

Partial Least Square (PLS)

Partial least squares (PLS)

- Partial Least Squares is the one method to solve simultaneous equations. (PLS1)

- $y = XB$

- $y: \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \quad X: \begin{pmatrix} x_{11} & x_{12} & \cdot & \cdot & x_{1m} \\ x_{21} & x_{22} & \cdot & \cdot & x_{2m} \\ & & \cdot & & \\ & & \cdot & & \\ x_{n1} & x_{n2} & \cdot & \cdot & x_{nm} \end{pmatrix}$

- $B: \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_m \end{pmatrix}$

- $y_1 = b_1 x_{11} + b_2 x_{12} + \cdot \cdot + b_m x_{1m}$

- 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 maximize covariance between T and y .

$$w = \frac{\mathbf{x}^T \mathbf{y}}{\|\mathbf{x}^T \mathbf{y}\|} \quad \mathbf{b} = \mathbf{W}(\mathbf{P}^T \mathbf{W})^{-1} \mathbf{q}$$

Object of PLS

- PLS can solve the equation

- $Y = XB$

- In this case,

- Y: user input

- X: m/z Intensity

- B: regression coefficient

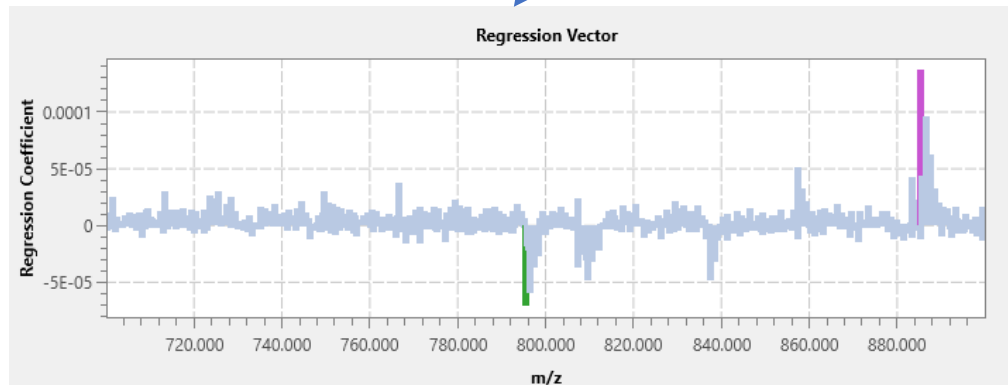
PLS Parameter

Number of Latent Variables: Auto Manual (5)

Pre-processing: Pareto Scale

ROI List

No.	File Name	ROI Name	Attribute	Y value
1	Testicle_9AA_P1_SL_5x_1...	ROI001	Group A	1.00000
2	Testicle_9AA_P1_SL_5x_1...	ROI002	Group B	0.00000
3	Testicle_9AA_P1_SL_5x_1...	ROI003	Group C	0.00000



Data Matrix Table

No.	Use	Tag	Label	m/z	ROI001	ROI002	ROI003
1	<input checked="" type="checkbox"/>		699.9849-700.1849	700.0849	1335.372	955.008	719.154
2	<input checked="" type="checkbox"/>		700.1849-700.3849	700.2849	3233.055	2285.856	4259.140
3	<input checked="" type="checkbox"/>		700.3849-700.5849	700.4849	7135.789	6658.481	6215.483
4	<input checked="" type="checkbox"/>		700.5849-700.7849	700.6849	350.186	557.643	704.661
5	<input checked="" type="checkbox"/>		700.7849-700.9849	700.8849	599.713	535.929	1297.413
6	<input checked="" type="checkbox"/>		700.9849-701.1849	701.0849	1603.896	1003.419	1719.029
7	<input checked="" type="checkbox"/>		701.1849-701.3849	701.2849	3562.864	3135.136	6112.206
8	<input checked="" type="checkbox"/>		701.3849-701.5849	701.4849	4053.940	4716.231	11056.985
9	<input checked="" type="checkbox"/>		701.5849-701.7849	701.6849	364.000	440.763	147.480
10	<input checked="" type="checkbox"/>		701.7849-701.9849	701.8849	547.404	453.994	1172.073
11	<input checked="" type="checkbox"/>		701.9849-702.1849	702.0849	1298.887	1064.758	1399.292
12	<input checked="" type="checkbox"/>		702.1849-702.3849	702.2849	2988.290	1353.019	2972.140
13	<input checked="" type="checkbox"/>		702.3849-702.5849	702.4849	2129.094	2368.437	5835.236
14	<input checked="" type="checkbox"/>		702.5849-702.7849	702.6849	205.491	299.329	127.194
15	<input checked="" type="checkbox"/>		702.7849-702.9849	702.8849	254.150	323.080	207.405
16	<input checked="" type="checkbox"/>		702.9849-703.1849	703.0849	1143.333	1304.598	1899.105
17	<input checked="" type="checkbox"/>		703.1849-703.3849	703.2849	2979.481	2536.971	3065.977
18	<input checked="" type="checkbox"/>		703.3849-703.5849	703.4849	4640.529	3625.504	6333.597
19	<input checked="" type="checkbox"/>		703.5849-703.7849	703.6849	383.706	380.487	874.887
20	<input checked="" type="checkbox"/>		703.7849-703.9849	703.8849	476.825	328.199	732.413

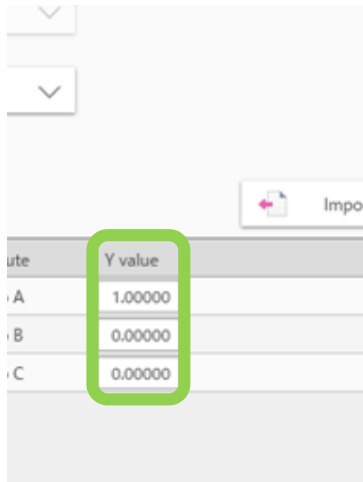
In IMAGEREVEAL MS,

y : User input

X: signal intensity of each m/z

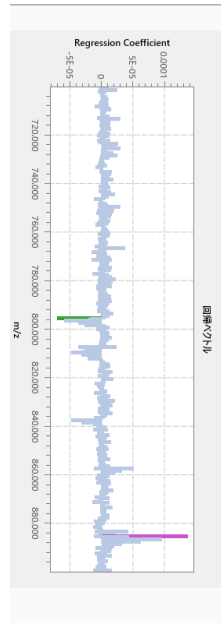
B: calculated

$$y = X B$$



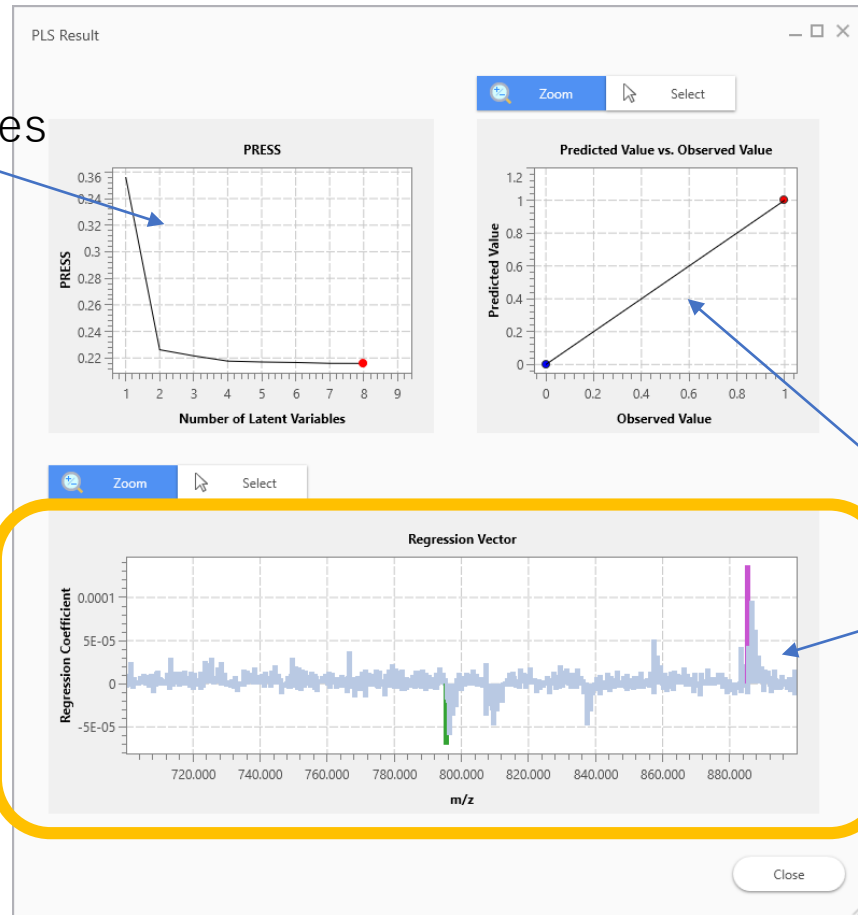
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m/z	Intensity	Label
100.0000	100.0000	100.0000
101.0000	101.0000	101.0000
102.0000	102.0000	102.0000
103.0000	103.0000	103.0000
104.0000	104.0000	104.0000
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199.0000	199.0000	199.0000
200.0000	200.0000	200.0000

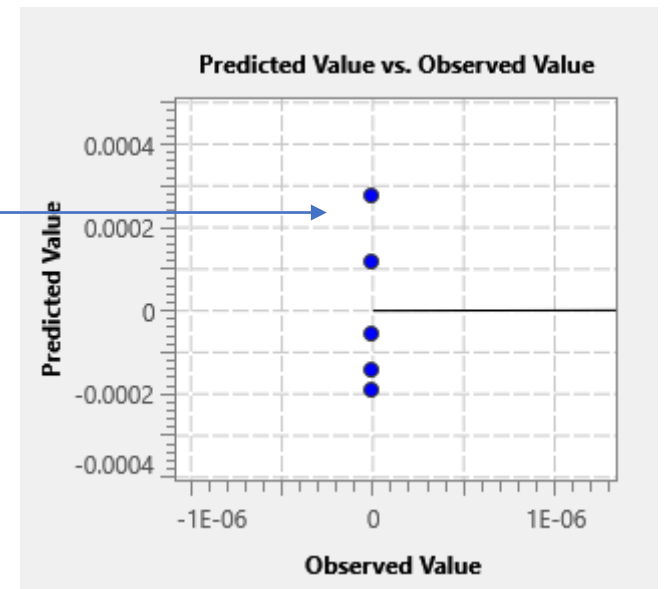


PLS result

How many Latent variables are good to predict.



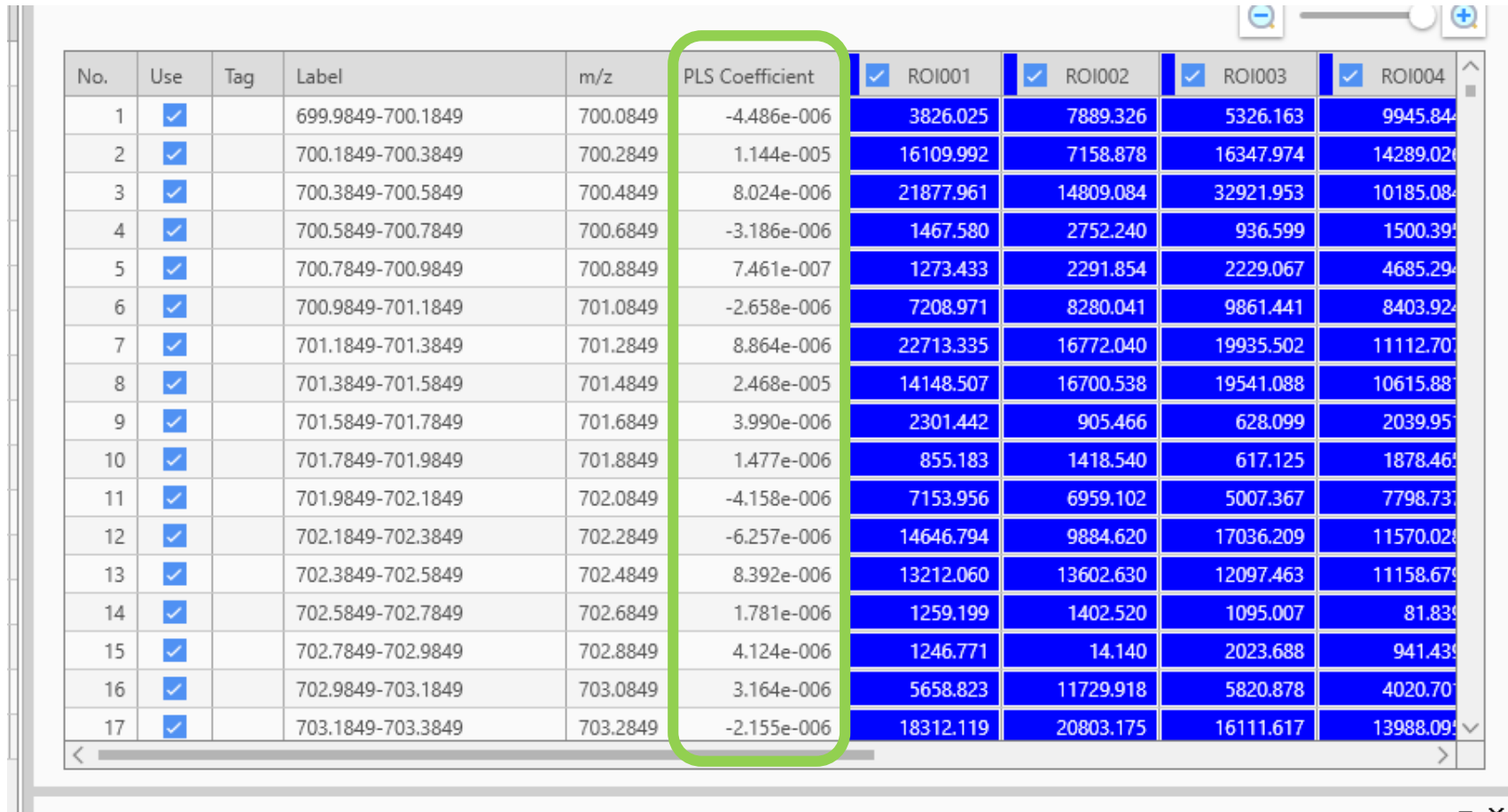
“predicted” means “calculated”



“Observed” means “input”

$$Y = XB$$

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



The screenshot displays a software window containing a table with 17 rows and 10 columns. The columns are: No., Use, Tag, Label, m/z, PLS Coefficient, ROI001, ROI002, ROI003, and ROI004. The 'PLS Coefficient' column is highlighted with a green rectangular box. Each row contains numerical data for these columns. The 'Use' column contains blue checkmarks, and the ROI columns also contain blue checkmarks in their headers.

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