

Metabolite	<sup>1</sup> H chemical shift (ppm relative to DSS) and multiplicity <sup>a</sup>
1-Methylnicotinamide	9.26(br s), 8.95(m), 8.88(m), 4.47(s)
1,6-Anhydro-β-D Glucose	5.44(m), 4.98(dd)
2-Aminobutyrate	0.97(t)
2-Hydroxyisobutyrate	1.35(s)
2-Oxoglutarate	3.00(t), 3.00(t)
3-Hydroxyisovalerate	2.36(s), 1.26(s)
3-Indoxysulfate	7.69(m), 7.49(m), 7.26(m), 7.19(m)
4-Hydroxyphenylacetate	7.15(m), 6.85(m), 3.44(s)
4-Pyridoxate	7.86(s), 2.44(s)
Acetate	1.91(s)
Acetone	2.22(s)
Alanine	1.47(d)
Asparagine	2.95(dd), 2.85(dd)
Betaine	3.25(br s)
Carnitine	3.21(br s), 2.43(br s)
Choline	3.19(br s)
cis-Aconitate	3.12(d), 5.74(t)
Citrate	2.53(d), 2.68(d)
Creatinine	3.03(br s), 4.05(br s)
Dimethylamine	2.72(s)
Ethanolamine	3.14(m)
Ethylmalonate	1.70(m), 0.87(t)
Formate	8.44(s)
Fucose	5.20(d), 4.55(d), 1.24(d)
Glucose	5.23(d), 4.63(d), 3.23(m)
Glutamine	2.43(m), 2.46(m)
Glycine	3.55(s)
Hippurate	7.82(m), 7.63(M), 7.54(m), 3.96(d)
Histidine	7.85(br s), 7.08(br s)
Hypoxanthine	8.20(s), 8.18(s)
Isoleucine	1.00(d), 0.93(t)
Lactate	1.32(d)
Leucine	0.95(d), 0.94(d)
Lysine	3.02(m), 1.71(m)
N,N-Dimethylglycine	2.91(s)
O-Acetylcarnitine	3.18(br s), 2.13(s)
Pantothenate	0.92(s), 0.88(s)
π-Methylhistidine	8.07(br s), 7.12(br s), 3.73(s)
Pyroglutamate	2.39(m)
Succinate	2.40(s)
Sucrose	5.40(d), 4.21(d)
τ-methylhistidine	7.72(br s), 7.02(br s)
Taurine	3.42(t), 3.25(t)
Threonine	1.32(d)
trans-Aconitate	6.58(t), 3.44(d)
Trigonelline	9.11(br s), 8.82(m), 4.42(s)
Trimethylamine-N-oxide	3.25(s)
Tryptophan	7.71(m)
Tyrosine	7.18(m), 6.88(m)
Urea	5.77(br s)
Valine	1.03(d), 0.98(d)
Xylose	4.57(d)

<sup>a</sup> s (singlet), br s (broad singlet), d (doublet), dd (doublet of doublets), t (triplet)