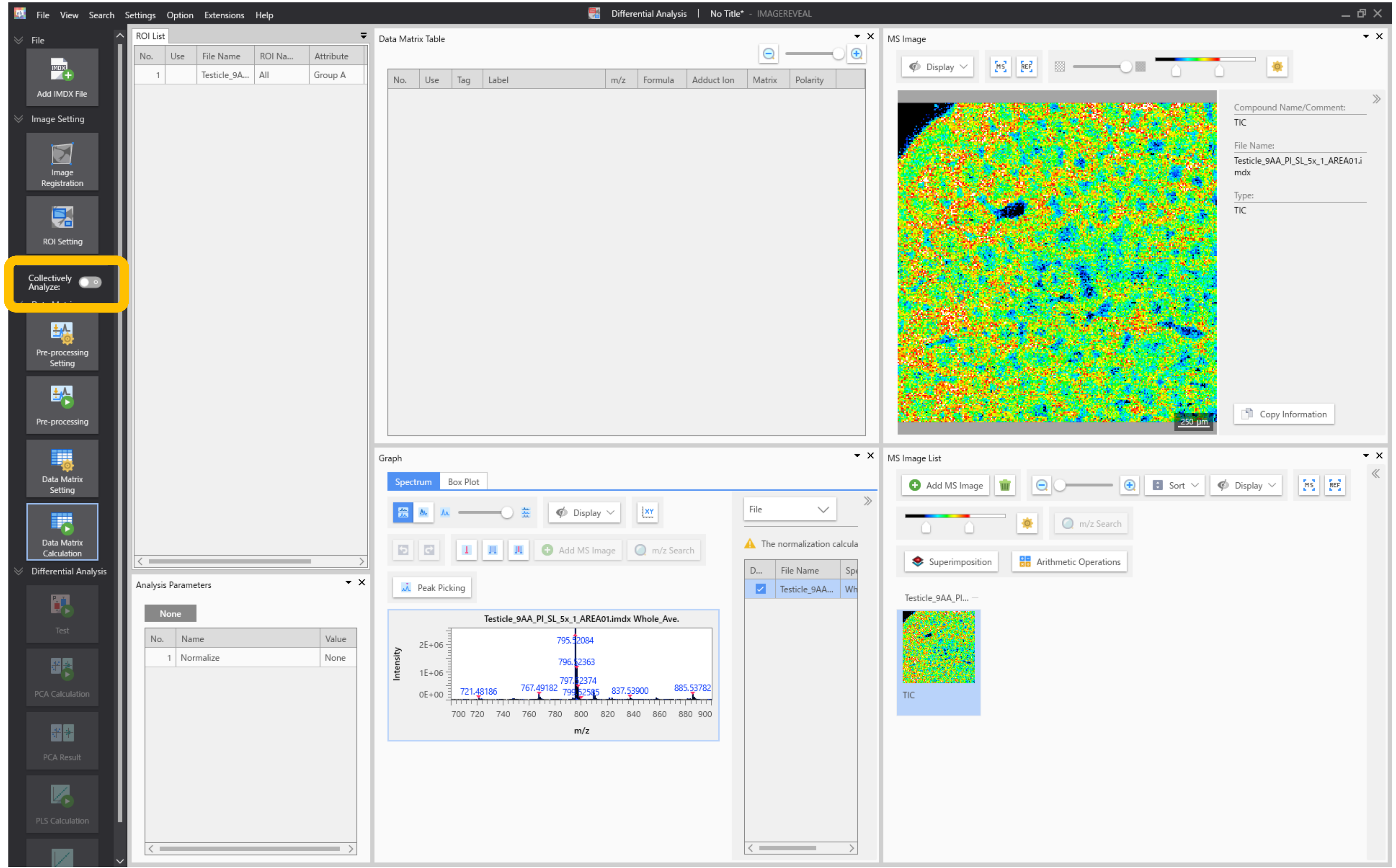
Collective analysis

The collective analysis function has been added in version 1.1



ROI List

No.	Use	File Name	ROI Na...	Attribute
1		Testicle_9A...	All	Group A

Data Matrix Table

No.	Use	Tag	Label	m/z	Formula	Adduct Ion	Matrix	Polarity

Compound Name/Comment:
TIC
File Name:
Testicle_9AA_PI_SL_5x_1_AREA01.imdx
Type:
TIC

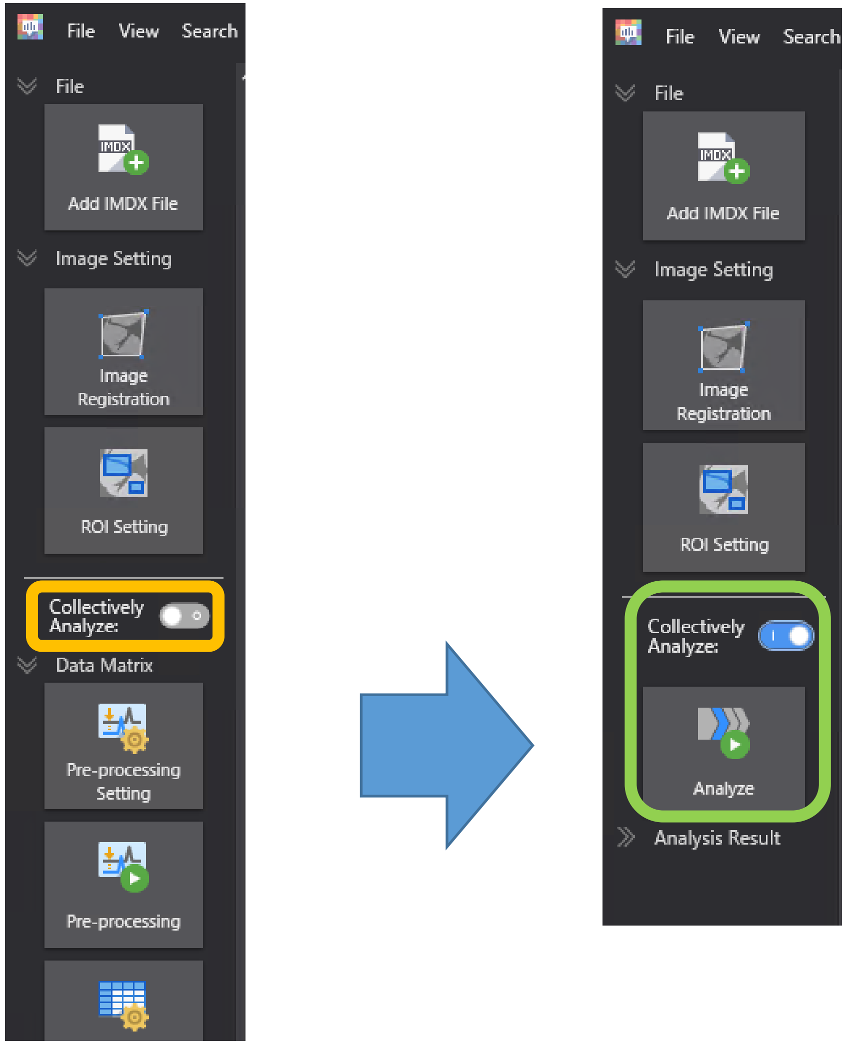
Analysis Parameters

No.	Name	Value
1	Normalize	None

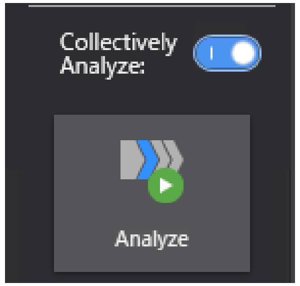
The normalization calcula

D...	File Name	Spe
☑	Testicle_9AA...	Wh

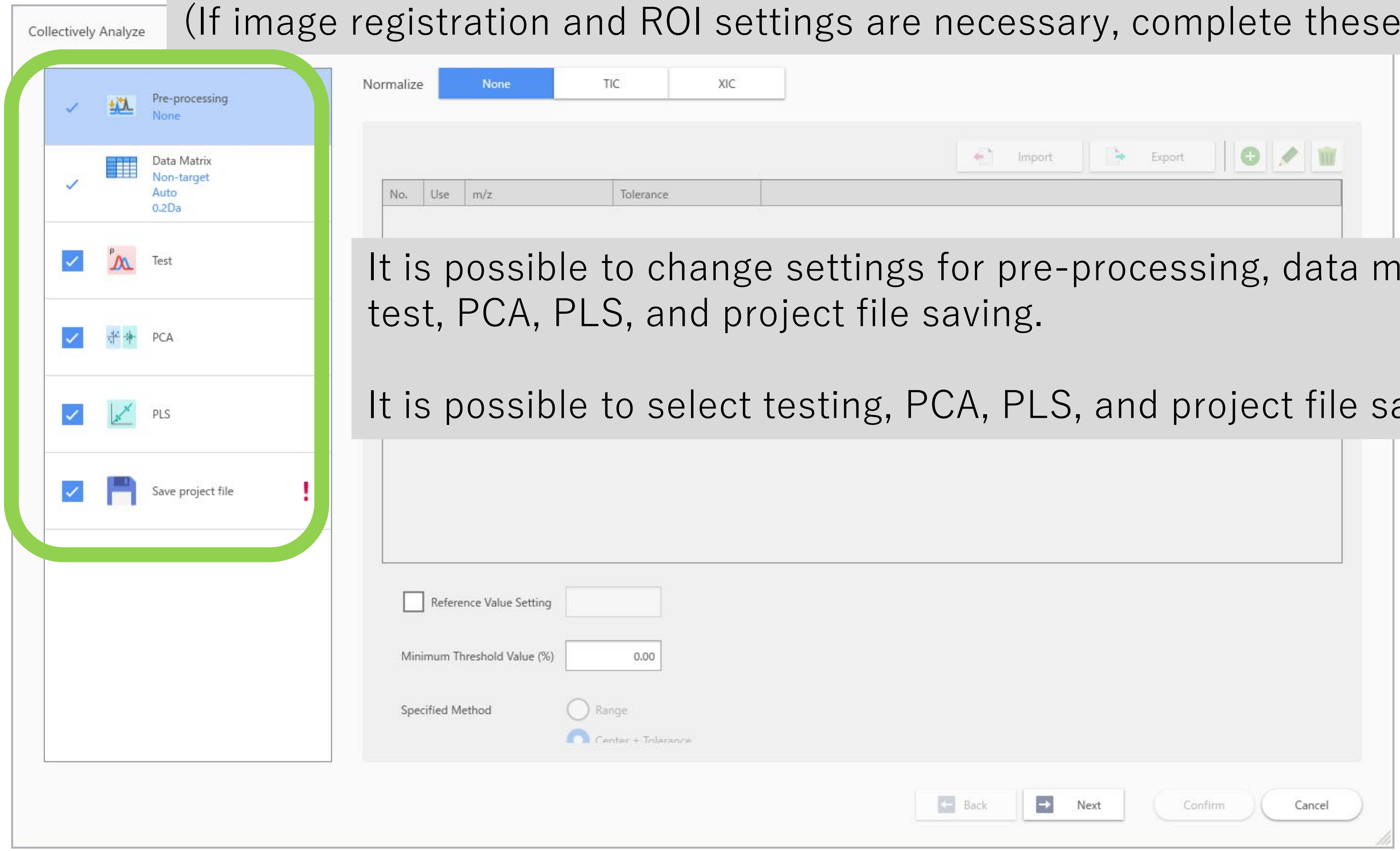
Switch on the “collective analysis” and the contents of the menu bar changes



Collective analysis settings screen



(If image registration and ROI settings are necessary, complete these beforehand)



✓ Pre-processing
None

✓ Data Matrix
Non-target
Auto
0.2Da

☑ Test

☑ PCA

☑ PLS

☑ Save project file !

Normalize: **None** | TIC | XIC

No.	Use	m/z	Tolerance

☐ Reference Value Setting

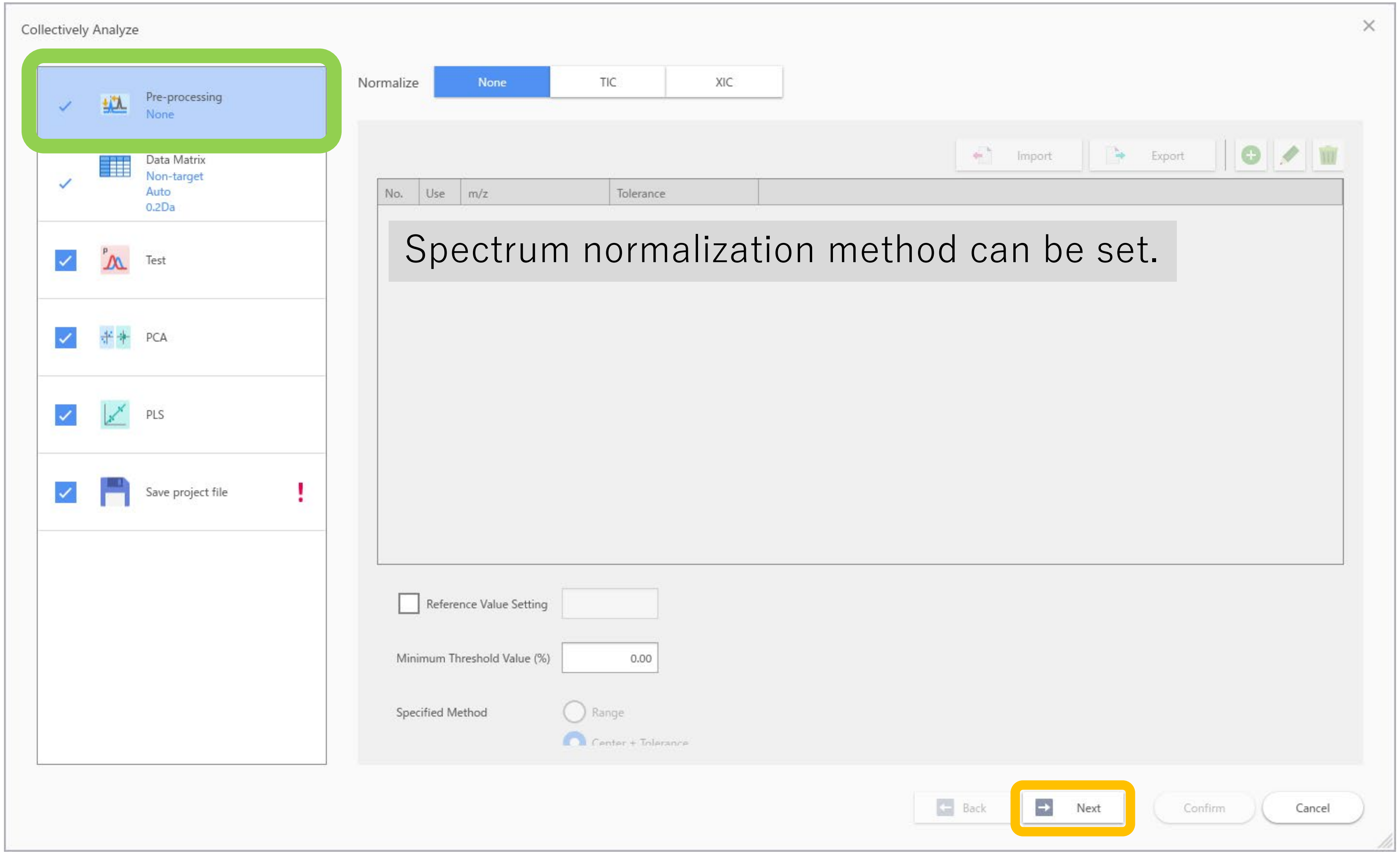
Minimum Threshold Value (%) 0.00

Specified Method ○ Range ● Center + Tolerance

It is possible to change settings for pre-processing, data matrix settings, test, PCA, PLS, and project file saving.

It is possible to select testing, PCA, PLS, and project file saving.

1. Pre-processing (normalization)



Collectively Analyze

- ✓ Pre-processing: None
- ✓ Data Matrix: Non-target, Auto, 0.2Da
- ☑ Test
- ☑ PCA
- ☑ PLS
- ☑ Save project file !

Normalize: **None** | TIC | XIC

No.	Use	m/z	Tolerance

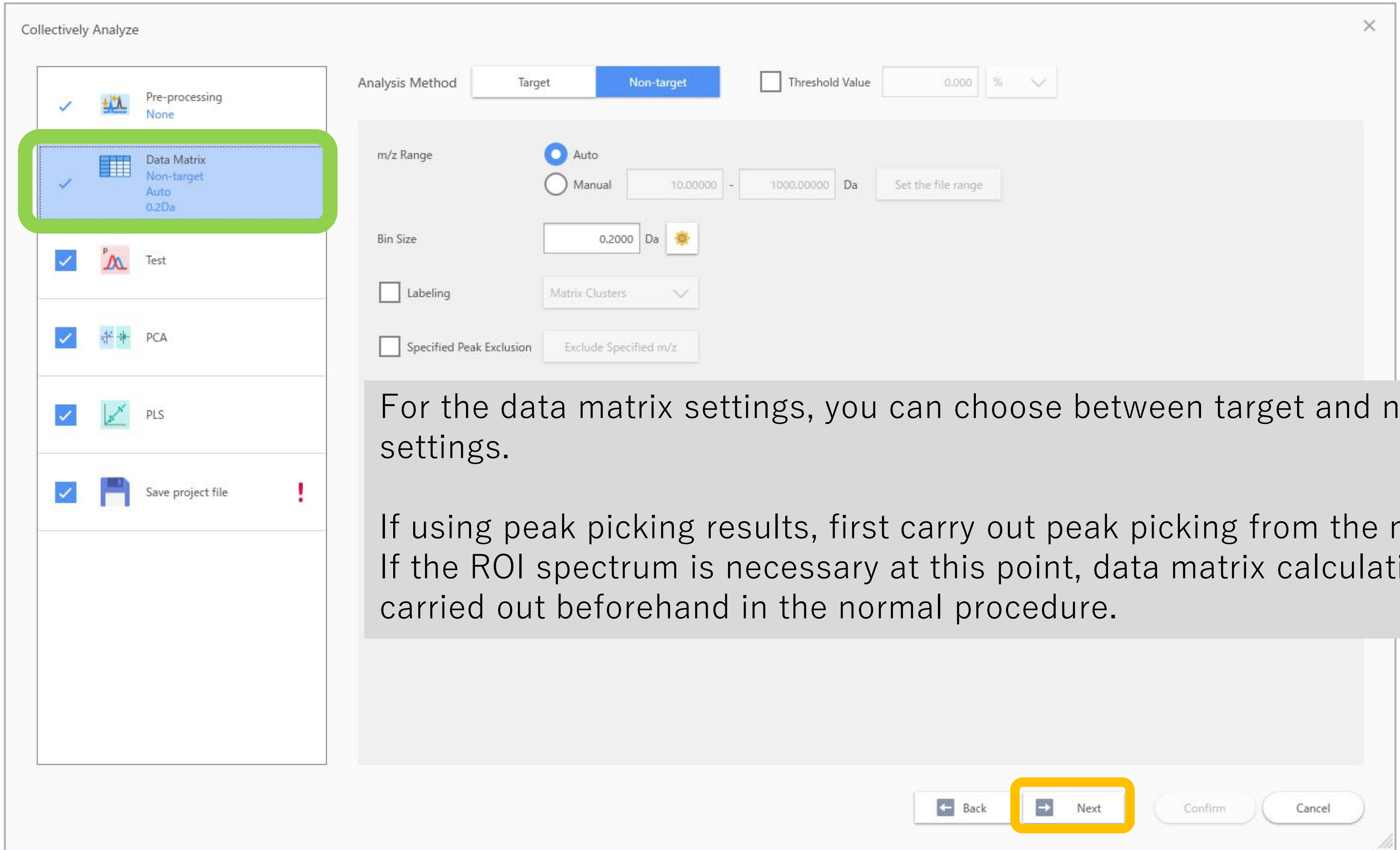
☐ Reference Value Setting

Minimum Threshold Value (%): 0.00

Specified Method: ○ Range ● Center + Tolerance

Spectrum normalization method can be set.

2. Data matrix settings


Collectively Analyze

✓ Pre-processing
None

✓ Data Matrix
Non-target
Auto
0.2Da

☑ Test

☑ PCA

☑ PLS

☑ Save project file !

Analysis Method: Target / **Non-target**

☐ Threshold Value 0.000 %

m/z Range: ● Auto
○ Manual 10.00000 - 1000.00000 Da

Bin Size: 0.2000 Da

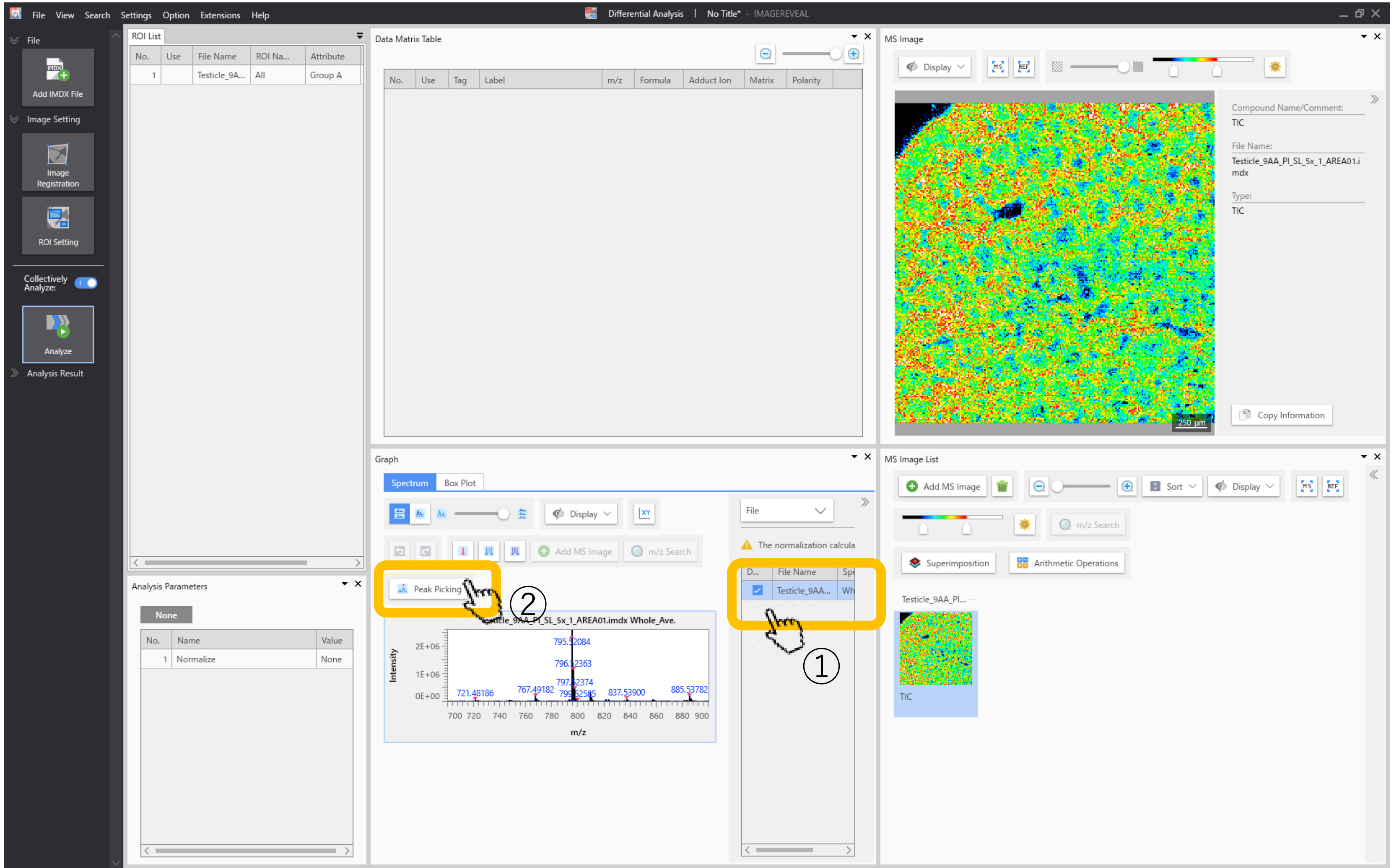
☐ Labeling: Matrix Clusters

☐ Specified Peak Exclusion: Exclude Specified m/z

For the data matrix settings, you can choose between target and non-target settings.

If using peak picking results, first carry out peak picking from the main window.
If the ROI spectrum is necessary at this point, data matrix calculations should be carried out beforehand in the normal procedure.

If peak picking is necessary:



No.	Use	File Name	ROI Na...	Attribute
1		Testicle_9A...	All	Group A

No.	Use	Tag	Label	m/z	Formula	Adduct Ion	Matrix	Polarity

Compound Name/Comment:
TIC
File Name:
Testicle_9AA_PI_SL_5x_1_AREA01.imdx
Type:
TIC

Analysis Parameters

None

No.	Name	Value
1	Normalize	None

File

The normalization calcula

D...	File Name	Spe
☑	Testicle_9AA...	Wh

Testicle_9AA_PI_SL_5x_1_AREA01.imdx Whole_Ave.

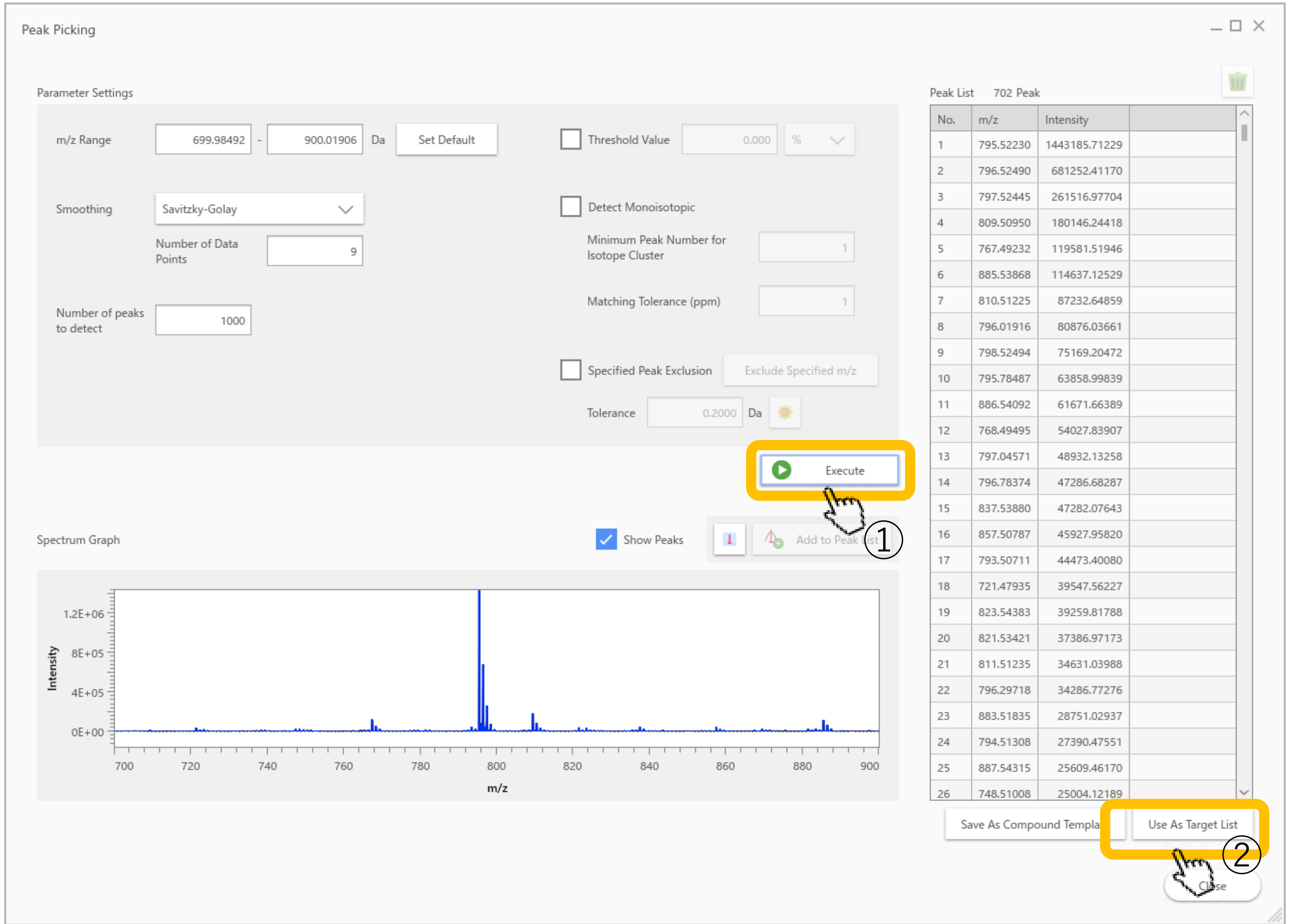
795.52084, 796.52363, 797.52374, 798.52585, 721.48186, 767.49182, 837.53900, 885.53782

Testicle_9AA_PI...

TIC

2. Data matrix settings

Peak picking


Peak Picking

Parameter Settings

m/z Range 699.98492 - 900.01906 Da

Smoothing: Savitzky-Golay

Number of Data Points: 9

Number of peaks to detect: 1000

☐ Threshold Value 0.000 %

☐ Detect Monoisotopic

Minimum Peak Number for Isotope Cluster: 1

Matching Tolerance (ppm): 1

☐ Specified Peak Exclusion

Tolerance 0.2000 Da

① Execute

Spectrum Graph ☑ Show Peaks

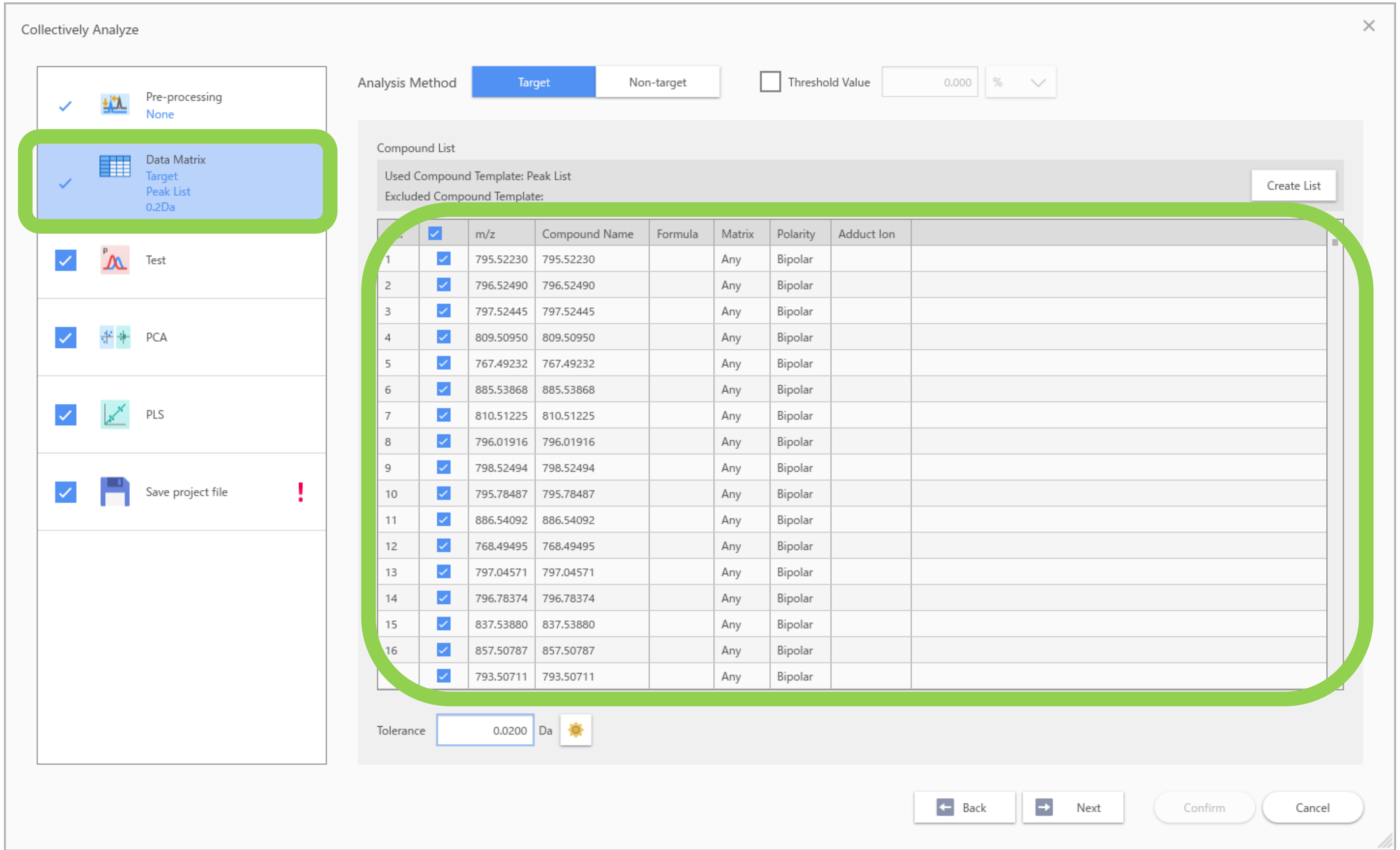
Peak List 702 Peak

No.	m/z	Intensity
1	795.52230	1443185.71229
2	796.52490	681252.41170
3	797.52445	261516.97704
4	809.50950	180146.24418
5	767.49232	119581.51946
6	885.53868	114637.12529
7	810.51225	87232.64859
8	796.01916	80876.03661
9	798.52494	75169.20472
10	795.78487	63858.99839
11	886.54092	61671.66389
12	768.49495	54027.83907
13	797.04571	48932.13258
14	796.78374	47286.68287
15	837.53880	47282.07643
16	857.50787	45927.95820
17	793.50711	44473.40080
18	721.47935	39547.56227
19	823.54383	39259.81788
20	821.53421	37386.97173
21	811.51235	34631.03988
22	796.29718	34286.77276
23	883.51835	28751.02937
24	794.51308	27390.47551
25	887.54315	25609.46170
26	748.51008	25004.12189

② Use As Target List

2. Data matrix settings

The peak picking results are automatically input and become target peaks



Analysis Method: Target

☐ Threshold Value 0.000 %

Compound List

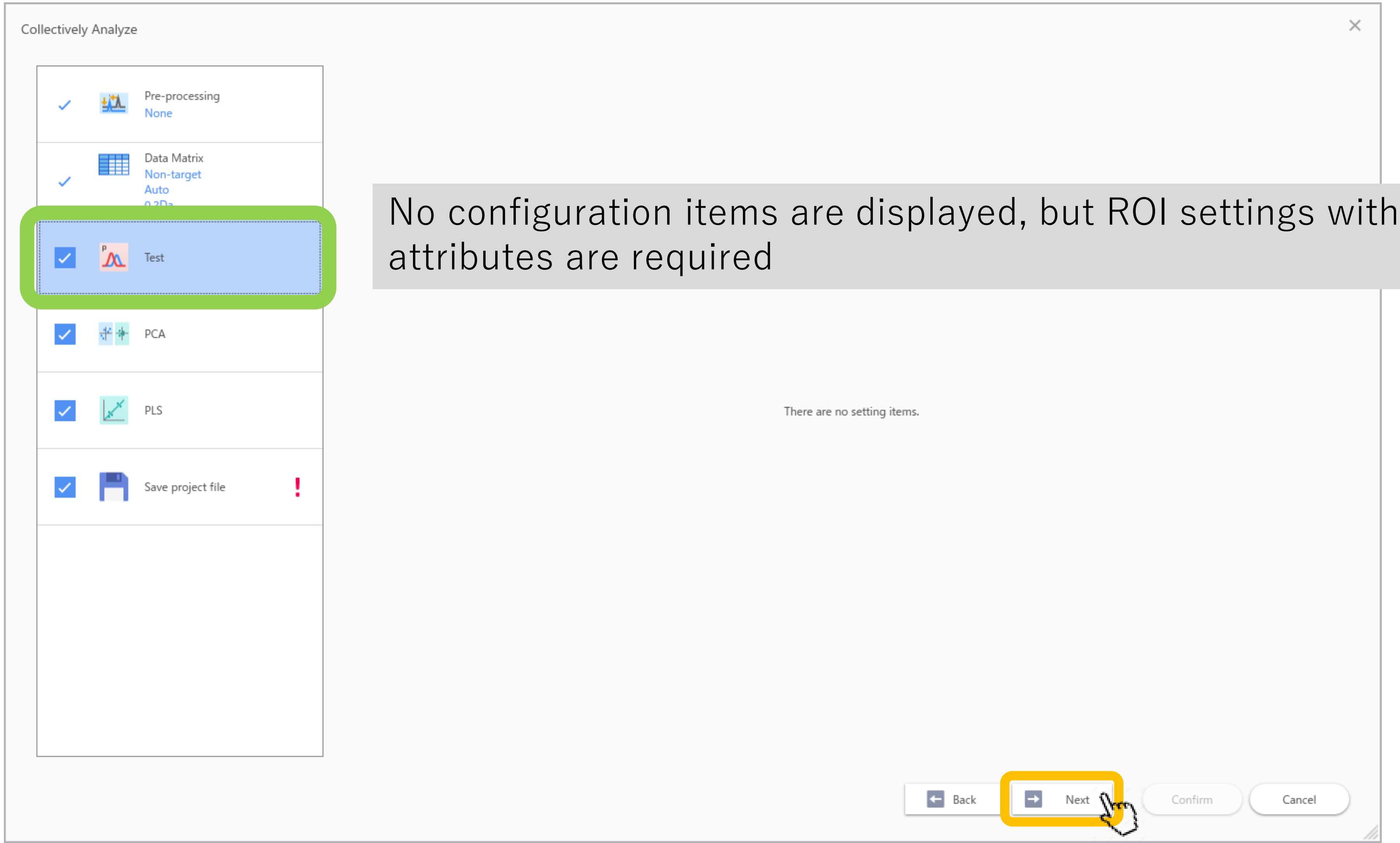
Used Compound Template: Peak List

Excluded Compound Template:

	☑	m/z	Compound Name	Formula	Matrix	Polarity	Adduct Ion
1	☑	795.52230	795.52230		Any	Bipolar	
2	☑	796.52490	796.52490		Any	Bipolar	
3	☑	797.52445	797.52445		Any	Bipolar	
4	☑	809.50950	809.50950		Any	Bipolar	
5	☑	767.49232	767.49232		Any	Bipolar	
6	☑	885.53868	885.53868		Any	Bipolar	
7	☑	810.51225	810.51225		Any	Bipolar	
8	☑	796.01916	796.01916		Any	Bipolar	
9	☑	798.52494	798.52494		Any	Bipolar	
10	☑	795.78487	795.78487		Any	Bipolar	
11	☑	886.54092	886.54092		Any	Bipolar	
12	☑	768.49495	768.49495		Any	Bipolar	
13	☑	797.04571	797.04571		Any	Bipolar	
14	☑	796.78374	796.78374		Any	Bipolar	
15	☑	837.53880	837.53880		Any	Bipolar	
16	☑	857.50787	857.50787		Any	Bipolar	
	☑	793.50711	793.50711		Any	Bipolar	

Tolerance 0.0200 Da

3. Test


Collectively Analyze

Pre-processing
None

Data Matrix
Non-target
Auto

☑ Test

☑ PCA

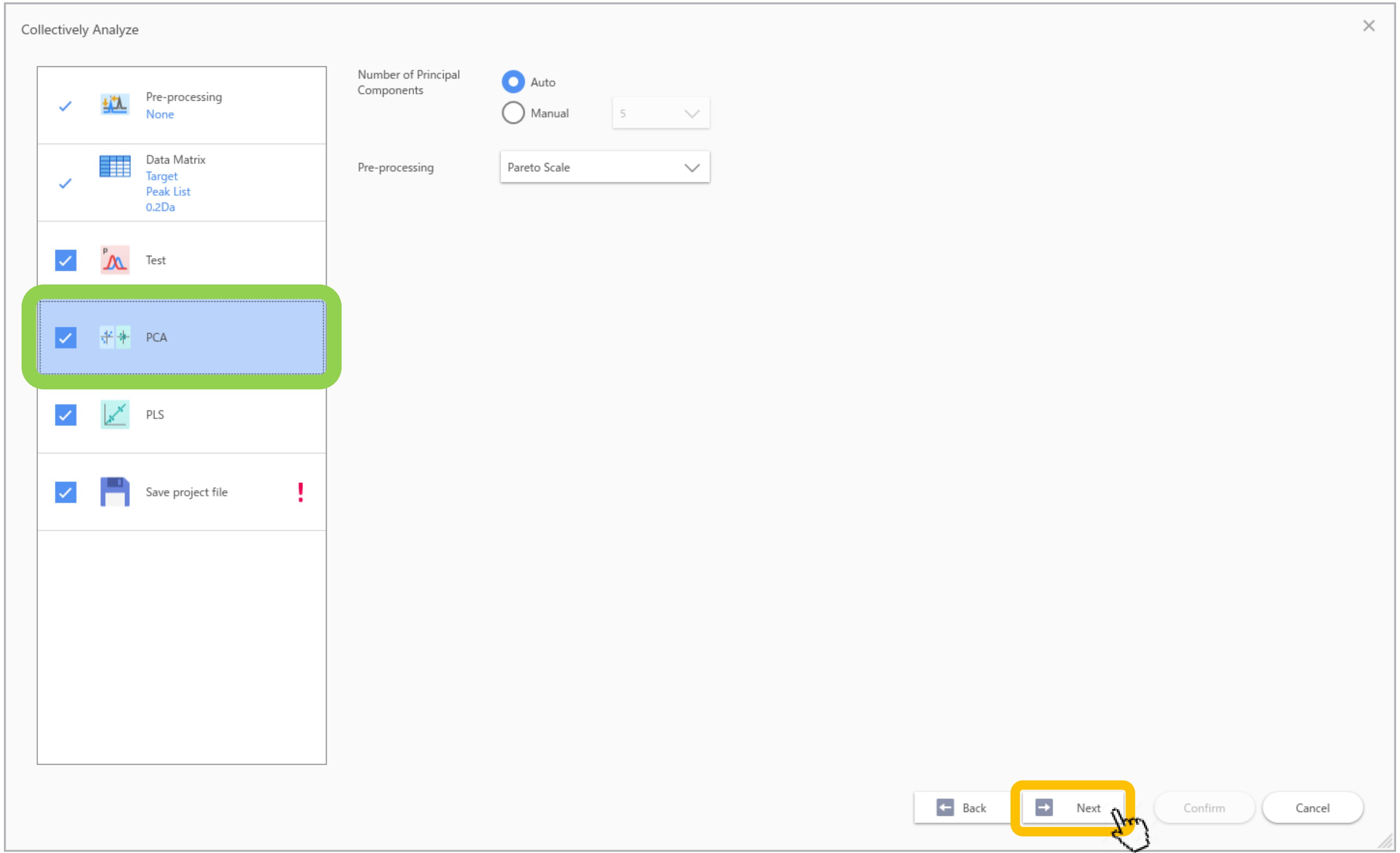
☑ PLS

☑ Save project file !

There are no setting items.

No configuration items are displayed, but ROI settings with two or more attributes are required

PCA



Collectively Analyze

✓ Pre-processing
None

✓ Data Matrix
Target
Peak List
0.2Da

☑ Test

☑ PCA

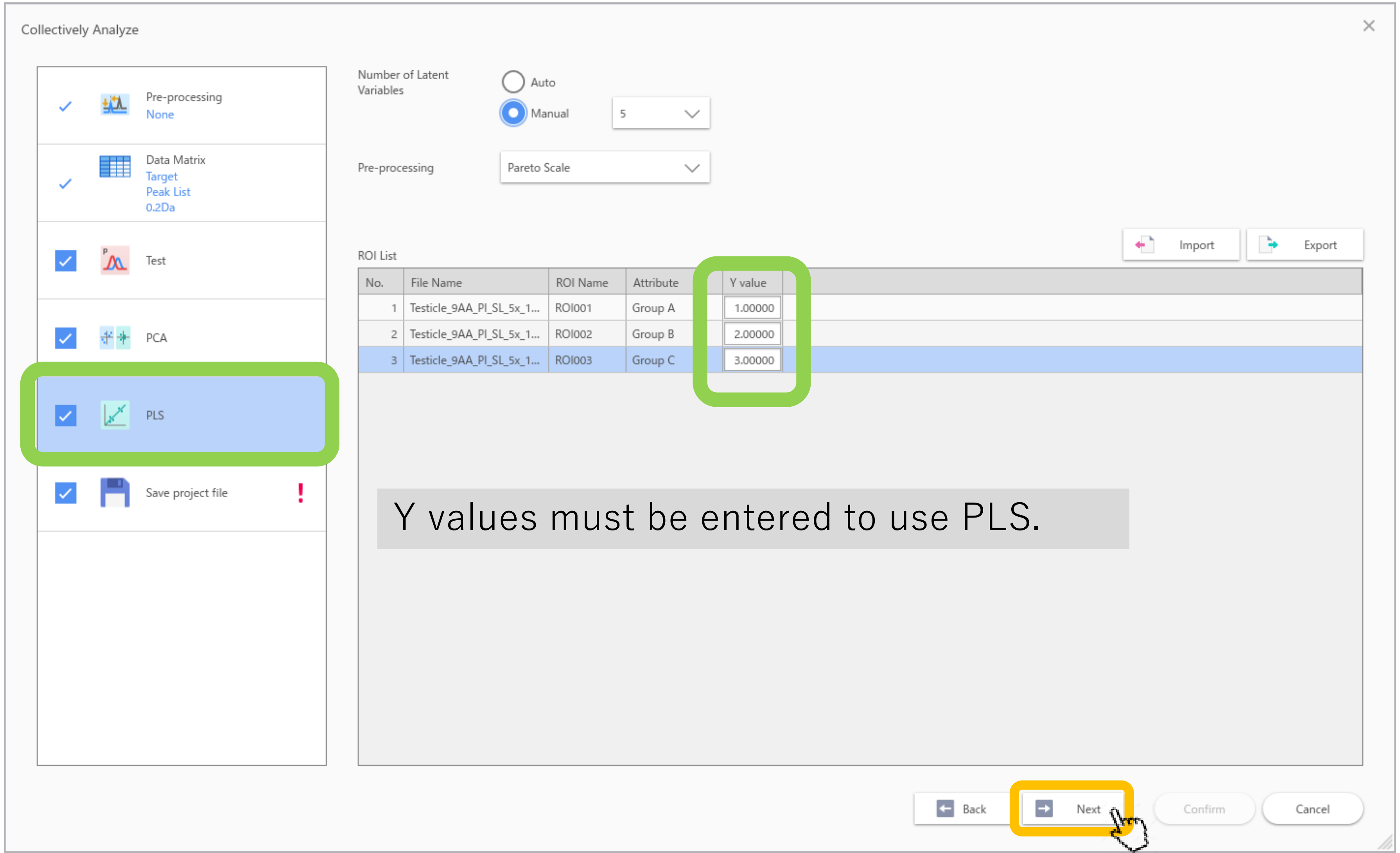
☑ PLS

☑ Save project file !

Number of Principal Components: ● Auto ○ Manual 5

Pre-processing: Pareto Scale

PLS



Collectively Analyze

- ✓ Pre-processing None
- ✓ Data Matrix Target Peak List 0.2Da
- ☑ Test
- ☑ PCA
- ☑ PLS
- ☑ Save project file !

Number of Latent Variables: ○ Auto ● Manual 5

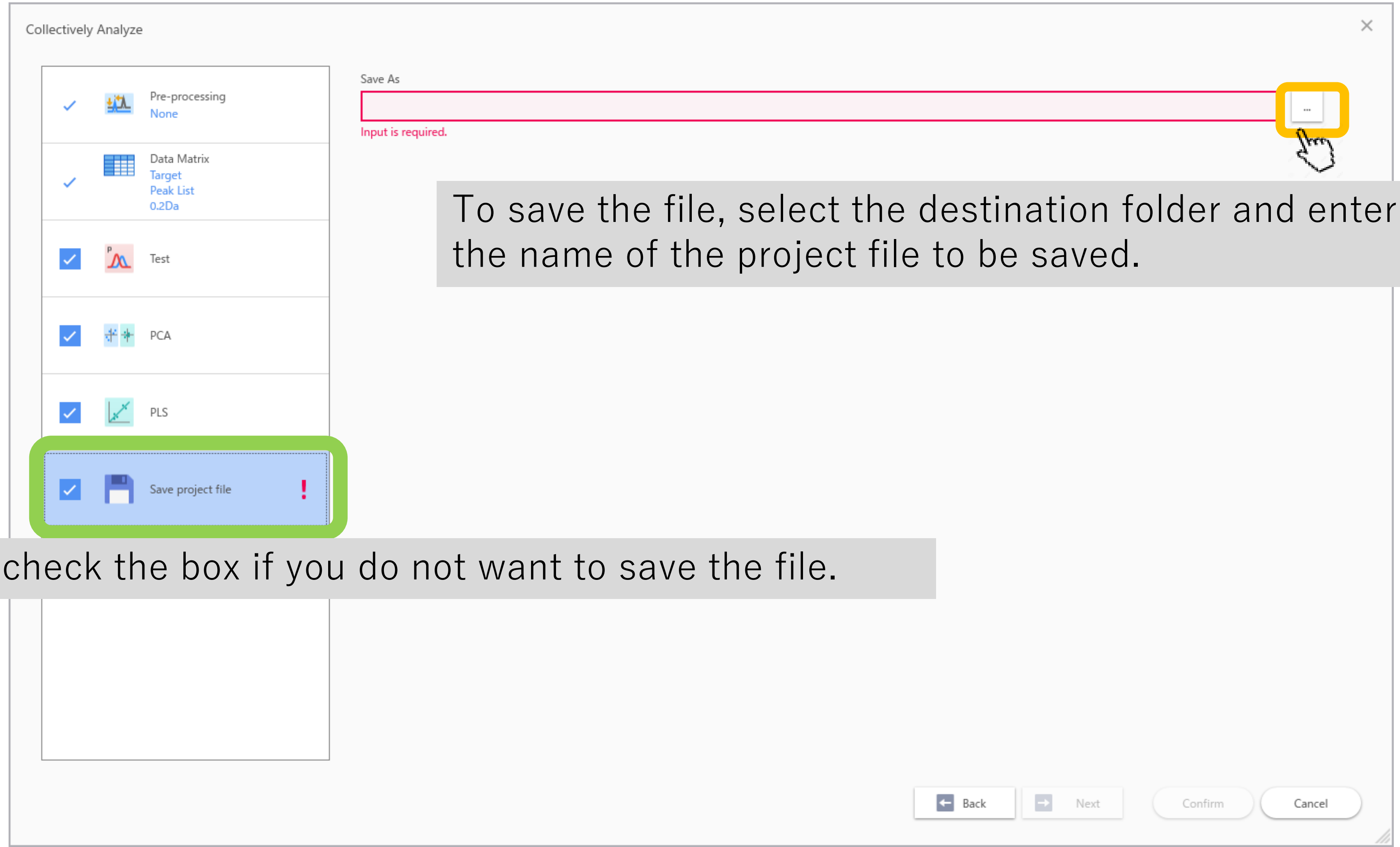
Pre-processing: Pareto Scale

ROI List

No.	File Name	ROI Name	Attribute	Y value
1	Testicle_9AA_PI_SL_5x_1...	ROI001	Group A	1.00000
2	Testicle_9AA_PI_SL_5x_1...	ROI002	Group B	2.00000
3	Testicle_9AA_PI_SL_5x_1...	ROI003	Group C	3.00000

Y values must be entered to use PLS.

Saving a project file

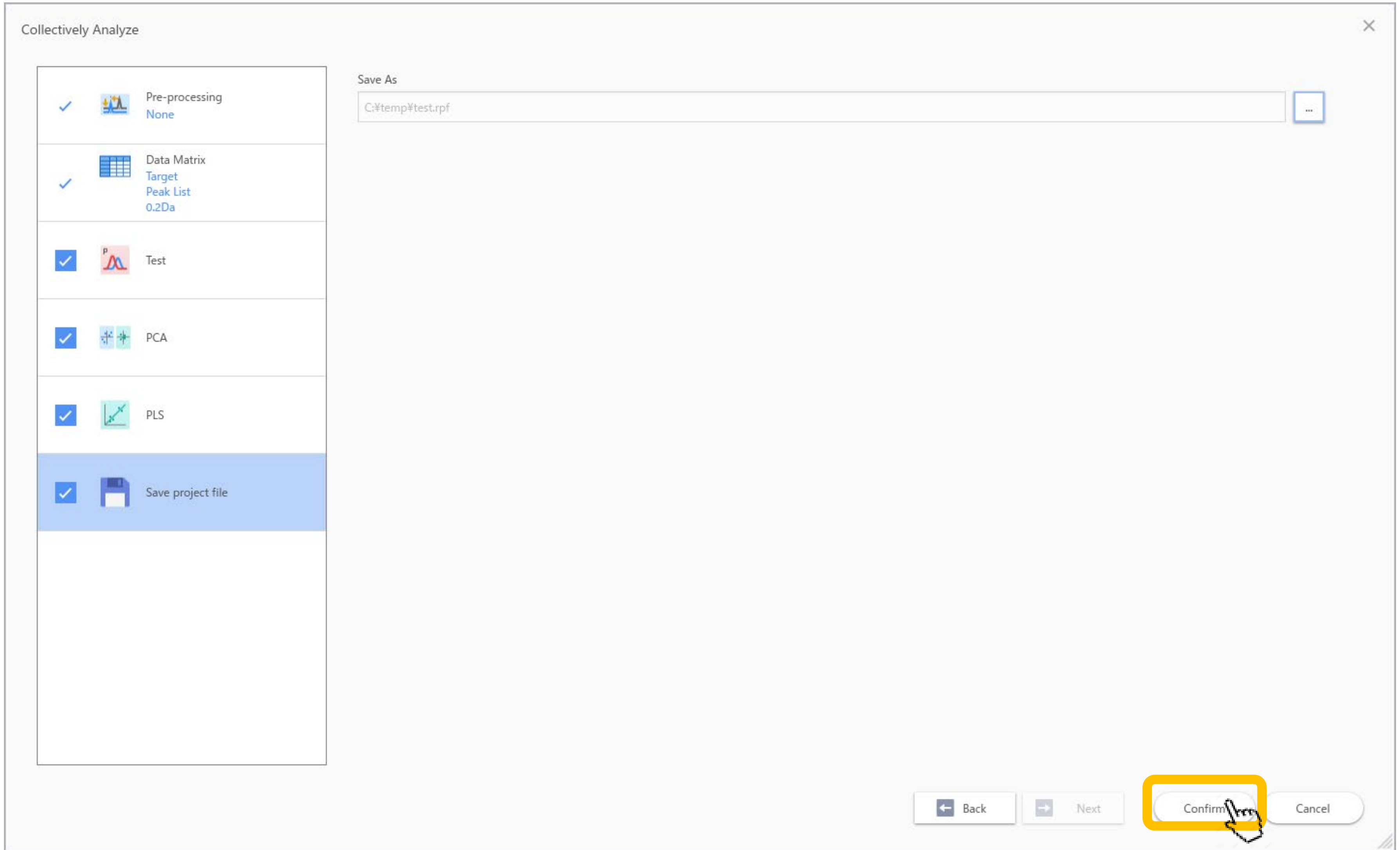


Input is required.

To save the file, select the destination folder and enter the name of the project file to be saved.

Uncheck the box if you do not want to save the file.

Once all settings are complete, click “Confirm”



Collectively Analyze

✓ Pre-processing
None

✓ Data Matrix
Target
Peak List
0.2Da

☑ Test

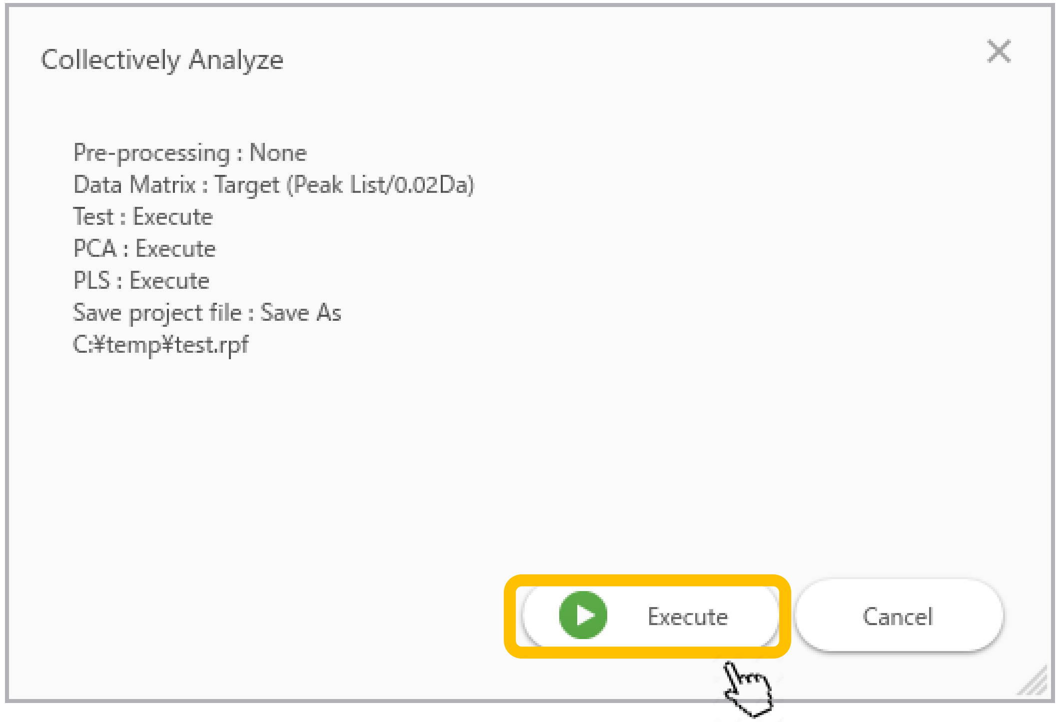
☑ PCA

☑ PLS

☑ Save project file

Save As: C:¥temp¥test.rpf

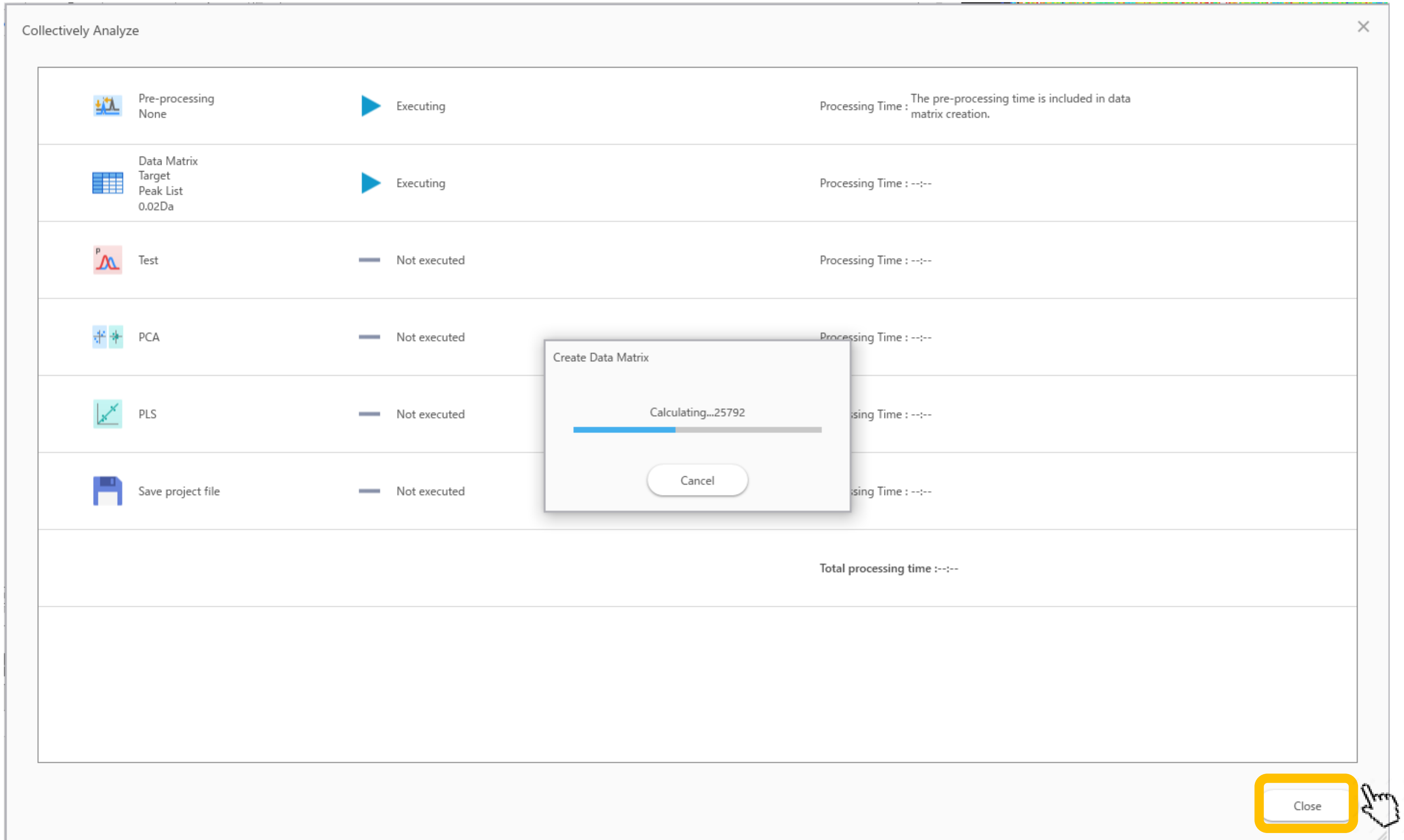
A confirmation window appears



Collectively Analyze

Pre-processing : None
Data Matrix : Target (Peak List/0.02Da)
Test : Execute
PCA : Execute
PLS : Execute
Save project file : Save As
C:¥temp¥test.rpf

The execution details are displayed.



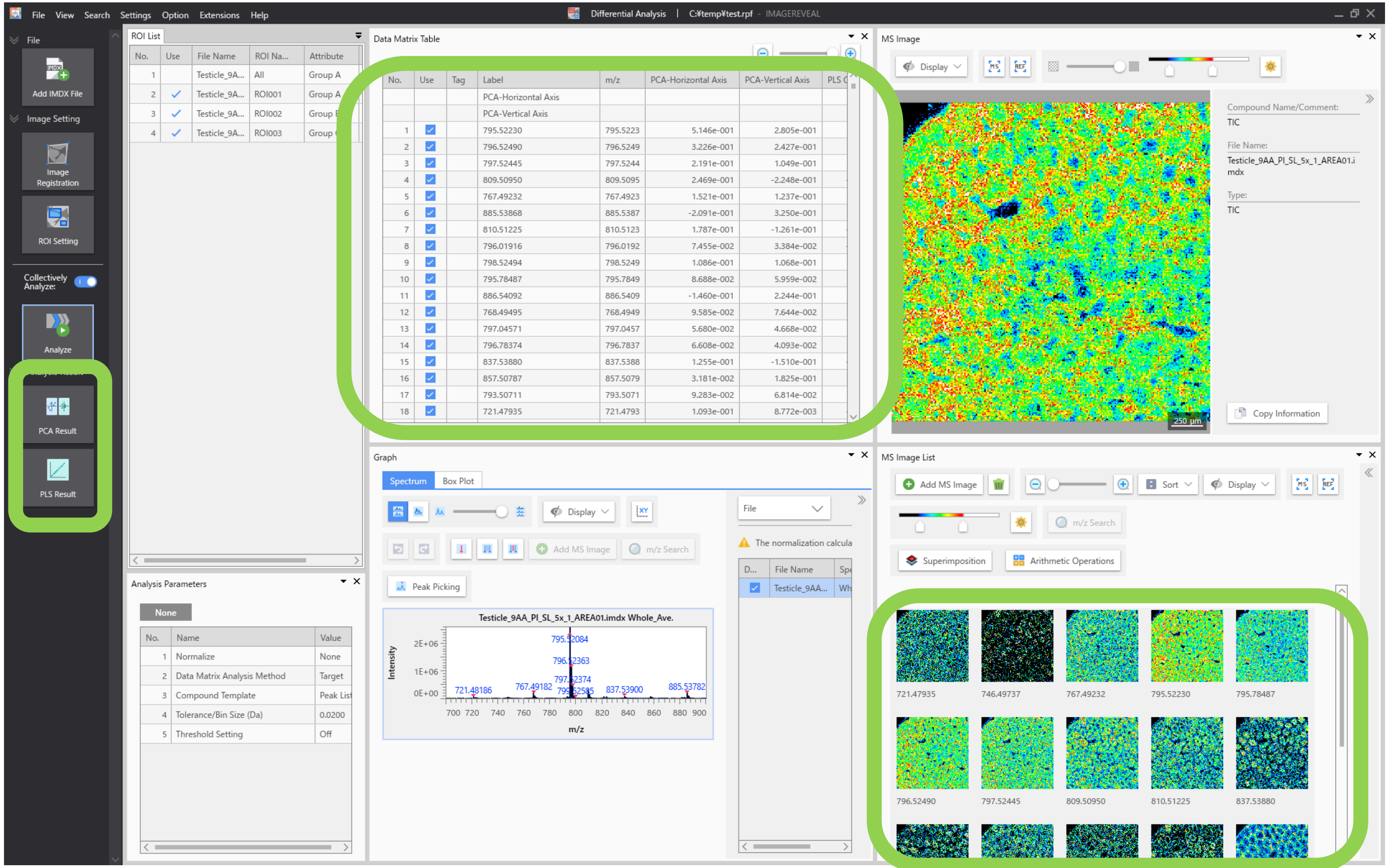
Collectively Analyze

Pre-processing None	Executing	Processing Time : The pre-processing time is included in data matrix creation.
Data Matrix Target Peak List 0.02Da	Executing	Processing Time : --:--
Test	Not executed	Processing Time : --:--
PCA	Not executed	Processing Time : --:--
PLS	Not executed	Processing Time : --:--
Save project file	Not executed	Processing Time : --:--
		Total processing time :--:--

Create Data Matrix

Calculating...25792

Once the process is complete, analysis results appear on the main window



ROI List

No.	Use	File Name	ROI Na...	Attribute
1		Testicle_9A...	All	Group A
2	✓	Testicle_9A...	ROI001	Group A
3	✓	Testicle_9A...	ROI002	Group
4	✓	Testicle_9A...	ROI003	Group

Data Matrix Table

No.	Use	Tag	Label	m/z	PCA-Horizontal Axis	PCA-Vertical Axis	PLS
			PCA-Horizontal Axis				
			PCA-Vertical Axis				
1	☑		795.52230	795.5223	5.146e-001	2.805e-001	
2	☑		796.52490	796.5249	3.226e-001	2.427e-001	
3	☑		797.52445	797.5244	2.191e-001	1.049e-001	
4	☑		809.50950	809.5095	2.469e-001	-2.248e-001	
5	☑		767.49232	767.4923	1.521e-001	1.237e-001	
6	☑		885.53868	885.5387	-2.091e-001	3.250e-001	
7	☑		810.51225	810.5123	1.787e-001	-1.261e-001	
8	☑		796.01916	796.0192	7.455e-002	3.384e-002	
9	☑		798.52494	798.5249	1.086e-001	1.068e-001	
10	☑		795.78487	795.7849	8.688e-002	5.959e-002	
11	☑		886.54092	886.5409	-1.460e-001	2.244e-001	
12	☑		768.49495	768.4949	9.585e-002	7.644e-002	
13	☑		797.04571	797.0457	5.680e-002	4.668e-002	
14	☑		796.78374	796.7837	6.608e-002	4.093e-002	
15	☑		837.53880	837.5388	1.255e-001	-1.510e-001	
16	☑		857.50787	857.5079	3.181e-002	1.825e-001	
17	☑		793.50711	793.5071	9.283e-002	6.814e-002	
18	☑		721.47935	721.4793	1.093e-001	8.772e-003	

Compound Name/Comment:
TIC

File Name:
Testicle_9AA_PI_SL_5x_1_AREA01.imdx

Type:
TIC

Analysis Parameters

None

No.	Name	Value
1	Normalize	None
2	Data Matrix Analysis Method	Target
3	Compound Template	Peak List
4	Tolerance/Bin Size (Da)	0.0200
5	Threshold Setting	Off

The normalization calcula

D...	File Name	Spe
☑	Testicle_9AA...	Wh