Creating a data matrix

What is a data matrix?

- Before processing data with IMAGEREVEAL MS, the necessary information is isolated from the data file
  - This is referred to as a “data matrix”
  - The reason for creating a data matrix is that MS imaging files are large and directly processing the original file would take a long time.
- The data is isolated according to the “data matrix settings”
  - The settings relate to MS peak types and widths
- We recommend saving the data matrices to an SSD, because it much faster than saving them to an HDD.

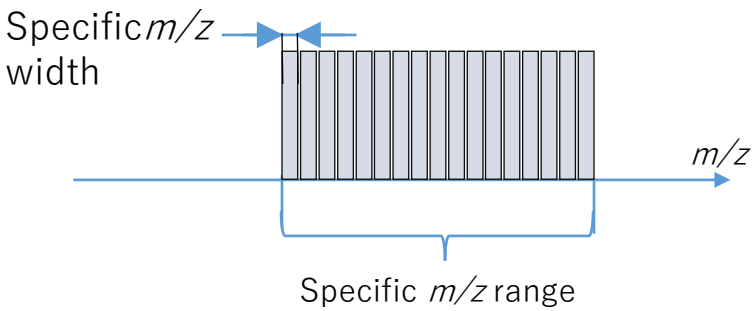
Choosing peaks for processing

Non-target: Whole *m/z* range
Target: Specified *m/z* values
} Set from “data matrix settings”

Peak picking: Select peaks from the mass spectrum → Set from “Peak picking”

Non-target

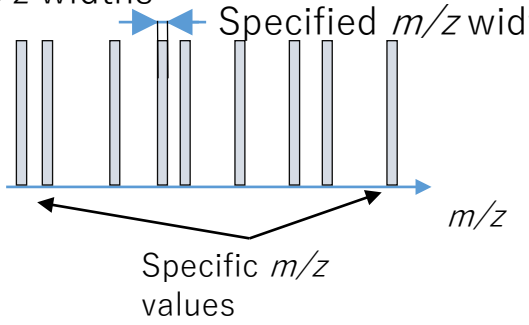
Divide a specific *m/z* into specified *m/z* widths



Target

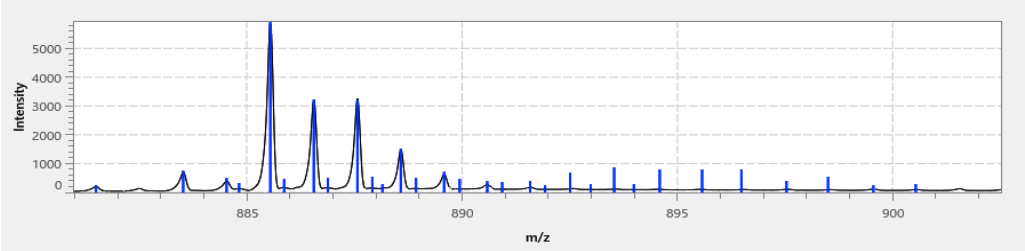
Table of compounds

Cut out specific *m/z* values with specified *m/z* widths

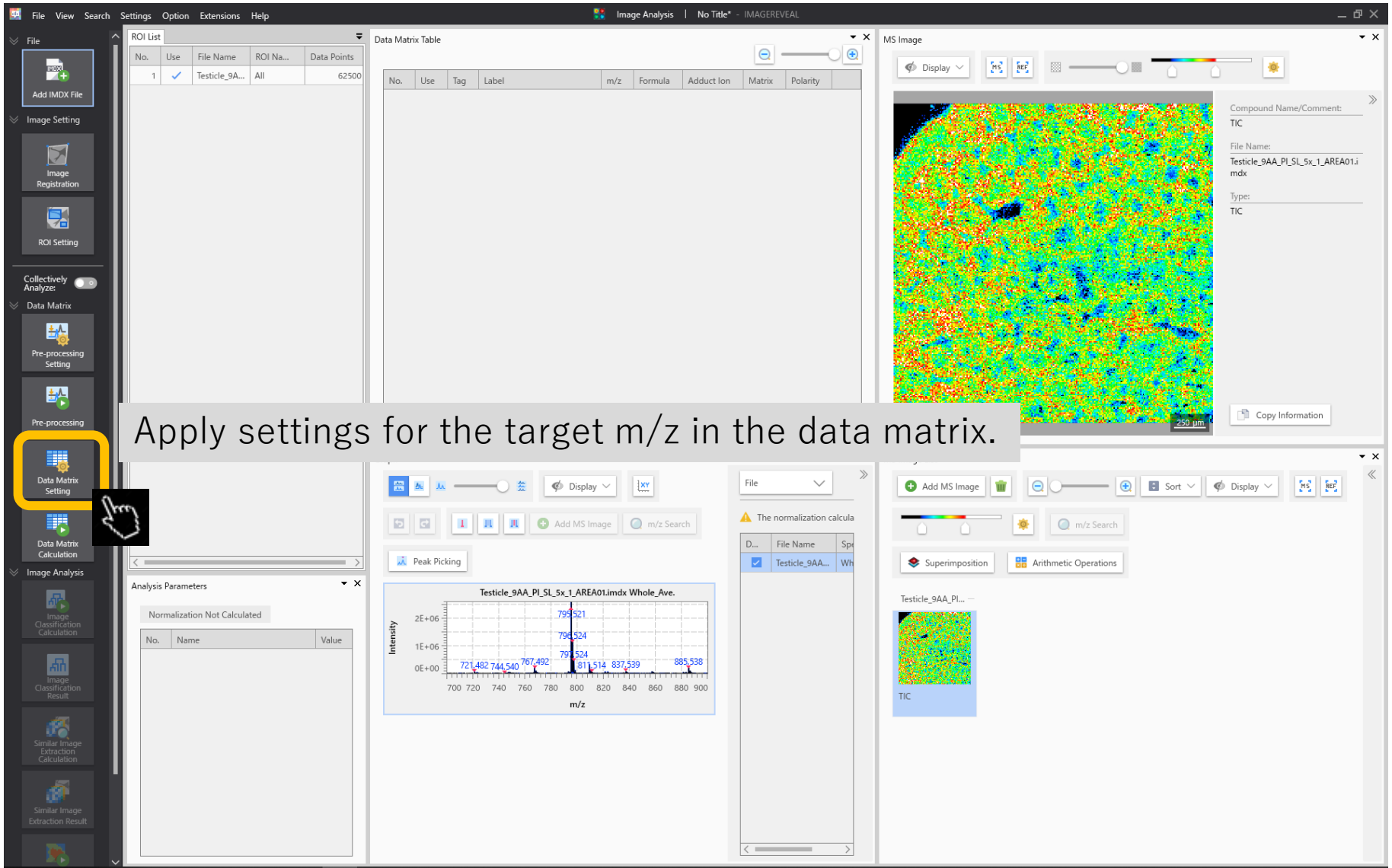


Peak picking

Target based on the measured spectrum

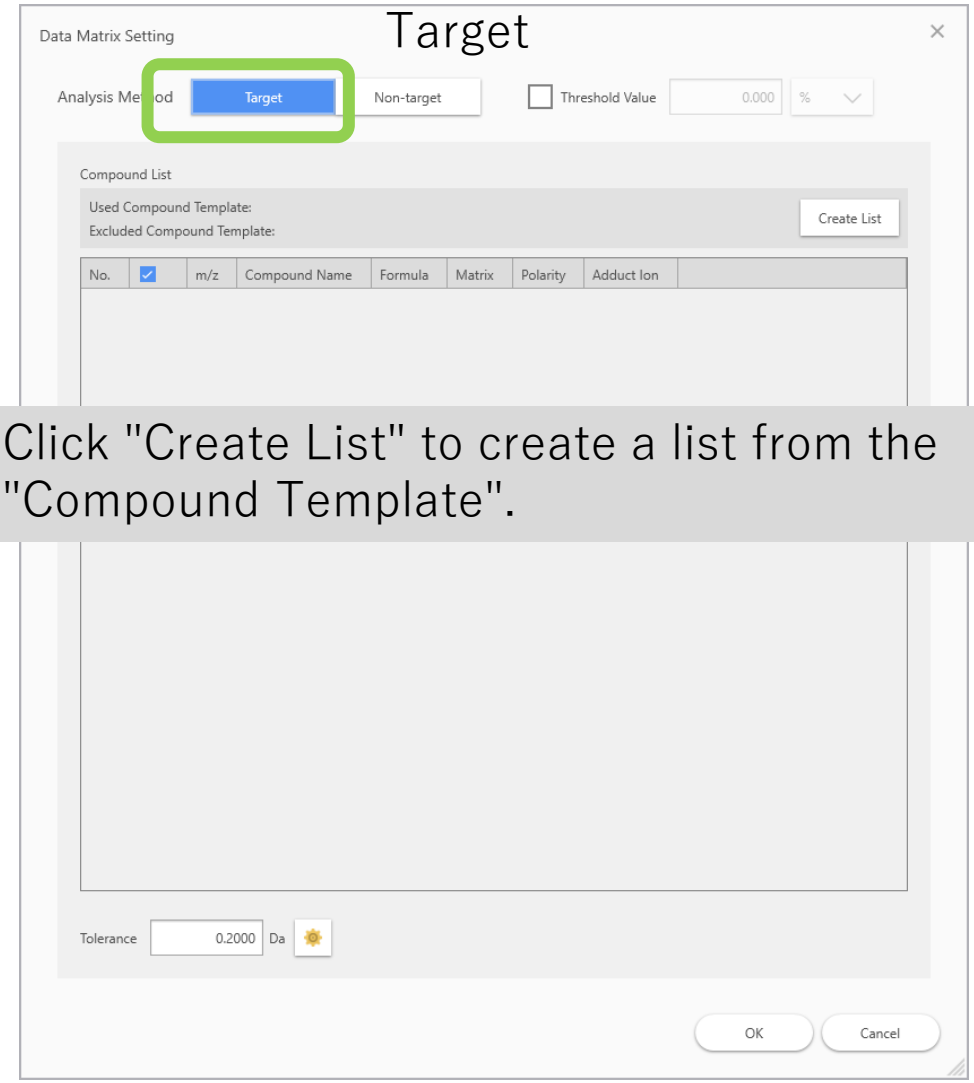


Data matrix settings (target, non-target)



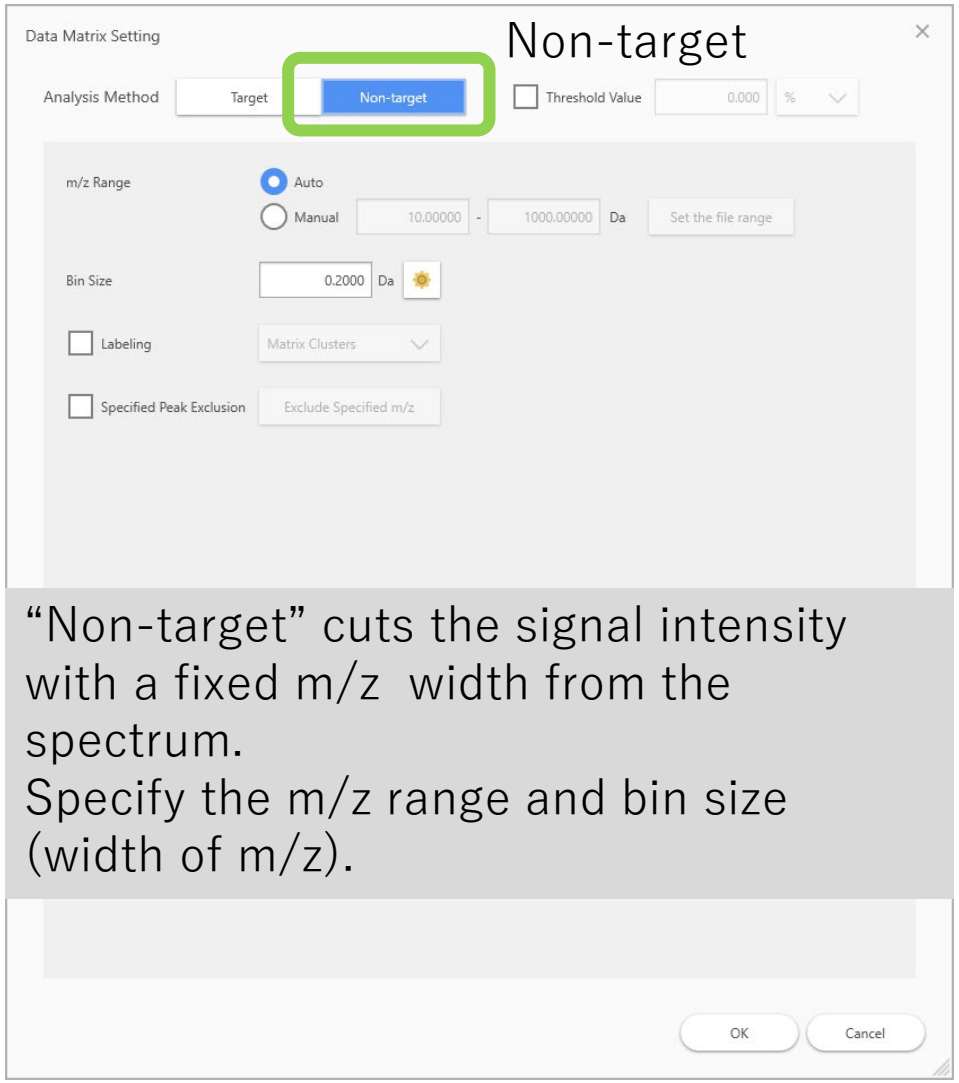
Data matrix settings (choose target or non-target)

Target



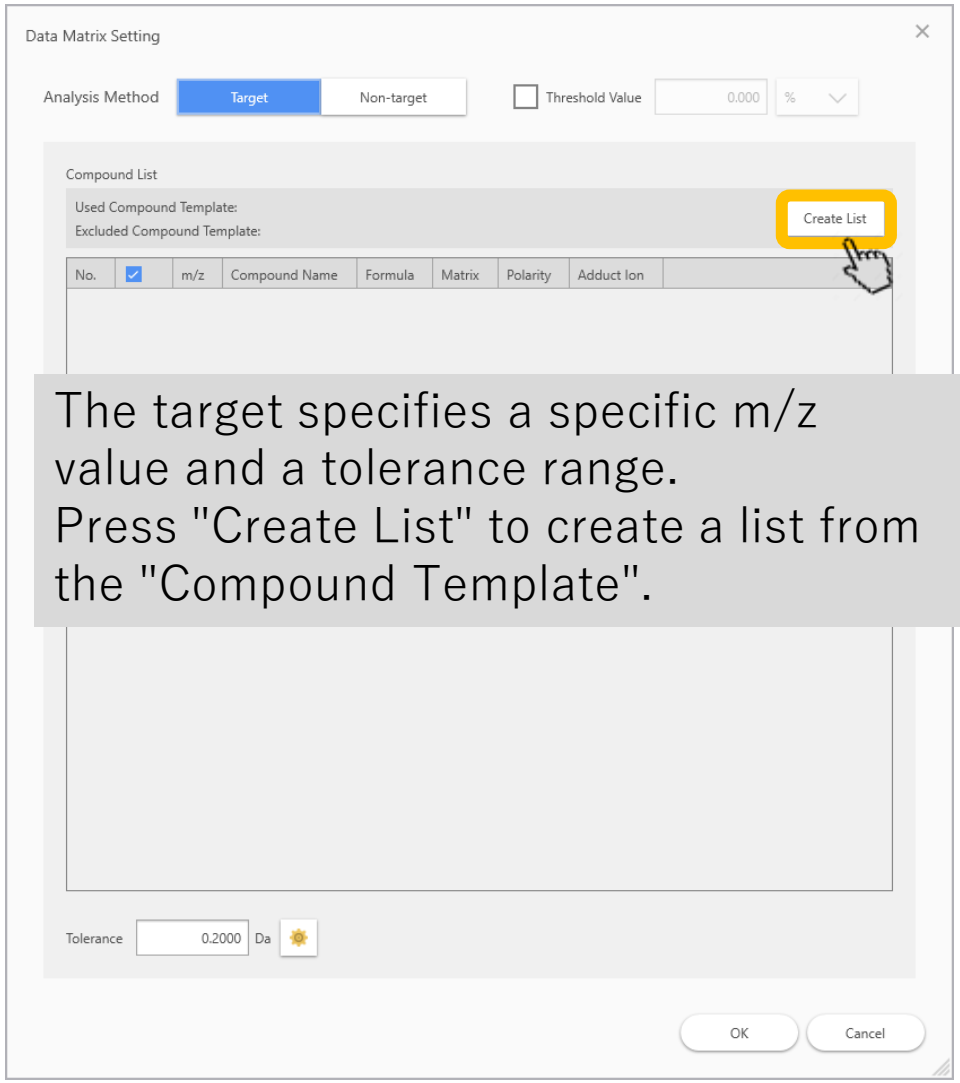
Click "Create List" to create a list from the "Compound Template".

Non-target

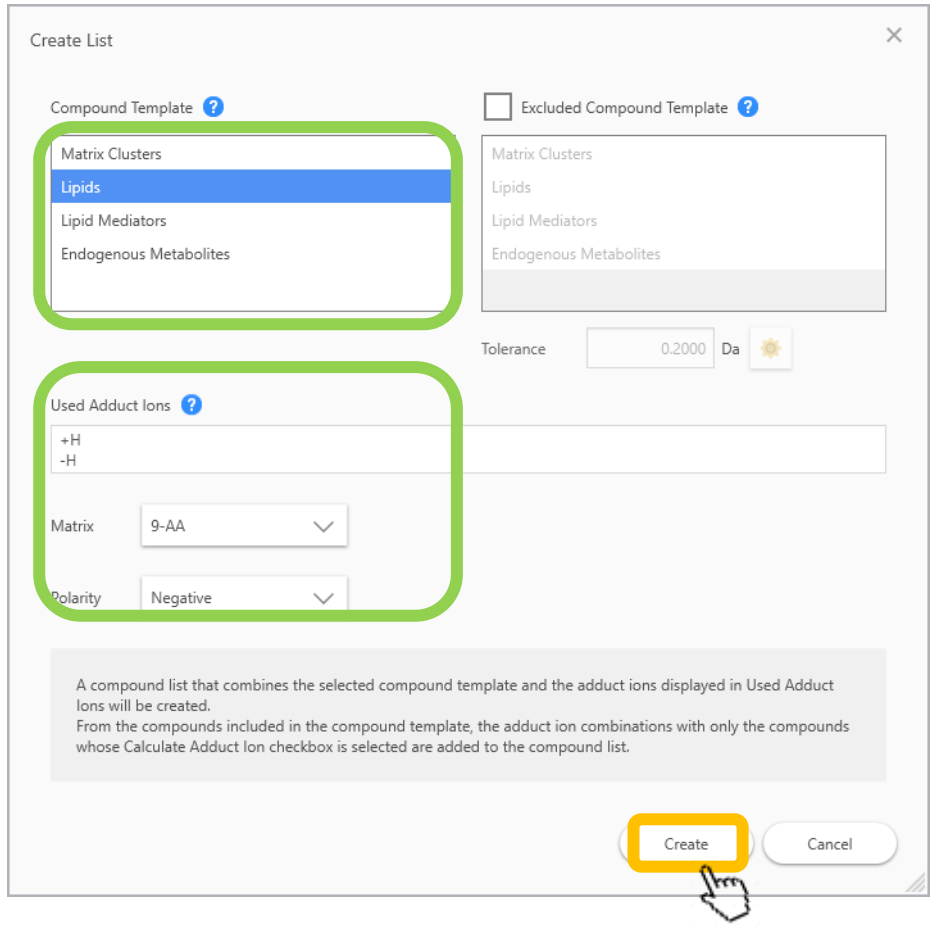


“Non-target” cuts the signal intensity with a fixed m/z width from the spectrum.
Specify the m/z range and bin size (width of m/z).

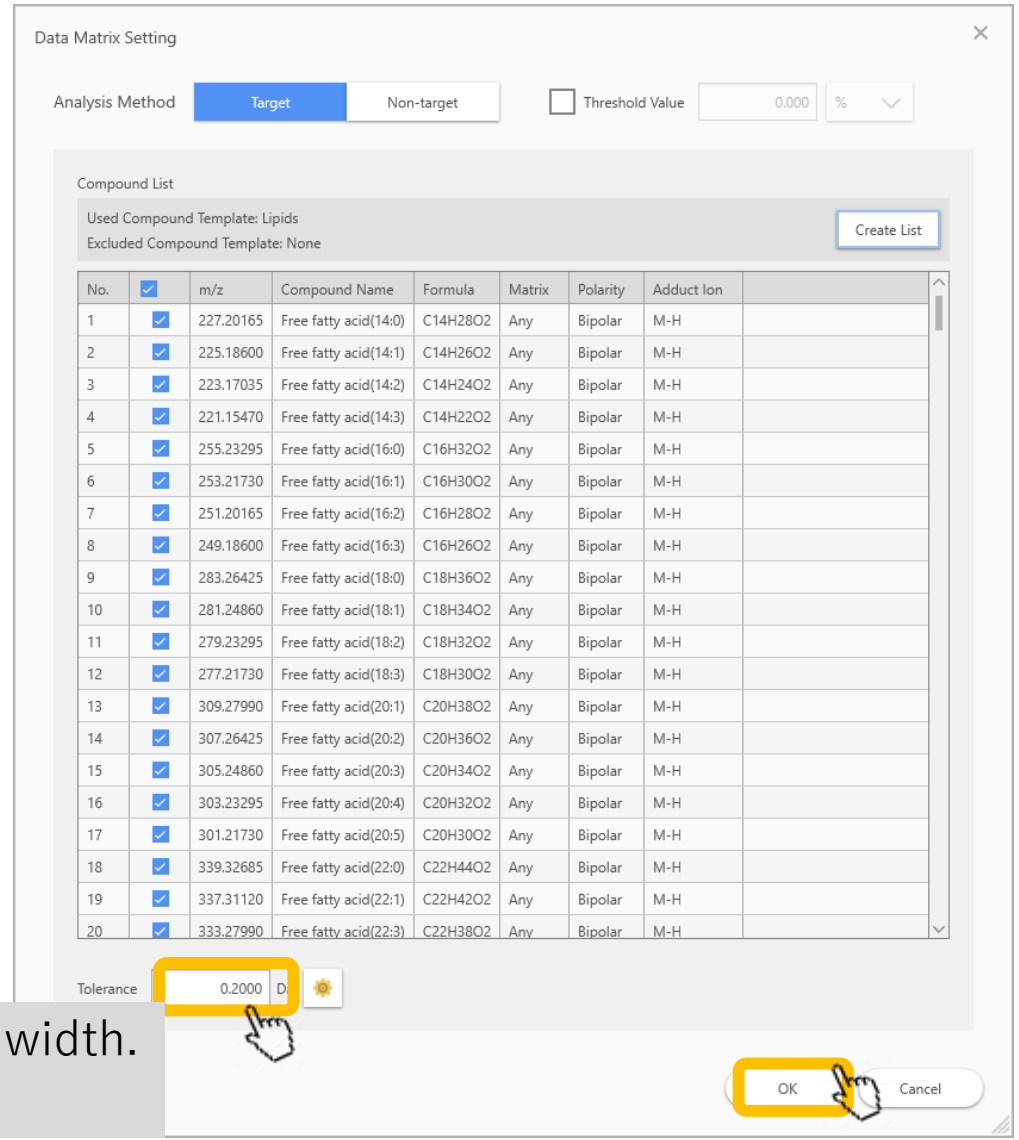
Data matrix settings (target)



The target specifies a specific m/z value and a tolerance range.
Press "Create List" to create a list from the "Compound Template".

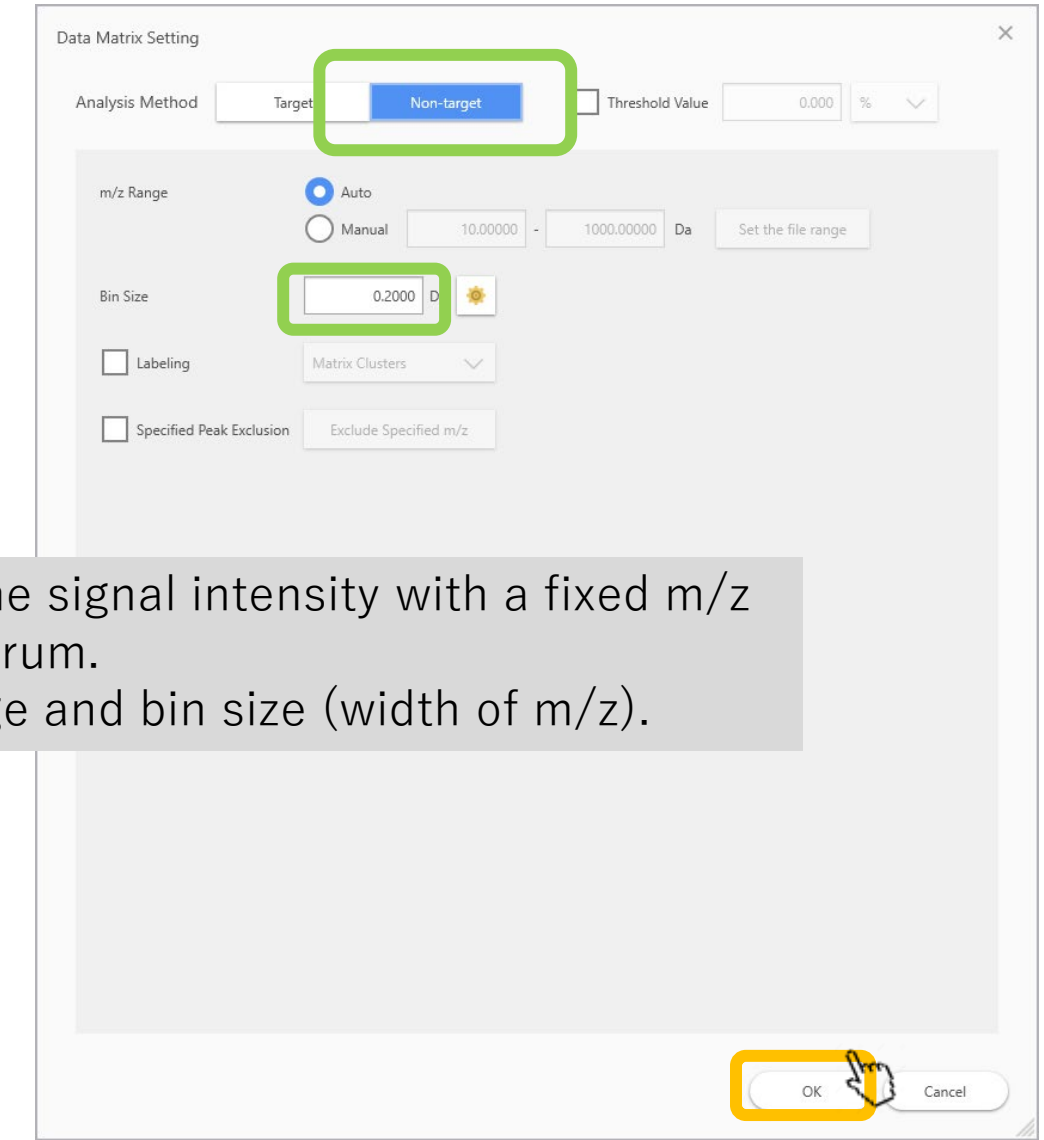


Data matrix settings (target)



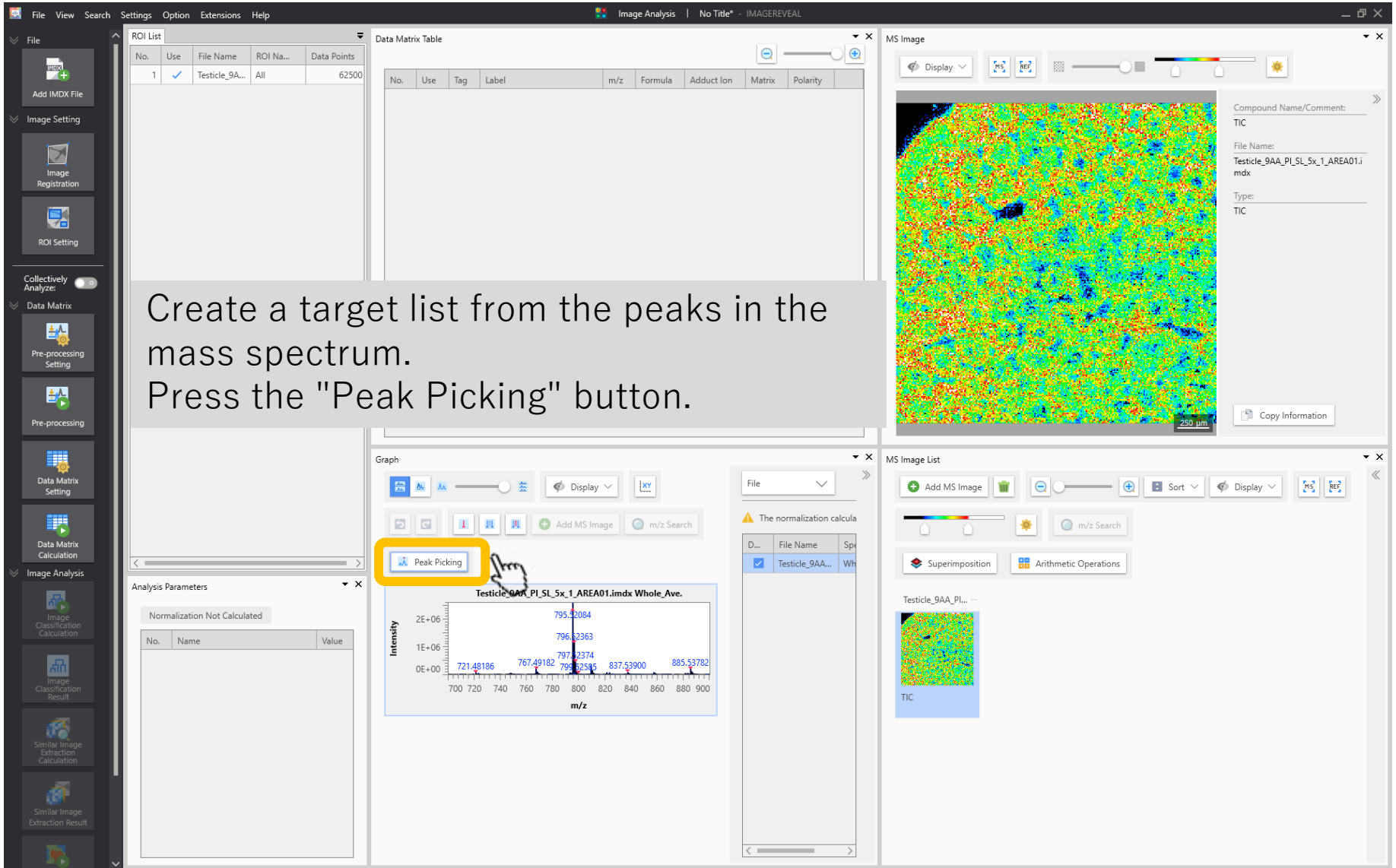
Specifies the allowable width. (Tolerance)

Data matrix settings (non-target)



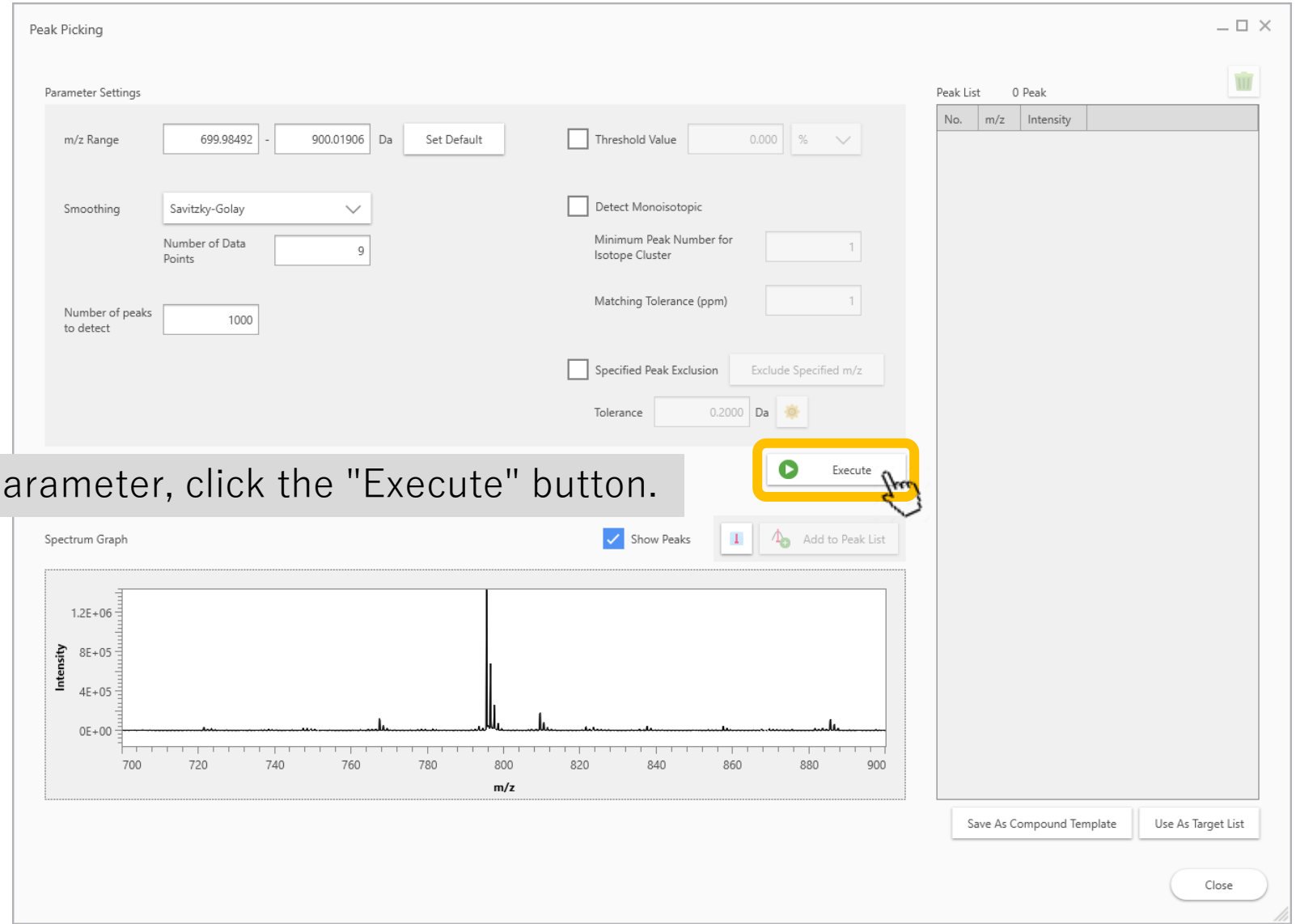
“Non-target “ cuts the signal intensity with a fixed m/z width from the spectrum.
Specify the m/z range and bin size (width of m/z).

Create a target list through peak picking

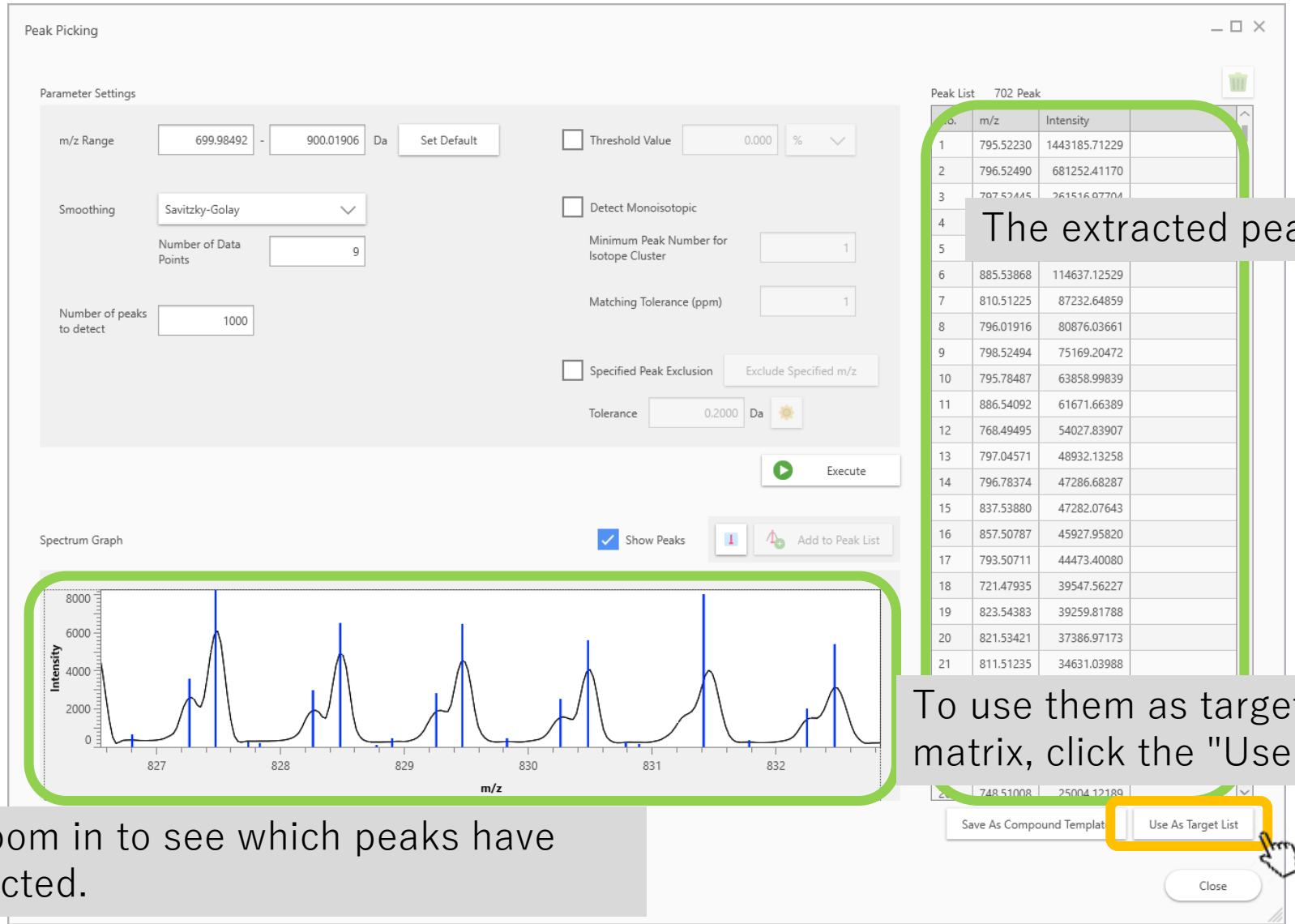


Create a target list through peak picking

After setting each parameter, click the "Execute" button.



Create a target list through peak picking

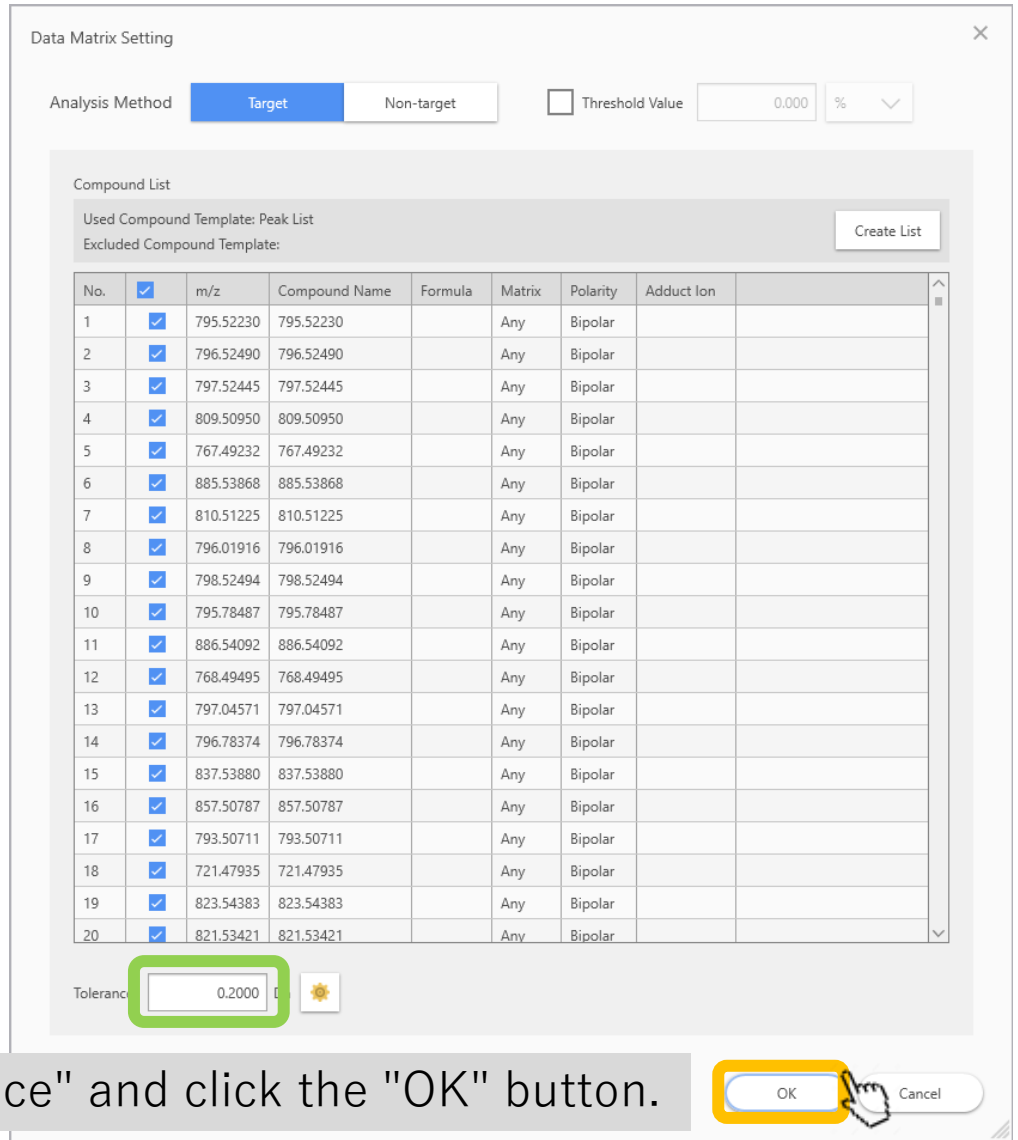


The extracted peaks will be displayed.

To use them as targets for creating a data matrix, click the "Use as target list" button.

You can zoom in to see which peaks have been extracted.

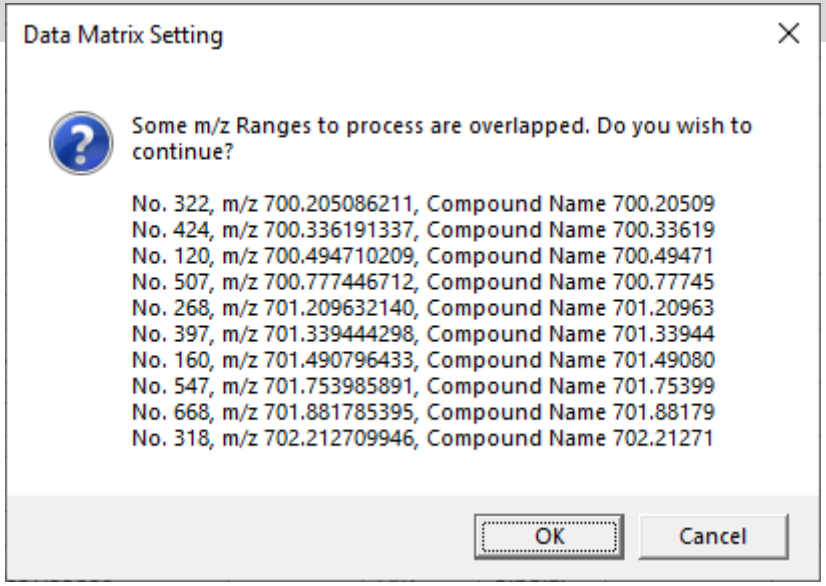
Create a target list through peak picking



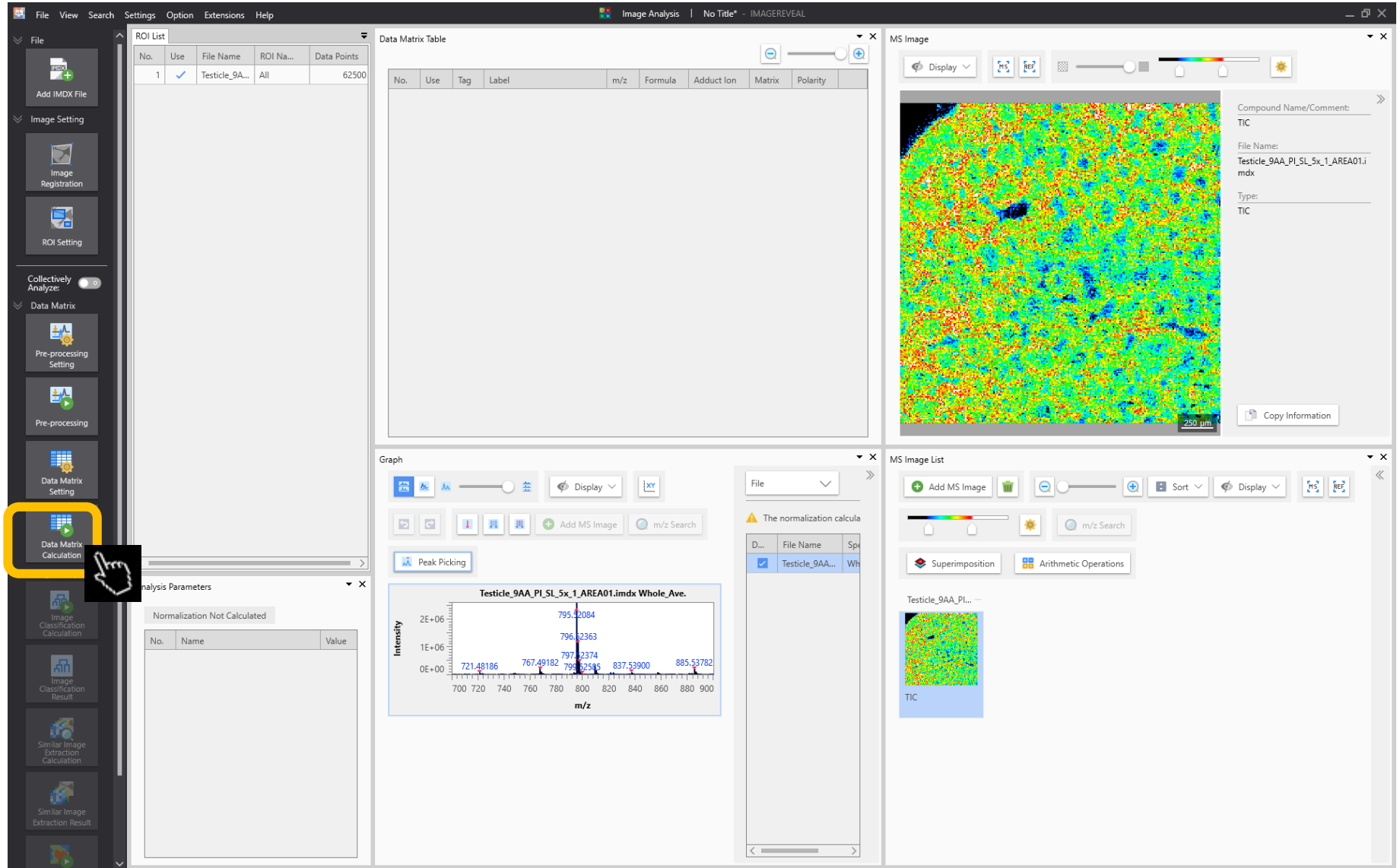
Enter the “Tolerance" and click the "OK" button.

Create a target list through peak picking

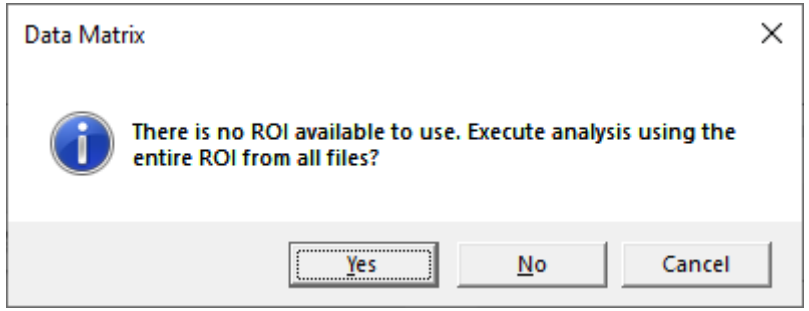
Depending on the tolerance, m/z widths of nearby peaks may be overlapped.
In this case, a warning will appear.
Unless the overlap is a problem, click the "OK" button.
If it is a problem, click the “cancel” button and adjust the tolerance value.



Once the data matrix settings are complete, move onto the matrix calculations

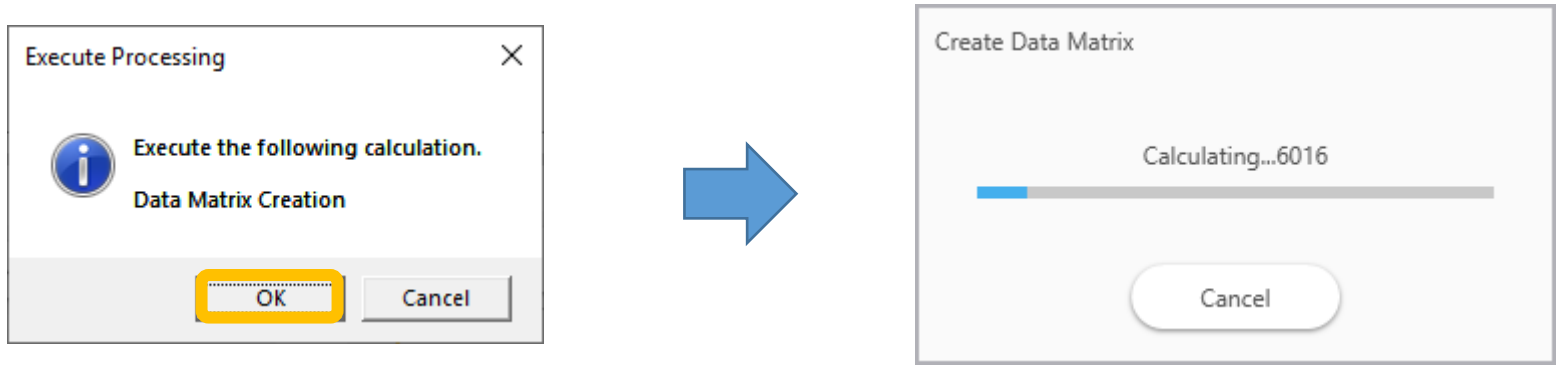


If there are no ROI settings, a window will appear to verify



If you wish to process the entire measurement region, click “Yes”

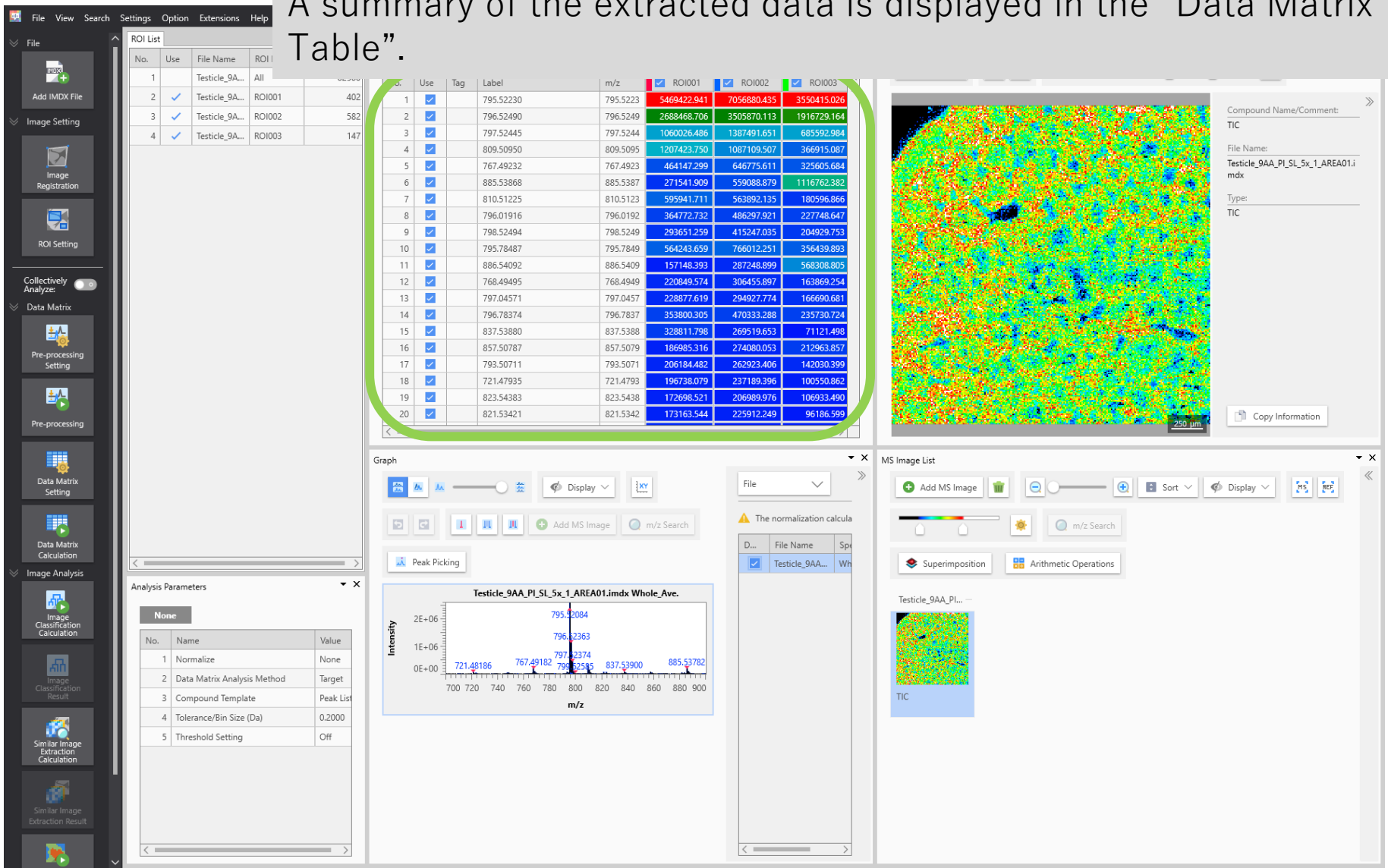
A window will appear to start calculations to create a data matrix



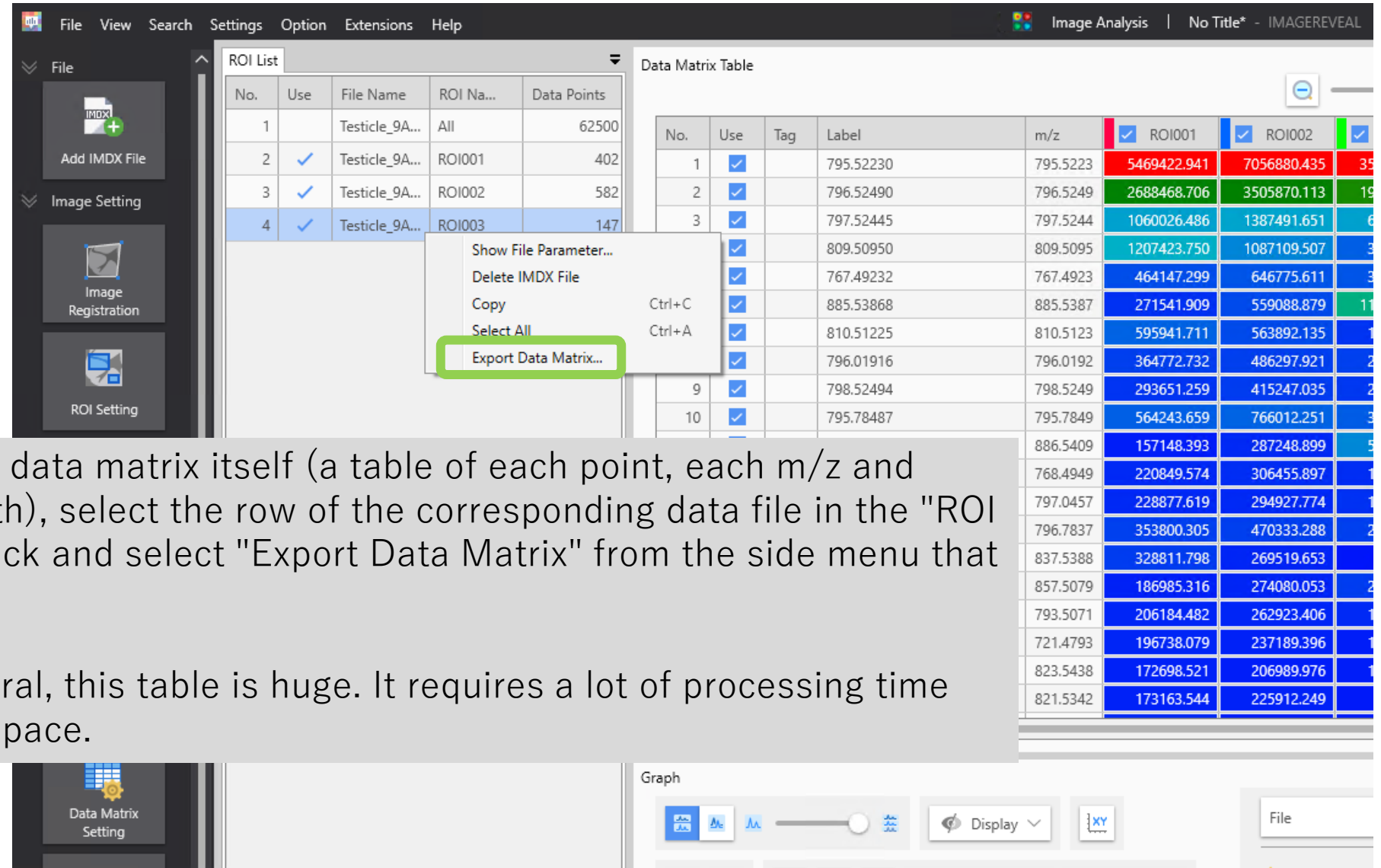
Click “OK” to begin calculations.

Data matrix calculations are complete

A summary of the extracted data is displayed in the “Data Matrix Table”.



Export the data matrix



To export the data matrix itself (a table of each point, each m/z and signal strength), select the row of the corresponding data file in the "ROI List", right-click and select "Export Data Matrix" from the side menu that appears.

Note: In general, this table is huge. It requires a lot of processing time and storage space.