

Supplementary Table 2. Metabolomics of 786-O VHL-deficient and –restored cells upon cystine deprivation

PARAM_GROUP_DESC	PLATFORM	SUPER_PATHWAY	SUB_PATHWAY	Vec+Cys 18h	Vec+Cys 18h	Vec+Cys 18h	Vec+Cys 18h	Vec-Cys 18h	Vec-Cys 18h	Vec-Cys 18h	Vec-Cys 18h	VHL+Cys 18h	VHL+Cys 18h	VHL+Cys 18h	VHL+Cys 18h	VHL-Cys 18h	VHL-Cys 18h	VHL-Cys 18h	VHL-Cys 18h
BIOCHEMICAL																			
1-arachidonoylglycerophosphoethanolamine*	LC/MS Neg	Lipid	Lysolipid	1.45	1.24	2.97	1.67	1.71	0.81	0.99	1.1	1.11	2.96	1.83	1.33	1.06	1.4	1.15	1.01
1-methylnicotinamide	LC/MS Pos	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	2.03	1.93	2.55	2.23	0.88	1.03	0.98	0.91	1.52	2.15	1.77	2.02	1.34	1.13	1.53	1.35
1-myristoylglycerophosphocholine	LC/MS Pos	Lipid	Lysolipid	1.86	0.43	2.3	0.43	0.43	0.43	0.43	0.43	0.43	0.49	0.43	0.43	0.96	0.43	0.43	0.43
1-oleoylglycerophosphocholine	LC/MS Pos	Lipid	Lysolipid	2.26	0.08	3.21	0.85	1.1	0.08	0.54	0.08	1.01	2.06	1.74	0.08	1.2	0.08	0.08	0.08
1-oleoylglycerophosphoinositol*	LC/MS Neg	Lipid	Lysolipid	0.71	0.38	1.39	0.38	0.38	0.63	0.62	0.38	0.91	0.86	0.75	0.38	0.41	0.68	0.94	0.59
1-palmitoylglycerophosphocholine	LC/MS Pos	Lipid	Lysolipid	3.32	1	4.25	6.11	1.72	0.69	0.66	1.41	1.48	14.29	2.06	1.16	2	0.73	0.19	0.7
1-stearoylglycerophosphocholine	LC/MS Pos	Lipid	Lysolipid	2.95	0.16	3.31	1.9	1.91	0.16	0.93	0.4	1.08	8.69	1.88	0.16	1.37	0.16	0.27	0.39
1-stearoylglycerophosphoethanolamine	LC/MS Pos	Lipid	Lysolipid	1.94	0.39	1.45	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.39	0.76	0.39	0.39	0.39
1-stearoylglycerophosphoinositol	LC/MS Neg	Lipid	Lysolipid	0.43	0.97	0.82	1.12	0.28	0.49	0.45	0.34	1.35	1.75	0.7	2	0.98	1.17	1.18	1.01
2-aminoadipate	GC/MS	Amino acid	Lysine metabolism	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21
2-aminobutyrate	GC/MS	Amino acid	Butanoate metabolism	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54
2-arachidonoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	3.34	0.51	3.33	2.16	1.52	0.06	0.62	0.39	1.26	6.11	2.35	0.67	3.45	0.06	0.25	0.2
2-arachidonoylglycerophosphoethanolamine*	LC/MS Pos	Lipid	Lysolipid	5.2	1.74	6.15	5.61	1.97	0.58	1.3	2.24	1.97	16.62	2.73	1.41	3.2	0.69	0.29	0.63
2-docosahexaenoylglycerophosphoethanolamine*	LC/MS Pos	Lipid	Lysolipid	14.17	0.67	16.28	2.55	4.01	1.14	2.43	0.84	5.83	9.82	8.85	0.68	11.82	0.14	0.85	0.14
2-docosapentaenoylglycerophosphoethanolamine*	LC/MS Pos	Lipid	Lysolipid	4.96	0.13	7.12	0.21	1.83	0.13	1	0.13	2.31	1.45	3.06	0.13	2.9	0.13	0.29	0.13
2-hydroxyglutarate	GC/MS	Lipid	Fatty acid, dicarboxylate	1.58	1.39	1.45	0.1	0.52	0.72	0.49	0.92	0.1	0.1	0.1	1.25	0.49	0.53	0.1	0.71
2-methylbutyrylcarnitine (C5)	LC/MS Pos	Amino acid	Valine, leucine and isoleucine metabolism	1.21	1.04	1.41	1.18	0.25	0.57	0.53	0.25	0.81	0.25	0.57	0.25	0.58	0.25	0.25	0.63
2-myristoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	4.68	0.24	3.96	1.31	1.4	0.24	0.99	0.24	1.09	2.23	1.83	0.24	1.49	0.24	0.45	0.24
2-oleoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	8.66	0.08	9.19	1.32	4.15	0.08	1.21	0.19	3.41	4.28	4.24	0.08	5.23	0.08	0.29	0.08
2-oleoylglycerophosphoethanolamine*	LC/MS Pos	Lipid	Lysolipid	4.45	0.35	4.17	0.96	1.75	0.12	0.69	0.14	1.5	3.07	2.01	0.12	1.95	0.12	0.15	0.12
2-oleoylglycerophosphoinositol*	LC/MS Neg	Lipid	Lysolipid	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54	0.54
2-palmitoleoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	3.18	0.18	2.6	0.18	0.86	0.18	0.46	0.18	0.58	1.37	1.54	0.18	1.47	0.18	0.18	0.18
2-palmitoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	2.61	0.04	3.49	1.78	1.21	0.04	0.52	0.04	1.1	2.85	1.16	0.04	1.66	0.04	0.1	0.04
2-palmitoylglycerophosphoethanolamine*	LC/MS Pos	Lipid	Lysolipid	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17
2-stearoylglycerophosphocholine*	LC/MS Pos	Lipid	Lysolipid	1.22	0.47	1.72	1.89	0.47	0.47	0.47	0.47	0.47	2.81	1.19	0.47	0.9	0.47	0.47	0.47
3-(4-hydroxyphenyl)lactate	LC/MS Neg	Amino acid	Phenylalanine & tyrosine metabolism	0.68	0.69	0.88	0.78	0.43	0.4	0.46	0.55	0.76	1.19	0.9	1.05	0.76	0.71	0.87	0.78
3-methyl-2-oxobutyrate	LC/MS Neg	Amino acid	Valine, leucine and isoleucine metabolism	1.85	0.91	1.38	1.54	0.65	0.6	0.78	1.01	0.84	1.59	1.29	1.23	0.78	0.68	0.89	0.99
3-methyl-2-oxovalerate	LC/MS Neg	Amino acid	Valine, leucine and isoleucine metabolism	1.23	0.98	1.59	1.3	0.62	0.62	0.64	0.78	0.92	1.4	1.21	1.09	0.96	0.85	1	0.84
3-phosphoglycerate	GC/MS	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	1.97	1.77	0.83	1.01	0.57	0.56	0.71	0.62	0.57	0.73	0.91	0.75	0.68	0.99	0.95	0.44
4-methyl-2-oxopentanoate	LC/MS Neg	Amino acid	Valine, leucine and isoleucine metabolism	1	1.01	1.36	1.06	0.54	0.63	0.52	0.73	0.77	1.2	1.05	1	0.86	0.76	0.92	0.87
5-aminovalerate	LC/MS Pos	Amino acid	Urea cycle; arginine-, proline-, metabolism	2.72	2.97	1.9	1.49	0.58	0.51	1.23	0.53	1.53	2.55	2.43	1.95	1.09	0.91	1.38	1.34
5-methylthioadenosine (MTA)	LC/MS Pos	Amino acid	Polyamine metabolism	1.38	1.51	1.67	1.1	0.64	0.64	0.56	0.79	0.52	0.87	1	0.87	0.6	0.63	0.76	0.51
5-oxoproline	LC/MS Neg	Amino acid	Glutathione metabolism	0.39	0.42	0.49	0.41	0.21	0.21	0.23	0.21	0.22	0.36	0.25	0.32	0.22	0.22	0.25	0.22
acetyl CoA	LC/MS Neg	Cofactors and vitamins	Pantothenate and CoA metabolism	0.5	1.1	0.06	1.11	1.28	1.12	1.4	1.23	0.53	0.76	0.31	1.02	1.99	1.77	2.29	1.79
acetylphosphate	GC/MS	Energy	Oxidative phosphorylation	1.03	1.47	1.2	1.67	0.5	0.67	0.6	0.54	0.63	1.09	0.78	1.08	0.59	0.76	0.93	0.63
adenine	GC/MS	Nucleotide	Purine metabolism; adenine containing	1.26	1	1.1	1.23	0.48	0.57	0.93	0.55	0.71	1	0.94	0.66	0.69	0.66	1.02	0.84
adenosine	LC/MS Pos	Nucleotide	Purine metabolism; adenine containing	0.43	0.83	0.7	0.43	0.43	0.67	0.99	0.59	0.71	1.01	1.18	0.84	0.63	0.45	0.93	0.89
adenosine 5'-monophosphate (AMP)	LC/MS Pos	Nucleotide	Purine metabolism; adenine containing	1.02	0.91	1.09	0.78	0.42	0.55	0.54	0.51	0.95	1.39	1.04	1.45	0.58	0.46	0.66	0.48
alanine	GC/MS	Amino acid	Alanine and aspartate metabolism	1.22	1.01	1.29	0.98	0.41	0.61	0.57	0.43	0.74	0.96	0.8	0.83	0.81	0.85	0.88	0.72
allantoin	GC/MS	Nucleotide	Purine metabolism, urate metabolism	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
alpha-ketoglutarate	GC/MS	Energy	Krebs cycle	2.76	4.48	3.31	2.77	0.9	1.25	0.75	0.71	0.95	1.47	1.44	1.14	0.39	0.79	0.88	0.74
arabitol	GC/MS	Carbohydrate	Nucleotide sugars, pentose metabolism	0.25	0.93	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.29	0.25	0.25
arachidonate (20:4n6)	LC/MS Neg	Lipid	Long chain fatty acid	1.1	1.41	1.36	1.42	0.9	1.31	1.05	0.88	0.58	1.11	0.83	1.42	0.47	0.85	0.86	0.73
arginine	LC/MS Pos	Amino acid	Urea cycle; arginine-, proline-, metabolism	1.76	1.97	2.27	2.14	0.74	0.88	0.9	0.86	1.11	1.74	1.29	1.54	0.93	0.81	0.98	0.95
asparagine	GC/MS	Amino acid	Alanine and aspartate metabolism	0.2	0.2	0.2	0.37	0.65	0.75	0.67	0.96	0.2	0.96	1	0.67	1	1.32	1.22	1.03
aspartate	GC/MS	Amino acid	Alanine and aspartate metabolism	1.14	1.41	1.34	1.21	0.79	0.76	0.64	0.73	0.81	1.35	0.9	1	0.99	0.97	1.18	1.03
azelate (nonanedioate)	LC/MS Neg	Lipid	Fatty acid, dicarboxylate	2.61	1.82	2.23	2.77	0.72	0.81	1.01	0.94	1.47	1.99	1.35	1.94	0.82	0.74	0.92	1.15
beta-alanine	GC/MS	Amino acid	Alanine and aspartate metabolism	3.23	1.85	2.82	4.22	0.3	0.86	0.56	0.37	1.38	3.03	1.26	2.38	0.72	0.58	0.68	0.61
betaine	LC/MS Pos	Amino acid	Glycine, serine and threonine metabolism	0.71	0.98	0.75	0.08	0.08	0.08	0.08	0.21	0.67	1.12	0.72	0.92	0.51	0.49	0.43	0.41
butyrylcarnitine	LC/MS Pos	Lipid	Fatty acid metabolism (also BCAA metabolism)	0.75	0.65	1.06	0.64	0.14	0.2	0.18	0.18	0.42	0.56	0.4	0.47	0.09	0.11	0.13	0.12
carnitine	LC/MS Pos	Lipid	Carnitine metabolism	0.74	0.78	0.95	0.68	0.29	0.28	0.27	0.26	0.35	0.61	0.4	0.56	0.25	0.25	0.32	0.3
cholesterol	GC/MS	Lipid	Sterol/Steroid	1	1.69	1.61	1.71	0.58	0.85	0.6	0.52	0.73	1.11	1.05	1.44	0.61	0.88	0.83	0.95
choline phosphate	LC/MS Pos	Lipid	Glycerolipid metabolism	1.6	1.82	2.15	1.94	0.58	0.71	0.68	0.59	0.88	1.26	0.91	1.08	0.63	0.52	0.69	0.63
citrate	GC/MS	Energy	Krebs cycle	1.15	1	1.39	1.12	0.41	0.38	0.25	0.47	0.9	1.36	0.87	1.23	0.55	0.42	0.51	0.46
coenzyme A	LC/MS Neg	Cofactors and vitamins	Pantothenate and CoA metabolism	1.29	1.38	1.62	1.31	0.14	0.24	0.14	0.18	0.94	1.45	1.1	1.23	0.14	0.22	0.2	0.27
creatine	LC/MS Pos	Amino acid	Creatine metabolism	1.49	1.45	1.87	1.59	0.58	0.72	0.67	0.58	0.93	1.32	1.05	1.23	0.7	0.62	0.83	0.7
creatine phosphate	LC/MS Neg	Amino acid	Creatine metabolism	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.08	0.15	0.1	0.13	0.08	0.08	0.08	0.08
creatinine																			

glutamine	LC/MS Pos	Amino acid	Glutamate metabolism	1.06	1.17	1.34	1.38	0.82	0.98	0.95	0.82	0.98	1.4	0.96	1.17	1.36	1.04	1.42	1.41
glutathione, oxidized (GSSG)	LC/MS Pos	Amino acid	Glutathione metabolism	2.19	2.09	2.68	2.31	0.01	0.02	0.01	0.01	1.36	2.46	1.79	1.92	0.01	0.01	0.01	0.01
glutathione, reduced (GSH)	LC/MS Pos	Amino acid	Glutathione metabolism	2.71	2.51	3.08	2.76	0	0.01	0	0	1.74	2.43	1.82	2.46	0.01	0.01	0.01	0.01
glycerol 2-phosphate	GC/MS	Xenobiotics	Chemical	1.03	2.47	2.74	1.94	1.19	1.27	0.94	0.79	0.34	0.76	0.3	0.3	0.37	0.3	1.01	0.3
glycerol 3-phosphate (G3P)	GC/MS	Lipid	Glycerolipid metabolism	1.64	1.9	2.3	2.11	0.93	0.82	1.04	0.96	0.4	0.44	0.46	0.41	0.33	0.33	0.54	0.26
glycerophosphorylcholine (GPC)	LC/MS Pos	Lipid	Glycerolipid metabolism	3.02	3.13	3.93	3.65	1.61	1.79	1.81	1.66	0.38	0.59	0.42	0.52	0.35	0.32	0.38	0.35
glycine	GC/MS	Amino acid	Glycine, serine and threonine metabolism	0.48	0.49	0.61	0.51	0.39	0.38	0.39	0.39	0.49	0.76	0.61	0.64	0.61	0.62	0.76	0.65
guanosine 5'-triphosphate	LC/MS Neg	Nucleotide	Purine metabolism, guanine containing	2.07	2.03	2.18	2	0.69	1	0.95	0.9	1.24	1.9	1.21	1.54	1.04	0.88	1.07	1.11
hippurate	LC/MS Neg	Xenobiotics	Benzoate metabolism	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76
histidine	LC/MS Neg	Amino acid	Histidine metabolism	0.88	0.92	1	0.86	0.74	0.68	0.78	0.63	0.88	0.92	1.15	0.88	1.09	0.89	1.27	0.9
homocystine	LC/MS Pos	Amino acid	Cysteine, methionine, SAM, taurine metabolism	1.78	2.34	2.67	2.17	1.02	1.26	1.26	1.1	1.29	2.28	1.42	1.88	1.17	0.89	1.33	0.82
hypotaurine	GC/MS	Amino acid	Cysteine, methionine, SAM, taurine metabolism	1.1	0.67	1.01	0.82	0.07	0.24	0.07	0.19	0.26	0.35	0.28	0.53	0.2	0.25	0.07	0.27
inosine	LC/MS Neg	Nucleotide	Purine metabolism, (hypo)xanthine/inosine containing	0.25	0.25	0.25	0.25	0.25	0.43	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.47	0.75
inositol 1-phosphate (I1P)	GC/MS	Lipid	Inositol metabolism	0.87	1.09	0.52	0.67	0.56	0.6	0.59	0.39	0.98	1.38	1.01	0.61	0.6	0.75	0.71	0.61
Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,	LC/MS Neg	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	3.02	2.96	3.52	2.96	0.83	1.01	0.99	0.96	1.15	2.01	1.34	1.47	0.77	0.72	0.71	0.71
isobutyrylcarnitine	LC/MS Pos	Amino acid	Valine, leucine and isoleucine metabolism	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
isoleucine	LC/MS Pos	Amino acid	Valine, leucine and isoleucine metabolism	0.88	0.84	0.87	0.94	0.47	0.62	0.64	0.65	0.79	1.25	0.81	1.12	0.86	0.72	0.91	0.92
isovalerylcarnitine	LC/MS Pos	Amino acid	Valine, leucine and isoleucine metabolism	0.24	1	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	0.24	1.27
kyurenine	LC/MS Pos	Amino acid	Tryptophan metabolism	1.12	0.34	1.71	0.34	0.34	0.34	1.29	0.34	0.85	0.34	1.07	1.56	0.82	0.72	0.94	0.55
lactate	GC/MS	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	0.94	0.93	1.39	1.03	0.44	0.39	0.53	0.45	0.73	0.94	0.82	0.98	0.49	0.47	0.62	0.53
lathosterol	GC/MS	Lipid	Sterol/Steroid	0.66	0.2	0.2	0.2	0.57	0.2	0.2	0.2	1.08	0.2	0.2	0.42	0.2	0.2	0.2	0.2
leucine	LC/MS Pos	Amino acid	Valine, leucine and isoleucine metabolism	0.88	0.84	0.87	0.92	0.47	0.62	0.61	0.65	0.76	1.22	0.8	1.12	0.79	0.86	0.95	0.92
lysine	GC/MS	Amino acid	Lysine metabolism	0.63	0.8	0.56	0.85	0.51	0.92	0.67	0.72	0.39	0.68	0.7	0.63	0.49	0.67	0.49	0.66
malate	GC/MS	Energy	Krebs cycle	1.8	2.27	2.57	2.09	0.59	0.62	0.57	0.77	0.99	1.63	1.03	1.35	0.64	0.63	0.79	0.65
methionine	LC/MS Pos	Amino acid	Cysteine, methionine, SAM, taurine metabolism	1.21	0.99	1.23	1.16	0.64	0.72	0.75	0.77	0.92	1.32	0.93	1.17	0.83	0.83	1	0.89
myo-inositol	GC/MS	Lipid	Inositol metabolism	0.65	0.62	0.81	0.64	0.27	0.25	0.25	0.27	0.25	0.39	0.31	0.32	0.22	0.19	0.23	0.19
N-acetyl-aspartyl-glutamate (NAAG)	LC/MS Pos	Amino acid	Glutamate metabolism	0.75	0.65	0.86	0.88	0.34	0.36	0.35	0.53	1	1.6	1.17	1.31	0.74	0.56	0.96	0.78
N-acetylaniline	LC/MS Neg	Amino acid	Alanine and aspartate metabolism	0.22	1.04	1.29	0.96	0.36	0.54	0.22	0.22	0.72	0.22	0.81	0.7	0.22	0.22	0.22	0.22
N-acetylaspartate (NAA)	GC/MS	Amino acid	Alanine and aspartate metabolism	1.15	1.49	1.25	1.17	0.5	0.42	0.45	0.28	0.97	1.41	1.32	1.44	0.65	0.84	0.99	0.83
N-acetylglutamate	LC/MS Neg	Amino acid	Glutamate metabolism	1.65	2.15	2.64	2.08	0.81	0.81	0.97	0.96	1.56	2.16	1.66	2.34	1.04	0.81	1.19	1.2
N-acetylglutamine	LC/MS Pos	Amino acid	Glutamate metabolism	0.29	0.29	1.13	0.29	0.29	0.29	0.29	0.29	0.75	0.79	0.87	0.29	0.29	0.29	0.29	0.29
N-acetylmethionine	LC/MS Neg	Amino acid	Cysteine, methionine, SAM, taurine metabolism	1.34	1.34	2.03	1.58	0.3	0.31	0.33	0.32	0.94	1.54	0.88	0.89	0.3	0.28	0.49	0.37
N-acetylneuraminate	GC/MS	Carbohydrate	Aminosugars metabolism	0.33	0.33	0.96	0.58	0.33	0.33	0.33	0.33	0.92	1.89	0.38	0.33	0.33	0.74	0.51	0.42
N-acetyls erine	GC/MS	Amino acid	Glycine, serine and threonine metabolism	1.54	0.11	1.42	0.69	0.31	0.33	0.11	0.48	0.68	1.71	1.32	0.8	0.4	0.33	0.45	0.26
N-acetylthreonine	LC/MS Neg	Amino acid	Glycine, serine and threonine metabolism	1.18	1.2	1.02	1.22	0.22	0.24	0.22	0.22	0.53	1.07	0.64	0.86	0.29	0.28	0.41	0.44
N-carbamoylaspartate	LC/MS Pos	Amino acid	Alanine and aspartate metabolism	1.24	1.2	2.61	1.61	0.46	0.46	0.46	0.46	0.74	0.82	0.81	1.52	0.46	0.69	0.46	0.51
nicotinamide	LC/MS Pos	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.94	1.47	1.9	0.64	0.69	0.8	1.14	0.62	0.91	1.26	1.24	1.38	0.72	0.81	1	1.01
nicotinamide adenine dinucleotide (NAD+)	LC/MS Pos	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	0.88	0.95	1.2	0.96	0.38	0.44	0.45	0.42	0.84	1.31	1.03	1.25	0.69	0.67	0.82	0.72
nicotinamide adenine dinucleotide reduced (NADH)	LC/MS Neg	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	1.89	1.86	1.89	2.17	0.43	1.03	0.77	0.97	1.46	5.18	1.9	2.84	0.93	1.59	1.07	1.98
ophthalmate	LC/MS Neg	Amino acid	Glutathione metabolism	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35
ornithine	GC/MS	Amino acid	Urea cycle; arginine-, proline-, metabolism	1.06	2.01	0.96	1.09	0.71	0.82	0.79	0.54	1.94	2.83	1.76	2.02	1.72	1.79	2.09	2.02
p-toluic acid	GC/MS	Amino acid	Phenylalanine & tyrosine metabolism	0.49	0.49	0.49	0.49	0.81	0.49	0.79	0.49	0.49	0.49	0.49	0.49	0.49	0.85	0.49	0.49
palmitoyl sphingomyelin	GC/MS	Lipid	Sphingolipid	6.93	1.07	1.3	0.96	0.54	0.52	0.54	0.48	0.82	1.02	0.85	1.12	0.6	0.69	0.62	0.72
pantothenate	LC/MS Pos	Cofactors and vitamins	Pantothenate and CoA metabolism	0.29	5.87	7	6.92	1.72	2.18	2.27	2.29	4	6.31	4.4	5.96	2.84	2.82	3.36	3.04
penicillin G	LC/MS Pos	Xenobiotics	Drug	1.07	0.99	1.12	1.14	1.34	1.44	1.54	1.72	0.82	0.95	0.74	1.09	1.44	1.23	1.44	1.46
phenol red	LC/MS Neg	Xenobiotics	Chemical	0.99	1.01	0.99	1.01	0.99	1.01	0.99	1.01	0.99	1.01	0.99	1.01	0.99	1.01	0.99	1.01
phenylacetylglucine	LC/MS Neg	Amino acid	Phenylalanine & tyrosine metabolism	0.72	0.65	0.89	0.69	0.24	0.4	0.36	0.29	0.52	1	0.46	0.41	0.27	0.32	0.42	0.32
phenylalanine	LC/MS Pos	Amino acid	Phenylalanine & tyrosine metabolism	0.8	0.77	0.82	0.88	0.39	0.59	0.54	0.64	0.79	1.18	0.76	1.17	0.76	0.77	0.8	0.86
phosphate	GC/MS	Energy	Oxidative phosphorylation	1.73	1.92	2.06	1.88	1.11	0.99	1.05	1.22	1.05	1.76	1.52	1.49	0.86	1.1	1.14	0.99
phosphoethanolamine	GC/MS	Lipid	Glycerolipid metabolism	0.3	0.58	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
pro-hydroxy-pro	LC/MS Pos	Peptide	Dipeptide	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
proline	LC/MS Pos	Amino acid	Urea cycle; arginine-, proline-, metabolism	1.69	1.91	2.18	1.99	0.85	1.01	0.99	0.9	1.11	1.68	1.3	1.59	0.99	0.91	1.24	1.06
propionylcarnitine	LC/MS Pos	Lipid	Fatty acid metabolism (also BCAA metabolism)	0.96	0.89	1.04	1.11	0.28	0.31	0.48	0.44	0.33	0.46	0.4	0.51	0.24	0.26	0.25	0.26
pseudouridine	LC/MS Neg	Nucleotide	Pyrimidine metabolism, uracil containing	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35	0.35
putrescine	GC/MS	Amino acid	Polyamine metabolism	1.16	1.38	0.98	0.91	0.23	0.43	0.42	0.37	1.45	2.75	2.01	2.23	0.98	1.4	1.29	1.02
pyridoxine (Vitamin B6)	LC/MS Neg	Cofactors and vitamins	Vitamin B6 metabolism	1.16	1.1	0.8	0.83	0.46	0.42	0.46	0.45	0.69	0.76	0.78	0.8	0.63	0.44	0.86	0.55
pyroglutamine*	LC/MS Pos	Amino acid	Glutamate metabolism	3.86	3.56	4.4	2.81	1.33	1.65	1.44	1.15	2.11	2.43	2.4	2.77	1.33	1.21	2.05	1.73
pyrophosphate (PPi)	GC/MS	Energy	Oxidative phosphorylation	2.07	1.87	0.97	1.29	0.07	0.29	0.57	0.29	1.01	1.2	0.45	0.92	0.47	0.57	0.67	0.47
ribitol	GC/MS	Carbohydrate	Nucleotide sugars, pentose metabolism	1.48	2.02	2.62	1.72	0.88	0.86	0.35	1.08	1.14	2.46	1.77	2.05	1.09	1.74	1.31	1.38
S-adenosylhomocysteine (SAH)	LC/MS Neg	Amino acid	Cysteine, methionine, SAM, taurine metabolism	2.68	2.22	3.44	3.18	0.4	0.67	0.51	0.4	1.84	4.01	2.19	3.48	0.69	0.97	0.95	0.95
S-lactoylglutathione	LC/MS Neg	Amino acid	Glutathione metabolism	1.35	1.9	1.36	2.08	0.13	0.13	0.13	0.13	0.94	1.08	0.65	1.12	0.13	0.13	0.13	0.13
scyllo-inositol	GC/MS	Lipid	Inositol metabolism	0.26	0.72	0.24	0.05	0.05	0.1	0.05	0.05	0.05	0.05	0.05	0.05	0.11	0.05	0.05	0.19
serine	GC/MS	Amino acid	Glycine, serine and threonine metabolism	0.68	0.88	0.9	0.68	0.58	0.46	0.5	0.52	0.59	0.78	0.6	0.61	0.67	0.65	0.82	0.73
sorbitol	GC/MS	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	2.44	1.38	1.72	1.63	1.27	0.94	0.63	1	3.64	5.46	3.86	4.17	10.13	6.49	10.62	5.22
sphingosine	LC/MS Pos	Lipid	Sphingolipid	3.63	0.31	4.22	0.31	1.4	0.31	0.86	0.31	1.63	2.78	2.23	0.31	1.67	0.31	0.31	0.31
streptomycin	LC/MS Pos	Xenobiotics	Drug	1.38	1.41	0.47	0.47	0.52	1.69	0.47	0.61	0.83	0.47	0.47	0.99	0.61	1	1.29	1.23
taurine	GC/MS	Amino acid	Cysteine, methionine, SAM, taurine metabolism	0.73	0.7	1.01	0.96	0.43	0.										