

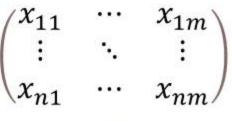
Pre-Processing

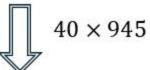
Baseline Correction

Auto-Scaling

Log-Transformation

Feature-Matrix





Test

 $y = X\beta + \epsilon$ Model Evaluation
RMSEP
LoA
95% Limits

PLS Model Building

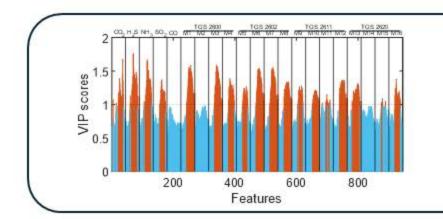
Leave-One-Block-Out CV

 LV_i ; $i=1\cdots 4$

Leave-One-Sample-Out



RMSECV



Feature Analysis

4:

$$\mathit{VIP}^1_{score} > 1$$

:

 $VIP^m_{score} > 1$

$$v_{j} = \sqrt{\frac{p \sum_{a=1}^{A} \left[SS_{a} \left(\frac{w_{aj}}{\|w_{a}\|} \right)^{2} \right]}{\sum_{a=1}^{A} SS_{a}}}$$