

1 **Supplementary Table 1.** ¹H NMR data for metabolites in rat plasma and urine

Keys	Metabolites	Moieties	$\delta^1\text{H}$ (multiplicity)	Samples
1	Lipid	$\text{CH}_3(\text{CH}_2)_n, \text{CH}_3\text{CH}_2\text{CH}_2\text{C}=\text{}$	0.86(t), 0.88(t)	P
		$(\text{CH}_2)_n, \text{CH}_2\text{C}=\text{O}, -\text{CH}=\text{CH}-$	1.27(m), 2.0(m), 5.30(m)	
2	Leucine	$\alpha\text{CH}, \beta\text{CH}_2, \gamma\text{CH}$	3.72(t), 1.71(m), 1.72(m)	P
		$\delta\text{CH}_3, \delta\text{CH}_3'$	0.95(dd), 0.96(dd)	
3	Isoleucine	$\alpha\text{CH}, \beta\text{CH}, \beta\text{CH}_3'$	3.67(d), 1.99(m), 1.01(d)	P
		$\gamma\text{CH}_2, \gamma\text{CH}_2', \delta\text{CH}_3$	1.25(m), 1.46(m), 0.94(t)	
4	Valine	$\alpha\text{CH}, \beta\text{CH}, \gamma\text{CH}_3, \gamma\text{CH}_3'$	3.61(d), 2.30(m), 1.05(d), 0.99(d)	P,U
5	Lactate	$\alpha\text{CH}, \beta\text{CH}_3$	4.12(q), 1.33(d)	P,U
6	Ether	CH_2, CH_3	3.66(q), 1.18(t)	P
7	3-Hydroxybutyrate	$\alpha\text{CH}_2, \alpha\text{CH}_2', \beta\text{CH}, \gamma\text{CH}_3$	2.32(dd), 2.41(dd), 4.16(m), 1.21(d)	P

8	Alanine	αCH , βCH_3	3.78(q), 1.48(d)	P,U
9	Arginine	αCH , βCH_2 , γCH_2 , δCH_2	3.74(t), 1.89(m), 1.68(m), 3.23(t)	P
10	Acetate	CH_3	1.93(s)	P,U
11	N-acetyl-glycoprotein	CH_3	2.05(s)	P,U
12	O-acetyl-glycoprotein	CH_3	2.14(s)	P
13	Pyruvate	CH_3	2.38(s)	P,U
14	Glutamate	αCH , βCH_2 , γCH_2	3.75(m), 2.08(m), 2.36(m)	P
15	Glutamine	αCH , βCH_2 , γCH_2	3.77(m), 2.18(m), 2.45(m)	P
16	Citrate	CH_2 , CH_2'	2.72(d), 2.54(d)	P,U
17	Methionine	αCH , βCH_2 , γCH_2 , S- CH_3	3.84(t), 2.12(m), 2.54(t), 2.10(s)	P
18	2-Oxoglutarate	βCH_2 , γCH_2	2.46(t), 3.03(t)	P,U
19	Dimethylglycine	CH_3 , CH_2	2.92(s), 3.71(s)	P,U
20	Creatine	CH_3 , CH_2	3.04(s), 3.92(s)	P,U

21	Asparagine	αCH , βCH_2 , $\beta\text{CH}_2'$	3.97(m), 2.83(dd), 2.94(dd)	P
22	Acetone	CH_3	2.24(s)	P
23	Acetoacetate	CH_3	2.28(s)	U
24	DMSO ₂	CH_3	3.17(s)	U
25	Choline	αCH_2 , βCH_2 , N- CH_3	4.07(t), 3.53(t), 3.21(s)	P
26	O-phosphocholine	αCH_2 , βCH_2 , N- CH_3	4.22(t), 3.60(t), 3.21(s)	P
27	Trimethylamine N-oxide	N- CH_3	3.23(s)	P
28	Betaine	CH_2 , N- CH_3	3.25(s), 3.94(s)	P,U
29	Glycerol	CH_2	3.56(dd)	P,U
30	Glycine	CH_2	3.58(s)	P,U
31	β -Glucose	1-CH, 2-CH, 3-CH, 4-CH 5-CH, 6-CH, 6-CH'	4.66(d), 3.27(dd), 3.48(t), 3.42(dd)	P,U
			3.47(m), 3.72(dd), 3.90(dd)	

32	α -Glucose	1-CH, 2-CH, 3-CH 4-CH, 5-CH, 6-CH	5.24(d), 3.54(dd), 3.72(dd) 3.42(dd), 3.84(m), 3.78(m)	P,U
33	Taurine	CH ₂ ,CH ₂ '	3.43(t), 3.26(t)	U
34	Uracil	5-CH, 6-CH	5.81(d), 7.55(d)	U
35	Xanthosine	2-CH, 2'-CH 3-CH, 4-CH	7.88(s), 5.85(d) 4.72(m), 4.41(m)	P
36	Hippurate	2,6-CH, 3,5-CH 4-CH, CH ₂	7.53(d),7.62(m) 7.82(m), 3.98(d)	P,U
37	Fumarate	CH	6.53(s)	P,U
38	Tyrosine	2,6-CH, 3,5-CH	7.19(d), 6.89(d)	P,U
39	Histidine	2-CH, 4-CH	7.86(s), 7.04(s)	P,U
40	Phenylalanine	2,6-CH,3,5-CH, 4-CH	7.33(m), 7.42(m), 7.36(m)	P
41	Formate	CH	8.47(s)	P,U
42	Xanthine	CH	7.82(s)	P
43	Cytidine	2-CH, 3-CH	7.85(s), 6.08(s)	P,U

44	Hypoxanthine	2-CH, 7-CH	8.22(s), 8.20(s)	U
45	Tyramine	CH, CH'	7.22(dd), 6.88(dd)	U
		CH ₂ , CH ₂ '	3.21(t), 2.91(t)	
46	Succinate	CH ₂	2.42(s)	U
47	Cis-Aconitate	CH, CH ₂	5.71(s), 3.15(s)	U
48	Urea	CH ₂	5.82(s)	U
49	Allantion	CH	5.39(s)	U
50	Indoxyl sulfate	4-CH, 5-CH, 6-CH	7.50(m), 7.21(m), 7.29(m)	U
		7-CH, CH ₃	7.71(m), 7.38(s)	
51	Bile acids	CH ₃	0.73(s)	U
52	DMSO	CH ₃	2.73(s)	U
53	Methanol	CH ₃	3.36(s)	U
54	Hydroquinone	CH	6.80(s)	U
55	Dimethylamine	CH ₃	2.74(s)	U
56	Dihydroxyacetone	CH ₃	4.46(s)	U

57	Malate	CH, CH ₂ , CH ₂ '	4.31(dd), 2.38(m), 2.65(m)	U
58	Butyrate	αCH ₂ , βCH ₂ , γCH ₃	2.15(t), 1.56(m), 0.92(t)	U
59	Carnitine	αCH ₂ , βCH, γCH ₂ N-CH ₃	2.40(m), 4.56(m), 3.41(m) 3.25(s)	U
60	Phenylacetylglycine	CH ₂ , CH ₂ , 2,6-CH, 3,5-CH, 4-CH	3.69(s), 3.77(s), 7.34(m) 7.41(m), 7.36(m)	U
61	2-Oxobutyrate	CH ₂ , CH ₃	2.75(q), 1.05(t)	U
62	Ethanol	CH ₃ , CH ₂	1.19(t), 3.67(q)	U
63	Ethylmalonate	CH, CH ₂ , CH ₃	2.99(t), 1.71(m), 0.89(t)	U
64	Isovaleryglycine	CH, CH ₂ , CH ₃	1.94(m), 2.02(d), 0.93(d)	U
65	3-Methyl-2-oxovalerate	βCH, βCH ₃ , γCH, δCH ₃	2.92(m), 1.46(m), 1.68(m), 1.10(d)	U
66	2-Ketoisovalerate	CH, CH ₃	3.03(m), 1.13(d)	U
67	Methylmalonate	CH, CH ₃	3.17(q), 1.25(d)	U
68	3-Hydroxyisovalerate	CH, CH ₃	2.36(s), 1.27(s)	U

69	Threonine	α CH, β CH, γ CH ₃	3.59(d), 4.25(m), 1.32(d)	U
70	N-Acetylglutamate	α CH, β CH ₂	4.13(m), 1.86(m)	U
		β CH ₂ , γ CH ₂	2.02(m), 2.23(m)	
71	Creatinine	CH ₃ , CH ₂	3.05(s), 4.07(s)	P,U
72	Trimethylamine	N-CH ₃	2.88(s)	U
73	Trigonelline	2-CH, 4-CH, 5-CH	9.14(s), 8.85(m), 8.09(m)	U
		6-CH, CH ₃	8.85(m), 4.43(s)	
74	Benzoate	2,6-CH, 3,5-CH, 4-CH	7.87(d), 7.49(d), 7.57(t)	U

2 Note: s, singlet; d, doublet; t, quartet; m, multiplet; dd, doublet of doublets; P, plasma; U, urine

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