Partial Least Square (PLS)

Partial least squares (PLS)

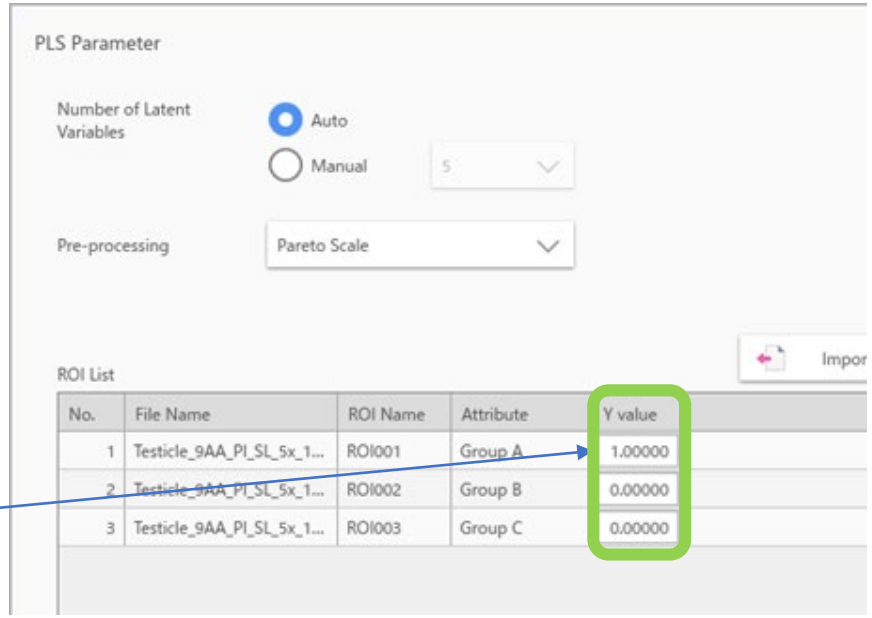
- Partial Least Squares is the one method to solve simultaneous equations. (PLS1)
  - y =XB
    - y: $\begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_n \end{pmatrix}$ X: $\begin{pmatrix} x_{11}\, x_{12} & \cdot & \cdot & x_{1m} \\ x_{21}\, x_{22} & \cdot & \cdot & x_{2m} \\ & & \cdot & \\ & & \cdot & \\ x_{\mathrm{n1}}\, x_{\mathrm{n2}} & \cdot & \cdot & x_{nm} \end{pmatrix}$
    - B: $\begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_m \end{pmatrix}$
    - $y_1 = b_1\, x_{11} + b_2\, x_{12} + \cdot\ \cdot + b_{\mathrm{m}} x_{1m}$

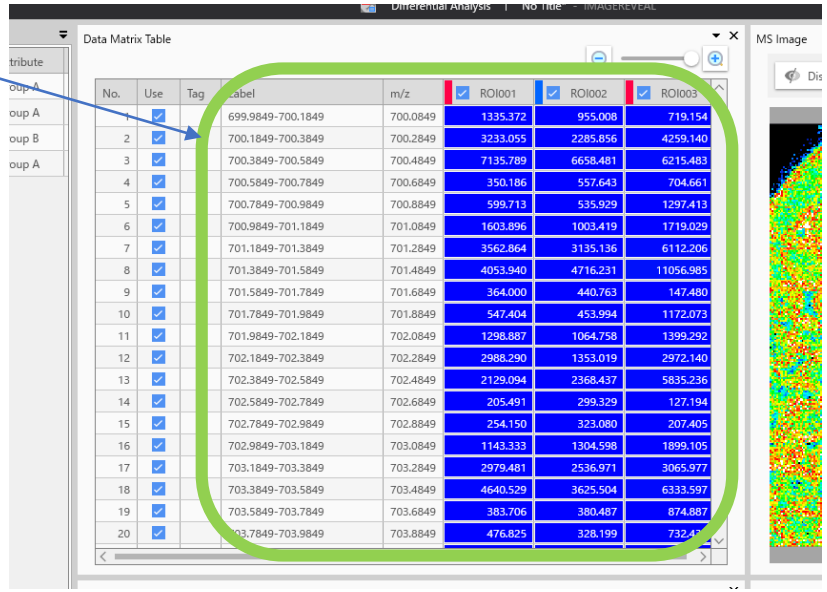
- PLS1 tries to find a linear decomposition of X and y such that
  - $X=TP^t+E$ and $y=Tq+f$, where
  - T: Scores
  - P: X loadings q: y loadings
  - E: X residuals f: y residuals
- Decomposition is finalized so as to <u>maximize covariance between T and y.</u>

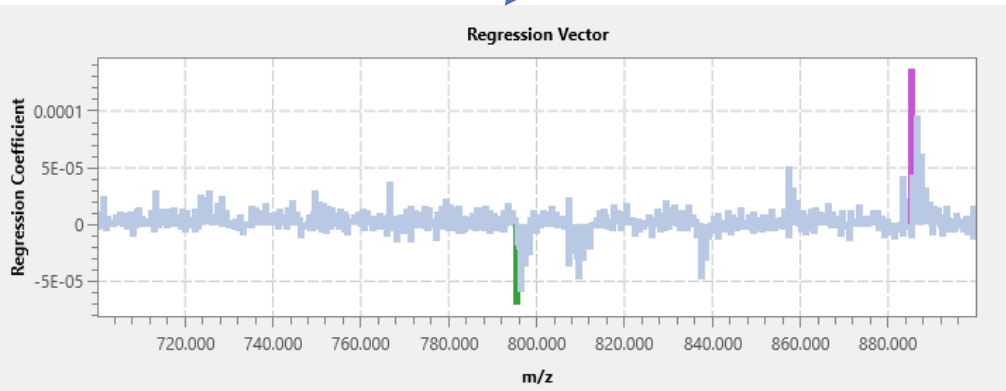
$$w = \frac{\mathbf{X}^{\mathrm{T}}\mathbf{y}}{\|\mathbf{X}^{\mathrm{T}}\mathbf{y}\|} \qquad \mathbf{b} = \mathbf{W}\left(\mathbf{P}^{\mathrm{T}}\mathbf{W}\right)^{-1}\mathbf{q}$$

Object of PLS

- PLS can solve the equation
  - Y = XB
    - In this case,
      - Y: user input
      - X: m/z Intensity
      - B: regression coefficient



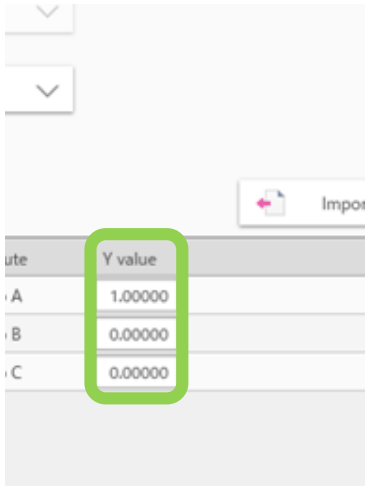




In IMAGEREVEAL MS,

y : User input
X: signal intensity of each m/z
B: calculated

$$y = X B$$



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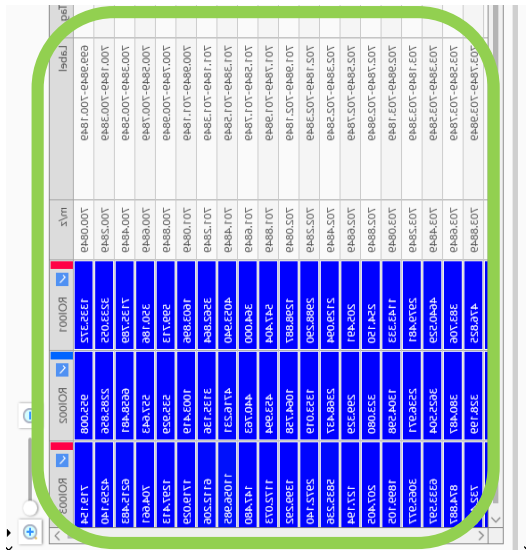
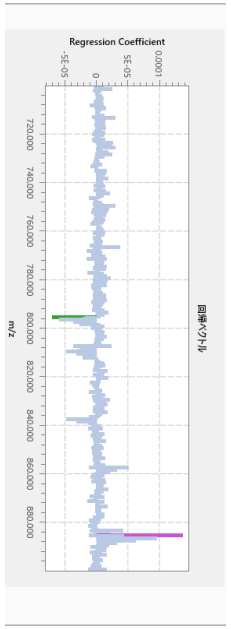
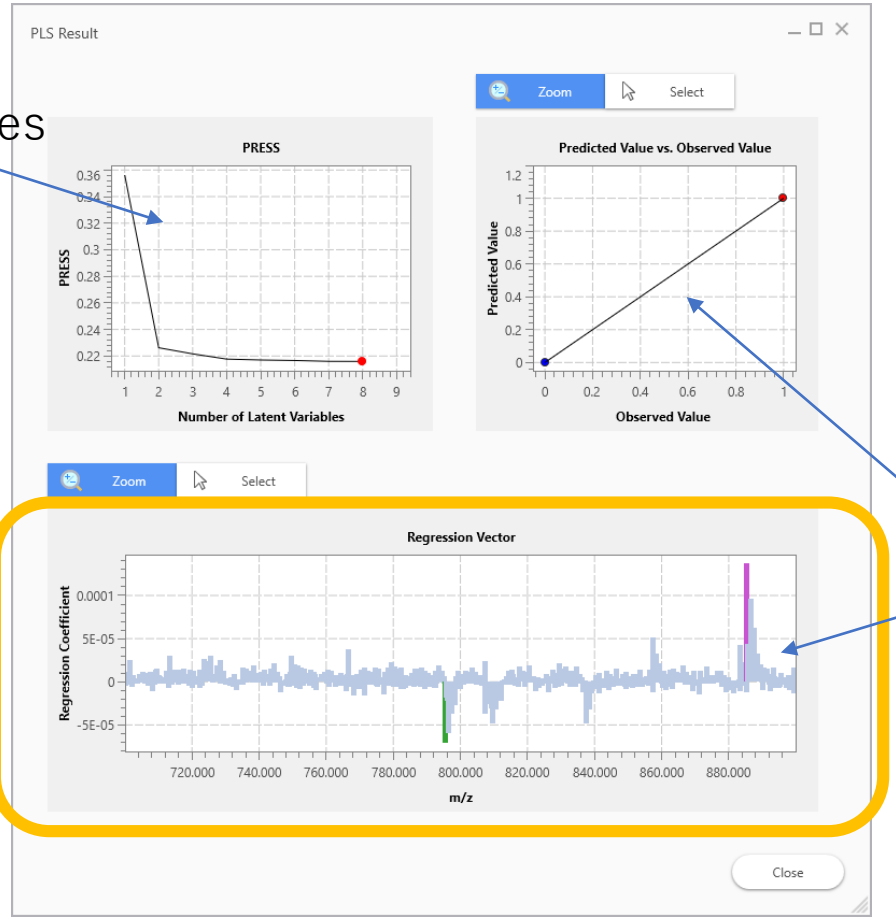




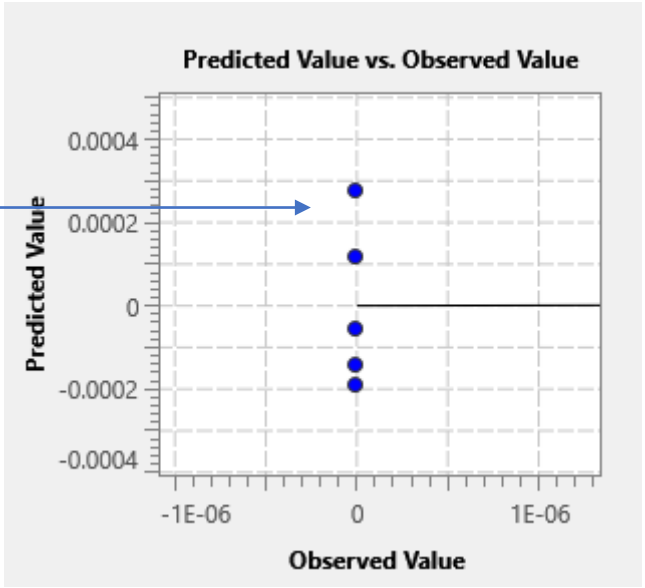
PLS result

How many Latent variables are good to predict.



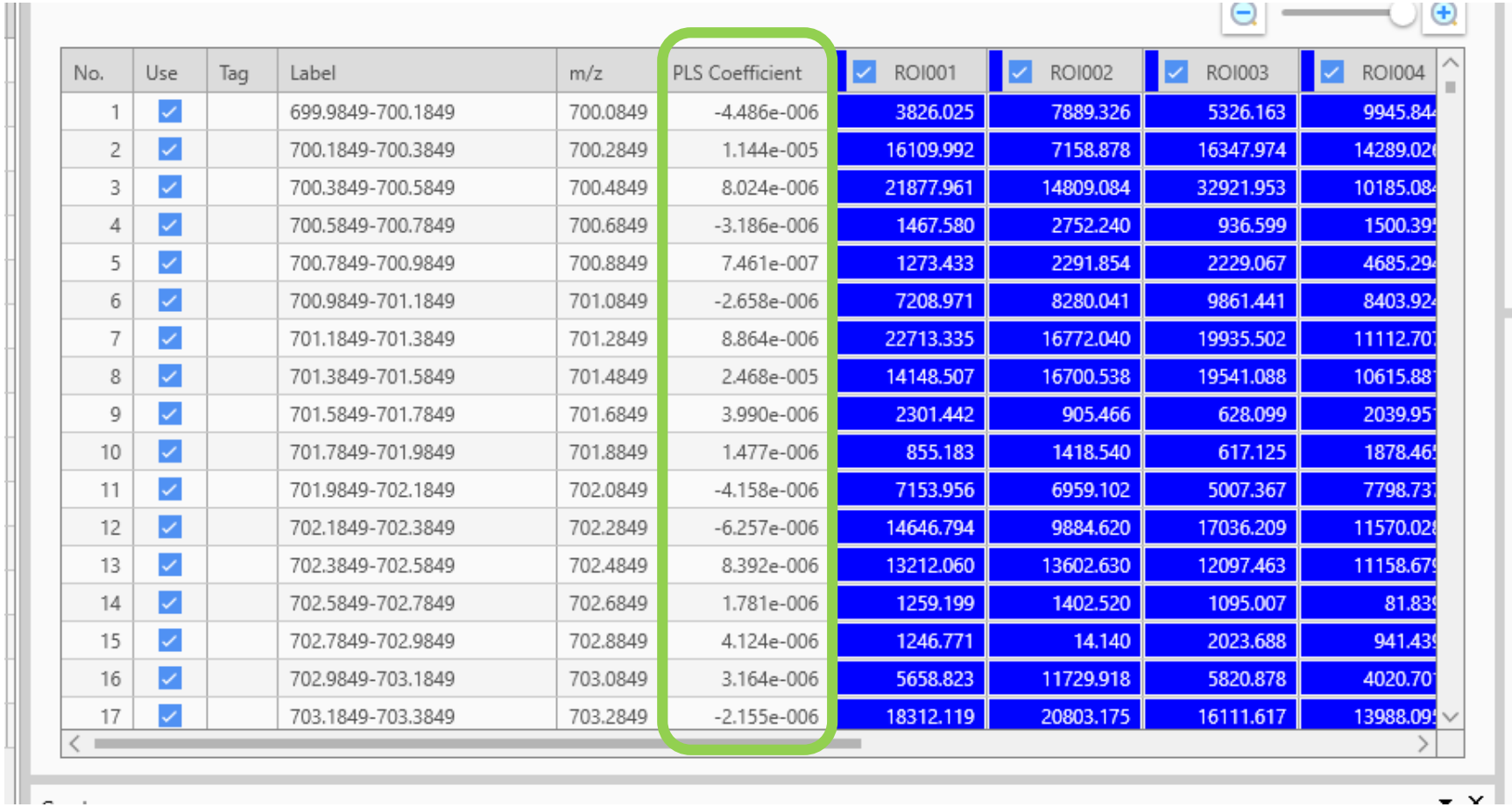
Y = XB

“predicted” means “calculated”



“Observed” means “input”

Regression coefficient is described in the “Data Matrix Table”.



No.	Use	Tag	Label	m/z	PLS Coefficient	ROI001	ROI002	ROI003	ROI004
1	✓		699.9849-700.1849	700.0849	-4.486e-006	3826.025	7889.326	5326.163	9945.84
2	✓		700.1849-700.3849	700.2849	1.144e-005	16109.992	7158.878	16347.974	14289.02
3	✓		700.3849-700.5849	700.4849	8.024e-006	21877.961	14809.084	32921.953	10185.08
4	✓		700.5849-700.7849	700.6849	-3.186e-006	1467.580	2752.240	936.599	1500.39
5	✓		700.7849-700.9849	700.8849	7.461e-007	1273.433	2291.854	2229.067	4685.29
6	✓		700.9849-701.1849	701.0849	-2.658e-006	7208.971	8280.041	9861.441	8403.92
7	✓		701.1849-701.3849	701.2849	8.864e-006	22713.335	16772.040	19935.502	11112.70
8	✓		701.3849-701.5849	701.4849	2.468e-005	14148.507	16700.538	19541.088	10615.88
9	✓		701.5849-701.7849	701.6849	3.990e-006	2301.442	905.466	628.099	2039.95
10	✓		701.7849-701.9849	701.8849	1.477e-006	855.183	1418.540	617.125	1878.46
11	✓		701.9849-702.1849	702.0849	-4.158e-006	7153.956	6959.102	5007.367	7798.73
12	✓		702.1849-702.3849	702.2849	-6.257e-006	14646.794	9884.620	17036.209	11570.02
13	✓		702.3849-702.5849	702.4849	8.392e-006	13212.060	13602.630	12097.463	11158.67
14	✓		702.5849-702.7849	702.6849	1.781e-006	1259.199	1402.520	1095.007	81.83
15	✓		702.7849-702.9849	702.8849	4.124e-006	1246.771	14.140	2023.688	941.43
16	✓		702.9849-703.1849	703.0849	3.164e-006	5658.823	11729.918	5820.878	4020.70
17	✓		703.1849-703.3849	703.2849	-2.155e-006	18312.119	20803.175	16111.617	13988.09