

Supplement S1

Results from discriminatory analysis via cross-validated Random Forest for further combinations of groups, not included in the main manuscript with the most important metabolites responsible for discrimination

tested system	Features ranked by their contributions to classification accuracy	discriminatory performance - OOB error	AUC value (for binary systems)
A-B-C-ctrl	hippurate, citrate, hypoxanthine, pyruvate, carnitine, alanine, acetate, formate	0.207	-
A-B-C	hippurate, citrate, hypoxanthine, carnitine, alanine, acetone, acetate, formate	0.176	-
A-B	hypoxanthine, alanine, formate, hippurate, carnitine, citrate	0.196	0.913
A-C	hippurate, citrate, alanine, acetone, carnitine, tyrosine, glycine	0.08	0.976
B- C	carnitine, citrate, hypoxanthine, acetone, hippurate, formate, alanine	0.09	0.933