

Calculations combining multiple images

Select the images that you want to use in the calculations

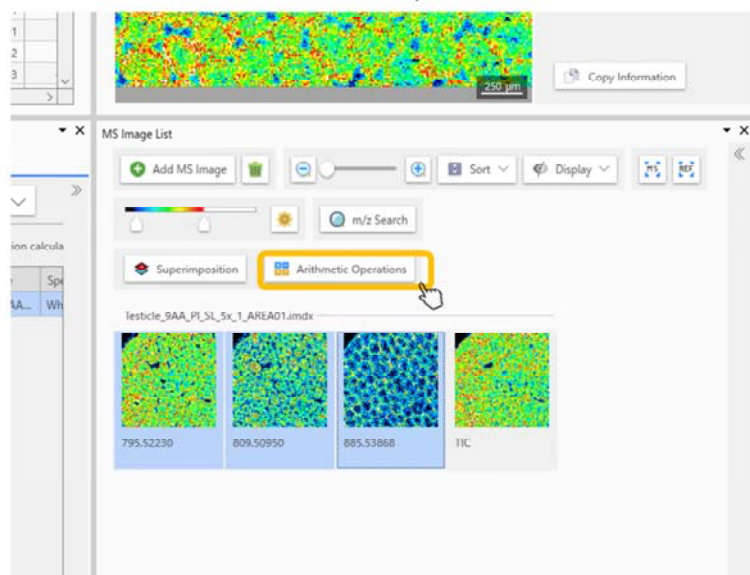
The screenshot displays a software interface with several panels. On the left is a sidebar with navigation icons. The main area is divided into four sections:

- Data Matrix Table:** A table with columns: ID#, User, Log, Label, PCA Principal Data, PCA Principal Axis, and PCA Principal Axis. It contains 18 rows of data.
- Heatmap:** A large square heatmap with a color scale from blue to red, representing data values across a spatial grid.
- Image Selection Panel:** A panel titled 'Add New Image' showing a row of four small image thumbnails. A yellow box highlights the first three thumbnails, and a hand cursor points to the word 'select' next to them.
- Analysis Parameters:** A panel on the bottom left with a table of parameters and their values.

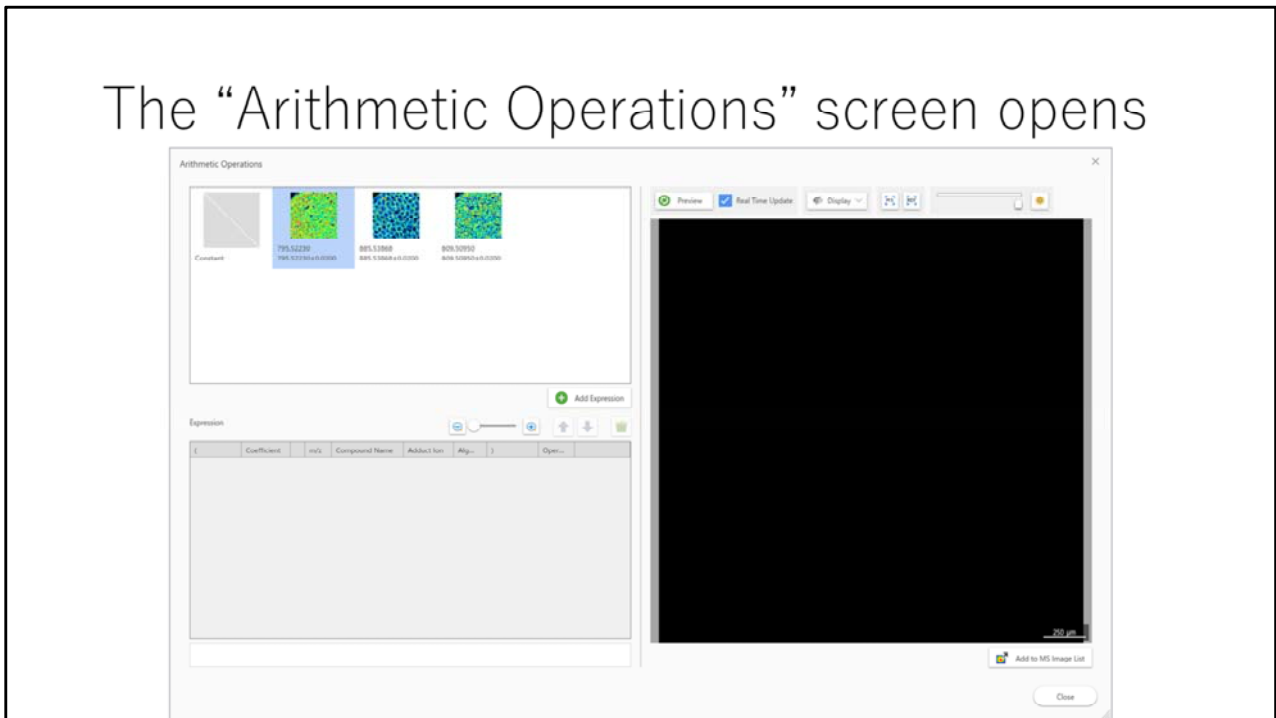
ID#	User	Log	Label	PCA Principal Data	PCA Principal Axis	PCA Principal Axis
1			PCA Principal Data			
2			PCA Principal Axis			
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						
16						
17						
18						

ID#	Name	Value
1	Iteration	None
2	Data Matrix Analysis Method	Target
3	Computational Template	Peak List
4	Subtraction/Residual Size (Std)	0.0001
5	Threshold Setting	Off

Click the “Arithmetic Operations” button

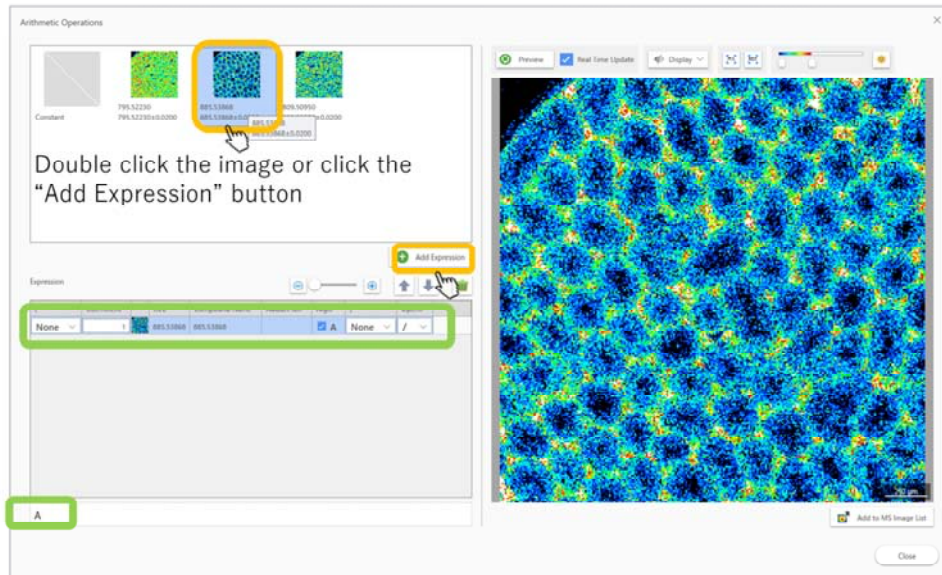


The “Arithmetic Operations” screen opens



The image you select appears on the right

Double click on the image to add an expression



Add the m/z to be used in the calculations to the command.

Change the order, operators, brackets, coefficients etc. to create the necessary expressions.

(Coefficient	m/z	Compound Name	Adduct Ion	Alg...)	Oper...
None	1	885.53868	885.53868		<input checked="" type="checkbox"/> A	None /	
None	1	795.52230	795.52230		<input checked="" type="checkbox"/> B	None /	
None	1	809.50950	809.50950		<input checked="" type="checkbox"/> C	None /	

A/B/C

Change the order, operators, brackets, coefficients etc. to create the necessary expressions.

Example of (A+B)/C

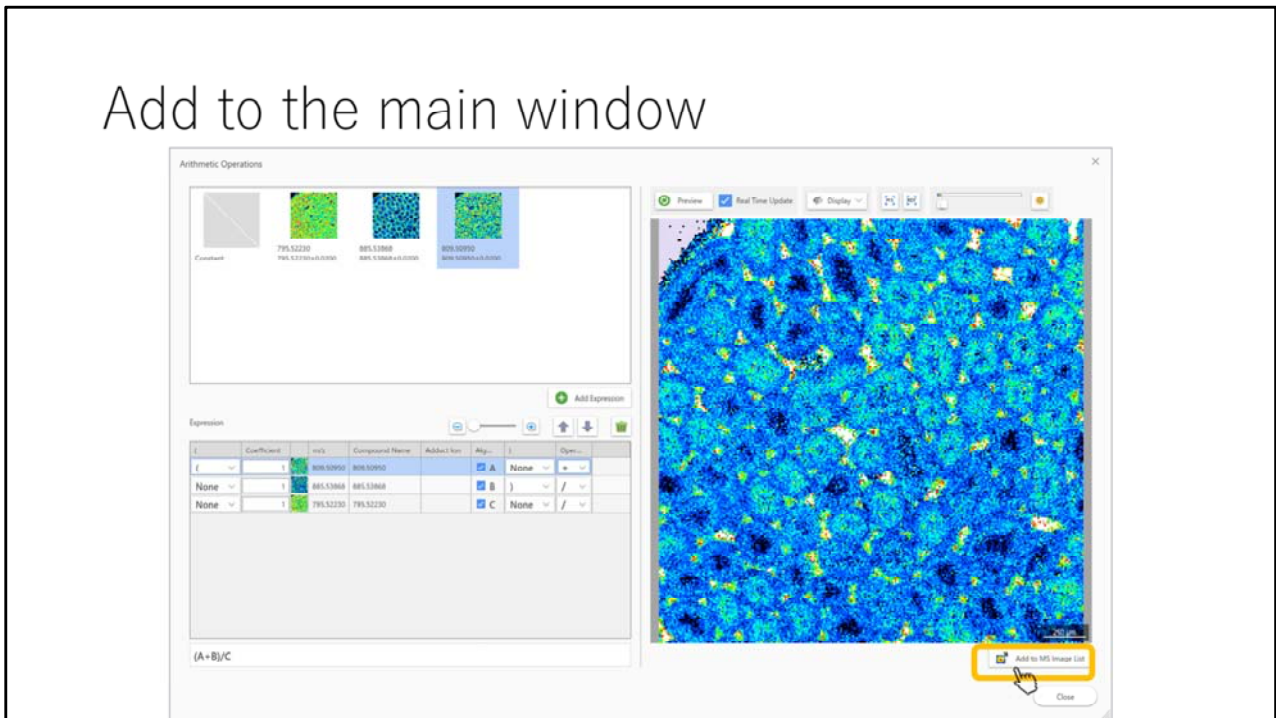
Expression

(Coefficient	m/z	Compound Name	Adduct Ion	Alg...)	Oper...
(1	809.50950	809.50950		<input checked="" type="checkbox"/> A	None	+
None	1	885.53868	885.53868		<input checked="" type="checkbox"/> B)	/
None	1	795.52230	795.52230		<input checked="" type="checkbox"/> C	None	/

(A+B)/C

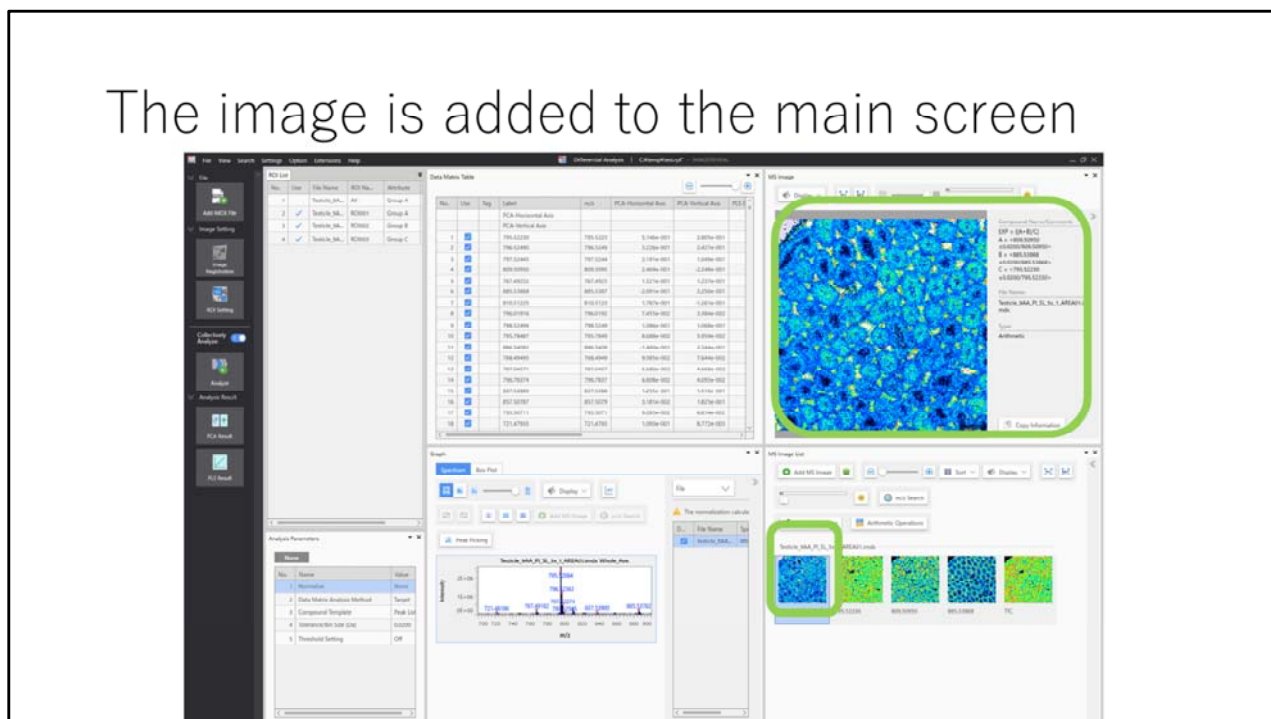
Example of (A+B)/C

Add to the main window



The image created can be added to the list of MS images on the main window

The image is added to the main screen



The information about the calculations is included in a comment. The expression is displayed as a compound name.