

Pre-Processing

Baseline Correction

Auto-Scaling

Log-Transformation

Feature-Matrix

 x_{1m} x_{nm}



Test

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

PLS Model Building

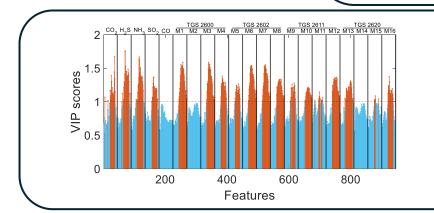
Leave-One-Block-Out CV

 LV_i ; $i = 1 \cdots 4$

Leave-One-Sample-Out



RMSECV



Feature Analysis

4 :

$$VIP_{score}^1 > 1$$

 $VIP^m_{score} > 1$

$$v_j = \sqrt{\frac{p \sum_{a=1}^{A} \left[SS_a \left(\frac{w_{aj}}{\|w_a\|} \right)^2 \right]}{\sum_{a=1}^{A} SS_a}}$$