

Table S1. AUC of ROC; sensitivity and specificity at optimal cut-off value for each metabolite and the machine learning model.

Model	Train set		
	AUC	Specificity	Sensitivity
Taurocholic acid	0.8421	0.6667	0.9474
Uracil	0.8399	0.8333	0.8421
Biliverdin	0.8289	0.6667	0.9474
Histidine	0.8180	0.8750	0.6842
Tauroursodeoxycholic acid	0.8048	0.6250	0.8947
Pyrroline hydroxycarboxylic acid	0.8026	1.0000	0.6316
Phenylalanine	0.8004	0.9583	0.5789
Random forest model (RF)	1.0000	1.0000	1.0000