

Supplementary dataset S3: PCA and OPLS models summaries.

Cumulative proportion of variation in the dataset explained by each component in the PCA model

Component No.	Cumulative fraction of the sum of squares explained by the component(s): "R2X(cum)"
Comp[1]	0.159543
Comp[2]	0.302585
Comp[3]	0.407947
Comp[4]	0.506009
Comp[5]	0.575514
Comp[6]	0.638655
Comp[7]	0.693675
Comp[8]	0.744602
Comp[9]	0.785956

OPLS model summary

OPLS model: 1 predictive component & 1, 2 or 3 orthogonal component	Fraction of the variation explained by the model: "R2Y(cum)"	Fraction of of the variation related to TWG that can be predicted by the model: "Q2(cum)"
Comp[1+0]	0.676476	0.399173
Comp[1+1]	0.861713	0.545341
Comp[1+2]	0.915427	0.656604
Comp[1+3]	0.943066	0.747226