

OPLS-DA model	Outliers included	Outliers excluded (see manuscript)
Metabolomics data	$R^2Y = 0.76$; $Q^2 = 0.68$	$R^2Y = 0.75$; $Q^2 = 0.68$
Cytokine/chemokine data	$R^2Y = 0.72$; $Q^2 = 0.61$	$R^2Y = 0.74$; $Q^2 = 0.66$
Combined dataset	$R^2Y = 0.85$; $Q^2 = 0.72$	$R^2Y = 0.85$; $Q^2 = 0.74$