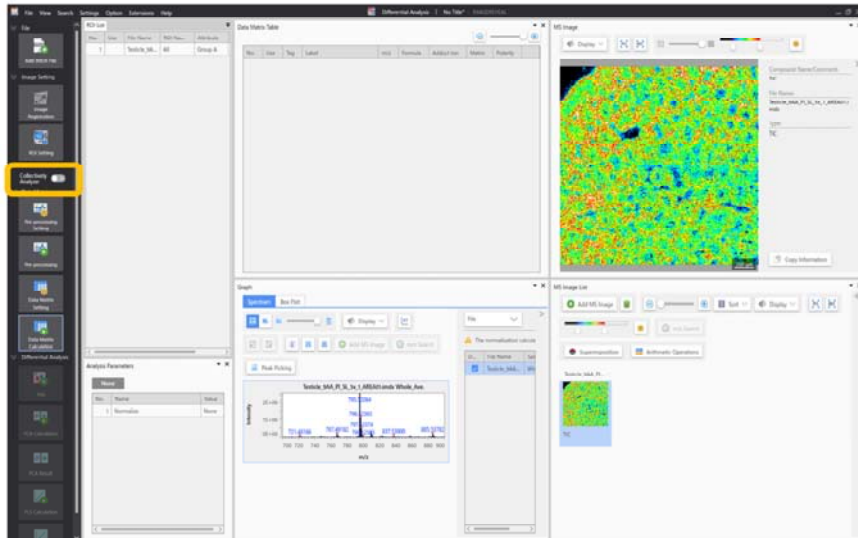
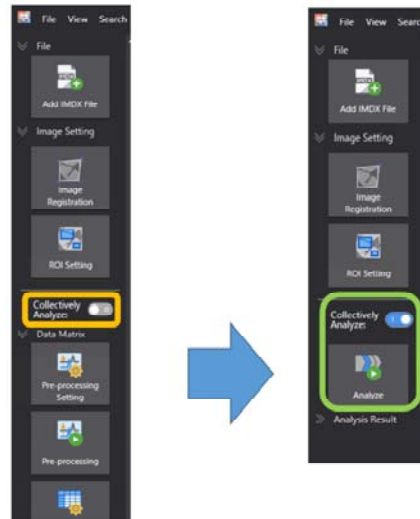


Collective analysis

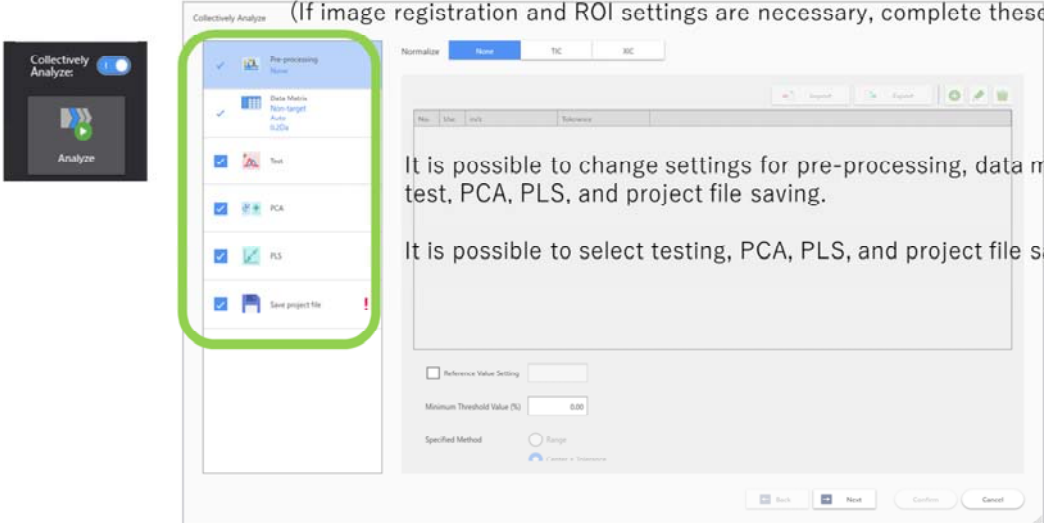
The collective analysis function has been added in version 1.1



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)

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

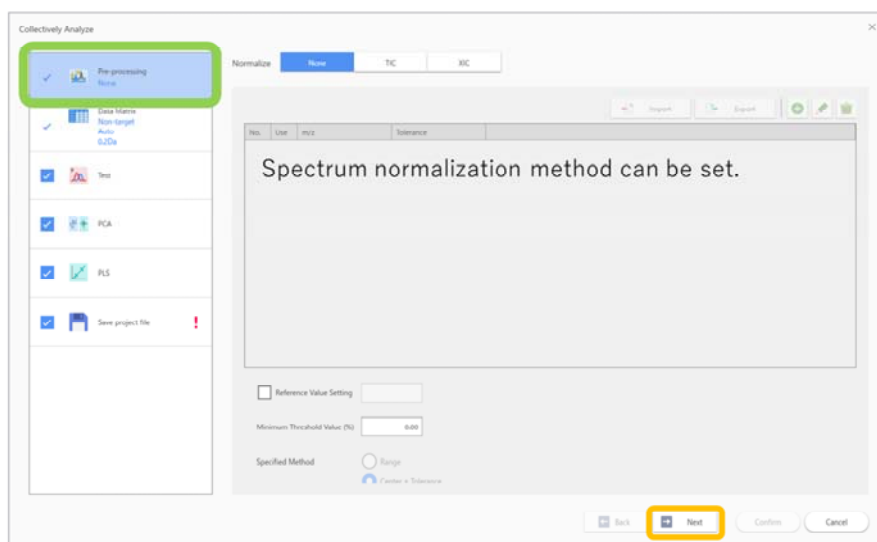
It is possible to select testing, PCA, PLS, and project file saving.

If image registration and ROI settings are necessary complete these beforehand.

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

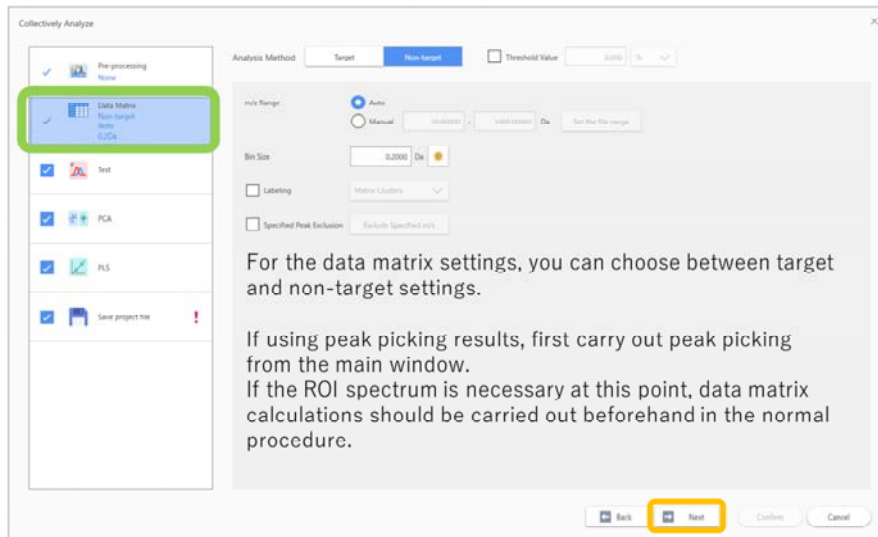
It is possible to select testing, PCA, PLS, and project file saving.

1. Pre-processing (normalization)



Spectrum normalization method can be set.

2. Data matrix settings



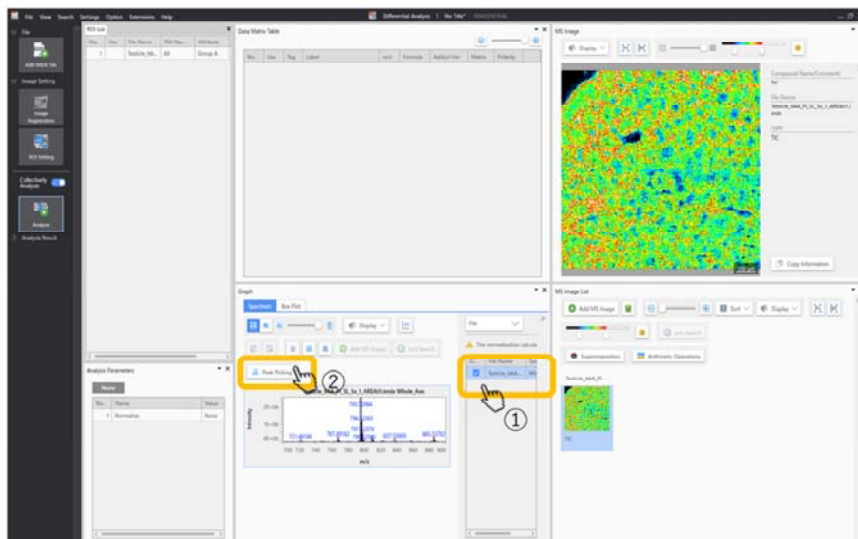
For the data matrix settings, you can choose between target and non-target settings.

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.

2. Data matrix settings

If peak picking is necessary:



Display the spectrum and click the peak picking button

2. Data matrix settings

Peak picking

The screenshot displays the 'Peak Picking' software interface. It is divided into three main sections: 'Parameter Settings', 'Spectrum Graph', and 'Peak List'.

Parameter Settings: This section contains various controls for the peak picking process. The 'm/z Range' is set from 699.80452 to 900.01956. The 'Smoothing' is set to 'Savitzky-Golay'. The 'Number of Data Points' is 8, and the 'Number of peaks to detect' is 1000. There are checkboxes for 'Threshold Value' (set to 0.000), 'Direct Monochromator', 'Specified Peak Exclusion', and 'Show Peaks'. A green 'Execute' button is highlighted with a yellow box and a hand icon.

Spectrum Graph: This section shows a mass spectrum plot with 'Intensity' on the y-axis (ranging from 0E+00 to 1.2E+06) and 'm/z' on the x-axis (ranging from 700 to 900). A prominent peak is visible at approximately m/z 796. A 'Save as Compound Template' button is highlighted with a yellow box and a hand icon.

Peak List: This section displays a table of detected peaks. The table has columns for 'No.', 'm/z', and 'Intensity'. The data is as follows:

No.	m/z	Intensity
1	795.52230	1440185.71229
2	796.50490	461252.41170
3	797.53445	281516.97704
4	805.50950	180746.24418
5	787.49322	119581.51946
6	885.63668	114637.13939
7	815.51225	87232.64859
8	796.01916	80876.03661
9	796.52494	75169.20412
10	795.78487	63858.99839
11	886.54002	61671.86389
12	768.49493	54627.03987
13	767.54271	48933.10354
14	796.76274	47361.88287
15	855.53880	47262.07643
16	852.58182	45931.85620
17	793.50711	44473.40280
18	721.47975	39547.56227
19	823.54383	38298.81788
20	821.63421	37946.87179
21	811.51225	34631.03888
22	796.29718	34286.72776
23	884.51825	28711.02987
24	794.51388	27893.47351
25	887.54315	25629.48170
26	748.51908	23054.12189

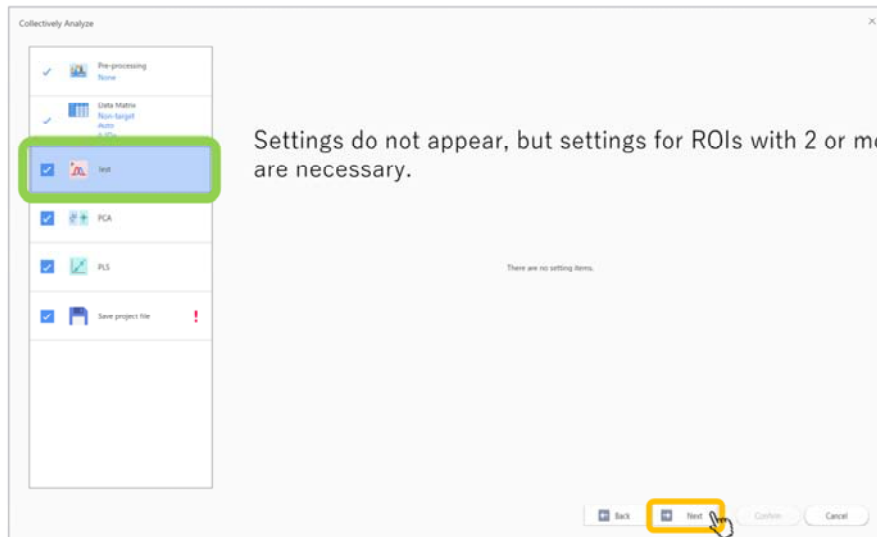
2. Data matrix settings

The peak picking results are automatically input and become target peaks

The screenshot displays the 'Collectively Analyze' software interface. On the left, a sidebar contains several options: 'Pre-processing' (checked), 'Data Matrix' (checked and highlighted with a green box), 'Test' (checked), 'PCA' (checked), 'PLS' (checked), and 'Save project file' (checked). The main window shows the 'Analysis Method' set to 'Target' and a 'Threshold Value' of 0.000. Below this is a 'Compound List' table with columns for 'm/z', 'Compound Name', 'Formula', 'Matrix', 'Polarity', and 'Adduct Ion'. The table contains 16 rows of data, with the first row highlighted in blue. A green rounded rectangle highlights the entire 'Compound List' table. At the bottom of the window, there are 'Back', 'Next', 'Confirm', and 'Cancel' buttons.

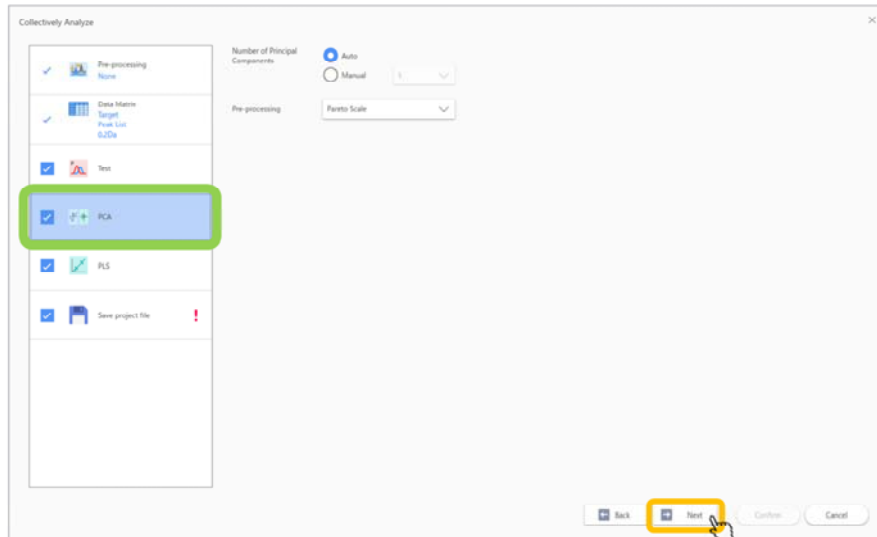
	m/z	Compound Name	Formula	Matrix	Polarity	Adduct Ion
1	795.52281	795.52230		Any	Bipolar	
2	796.52445	796.52400		Any	Bipolar	
3	797.52445	797.52445		Any	Bipolar	
4	805.50950	805.50950		Any	Bipolar	
5	767.49232	767.49232		Any	Bipolar	
6	865.53866	865.53866		Any	Bipolar	
7	810.51225	810.51225		Any	Bipolar	
8	796.01916	796.01916		Any	Bipolar	
9	798.52494	798.52494		Any	Bipolar	
10	793.78487	793.78487		Any	Bipolar	
11	886.64992	886.64992		Any	Bipolar	
12	768.49495	768.49495		Any	Bipolar	
13	797.04571	797.04571		Any	Bipolar	
14	796.78374	796.78374		Any	Bipolar	
15	837.63860	837.63860		Any	Bipolar	
16	857.60787	857.60787		Any	Bipolar	
	793.50711	793.50711		Any	Bipolar	

3. Test



Settings do not appear, but settings for ROIs with 2 or more attributes are necessary.

PCA



PLS

Collectively Analyze

Number of Latent Variables: Auto Manual 1

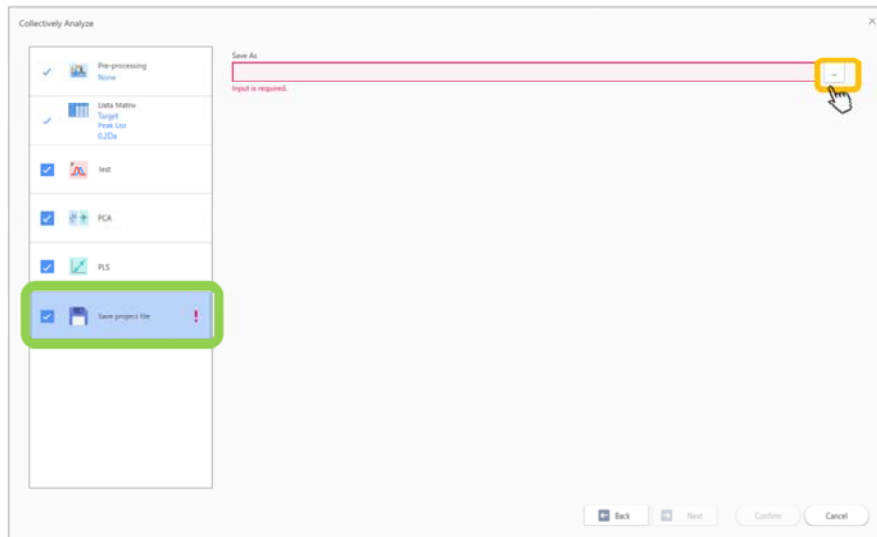
Pre-processing: Pareto Scale

Y values must be entered to use PLS.

No.	File Name	ROI Name	Attribute	Y value
1	Testfile_MAA_PL_S1_Sc_1...	ROI001	Group A	1.00000
2	Testfile_MAA_PL_S1_Sc_1...	ROI002	Group B	2.00000
3	Testfile_MAA_PL_S1_Sc_1...	ROI003	Group C	3.00000

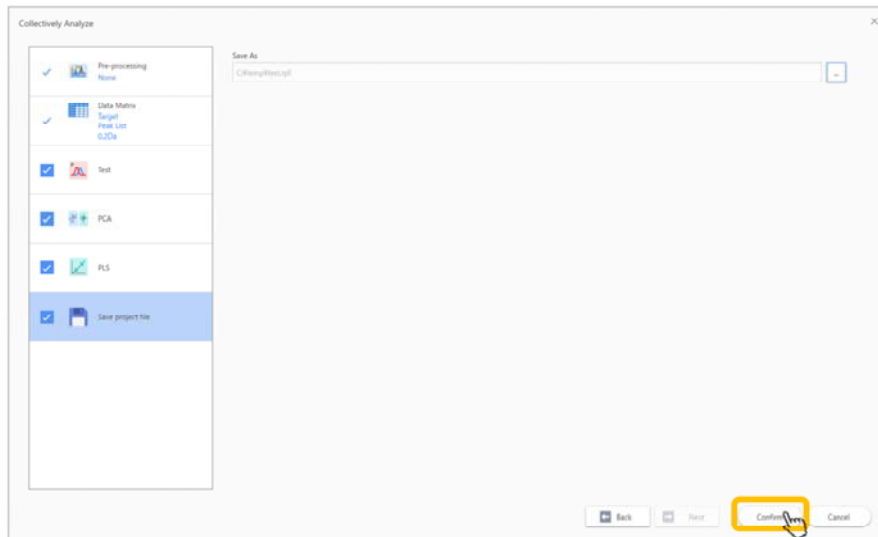
Buttons: Back, Next, Confirm, Cancel

Saving a project file

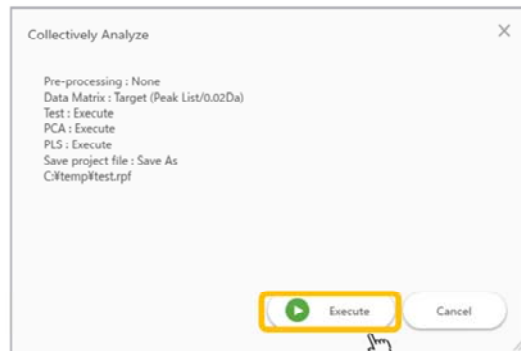


Select the folder to save the file in and type in a file name.

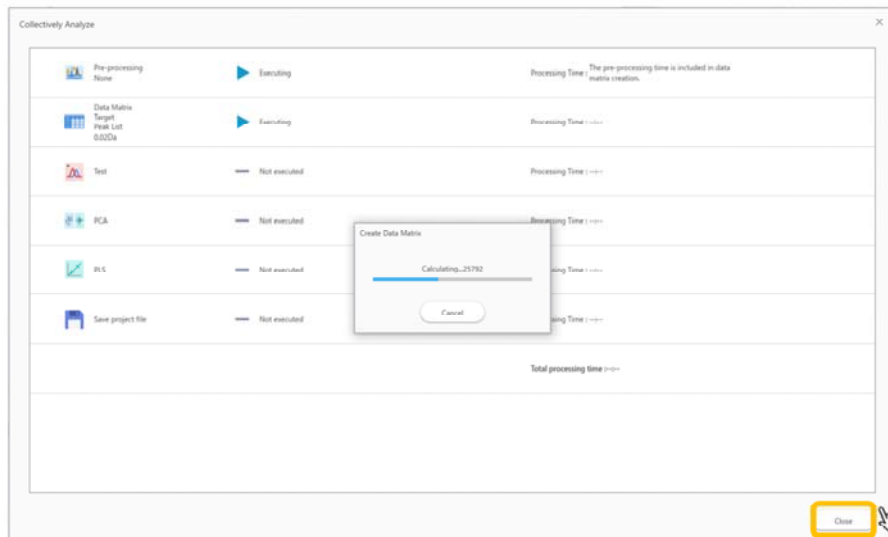
Once all settings are complete, click “Confirm”



A confirmation window appears



The contents to be executed are displayed



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

