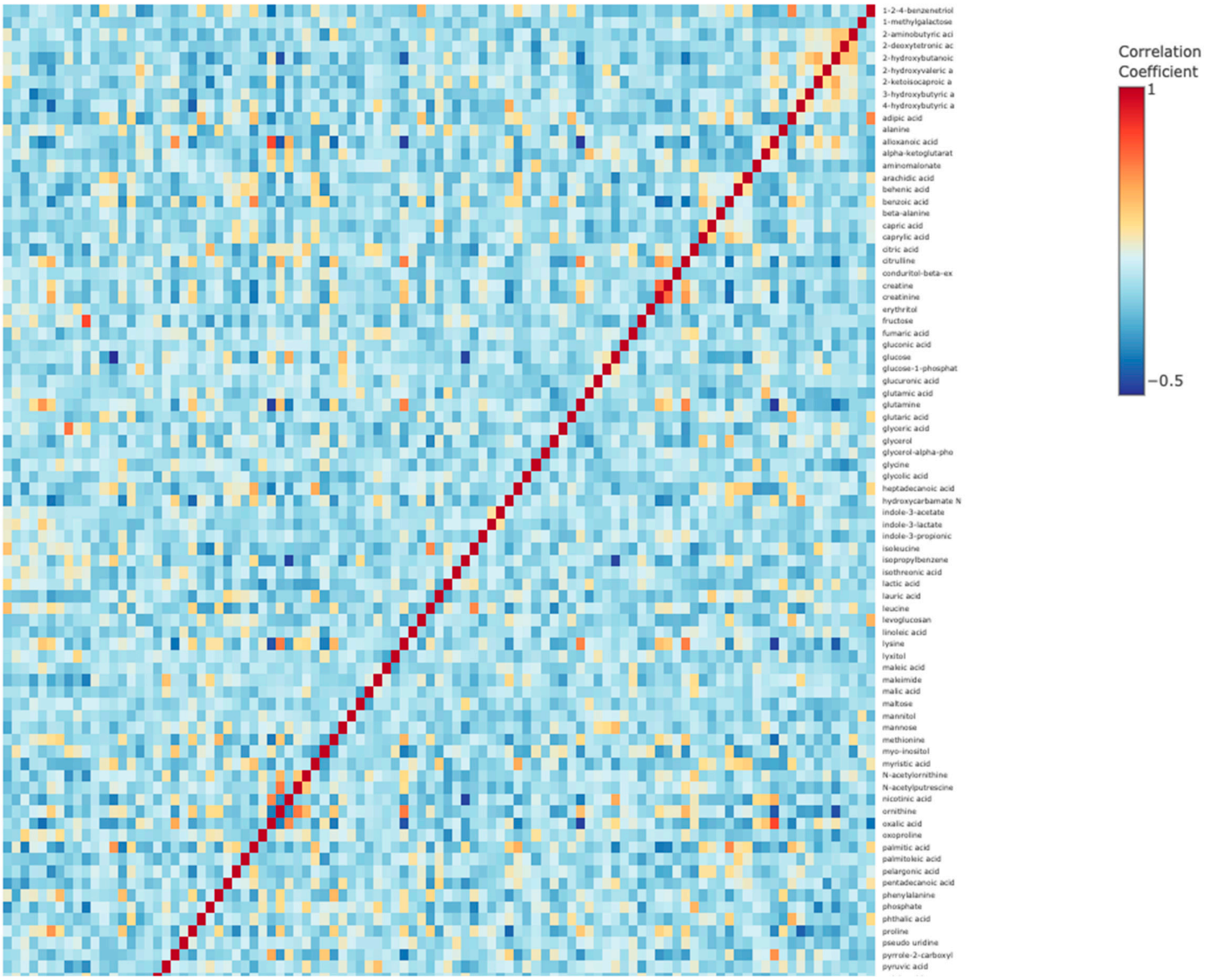


Figure S1. Correlation heatmap analysis results.

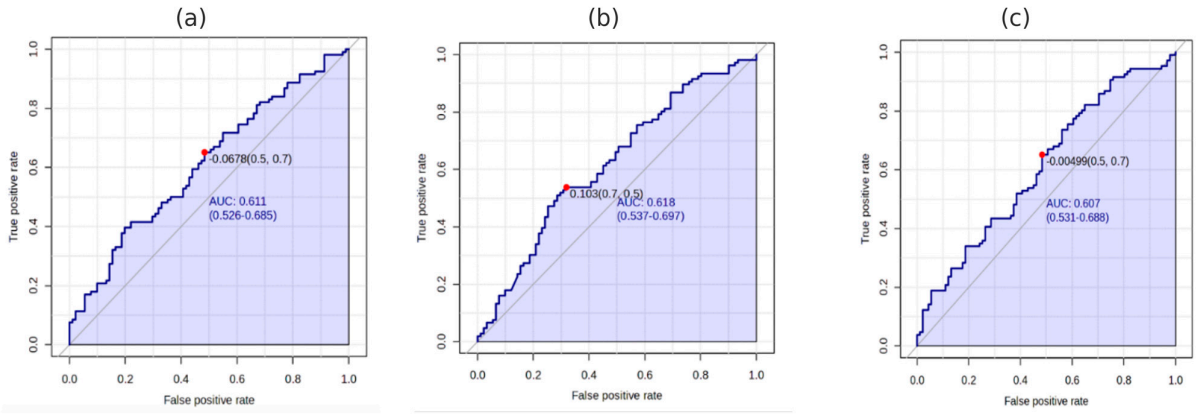


Figure S2. Univariate ROC curves of the first three biomarker candidate compounds in the TPOT SHAP plot.