

**Supplemental Table 4.** Measurement results of two mass spectrometers

Compound name	Relative area				KEGG ID
	1960	1975	1990	2005	
1-Methylnicotinamide	N.D.	6.2E-05	8.0E-05	6.9E-05	C02918
Perillic acid	N.D.	9.1E-05	1.1E-04	1.7E-04	C11924
Phosphocreatine	N.D.	7.0E-05	8.1E-05	7.0E-05	C02305
Asylcarnitine (fatty acid; 17:0)	N.D.	1.2E-05	1.1E-05	1.2E-05	No ID
GABA	N.D.	1.3E-04	1.1E-04	N.D.	C00334
S-Methylmethionine	N.D.	3.0E-04	1.2E-04	N.D.	C03172
Behenic acid	N.D.	6.3E-06	N.D.	N.D.	C08281
Hydroxyprogesterone caproate	6.9E-06	2.1E-05	2.6E-05	6.1E-05	C08148
2-Amino-2-(hydroxymethyl)-1,3-propanediol	2.3E-04	6.2E-04	3.0E-03	1.2E-03	C07182
Stachydrine	9.2E-04	2.4E-03	2.0E-03	1.7E-03	C10172
Dihydroxyacetone phosphate	7.9E-05	1.6E-04	2.0E-04	1.7E-04	C00111
Deoxycholic acid	2.2E-05	4.1E-05	9.1E-06	1.9E-05	C04483
Ribose 5-phosphate	1.4E-04	2.5E-04	2.7E-04	2.8E-04	C00117
Asylcarnitine (fatty acid; 15:0)	1.2E-05	2.1E-05	1.6E-05	1.5E-05	No ID
Ribulose 5-phosphate	8.9E-04	1.4E-03	1.7E-03	1.4E-03	C00199, C01101
Taurodeoxycholic acid	5.9E-06	9.2E-06	8.5E-06	7.5E-06	C05463
Asylcarnitine (fatty acid; 18:2)	6.3E-05	9.7E-05	3.8E-05	9.5E-05	No ID
<i>cis</i> -5,8,11,14,17-Eicosapentaenoic acid	5.8E-04	8.7E-04	7.7E-04	1.2E-03	C06428
Glucose 6-phosphate	2.3E-04	3.4E-04	3.6E-04	4.5E-04	C00668, C01172, C00092
Heptadecanoic acid	4.5E-05	6.6E-05	7.0E-05	7.0E-05	No ID
2-Aminoadipic acid	5.7E-04	8.2E-04	7.7E-04	5.0E-04	C00956
Sedoheptulose 7-phosphate	5.2E-05	7.4E-05	1.2E-04	1.6E-04	C05382
Fatty acid (24:5)	1.4E-05	2.0E-05	1.8E-05	1.6E-05	No ID
21-Deoxycortisol Corticosterone	2.2E-04	3.1E-04	1.4E-04	2.2E-04	C05497 C02140
Fatty acid (22:5)	5.7E-04	8.0E-04	7.3E-04	7.9E-04	No ID
Asylcarnitine (fatty acid; 16:2)	4.0E-05	5.5E-05	3.0E-05	3.8E-05	No ID
1-Methyl-4-imidazoleacetic acid	1.6E-04	2.2E-04	1.6E-04	2.0E-04	C05828
Imidazolelactic acid	7.5E-05	1.0E-04	8.8E-05	9.1E-05	C05568
Benzoic acid	2.6E-04	3.4E-04	2.4E-04	2.6E-04	C00180

Phenaceturic acid	1.2E-04	1.5E-04	9.9E-05	1.3E-04	C05598
Pentadecanoic acid	1.2E-05	1.5E-05	1.7E-05	1.5E-05	No ID
Fatty acid (17:0)	2.4E-05	3.1E-05	3.9E-05	N.D.	No ID
<i>N,N</i> -Dimethylglycine	4.8E-03	6.3E-03	5.9E-03	5.1E-03	C01026
Pipecolic acid	1.5E-03	1.9E-03	2.0E-03	1.9E-03	C00408
<i>Unknown compound</i>	2.9E-04	3.7E-04	4.5E-04	4.6E-04	No ID
Urocanic acid	2.9E-04	3.7E-04	3.2E-04	3.7E-04	C00785
Threonic acid	1.4E-03	1.8E-03	1.5E-03	1.5E-03	C01620
Phosphoenolpyruvic acid	1.4E-04	1.8E-04	1.7E-04	2.3E-04	C00074
Ophthalmic acid	2.3E-04	2.9E-04	2.2E-04	2.1E-04	No ID
Fructose 6-phosphate	4.6E-05	5.6E-05	6.2E-05	7.3E-05	C05345, C00085
15(S)-HETE	1.7E-03	2.1E-03	2.2E-03	1.7E-03	C04742
<i>N</i> -Methylphenylethanolamine	1.7E-05	2.0E-05	2.0E-05	1.9E-05	C03711
Nervonic acid	1.7E-05	2.0E-05	1.4E-05	1.5E-05	C08323
Trigonelline	1.7E-04	2.0E-04	1.4E-04	1.3E-04	C01004
Asylcarnitine (fatty acid; 18:0)	1.8E-04	2.1E-04	1.7E-04	1.7E-04	No ID
Mucic acid	2.1E-04	2.5E-04	2.5E-04	1.8E-04	C00879, C01807
Asylcarnitine (fatty acid; 14:2)	3.4E-05	4.0E-05	2.4E-05	3.0E-05	No ID
2-Hydroxybutyric acid	2.7E-03	3.1E-03	2.5E-03	2.3E-03	C05984
Urea	6.2E-01	7.1E-01	7.1E-01	7.5E-01	C00086
2-Hydroxyvaleric acid	2.0E-03	2.3E-03	2.1E-03	2.0E-03	No ID
Fatty acid (16:2)	4.2E-05	4.8E-05	4.2E-05	4.1E-05	No ID
Linolenic acid	9.1E-04	1.0E-03	1.1E-03	1.1E-03	C06427
Cystathionine	1.9E-04	2.2E-04	2.5E-04	2.4E-04	C00542, C02291
3-Phosphoglyceric acid	1.9E-04	2.1E-04	2.5E-04	2.6E-04	C00197
Linoleic acid	1.2E-02	1.3E-02	1.3E-02	1.2E-02	C01595
Methionine sulfoxide	6.2E-04	6.9E-04	6.0E-04	6.2E-04	C02989
<i>N</i> -Glycolylneuraminic acid	6.0E-05	6.7E-05	4.5E-05	8.2E-05	C03410
Gluconolactone	7.7E-04	8.6E-04	7.1E-04	7.3E-04	C00198
Ethanolamine phosphate	2.3E-04	2.5E-04	2.7E-04	3.0E-04	C00346
SDMA	1.4E-04	1.6E-04	1.4E-04	1.5E-04	No ID
2'-Deoxycytidine	1.5E-04	1.6E-04	1.5E-04	1.3E-04	C00881
ADMA	3.1E-04	3.4E-04	3.2E-04	3.0E-04	C03626
Pyruvic acid	1.4E-03	1.5E-03	1.7E-03	1.4E-03	C00022
Hypotaurine	3.9E-04	4.2E-04	4.9E-04	4.7E-04	C00519

Taurine	1.9E-02	2.1E-02	1.9E-02	2.0E-02	C00245
Fatty acid (19:0)	1.6E-05	1.8E-05	1.5E-05	1.9E-05	No ID
Homovanillic acid	8.0E-05	8.5E-05	6.7E-05	9.6E-05	C05582
Pantothenic acid	5.6E-05	5.9E-05	5.8E-05	6.2E-05	C00864
<i>cis</i> -11,14-Eicosadienoic acid	9.7E-05	1.0E-04	9.7E-05	9.8E-05	C16525
Sarcosine	5.2E-04	5.5E-04	4.3E-04	4.3E-04	C00213
Linoleyl ethanolamide	1.4E-05	1.5E-05	1.8E-05	1.7E-05	No ID
Fatty acid (12:0)	1.5E-05	1.6E-05	1.6E-05	2.1E-05	No ID
Ethyl arachidonate	1.4E-04	1.5E-04	1.8E-04	1.4E-04	No ID
Uric acid	1.2E-02	1.2E-02	1.3E-02	1.3E-02	C00366
Succinic acid	9.5E-04	9.9E-04	1.0E-03	1.2E-03	C00042
Fatty acid (19:2)	1.1E-05	1.2E-05	1.0E-05	1.0E-05	No ID
Palmitoylcarnitine	1.2E-03	1.3E-03	7.3E-04	9.4E-04	C02990
Carnitine	8.8E-03	9.1E-03	9.1E-03	9.1E-03	C00318, C00487, C15025
Cholesterol	7.5E-03	7.8E-03	7.7E-03	8.2E-03	C00187
Cytidine	6.7E-04	7.0E-04	6.5E-04	7.6E-04	C00475
Betaine	3.1E-02	3.2E-02	2.7E-02	2.7E-02	C00719
5-Oxoproline	9.4E-04	9.7E-04	7.5E-04	9.6E-04	C01879
<i>cis</i> -4,7,10,13,16,19-Docosahexaenoic acid	1.1E-02	1.1E-02	1.1E-02	1.2E-02	C06429
Lactic acid	2.5E-01	2.6E-01	2.6E-01	2.7E-01	C00186, C00256, C01432
Glu	1.2E-02	1.3E-02	1.3E-02	1.6E-02	C00025, C00217, C00302
6-Hydroxyhexanoic acid	8.2E-05	8.4E-05	6.4E-05	7.9E-05	C06103
2-Aminoisobutyric acid 2-Aminobutyric acid	5.0E-03	5.1E-03	4.6E-03	3.5E-03	C03665 C02261, C02356
Phe	3.4E-02	3.5E-02	3.4E-02	3.8E-02	C00079, C02057, C02265
Stearoyl ethanolamide	3.3E-05	3.4E-05	3.8E-05	3.8E-05	No ID
Spermidine	8.0E-05	8.2E-05	7.3E-05	1.0E-04	C00315
Citrulline	1.1E-02	1.2E-02	1.0E-02	1.1E-02	C00327
Creatinine	1.9E-03	1.9E-03	1.9E-03	1.9E-03	C00791
3-Methylhistidine	3.8E-03	3.9E-03	3.9E-03	3.9E-03	C01152
Guanidoacetic acid	3.2E-04	3.2E-04	3.1E-04	3.6E-04	C00581
Glutathione (GSSG)_divalent	6.5E-04	6.5E-04	7.7E-04	7.7E-04	C00127
Asp	2.8E-03	2.9E-03	2.8E-03	4.0E-03	C00049, C00402, C16433
Glucuronic acid	2.3E-04	2.3E-04	2.0E-04	2.2E-04	C00191

Stearidonic acid	6.8E-05	6.9E-05	5.8E-05	6.7E-05	C16300
5-Hydroxylysine	1.5E-04	1.5E-04	1.7E-04	1.5E-04	C16741
$\gamma$ -Butyrobetaine	4.8E-04	4.8E-04	5.6E-04	6.7E-04	C01181
Asylcarnitine (fatty acid; 20:0)	8.2E-06	8.3E-06	N.D.	N.D.	No ID
Fatty acid (22:4)	3.0E-04	3.0E-04	3.0E-04	2.4E-04	No ID
Nicotinamide	1.5E-03	1.5E-03	1.6E-03	1.4E-03	C00153
<i>O</i> -Acetylcarnitine	2.8E-02	2.8E-02	3.1E-02	2.9E-02	C02571
<i>Unknown compound</i>	5.6E-05	5.6E-05	4.4E-05	5.3E-05	No ID
Asylcarnitine (fatty acid; 14:0)	8.2E-04	8.2E-04	4.7E-04	4.6E-04	No ID
Gly	3.5E-02	3.5E-02	3.8E-02	4.0E-02	C00037
Asylcarnitine (fatty acid; 20:1)	3.4E-05	3.4E-05	2.3E-05	2.3E-05	No ID
5-Hydroxytryptophan	9.2E-06	9.2E-06	8.8E-06	8.7E-06	C00643
Glycerol 3-phosphate	1.2E-03	1.2E-03	1.1E-03	1.2E-03	C00093
2-Hydroxyisobutyric acid	1.1E-03	1.1E-03	1.2E-03	9.9E-04	No ID
Met	8.8E-03	8.8E-03	1.0E-02	9.7E-03	C00073, C00855, C01733
<i>N</i> -Acetylglycine	5.7E-04	5.6E-04	6.1E-04	6.9E-04	No ID
Hecogenin	1.1E-05	1.1E-05	1.5E-05	1.5E-05	C08902
Dyphylline	7.4E-03	7.3E-03	7.4E-03	7.8E-03	C07819
Leu	1.2E-01	1.2E-01	1.2E-01	1.3E-01	C00123, C01570, C16439
Ala	4.1E-02	4.0E-02	4.4E-02	4.4E-02	C00041, C00133, C01401
Sitosterol	1.0E-05	9.9E-06	9.3E-06	8.3E-06	C01753
<i>S</i> -Sulfocysteine	2.4E-04	2.3E-04	2.4E-04	2.2E-04	C05824
Arachidonic acid	5.7E-03	5.6E-03	5.6E-03	5.2E-03	C00219
Sphinganine	2.1E-05	2.1E-05	2.1E-05	2.3E-05	C00836
Isethionic acid	4.9E-04	4.8E-04	6.0E-04	6.2E-04	C05123
Asn	7.2E-03	7.0E-03	6.9E-03	6.8E-03	C00152, C01905, C16438
Trp	2.0E-02	2.0E-02	2.2E-02	2.5E-02	C00078, C00525, C00806
Cholesterol sulfate	4.5E-04	4.4E-04	4.0E-04	4.3E-04	C18043
Val	1.1E-01	1.0E-01	1.1E-01	1.1E-01	C00183, C06417, C16436
Cysteine glutathione disulfide	4.9E-04	4.7E-04	4.9E-04	4.9E-04	C05526
<i>N</i> <sup>6</sup> , <i>N</i> <sup>6</sup> , <i>N</i> <sup>6</sup> -Trimethyllysine	3.6E-04	3.5E-04	3.7E-04	3.4E-04	C03793
Anserine_divalent	3.4E-04	3.3E-04	2.9E-04	3.5E-04	C01262
Stearic acid	1.9E-03	1.8E-03	1.7E-03	1.7E-03	C01530
4-Methyl-2-oxovaleric acid 3-Methyl-2-oxovaleric acid	2.5E-03	2.5E-03	2.5E-03	2.6E-03	C00233 C00671, C03465

2-Oxoglutaric acid	1.4E-03	1.4E-03	1.4E-03	1.4E-03	C00026
Palmitoylethanolamide	4.6E-05	4.5E-05	4.9E-05	5.1E-05	No ID
Serotonin	2.1E-04	2.0E-04	1.9E-04	1.9E-04	C00780
Ile	6.8E-02	6.5E-02	6.4E-02	7.2E-02	C00407, C06418, C16434
<i>N</i> -Ethylmaleimide_+H <sub>2</sub> O	3.1E-04	3.0E-04	3.0E-04	3.7E-04	C02441
Uridine	1.8E-03	1.8E-03	1.8E-03	1.9E-03	C00299
Lauric acid	1.2E-03	1.2E-03	1.1E-03	1.2E-03	C02679
2-Hydroxyglutaric acid	2.7E-04	2.6E-04	2.4E-04	2.5E-04	C02630, C01087, C03196
Pro	3.5E-02	3.4E-02	3.4E-02	3.5E-02	C00148, C00763, C16435
Erucic acid	5.6E-05	5.4E-05	4.1E-05	4.5E-05	C08316
Asylcarnitine (fatty acid; 18:1)	1.2E-03	1.2E-03	5.7E-04	9.9E-04	No ID
Fatty acid (17:1)	1.1E-04	1.1E-04	1.2E-04	1.1E-04	No ID
Choline	2.3E-02	2.1E-02	2.2E-02	2.4E-02	C00114
Ethanolamine	2.2E-03	2.1E-03	2.4E-03	2.3E-03	C00189
Fatty acid (16:3)	2.2E-05	2.1E-05	2.1E-05	1.7E-05	No ID
Malic acid	3.8E-03	3.6E-03	3.3E-03	3.9E-03	C00149, C00497, C00711
Decanoic acid	2.2E-04	2.1E-04	1.9E-04	2.0E-04	C01571
3-Aminobutyric acid	2.1E-04	2.0E-04	2.7E-04	2.9E-04	No ID
<i>N</i> <sup>5</sup> -Ethylglutamine	3.6E-04	3.4E-04	3.4E-04	3.8E-04	C01047
Thr	4.6E-02	4.3E-02	4.1E-02	4.4E-02	C00188, C00820
Gln	1.3E-01	1.2E-01	1.2E-01	1.2E-01	C00064, C00303, C00819
His	1.9E-02	1.7E-02	1.7E-02	1.7E-02	C00135, C00768, C06419
Creatine	1.0E-01	9.2E-02	9.0E-02	9.7E-02	C00300
Asylcarnitine (fatty acid; 12:0)	1.5E-04	1.4E-04	7.7E-05	8.6E-05	No ID
Homoserine	1.6E-04	1.5E-04	1.7E-04	1.6E-04	C00263
Arg	3.8E-02	3.5E-02	3.3E-02	3.6E-02	C00062, C00792
Sphingosine	4.9E-05	4.5E-05	4.6E-05	5.3E-05	C00319
2-Hydroxy-4-methylvaleric acid	3.1E-04	2.9E-04	3.0E-04	3.4E-04	C03264
4-Acetamidobutanoic acid	2.1E-04	2.0E-04	1.6E-04	2.4E-04	C02946
<i>S</i> -Methylcysteine	3.6E-04	3.3E-04	3.7E-04	3.4E-04	No ID
Glyceric acid	5.1E-04	4.7E-04	4.9E-04	5.0E-04	C00258
Citric acid	2.8E-02	2.6E-02	2.4E-02	2.7E-02	C00158
2-Oxoisovaleric acid	7.9E-04	7.2E-04	7.6E-04	7.3E-04	C00141
Octanoic acid	2.2E-04	2.0E-04	1.4E-04	1.8E-04	C06423
Isovalerylalanine	1.3E-03	1.1E-03	8.2E-04	9.3E-04	No ID

Fatty acid (14:2)	1.3E-05	1.1E-05	1.1E-05	1.1E-05	No ID
<i>N</i> <sup>6</sup> -Acetyllysine	2.9E-04	2.7E-04	2.4E-04	2.7E-04	C02727
Ornithine	1.8E-02	1.6E-02	1.7E-02	1.9E-02	C00077, C00515, C01602
Myristic acid	3.0E-04	2.7E-04	2.8E-04	2.5E-04	C06424
Campesterol	2.6E-05	2.3E-05	2.3E-05	2.4E-05	C01789
Isocitric acid	1.4E-03	1.2E-03	1.2E-03	1.2E-03	C00311
Gluconic acid	1.5E-03	1.3E-03	1.2E-03	1.3E-03	C00257
Glycerophosphocholine	1.1E-02	1.0E-02	9.9E-03	9.8E-03	C00670
<i>N</i> -Acetylaspartic acid	8.6E-05	7.6E-05	8.5E-05	1.0E-04	C01042
<i>cis</i> -8,11,14-Eicosatrienoic acid	3.4E-04	3.0E-04	3.3E-04	3.1E-04	C03242
Kynurenine	2.2E-04	1.9E-04	1.5E-04	2.3E-04	C00328, C01718
<i>Unknown compound</i>	1.1E-03	9.9E-04	7.4E-04	8.3E-04	No ID
Fatty acid (19:1)	7.5E-05	6.5E-05	6.3E-05	5.7E-05	No ID
Butyrylcarnitine	2.7E-04	2.4E-04	2.0E-04	2.3E-04	C02862
<i>N</i> <sub>ω</sub> -Methylarginine	5.1E-05	4.4E-05	7.2E-05	3.5E-05	No ID
Ser	2.3E-02	2.0E-02	2.0E-02	2.1E-02	C00065, C00716, C00740
3-Indoxylsulfuric acid	5.0E-04	4.3E-04	3.1E-04	4.3E-04	No ID
β-Ala	9.7E-04	8.3E-04	8.8E-04	7.7E-04	C00099
Palmitic acid	9.9E-03	8.4E-03	7.9E-03	7.5E-03	C00249
Hexanoic acid	2.8E-04	2.3E-04	2.2E-04	2.9E-04	C01585
Hydroxyproline	8.3E-03	6.9E-03	6.8E-03	7.0E-03	C01157
Trimethylamine <i>N</i> -oxide	4.4E-04	3.7E-04	2.3E-04	3.1E-04	C01104
<i>N</i> -Acetylhistidine	7.9E-05	6.5E-05	6.9E-05	N.D.	C02997
Ricinoleic acid	4.3E-05	3.5E-05	3.7E-05	3.5E-05	C08365
3-Hydroxytetradecanoic acid	1.6E-05	1.3E-05	1.2E-05	1.2E-05	No ID
<i>cis</i> -11-Eicosenoic acid	7.9E-04	6.4E-04	5.1E-04	5.0E-04	C16526
<i>Unknown compound</i>	7.6E-04	6.2E-04	7.4E-04	9.6E-04	No ID
Asylcarnitine (fatty acid; 12:1)	4.5E-05	3.7E-05	1.7E-05	2.4E-05	No ID
5-Methoxyindoleacetic acid	1.5E-04	1.2E-04	1.2E-04	1.3E-04	No ID
<i>N</i> <sup>6</sup> -Methyllysine	5.0E-04	4.0E-04	4.8E-04	4.8E-04	C02728
Putrescine	1.8E-04	1.4E-04	1.6E-04	1.7E-04	C00134
Pelargonic acid	2.6E-04	2.0E-04	2.1E-04	2.3E-04	C01601
Oleoylethanolamine	8.4E-05	6.6E-05	7.6E-05	7.4E-05	No ID
Cystine	7.4E-04	5.9E-04	6.2E-04	5.9E-04	C00491, C01420
Arachidic acid	5.4E-05	4.2E-05	2.8E-05	2.8E-05	C06425

Myristoleic acid	8.4E-04	6.6E-04	4.2E-04	5.6E-04	C08322
Oleic acid	5.9E-03	4.7E-03	4.2E-03	3.9E-03	C00712
Guanosine	3.8E-04	3.0E-04	3.1E-04	2.8E-04	C00387
<i>Unknown compound</i>	2.7E-04	2.1E-04	2.6E-04	3.1E-04	No ID
Tyr	1.9E-02	1.5E-02	1.5E-02	1.6E-02	C00082, C01536, C06420
Lys	7.8E-02	6.1E-02	6.3E-02	6.5E-02	C00047, C00739, C16440
Histamine	5.7E-05	4.3E-05	5.7E-05	5.8E-05	C00388
Indole-3-carboxaldehyde	7.7E-05	5.9E-05	7.0E-05	6.8E-05	C11002
<i>cis</i> -Aconitic acid	9.5E-04	7.1E-04	7.6E-04	9.6E-04	C00417
<i>O</i> -Succinylhomoserine	8.9E-05	6.6E-05	6.7E-05	8.3E-05	C01118
Asylcarnitine (fatty acid; 16:1)	5.4E-04	4.0E-04	2.0E-04	2.6E-04	No ID
Hypoxanthine	8.6E-04	6.4E-04	8.4E-04	1.0E-03	C00262
Taurocholic acid	1.5E-05	1.1E-05	9.6E-06	N.D.	C05122
Cholic acid	8.2E-05	6.1E-05	1.3E-05	3.8E-05	C00695
3-Hydroxybutyric acid	2.5E-01	1.8E-01	2.1E-01	2.2E-01	C01089, C03197
Fatty acid (14:1)-2	7.0E-05	5.1E-05	4.1E-05	4.1E-05	No ID
Inosine	2.7E-03	2.0E-03	3.2E-03	2.6E-03	C00294
Glycerol	1.5E-01	1.1E-01	1.1E-01	1.4E-01	C00116
11-Aminoundecanoic acid	7.2E-05	5.2E-05	6.3E-05	7.7E-05	C19325
$\alpha$ -Tocopherol	5.6E-05	3.9E-05	3.5E-05	2.3E-05	C02477
Asylcarnitine (fatty acid; 14:1)	1.1E-04	7.3E-05	3.1E-05	4.5E-05	No ID
Fatty acid (14:1)-1	4.2E-05	2.8E-05	N.D.	2.7E-05	No ID
<i>Unknown compound</i>	3.6E-04	2.3E-04	2.2E-04	2.4E-04	No ID
Carnosine	7.1E-05	4.5E-05	4.9E-05	5.5E-05	C00386
10-Hydroxydecanoic acid	1.5E-04	9.1E-05	8.7E-05	1.1E-04	C02774
Diethanolamine	1.0E-04	6.1E-05	1.5E-04	1.4E-04	C06772
8-Hydroxyoctanoic acid	2.2E-04	1.3E-04	1.2E-04	1.3E-04	No ID
Palmitoleic acid	4.5E-03	2.6E-03	2.5E-03	2.0E-03	C08362
Erythrose 4-phosphate	1.1E-03	6.2E-04	7.8E-04	7.1E-04	C00279, C03604
Acetoacetic acid	9.5E-03	4.8E-03	6.9E-03	6.4E-03	C00164
<i>Unknown compound</i>	7.3E-04	3.5E-04	5.9E-04	7.3E-04	No ID
Testosterone	2.5E-05	1.1E-05	1.7E-05	8.8E-06	C00535
Fatty acid (20:3)	8.1E-04	3.4E-04	3.1E-04	3.1E-04	No ID
Triethanolamine	1.1E-04	3.9E-05	9.5E-05	1.9E-04	C06771
1-Methylhistamine	4.5E-05	N.D.	6.3E-05	N.D.	C05127

Hexylamine	1.0E-04	N.D.	1.4E-04	1.6E-04	C08306
Adipic acid	6.5E-05	N.D.	N.D.	2.6E-04	C06104
<i>O</i> -Acetylhomoserine	3.1E-06	N.D.	N.D.	3.5E-06	C01077
Fatty acid (22:3)	1.1E-05	N.D.	N.D.	N.D.	No ID
Isovalerylcarnitine	N.D.	N.D.	9.0E-05	9.7E-05	No ID
Ascorbic acid	N.D.	N.D.	N.D.	4.5E-05	C00072

N.D., not determined.