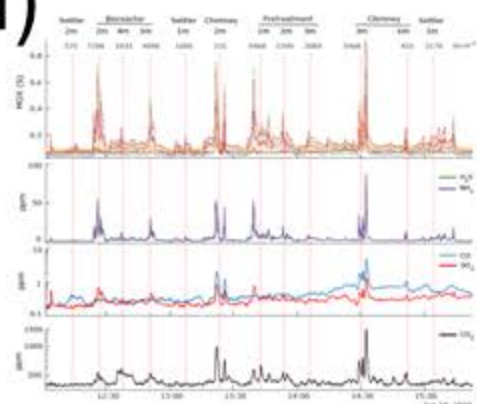
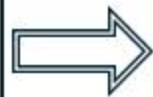


a)



RAW  
DATA



## Pre-Processing

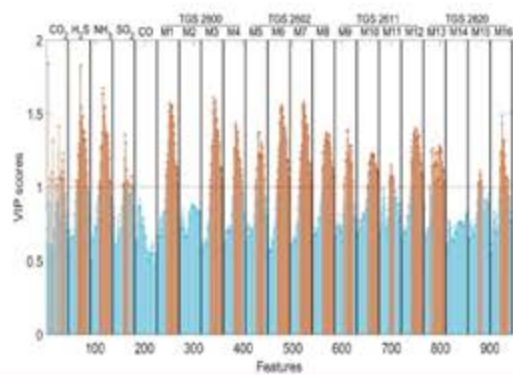
Log-  
Transformation

Auto-Scaling

Feature-Matrix

$$\begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$$

73 × 945



## Feature Selection

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

$\vdots$

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

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

## PLS Model Building

Leave-One-Block-Out CV

$LV_i; i = 1 \dots 4$

Leave-One-  
Sample-Out



RMSECV

$\vdots 4$

Model Evaluation

RMSEP

LoA

95% Limits

$$y_1 = X\beta_1 + \epsilon$$

$\vdots 4$

$$y_p = X\beta_p + \epsilon$$