915
indoleacetoylcarnitine	1.58	1.59	3.88	0.141240.292120.099760.259600.017990.14932 5234 608 3583 3011 9153 7958
5-hydroxyindole sulfate	0.68	0.62	2.17	0.438910.527990.080400.246540.197150.26291 0316 6766 6119 6513 5563 4591
3-indoxyl sulfate	0.85	0.76	1.5	0.909480.681540.860760.553230.017710.14932 999 1341 2315 6525 1234 7958
6-bromotryptophan	0.9	0.87	1.1	0.068970.199000.068800.235120.153060.23324 3741 0661 1597 1437 4544 7518
1-carboxyethylleucine	0.89	0.81	1.08	0.211390.370770.058590.223880.787670.55853 935 3325 7703 2146 5723 2215
alpha-hydroxyisocaproate	0.88	0.88	0.96	0.009720.091950.228980.352180.759870.54615 0701 3548 1997 1402 5659 6183
isovaleryl glycine	0.94	0.75	0.96	0.324960.454700.027780.201000.589510.46947 5684 1605 1155 9166 4623 6062
isovalerylcarnitine (C5)	1.32	1.44	1.85	0.022380.120570.041300.204300.011350.13539 0322 0985 779 6918 0164 9681
beta-hydroxyisovalerate	1.08	0.87	1.6	0.418100.521360.085670.249170.008520.13469 8712 3947 7252 401 6846 0715
3-methylglutaconate	0.88	0.96	1.22	0.005340.063010.556670.473040.027300.15765 1269 1514 7081 7144 7626 4649
N-acetyl isoleucine	0.57	0.62	3.21	0.017050.108140.163340.319560.083530.19805 4965 5927 0615 2564 4145 4444
1-carboxyethylisoleucine	0.9	0.74	0.96	0.208250.369100.067510.235120.332900.35014 5065 1724 3176 1437 8188 1495
2-hydroxy-3-methylvalerate	0.93	0.9	1.04	0.038530.149240.439340.427270.934050.59744 7114 289 1798 4271 9393 6399
2-methylbutyrylcarnitine (C5)	0.8	1.04	1.4	0.011990.095650.570860.477930.068530.18874 3686 178 0271 7813 2748 5601
tiglylcarnitine (C5:1-DC)	0.8	0.8	0.88	0.001540.039770.077500.244920.379280.37610 8861 9476 5627 1099 4134 0334
3-hydroxy-2-ethylpropionate	0.9	0.99	1.43	0.063860.192180.885360.558600.065960.18874 2007 4883 5669 8522 4564 5601
ethylmalonate	0.91	0.82	1.07	0.060570.186910.035830.204300.316330.33837 313 2842 9841 6918 9154 7979
methylsuccinate	0.95	0.83	1.1	0.425780.522020.015960.153810.097380.20282 6126 9768 3196 5112 9387 035
N-acetylvaline	0.9	0.85	1.1	0.079090.211280.129610.283120.241020.29194 0488 6252 7665 0417 5771 0619

1-carboxyethylvaline	0.91	0.83	1.06	0.330820.458880.131570.283120.025550.15765 5748 8004 288 0417 5263 4649
alpha-hydroxyisovalerate	0.85	0.91	1.09	0.000330.023660.099360.259600.685790.51613 5036 4592 6123 3011 7423 8658
isobutyrylcarnitine (C4)	0.82	0.95	1.17	0.003870.058840.737480.524410.351920.36092 4929 1112 4904 3525 0898 854
methionine	1.12	1.07	1.26	0.012460.096170.160060.318000.001070.06744 9937 228 1167 8092 3161 0674
N-acetylmethionine	0.87	0.83	1.16	0.010850.095580.015730.153810.025720.15765 5207 3799 4523 5112 8736 4649
N-formylmethionine	0.89	0.91	1.17	0.002210.044430.043530.204300.011250.13539 3627 422 8597 6918 3124 9681
S-methylmethionine	1.34	1.44	1.25	0.244880.401430.024120.185950.309710.33333 1209 3424 0673 5146 1829 3728
methionine sulfone	1.12	1.09	1.22	0.022520.120570.191280.337300.015710.14770 2129 0985 4905 8644 8841 0418
methionine sulfoxide	1.17	1.06	1.24	0.001650.039770.420700.425810.003940.11035 4511 9476 1765 1742 7147 0299
N-acetylmethionine sulfoxide	0.83	0.78	1.16	0.034480.138620.339540.396740.854540.57980 0923 355 4384 2525 8992 4408
S-adenosylhomocysteine (SAH)	1.47	1.07	1.41	0.080700.214090.457250.431610.024580.15765 9609 0873 2902 4187 3598 4649
cystathionine	0.93	0.94	1.4	0.138070.287620.497730.443720.011020.13539 3003 7054 0691 1097 5386 9681
lanthionine	0.91	0.9	1.26	0.076390.207460.086000.249170.060530.18785 9293 731 4523 401 1745 1722
cysteine sulfinic acid	0.87	0.9	0.92	0.049940.169520.121810.280270.404960.38578 494 8728 5941 9855 3606 3066
hypotaurine	0.91	0.93	1.12	0.074960.207460.528930.465040.108940.20601 4682 731 6569 5909 3483 8928
N-acetyltaurine	0.91	0.91	1.05	0.036350.143660.123320.280270.176680.24426 0782 8527 5238 9855 3019 7837
succinoyltaurine	0.86	0.85	1.28	0.093620.235240.177560.331960.022070.15765 1611 3938 3981 2142 9993 4649
argininosuccinate	0.76	0.79	1.05	0.041130.154850.122130.280270.847810.57833 3301 5191 0624 9855 7705 8356
urea	0.99	0.93	1.11	0.836620.667460.042400.204300.106890.20601 7303 9362 5413 6918 1929 8928
citrulline	0.96	0.97	1.17	0.482440.537430.655350.503650.095290.20282 9096 0697 4376 8993 0324 035
homocitrulline	0.89	0.94	1.24	0.097910.239390.366630.404180.073450.18874 0409 6389 0201 1603 386 5601
proline	1.05	0.99	1.08	0.096810.238300.755110.527860.373200.37227 4785 8523 9111 6231 1257 1307
dimethylarginine (SDMA + ADMA)	0.95	0.95	1.08	0.014440.100300.363940.404180.080470.19545 9911 9412 7429 1603 556 2245
N-acetylarginine	0.81	0.92	1.16	0.055080.177580.530890.465040.239890.29131 6761 0363 3412 5909 2631 5484
N-delta-acetylornithine	0.95	0.89	0.92	0.311970.448920.015260.153810.939500.60016 4296 6427 2135 5112 2986 4682
trans-4-hydroxyproline	0.65	0.68	0.63	2.546380.003670.003230.077750.002000.10092 E-05 3363 0244 258 7448 3243
pro-hydroxy-pro	1.09	1.04	1.22	0.574050.580110.257160.358690.141740.22479 1683 7034 1103 8521 0841 298

N-methylproline	0.72	0.93	0.97	0.00257	0.04761	0.71720	0.51698	0.81575	0.56802
N,N,N-trimethyl-alanylproline betaine (TMAP)	0.87	1.06	1.42	7356	4135	8225	4541	8148	9937
N-monomethylarginine	0.93	0.96	1.04	0.01899	0.11070	0.54140	0.46759	0.03335	0.16246
argininate	0.89	1.49	2.83	3985	8667	9876	0689	3313	7472
guanidinoacetate	1.2	1.13	1.42	0.07538	0.20746	0.44895	0.42892	0.43088	0.40041
creatine	1.01	0.94	1.45	7942	731	6071	5104	6663	7259
creatinine	0.95	0.98	1.05	0.45454	0.52976	0.06372	0.23240	0.07105	0.18874
putrescine	1.22	1.06	1.29	5979	1636	5134	5414	1886	5601
N-acetylputrescine	1.09	0.76	1.42	0.02207	0.12057	0.21853	0.34891	0.06183	0.18874
N-carbamoylputrescine	1.35	1.56	1.76	9095	0985	8303	5076	715	5601
N-acetyl-isoputrescine	0.91	0.92	1.11	0.96973	0.69598	0.30483	0.38103	0.00417	0.11035
N('1)-acetylspermidine	1.13	1.08	1.25	4363	1136	0304	16	0423	0299
5-methylthioadenosine (MTA)	1.05	0.93	1.34	0.00746	0.07556	0.59172	0.48445	0.09843	0.20282
4-acetamidobutanoate	0.84	0.84	1.93	4181	2799	6032	4247	609	035
glutathione, oxidized (GSSG)	0.77	0.99	1.37	0.18824	0.34703	0.43562	0.42654	0.09752	0.20282
cysteine-glutathione disulfide	0.96	0.99	1.19	2268	5211	6288	8407	6437	035
S-methylglutathione	0.95	1.04	1.8	0.13763	0.28762	0.55536	0.47304	0.03608	0.16246
cysteinylglycine disulfide	1.15	1.19	1.21	5913	7054	9399	7144	3577	7472
5-oxoproline	0.9	0.88	0.96	0.06769	0.19823	0.02433	0.18595	0.05621	0.18785
2-aminobutyrate	0.91	1.1	1.08	7806	1369	5447	5146	4865	1722
2-hydroxybutyrate/2-hydroxyisobutyrate	0.8	0.84	0.86	0.00414	0.06096	0.40777	0.42035	0.10817	0.20601
Ophthalmate	0.71	0.94	1.55	9482	9448	4043	1028	8092	8928
gamma-glutamylfelynylglycine	0.86	0.85	0.9	0.10565	0.25183	0.34960	0.40268	0.06012	0.18785
gamma-glutamylalanine	1	1.13	0.74	4593	499	4253	1864	7673	1722
gamma-glutamylglutamate	0.96	0.87	1.4	0.47817	0.53681	0.22000	0.34891	0.09318	0.20282
gamma-glutamylglutamine	0.94	0.95	1.12	7598	7714	7778	5076	0839	035
gamma-glutamylglycine	0.87	0.94	1.07	0.05905	0.18519	0.60984	0.49192	0.04172	0.17629
				3409	4414	505	6624	8642	2683
				0.07694	0.20746	0.91212	0.56658	0.04715	0.18266
				1867	731	6017	172	5172	1208
				0.57070	0.57875	0.81662	0.54297	0.01186	0.13541
				2599	9744	4131	128	1967	4007
				0.48695	0.53923	0.68678	0.51163	0.02499	0.15765
				9546	6729	5453	0265	473	4649
				0.08959	0.22875	0.03297	0.20430	0.06938	0.18874
				5544	9272	7136	6918	9423	5601
				0.05946	0.18546	0.03196	0.20430	0.59129	0.46962
				066	3618	5397	6918	4051	0235
				0.05982	0.18560	0.23558	0.35281	0.47434	0.42117
				6468	1359	4037	5194	8729	6529
				0.01256	0.09617	0.07081	0.23512	0.52031	0.43953
				9597	228	9167	1437	2339	2946
				0.02851	0.13162	0.74552	0.52568	0.18206	0.24824
				2311	0382	1459	0595	7806	2476
				0.01649	0.10577	0.25099	0.35573	0.08249	0.19805
				806	6962	5595	5911	7561	4444
				0.56084	0.57585	0.06573	0.23512	0.05190	0.18506
				3007	8067	3923	1437	4036	7015
				0.57050	0.57875	0.14007	0.29576	0.06697	0.18874
				9264	9744	8399	4293	9144	5601
				0.10798	0.25245	0.26948	0.36111	0.00391	0.11035
				8882	0363	6436	0456	6991	0299
				0.02822	0.13136	0.60695	0.49192	0.49610	0.43077
				8349	0421	5581	6624	9395	0436

gamma-glutamylhistidine	0.91	1.02	1.13	0.017690.109790.617240.492940.241560.29194 5583 5027 764 256 8806 0619
gamma-glutamylisoleucine	0.85	1.02	1.05	0.039780.152320.908650.565150.647380.49463 0538 6081 4957 4847 868 6556
gamma-glutamylleucine	0.88	0.98	1.1	0.041320.154850.673020.505820.324890.34387 813 5191 1079 8125 3229 0965
gamma-glutamyl-epsilon-lysine	0.76	0.9	1.19	0.001980.044430.216540.348910.027530.15765 0051 422 4716 5076 2793 4649
gamma-glutamylmethionine	1.08	1.15	1.47	0.479260.536990.076800.244920.009140.13469 6466 5375 5292 1099 0566 0715
gamma-glutamylphenylalanine	0.92	0.95	1.13	0.057250.182540.478170.435200.032430.16246 9919 6239 1444 2513 7553 7472
gamma-glutamylvaline	0.87	1	1.09	0.070520.201450.743520.525680.382910.37746 2187 3648 5031 0595 307 5285
gamma-glutamylserine	0.98	1	1.29	0.355110.480180.809430.542720.095950.20282 8449 0799 2914 9304 7644 035
gamma-glutamylcitrulline	0.86	0.88	1.22	0.153000.304450.359640.404180.103050.20601 8457 1536 54 1603 2097 8928
gamma-glutamyl-2-aminobutyrate	0.88	1.26	1.23	0.064520.192920.097680.257850.126310.21914 8216 7031 126 7023 3041 2586
Leucylhydroxyproline	1.68	1.27	1.52	0.002230.044430.012340.153810.072360.18874 3134 422 6677 5112 1165 5601
felinylglycine	0.87	0.97	0.83	0.031940.138130.899800.561820.023310.15765 571 8448 7096 9389 8156 4649
isoleucylglycine	1.33	1.12	1.93	0.049840.169520.469210.433550.073800.18874 6045 8728 3358 2866 0736 5601
phenylacetylalanine	2.08	1.06	1.52	0.026130.127360.477730.435200.169010.24358 998 1579 0689 2513 8975 9669
phenylacetylglutamate	1.69	1.18	2.17	0.033260.138620.150310.307920.007170.12793 0505 355 5814 5906 746 2774
phenylacetylglutamine	1.83	1.18	1.99	0.108390.252450.416450.425810.058840.18785 2238 0363 3106 1742 9876 1722
4-hydroxyphenylacetyl glycine	0.66	0.55	0.59	0.046400.164480.264200.358690.233100.28793 7894 9242 5739 8521 0674 6103
phenylacetylserine	2.02	1.26	2.12	0.051860.172010.259570.358690.036330.16246 9663 4441 3811 8521 8759 7472
1,5-anhydroglucitol (1,5-AG)	0.65	0.86	0.73	0.019370.110770.633150.497640.148070.22967 4568 2471 3562 4204 4806 4679
ribonate	0.84	0.82	1.06	0.033060.138620.010660.142650.866480.58262 8478 355 8092 7194 5912 0204
arabonate/xylonate	0.88	0.8	1.12	0.053790.175370.259760.358690.034850.16246 3521 0861 0346 8521 5314 7472
sedoheptulose	0.84	0.85	1	0.034320.138620.211600.348910.966900.60388 9637 355 4818 5076 5508 0894
glucuronate	1.01	0.92	1.4	0.438950.527990.220660.348910.034850.16246 4521 6766 3996 5076 3609 7472
N-acetylglucosaminylasparagine	0.85	0.89	1.51	0.011830.095650.095240.257850.128800.22026 971 178 0611 7023 9588 6201
N-acetylglucosamine/N-acetylgalactosamine	0.89	0.89	1.17	0.014780.100380.036400.204300.182200.24824 7458 6505 1097 6918 2973 2476
citrate	0.93	0.93	1.09	0.071390.202240.249710.355730.044610.18235 3467 7188 9931 5911 504 731
aconitate [cis or trans]	0.88	0.88	1.08	0.002860.047610.049830.213130.175770.24426 8733 4135 3642 8329 7522 7837

isocitrate	0.82	0.91	1.21	0.000590.034580.127440.283120.077730.19080 9429 9023 5676 0417 1126 3079
succinylcarnitine (C4-DC)	0.88	0.92	1.03	0.031270.136730.418150.425810.372690.37227 9568 7473 8037 1742 9166 1307
fumarate	0.92	0.82	0.95	0.199690.362940.077360.244920.952880.60105 2456 3791 0186 1099 9486 1521
malate	0.87	0.84	0.98	0.005140.063010.069250.235120.881060.58494 4715 1514 1866 1437 5396 1523
2-methylcitrate/homocitrate	1.11	0.9	1.34	0.403050.513830.186370.332910.015050.14770 9327 1414 143 3203 0816 0418
Malonylcarnitine	0.58	0.9	0.89	0.002100.044430.804340.542310.510260.43480 3211 422 734 9019 8853 452
Malonate	0.85	1.51	1.2	0.013820.097570.818070.542970.207960.27016 3204 7835 7519 128 3788 1686
caproate (6:0)	0.85	0.93	0.89	0.021460.120570.186710.332910.323550.34387 26 0985 7647 3203 8484 0965
heptanoate (7:0)	0.75	0.84	0.91	0.003050.047610.097510.257850.576740.46319 163 4135 9575 7023 9851 1051
caprylate (8:0)	0.8	0.91	0.9	0.043810.158820.359980.404180.562190.45831 1921 0276 6565 1603 8149 7397
pelargonate (9:0)	0.84	0.89	0.87	0.071500.202240.115070.275070.592920.46997 0969 7188 3923 1601 0989 7996
caprate (10:0)	0.85	0.89	1.01	0.015480.101560.058510.223880.881930.58494 921 5763 7691 2146 1095 1523
undecanoate (11:0)	0.87	0.89	0.94	0.042780.156960.131650.283120.673940.50977 5897 9701 3655 0417 9087 0766
tetradecadienoate (14:2)	0.74	0.92	0.94	0.013860.097570.090530.251300.912290.59370 6418 7835 3386 6182 6594 7969
heptadecatrienoate (17:3)	1.01	0.81	0.92	0.900480.681540.177260.331960.919940.59370 2562 1341 5694 2142 8115 7969
stearidonate (18:4n3)	0.95	0.84	0.99	0.496820.542960.051830.216980.721540.53382 863 6986 3586 1564 3681 1315
(11 or 12)-methyltridecanoate (a14:0 or i14:0)	0.9	0.8	0.91	0.013480.097570.000310.021960.543130.44955 6856 7835 9368 3535 695 473
branched-chain fatty acid 16:0	1.06	0.82	1.05	0.464850.529760.079840.246390.879910.58494 6699 1636 5305 6311 1354 1523
glutarate (C5-DC)	0.81	0.92	0.78	0.010490.094640.186380.332910.400070.38457 766 8395 6094 3203 2447 7574
adipate (C6-DC)	0.87	0.89	0.82	0.101020.243900.086050.249170.380110.37617 2384 4854 1743 401 0164 7462
Maleate	0.91	0.77	1.09	0.200320.362940.063210.232310.369070.36962 2157 3791 8526 78 6668 3756
pimelate (C7-DC)	0.91	0.87	0.75	0.253970.407220.057270.223880.277670.31504 3835 9788 3328 2146 9088 8798
suberate (C8-DC)	0.89	0.87	0.83	0.165970.322460.045410.204320.408230.38578 5448 912 4074 2457 2701 3066
azelate (C9-DC)	0.88	0.9	0.84	0.116180.261290.091650.252110.456020.41530 0565 8366 0373 9017 1553 901
sebacate (C10-DC)	0.84	0.86	0.82	0.051630.172010.034160.204300.482660.42571 8038 4441 9563 6918 7139 5907
undecanedioate (C11-DC)	0.84	0.87	0.83	0.074570.207460.066140.235120.474450.42117 0349 731 577 1437 693 6529
tridecanedioate (C13-DC)	0.84	0.85	0.86	0.063370.192180.057660.223880.554830.45467 2712 4883 033 2146 2724 0441

dodecanedioate (C12-DC)	0.83	0.86	0.83	0.042980.156960.067850.235120.486680.42615 0571 9701 4038 1437 5325 6545
dodecadienoate (12:2)	0.76	0.96	1	0.010420.094640.378230.408230.873520.58476 3048 8395 1099 3249 7568 811
tridecanedioate (C13:1-DC)	0.77	0.88	1.01	0.025950.127360.171100.327350.450430.41173 2686 1579 9321 1976 7656 6153
tetradecanedioate (C14-DC)	0.86	0.85	1.02	0.006300.068620.038690.204300.956850.60105 3563 9518 9438 6918 4209 1521
branched chain 14:0 dicarboxylic acid	0.95	0.95	1.65	0.448290.529760.574560.478290.030230.16246 5485 1636 1913 4057 4582 7472
hexadecanedioate (C16-DC)	0.85	0.75	1.22	0.010390.094640.000190.015600.100740.20588 9806 8395 4518 6967 3488 6978
hexadecenedioate (C16:1-DC)	0.96	0.83	1.38	0.816500.665060.016520.153810.001030.06744 0948 1193 4144 5112 6353 0674
heptadecanedioate (C17-DC)	0.82	0.74	1.24	0.037300.146440.000950.057740.280470.31575 6982 4652 9551 1402 8161 6615
octadecanedioate (C18-DC)	0.84	0.83	1.27	0.012040.095650.033350.204300.225480.28262 9186 178 2131 6918 2511 0342
octadecenedioate (C18:1-DC)	0.85	0.73	1.24	0.143880.294650.008490.122470.304080.33115 6805 2872 0111 9891 7308 4014
octadecadienedioate (C18:2-DC)	0.89	0.77	1.19	0.054600.177000.006470.107490.035330.16246 1434 4693 5259 0126 4427 7472
nonadecanedioate (C19-DC)	0.79	0.88	1.32	0.001640.039770.245870.355500.233690.28796 8726 9476 4836 7058 5307 3094
eicosanedioate (C20-DC)	0.84	0.89	1.36	0.004630.061660.261180.358690.153660.23324 6249 0247 482 8521 0746 7518
docosadioate (C22-DC)	0.83	0.75	1.35	0.000360.023660.016280.153810.304310.33115 9097 4592 4086 5112 6147 4014
2-aminoheptanoate	0.88	0.82	1.12	0.075230.207460.060080.227730.214360.27423 0555 731 0082 8371 8958 0875
2-aminooctanoate	0.9	0.81	1.09	0.272110.419840.007870.118490.358110.36297 6412 0051 6433 1992 072 9959
butyrylcarnitine (C4)	0.96	1.05	1.8	0.777430.656810.549590.471620.070690.18874 353 5353 9806 3059 725 5601
Butyrylglycine	0.66	0.66	0.79	0.003050.047610.003950.086580.077260.19080 3071 4135 6983 6656 7719 3079
propionylcarnitine (C3)	0.86	0.95	1.19	0.248910.404620.624200.492940.411780.38768 7242 5746 1484 256 9218 6534
Propionylglycine	0.63	0.65	0.9	0.049930.169520.036550.204300.675300.50977 1454 8728 4827 6918 8402 0766
methylmalonate (MMA)	0.9	0.9	1.07	0.074380.207460.228260.352180.141110.22450 6453 731 9526 1402 1774 3528
2-methylmalonylcarnitine (C4-DC)	0.84	0.74	0.91	0.310400.447780.016610.153810.639890.49039 6278 6748 4716 5112 1433 8867
Hexanoylglycine	0.53	0.67	0.66	0.001110.036730.097890.257850.135670.22345 2598 4416 3193 7023 8374 5259
3,4-methylene heptanoylglycine	0.76	0.7	0.55	0.009160.089670.267360.359520.059200.18785 9267 747 4611 6008 3155 1722
N-octanoylglycine	0.54	0.65	0.92	0.012100.095650.151610.307970.391000.37948 0831 178 9971 643 2219 6617
N-linoleoylglycine	1.25	0.96	0.69	0.315830.449990.964300.579730.060360.18785 2963 0312 5447 6878 347 1722
acetylcarnitine (C2)	0.86	1.08	1.38	0.067860.198230.145060.300040.131820.22239 0033 1369 6552 0232 4161 5377

octanoylcarnitine (C8)	0.9	0.91	1.3	0.226570.389100.088480.251300.259910.30539 3184 7823 2736 6182 7579 9567
decanoylcarnitine (C10)	0.93	0.93	1.69	0.365550.488990.313700.382090.096450.20282 6495 7465 4168 1342 4951 035
laurylcarnitine (C12)	0.94	1	1.72	0.236320.395580.964610.579730.096170.20282 9423 7774 5034 6878 6002 035
myristoylcarnitine (C14)	0.86	0.89	1.47	0.068020.198230.169650.326690.132550.22287 0759 1369 6692 3432 0183 2326
pentadecanoylcarnitine (C15)	0.92	0.87	1.49	0.416030.521360.105390.265070.074870.18874 8453 3947 397 6514 908 5601
palmitoylcarnitine (C16)	0.89	0.96	1.39	0.089550.228750.484550.435200.098340.20282 3321 9272 9115 2513 3827 035
arachidoylcarnitine (C20)	0.91	0.88	1.17	0.041700.155240.116850.277110.268320.31192 0804 3512 3811 2592 5717 6388
behenoylcarnitine (C22)	0.76	0.88	1.19	0.031010.136610.365580.404180.166260.24358 5681 8894 8115 1603 4006 9669
lignoceroylcarnitine (C24)	0.81	0.82	0.89	0.002150.044430.019340.166330.054090.18647 4803 422 9568 8451 2452 039
cerotoylcarnitine (C26)	0.62	0.8	0.91	0.001350.037270.103850.265070.567510.45971 6512 3914 2941 6514 4599 9939
butenoylcarnitine (C4:1)	0.94	0.96	0.87	0.454850.529760.815100.542720.508770.43480 2971 1636 2361 9304 3852 452
undecenoylcarnitine (C11:1)	1.01	0.88	1.36	0.578560.581620.011660.151810.027590.15765 7513 4756 8402 6533 0065 4649
palmitoleoylcarnitine (C16:1)	0.94	0.94	1.42	0.236950.395580.203430.343620.092880.20282 0322 7774 0135 1116 886 035
oleoylcarnitine (C18:1)	0.85	0.94	1.36	0.026150.127360.281660.368900.137340.22345 4182 1579 2475 9448 1586 5259
eicosenoylcarnitine (C20:1)	0.88	0.94	1.32	0.019380.110770.265250.358690.177540.24454 8869 2471 9024 8521 0771 1312
erucoylcarnitine (C22:1)	0.88	0.82	1.13	0.122710.267200.036950.204300.467160.42117 2614 4683 4642 6918 3895 6529
nervonoylcarnitine (C24:1)	0.75	0.82	1.29	0.004220.060960.018200.162270.176850.24426 6409 9448 2545 356 6354 7837
ximenoylcarnitine (C26:1)	0.61	0.72	0.76	0.000140.011690.002040.066390.107430.20601 1883 5858 2223 0469 2421 8928
linoleoylcarnitine (C18:2)	0.83	0.91	1.42	0.024710.127360.235360.352810.091850.20282 6161 1579 4696 5194 847 035
linolenoylcarnitine (C18:3)	0.81	0.85	1.67	0.034450.138620.118880.278350.252920.30289 051 355 4939 0496 8723 3355
dihomo-linoleoylcarnitine (C20:2)	0.83	0.9	1.36	0.025660.127360.151240.307970.095190.20282 858 1579 7784 643 7848 035
arachidonoylcarnitine (C20:4)	0.87	0.9	1.57	0.136370.286670.172850.327350.071480.18874 6196 1813 6335 1976 8055 5601
dihomo-linolenoylcarnitine (C20:3n3 or 6)	0.77	0.9	1.52	0.026670.127360.299420.377330.027480.15765 3313 1579 0677 5653 0662 4649
adrenoylcarnitine (C22:4)	0.72	0.78	1.3	0.013380.097570.019090.166330.280740.31575 1633 7835 9664 8451 5613 6615
docosapentaenoylcarnitine (C22:5n3)	0.94	0.96	1.58	0.457110.529760.434860.426540.010440.13539 6806 1636 7034 8407 3828 9681
docosahexaenoylcarnitine (C22:6)	0.87	0.93	1.44	0.118450.263910.214820.348910.000840.06744 8478 6849 8997 5076 9103 0674
adipoylcarnitine (C6-DC)	0.81	0.8	1.05	0.004660.061660.040280.204300.541070.44888 9152 0247 802 6918 3564 0452

suberoylcarnitine (C8-DC)	0.69	0.68	0.52	0.004860.062400.189930.336150.093790.2028263941572230748316602035
octadecenedioylcarnitine (C18:1-DC)	0.87	0.87	1.37	0.456410.529760.186090.332910.087640.20121509516360388320399952418
(R)-3-hydroxybutyrylcarnitine	0.38	1.03	1.68	0.012660.096170.395440.420230.128740.2202666792284189905727856201
(S)-3-hydroxybutyrylcarnitine	0.75	0.98	1.15	0.088130.227430.492900.440230.826610.571630535258072047648241011
3-hydroxyoleoylcarnitine	0.81	0.89	1.23	0.002870.047610.070440.235120.435150.40214827441356038143706259668
Deoxycarnitine	0.99	1.09	1.47	0.764540.654570.450630.428920.059610.18785646230222964510421221722
Carnitine	1.04	1.13	1.39	0.571780.578840.075770.244920.047500.182669709497383109914021208
3-hydroxybutyrate (BHBA)	0.78	1	1.1	0.026110.127360.930530.569210.660230.50216799915794095460382774771
palmitoylcholine	0.88	1.12	1.3	0.537140.564330.837800.549400.059770.1878589131903904197019791722
Oleoylcholine	0.92	1.14	1.33	0.624370.604880.848810.549400.077150.190809038756351970166593079
Stearoylcholine	0.95	1.18	1.35	0.707900.632540.717370.516980.050750.1850676084222298454154467015
docosa-hexaenoylcholine	0.9	1.29	1.52	0.485320.539230.375590.406650.025110.1576549867296981961563474649
Arachidonoylcholine	0.98	1.21	1.44	0.787330.660460.575250.478290.035420.16246263401679939405721417472
alpha-hydroxycaproate	0.89	0.75	1.04	0.424220.522020.083180.247200.708090.52757835297687747301757568826
2-hydroxyheptanoate	0.87	0.9	0.83	0.136620.286670.471840.435140.037850.16585084118134799909782147635
2-hydroxyoctanoate	0.72	0.87	1.13	0.008940.088950.001540.066390.289240.32171121547768229046954927856
2-hydroxydecanoate	0.85	0.77	1.17	0.047130.165110.028570.201000.308770.33333131804468541916665613728
2-hydroxylaurate	0.83	0.85	1.07	0.006890.071010.006230.107140.839050.57640223386851623022625247059
2-hydroxymyristate	1.1	0.77	0.85	0.682360.625980.036930.204300.472510.42117424884940672691829646529
3-hydroxyhexanoate	0.82	1.04	1	0.040120.152320.956510.578970.945850.60105519260813808571223391521
3-hydroxyoctanoate	0.75	1.11	0.86	0.011000.095580.763870.529870.733650.54003538937997654539493483566
3-hydroxydecanoate	0.78	1	0.99	0.002780.047610.608980.491920.809560.56558376541356276662492655765
3-hydroxysebacate	0.76	0.89	1	0.012890.096660.222420.348910.911150.59370861514012835507642247969
3-hydroxylaurate	0.79	0.96	0.94	0.032070.138130.273040.361110.776010.5528688398448361804565098188
3-hydroxymyristate	0.85	0.92	1.09	0.095600.236770.171540.327350.521880.4395367636722969197645462946
8-hydroxyoctanoate	0.88	0.85	0.81	0.156320.307860.035300.204300.353370.3609259227688542669180236854
16-hydroxypalmitate	0.85	0.85	1.12	0.001340.037270.087540.250850.407860.38578760239144751932507723066

13-HODE + 9-HODE	0.82	0.77	1.09	0.122450.267200.009160.125990.609900.47910 1405 4683 044 6273 4233 2764
hydroxy-undecanedioate (OH-C11:0-DC)	0.85	0.93	0.86	0.095110.236570.313930.382090.516070.43775 8291 9324 4358 1342 4281 1815
9,10-DiHOME	0.92	0.82	1.11	0.679020.625980.062750.232310.397930.38325 9522 8494 9596 78 2594 3396
2S,3R-dihydroxybutyrate	0.9	1	0.97	0.093430.235240.973720.580810.995060.61306 1313 3938 6105 652 7307 8922
Azelaoyltaurine	0.81	0.77	1.24	0.032780.138620.030330.204300.083910.19805 7174 355 7195 6918 0671 4444
Hexanoyltaurine	0.75	0.83	1.14	0.005350.063010.069930.235120.166690.24358 0757 1514 8509 1437 0376 9669
myo-inositol	1.38	0.97	1.35	0.018260.110020.991630.587170.468930.42117 2408 535 2218 7628 9737 6529
choline phosphate	0.98	1.01	1.19	0.679620.625980.725230.519110.073790.18874 6961 8494 5634 7628 6119 5601
glycerophosphorylcholine (GPC)	0.97	0.95	1.16	0.742180.644010.590950.484450.003660.11035 9107 1559 5643 4247 7854 0299
Glycerophosphoethanolamine	0.92	0.9	1.06	0.040050.152320.119110.278350.016740.14770 0553 6081 0433 0496 5942 0418
1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	0.96	0.96	1.21	0.839420.667460.300880.378190.081620.19730 6516 9362 8769 573 9999 2894
1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)	1.01	0.88	1.68	0.627670.604880.079290.246270.042800.17785 4996 75 5761 9175 5635 3564
1,2-dipalmitoyl-GPC (16:0/16:0)	1.01	0.94	1.11	0.562710.575850.145210.300040.016670.14770 0461 8067 9854 0232 2231 0418
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)	0.98	0.91	1.27	0.820440.665060.013770.153810.020190.14932 2099 1193 5891 5112 7752 7958
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	1.07	0.92	1.17	0.068360.198230.115420.275070.091790.20282 3569 1369 1764 1601 0917 035
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	0.95	0.93	1.15	0.181750.340540.028810.201000.073090.18874 0528 7669 0814 9166 4458 5601
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	0.96	0.94	1.05	0.027270.127970.039530.204300.243520.29289 9975 9256 0621 6918 6799 8724
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	0.98	0.98	1.2	0.814310.665060.601730.490140.049270.18462 6151 1193 0479 4289 3257 9535
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)	0.98	0.9	1.28	0.930450.684820.023890.185950.034590.16246 2924 4161 6959 5146 8987 7472
1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)	1.06	0.88	1.55	0.469550.533350.036590.204300.019980.14932 0514 8647 7042 6918 2069 7958
1-stearoyl-2-oleoyl-GPC (18:0/18:1)	1.02	0.95	1.19	0.453110.529760.262180.358690.033400.16246 1603 1636 8217 8521 0916 7472
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)	1.01	0.96	1.06	0.488420.539230.272860.361110.058450.18785 2007 6729 8421 0456 9601 1722
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	1.05	1.01	1.15	0.049590.169520.864460.553980.034610.16246 1122 8728 6801 5264 0157 7472
1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	1.02	1.03	1.2	0.457570.529760.716620.516980.096650.20282 2935 1636 166 4541 4019 035
1-oleoyl-2-linoleoyl-GPC (18:1/18:2)	1.03	0.96	1.1	0.172960.331570.289720.369950.051210.18506 1252 5976 4819 9145 6764 7015
1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)	1.13	1.11	1.33	0.018890.110700.308120.382090.028720.15852 1396 8667 5707 1342 1895 2177
1,2-dilinoleoyl-GPC (18:2/18:2)	1.01	0.91	1.21	0.528620.559460.090390.251300.040250.17296 0833 3841 1307 6182 3177 6222

1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)	1.04	0.89	1.44	0.491000.540690.025410.189430.036510.16246 2244 5708 0905 245 7233 7472
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)	1.12	0.98	1.4	0.101830.244830.634980.497850.035260.16246 1383 3664 0393 3267 3769 7472
1,2-dilinolenoyl-GPC (18:3/18:3)	1.07	0.77	2.62	0.461850.529760.013140.153810.105900.20601 6501 1636 2326 5112 363 8928
1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)	0.86	0.71	1.08	0.213800.371590.072060.235990.522810.43953 0305 5946 3864 8708 2083 2946
1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)	0.92	0.77	1.34	0.318040.451590.339320.396740.069670.18874 7489 1034 8603 2525 7531 5601
1-stearoyl-2-oleoyl-GPE (18:0/18:1)	1.18	0.82	1.7	0.164240.320170.045010.204320.016620.14770 0637 664 6293 2457 2983 0418
1-stearoyl-2-linoleoyl-GPE (18:0/18:2)	0.97	0.77	1.3	0.710160.632540.061800.230640.034210.16246 2714 422 6099 8714 2298 7472
1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	0.96	0.69	1.21	0.421010.522020.005740.102360.063120.18874 4169 9768 1126 2942 0977 5601
1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)	1.01	0.78	1.23	0.649080.618060.030830.204300.012120.13541 8605 2071 9836 6918 0739 4007
1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	0.97	0.87	0.71	0.383330.499140.016540.153810.106570.20601 1326 771 6384 5112 9258 8928
1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)	0.82	0.85	1.21	0.021590.120570.186560.332910.069000.18874 0722 0985 2208 3203 2179 5601
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	0.97	0.94	1.22	0.653440.620160.421300.425810.046030.18266 2558 0317 405 1742 4216 1208
1-palmitoyl-GPA (16:0)	0.67	0.87	1.35	0.061860.189890.565750.477090.204570.26756 7292 0828 398 9929 7795 1383
1-linoleoyl-GPA (18:2)	0.67	0.78	0.87	4.6544E0.004470.113620.274860.075080.18874 -05 6239 1475 3304 6149 5601
1-palmitoleoyl-GPC (16:1)	0.97	0.88	1.4	0.903650.681540.103780.265070.051510.18506 968 1341 1257 6514 4701 7015
1-stearoyl-GPC (18:0)	1.02	0.97	1.23	0.560700.575850.534940.465680.064630.18874 9312 8067 3966 5354 3175 5601
1-oleoyl-GPC (18:1)	1.03	0.94	1.39	0.452480.529760.313040.382090.023060.15765 8019 1636 0751 1342 8279 4649
1-linoleoyl-GPC (18:2)	1.02	0.96	1.38	0.671610.625980.368430.404180.006650.12793 6344 8494 7121 1603 2064 2774
1-linolenoyl-GPC (18:3)	1.05	0.88	1.49	0.538670.564330.090760.251300.030880.16246 4567 1903 2625 6182 8253 7472
1-arachidonoyl-GPC (20:4n6)	1.09	1.07	1.65	0.286070.429880.516000.457470.008890.13469 4065 0746 9475 4893 9896 0715
1-palmitoyl-GPE (16:0)	0.9	0.84	1.26	0.116370.261290.001680.066390.110210.20601 7517 8366 8895 0469 3375 8928
1-stearoyl-GPE (18:0)	0.91	0.86	1.4	0.222180.383850.003810.086580.064460.18874 3121 3344 8577 6656 3754 5601
1-oleoyl-GPE (18:1)	1.14	0.97	1.63	0.109180.252450.299060.377330.002880.11035 689 0363 3733 5653 9141 0299
1-linoleoyl-GPE (18:2)	1.05	0.92	1.43	0.421490.522020.245230.355500.006390.12793 6161 9768 1772 7058 0793 2774
1-arachidonoyl-GPE (20:4n6)	0.96	0.83	1.41	0.724990.637720.001280.066390.025040.15765 8222 5575 323 0469 9743 4649
1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)	1.06	0.89	1.13	0.169180.327340.023050.185950.359970.36413 3154 9933 9923 5146 3894 4325
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)	0.93	0.89	1.36	0.143900.294650.052800.217260.070570.18874 1043 2872 2772 0251 3125 5601

1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	0.95	0.76	1.13	0.784640.660010.002480.066390.188470.254038869 2209 2383 0469 6357 5873
1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)	0.98	0.81	1.12	0.935490.686780.022920.185950.176300.244266571 4343 068 5146 944 7837
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)	0.94	0.9	1.21	0.247410.404440.042960.204300.093520.20282706 1459 5123 6918 4163 035
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)	1.01	0.96	1.32	0.795750.663030.479580.435200.087130.200938861 4033 6873 2513 1071 8688
1-(1-enyl-palmitoyl)-GPC (P-16:0)	1	0.93	1.4	0.770130.655440.238920.352810.067510.188746511 8768 1626 5194 232 5601
1-(1-enyl-palmitoyl)-GPE (P-16:0)	0.98	0.95	1.31	0.802650.663190.460220.431670.093280.202822969 2571 315 8512 8096 035
1-(1-enyl-oleoyl)-GPE (P-18:1)	0.84	0.88	1.37	0.731050.639310.297900.377330.085310.198828442 6219 9415 5653 5895 7981
1-(1-enyl-stearoyl)-GPE (P-18:0)	1	0.92	1.3	0.591210.587040.306970.381860.053750.186476762 5929 7992 1341 1411 039
glycerol 3-phosphate	0.91	0.86	1.12	0.022560.120570.068820.235120.442930.407096584 0985 1716 1437 486 8533
palmitoleoyl-linoleoyl-glycerol (16:1/18:2)	0.96	0.57	1.68	0.900480.681540.007830.118490.116860.211026222 1341 255 1992 119 3415
oleoyl-linoleoyl-glycerol (18:1/18:2)	0.89	0.66	1.65	0.260170.414720.016170.153810.070240.188748078 7527 7623 5112 1906 5601
oleoyl-linoleoyl-glycerol (18:1/18:2)	0.93	0.63	1.52	0.577860.581620.004700.094440.288620.321711619 4756 861 7584 9514 7856
linoleoyl-linoleoyl-glycerol (18:2/18:2)	0.8	0.68	1.65	0.047210.165110.049270.213130.078040.190802583 0446 4186 8329 9137 3079
oleoyl-arachidonoyl-glycerol (18:1/20:4)	0.83	0.76	1.9	0.077940.209190.159520.318000.708340.527575681 6458 7122 8092 3851 8826
oleoyl-arachidonoyl-glycerol (18:1/20:4)	0.85	0.81	1.95	0.296490.439810.082690.247200.448020.410274396 2551 6801 3017 0439 2573
linoleoyl-arachidonoyl-glycerol (18:2/20:4)	0.85	0.88	1.74	0.108840.252450.467050.433220.047050.182668577 0363 6248 2741 8386 1208
Sphinganine	1	1.1	1.16	0.978770.698980.040910.204300.253050.302891956 9881 3916 6918 5026 3355
N-palmitoyl-sphinganine (d18:0/16:0)	1.2	0.91	1.73	0.053770.175370.261110.358690.009640.134690054 0861 9902 8521 4798 0715
N-palmitoyl-sphingosine (d18:1/16:0)	0.89	0.88	1.57	0.462880.529760.172130.327350.031150.162465233 1636 1322 1976 1135 7472
N-palmitoyl-phytosphingosine (t18:0/16:0)	0.91	0.93	1.89	0.657740.620160.386400.412450.024200.15765062 0317 5321 4431 3835 4649
N-stearoyl-sphingosine (d18:1/18:0)	0.96	0.93	1.45	0.667400.625980.313110.382090.023410.15765909 8494 2332 1342 7633 4649
N-palmitoyl-heptadecasphingosine (d17:1/16:0)	0.9	0.73	2.04	0.925500.682920.076140.244920.024680.157653461 3451 0082 1099 0413 4649
ceramide (d18:1/17:0, d17:1/18:0)	0.9	0.74	2.17	0.847510.667630.284310.368920.034690.162465392 0561 475 2293 5739 7472
ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)	0.98	0.9	1.51	0.997520.705510.188780.335350.002500.106709358 1689 4244 5838 4733 8392
ceramide (d18:2/24:1, d18:1/24:2)	0.94	0.87	1.72	0.455390.529760.195600.342290.038510.166939193 1636 4654 5303 8537 9378
glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	0.97	0.88	1.32	0.827700.665060.060860.228910.065460.188748615 1193 5888 4557 7106 5601
glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	0.95	0.88	1.37	0.627010.604880.050100.213130.126050.219146734 75 9085 8329 8836 2586

glycosyl ceramide (d18:1/20:0, d16:1/22:0)	0.95	0.89	1.33	0.578280.581620.025570.189430.170770.24358 5419 4756 7513 245 3679 9669
glycosyl ceramide (d18:2/24:1, d18:1/24:2)	0.98	0.93	1.49	0.733080.639310.250950.355730.067450.18874 9515 6219 6326 5911 9305 5601
myristoyl dihydrosphingomyelin (d18:0/14:0)	1.14	1.03	1.54	0.080880.214090.929630.569210.035950.16246 2379 0873 6214 4603 2499 7472
palmitoyl dihydrosphingomyelin (d18:0/16:0)	1.13	0.98	1.27	0.018300.110020.456360.431610.057250.18785 4727 535 3078 4187 5352 1722
behenoyl dihydrosphingomyelin (d18:0/22:0)	1.03	0.94	1.35	0.301860.443220.223500.349330.085590.19882 9456 8168 618 9937 9838 7981
sphingomyelin (d18:0/18:0, d19:0/17:0)	1.1	0.94	1.38	0.196300.359600.212070.348910.097940.20282 6282 3885 2199 5076 7326 035
sphingomyelin (d18:0/20:0, d16:0/22:0)	1.07	0.89	1.41	0.210330.370020.044410.204300.068770.18874 2585 7028 0057 6918 8277 5601
sphingomyelin (d17:1/14:0, d16:1/15:0)	1	0.94	1.51	0.438750.527990.349640.402680.037930.16585 4124 6766 6298 1864 9037 7635
sphingomyelin (d18:1/14:0, d16:1/16:0)	1.01	0.95	1.3	0.604750.594480.364710.404180.094930.20282 1393 3094 0491 1603 9192 035
sphingomyelin (d18:2/14:0, d18:1/14:1)	1.09	0.98	1.52	0.149180.300030.539710.467590.089190.20282 8836 244 3528 0689 4022 035
sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)	0.96	0.91	1.33	0.943670.689710.234270.352810.090870.20282 2267 725 6313 5194 638 035
sphingomyelin (d17:2/16:0, d18:2/15:0)	0.98	0.9	1.5	0.537380.564330.235760.352810.047590.18266 2431 1903 7234 5194 6018 1208
sphingomyelin (d18:1/20:0, d16:1/22:0)	1	0.91	1.22	0.781790.658570.083030.247200.105490.20601 8907 4968 3354 3017 6161 8928
sphingomyelin (d18:1/20:1, d18:2/20:0)	1.01	0.97	1.2	0.706220.632540.422110.425810.073280.18874 7629 422 8686 1742 0346 5601
sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)	0.92	0.93	1.34	0.473860.536140.315090.382090.078180.19080 4625 819 9915 1342 1788 3079
sphingomyelin (d18:2/21:0, d16:2/23:0)	0.94	0.93	1.4	0.710330.632540.483130.435200.093290.20282 8192 422 6691 2513 5511 035
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)	1.02	0.91	1.28	0.525410.557310.081720.247200.109420.20601 2226 6635 2216 3017 3829 8928
sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)	0.98	0.92	1.24	0.800280.663190.058490.223880.170140.24358 2841 2571 9779 2146 9309 9669
sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)	0.93	0.93	1.37	0.552440.572310.288260.369070.083270.19805 7826 721 4179 298 3807 4444
sphingomyelin (d18:1/24:1, d18:2/24:0)	1.03	0.92	1.3	0.495230.542250.098020.257850.109380.20601 7552 515 134 7023 297 8928
sphingomyelin (d18:2/24:1, d18:1/24:2)	1.01	0.91	1.28	0.587340.586080.052410.217260.124010.21802 1406 7964 6664 0251 0852 6177
sphingosine 1-phosphate	1.02	1.04	1.42	0.717280.635430.775000.533090.019060.14932 3583 2938 2151 6551 575 7958
3-hydroxy-3-methylglutarate	0.92	0.93	1.13	0.011830.095650.225040.349470.148720.22967 5123 178 7124 9085 5489 4679
Cholesterol	1.01	0.93	1.34	0.905530.681540.251110.355730.015600.14770 5913 1341 4631 5911 0637 0418
beta-sitosterol	0.96	0.77	1.37	0.643540.615800.005380.102360.066530.18874 3714 0262 7656 2942 482 5601
Campesterol	0.93	0.86	1.35	0.187220.347030.020160.170270.002540.10670 4133 5211 1739 9576 7023 8392
5alpha-pregnan-3alpha,20beta-diol disulfate	0.63	0.8	0.66	0.030220.135180.450480.428920.111900.20608 1029 2436 0793 5104 6907 2563

Taurocholate	0.85	1.89	1.32	0.472980.536140.086430.249170.327580.34588 5265 819 9012 401 6281 4915
Deoxycholate	1.45	0.9	1.87	0.432810.527160.843080.549400.072950.18874 4259 9475 4398 9701 96 5601
tauroolithocholate 3-sulfate	0.89	0.93	1.23	0.315480.449990.843600.549400.058840.18785 9448 0312 3129 9701 4049 1722
N1-methylinosine	0.94	0.98	1.04	0.056600.181440.903580.562720.635160.48792 0128 5265 1476 6338 1329 7107
Urate	0.82	0.91	1.19	0.238580.396280.401600.420350.011170.13539 8932 6516 6355 1028 0651 9681
Allantoin	0.88	0.89	1.02	0.076640.207460.232590.352810.485820.42615 9013 731 9777 5194 6079 6545
allantoic acid	0.64	0.82	0.79	0.053750.175370.212760.348910.259990.30539 2295 0861 0975 5076 5112 9567
1-methylhypoxanthine	0.84	0.77	1.11	0.030480.135330.012830.153810.196670.26291 8942 1759 1403 5112 8548 4591
N1-methyladenosine	0.96	0.9	1.16	0.191810.352490.039030.204300.005390.12793 4596 4816 5055 6918 3902 2774
N6-carbamoylthreonyladenosine	0.88	0.9	1.06	0.026920.127360.263060.358690.464920.42114 7593 1579 4438 8521 4343 9515
N6-succinyladenosine	0.79	0.82	0.95	0.018730.110700.437700.426540.551950.45405 3758 8667 9383 8407 4338 6179
7-methylguanine	0.94	0.93	1.16	0.045970.164480.123660.280270.027430.15765 6293 9242 7099 9855 2435 4649
N2,N2-dimethylguanosine	0.84	0.95	1.36	0.106050.251830.415390.425810.066390.18874 2672 499 5887 1742 1818 5601
N2,N2-dimethylguanine	1.02	0.92	1.06	0.563840.575850.407550.420350.054020.18647 9463 8067 4544 1028 8857 039
Uracil	0.9	0.81	1.29	0.518090.554610.089890.251300.434340.40214 7528 7586 6064 6182 9828 8846
5,6-dihydrouridine	0.94	0.88	1.08	0.034590.138620.047370.209210.054150.18647 384 355 1729 9498 2154 039
2'-O-methyluridine	0.92	0.95	1.12	0.050840.171320.475910.435200.113690.20860 695 6585 5174 2513 2878 7394
2'-deoxyuridine	0.75	0.77	1.02	0.042260.156350.254370.358060.880950.58494 9016 0139 6428 3602 3472 1523
3-ureidoisobutyrate	0.92	0.89	1.09	0.014600.100300.118540.278350.055450.18785 2265 9412 8862 0496 2665 1722
3-ureidopropionate	0.93	0.95	1.06	0.011390.095650.045980.204980.130090.22096 9815 178 6634 2734 5511 2005
N-acetyl-beta-alanine	0.96	0.98	1.3	0.542880.567500.788630.535490.010230.13539 7735 7603 1905 1275 243 9681
3-(3-amino-3-carboxypropyl)uridine	0.78	0.79	1.17	0.009570.091950.031760.204300.092640.20282 281 3548 1052 6918 8042 035
Cytidine	0.85	0.93	1.32	0.088280.227430.288140.369070.140080.22428 8691 5258 86 298 465 8963
5-methylcytidine	0.93	0.96	1.11	0.210160.370020.579090.480650.059080.18785 2159 7028 3959 1673 2732 1722
N4-acetylcytidine	0.93	0.95	0.95	0.026720.127360.450840.428920.845320.57821 7862 1579 0128 5104 9946 0425
2'-deoxycytidine	0.92	0.93	1.09	0.025360.127360.070740.235120.019690.14932 979 1579 0726 1437 3262 7958
5-methyl-2'-deoxycytidine	1.15	1	1.2	0.006530.069860.690650.512600.085750.19882 8434 8387 0206 3558 806 7981

5-hydroxymethylcytidine	0.94	1.34	0.99	0.048780.169520.328010.391130.858660.580918188728676402357110098
5-hydroxymethyl-2'-deoxycytidine	0.94	0.98	1.11	0.069380.199190.600690.490120.083900.19805586137272408803964574444
3-aminoisobutyrate	1.31	1.24	1.12	0.126890.272200.017930.162270.389170.3794857254588419835674366617
nicotinate ribonucleoside	0.56	0.68	1.15	0.384070.499140.043760.204300.535960.4468508277713735691880567032
Nicotinamide	0.9	0.89	1.19	0.098830.240640.002090.066390.189100.2541961420195292046915156992
nicotinamide riboside	0.87	0.8	1.03	0.709810.632540.044560.204300.892010.5885738644221824691879017333
trigonelline (N'-methylnicotinate)	1.04	1.03	1.25	0.403380.513830.736080.524410.042470.17785349314146744352505533564
N1-Methyl-2-pyridone-5-carboxamide	1.13	0.94	1.13	0.093760.235240.625250.492940.347910.360926033393886412564857854
Pantothenate	0.93	1.04	0.97	0.058980.185190.178590.331960.672060.5096188944148951214224676072
ascorbic acid 3-sulfate	0.82	0.81	1.16	0.087140.227120.434970.426540.220240.27884954624841366840740258593
Threonate	0.91	0.9	1.17	0.092920.235240.153470.310430.184650.25023883839385364532473810224
oxalate (ethanedioate)	0.92	0.93	1	0.085200.224500.235600.352810.946190.60105737790317146519474161521
gulonate	0.92	0.77	1.1	0.005350.063010.180280.332530.144060.22628015915149574665308280918
alpha-tocopherol	1.1	0.97	1.06	0.015980.103620.465500.433220.203120.26732279247190423274110934439
alpha-tocotrienol	1.07	0.99	1.43	0.613020.599540.893540.560600.015020.1477005857752578689271840418
gamma-tocotrienol	1.13	1.32	0.44	0.099780.241920.252220.356070.054050.186474042729419732109708039
gamma-tocopherol/beta-tocopherol	1.14	0.99	1.39	0.181770.340540.621280.492940.008560.1346923817669385925645480715
Pterin	0.93	0.78	1.16	0.612390.599540.096730.257850.099520.20422235677521352702361699374
Heme	0.46	0.59	0.79	0.426100.522020.031000.204300.650040.4959138369768209669185572883
Biliverdin	0.65	0.95	1.07	0.076330.207460.667190.505810.866580.582624067313393002190790204
retinol (Vitamin A)	0.96	0.97	1.26	0.124240.269530.654970.503650.074070.18874844218225152899356835601
carotene diol (1)	1.02	0.95	1.36	0.914620.681990.423520.425810.048030.18293579160864874174219827852
carotene diol (2)	1.07	0.97	1.21	0.273150.420310.644460.501170.154030.233241636343434495709927518
beta-cryptoxanthin	0.95	0.78	1.26	0.592090.587040.129850.283120.011580.13539900859291653041708149681
pyridoxine (Vitamin B6)	0.68	0.78	1.12	0.589100.586080.050470.213130.625770.48283141279642753832992616437
Pyridoxamine	0.94	0.59	1.04	0.359060.482950.038240.204300.972510.60622051499161344691854693646
Pyridoxal	1.07	1	1.23	0.264470.416970.820130.542970.012470.1363482064539109812856549172

Pyridoxate	0.99	0.9	1.46	0.655590.620160.397720.420350.018510.14932 0677 0317 9529 1028 6066 7958
4-allylcatechol sulfate	3.58	2.86	2.92	3.536760.004088.149720.000980.014410.14770 E-05 1657 E-06 0826 2119 0418
4-acetylphenol sulfate	1.65	0.97	1.48	0.076750.207460.466930.433220.405880.38578 0277 731 4125 2741 8327 3066
4-ethylphenylsulfate	1.31	0.99	2.57	0.236780.395580.796940.539890.027700.15765 5736 7774 3771 8054 4806 4649
Theophylline	35.37	44.08	42.57	8.74E- 5.05E- 8E-11 3.807E- 1.231620.00619 12 09 08 E-05 1873
2-oxindole-3-acetate	0.95	0.78	1.58	0.518900.554610.077840.244920.019070.14932 9392 7586 0965 1099 4105 7958
beta-guanidinopropanoate	1.18	1.23	1.71	0.097050.238300.122870.280270.018780.14932 2495 8523 0609 9855 8592 7958
dihydrocaffeate sulfate	1.66	0.42	2.65	0.276650.422330.410980.422750.071790.18874 8986 1731 3689 4413 109 5601
Cinnamoylglycine	0.55	0.65	2.72	0.044030.158820.930550.569210.175380.24426 7758 0276 3503 4603 4588 7837
Ergothioneine	1.25	1.18	1.49	0.005860.067710.028000.201000.007370.12793 7643 6481 892 9166 96 2774
Erythritol	0.99	0.81	0.86	0.907530.681540.389680.415030.019930.14932 4913 1341 5355 533 9828 7958
Homostachydrine	0.96	0.97	1.29	0.424270.522020.571860.477950.028220.15765 851 9768 9867 185 2942 4649
indolin-2-one	0.99	0.7	1.64	0.775840.656810.015270.153810.074780.18874 0453 5353 12 5112 2827 5601
Mannonate	0.89	0.85	0.93	0.026560.127360.055530.222790.616150.48100 7253 1579 6039 3784 3117 5215
methyl indole-3-acetate	0.9	0.8	2.07	0.314920.449990.354070.404180.000960.06744 8704 0312 7028 1603 6897 0674
Stachydrine	0.92	0.85	1.13	0.038350.149240.127820.283120.209540.27081 1725 289 6271 0417 4061 5026
Tartarate	0.59	0.93	1.22	0.033570.138620.841370.549400.255090.30319 9036 355 7193 9701 9229 0633
4-vinylguaiacol sulfate	0.85	0.84	0.83	0.229870.390130.989420.587170.065140.18874 7743 8436 516 7628 8978 5601
Pyrraline	0.9	0.76	1.04	0.279550.424500.071320.235180.844960.57821 3664 4525 7984 8731 4059 0425
eugenol sulfate	33.99	28.82	21.9	7.06E- 2.036469.6877E0.000230.005830.12793 09 E-06 -07 3185 5333 2774
(2,4 or 2,5)-dimethylphenol sulfate	0.6	0.71	0.73	0.001070.036730.148160.304820.313450.33600 9852 4416 9362 5975 1737 4304
tartronate (hydroxymalonate)	0.94	0.87	1.01	0.234670.395580.090830.251300.847000.57833 803 7774 2863 6182 9083 8356
(S)-a-amino-omega-caprolactam	0.97	0.94	1.12	0.320490.451590.213800.348910.058780.18785 7386 1034 7277 5076 0707 1722
Salicylate	1.43	0.9	1.57	0.094660.236460.959780.579000.229410.28548 1156 1563 599 3158 4347 6917
2,6-dihydroxybenzoic acid	1.08	0.82	1.19	0.830700.665060.283380.368900.028160.15765 2428 1193 8183 9448 2975 4649
sulfate	0.93	0.9	1.05	0.015050.100990.001720.066390.018950.14932 201 428 5458 0469 2995 7958
O-sulfo-L-tyrosine	0.94	0.87	1.22	0.120470.264820.041570.204300.041000.17470 8986 94 8312 6918 6301 9125

Ectoine	1.15	1.09	1.74	0.27848	0.42399	0.78364	0.53549	0.04884	0.18462
				5031	758	4856	1275	7657	9535
1,2,3-benzenetriol sulfate (2)	11.31	2.23	15.29	0.00120	0.03673	0.01366	0.15381	0.00936	0.13469
				2898	4416	0554	5112	1435	0715
3-hydroxypyridine sulfate	1.16	0.67	1.95	0.61850	0.60185	0.04828	0.21131	0.13640	0.22345
				4072	0467	5281	557	0431	5259
6-hydroxyindole sulfate	0.72	0.65	1.8	0.76982	0.65544	0.71636	0.51698	0.05978	0.18785
				4817	8768	2442	4541	0856	1722
glycine conjugate of C10H14O2 (1)	0.8	0.72	0.89	0.01109	0.09558	0.05501	0.22256	0.81966	0.56838
				8348	3799	7378	7807	4099	8012
branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (1)	0.85	0.94	1.37	0.03445	0.13862	0.43570	0.42654	0.07493	0.18874
				7902	355	5267	8407	9513	5601
branched-chain, straight-chain, or cyclopropyl 12:1 fatty acid	0.63	0.75	1.03	0.17018	0.32734	0.02319	0.18595	0.76756	0.54813
				9507	9933	1077	5146	1062	4677