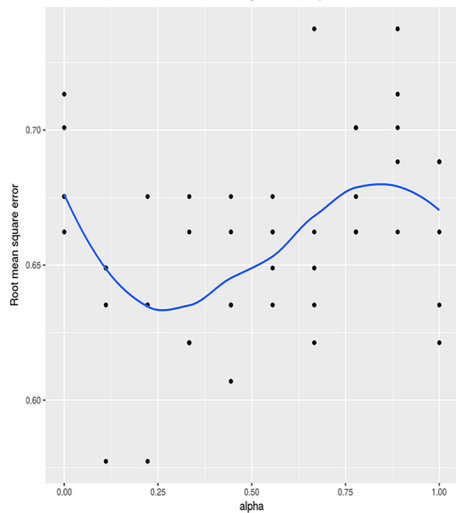
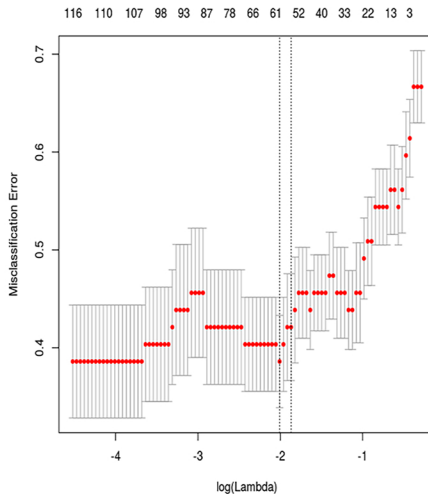
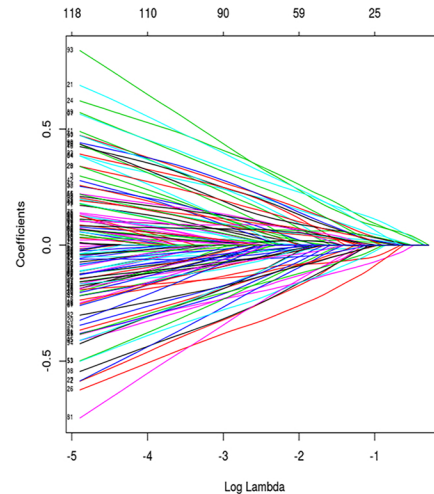


**A**

Cross validation best RMSE for differing values of alpha

**B****C**

Supplementary Figure 2: Selection of metabolites using elastic net regularization. (A) Tuning alpha parameter, the parameter representing the degree of mixing between lasso ( $\alpha=1$ ) and the ridge regularization ( $\alpha=0$ ). Y-axis is the root mean square error of the 10-fold cross-validation. We selected  $\alpha=0.22$  as it gave us the minimum error. (B) Tuning lambda, the parameter controlling the shrunk rate of coefficients in the linear model. Y-axis is the misclassification error of the 10-fold cross validation. X-axis is the range of lambda, with the optimal  $\lambda=0.008$  as it gave us the minimum misclassification error. (C) The shrinkage coefficients of the metabolites using tuned alpha and lambda. Only metabolites with non-zero coefficient were selected.