Supplementary Figures

Supplementary Figure S1. Principal component analysis of samples. First two principal components are shown. Samples outside [$\mu \pm 5SD$] are labelled outliers. The dotted lines represent $\mu \pm 5SD$.

Supplementary Figure S2. Mean decrease in accuracy (variable importance) of the random forest model trained on all metabolites.

Supplementary Figure S3. Non-zero coefficients of metabolites in the LASSO model. Absolute value of the coefficients are plotted to identify knee point to select a subset of metabolites to develop metabolic risk score.