

Supplemental Table 1. Plasma metabolites detected in the CE-TOFMS

Compound name	Relative area						Mean		Comparative analysis	
	SDC1	SDC2	SDC3	0-4LD1	0-4LD2	0-4LD3	SDC	0-4LD	Ratio [*]	<i>P</i> -value [†]
Adenosine	8.1E-05	7.1E-05	1.7E-04	9.5E-04	1.4E-03	3.1E-03	1.1E-04	1.8E-03	17	0.0611
Inosine	1.7E-04	2.2E-04	1.3E-03	4.8E-03	2.5E-03	3.9E-03	5.5E-04	3.8E-03	6.8	0.0133 #
IMP	4.8E-05	N.D.	6.3E-05	4.4E-04	1.3E-04	5.2E-04	5.6E-05	3.7E-04	6.6	0.1375
Serotonin	8.1E-04	5.9E-04	1.7E-03	5.9E-03	3.8E-03	7.0E-03	1.0E-03	5.6E-03	5.4	0.0099 ##
3-(4)Hydroxyphenyl)propionic acid	3.1E-04	3.6E-04	2.6E-04	1.1E-03	1.4E-03	1.3E-03	3.1E-04	1.2E-03	4.0	0.0006 ###
1-Methylhistamine	4.8E-05	4.5E-05	6.6E-05	1.7E-04	1.6E-04	1.9E-04	5.3E-05	1.7E-04	3.3	0.0002 ###
Guanosine	3.1E-05	N.D.	7.9E-05	1.8E-04	1.3E-04	1.7E-04	5.5E-05	1.6E-04	2.9	0.0342 #
4-Acetamidobutanoic acid	3.4E-04	2.8E-04	3.5E-04	6.1E-04	5.9E-04	6.2E-04	3.2E-04	6.1E-04	1.9	0.0003 ###
Phosphoenolpyruvic acid	1.9E-04	1.3E-04	1.5E-04	3.3E-04	2.1E-04	3.2E-04	1.5E-04	2.9E-04	1.9	0.0352 #
β-Ala	3.7E-04	3.8E-04	3.9E-04	5.9E-04	6.0E-04	8.1E-04	3.8E-04	6.6E-04	1.7	0.0187 #
Phosphorylcholine	5.6E-04	7.1E-04	5.7E-04	1.1E-03	9.2E-04	1.2E-03	6.1E-04	1.1E-03	1.7	0.0080 ##
Pyruvic acid	5.3E-03	4.9E-03	4.3E-03	6.8E-03	8.3E-03	9.5E-03	4.8E-03	8.2E-03	1.7	0.0157 #
Isovalerylalanine-1	1.8E-04	1.8E-04	5.5E-04	8.5E-04	4.2E-04	2.2E-04	3.0E-04	5.0E-04	1.6	0.4376
N-Acetylleucine-1										
Glycerophosphocholine	2.2E-03	1.5E-03	2.2E-03	3.1E-03	2.6E-03	3.9E-03	2.0E-03	3.2E-03	1.6	0.0505
N-Formylmethionine	1.1E-04	8.2E-05	9.9E-05	1.3E-04	1.7E-04	1.6E-04	9.6E-05	1.5E-04	1.6	0.0174 #
Anserine_divalent	6.7E-04	5.5E-04	7.1E-04	1.1E-03	7.5E-04	1.2E-03	6.4E-04	1.0E-03	1.6	0.0631
Isovalerylalanine-2										
N-Acetylleucine-2	2.2E-04	2.9E-04	1.9E-04	3.2E-04	3.6E-04	4.3E-04	2.3E-04	3.7E-04	1.6	0.0340 #
N-Acetylaspartic acid	1.6E-04	2.4E-04	3.8E-04	5.3E-04	2.8E-04	4.1E-04	2.6E-04	4.0E-04	1.6	0.1989
Ethanolamine phosphate	1.9E-04	2.9E-04	3.0E-04	4.1E-04	3.9E-04	4.1E-04	2.6E-04	4.0E-04	1.6	0.0171 #
Ribulose 5-phosphate	1.2E-03	8.4E-04	1.7E-03	2.4E-03	1.5E-03	1.9E-03	1.3E-03	2.0E-03	1.6	0.1197
1-Methyladenosine	5.4E-05	5.1E-05	4.4E-05	9.4E-05	6.1E-05	7.2E-05	5.0E-05	7.6E-05	1.5	0.0601
Taurine	1.9E-02	1.7E-02	1.7E-02	3.0E-02	2.0E-02	2.9E-02	1.8E-02	2.6E-02	1.5	0.0627
Glycerol 3-phosphate	8.7E-04	8.7E-04	9.8E-04	1.3E-03	1.1E-03	1.6E-03	9.1E-04	1.3E-03	1.5	0.0333 #
Homocarnosine	1.9E-04	1.9E-04	2.0E-04	3.7E-04	2.0E-04	2.9E-04	2.0E-04	2.9E-04	1.5	0.1443
p-Hydroxybenzoic acid	3.0E-04	3.6E-04	1.9E-04	4.0E-04	4.0E-04	4.2E-04	2.8E-04	4.1E-04	1.4	0.0772
Spermidine	3.1E-05	4.7E-05	7.5E-05	8.9E-05	5.3E-05	7.7E-05	5.1E-05	7.3E-05	1.4	0.2601
N-Acetylasparagine	7.9E-05	8.5E-05	N.D.	9.4E-05	1.4E-04	1.2E-04	8.2E-05	1.2E-04	1.4	0.1159
Guanidinosuccinic acid	1.3E-04	1.2E-04	1.4E-04	2.0E-04	1.9E-04	1.7E-04	1.3E-04	1.9E-04	1.4	0.0031 ##
Creatine	7.0E-02	6.3E-02	6.2E-02	1.1E-01	6.6E-02	1.0E-01	6.5E-02	9.2E-02	1.4	0.1207
Carnosine	2.4E-04	2.5E-04	2.6E-04	4.1E-04	2.5E-04	3.9E-04	2.5E-04	3.5E-04	1.4	0.1144
Thiamine phosphate	6.8E-05	6.4E-05	6.9E-05	9.4E-05	7.9E-05	1.1E-04	6.7E-05	9.4E-05	1.4	0.0396 #
Phenylpyruvic acid	1.3E-04	1.6E-04	N.D.	N.D.	2.1E-04	2.0E-04	1.5E-04	2.0E-04	1.4	0.0636
Diethanolamine	1.9E-04	2.3E-04	1.7E-04	2.6E-04	2.8E-04	2.7E-04	2.0E-04	2.7E-04	1.4	0.0169 #
Glu	1.4E-02	1.6E-02	1.2E-02	2.0E-02	1.6E-02	2.1E-02	1.4E-02	1.9E-02	1.4	0.0516
Ectoine	5.5E-04	5.1E-04	3.3E-04	4.0E-04	6.8E-04	8.0E-04	4.6E-04	6.3E-04	1.4	0.2910
Galactosamine										
Glucosamine	1.0E-04	1.2E-04	9.7E-05	1.6E-04	1.3E-04	N.D.	1.1E-04	1.4E-04	1.4	0.0946
N-Acetyltryptophan	1.4E-04	1.5E-04	1.2E-04	1.8E-04	1.8E-04	1.9E-04	1.4E-04	1.8E-04	1.3	0.0086 ##
Homocitrulline	4.8E-04	3.6E-04	3.8E-04	5.5E-04	5.9E-04	4.8E-04	4.1E-04	5.4E-04	1.3	0.0557
N-Acetylglutamine	1.7E-04	1.5E-04	1.2E-04	1.7E-04	1.4E-04	2.7E-04	1.4E-04	1.9E-04	1.3	0.3203
N-Acetylglycine	5.2E-04	4.8E-04	7.0E-04	9.8E-04	6.1E-04	6.3E-04	5.6E-04	7.4E-04	1.3	0.2763
XA0013	3.3E-03	3.4E-03	2.9E-03	3.8E-03	3.8E-03	4.8E-03	3.2E-03	4.1E-03	1.3	0.0724
Asp	2.4E-03	5.0E-03	2.3E-03	4.4E-03	3.0E-03	5.0E-03	3.2E-03	4.1E-03	1.3	0.4388
Choline	1.3E-02	1.4E-02	1.1E-02	1.7E-02	1.4E-02	1.7E-02	1.3E-02	1.6E-02	1.3	0.0581

Supplemental Table 1 (Continued)

Compound name	Relative area						Mean		Comparative analysis	
	SDC1	SDC2	SDC3	0-4LD1	0-4LD2	0-4LD3	SDC	0-4LD	Ratio [*]	<i>P</i> -value [†]
3-Ureidopropionic acid	1.4E-04	2.9E-04	1.9E-04	2.0E-04	3.3E-04	2.5E-04	2.1E-04	2.6E-04	1.3	0.4146
Isocitric acid	2.1E-03	2.1E-03	2.3E-03	2.7E-03	2.6E-03	2.7E-03	2.2E-03	2.7E-03	1.2	0.0009 ###
Ile	5.6E-02	6.7E-02	5.0E-02	6.8E-02	6.7E-02	7.6E-02	5.7E-02	7.1E-02	1.2	0.0833
<i>S</i> -Sulfocysteine	3.4E-04	6.1E-04	5.9E-04	5.9E-04	4.8E-04	8.2E-04	5.1E-04	6.3E-04	1.2	0.4305
Val	9.9E-02	1.1E-01	8.4E-02	1.1E-01	1.2E-01	1.3E-01	9.8E-02	1.2E-01	1.2	0.1110
Leu	9.8E-02	1.1E-01	8.4E-02	1.1E-01	1.2E-01	1.3E-01	9.8E-02	1.2E-01	1.2	0.0769
Trigonelline	2.6E-03	2.4E-03	1.5E-03	1.8E-03	2.8E-03	3.3E-03	2.2E-03	2.6E-03	1.2	0.4396
Pipecolic acid	2.2E-03	2.1E-03	2.1E-03	2.7E-03	2.3E-03	2.8E-03	2.1E-03	2.6E-03	1.2	0.0301 #
2-Oxoglutaric acid	6.3E-03	7.5E-03	6.8E-03	7.0E-03	9.3E-03	8.5E-03	6.9E-03	8.3E-03	1.2	0.1369
Ethanolamine	1.3E-03	1.4E-03	1.1E-03	1.5E-03	1.4E-03	1.7E-03	1.3E-03	1.5E-03	1.2	0.0847
Arg	3.6E-02	4.5E-02	3.4E-02	3.6E-02	4.3E-02	5.8E-02	3.9E-02	4.6E-02	1.2	0.3610
1-Methyl-4-imidazoleacetic acid	2.1E-04	3.7E-04	2.3E-04	3.3E-04	2.3E-04	4.0E-04	2.7E-04	3.2E-04	1.2	0.5017
<i>O</i> -Acetylhomoserine										
2-Aminoadipic acid	1.2E-03	1.6E-03	1.4E-03	1.7E-03	1.5E-03	1.7E-03	1.4E-03	1.7E-03	1.2	0.0862
XA0012	2.8E-04	2.3E-04	2.4E-04	3.1E-04	3.1E-04	2.8E-04	2.5E-04	3.0E-04	1.2	0.0484 #
Isethionic acid	7.5E-04	5.5E-04	6.0E-04	8.9E-04	7.5E-04	6.1E-04	6.3E-04	7.5E-04	1.2	0.3130
Thiamine	1.0E-04	9.7E-05	1.2E-04	1.3E-04	1.5E-04	1.1E-04	1.1E-04	1.3E-04	1.2	0.2281
<i>N</i> ⁵ -Ethylglutamine	2.1E-03	1.8E-03	1.5E-03	1.8E-03	2.2E-03	2.4E-03	1.8E-03	2.1E-03	1.2	0.2348
Terephthalic acid	2.4E-04	2.3E-04	2.4E-04	3.1E-04	2.5E-04	2.8E-04	2.4E-04	2.8E-04	1.2	0.0557
11-Aminoundecanoic acid	8.8E-05	2.1E-04	1.3E-04	2.2E-04	1.7E-04	1.1E-04	1.4E-04	1.7E-04	1.2	0.6395
3-Phosphoglyceric acid	3.4E-04	1.8E-04	3.4E-04	4.5E-04	2.3E-04	3.3E-04	2.8E-04	3.3E-04	1.2	0.5916
Kynurenine	4.3E-04	3.6E-04	3.7E-04	3.9E-04	5.2E-04	4.5E-04	3.9E-04	4.5E-04	1.2	0.2233
Trimethylamine <i>N</i> -oxide	3.4E-03	3.0E-03	3.2E-03	3.2E-03	3.8E-03	4.2E-03	3.2E-03	3.7E-03	1.2	0.1486
<i>cis</i> -Aconitic acid	2.1E-03	1.9E-03	2.0E-03	2.0E-03	2.4E-03	2.5E-03	2.0E-03	2.3E-03	1.2	0.1308
<i>N</i> -Acetylmethionine	1.2E-04	1.4E-04	6.6E-05	1.0E-04	1.4E-04	1.3E-04	1.1E-04	1.2E-04	1.2	0.5121
<i>N</i> -Acetylgalactosamine										
<i>N</i> -Acetylmannosamine	N.D.	3.0E-04	3.6E-04	3.9E-04	3.5E-04	4.1E-04	3.3E-04	3.8E-04	1.2	0.1780
<i>N</i> -Acetylglucosamine										
Urocanic acid	1.8E-04	4.5E-04	2.1E-04	3.9E-04	2.0E-04	3.8E-04	2.8E-04	3.2E-04	1.2	0.6972
Nicotinamide	4.3E-04	4.6E-04	6.5E-04	7.2E-04	4.7E-04	5.8E-04	5.1E-04	5.9E-04	1.1	0.4907
2'-Deoxycytidine	2.7E-04	2.8E-04	2.4E-04	2.9E-04	2.9E-04	3.2E-04	2.6E-04	3.0E-04	1.1	0.0651
4-Guanidinobutyric acid	7.0E-04	6.5E-04	3.3E-04	4.5E-04	7.8E-04	6.9E-04	5.6E-04	6.4E-04	1.1	0.6306
XC0001	6.0E-05	N.D.	8.7E-05	7.6E-05	8.4E-05	9.2E-05	7.3E-05	8.4E-05	1.1	0.4456
5-Oxoproline	1.0E-03	1.5E-03	1.0E-03	1.4E-03	9.5E-04	1.6E-03	1.2E-03	1.3E-03	1.1	0.5721
Homovanillic acid	2.1E-04	2.5E-04	1.8E-04	2.4E-04	2.6E-04	2.3E-04	2.2E-04	2.5E-04	1.1	0.2688
Urea	9.0E-01	9.3E-01	8.8E-01	9.5E-01	1.1E+00	1.1E+00	9.0E-01	1.0E+00	1.1	0.0427 #
<i>N</i> -Acetylhistidine	1.7E-04	1.8E-04	9.7E-05	1.3E-04	1.7E-04	2.0E-04	1.5E-04	1.6E-04	1.1	0.6175
Met	1.0E-02	1.1E-02	8.5E-03	9.1E-03	1.2E-02	1.3E-02	9.9E-03	1.1E-02	1.1	0.4034
Carboxymethyllysine	1.9E-04	1.2E-04	1.0E-04	1.5E-04	1.6E-04	1.4E-04	1.4E-04	1.5E-04	1.1	0.5731
XC0016	3.8E-04	3.3E-04	2.8E-04	3.2E-04	3.8E-04	4.0E-04	3.3E-04	3.7E-04	1.1	0.3669
Pantothenic acid	2.5E-04	2.2E-04	2.2E-04	2.6E-04	2.7E-04	2.4E-04	2.3E-04	2.6E-04	1.1	0.1481
3-Indoxylsulfuric acid	4.5E-03	6.3E-03	4.6E-03	4.4E-03	5.2E-03	7.3E-03	5.1E-03	5.7E-03	1.1	0.6362
Pro	3.2E-02	3.9E-02	2.2E-02	2.8E-02	3.2E-02	4.2E-02	3.1E-02	3.4E-02	1.1	0.6543
Lys	6.2E-02	7.8E-02	5.6E-02	6.4E-02	6.4E-02	8.8E-02	6.5E-02	7.2E-02	1.1	0.5510
2-Oxoisovaleric acid	8.5E-04	9.8E-04	1.4E-03	1.2E-03	1.1E-03	1.2E-03	1.1E-03	1.2E-03	1.1	0.5752
2-Hydroxyglutaric acid	6.1E-04	7.1E-04	5.2E-04	4.8E-04	7.2E-04	7.9E-04	6.1E-04	6.7E-04	1.1	0.6330
5-Hydroxylysine	4.0E-04	5.2E-04	2.8E-04	2.8E-04	4.4E-04	6.0E-04	4.0E-04	4.4E-04	1.1	0.7632

Supplemental Table 1 (Continued)

Compound name	Relative area						Mean		Comparative analysis		
	SDC1	SDC2	SDC3	0-4LD1	0-4LD2	0-4LD3	SDC	0-4LD	Ratio [*]	<i>P</i> -value [†]	
Hypotaurine	1.1E-03	1.3E-03	1.3E-03	1.2E-03	1.4E-03	1.5E-03	1.2E-03	1.4E-03	1.1	0.3575	
Creatinine	3.8E-03	3.6E-03	3.7E-03	3.9E-03	4.1E-03	4.1E-03	3.7E-03	4.0E-03	1.1	0.0281	#
Trp	4.3E-02	4.1E-02	3.4E-02	4.1E-02	4.4E-02	4.3E-02	4.0E-02	4.3E-02	1.1	0.3349	
Citric acid	4.1E-02	4.2E-02	4.8E-02	4.7E-02	4.6E-02	4.8E-02	4.4E-02	4.7E-02	1.1	0.2059	
Cytidine	5.1E-04	5.3E-04	5.0E-04	6.5E-04	5.1E-04	4.9E-04	5.1E-04	5.5E-04	1.1	0.5050	
Thr	3.6E-02	4.1E-02	3.0E-02	3.2E-02	3.5E-02	4.7E-02	3.6E-02	3.8E-02	1.1	0.6919	
Ornithine	2.0E-02	2.7E-02	1.5E-02	1.7E-02	2.0E-02	2.8E-02	2.0E-02	2.2E-02	1.1	0.8035	
Tyr	3.0E-02	3.3E-02	2.0E-02	2.3E-02	3.0E-02	3.4E-02	2.8E-02	2.9E-02	1.1	0.7879	
<i>N</i> _ω -Methylarginine	1.2E-04	1.2E-04	8.8E-05	9.9E-05	1.1E-04	1.4E-04	1.1E-04	1.2E-04	1.1	0.7370	
Putrescine	1.6E-04	1.6E-04	1.1E-04	1.4E-04	1.6E-04	1.4E-04	1.4E-04	1.5E-04	1.1	0.7015	
XC0040	1.8E-04	1.9E-04	1.2E-04	N.D.	1.8E-04	1.6E-04	1.6E-04	1.7E-04	1.0	0.8246	
γ-Glu-Val-Gly	1.2E-04	7.3E-05	9.2E-05	6.8E-05	1.3E-04	1.1E-04	9.6E-05	1.0E-04	1.0	0.8694	
XA0035	2.8E-04	2.6E-04	3.3E-04	3.2E-04	3.0E-04	2.9E-04	2.9E-04	3.0E-04	1.0	0.6472	
Cysteine glutathione disulfide	5.1E-03	5.6E-03	6.0E-03	5.3E-03	6.9E-03	5.0E-03	5.6E-03	5.7E-03	1.0	0.7702	
Butyrylcarnitine	1.8E-03	1.8E-03	1.2E-03	1.2E-03	2.0E-03	1.8E-03	1.6E-03	1.7E-03	1.0	0.8613	
Ophthalmic acid	2.5E-04	2.3E-04	1.9E-04	1.6E-04	3.6E-04	1.7E-04	2.2E-04	2.3E-04	1.0	0.9216	
XA0004	6.1E-05	7.8E-05	5.6E-05	N.D.	6.1E-05	7.3E-05	6.5E-05	6.7E-05	1.0	0.8853	
Phe	3.3E-02	4.0E-02	2.7E-02	3.0E-02	3.5E-02	3.7E-02	3.3E-02	3.4E-02	1.0	0.8782	
Uridine	1.2E-03	1.4E-03	1.5E-03	1.5E-03	1.3E-03	1.3E-03	1.4E-03	1.4E-03	1.0	0.7492	
Asn	6.7E-03	9.6E-03	5.8E-03	7.2E-03	6.6E-03	8.9E-03	7.4E-03	7.6E-03	1.0	0.9073	
Cystathionine	2.5E-04	2.2E-04	2.2E-04	2.1E-04	2.3E-04	2.7E-04	2.3E-04	2.4E-04	1.0	0.8164	
Gly	4.7E-02	5.1E-02	4.5E-02	5.0E-02	4.1E-02	5.5E-02	4.8E-02	4.9E-02	1.0	0.8410	
<i>S</i> -Adenosylmethionine	3.8E-05	2.6E-05	5.3E-05	4.4E-05	3.6E-05	3.9E-05	3.9E-05	4.0E-05	1.0	0.9297	
Glucuronic acid	5.1E-04	4.2E-04	5.0E-04	4.9E-04	4.3E-04	5.2E-04	4.7E-04	4.8E-04	1.0	0.8426	
Galacturonic acid											
SDMA	1.5E-04	1.8E-04	1.5E-04	1.8E-04	1.6E-04	1.5E-04	1.6E-04	1.6E-04	1.0	0.8780	
5-Methoxyindoleacetic acid	2.2E-04	2.6E-04	2.2E-04	1.4E-04	2.9E-04	2.9E-04	2.4E-04	2.4E-04	1.0	0.9541	
Gluconolactone	1.4E-03	1.1E-03	1.2E-03	1.3E-03	1.4E-03	1.2E-03	1.2E-03	1.3E-03	1.0	0.9689	
Cystine	1.5E-03	2.2E-03	2.4E-03	2.1E-03	2.4E-03	1.7E-03	2.1E-03	2.1E-03	1.0	0.9992	
Ala	5.6E-02	7.0E-02	4.3E-02	4.8E-02	5.5E-02	6.6E-02	5.6E-02	5.6E-02	1.0	0.9826	
Imidazolelactic acid	1.2E-04	9.4E-05	9.7E-05	1.0E-04	1.0E-04	1.1E-04	1.0E-04	1.0E-04	1.0	0.9603	
Glutathione (GSSG)_divalent	5.9E-03	6.1E-03	5.9E-03	5.2E-03	6.8E-03	5.8E-03	6.0E-03	5.9E-03	1.0	0.9399	
Lauric acid	2.8E-03	2.5E-03	2.5E-03	2.6E-03	2.4E-03	2.6E-03	2.6E-03	2.5E-03	1.0	0.8078	
2-Hydroxybutyric acid	1.4E-03	1.8E-03	2.1E-03	1.8E-03	1.8E-03	1.6E-03	1.8E-03	1.7E-03	1.0	0.9296	
<i>o</i> -Hydroxybenzoic acid	4.5E-04	6.0E-04	3.3E-04	2.1E-04	5.5E-04	6.1E-04	4.6E-04	4.5E-04	1.0	0.9722	
Lactic acid	4.0E-01	4.1E-01	3.4E-01	3.3E-01	4.0E-01	4.0E-01	3.8E-01	3.8E-01	1.0	0.8899	
Argininosuccinic acid	1.1E-04	1.5E-04	9.1E-05	8.6E-05	9.6E-05	1.7E-04	1.2E-04	1.2E-04	1.0	0.9534	
<i>N</i> -Acetylalanine	1.6E-04	1.5E-04	1.4E-04	1.6E-04	1.7E-04	1.1E-04	1.5E-04	1.5E-04	1.0	0.8993	
Gln	1.2E-01	1.2E-01	1.1E-01	1.3E-01	9.8E-02	1.1E-01	1.2E-01	1.1E-01	1.0	0.8321	
Phenaceturic acid	4.6E-04	3.7E-04	3.3E-04	4.1E-04	2.2E-04	5.1E-04	3.9E-04	3.8E-04	1.0	0.9408	
Stachydrine	1.0E-02	7.9E-03	6.7E-03	6.6E-03	8.9E-03	8.6E-03	8.2E-03	8.0E-03	1.0	0.8538	
<i>N</i> ⁶ -Acetyllysine	3.5E-04	3.6E-04	3.4E-04	3.2E-04	3.9E-04	3.2E-04	3.5E-04	3.4E-04	1.0	0.7033	
1-Methylhistidine											
3-Methylhistidine	4.1E-03	3.8E-03	4.0E-03	4.1E-03	3.4E-03	4.2E-03	4.0E-03	3.9E-03	1.0	0.6744	
<i>N</i> ⁶ -Methyllysine	3.2E-03	3.2E-03	2.9E-03	2.7E-03	3.1E-03	3.3E-03	3.1E-03	3.0E-03	1.0	0.6727	

Supplemental Table 1 (Continued)

Compound name	Relative area						Mean		Comparative analysis	
	SDC1	SDC2	SDC3	0-4LD1	0-4LD2	0-4LD3	SDC	0-4LD	Ratio*	P-value†
4-Methyl-2-oxovaleric acid	3.6E-03	3.3E-03	5.1E-03	4.4E-03	3.4E-03	3.7E-03	4.0E-03	3.8E-03	1.0	0.7927
3-Methyl-2-oxovaleric acid										
Myristoleic acid	6.7E-05	N.D.	7.9E-05	9.9E-05	N.D.	4.0E-05	7.3E-05	6.9E-05	1.0	0.9234
2'-Deoxyuridine	3.1E-04	2.4E-04	3.2E-04	2.6E-04	3.0E-04	2.6E-04	2.9E-04	2.7E-04	0.9	0.5866
Gluconic acid	2.8E-03	2.2E-03	2.6E-03	2.3E-03	2.4E-03	2.5E-03	2.5E-03	2.4E-03	0.9	0.4981
Uric acid	4.8E-03	3.5E-03	4.0E-03	3.8E-03	3.4E-03	4.4E-03	4.1E-03	3.9E-03	0.9	0.6418
<i>N,N</i> -Dimethylglycine	3.7E-03	3.3E-03	3.1E-03	3.1E-03	3.0E-03	3.4E-03	3.4E-03	3.2E-03	0.9	0.4084
Glycolic acid	3.6E-03	2.8E-03	4.0E-03	3.6E-03	3.1E-03	3.1E-03	3.5E-03	3.3E-03	0.9	0.6181
Ser	2.2E-02	2.4E-02	2.0E-02	2.0E-02	1.8E-02	2.4E-02	2.2E-02	2.1E-02	0.9	0.5203
Citrulline	1.9E-02	2.5E-02	1.9E-02	1.8E-02	1.6E-02	2.2E-02	2.1E-02	1.9E-02	0.9	0.5274
Thymidine	5.0E-04	4.7E-04	4.5E-04	3.9E-04	4.3E-04	4.7E-04	4.7E-04	4.3E-04	0.9	0.1861
Hydroxyproline	6.4E-03	7.2E-03	5.2E-03	4.8E-03	5.4E-03	6.7E-03	6.2E-03	5.6E-03	0.9	0.4879
XC0120	3.5E-05	6.1E-05	3.7E-05	3.8E-05	4.5E-05	3.6E-05	4.4E-05	4.0E-05	0.9	0.6443
Threonine acid	3.6E-03	2.9E-03	4.3E-03	3.7E-03	3.0E-03	3.0E-03	3.6E-03	3.2E-03	0.9	0.4971
Decanoic acid	3.1E-04	N.D.	2.6E-04	2.5E-04	N.D.	2.6E-04	2.8E-04	2.5E-04	0.9	0.3742
Succinic acid	5.4E-03	7.2E-03	5.7E-03	5.0E-03	5.6E-03	5.7E-03	6.1E-03	5.4E-03	0.9	0.3355
2-Hydroxyvaleric acid	3.5E-03	3.0E-03	4.0E-03	3.2E-03	2.8E-03	3.5E-03	3.5E-03	3.1E-03	0.9	0.3372
2-Aminoisobutyric acid										
2-Aminobutyric acid	1.6E-03	1.9E-03	1.5E-03	1.4E-03	1.4E-03	1.6E-03	1.7E-03	1.5E-03	0.9	0.2212
His	2.4E-02	2.6E-02	2.0E-02	2.1E-02	2.0E-02	2.2E-02	2.3E-02	2.1E-02	0.9	0.2259
2-Hydroxyisobutyric acid	1.3E-03	1.3E-03	1.7E-03	1.5E-03	9.6E-04	1.4E-03	1.4E-03	1.3E-03	0.9	0.4405
3-Hydroxybutyric acid	1.3E-02	1.6E-02	3.6E-02	2.8E-02	1.5E-02	1.4E-02	2.2E-02	1.9E-02	0.9	0.7876
Fumaric acid	1.2E-03	1.5E-03	1.1E-03	1.0E-03	9.4E-04	1.4E-03	1.3E-03	1.1E-03	0.9	0.4887
7,8-Dihydrobiopterin	N.D.	4.4E-05	5.6E-05	4.1E-05	4.7E-05	4.3E-05	5.0E-05	4.4E-05	0.9	0.3115
Carnitine	2.8E-02	2.4E-02	2.2E-02	2.2E-02	1.9E-02	2.3E-02	2.5E-02	2.2E-02	0.9	0.1969
Malic acid	1.6E-02	2.4E-02	1.7E-02	1.5E-02	1.4E-02	2.0E-02	1.9E-02	1.6E-02	0.9	0.4873
2-Hydroxy-4-methylvaleric acid	9.2E-04	8.0E-04	7.9E-04	7.5E-04	6.6E-04	7.6E-04	8.4E-04	7.2E-04	0.9	0.1060
Guanidoacetic acid	8.2E-04	1.1E-03	9.2E-04	7.4E-04	8.3E-04	8.7E-04	9.4E-04	8.1E-04	0.9	0.2137
Isovalerylcarnitine	3.0E-04	3.7E-04	2.5E-04	2.3E-04	2.5E-04	3.1E-04	3.1E-04	2.6E-04	0.8	0.3509
<i>N</i> -Acetylmuramic acid	9.5E-05	9.6E-05	N.D.	5.2E-05	7.7E-05	1.1E-04	9.5E-05	8.0E-05	0.8	0.5461
<i>O</i> -Acetylcarnitine	2.6E-02	2.3E-02	3.0E-02	2.7E-02	2.0E-02	1.9E-02	2.6E-02	2.2E-02	0.8	0.2280
GABA	2.3E-04	4.3E-04	1.6E-04	2.3E-04	2.3E-04	2.2E-04	2.7E-04	2.2E-04	0.8	0.5739
Glucose 6-phosphate	3.0E-04	3.3E-04	3.2E-04	3.0E-04	2.8E-04	1.9E-04	3.2E-04	2.6E-04	0.8	0.1626
Mucic acid	5.2E-04	4.6E-04	4.7E-04	4.1E-04	3.8E-04	3.7E-04	4.8E-04	3.8E-04	0.8	0.0146 #
Glyceric acid	7.5E-04	6.2E-04	5.9E-04	4.5E-04	5.2E-04	5.4E-04	6.6E-04	5.1E-04	0.8	0.0556
γ -Butyrobetaine	2.1E-03	2.0E-03	1.7E-03	1.5E-03	1.4E-03	1.5E-03	1.9E-03	1.5E-03	0.8	0.0261 #
Pyridoxal	1.2E-04	1.8E-04	1.3E-04	8.9E-05	1.2E-04	1.1E-04	1.4E-04	1.1E-04	0.7	0.1440
Sarcosine	7.3E-04	7.5E-04	N.D.	3.8E-04	5.1E-04	7.7E-04	7.4E-04	5.5E-04	0.7	0.2868
XC0061	1.8E-03	2.0E-03	1.2E-03	1.1E-03	1.3E-03	1.2E-03	1.7E-03	1.2E-03	0.7	0.1317
Betaine	5.1E-02	4.1E-02	3.5E-02	2.7E-02	2.8E-02	3.0E-02	4.2E-02	2.8E-02	0.7	0.0386 #
<i>S</i> -Methylmethionine	1.5E-04	1.2E-04	1.3E-04	7.9E-05	9.6E-05	9.4E-05	1.4E-04	9.0E-05	0.7	0.0129 #
Glycerol	3.3E-02	3.2E-02	4.8E-02	2.5E-02	2.2E-02	2.3E-02	3.7E-02	2.4E-02	0.6	0.0558
<i>N</i> -Acetyl- β -alanine	N.D.	6.3E-05	7.5E-05	3.4E-05	2.6E-05	N.D.	6.9E-05	3.0E-05	0.4	0.0352 #
<i>N</i> -Acetylphenylalanine	2.5E-04	3.3E-04	2.0E-04	1.1E-04	1.1E-04	1.3E-04	2.6E-04	1.1E-04	0.4	0.0184 #
Phosphocreatine	5.6E-04	4.3E-04	4.4E-04	8.0E-05	2.6E-04	1.2E-04	4.8E-04	1.5E-04	0.3	0.0080 ##
3-Phenylpropionic acid	7.7E-04	1.0E-03	7.6E-04	2.1E-04	1.9E-04	2.6E-04	8.5E-04	2.2E-04	0.3	0.0016 ##
Cholic acid	5.9E-04	5.1E-03	5.0E-04	4.7E-04	2.6E-04	5.8E-04	2.1E-03	4.4E-04	0.2	0.3461

Supplemental Table 1 (Continued)

Compound name	Relative area						Mean		Comparative analysis	
	SDC1	SDC2	SDC3	0-4LD1	0-4LD2	0-4LD3	SDC	0-4LD	Ratio ^a	P-value [†]
Taurocholic acid	3.9E-04	3.5E-03	2.1E-04	2.0E-04	2.3E-04	1.8E-04	1.4E-03	2.0E-04	0.15	0.3400
Hippuric acid	2.0E-03	1.6E-03	1.5E-03	1.0E-04	1.3E-04	1.7E-04	1.7E-03	1.4E-04	0.08	0.0005 ###
1-Methylnicotinamide	N.D.	N.D.	N.D.	N.D.	7.7E-05	8.5E-05	N.D.	8.1E-05	-	-
5-Aminovaleric acid	N.D.	N.D.	N.D.	N.D.	N.D.	1.1E-03	N.D.	1.1E-03	-	-
6-Aminohexanoic acid	N.D.	N.D.	N.D.	N.D.	2.5E-04	2.8E-04	N.D.	2.6E-04	-	-
ADP	N.D.	N.D.	N.D.	3.3E-04	3.1E-04	5.7E-04	N.D.	4.0E-04	-	-
ATP	N.D.	N.D.	N.D.	N.D.	N.D.	7.1E-05	N.D.	7.1E-05	-	-
Adipic acid	N.D.	N.D.	N.D.	N.D.	N.D.	1.0E-04	N.D.	1.0E-04	-	-
Cyclohexylamine	N.D.	N.D.	N.D.	N.D.	5.7E-05	N.D.	N.D.	5.7E-05	-	-
Cytosine	N.D.	N.D.	N.D.	N.D.	N.D.	2.2E-04	N.D.	2.2E-04	-	-
Dihydroxyacetone phosphate	N.D.	N.D.	N.D.	5.9E-04	1.9E-04	4.3E-04	N.D.	4.0E-04	-	-
N-Ethylmaleimide_+H ₂ O	N.D.	N.D.	N.D.	1.9E-04	N.D.	N.D.	N.D.	1.9E-04	-	-
γ-Glu-2-aminobutyric acid	N.D.	N.D.	N.D.	N.D.	N.D.	6.7E-05	N.D.	6.7E-05	-	-
2,6-Diaminopimelic acid	N.D.	1.3E-04	N.D.	N.D.	N.D.	N.D.	1.3E-04	N.D.	-	-
8-Hydroxyoctanoic acid	5.4E-05	N.D.	N.D.	N.D.	N.D.	N.D.	5.4E-05	N.D.	-	-
2-Hydroxyoctanoic acid	5.4E-05	N.D.	N.D.	N.D.	N.D.	N.D.	5.4E-05	N.D.	-	-
Acetoacetic acid	N.D.	N.D.	2.9E-04	N.D.	N.D.	N.D.	2.9E-04	N.D.	-	-
Glutaric acid	N.D.	3.5E-04	N.D.	N.D.	N.D.	N.D.	3.5E-04	N.D.	-	-
Isobutyric acid	N.D.	2.9E-03	N.D.	N.D.	N.D.	N.D.	2.9E-03	N.D.	-	-
Butyric acid	N.D.	2.9E-03	N.D.	N.D.	N.D.	N.D.	2.9E-03	N.D.	-	-
Piperidine	N.D.	N.D.	3.3E-05	N.D.	N.D.	N.D.	3.3E-05	N.D.	-	-
Propionic acid	N.D.	1.4E-03	N.D.	N.D.	N.D.	N.D.	1.4E-03	N.D.	-	-
XC0065	5.8E-05	N.D.	N.D.	N.D.	N.D.	N.D.	5.8E-05	N.D.	-	-
AMP	N.D.	N.D.	2.4E-04	4.3E-03	2.3E-03	4.9E-03	2.4E-04	3.8E-03	16	-
GMP	N.D.	N.D.	1.4E-04	8.1E-04	5.1E-04	9.1E-04	1.4E-04	7.4E-04	5.3	-
UMP	N.D.	N.D.	8.8E-05	3.3E-04	2.0E-04	5.4E-04	8.8E-05	3.5E-04	4.0	-
XC0126	N.D.	3.6E-05	N.D.	6.5E-05	7.7E-05	5.3E-05	3.6E-05	6.5E-05	1.8	-
XA0017	N.D.	N.D.	5.6E-05	1.1E-04	8.8E-05	N.D.	5.6E-05	1.0E-04	1.8	-
Hypoxanthine	N.D.	N.D.	5.0E-04	1.2E-03	6.5E-04	5.5E-04	5.0E-04	8.0E-04	1.6	-
p-Coumaric acid	N.D.	8.0E-05	N.D.	1.2E-04	1.6E-04	9.2E-05	8.0E-05	1.2E-04	1.5	-
Glucaric acid	6.6E-05	N.D.	N.D.	6.4E-05	N.D.	1.1E-04	6.6E-05	8.9E-05	1.4	-
Xanthine	N.D.	N.D.	4.9E-04	9.0E-04	5.5E-04	4.2E-04	4.9E-04	6.2E-04	1.3	-
2,5-Dihydroxybenzoic acid	N.D.	6.0E-05	N.D.	N.D.	7.2E-05	N.D.	6.0E-05	7.2E-05	1.2	-
Fructose 6-phosphate	N.D.	6.8E-05	N.D.	N.D.	7.3E-05	8.4E-05	6.8E-05	7.9E-05	1.2	-
3-Hydroxykynurenine	5.9E-05	N.D.	N.D.	5.7E-05	7.5E-05	N.D.	5.9E-05	6.6E-05	1.1	-
Triethanolamine	N.D.	8.8E-05	7.5E-05	8.3E-05	N.D.	N.D.	8.2E-05	8.3E-05	1.0	-
XA0027	N.D.	3.4E-04	N.D.	3.3E-04	3.2E-04	N.D.	3.4E-04	3.3E-04	1.0	-
XA0002	5.0E-04	N.D.	N.D.	N.D.	N.D.	4.2E-04	5.0E-04	4.2E-04	0.8	-
Pelargonic acid	4.3E-04	N.D.	N.D.	3.8E-04	3.7E-04	3.3E-04	4.3E-04	3.6E-04	0.8	-
N ⁸ -Acetylspermidine	N.D.	5.4E-05	3.8E-05	3.7E-05	N.D.	N.D.	4.6E-05	3.7E-05	0.8	-
XA0036	8.4E-05	N.D.	N.D.	6.7E-05	N.D.	4.6E-05	8.4E-05	5.6E-05	0.7	-
Ascorbate 2-sulfate	8.4E-05	N.D.	N.D.	6.7E-05	N.D.	4.6E-05	8.4E-05	5.6E-05	0.7	-
Indole-3-acetic acid	9.5E-05	9.8E-05	N.D.	6.2E-05	N.D.	N.D.	9.7E-05	6.2E-05	0.6	-

*Ratio of 0-4LD to SDC

†t-test, #p < 0.05, ##p < 0.01, ###p < 0.001