



Figure S4. OPLS-DA model validation diagram. The abscissa represents the model accuracy. The ordinate is the model classification effect frequency. The model performs 200 random arrangements and combination experiments on the data. If  $P = 0.02$  for  $Q^2$ , the prediction ability of four random grouping models in this permutation test is better than that of the OPLS-DA model. If  $P = 0.545$  for  $R^2Y$ , there are 109 random grouping models in the permutation test and their rate of interpretation for the Y matrix is better than that of the OPLS-DA model. In general, the model is optimal at  $P < 0.05$ .