# Find components that differ between regions

# Example

Extract components “A”, ”B” and “C”, which differ in intensity between regions

# Steps

1. ROI settings for “A”,”B” and ”C”
2. Data matrix table calculations
3. Testing
4. PCA
5. PLS

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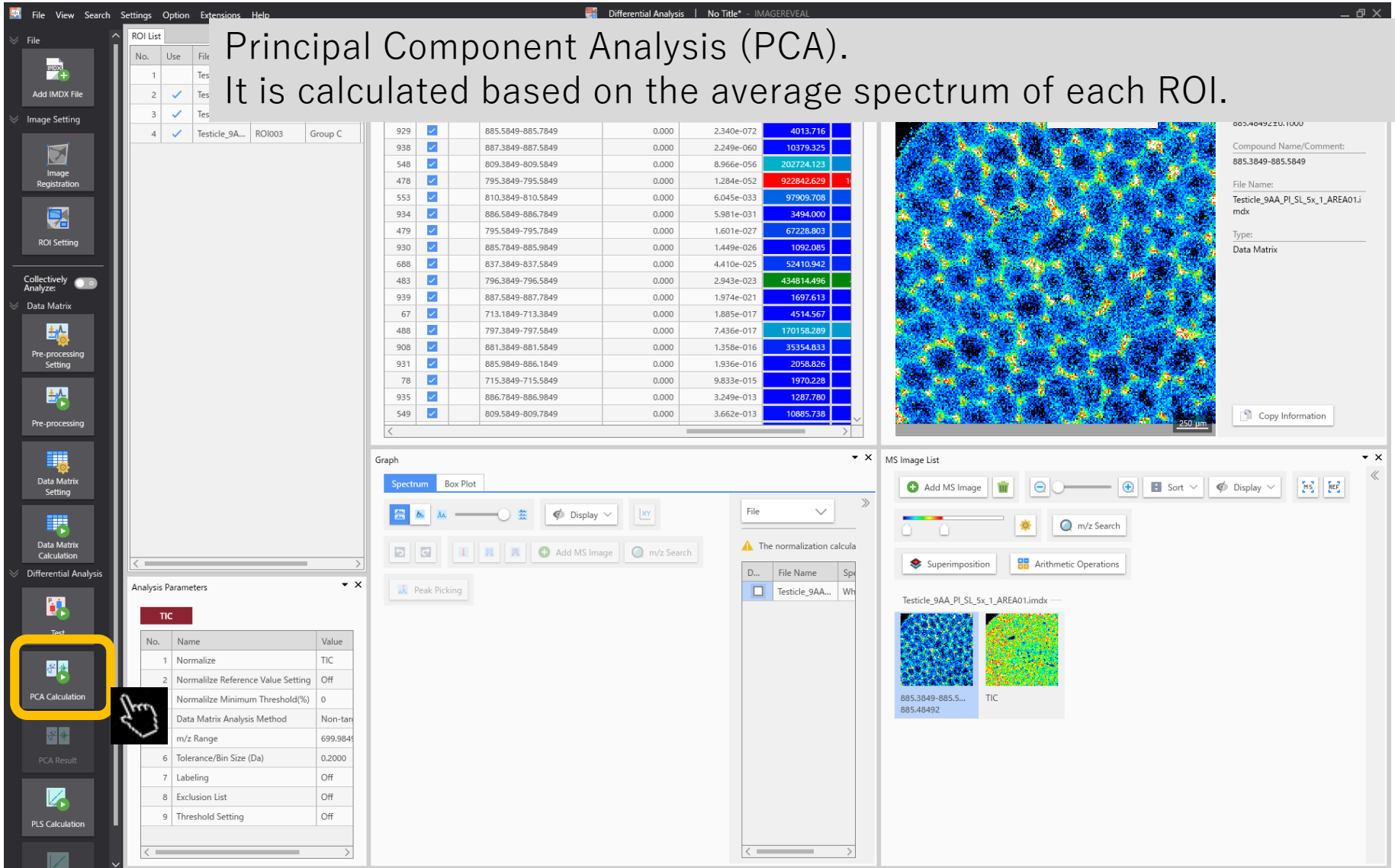
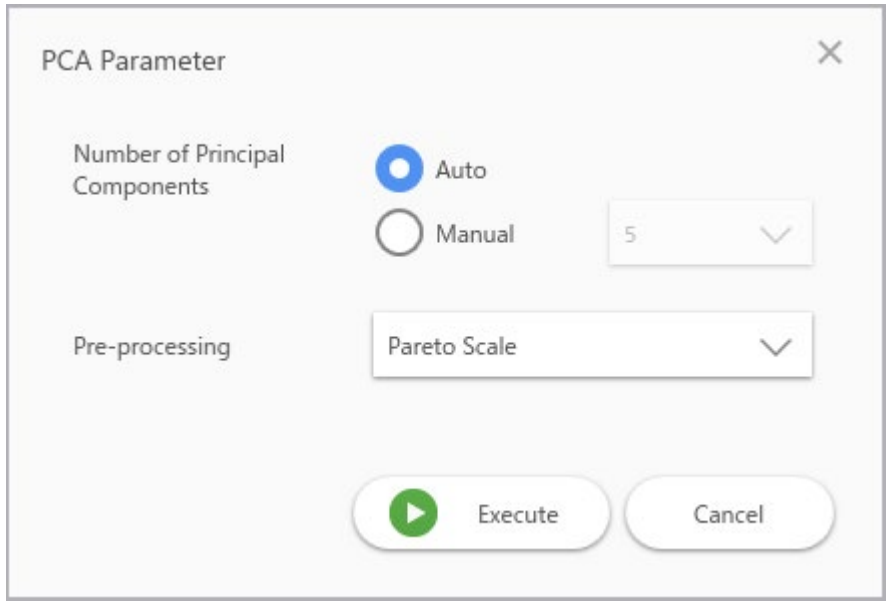
# 4.1 PCA (Principal Component Analysis)

Principal Component Analysis (PCA).
It is calculated based on the average spectrum of each ROI.



# 4.2 PCA parameter settings

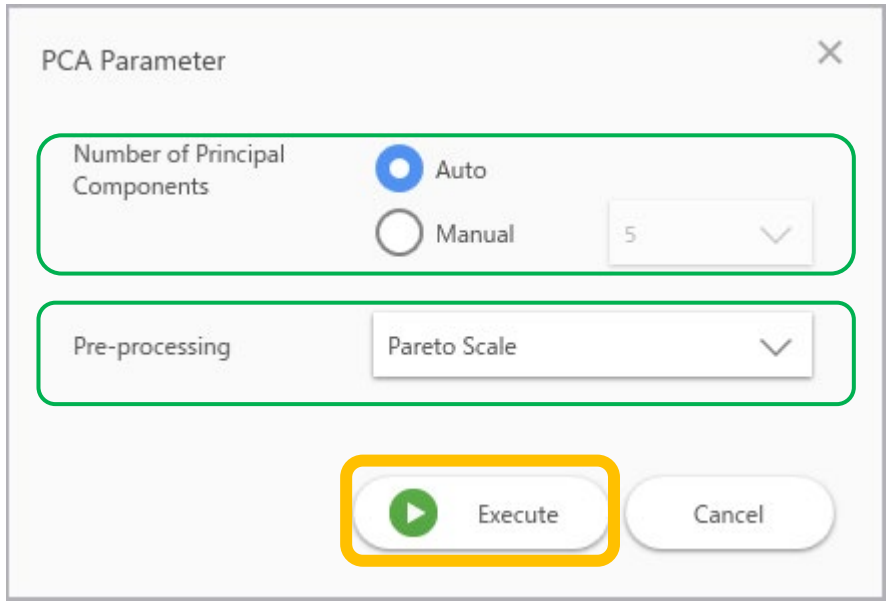
In general these settings are fine.



# 4.3 PCA parameter settings

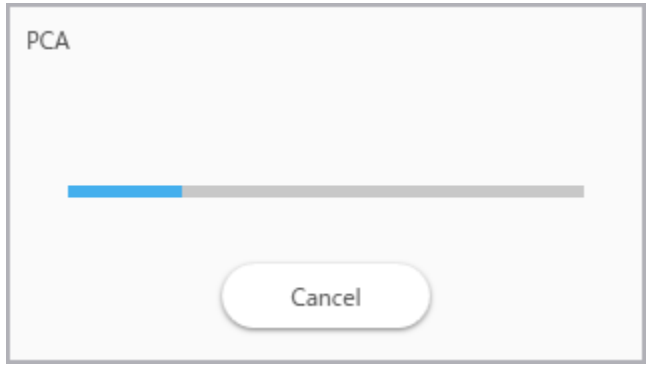
Number of axes

Processing of signal intensity

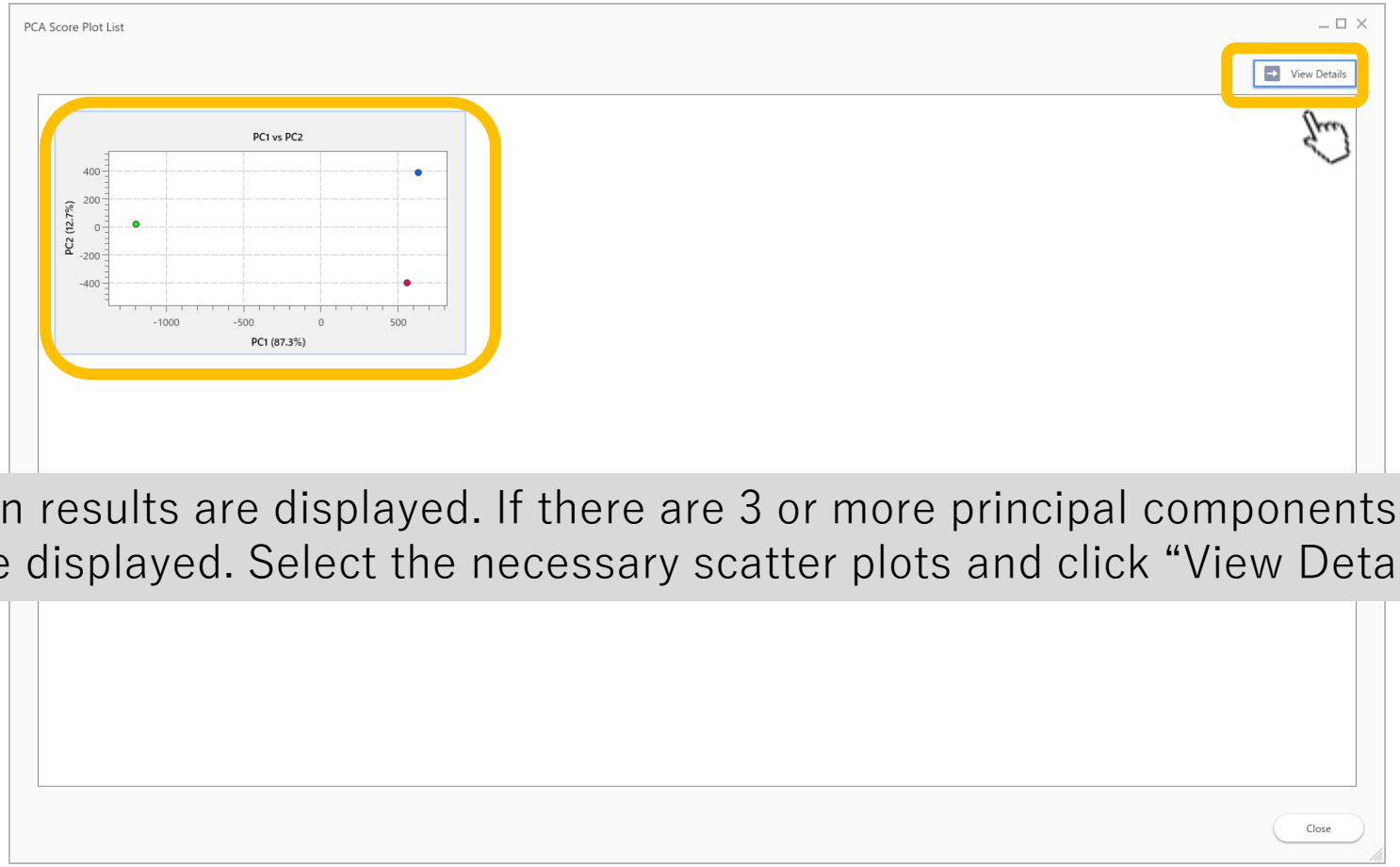



Select from the “Pre-processing” menu to change the way the signal intensity is handled.
・“None”: Signal intensity remains as-is
・“Centre”: Sets the average of signal intensities for each m/z within the ROIs to 0
・“Autoscale”: In addition to centring, sets the standard deviation of changes between ROIs to 1
・“Pareto scale”: In addition to centring, divides the changes between ROIs by the square root of the standard deviation. The result is in between “centre” and “autoscale”.

# 4.4 PCA calculations



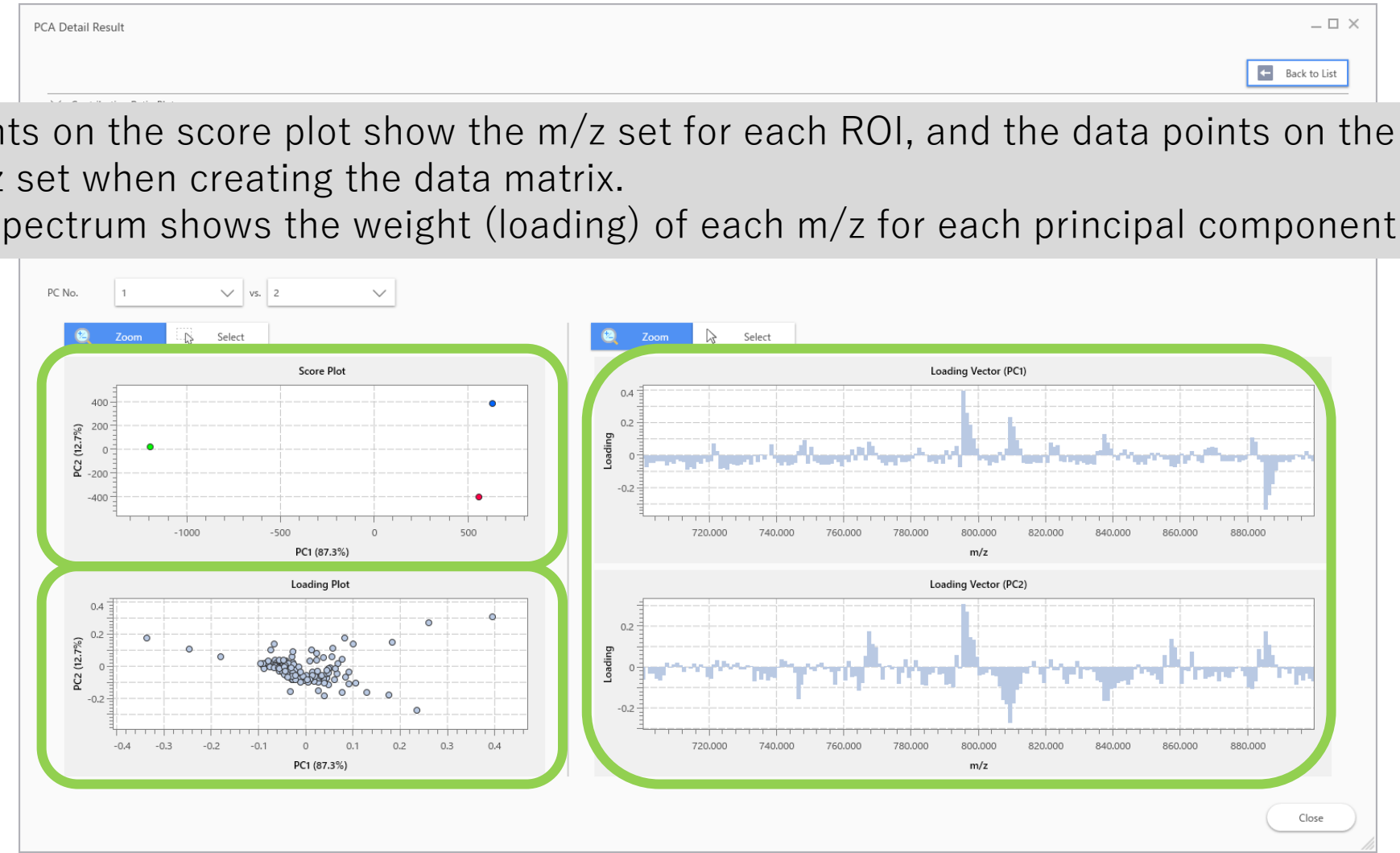
# 4.5 PCA results at a glance



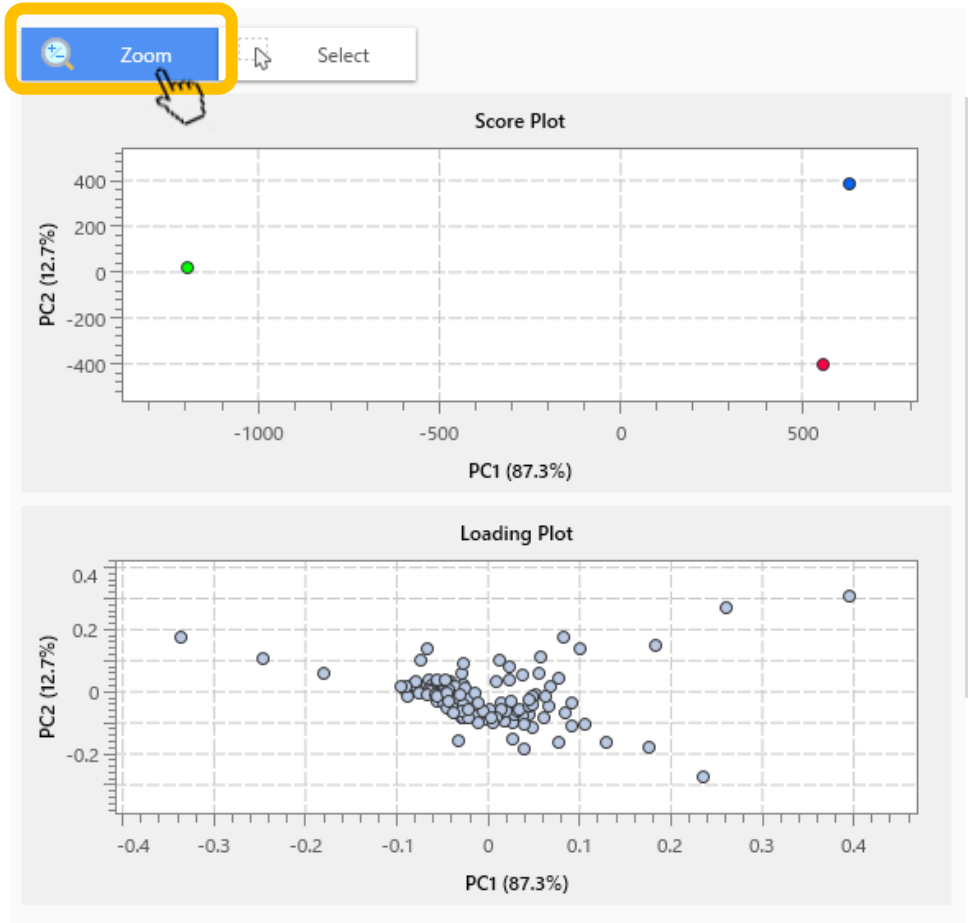

The PCA calculation results are displayed. If there are 3 or more principal components axes, multiple scatter plots will be displayed. Select the necessary scatter plots and click “View Details”.

# 4.6 PCA results screen

The data points on the score plot show the m/z set for each ROI, and the data points on the loading plot show the m/z set when creating the data matrix.
The loading spectrum shows the weight (loading) of each m/z for each principal component (PC).



# 4.7 PCA results screen, zooming

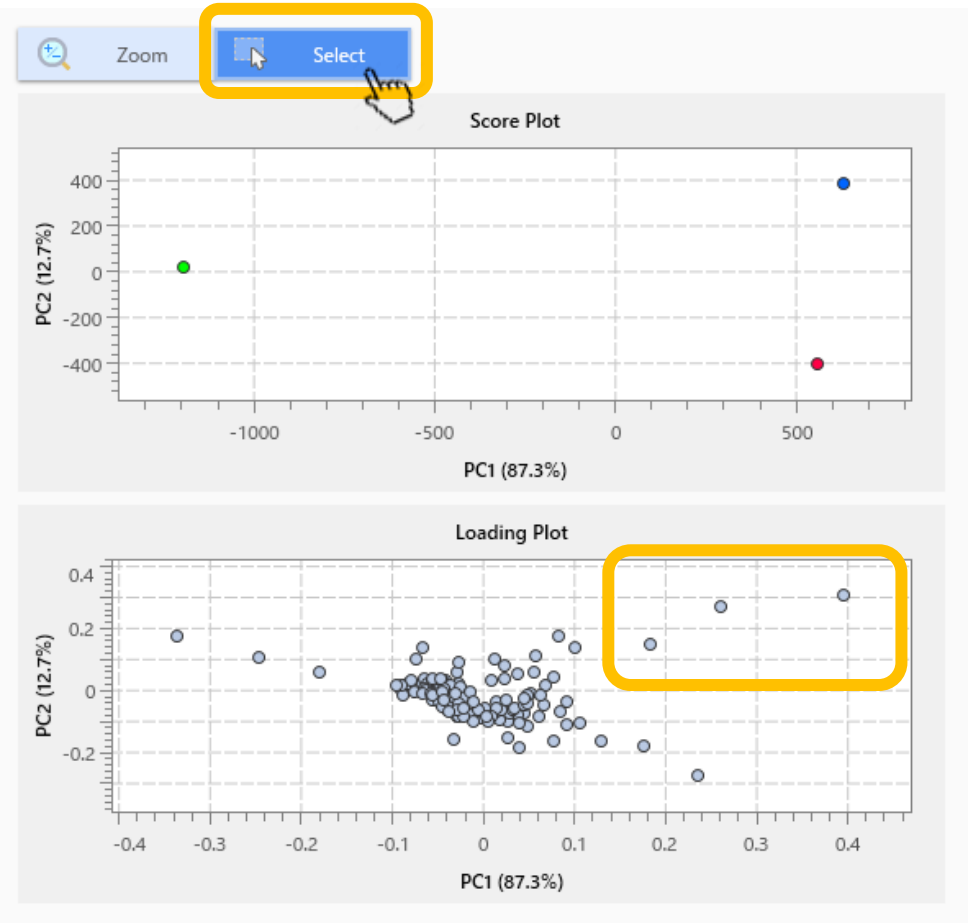



The data points on the score plot show the m/z set for each ROI, and the data points on the loading plot show the m/z set when creating the data matrix.

The loading spectrum shows the weight (loading) of each m/z for each principal component (PC).

If “Zoom” is selected, dragging the cursor over the plot will zoom in or out.
The mouse wheel can also be used to zoom in or out.

# 4.8 Selecting data points

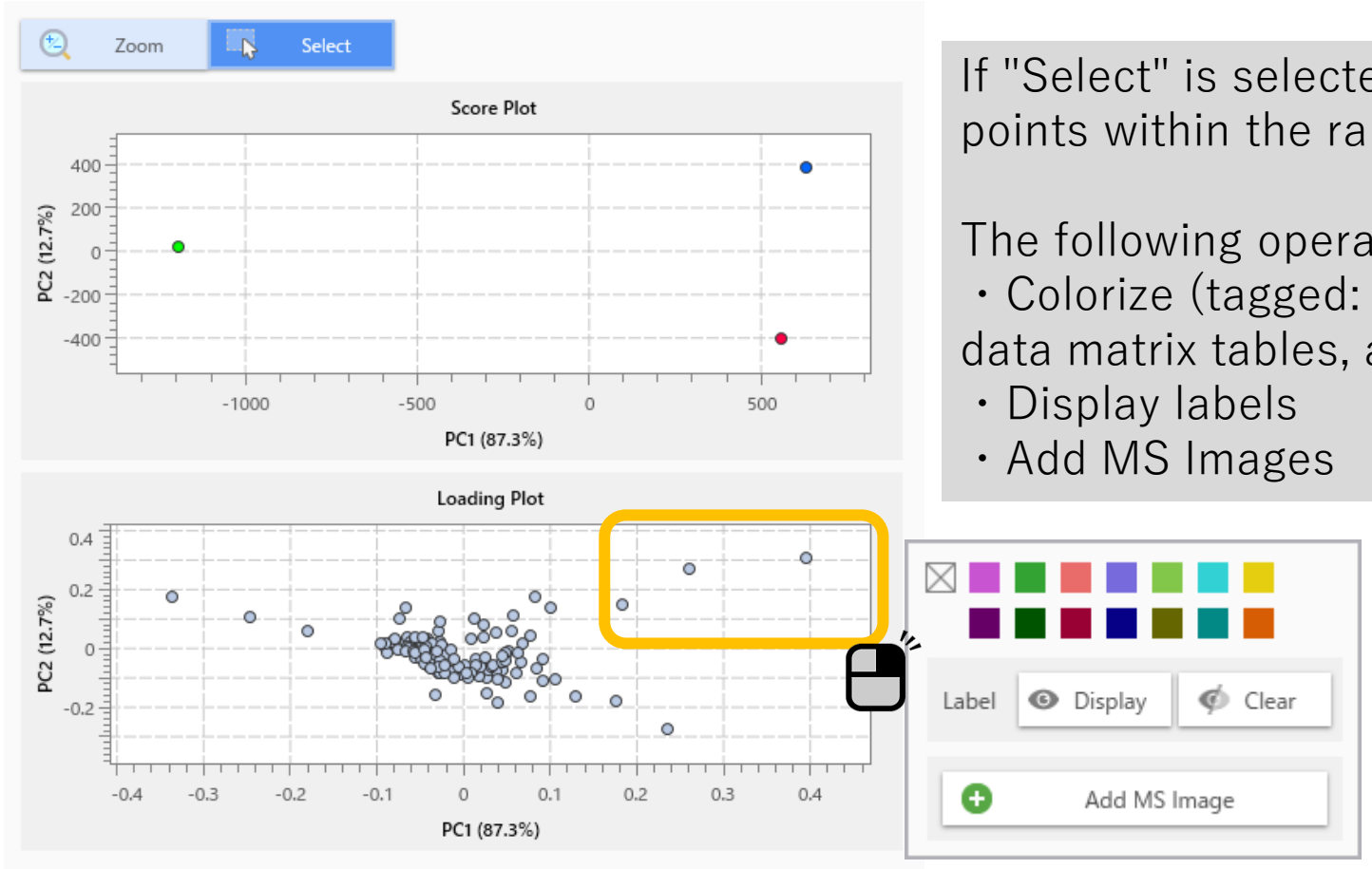



If “Select” is selected, dragging the cursor over the plots will highlight the data points within that area.

The following operations are possible using the sidebar.

- Add colours (tagging: these colours will also be applied to other graphs, data matrices, and MS image list)
- Show labels
- Add MS image

# 4.9 Add colours to data points (tagging)



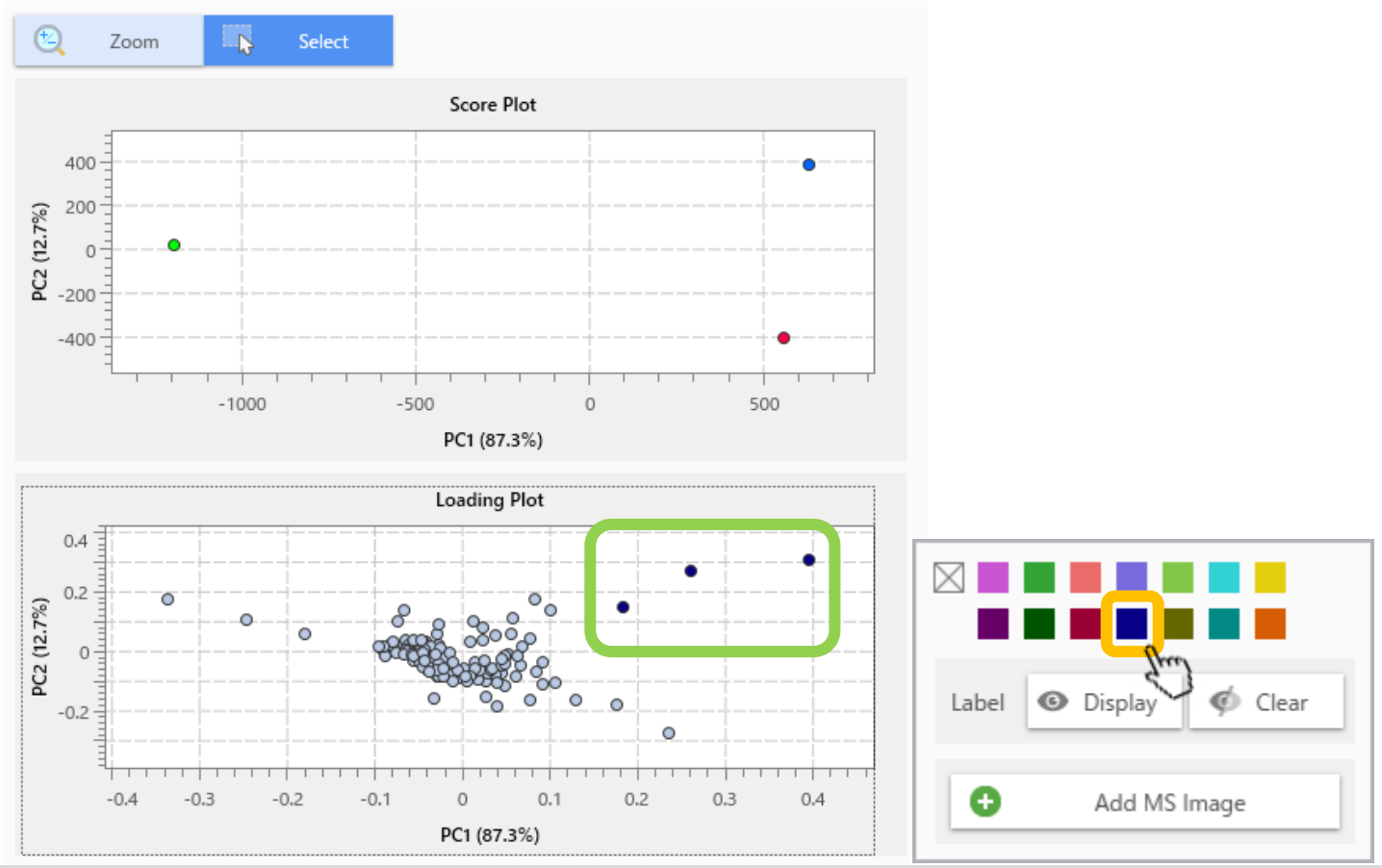




If "Select" is selected, dragging on the plot will select data points within the range.

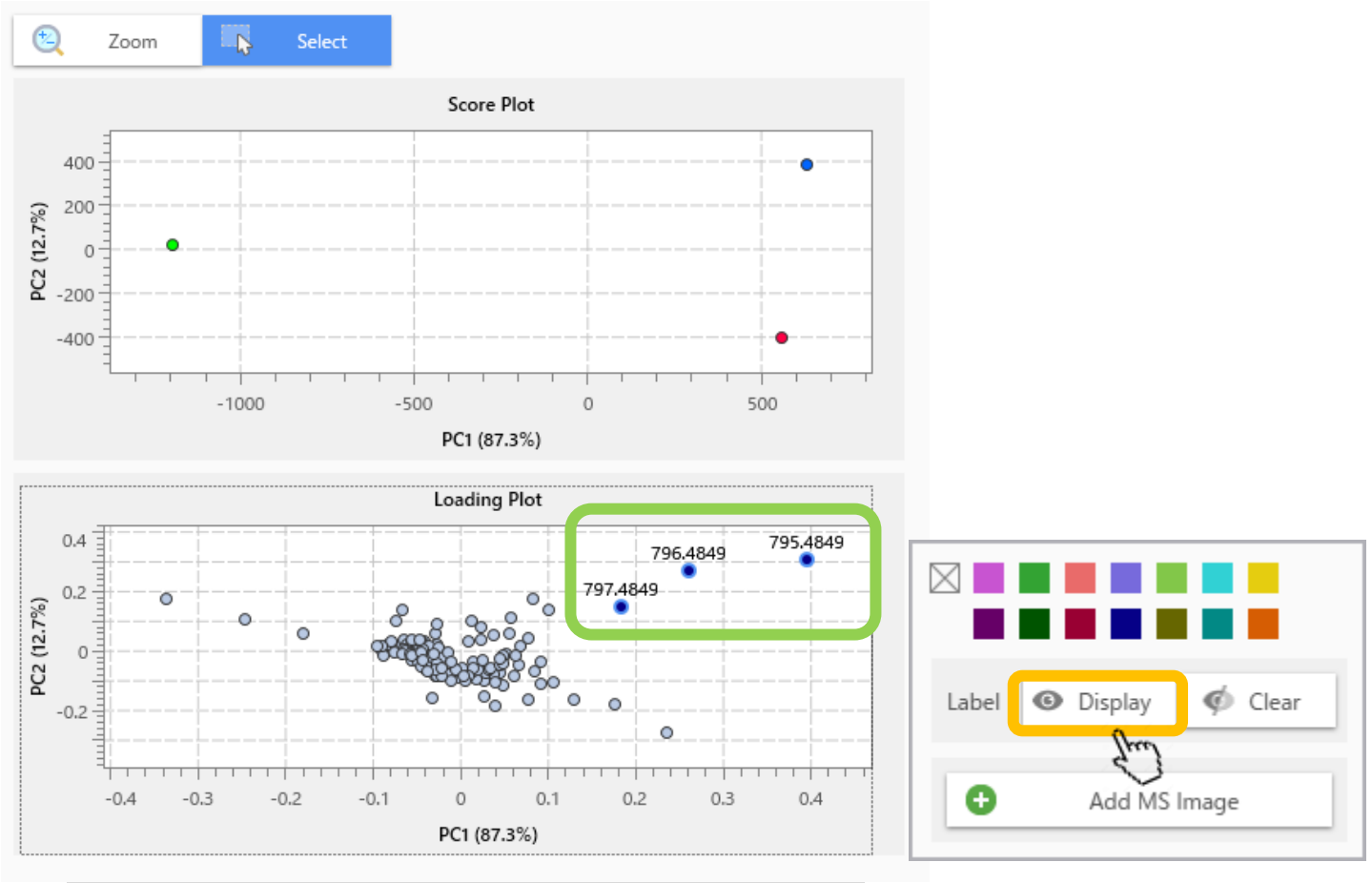
The following operations are available from the side menu
・Colorize (tagged: this color will be the same in other graphs, data matrix tables, and MS ImageList)
・Display labels
・Add MS Images

# 4.10 Add colours to data points (tagging)



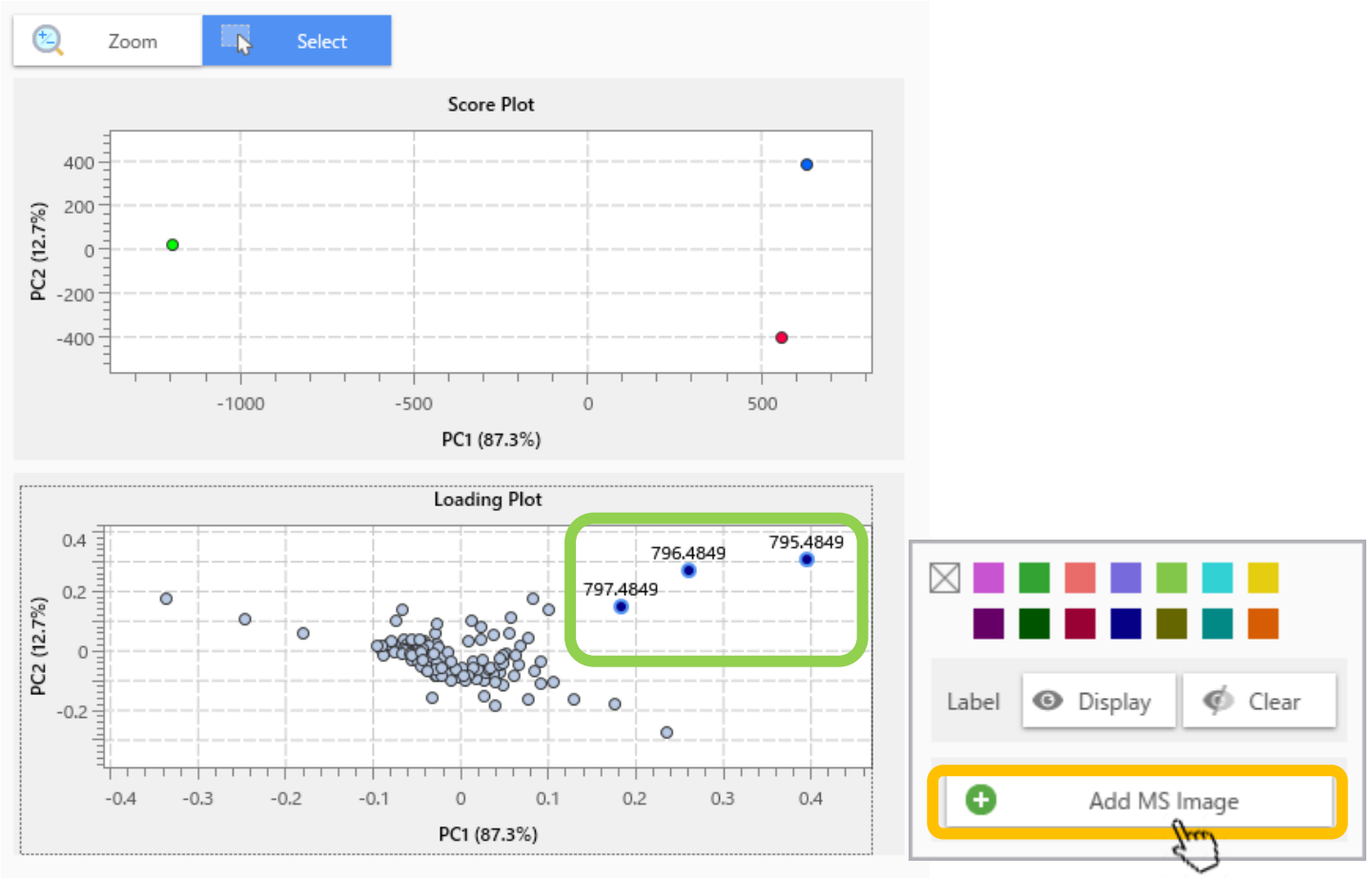

Colours of the selected data points can be changed.
These colours will be applied to other graphs, the data matrix tables and the MS image list.

# 4.11 Display data point labels



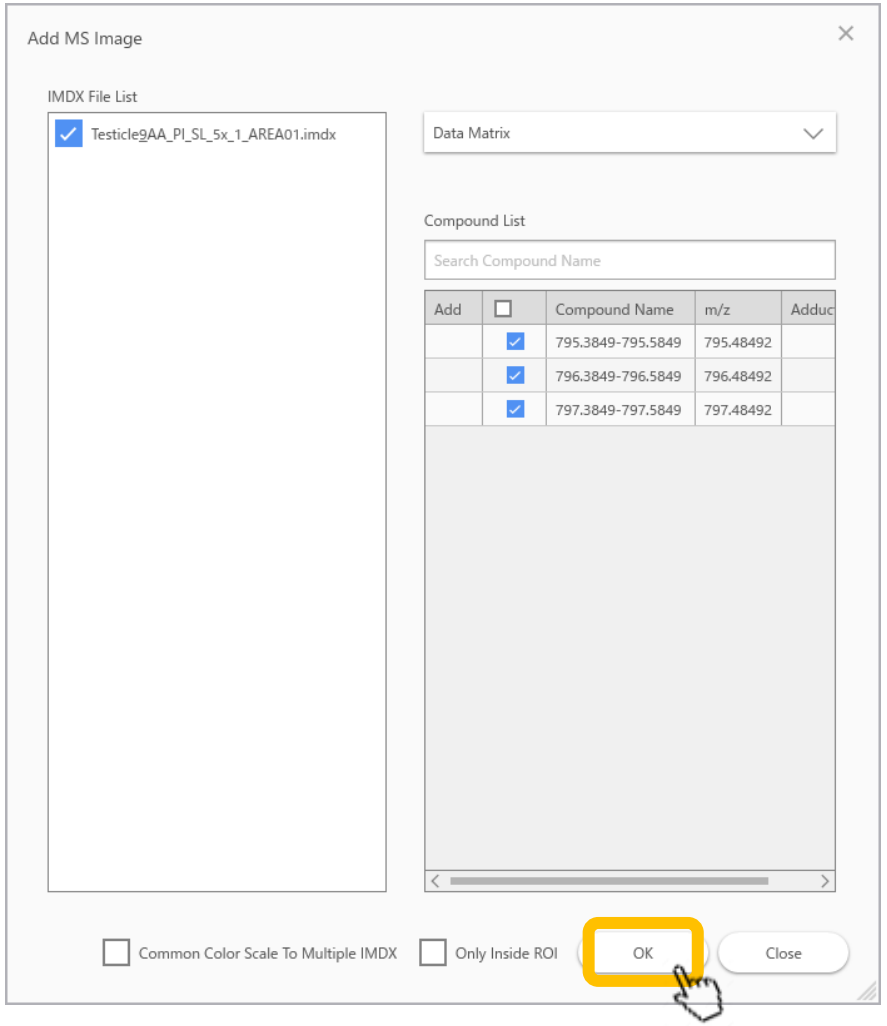

Labels for data points are displayed.

# 4.12 Create an MS image from the data points

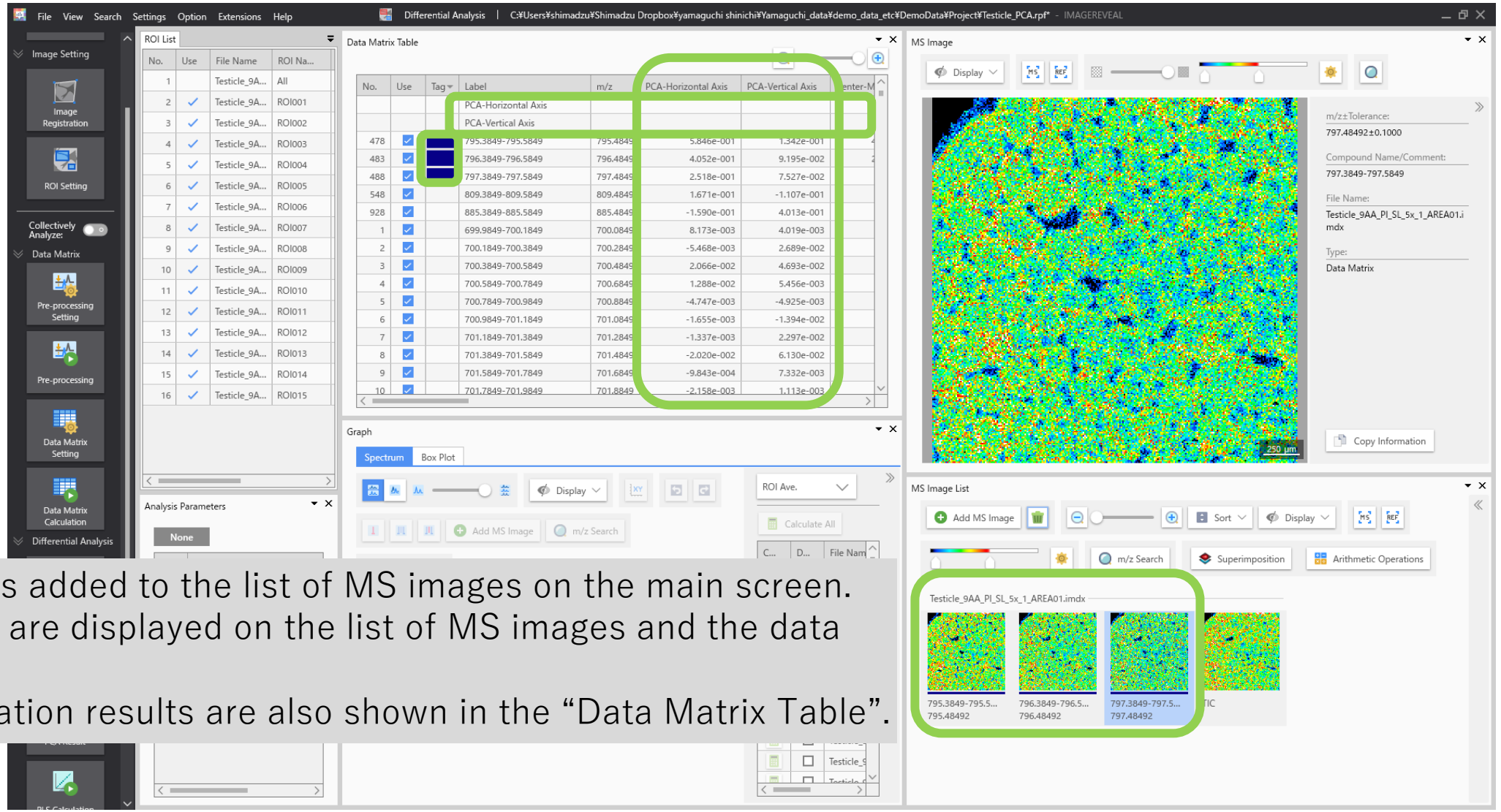



Adds the MS image of the selected data points to the main screen.

# 4.13 Add MS image



# 4.14 Results are displayed on the main screen




The MS image is added to the list of MS images on the main screen.
The tag colours are displayed on the list of MS images and the data matrix table.
The PCA calculation results are also shown in the “Data Matrix Table”.