

Supplementary Table S1. Spearman correlations for metabolites overlapping across GC-MS and ¹H-NMR.*

	N	Correlation Coefficient	pValue
Hippurate	37	0.51	0.001
Alanine	37	0.48	0.002
Hypoxanthine	37	0.46	0.004
Valine	37	0.43	0.008
4-Hydroxyphenylacetate	34	0.41	0.02
Citrate	37	0.39	0.02
Homovanillate	36	0.36	0.03
myo-Inositol	36	0.36	0.03
3-Hydroxyisobutyrate	37	0.35	0.03
Indole-3-acetate	36	0.34	0.04
Threonine	37	0.30	0.07
Xanthurenate	26	-0.34	0.08
4-Hydroxy-3-methoxymandelate	29	-0.32	0.08
Arabinose	37	0.28	0.09
2-Hydroxyphenylacetate	20	0.37	0.10
Mannitol	37	0.23	0.17
Glutamine	37	0.20	0.23
Tyrosine	37	0.16	0.34
Histidine	37	0.12	0.46
N-Acetylglucosamine	44	-0.10	0.47
Glutamate	36	0.11	0.53
Glucose	37	-0.10	0.53
Glycolate	37	-0.09	0.56
Tartrate	37	0.07	0.65
3-Aminoisobutyrate	36	0.14	0.69
Pyroglutamate	37	-0.13	0.73
Asparagine	37	-0.06	0.74
5-Hydroxyindole-3-acetate	31	0.03	0.87
Gluconate	37	-0.03	0.87
Lactate	37	-0.01	0.95
Fructose	36	-0.01	0.97
2-Hydroxyglutarate	3	NA	
2-Phosphoglycerate	3	NA	
Lysine	1	NA	

*significant pValues are bold