

Online Supporting Material

Supplemental Table 6. Stool metabolites that differed ($P \leq 0.10$) between C and U mice at d 16 of age¹

Metabolite	Method	FC	P	Q	Pathway
Kynurenate	LC/MS neg	3.22	0.0016	0.0146	Tryptophan metabolism
Taurolithocholate 3-sulfate	LC/MS neg	3.13	0.0011	0.0114	Bile acid metabolism
Oxamate	GC/MS	2.57	0.0079	0.0257	Chemical
Undecanedioate	LC/MS neg	2.51	6.05×10^{-5}	0.0023	Fatty acid, dicarboxylate
Agmatine	GC/MS	2.30	0.0235	0.0456	Polyamine metabolism
1-stearoylglycerophosphoinositol	LC/MS neg	2.29	0.0711	0.0813	Lysolipid
1-stearoylglycerophosphoglycerol	LC/MS neg	2.21	0.0178	0.0406	Lysolipid
Lathosterol	GC/MS	1.92	0.0012	0.0114	Sterol/Steroid
Myristate (14:0)	LC/MS neg	1.89	0.0073	0.0252	Long chain fatty acid
Laurate (12:0)	LC/MS neg	1.86	0.0575	0.071	Medium chain fatty acid
2-palmitoylglycerophosphoethanolamine	LC/MS neg	1.78	0.0632	0.0762	Lysolipid
Putrescine	GC/MS	1.68	0.0319	0.0558	Polyamine metabolism
1-palmitoylglycerophosphoethanolamine	LC/MS neg	1.63	0.0634	0.0762	Lysolipid
19-methylarachidic acid	GC/MS	1.61	0.0185	0.0406	Fatty acid, branched
Docosadienoate (22:2n6)	LC/MS neg	1.60	0.0243	0.0458	Long chain fatty acid
Pregnen-diol disulfate	LC/MS neg	1.52	0.0302	0.0547	Sterol/Steroid
D-urobilin	LC/MS pos	1.52	0.0603	0.0738	Hemoglobin and porphyrin metabolism
7-methylguanine	GC/MS	1.52	0.0872	0.0897	Purine metabolism, guanine containing
Heneicosanoate (21:0)	GC/MS	1.46	0.0729	0.0821	Long chain fatty acid
Erucate (22:1n9)	GC/MS	1.45	0.0369	0.0594	Long chain fatty acid
Arachidate (20:0)	GC/MS	1.43	0.0336	0.0573	Long chain fatty acid
N2-acetylysine	LC/MS pos	1.41	0.0235	0.0456	Lysine metabolism
Palmitate (16:0)	LC/MS neg	1.28	0.0167	0.0403	Long chain fatty acid
2-hydroxybutyrate (AHB)	GC/MS	1.26	0.0842	0.0897	Cysteine, methionine, SAM, taurine metabolism
Glutamate	LC/MS pos	0.86	0.038	0.0594	Glutamate metabolism
Creatine	LC/MS pos	0.81	0.034	0.0576	Creatine metabolism
Fucosterol	GC/MS	0.79	0.089	0.091	Sterol/Steroid
Adenine	GC/MS	0.79	0.0922	0.0934	Purine metabolism, adenine containing
Leucylglutamate	LC/MS pos	0.79	0.0956	0.0963	Dipeptide
Xanthine	LC/MS neg	0.78	0.0377	0.0594	Purine metabolism, (hypo)xanthine/inosine containing
Allo-threonine	GC/MS	0.77	0.0189	0.0406	Glycine, serine and threonine metabolism
Nicotinate	LC/MS neg	0.77	0.0498	0.0651	Nicotinate and nicotinamide metabolism
4-hydroxycinnamate	LC/MS neg	0.77	0.0798	0.0862	Phenylalanine & tyrosine metabolism
Proline	LC/MS pos	0.76	0.0258	0.0477	Urea cycle; arginine-, proline-, metabolism
β -hydroxypyruvate	GC/MS	0.76	0.0969	0.0965	Glycine, serine and threonine metabolism
Pyridoxamine	LC/MS pos	0.75	0.0472	0.0642	Vitamin B6 metabolism
Lactate	GC/MS	0.75	0.0773	0.0847	Glycolysis, gluconeogenesis, pyruvate metabolism
Taurine	GC/MS	0.74	0.0552	0.0699	Cysteine, methionine, SAM, taurine metabolism
Glycerate	GC/MS	0.74	0.0742	0.0828	Glycolysis, gluconeogenesis, pyruvate metabolism
Myo-inositol	GC/MS	0.74	0.0749	0.0831	Inositol metabolism
N-acetylaspartate (NAA)	LC/MS neg	0.73	0.027	0.0493	Alanine and aspartate metabolism
Aspartyllleucine	LC/MS pos	0.73	0.0476	0.0642	Dipeptide
Phenylalanylsoleucine	LC/MS pos	0.73	0.0703	0.0808	Dipeptide
Glycylsoleucine	LC/MS pos	0.73	0.0757	0.0834	Dipeptide
Homoserine	GC/MS	0.73	0.0801	0.0862	Glycine, serine and threonine metabolism
Uracil	GC/MS	0.73	0.0867	0.0897	Pyrimidine metabolism, uracil containing
Deoxycarnitine	LC/MS pos	0.72	0.0002	0.0072	Carnitine metabolism
Methionine sulfoxide	LC/MS pos	0.72	0.0061	0.0236	Cysteine, methionine, SAM, taurine metabolism
2-hydroxyglutarate	GC/MS	0.72	0.0573	0.071	Fatty acid, dicarboxylate
Mannose	GC/MS	0.72	0.0685	0.0798	Fructose, mannose, galactose, starch, sucrose metabolism
Ribose	GC/MS	0.72	0.0868	0.0897	Nucleotide sugars, pentose metabolism
Glycerol 3-phosphate (G3P)	GC/MS	0.71	0.0437	0.0631	Glycerolipid metabolism

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Trans-urocanate	LC/MS pos	0.71	0.0663	0.078	Histidine metabolism
N6-acetyllysine	LC/MS pos	0.71	0.0982	0.0972	Lysine metabolism
Pipecolate	GC/MS	0.70	0.0394	0.0598	Lysine metabolism
Alanine	GC/MS	0.70	0.0517	0.0669	Alanine and aspartate metabolism
Homocysteine	GC/MS	0.70	0.0656	0.0778	Cysteine, methionine, SAM, taurine metabolism
Vanillate	GC/MS	0.70	0.0732	0.0821	Food component/Plant
Hypotaurine	GC/MS	0.70	0.0799	0.0862	Cysteine, methionine, SAM, taurine metabolism
γ -glutamylthreonine	LC/MS pos	0.69	0.0129	0.0353	γ -glutamyl
Histidine	LC/MS neg	0.69	0.024	0.0456	Histidine metabolism
Linoleate (18:2n6)	LC/MS neg	0.69	0.047	0.0642	Essential fatty acid
Conjugated linoleate (18:2n7; 9Z,11E)	GC/MS	0.69	0.0563	0.0709	Long chain fatty acid
3-(4-hydroxyphenyl)lactate	LC/MS neg	0.69	0.0716	0.0813	Phenylalanine & tyrosine metabolism
Serine	GC/MS	0.69	0.0866	0.0897	Glycine, serine and threonine metabolism
Tyrosylisoleucine	LC/MS pos	0.69	0.0919	0.0934	Dipeptide
γ -glutamyltyrosine	LC/MS pos	0.68	0.0024	0.016	γ -glutamyl
γ -glutamylglutamate	LC/MS pos	0.68	0.0057	0.0236	γ -glutamyl
α -tocopherol	GC/MS	0.68	0.0078	0.0257	Tocopherol metabolism
Phenylalanine	LC/MS pos	0.68	0.0123	0.0341	Phenylalanine & tyrosine metabolism
4-hydroxymandelate	GC/MS	0.68	0.0328	0.0565	Benzoate metabolism
Isoleucine	LC/MS pos	0.67	0.0217	0.045	Valine, leucine and isoleucine metabolism
Glycylvaline	LC/MS pos	0.67	0.032	0.0558	Dipeptide
Urate	GC/MS	0.67	0.0483	0.0642	Purine metabolism, urate metabolism
Cytosine	GC/MS	0.67	0.0567	0.0709	Pyrimidine metabolism, cytidine containing
1-linoleoylglycerol (1-monolinolein)	GC/MS	0.67	0.0624	0.076	Monoacylglycerol
Phenylalanylglutamate	LC/MS pos	0.67	0.0856	0.0897	Dipeptide
N-acetylglucosamine	GC/MS	0.67	0.0963	0.0964	Aminosugars metabolism
Pyridoxal	LC/MS pos	0.66	0.0018	0.0146	Pyridoxal metabolism
3,4-dihydroxybenzoate	GC/MS	0.66	0.0435	0.0631	Benzoate metabolism
2-aminopentanoate	GC/MS	0.66	0.0443	0.0634	Lysine metabolism
Fumarate	GC/MS	0.66	0.0648	0.0774	Krebs cycle
Tyrosylleucine	LC/MS pos	0.66	0.07	0.0808	Dipeptide
Adenosine	LC/MS pos	0.65	0.0027	0.0163	Purine metabolism, adenine containing
Tryptophan	LC/MS pos	0.65	0.0187	0.0406	Tryptophan metabolism
Glycylleucine	LC/MS pos	0.65	0.0259	0.0477	Dipeptide
N-acetylserine	GC/MS	0.65	0.0396	0.0598	Glycine, serine and threonine metabolism
Glycerol 2-phosphate	GC/MS	0.65	0.0552	0.0699	Chemical
γ -glutamylphenylalanine	LC/MS pos	0.64	0.002	0.0146	γ -glutamyl
N-acetylneuraminate	LC/MS pos	0.64	0.0089	0.0284	Aminosugars metabolism
2-hydroxystearate	LC/MS neg	0.64	0.0136	0.0366	Fatty acid, monohydroxy
Glycerol	GC/MS	0.64	0.0187	0.0406	Glycerolipid metabolism
γ -glutamylmethionine	LC/MS pos	0.63	0.0045	0.0222	γ -glutamyl
Glycylglycine	GC/MS	0.63	0.017	0.0405	Dipeptide
Diaminopimelate	GC/MS	0.63	0.0415	0.0613	Lysine metabolism
N-acetylmethionine	LC/MS neg	0.63	0.0452	0.0642	Cysteine, methionine, SAM, taurine metabolism
Tyrosine	LC/MS pos	0.62	0.0024	0.016	Phenylalanine & tyrosine metabolism
Valine	LC/MS pos	0.62	0.0111	0.0323	Valine, leucine and isoleucine metabolism
Cis-vaccenate (18:1n7)	GC/MS	0.62	0.0114	0.0327	Long chain fatty acid
Pyruvate	GC/MS	0.62	0.0159	0.039	Glycolysis, gluconeogenesis, pyruvate metabolism
Galactose	GC/MS	0.62	0.0495	0.0651	Fructose, mannose, galactose, starch, sucrose metabolism
Glycylproline	LC/MS pos	0.61	0.0009	0.0114	Dipeptide
Methionine	LC/MS pos	0.61	0.0098	0.0293	Cysteine, methionine, SAM, taurine metabolism
Methylphosphate	GC/MS	0.61	0.0147	0.0374	Purine and pyrimidine metabolism
4-hydroxyphenylpyruvate	LC/MS neg	0.61	0.0371	0.0594	Phenylalanine & tyrosine metabolism
3-phenylpropionate (hydrocinnamate)	GC/MS	0.61	0.0377	0.0594	Phenylalanine & tyrosine metabolism
Arginylisoleucine	LC/MS pos	0.61	0.0478	0.0642	Dipeptide
Aspartate	GC/MS	0.61	0.0482	0.0642	Alanine and aspartate metabolism
Leucine	LC/MS pos	0.60	0.0074	0.0252	Valine, leucine and isoleucine metabolism

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Phosphoethanolamine	GC/MS	0.60	0.0206	0.0432	Glycerolipid metabolism
N-acetyl muramate	LC/MS neg	0.60	0.036	0.0593	Fructose, mannose, galactose, starch, sucrose metabolism
Fucose	GC/MS	0.60	0.0395	0.0598	Aminosugars metabolism
Syringic acid	GC/MS	0.60	0.0398	0.0598	Food component/Plant
Threonylsoleucine	LC/MS pos	0.59	0.0478	0.0642	Dipeptide
Hexadecanedioate	LC/MS neg	0.58	0.001	0.0114	Fatty acid, dicarboxylate
γ -glutamylleucine	LC/MS pos	0.58	0.0019	0.0146	γ -glutamyl
γ -tocopherol	GC/MS	0.57	0.0231	0.0456	Tocopherol metabolism
Ornithine	GC/MS	0.57	0.05	0.0651	Urea cycle; arginine-, proline-, metabolism
Histidylvaline	LC/MS pos	0.57	0.0534	0.0686	Dipeptide
O-acetylserine	GC/MS	0.57	0.0666	0.078	Glycine, serine and threonine metabolism
Sorbitol	GC/MS	0.56	1.02 x 10 ⁻⁵	0.0006	Fructose, mannose, galactose, starch, sucrose metabolism
3-hydroxypyridine	GC/MS	0.56	0.0003	0.0072	Chemical
Glycyltyrosine	LC/MS pos	0.56	0.0062	0.0236	Dipeptide
Glucose	GC/MS	0.56	0.0074	0.0252	Glycolysis, gluconeogenesis, pyruvate metabolism
Tryptophylleucine	LC/MS pos	0.56	0.0319	0.0558	Dipeptide
Histidylsoleucine	LC/MS pos	0.55	0.0096	0.0293	Dipeptide
Thymine	GC/MS	0.55	0.0238	0.0456	Pyrimidine metabolism, thymine containing
2-deoxyribose	GC/MS	0.55	0.0356	0.0591	Nucleotide sugars, pentose metabolism
N-acetylmannosamine	GC/MS	0.55	0.0369	0.0594	Aminosugars metabolism
Sarcosine (N-Methylglycine)	GC/MS	0.54	0.0146	0.0374	Glycine, serine and threonine metabolism
3-methyl-2-oxobutyrate	LC/MS neg	0.54	0.0172	0.0405	Valine, leucine and isoleucine metabolism
2-hydroxypalmitate	LC/MS neg	0.54	0.0422	0.062	Fatty acid, monohydroxy
Campesterol	GC/MS	0.53	0.0034	0.0179	Sterol/Steroid
Linolenate [α or γ ; (18:3n3 or 6)]	LC/MS neg	0.53	0.0236	0.0456	Essential fatty acid
Phenylalanyl aspartate	LC/MS pos	0.53	0.0461	0.0642	Dipeptide
Val-val-val	LC/MS pos	0.52	0.0011	0.0114	Polypeptide
4-methylthio-2-oxobutanoate	GC/MS	0.52	0.0062	0.0236	Cysteine, methionine, SAM, taurine metabolism
β -tocotrienol	GC/MS	0.52	0.0139	0.0369	Tocopherol metabolism
4-hydroxy-2-oxogluutaric acid	GC/MS	0.52	0.0159	0.039	Fatty acid, dicarboxylate
2-oleoylglycerol (2-monolein)	GC/MS	0.52	0.0188	0.0406	Monoacylglycerol
Tyrosylvaline	LC/MS pos	0.52	0.0455	0.0642	Dipeptide
Isobar: betaine aldehyde, N-methyldiethanolamine	LC/MS pos	0.52	0.0854	0.0897	Glycine, serine and threonine metabolism
Tyrosylglutamate	LC/MS pos	0.51	0.0181	0.0406	Dipeptide
2-linoleoylglycerol (2-monolinolein)	GC/MS	0.51	0.0352	0.0591	Monoacylglycerol
α -hydroxyisovalerate	GC/MS	0.50	0.0031	0.0178	Valine, leucine and isoleucine metabolism
N-acetylgalactosamine	GC/MS	0.50	0.022	0.0451	Aminosugars metabolism
3-methyl-2-oxovalerate	LC/MS neg	0.50	0.0223	0.0451	Valine, leucine and isoleucine metabolism
Histidylleucine	LC/MS pos	0.50	0.0312	0.0558	Dipeptide
Lysylvaline	LC/MS pos	0.50	0.041	0.061	Dipeptide
L-uroporphobilin	LC/MS pos	0.49	0.0175	0.0406	Hemoglobin and porphyrin metabolism
Phenylpyruvate	LC/MS neg	0.48	0.0051	0.0236	Phenylalanine & tyrosine metabolism
Dihydrocholesterol	GC/MS	0.48	0.0052	0.0236	Sterol/Steroid
Xylulose	GC/MS	0.48	0.0102	0.0301	Nucleotide sugars, pentose metabolism
3,4-dihydroxyphenylacetate	GC/MS	0.48	0.0151	0.0381	Phenylalanine & tyrosine metabolism
4-methyl-2-oxopentanoate	LC/MS neg	0.47	0.0141	0.0369	Valine, leucine and isoleucine metabolism
γ -glutamylsoleucine	LC/MS pos	0.46	0.0004	0.0087	γ -glutamyl
Phenyllactate (PLA)	LC/MS neg	0.46	0.0033	0.0179	Phenylalanine & tyrosine metabolism
Lysylsoleucine	LC/MS pos	0.46	0.0067	0.0251	Dipeptide
Hyocholate	LC/MS neg	0.46	0.0071	0.0252	Bile acid metabolism
Campestanol	GC/MS	0.45	0.0004	0.0087	Food component/Plant
Cytidine	LC/MS pos	0.45	0.0036	0.0179	Pyrimidine metabolism, cytidine containing
Cholatole	LC/MS neg	0.45	0.02	0.0422	Bile acid metabolism
Lysylleucine	LC/MS pos	0.44	0.0019	0.0146	Dipeptide
Oleic ethanolamide	LC/MS neg	0.44	0.0119	0.0335	Endocannabinoid
5 α -pregnan-3 α ,20 β -diol disulfate 1	LC/MS neg	0.44	0.0394	0.0598	Sterol/Steroid

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Ribulose	GC/MS	0.43	0.0075	0.0252	Nucleotide sugars, pentose metabolism
2-hydroxy-3-methylvalerate	GC/MS	0.41	0.0006	0.0112	Valine, leucine and isoleucine metabolism
3-dehydrocholate	LC/MS pos	0.41	0.0026	0.0163	Bile acid metabolism
α -ketoglutarate	GC/MS	0.40	0.0091	0.0287	Krebs cycle
Sitostanol	GC/MS	0.39	0.0011	0.0114	Food component/Plant
Iduronic acid	GC/MS	0.39	0.003	0.0175	Aminosugars metabolism
Arginine	LC/MS pos	0.38	0.0051	0.0236	Urea cycle; arginine-, proline-, metabolism
α -glutamyllysine	GC/MS	0.38	0.0059	0.0236	Dipeptide
α -hydroxyisocaproate	GC/MS	0.36	0.0014	0.0127	Valine, leucine and isoleucine metabolism
12,13-hydroxyoctadec-9(Z)-enoate	LC/MS neg	0.36	0.002	0.0147	Fatty acid, dihydroxy
Ferulate	LC/MS neg	0.36	0.0053	0.0236	Food component/Plant
Biliverdin	LC/MS pos	0.36	0.0872	0.0897	Hemoglobin and porphyrin metabolism
β -muricholate	LC/MS pos	0.34	0.0027	0.0163	Bile acid metabolism
3-(3-hydroxyphenyl)propionate	GC/MS	0.34	0.0094	0.0292	Phenylalanine & tyrosine metabolism
3-(4-hydroxyphenyl)propionate	GC/MS	0.33	0.0011	0.0114	Phenylalanine & tyrosine metabolism
2-oxindole-3-acetate	LC/MS pos	0.29	0.0059	0.0236	Food component/Plant
Dihydroferulic acid	LC/MS neg	0.26	0.0007	0.0113	Food component/Plant
Arabinose	GC/MS	0.25	0.0055	0.0236	Nucleotide sugars, pentose metabolism
Leu-leu-leu	LC/MS pos	0.24	2.70×10^{-6}	0.0003	Polypeptide
α -muricholate	LC/MS pos	0.22	0.0007	0.0113	Bile acid metabolism
Chenodeoxycholate	LC/MS neg	0.20	3.71×10^{-5}	0.0017	Bile acid metabolism
Xylose	GC/MS	0.18	0.0035	0.0179	Nucleotide sugars, pentose metabolism
Deoxycholate	LC/MS neg	0.06	3.49×10^{-6}	0.0003	Bile acid metabolism

¹C, control mice; FC, fold-change for concentration of metabolites derived from U mice in relation to C; GC, gas chromatography; LC, liquid chromatography; MS, mass spectrometry; P, P value; Q, Q value; U, undernourished mice.