Table S1 NMR data for metabolites detected in feces on day 42

| Keys | Metabolites | $\delta^{1}H$ (ppm) | $\delta^{13}C$ (ppm) |
|---|---|---|---|
| F1 | 1,3-Dihydroxyacetone | 4.420(s), 3.571(s) | 67.5 |
| F2 | 2-Ketoisovalerate | 1.130(d), 3.027(m) | 18.8, 39.5 |
| F3 | 3-Methyl-2-ketovalerate | 0.888(t), 1.102(d), 1.461(m), 1.731(m), 2.939(m) | 13.3 |
| F4 | 3-Methyl-2-oxovalerate | 0.898(t), 1.103(d), 1.448(m), 1.671(m), 2.926(m) | 13.2, 16.4, 26.8, 26.8, 45.9 |
| F5 | 5-Aminovalerate | 1.620(m), 1.650(m), 2.240(t), 3.021(t) | 25.6, 29.7, 39.3, 41.4 |
| F6 | Acetate | 1.924(s) | 26.5 |
| F7 | Adenine | 8.190(s), 8.211(s) | 144.2, 156.2 |
| F8 | Alanine | 1.488(d), 3.787(m) | 18.3, 53.3 |
| F9 | Arginine | 1.698(m), 1.925(m), 3.248(t), 3.760(t) | 30.5,30.5,44.6,57.5 |
| F10 | Aspartate | 2.683(dd), 2.80(dd), 3.91(dd) | 39.3, 39.3, 55.1 |
| F11 | Butyrate | 0.903(t), 1.561(m), 2.157(t) | 16.0, 22.1, 42.3 |
| F12 | Cadaverine | 1.483(d), 1.724(m), 3.022(t) | 25.9, 29.4, 41.4 |
| F13 | Caproate | 0.887(t),1.309(m), 1.556(m), 2.178(t) | 16.2,32.6,23.6,29.1,39.5 |
| F14 | Choline | 3.204(s), 3.519(t), 4.061(m) | 56.9, 70.1, 58.2 |
| F15 | Citrulline | 1.57(m), 1.88(m), 3.149(m), 3.665(m) | —, —, 42.0, 57.9 |
| F16 | Creatine | 3.050(s), 3.929(s) | 40.1, 56.2 |
| F17 | Deoxycholic Acid | 0.720(s) | — |
| F18 | Ethanolamine | 3.134(d), 3.817(d) | 45.4, 60.2 |
| F19 | Fatty acids and fatty acyl chains | 0.882(t) | 16.8 |
| F20 | Formate | 8.463(s) | 172.0 |
| F21 | Fumarate | 6.524(s) | 137.5 |
| F22 | Glutamine | 2.155(m), 2.447(m), 3.773(t) | 29.53, 32.96, 57.10 |
| F23 | Glutarate | 2.181(t) | —, 39.44 |
| F24 | Glycine | 3.570(s) | 44.5 |
| F25 | Hypoxanthine | 8.197(s), 8.216(s) | 149.4, 143.2 |
| F26 | Isocaproate | 0.882(d), 1.449(m), 1.483(d), 2.191(t) | —, 37.56, 30.7, 39.3 |
| F27 | Isoleucine | 0.943(t), 1.00(d), 1.267(m), 1.470(m), 1.984(m), 3.676(d) | 14.7, 17.2, 26.8, 26.8, 62.4 |
| F28 | Lactate | 1.34(d), 4.123(d） | 22.9, 71.4 |
| F29 | Leucine | 0.96(d), 0.97(d), 1.696(m), 1.721(m), 1.738(m), 3.740(m) | 23.4, 24.3, 26.6, 56.9 |
| F30 | Lycine | 1.483(m), 1.724(m), 1.896(m), 3.027(t), 3.765(t) | 23.44, 29.72, —, 41.5, 57.58 |
| F31 | Malonate | 3.110(s) | 50.1 |
| F32 | Mcthylamine | 2.618(s) | 27.6 |
| F33 | Methanol | 3.356(s) | 51.2 |

| | | | |
|---|---|---|---|
| F34 | Methionine | 2.146(s), 2.202(m), 2.646(t), 3.864(m) | 16.0, 31.3, 29.4,56.7 |
| F35 | Methylsuccinate | 1.104(d), 2.130(d), 2.633(m) | 20.68, 44.43, — |
| F36 | N, N-Dimethylglycine | 2.920(s), 3.714(s) | 46.1, 62.2 |
| F37 | N-Acety-glycoprotein | 2.032(s) | 24.5 |
| F38 | N-Acetyl group contained glycoprotrin | 2.042(s), 2.080(s) | — |
| F39 | N-Acetyl-D-glucosamine | 3.760(m), 3.872(m), 5.211(d) | — |
| F40 | N-Heptanoate | 1.556(m) | 30.2 |
| F41 | Nicotinate | 7.532(dd), 8.160(m), 8.617(dd), 8.946(s) | — |
| F42 | Phenylacetate | 3.542(s), 7.317(m), 7.375(m) | 47.2, 129.6, 131.1 |
| F43 | Phenylalanine | 3.131(dd), 3.290(dd), 3.982(dd), 7.330(m), 7.380(m), 7.430(m) | 38.9, 38.9, 58.9, 132.2, 129.8, 131.9 |
| F44 | 4-Hydroxyphenylacetate | 3.453(s), 6.867(d), 7.203(d) | 46.9, 118.2, 133.4 |
| F45 | Proline | 2.007(m), 2.070(dd), 2.357(m), 3.336(m), 3.462(d), 4.125(m) | 25.8, 32.1, 48.7, 48.7, 63.5 |
| F46 | Propionate | 1.060(t), 2.187(q) | 12.9, 33.3 |
| F47 | Pyruvate | 2.377(s) | 29.5 |
| F48 | Sarcosine | 2.704(s), 3.597(s) | 34.8, 53.7 |
| F49 | Serine | 3.828(dd), 3.949(dd), 3.981(dd) | 59.32, —, — |
| F50 | Succinate | 2.410(s) | 37.3 |
| F51 | Taurine | 3.259(t), 3.437(t) | 49.5, 37.5 |
| F52 | Taurochenodeoxycholate | 0.675(s), 0.960(s） | — |
| F53 | Taurocholic Acid (TCA) | 0.671(s) | —, 77.1 |
| F54 | Tayricholic | 0.671(s), 1.043(s), 1.354(m), 1.410(m), 1.730(m), 2.22(m), 2.30(m), 3.086(t), 3.574(m) | — |
| F55 | Tauro-β-Muricholic Acid (TβMCA) | 0.693(s) | — |
| F56 | Threonine | 1.338(d), 3.590(d), 4.258(m) | 23.5, 63.2, 68.2 |
| F57 | Trimethylamine | 2.880(s) | 47.4 |
| F58 | Trimethylamine N-Oxide | 3.261(s) | 61.5 |
| F59 | Tryptophan | 7.203(m), 7.289(m), 7.31(s), 7.548(m), 7.741(m) | 122.3, 124.9, 128.0, 115.2, 121.3, 92.5 |
| F60 | Tyrosine | 3.050(dd), 3.194(dd), 3.943(dd), 6.904(m), 7.196(m) | 37.9, 37.8, 59.4, 118.8, 133.4 |
| F61 | Uracil | 5.805(d), 7.540(d) | 104.2, 146.2 |
| F62 | Urocanate | 6.400(d), 7.310(d), 7.431(s), 7.894(s), | 133.4, 124.7, 141.4, 134.2 |
| F63 | Valerate | 0.899(t), 1.309(m), 2.178(d) | 16.4, 23.9, 39.6 |
| F64 | Xanthine | 7.900(s) | 141.8 |
| F65 | α-Arabinose | 5.213(d), 5.300(d), 4.510(d), 4.100(m), 3.890(m), | —, —, 72.3, 66.3, 93.9 |

| | | | |
|---|---|---|---|
| | | 3.663(m) | |
| F66 | α-Galactose | 3.816(m), 3.862(m), 3.998(m), 5.273(d) | 71.7, 73.3, 72.5, —, 95.3 |
| F67 | α-Glucose | 3.406(m), 3.590(dd), 3.733(m), 3.733(m), 3.846(m), 3.846(m), 5.520(d) | 72.4, 74.3, 75.4, —, —, 75.2, 94.9 |
| F68 | α-Ketoglutarat | 2.452(t), 3.010(t) | — |
| F69 | α-Ketoglutarate | 2.443(t), 3.011(t) | 33.4, 38.3 |
| F70 | α-Ketoisocaproate | 0.920(d), 2.066(m), 2.616(d) | — |
| F71 | α-Ketoisovalerate | 1.130(d), 3.020(m) | 18.8, 39.5 |
| F72 | α-Keto-β-methyl-valerate | 0.887(t), 1.104(d), 1.687(m), 2.923(m) | — |
| F73 | α-L-Fucose | 1.201(d), 3.771(m), 3.771(m), 3.872(m), 4.202(m), 5.211(d) | 17.8, 72.8, 72.8, 95.6 |
| F74 | α-Xylose | 5.190(d), 4.571(d), 3.922(q), 3.521(dd), 3.430(t), 3.316(t) | 99.7 |
| F75 | β-Arabinose | 3.520(dd), 3.670(t), 3.951(m), 3.863(dd), 4.522(d) | —, —, 72.3, 66.3, 93.9 |
| F76 | β-Galactose | 3.493(dd), 3.656(m), 3.937(m), 4.592(d) | 71.7, 73.3, 72.5, —, 95.3 |
| F77 | β-Glucose | 3.294(m), 3.515(m), 3.743(m), 3.909(dd), 4.656(d) | —, —, —, 63.26, 63.26, 98.3 |
| F78 | β-L-Fucose | 1.250(d), 3.452(m), 3.644(m), 3.805(m), 3.805(m), 4.562(d) | 17.8, 72.8, 72.8, 95.6 |

"—": The corresponding $^{13}C$ shift values are not found in the HSQC spectra, and the metabolites without $^{13}C$ shift values were assigned only based on the $^{1}H$ shift in the TOCSY spectrum.

Table S2 NMR data for metabolites detected in urine on day 42

| Keys | Metabolites | $\delta^{1}$H (ppm) | $\delta^{13}$C (ppm) |
|---|---|---|---|
| U1 | 2-Hydroxy-3-methylvalerate | 0.807(t), 0.931(d), 1.152(m), 1.353(m), 1.752(m), 3.876(d) | — |
| U2 | 2-Hydroxybutyrate | 0.899(m), 1.689(m), 3.996(d) | 10.7, 29.5, —, 76.1 |
| U3 | 2-Hydroxyisobutyrate | 1.143(s) | 30.0 |
| U4 | 2-Ketoglutarate | 2.440(t), 3.010(t) | 32.5, 40.4, 184.4, 208.1 |
| U5 | 2-Ketoisovalerate | 1.110(d), 3.020(m) | 18.8, 39.5 |
| U6 | 2-Methylglutarate | 1.071(d), 1.602(m), 1.754(m), 2.150(t), 2.240(m) | — |
| U7 | 2-Oxoglutarate | 2.431(t), 3.004(t) | 33.2, 39.0 |
| U8 | 3-Hydroxyisobutyrate | 1.061(d), 2.487(m), 3.525(m), 3.714(m) | 19.5, —, —, — |
| U9 | 3-Hydroxyisovalerate | 1.270(s), 2.380(s) | 30.2, 51.6 |
| U10 | 3-Methyl-2-oxovalerate | 0.899(t), 1.103(d), 1.438(m), 1.662(m), 2.928(m) | 13.2, 16.4, 26.8, 26.8, 45.9 |
| U11 | p-Cresol glucuronide | 7.231(d), 7.062(d), 2.301(s) | 22.3, 123.2, 135.6 |
| U12 | 4-Hydroxyphenylacetate | 6.871(d), 7.160(d), 3.451(s) | 46.9, 118.2, 133.4 |
| U13 | 5-Aminovalerate | 1.624(t), 1.650(t), 2.237(m), 3.022(m) | 25.6, 29.7, 39.3, 41.4 |
| U14 | Acetamide | 2.035(s) | 25.0 |
| U15 | Acetate | 1.921(s) | 26.5 |
| U16 | Acetoacetate | 2.270(s), 3.444(s), 2.372(s) | 32.3, — |
| U17 | Acetone | 2.240(s) | 28.2 |
| U18 | Acetylcarnitine | 2.151(s), 2.504(m), 2.631(m), 3.202(s), 3.621(d), 3.829(dd) | 22.4, 44.0, 44.0, 57.5, 70.9,70.9 |
| U19 | Adenine | 8.195(s), 8.213(s) | 144.3, 156.5 |
| U20 | Adipate | 2.192(t), 1.547(m) | — |
| U21 | Alanine | 3.785(q), 1.480(d) | 18.3, 53.3 |
| U22 | Allantoate | 5.290(s) | — |
| U23 | Allothreonine | 1.191(d), 4.265(m), 3.843(d) | 22.0,70.2 |
| U24 | Arginine | 3.778(m), 1.934(m), 1.735(m), 3.257(t) | 30.5, 30.5, 44.6, 57.5 |
| U25 | Aspartate | 2.666(dd), 2.805(dd), 3.900(dd) | 39.3, 39.3, 55.1 |
| U26 | Betaine | 3.273(s), 3.902(s) | 57.0, 68.0 |
| U27 | Butyrate | 0.940(t), 2.180(t), 1.588(m) | 16.0, 22.1, 42.3 |
| U28 | Cadaverine | 1.483(d), 1.724(m), 3.022(t) | 25.9, 29.4, 41.4 |
| U29 | Caproate | 0.887(t), 1.309(m), 1.556(m), 2.178(t) | 16.23, 32.69, 23.66, 29.05, 39.54 |
| U30 | Carnitine | 2.410(t), 3.230(s), 3.405(m), 4.554(m) | —, 57.51, 71.6, 66.38 |
| U31 | Choline | 3.211(s), 3.538(m), 4.076(m) | 57.2, 70.3, 57.2 |
| U32 | Citrate | 2.541(d), 2.660(d) | 46.5, 76.4, 181.5 |

| | | | |
|---|---|---|---|
| U33 | Creatine | 3.040(s), 3.933(s) | 40, 56.9, 160, 177.6 |
| U34 | Creatine phosphate | 3.032(s), 3.940(s) | 40.1, 56.2 |
| U35 | Creatinine | 3.050(s), 4.060(s) | 33.2, 59.2, 172.1, 191.9 |
| U36 | Cysteine | 3.051(s), 3.982(dd) | 27.8, 63.1 |
| U37 | Deoxycytidine | 6.270(t), 2.360(dd), 7.820(d), 6.052(d) | —, —, —, 145.7 |
| U38 | Desaminotyrosine | 2.463(t), 2.835(t), 6.859(d), 7.191(d) | 42.87, 33.72, 118.54, 132.6 |
| U39 | Dimethyl sulfone | 3.940(s) | — |
| U40 | Dimethylamine | 2.721(s) | 37.8 |
| U41 | Dimethylglycine | 2.921(s), 3.720(s) | 40.4, 62.6, 173.1 |
| U42 | Ethanol | 1.185(t), 3.656(q) | 19.54, — |
| U43 | Ethanolamine | 3.1349(d), 3.817(d) | 44.4, 60.2 |
| U44 | Formate | 8.461(s) | 172, — |
| U45 | Fucose | 1.250(d), 3.816(m), 5.214(d), 3.770(m) | 18.6, 73, 94.8, — |
| U46 | Fumarate | 6.920(s) | 138.6, 177.7 |
| U47 | Galactarate | 3.953(s), 4.160(s) | — |
| U48 | Galactonate | 4.260(s) | — |
| U49 | Glucuronate | 3.574(dd), 3.724(m), 4.070(d), 4.642(d), 5.243(d) | — |
| U50 | Glutamate | 3.781(t), 2.060(m), 2.358(m) | 57.7, 29.9, 36.8, 178 |
| U51 | Glutamine | 2.142(m), 2.463(m), 3.770(t) | 57.2, 29, 34, 175.4, 180.5 |
| U52 | Glutarate | 2.181(t) | 26.15, 39.44 |
| U53 | Glycerate 3-phosphate | 4.225(m), 4.064(d), 3.843(d) | 80.0, —, 64.5 |
| U54 | Glycerol | 3.551(t), 3.634(m), 3.767(m) | — |
| U55 | Glycerophosphocholine | 3.223(s), 3.689(m), 3.925(m), 4.317(dd) | 55.9,68.1,73.9,64.4 |
| U56 | Glycine | 3.563(s) | 44.4, 175.6 |
| U57 | Glycogen | 5.290(d), 3.600(d), 3.890(d), 3.700(dd), 3.863(d), 3.464(dd) | 102.6, 74.7, 63.8, 65.4, 63.6, 72.5 |
| U58 | Glycolate | 3.941(s) | 64.2 |
| U59 | Glycylproline | 3.941(s), 3.880(d) | 49.0, 42.7 |
| U60 | GPC | 3.241(s), 3.694(d), 4.139(m) | 56.9, 69.1, 62.5 |
| U61 | GSSG | 3.789(m), 2.554(m), 2.177(m), 3.320(dd), 4.660(t) | 56.4, 34.2, 29.7, 177.2. 41.9, 41.9, |
| U62 | Guanidoacetate | 3.800(s) | 47.7, 160.3, 178.3 |
| U63 | Guanine | 7.891(s) | 145.5, 168.5, 156.4, 81.8 |
| U64 | Hippurate | 3.961(d), 7.540(t), 7.620(t), 7.820(t), 8.521(s) | 132.1, 135.5, 130.2, 47.2 |
| U65 | Hypotaurine | 3.360(t), 2.662(t) | 37, 58.5 |

| | | | |
|---|---|---|---|
| U66 | Hypoxanthine | 8.201(s) | 145.6 |
| U67 | Indole-3-acetate | 3.681(s), 7.161(t), 7.216(t), 7.507(d), 7.635(d) | 36.65, 121.26, 126.49, 114.38, 121.37 |
| U68 | Isobutyrate | 1.053(d), 2.382(m) | 22.04, 39.32 |
| U69 | Isocaproate | 0.882(d), 1.449(m), 1.483(d), 2.191(t) | —, 37.57, —, 39.33 |
| U70 | Isoleucine | 0.936(t), 0.995(d), 1.249(m), 1.452(m),1.971(m), 3.655(d) | 62.3, 38.6, 27.5, 27.5, 17.9, 20.9, 178.1 |
| U71 | Isovalerylglycine | 0.925(d), 1.994(m), 2.166(d), 3.746(d) | 24.37, 30.2, 46.93, — |
| U72 | Ketoleucine | 0.944(s), 2.080(m), 2.817(d) | 24.32, 26.2, — |
| U73 | Lactate | 4.113(q), 1.332(d) | 71.4, 23.1, 185.5 |
| U74 | Lactose | 5.222(d), 4.676(d), 3.295(t) | 104.59, 98.91, — |
| U75 | Leucine | 3.751(d), 1.782(s), 1.590(m), 0.972(d) | 60.3, 42.8, 27.5, 24.6, 178.3 |
| U76 | Lysine | 3.761(t), 3.030(t), 1.626(m) | 64.1, 42.2, 33.4, 177 |
| U77 | Malate | 2.671(dd), 2.370(dd), 4.353(dd) | 45.8, 73.5, 183.6 |
| U78 | Malonate | 3.053(s) | 51.5 |
| U79 | Mannitol | 3.677(d), 3.770(m), 3.873(dd) | 65.37, 72.8, 66.69 |
| U80 | Methanol | 3.366(s) | 52.1 |
| U81 | Methionine | 3.875(m), 2.162(t), 2.650(s), 2.140 (s) | 57.2, 31.3, 29.4, 16.6, — |
| U82 | Methyl phosphate | 3.470(d) | 54.2 |
| U83 | Methylamine | 2.600(s) | 28.1 |
| U84 | Methylguanidine | 2.833(s) | 30.2, 158.7 |
| U85 | Methylsuccinate | 1.104(d), 2.134(d), 2.633(m) | 20.68, 44.43, — |
| U86 | N,N-dimethylglycine | 2.921(s), 3.713(s) | 40.4, 62.6, 173.1 |
| U87 | N6,N6,N6-trimethyllysine | 3.109(s) | 47.14 |
| U88 | N-Acetylglycine | 2.032(s), 3.740(d), 7.980(s) | 24.2, 46.1, — |
| U89 | NAG C | 2.042(s) | 23.2, 175.6 |
| U90 | N-Heptanoate | 1.309(m) | 30.22 |
| U91 | N-Methylhydantoin | 2.920(s), 4.080(s) | — |
| U92 | N-Nitrosodi Phenylacetylglycine | 3.010(s), 3.802(s) | 145.1, 167.8 |
| U93 | O-Acetylcholine | 2.143(s), 3.202(s), 3.711(t), 4.529(m) | 23.4, 56.8, 67.1, 60.2 |
| U94 | OAG | 2.140(s) | 21, 175.6 |
| U95 | Ornithine | 1.775(m), 1.828(m), 1.929(m), 3.044(t), 3.782(d) | 25.5, 25.5, —, 41.12, 56.81 |
| U96 | Oxypurinol | 8.210(s) | 129.09 |
| U97 | Pantothenate | 0.940(s), 0.900(s), 3.521(s), 3.400(s), 4.000(s), 3.450(t), 2.433(t) | 23.7, 22.2, 71.5, 78.7, 41.4, 177.8, 39.5, 39.5, 183 |
| U98 | PC | 3.224(s), 3.609(m), 4.173(m) | 56.9, 77.6, 61 |

| | | | |
|---|---|---|---|
| U99 | *p*-Cresol glucuronide | 2.299(s), 7.055(m), 7.237(m) | 133.3, 124.4, 22.7, 136.2 |
| U100 | *p*-Cresol sulfate | 2.347(s), 7.217(d), 7.293(d) | —, 121.61, 136.05 |
| U101 | Phenylacetate | 3.530(s) | 118.2, 133.4 |
| U102 | Phenylacetylglycine | 7.428(m), 7.369(m), 7.366(m), 3.650(s) | 130, 129.1, 40.8, 40.8, 177.4 |
| U103 | Phenylalanine | 7.320(dd), 7.420(dd), 7.368(m), 3.120(dd), 3.253(dd), 3.980(dd) | 38.9, 38.9, 58.9, 132.2, 129.8, 131.9 |
| U104 | Proline | 2.023(s), 2.354(m), 3.320(m), 3.398(m), 4.147(t) | 25.78, 32.11, 48.71, 48.71, 63.51 |
| U105 | Propionate | 1.061(t), 2.191(d) | 12.95, 33.35 |
| U106 | Pyruvate | 2.372(s) | 36.2, 172.9, 207.9 |
| U107 | Sarcosine | 2.762(s), 3.650(s) | 39.4, 50.9, 185.8 |
| U108 | Scyllo-inositol | 3.350(s) | 74.3 |
| U109 | Sebacate | 2.184(t), 1.567(m), 1.312(m) | 48.4, 28.4, 31.9 |
| U110 | Serine | 3.828(dd), 3.949(dd), 3.981(dd) | 59.32, —, — |
| U111 | Succinate | 2.412(s) | 37.6, 185.4 |
| U112 | Sucrose | 3.661(dd), 3.740(dd), 3.480(dd), 3.857(m), 4.104(d) | 75.5, 72.2, 75.3, 79.3, 76.9 |
| U113 | Tartrate | 4.573(s) | 77.38 |
| U114 | Taurine | 3.273(t), 3.421(t) | 38.1, 50.6 |
| U115 | Threonine | 3.600(d), 4.267(m), 1.330(d) | 25.6, 66.1, 68.7, 185.4 |
| U116 | Triglycerides | 5.212(m), 4.073(m), 4.281(m) | 69.9, 62.8, 62.8 |
| U117 | Trimethylamine | 2.882(s) | 47.6 |
| U118 | Trimethylamine N-Oxide | 3.266(s) | 61.5 |
| U119 | Tryptophan | 3.298(dd), 3.498(dd), 4.089(q), 7.204(t), 7.310(m), 7.507(d) | 119.5, 122.5, 125, 112.9 |
| U120 | Tyrosine | 6.911(d), 7.200(d), 3.941(dd), 3.202(dd), 3.073(dd) | 118.7, 133.7, 58.7, 38.2, 38.2 |
| U121 | Uracil | 5.805(d), 7.540(d) | 103.9, 146.4 |
| U122 | Urea | 5.792(s) | — |
| U123 | Urocanate | 7.318(d), 7.434(s), 7.885(s), 6.40(d) | 136.9, 132.1, 123.3, 133.4, 124.6 |
| U124 | Valerate | 0.899(t), 1.309(m), 2.168(d) | 16.4,23.9,39.6 |
| U125 | Valine | 3.622(d), 2.282(m), 1.050(d), 0.994 (d) | 63.2，32.0，21.2，19.5，177.9 |
| U126 | Xanthine | 7.901(s) | 144 |
| U127 | α-Arabinose | 3.850(dd), 3.906(m), 3.993(t), 4.023(d), 5.251(d) | —, —, 72.3, 66.37, 93.94 |

| | | | |
|---|---|---|---|
| U128 | α-Glucose | 5.241(d), 3.540(dd), 3.730(dd), 3.421(dd), 3.830(dd), 3.830(dd) | 95.4, 74.9, 76.2, 72.7, 74.4, 63.7 |
| U129 | α-Ketoglutarate | 2.443(t), 3.011(t) | 32.5, 40.4, 184.4, 208.1 |
| U130 | α-Ketoisocaproate | 0.920(s), 2.054(m), 2.616(d) | — |
| U131 | α-Ketoisovalerate | 1.127(d), 3.022(m) | —, 40.1 |
| U132 | α-Keto-β-methyl-valerate | 0.887(t), 1.104(d), 1.687(m), 2.923(m) | 13.2, 16.4, 26.8, 26.8, 45.9 |
| U133 | α-Xylose | 3.545(dd), 3.630(m), 3.671(t), 5.203(d) | — |
| U134 | β-Arabinose | 3.525(dd), 3.671(t), 3.856(dd), 3.945(m), 4.523(d) | —, 69.8, 70.6, —, 99.7 |
| U135 | β-Glucose | 4.450(d), 3.261(dd), 3.503(dd), 3.400(dd), 3.470(dd), 3.742(dd), 3.901(dd) | 99.3, 77.5, 79, 72.9, 79, 63.7 |

"—": The corresponding $^{13}C$ shift values are not found in the HSQC spectra, and the metabolites without $^{13}C$ shift values were assigned only based on the $^{1}H$ shift in the TOCSY spectrum.

Table S3 Summary table of differential metabolites during the whole experiment.

| □ | □ | Model vs Control | | | | | | | | | | | | SBS vs Model | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Day 7 | | | Day 14 | | | Day 28 | | | Day 42 | | | Day 28 | | | Day 42 | | |
| □ | Metabolites | FC | *P* | Trends | FC | *P* | Trends | FC | *P* | Trends | FC | *P* | Trends | FC | *P* | Trends | FC | *P* | Trends |
| **Energy metabolism** | Citrate (U) | 0.5332 | < 0.001 | ↓** | 0.4459 | 0.0023 | ↓** | 0.6369 | 0.0486 | ↓* | 0.6150 | 0.0499 | ↓* | | | | 2.4360 | 0.0100 | ↑** |
| | Oxoglutarate (U) | 0.6789 | < 0.001 | ↓** | 0.5711 | < 0.001 | ↓** | 0.6995 | 0.0465 | ↓* | 0.6766 | 0.0477 | ↓* | 1.7026 | 0.0041 | ↑** | 2.0975 | 0.0152 | ↑* |
| | Succinate (U) | 0.7420 | < 0.001 | ↓** | 0.6752 | 0.0020 | ↓** | 0.7237 | 0.0455 | ↓* | 0.6995 | 0.0465 | ↓* | | | | 2.0391 | 0.0004 | ↑** |
| | Fumarate (U) | 1.6145 | < 0.001 | ↑** | | | | | | | | | | | | | 2.0126 | 0.0217 | ↑* |
| | Malate (U) | 0.6944 | < 0.001 | ↓** | 0.5718 | < 0.001 | ↓** | 0.7242 | 0.0452 | ↓* | 0.7237 | 0.0455 | ↓* | | | | 2.2163 | 0.0099 | ↑** |
| | Malonate (U) | 1.2434 | 0.0147 | ↑* | 1.2434 | 0.0147 | ↑* | 1.2859 | 0.0435 | ↑* | 2.3968 | 0.0232 | ↑* | | | | 2.9945 | < 0.001 | ↑** |
| | Triglycerides (U) | 0.6715 | 0.0429 | ↓* | | | | | | | | | | | | | 3.4623 | < 0.001 | ↑** |
| | Pyruvate (U) | | | | | | | | | | 0.4215 | 0.0160 | ↓* | | | | 1.8860 | 0.0099 | ↑** |
| | Glucose (U) | | | | 1.2453 | < 0.001 | ↑** | 1.2295 | 0.0001 | ↑** | 1.2034 | 0.0001 | ↑** | | | | 2.6830 | < 0.001 | ↑** |
| | Glucose (F) | | | | | | | 1.2295 | 0.0001 | ↑** | | | | 0.7828 | 0.0072 | ↓** | | | |
| **Amino acids metabolism** | Phenylalanine (U) | 1.2318 | < 0.001 | ↑** | 1.2318 | < 0.001 | ↑** | 1.8527 | 0.0429 | ↑* | 3.2213 | 0.0081 | ↑** | | | | 2.5449 | 0.0002 | ↑** |
| | Aspartate (U) | 0.7586 | < 0.001 | ↓** | 0.6677 | 0.0001 | ↓** | 0.6690 | 0.0016 | ↓** | 2.5572 | 0.0197 | ↑* | | | | 2.3627 | 0.0075 | ↑** |
| | Lysine (U) | 0.7793 | < 0.001 | ↓** | 0.7688 | < 0.001 | ↓** | 0.7623 | 0.0010 | ↓** | | | | | | | 3.9820 | < 0.001 | ↑** |
| | Cysteine (U) | | | | 0.7922 | < 0.001 | ↓** | 0.7663 | 0.0009 | ↓** | | | | 4.3197 | < 0.001 | ↑** | 4.3197 | < 0.001 | ↑** |
| | Methionine (U) | 0.8076 | 0.0033 | ↓** | 0.6746 | 0.0034 | ↓** | 0.5238 | 0.0260 | ↓* | 0.5670 | 0.0162 | ↓* | | | | 2.2899 | 0.0074 | ↑** |
| | Leucine (U) | | | | | | | | | | | | | | | | 2.2732 | 0.0030 | ↑** |
| | Leucine (F) | | | | | | | | | | 0.752 | < 0.001 | ↓** | | | | 1.4215 | 0.0019 | ↑** |
| | Valine (F) | 0.8001 | 0.0033 | ↓** | 0.7998 | 0.0033 | ↓** | 0.8166 | 0.0001 | ↓** | 0.8313 | 0.0001 | ↓** | | | | 3.2501 | < 0.001 | ↑** |
| | Ornithine (U) | | | | 0.7940 | < 0.001 | ↓** | 0.7986 | 0.0006 | ↓** | 0.7994 | 0.0006 | ↓** | | | | 4.0211 | < 0.001 | ↑** |
| | Arginine (U) | | | | 0.8176 | < 0.001 | ↓** | 0.8034 | 0.0002 | ↓** | 0.7416 | 0.0166 | ↓* | | | | 3.6507 | < 0.001 | ↑** |
| | Glutamine (U) | | | | 0.7736 | < 0.001 | ↓** | 0.7789 | 0.0008 | ↓** | 0.5242 | 0.0273 | ↓* | | | | 1.8842 | 0.0030 | ↑** |
| **Nucleotides** | Uracil (F) | 0.4415 | 0.0094 | ↓** | 0.6760 | 0.0078 | ↓** | 0.4724 | 0.0448 | ↓* | 0.7789 | 0.0008 | ↓** | 3.0477 | < 0.001 | ↑** | | | |

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **metabolism** | Uracil (U) | | | | | | | | | | | | 2.0252 | 0.0003 | ↑** | 3.0477 | < 0.001 | ↑** |
| | Adenine (F) | 0.4738 | 0.0029 | ↓** | 0.5138 | 0.0001 | ↓** | 0.5377 | 0.0261 | ↓* | 0.5670 | 0.0162 | ↓* | | | | 1.7600 | 0.0040 | ↑** |
| | Adenine (U) | | | | 0.7541 | 0.0029 | ↓** | 0.5708 | 0.0087 | ↓** | 0.6168 | 0.0051 | ↓** | | | | 3.0295 | 0.0005 | ↑** |
| | Hypoxanthine | | | | 0.6739 | < 0.001 | ↓** | 0.6690 | 0.0016 | ↓** | 0.6895 | 0.0014 | ↓** | | | | 3.0578 | 0.0005 | ↑** |
| | Xanthine (F) | 0.6644 | 0.0004 | ↓** | 0.6244 | 0.0042 | ↓** | | | | | | | | | | | | |
| | Xanthine (U) | | | | 2.3340 | 0.0009 | ↑** | 2.5373 | 0.0001 | ↑** | | | | 0.5655 | 0.0461 | ↓* | | | |
| | Allantoate (U) | 1.2659 | 0.0116 | ↑* | 1.4336 | 0.0004 | ↑** | 3.4798 | 0.0079 | ↑** | | | | | | | | | |
| | Choline (U) | | | | | | 1.3118 | 0.7623 | 0.0010 | ↑** | 1.4053 | 0.0014 | ↑** | 0.7473 | 0.0014 | ↓** | 0.6785 | 0.0076 | ↓** |
| | TMA (U) | 1.4914 | 0.0463 | ↑* | 1.4441 | < 0.001 | ↑** | 1.2295 | 0.0001 | ↑** | 2.2788 | 0.0300 | ↑* | 0.6186 | 0.0143 | ↓* | 0.3957 | 0.0003 | ↓** |
| | Betaine (U) | 0.6114 | < 0.001 | ↓** | 0.6810 | 0.0009 | ↓** | 0.6361 | 0.0081 | ↓** | 0.6538 | 0.0260 | ↓* | | | | 2.7146 | 0.0002 | ↑** |
| | Creatine (U) | | | | 0.4180 | < 0.001 | ↓** | 0.4592 | 0.0313 | ↓* | 0.4865 | 0.0271 | ↓* | 2.2733 | 0.0023 | ↑** | 3.6723 | < 0.001 | ↑** |
| | Creatinine (U) | | | | 0.3118 | < 0.001 | ↓** | 0.7416 | 0.0166 | ↓* | 0.7663 | 0.0009 | ↓** | 2.8366 | 0.0001 | ↑** | 3.3632 | 0.0001 | ↑** |
| | Sarcosine (U) | | | | 1.2022 | 0.0218 | ↑* | | | | | | | | | | 3.5613 | < 0.001 | ↑** |
| **Gut** | Hippurate (U) | 1.2323 | 0.0102 | ↑* | 1.8611 | < 0.001 | ↑** | | | | 2.2660 | 0.0308 | ↑* | 2.2826 | < 0.001 | ↑** | 3.4987 | < 0.001 | ↑** |
| **Microbiota** | Acetone (U) | 0.5777 | < 0.001 | ↓** | 0.5088 | < 0.001 | ↓** | | | | | | | 1.8569 | 0.0021 | ↑** | 2.1440 | 0.0298 | ↑* |
| **and Host Co-** | Hypotaurine (U) | 0.5582 | < 0.001 | ↓** | 0.5225 | < 0.001 | ↓** | | | | | | | | | | 2.6967 | 0.0001 | ↑** |
| **metabolism** | Taurine (U) | 1.7218 | < 0.001 | ↑** | 1.7141 | 0.0014 | ↑** | 1.8011 | 0.0055 | ↑** | 1.7257 | 0.0106 | ↑* | | | | 0.6927 | < 0.001 | ↓** |
| | Taurine (F) | | | | | | | | | | | | | 0.7281 | 0.0039 | ↓** | | | |
| | Formate (U) | | | | 0.3835 | 0.0001 | ↓** | 0.6842 | 0.0277 | ↓* | 0.7937 | 0.0056 | ↓** | 2.6147 | 0.0015 | ↑** | 2.6147 | 0.0015 | ↑** |
| | Butyrate (F) | | | | 0.6794 | 0.0297 | ↓* | 0.6847 | 0.0189 | ↓* | | | | 1.7767 | 0.0014 | ↑** | | | |
| | Butyrate (U) | 0.7575 | < 0.001 | ↓** | 0.7729 | < 0.001 | ↓** | 0.6440 | 0.0371 | ↓* | | | | 2.0858 | 0.0008 | ↑** | 2.2291 | 0.0041 | ↑** |
| | Propionate (F) | | | | 1.4311 | 0.0010 | ↑** | | | | 1.2696 | 0.0001 | ↑** | 1.3151 | 0.0110 | ↑* | | | |
| | Propionate (U) | 0.7983 | 0.0015 | ↓** | | | | | | | 1.2859 | 0.0435 | ↑* | | | | | | |

Table S4 The metabolic pathway analysis results based on the altered metabolites from the model group compared with the control group on day 42.

| | Total | Hits | Raw *P* | Holm adjust | FDR | Impact |
|---|---|---|---|---|---|---|
| **Feces** | | | | | | |
| Propanoate metabolism | 23 | 2 | 0.002288 | 0.089228 | 0.054132 | 0 |
| Pantothenate and CoA biosynthesis | 19 | 4 | 0.002776 | 0.10549 | 0.054132 | 0 |
| beta-Alanine metabolism | 21 | 2 | 0.014567 | 0.53897 | 0.11647 | 0 |
| Valine, leucine and isoleucine biosynthesis | 8 | 6 | 0.019856 | 0.71481 | 0.11647 | 0 |
| Purine metabolism | 65 | 4 | 0.020742 | 0.72598 | 0.11647 | 0.03396 |
| Pyruvate metabolism | 22 | 4 | 0.027458 | 0.93357 | 0.11647 | 0.35147 |
| Glycerolipid metabolism | 16 | 1 | 0.02854 | 0.94182 | 0.11647 | 0 |
| Glycolysis / Gluconeogenesis | 26 | 4 | 0.029273 | 0.94182 | 0.11647 | 0.13055 |
| Glyoxylate and dicarboxylate metabolism | 32 | 6 | 0.02937 | 0.94182 | 0.11647 | 0.14815 |
| Valine, leucine and isoleucine degradation | 40 | 5 | 0.03648 | 1 | 0.12934 | 0.02168 |
| Glycine, serine and threonine metabolism | 33 | 9 | 0.045063 | 1 | 0.14645 | 0.67871 |
| Nitrogen metabolism | 39 | 2 | 0.076051 | 1 | 0.22815 | 0.0743 |
| Butanoate metabolism | 15 | 3 | 0.087249 | 1 | 0.24305 | 0 |
| Nicotinate and nicotinamide metabolism | 15 | 2 | 0.11583 | 1 | 0.30116 | 0 |
| Proline metabolism | 38 | 4 | 0.13625 | 1 | 0.33212 | 0.14778 |
| Histidine metabolism | 16 | 2 | 0.22634 | 1 | 0.51924 | 0.12295 |
| Arginine metabolism | 14 | 6 | 0.27031 | 1 | 0.54142 | 0.30457 |
| Pyrimidine metabolism | 6 | 1 | 0.27936 | 1 | 0.54142 | 0 |
| Primary bile acid biosynthesis | 46 | 3 | 0.30457 | 1 | 0.54142 | 0.02493 |
| Taurine and hypotaurine metabolism | 8 | 1 | 0.31159 | 1 | 0.54142 | 0.42857 |
| Sphingolipid metabolism | 21 | 1 | 0.31916 | 1 | 0.54142 | 0 |
| Cysteine and methionine | 33 | 3 | 0.3193 | 1 | 0.54142 | 0.1263 |

| | | | | | | |
|---|---|---|---|---|---|---|
| metabolism | | | | | | |
| Tryptophan metabolism | 41 | 1 | 0.35437 | 1 | 0.57586 | 0.14305 |
| Galactose metabolism | 27 | 1 | 0.38811 | 1 | 0.58217 | 0.02924 |
| Fructose and mannose metabolism | 20 | 1 | 0.38811 | 1 | 0.58217 | 0 |
| Porphyrin and chlorophyll metabolism | 30 | 1 | 0.48464 | 1 | 0.68264 | 0 |
| Tyrosine metabolism | 42 | 4 | 0.50396 | 1 | 0.68264 | 0.16435 |
| Citrate cycle (TCA cycle) | 20 | 4 | 0.52224 | 1 | 0.68264 | 0.16744 |
| Amino sugar and nucleotide sugar metabolism | 37 | 2 | 0.52511 | 1 | 0.68264 | 0.05035 |
| Alanine, aspartate and glutamate metabolism | 28 | 7 | 0.57344 | 1 | 0.72143 | 0.38782 |
| Pentose and glucuronate interconversions | 18 | 1 | 0.61333 | 1 | 0.74177 | 0 |
| D-Glutamine and D-glutamate metabolism | 6 | 2 | 0.64592 | 1 | 0.74177 | 0 |
| Glutathione metabolism | 28 | 2 | 0.64667 | 1 | 0.74177 | 0.08873 |
| Ubiquinone and other terpenoid-quinone biosynthesis | 9 | 1 | 0.75746 | 1 | 0.84403 | 0 |
| Selenocompound metabolism | 20 | 1 | 0.83991 | 1 | 0.89956 | 0 |
| Glycerophospholipid metabolism | 36 | 2 | 0.8726 | 1 | 0.89956 | 0.03906 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | 4 | 2 | 0.89226 | 1 | 0.89956 | 1 |
| Phenylalanine metabolism | 10 | 3 | 0.89956 | 1 | 0.89956 | 0.35714 |
| **Urine** | | | | | | |
| Purine metabolism | 66 | 6 | 0.000929 | 0.044598 | 0.044598 | 0.07017 |
| Propanoate metabolism | 23 | 3 | 0.002066 | 0.097112 | 0.049589 | 0 |
| Starch and sucrose metabolism | 18 | 1 | 0.01255 | 0.57728 | 0.13303 | 0.05023 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Ascorbate and aldarate metabolism | 10 | 1 | 0.016628 | 0.74828 | 0.13303 | 0.25 |
| Pentose and glucuronate interconversions | 18 | 1 | 0.016628 | 0.74828 | 0.13303 | 0.125 |
| Inositol phosphate metabolism | 30 | 1 | 0.016628 | 0.74828 | 0.13303 | 0 |
| Pyrimidine metabolism | 39 | 4 | 0.020855 | 0.87592 | 0.14301 | 0.08374 |
| Sphingolipid metabolism | 21 | 1 | 0.043169 | 1 | 0.25901 | 0 |
| Porphyrin and chlorophyll metabolism | 30 | 2 | 0.06506 | 1 | 0.34699 | 0 |
| Galactose metabolism | 27 | 4 | 0.086591 | 1 | 0.41564 | 0.17844 |
| Glycine, serine and threonine metabolism | 34 | 11 | 0.10551 | 1 | 0.46041 | 0.72659 |
| Fructose and mannose metabolism | 18 | 1 | 0.17104 | 1 | 0.57156 | 0 |
| Amino sugar and nucleotide sugar metabolism | 37 | 1 | 0.17104 | 1 | 0.57156 | 0 |
| Histidine metabolism | 16 | 3 | 0.17938 | 1 | 0.57156 | 0.12295 |
| Cysteine and methionine metabolism | 33 | 4 | 0.18768 | 1 | 0.57156 | 0.22222 |
| Thiamine metabolism | 7 | 1 | 0.19052 | 1 | 0.57156 | 0 |
| Glycerolipid metabolism | 16 | 1 | 0.21183 | 1 | 0.59716 | 0.23676 |
| beta-Alanine metabolism | 21 | 2 | 0.22938 | 1 | 0.59716 | 0 |
| Arginine and proline metabolism | 38 | 8 | 0.2397 | 1 | 0.59716 | 0.36787 |
| Pantothenate and CoA biosynthesis | 19 | 6 | 0.24882 | 1 | 0.59716 | 0.00714 |
| Glyoxylate and dicarboxylate metabolism | 32 | 9 | 0.27593 | 1 | 0.62064 | 0.1799 |
| Glutathione metabolism | 28 | 6 | 0.31221 | 1 | 0.62064 | 0.1388 |
| Tryptophan metabolism | 41 | 2 | 0.32129 | 1 | 0.62064 | 0.14305 |
| Taurine and hypotaurine metabolism | 8 | 3 | 0.32775 | 1 | 0.62064 | 0.71428 |
| Synthesis and degradation | 5 | 1 | 0.35835 | 1 | 0.62064 | 0.6 |

| | | | | | | |
|---|---|---|---|---|---|---|
| of ketone bodies | | | | | | |
| Nicotinate and nicotinamide metabolism | 15 | 2 | 0.37637 | 1 | 0.62064 | 0.1943 |
| Aminoacyl-tRNA biosynthesis | 48 | 18 | 0.37649 | 1 | 0.62064 | 0.16667 |
| Nitrogen metabolism | 6 | 2 | 0.38106 | 1 | 0.62064 | 0 |
| Phenylalanine metabolism | 12 | 5 | 0.39971 | 1 | 0.62064 | 0.35714 |
| Alanine, aspartate and glutamate metabolism | 28 | 9 | 0.42043 | 1 | 0.62064 | 0.58494 |
| Citrate cycle (TCA cycle) | 20 | 6 | 0.4298 | 1 | 0.62064 | 0.30194 |
| Arginine biosynthesis | 14 | 7 | 0.4631 | 1 | 0.62064 | 0.2538 |
| Pyruvate metabolism | 22 | 5 | 0.46458 | 1 | 0.62064 | 0.38257 |
| Butanoate metabolism | 15 | 5 | 0.47244 | 1 | 0.62064 | 0.11111 |
| Primary bile acid biosynthesis | 46 | 2 | 0.47498 | 1 | 0.62064 | 0.04478 |
| Lysine degradation | 25 | 1 | 0.47841 | 1 | 0.62064 | 0 |
| Biotin metabolism | 10 | 1 | 0.47841 | 1 | 0.62064 | 0 |
| Valine, leucine and isoleucine degradation | 40 | 8 | 0.50265 | 1 | 0.62598 | 0.07143 |
| Tyrosine metabolism | 42 | 5 | 0.51162 | 1 | 0.62598 | 0.16435 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | 4 | 2 | 0.52165 | 1 | 0.62598 | 1 |
| D-Glutamine and D-glutamate metabolism | 6 | 3 | 0.55993 | 1 | 0.65553 | 0.5 |
| Glycolysis / Gluconeogenesis | 26 | 5 | 0.58601 | 1 | 0.66972 | 0.13055 |
| Ether lipid metabolism | 20 | 1 | 0.6383 | 1 | 0.70815 | 0 |
| Fatty acid degradation | 39 | 1 | 0.6533 | 1 | 0.70815 | 0 |
| Glycerophospholipid metabolism | 36 | 4 | 0.66389 | 1 | 0.70815 | 0.0872 |
| Valine, leucine and isoleucine biosynthesis | 8 | 6 | 0.70017 | 1 | 0.73061 | 0 |
| Selenocompound metabolism | 20 | 1 | 0.77348 | 1 | 0.78993 | 0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ubiquinone and other terpenoid-quinone biosynthesis | 9 | 1 | 0.83967 | 1 | | 0.83967 | 0 |

Table S5. The metabolic pathway analysis results based on the altered metabolites from the SBS group compared with the model group on day 42.

| | Total | Hits | Raw *P* | Holm adjust | FDR | Impact |
|---|---|---|---|---|---|---|
| **Feces** | | | | | | |
| Primary bile acid biosynthesis | 146 | 3 | 0.000726 | 0.028333 | 0.014386 | 0.06763 |
| Aminoacyl-tRNA biosynthesis | 48 | 14 | 0.001621 | 0.061613 | 0.014386 | 0.16667 |
| Purine metabolism | 66 | 4 | 0.001653 | 0.061613 | 0.014386 | 0.05592 |
| Valine, leucine and isoleucine biosynthesis | 40 | 5 | 0.002347 | 0.084507 | 0.014386 | 0.02168 |
| Valine, leucine and isoleucine degradation | 8 | 4 | 0.002651 | 0.092778 | 0.014386 | 0 |
| Glycolysis / Gluconeogenesis | 32 | 6 | 0.002768 | 0.094119 | 0.014386 | 0.14815 |
| Pyruvate metabolism | 22 | 4 | 0.002889 | 0.095332 | 0.014386 | 0.35147 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | 26 | 4 | 0.002951 | 0.095332 | 0.014386 | 0.13055 |
| Pentose and glucuronate interconversions | 18 | 2 | 0.006914 | 0.21433 | 0.02996 | 0.07812 |
| Taurine and hypotaurine metabolism | 8 | 1 | 0.01098 | 0.32941 | 0.041915 | 0.42857 |
| Amino sugar and nucleotide sugar metabolism | 37 | 3 | 0.011822 | 0.34284 | 0.041915 | 0.06569 |
| Citrate cycle (TCA cycle) | 21 | 1 | 0.02533 | 0.70925 | 0.082323 | 0 |
| Cysteine and methionine metabolism | 33 | 3 | 0.034387 | 0.92844 | 0.10316 | 0.1263 |
| Ubiquinone and other terpenoid-quinone biosynthesis | 9 | 1 | 0.062677 | 1 | 0.16659 | 0 |
| Tyrosine metabolism | 42 | 4 | 0.064071 | 1 | 0.16659 | 0.16435 |
| Glycerolipid metabolism | 16 | 1 | 0.089859 | 1 | 0.20551 | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Phenylalanine metabolism | 12 | 3 | 0.094106 | 1 | 0.20551 | 0.35714 |
| Glyoxylate and dicarboxylate metabolism | 4 | 2 | 0.094852 | 1 | 0.20551 | 1 |
| Glycine, serine and threonine metabolism | 34 | 9 | 0.10903 | 1 | 0.2238 | 0.70251 |
| Glycerophospholipid metabolism | 36 | 2 | 0.11662 | 1 | 0.22741 | 0.03906 |
| Arginine biosynthesis | 14 | 6 | 0.12321 | 1 | 0.22881 | 0.30457 |
| Sphingolipid metabolism | 20 | 4 | 0.1595 | 1 | 0.28075 | 0.16744 |
| D-Glutamine and D-glutamate metabolism | 6 | 2 | 0.17052 | 1 | 0.28075 | 0 |
| Alanine, aspartate and glutamate metabolism | 28 | 7 | 0.17672 | 1 | 0.28075 | 0.38782 |
| Arginine and proline metabolism | 38 | 4 | 0.18502 | 1 | 0.28075 | 0.14778 |
| Histidine metabolism | 16 | 2 | 0.18717 | 1 | 0.28075 | 0.12295 |
| Nitrogen metabolism | 6 | 1 | 0.20088 | 1 | 0.29016 | 0 |
| Pyrimidine metabolism | 39 | 2 | 0.2109 | 1 | 0.29376 | 0.0743 |
| Nicotinate and nicotinamide metabolism | 15 | 2 | 0.24706 | 1 | 0.33225 | 0 |
| Galactose metabolism | 27 | 1 | 0.27616 | 1 | 0.34742 | 0.02924 |
| Fructose and mannose metabolism | 18 | 1 | 0.27616 | 1 | 0.34742 | 0 |
| beta-Alanine metabolism | 21 | 2 | 0.33517 | 1 | 0.40849 | 0 |
| Pantothenate and CoA biosynthesis | 19 | 3 | 0.35809 | 1 | 0.4232 | 0 |
| Selenocompound metabolism | 20 | 1 | 0.47018 | 1 | 0.53932 | 0 |
| Porphyrin and chlorophyll metabolism | 30 | 1 | 0.4942 | 1 | 0.55068 | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Propoate metabolism | 23 | 2 | 0.67914 | 1 | 0.73574 | 0 |
| Tryptophan metabolism | 41 | 1 | 0.74074 | 1 | 0.75638 | 0.14305 |
| Glutathione metabolism | 28 | 2 | 0.75379 | 1 | 0.75638 | 0.08873 |
| Butanoate metabolism | 15 | 3 | 0.75638 | 1 | 0.75638 | 0 |
| **Urine** | | | | | | |
| Arginine and proline metabolism | 38 | 8 | 7.21E-05 | 0.00346 | 0.002007 | 0.36787 |
| Glutathione metabolism | 28 | 6 | 8.36E-05 | 0.00393 | 0.002007 | 0.1388 |
| Butanoate metabolism | 15 | 5 | 0.000153 | 0.007026 | 0.002444 | 0.11111 |
| Aminoacyl-tRNA biosynthesis | 48 | 18 | 0.000316 | 0.014205 | 0.00354 | 0.16667 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | 4 | 2 | 0.000377 | 0.01657 | 0.00354 | 1 |
| Ubiquinone and other terpenoid-quinone biosynthesis | 9 | 1 | 0.000443 | 0.019027 | 0.00354 | 0 |
| Pantothenate and CoA biosynthesis | 19 | 7 | 0.000547 | 0.022987 | 0.003753 | 0.02857 |
| Arginine biosynthesis | 14 | 7 | 0.000663 | 0.027187 | 0.003979 | 0.2538 |
| D-Glutamine and D-glutamate metabolism | 6 | 3 | 0.0008 | 0.032009 | 0.004115 | 0.5 |
| Taurine and hypotaurine metabolism | 8 | 3 | 0.000857 | 0.033432 | 0.004115 | 0.71428 |
| Cysteine and methionine metabolism | 33 | 4 | 0.001124 | 0.042691 | 0.004902 | 0.22222 |
| Tyrosine metabolism | 42 | 5 | 0.001657 | 0.061322 | 0.006396 | 0.16435 |
| Thiamine metabolism | 7 | 1 | 0.00195 | 0.070211 | 0.006396 | 0 |
| Phenylalanine metabolism | 12 | 5 | 0.001988 | 0.070211 | 0.006396 | 0.35714 |
| Glycine, serine and threonine metabolism | 34 | 12 | 0.002025 | 0.070211 | 0.006396 | 0.72659 |
| Glycolysis / Gluconeogenesis | 26 | 5 | 0.002162 | 0.071331 | 0.006396 | 0.13055 |
| Primary bile acid | 46 | 2 | 0.002283 | 0.073044 | 0.006396 | 0.04478 |

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|---|---|---|---|---|---|---|
| biosynthesis | | | | | | |
| Lysine degradation | 25 | 2 | 0.002596 | 0.080465 | 0.006396 | 0 |
| Biotin metabolism | 10 | 1 | 0.002603 | 0.080465 | 0.006396 | 0 |
| Alanine, aspartate and glutamate metabolism | 28 | 9 | 0.002665 | 0.080465 | 0.006396 | 0.58494 |
| Citrate cycle (TCA cycle) | 20 | 6 | 0.002875 | 0.080502 | 0.006402 | 0.30194 |
| Valine, leucine and isoleucine biosynthesis | 8 | 6 | 0.002934 | 0.080502 | 0.006402 | 0 |
| Pentose and glucuronate interconversions | 18 | 2 | 0.003241 | 0.08427 | 0.006761 | 0.125 |
| Valine, leucine and isoleucine degradation | 40 | 7 | 0.00338 | 0.084508 | 0.006761 | 0.04879 |
| Sphingolipid metabolism | 21 | 1 | 0.003947 | 0.094733 | 0.007579 | 0 |
| Tryptophan metabolism | 41 | 2 | 0.004359 | 0.10026 | 0.008048 | 0.14305 |
| Glycerophospholipid metabolism | 36 | 4 | 0.004936 | 0.10859 | 0.008775 | 0.0872 |
| Fructose and mannose metabolism | 18 | 1 | 0.005355 | 0.11245 | 0.008863 | 0 |
| Amino sugar and nucleotide sugar metabolism | 37 | 1 | 0.005355 | 0.11245 | 0.008863 | 0 |
| Fatty acid degradation | 39 | 1 | 0.007207 | 0.13692 | 0.01153 | 0 |
| Ether lipid metabolism | 20 | 1 | 0.007807 | 0.14052 | 0.011712 | 0 |
| Galactose metabolism | 27 | 4 | 0.007871 | 0.14052 | 0.011712 | 0.17844 |
| Glyoxylate and dicarboxylate metabolism | 32 | 9 | 0.008117 | 0.14052 | 0.011712 | 0.1799 |
| Synthesis and degradation of ketone bodies | 5 | 1 | 0.008296 | 0.14052 | 0.011712 | 0.6 |
| Pyrimidine metabolism | 39 | 5 | 0.010006 | 0.14052 | 0.013723 | 0.08374 |
| Ascorbate and aldarate metabolism | 10 | 1 | 0.023451 | 0.30487 | 0.030117 | 0.25 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Inositol phosphate metabolism | 30 | 1 | 0.023451 | 0.30487 | 0.030117 | 0 |
| Starch and sucrose metabolism | 18 | 1 | 0.023842 | 0.30487 | 0.030117 | 0.05023 |
| Histidine metabolism | 16 | 3 | 0.053986 | 0.53986 | 0.066445 | 0.12295 |
| Glycerolipid metabolism | 16 | 1 | 0.056716 | 0.53986 | 0.068059 | 0.23676 |
| Nicotinate and nicotinamide metabolism | 15 | 1 | 0.059016 | 0.53986 | 0.069091 | 0 |
| beta-Alanine metabolism | 21 | 3 | 0.060793 | 0.53986 | 0.069478 | 0.39925 |
| Nitrogen metabolism | 6 | 2 | 0.071395 | 0.53986 | 0.079696 | 0 |
| Porphyrin and chlorophyll metabolism | 30 | 2 | 0.076027 | 0.53986 | 0.081454 | 0 |
| Purine metabolism | 66 | 6 | 0.076363 | 0.53986 | 0.081454 | 0.07017 |
| Pyruvate metabolism | 22 | 5 | 0.12848 | 0.53986 | 0.13407 | 0.38257 |
| Propanoate metabolism | 23 | 4 | 0.14103 | 0.53986 | 0.14404 | 0 |
| Selenocompound metabolism | 20 | 1 | 0.18842 | 0.53986 | 0.18842 | 0 |