Find components that differ between regions

Example

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

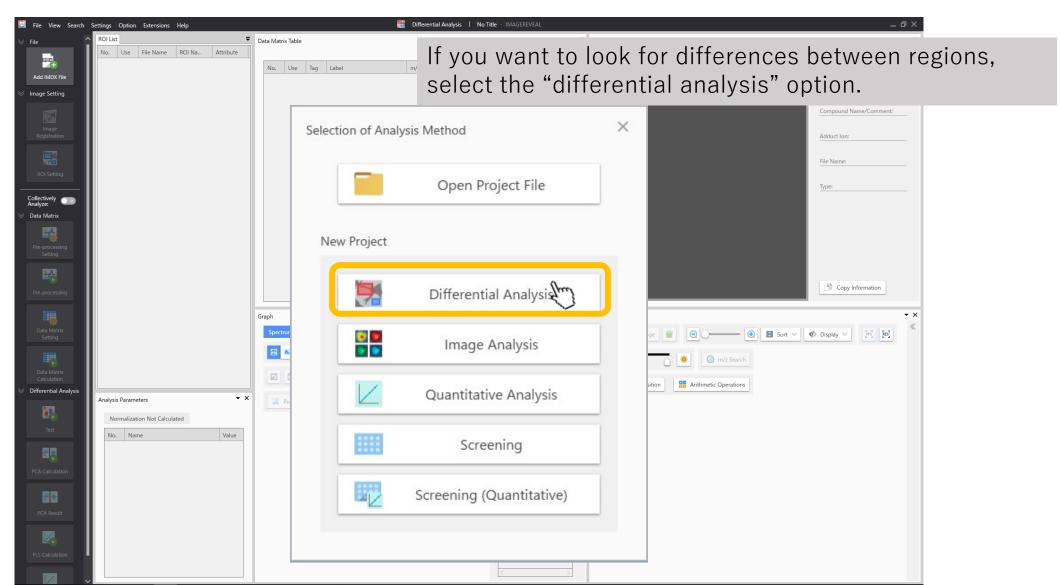
Steps

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

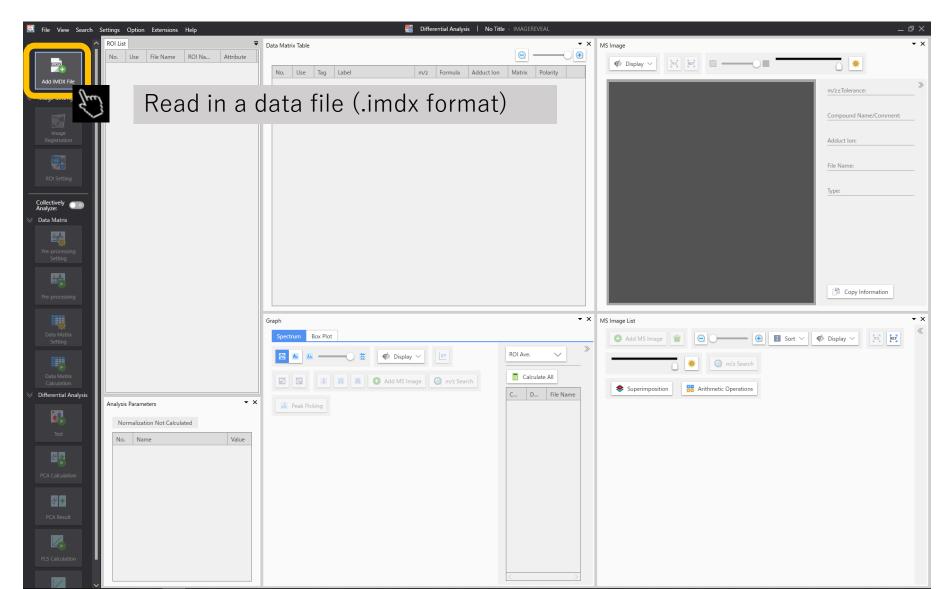
Steps

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

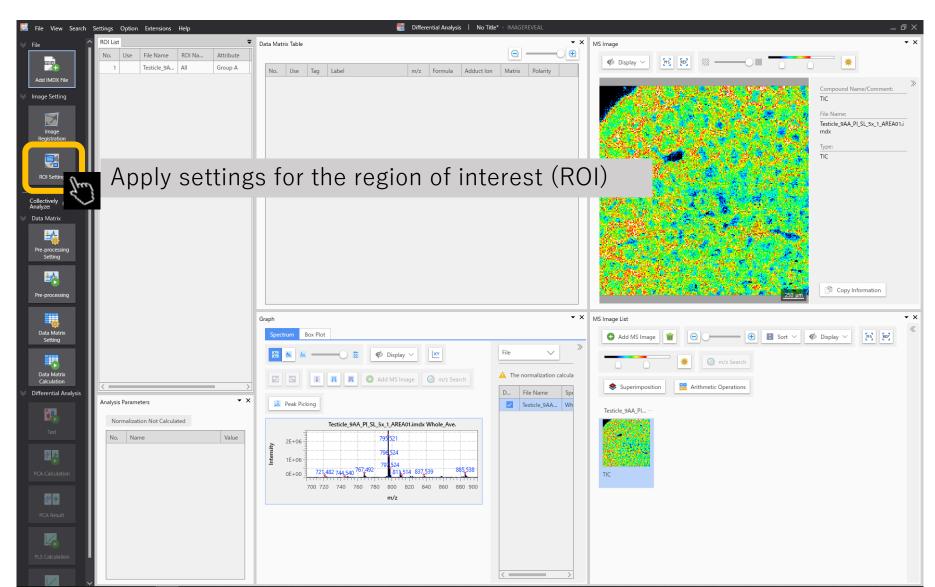
1.1 Select "Differential analysis"



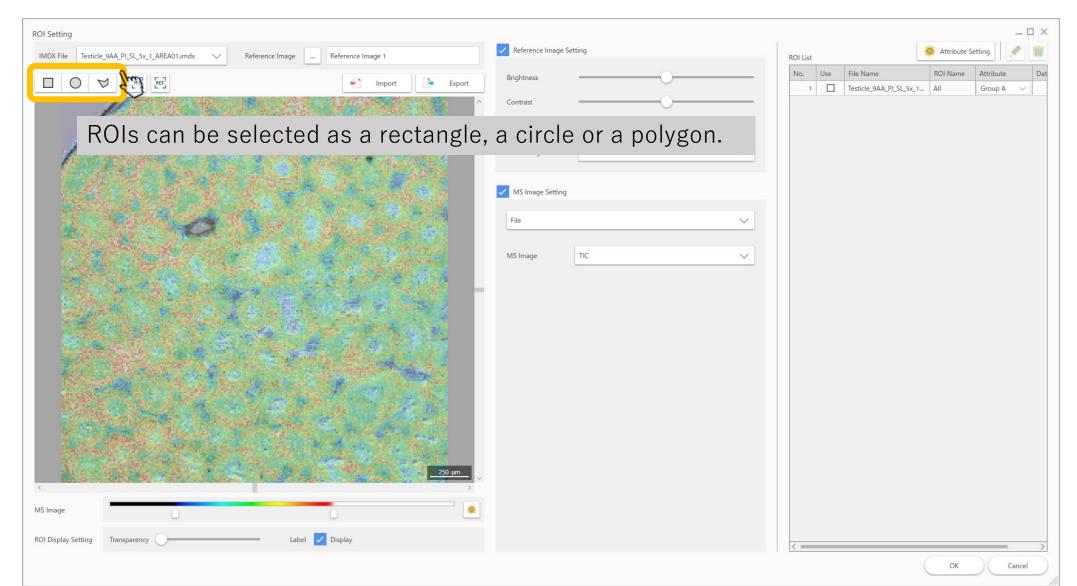
1.2 Add data file (.imdx)



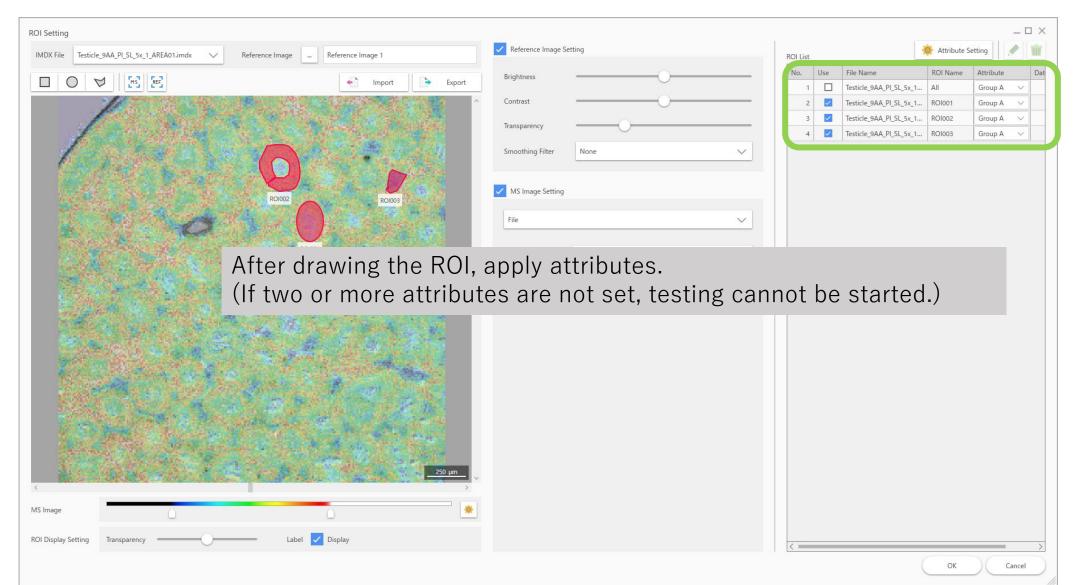
1.3 ROI settings



1.4 ROI settings



1.5 ROI settings

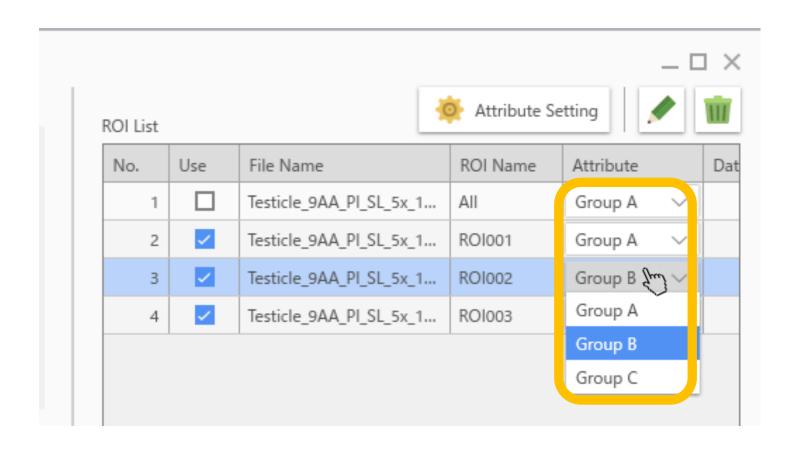


1.6 ROI settings

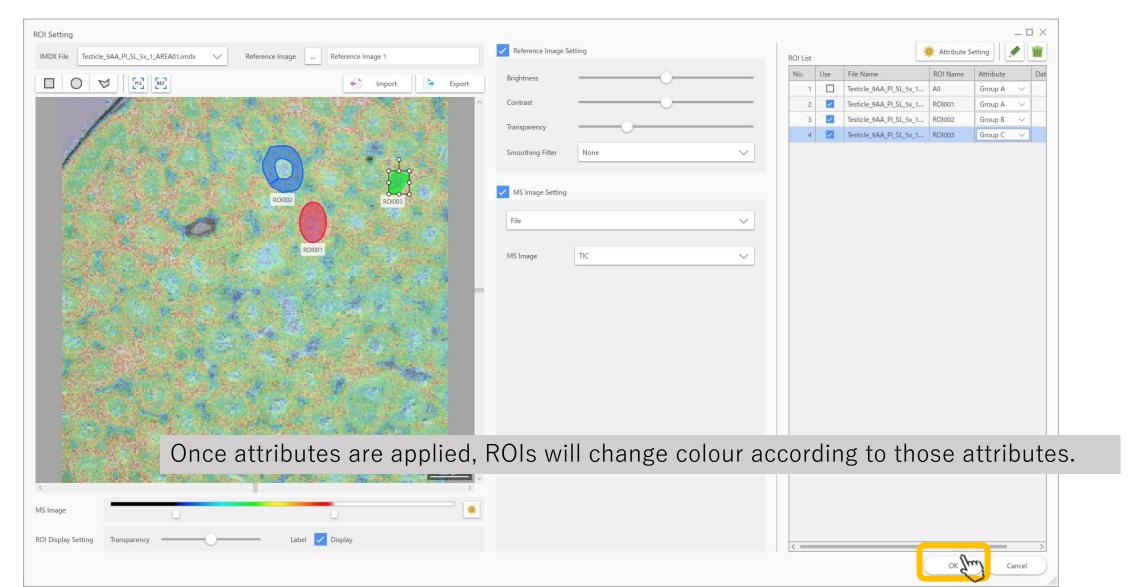
Select attributes for each ROI in the "Attributes" column. Attributes can be added or edited. The names of the ROIs can be changed.

No.	Use	File Name	ROI Name	Attribute	Dat
1		Testicle_9AA_PI_SL_5x_1	All	Group A V	
2	~	Testicle_9AA_PI_SL_5x_1	ROI001	Group A 🗸	
3	~	Testicle_9AA_PI_SL_5x_1	ROI002	Group A fm V	
4	~	Testicle_9AA_PI_SL_5x_1	ROI003	Group A V	

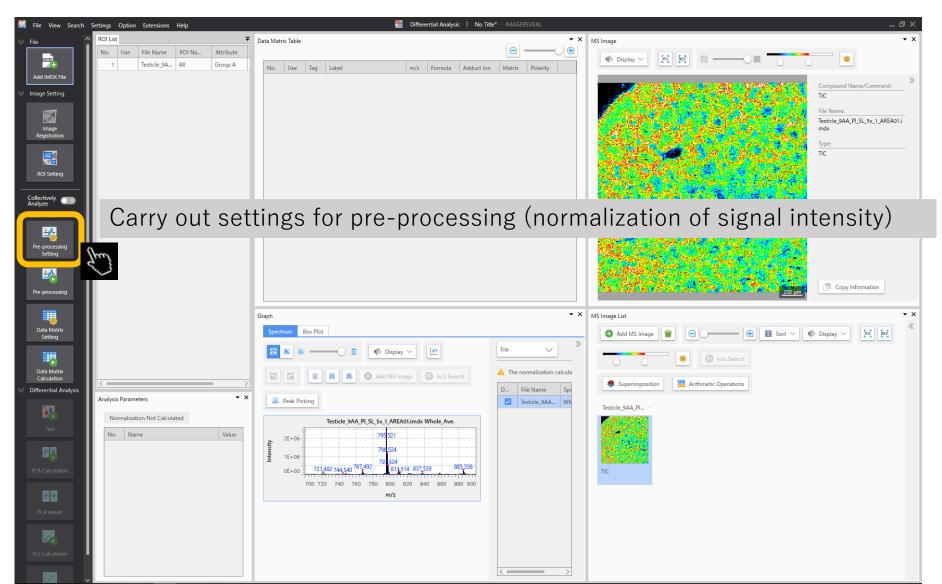
1.7 ROI settings



1.8 ROI settings



2.1 Pre-processing settings

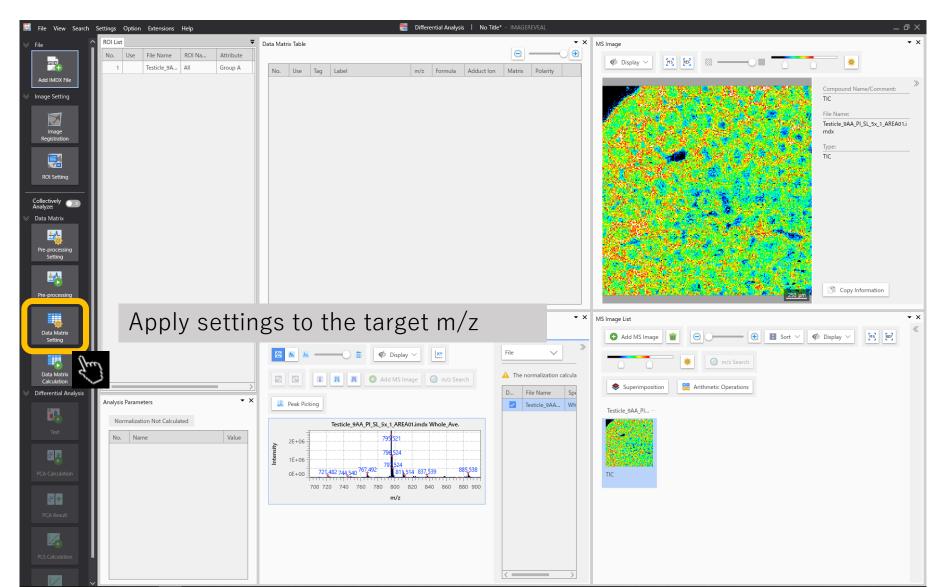


2.2 Pre-processing settings

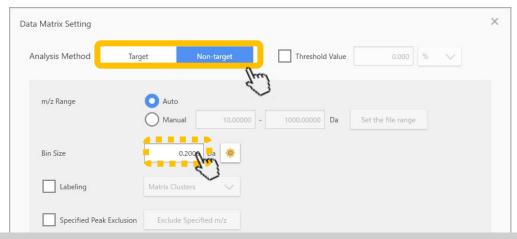


Set the "Normalize" criteria. TIC is generally used.

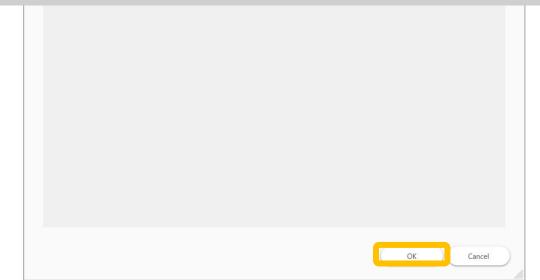
2.3 Data matrix settings



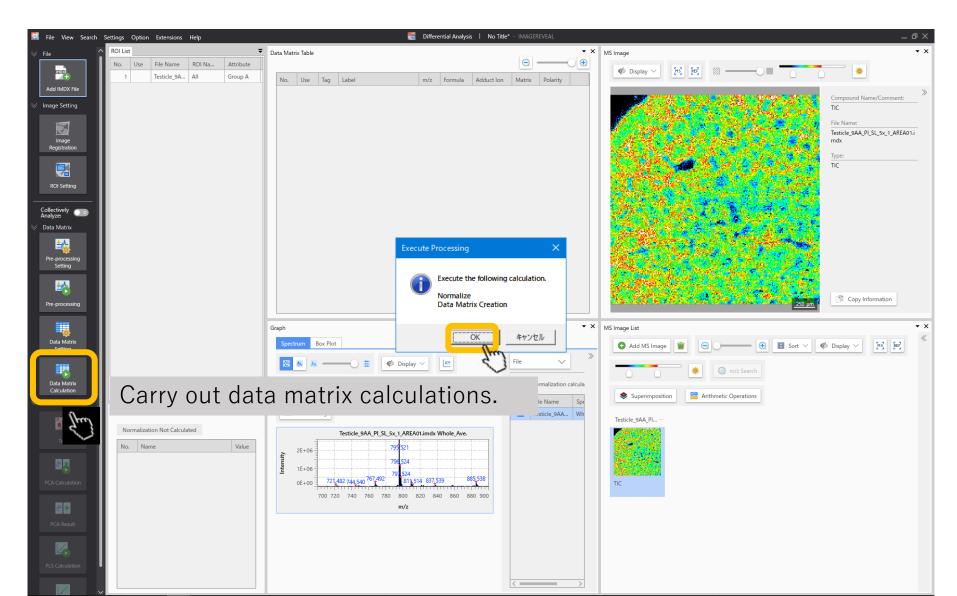
2.4 Data matrix settings



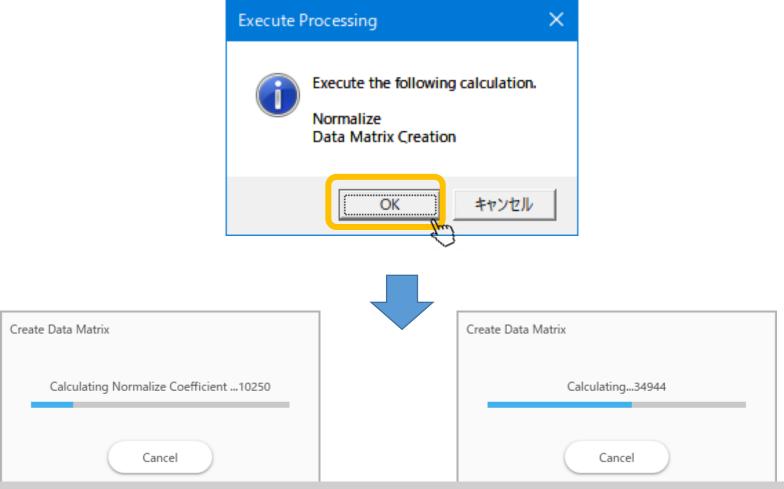
Non-target: cut out fixed widths of signal intensity from the spectrum. Target: specify particular m/z values and the tolerance width.



2.5 Data matrix calculations

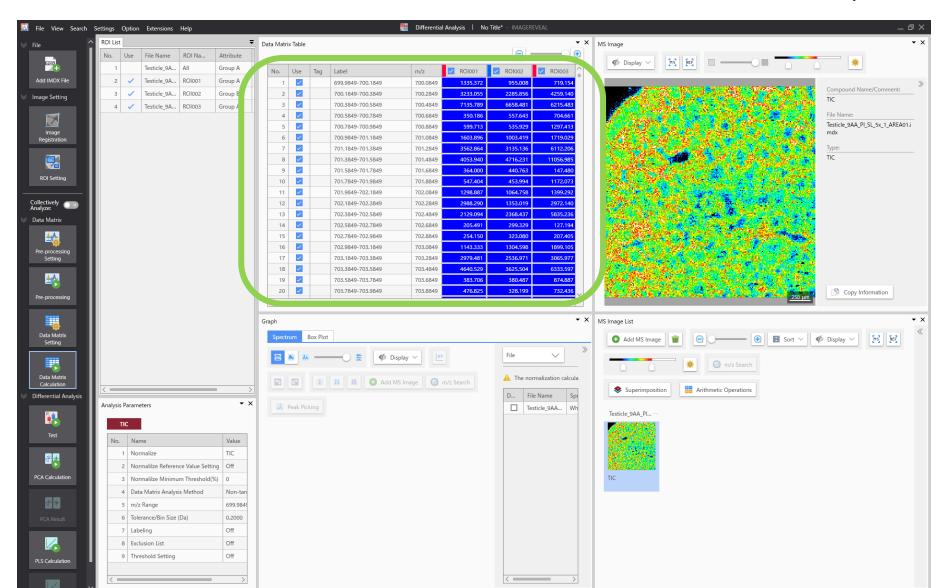


2.6 Running calculations



If pre-processing calculations have not yet been carried out, they will be run here at the same time. If there are a large number of target compounds, the calculations will take longer.

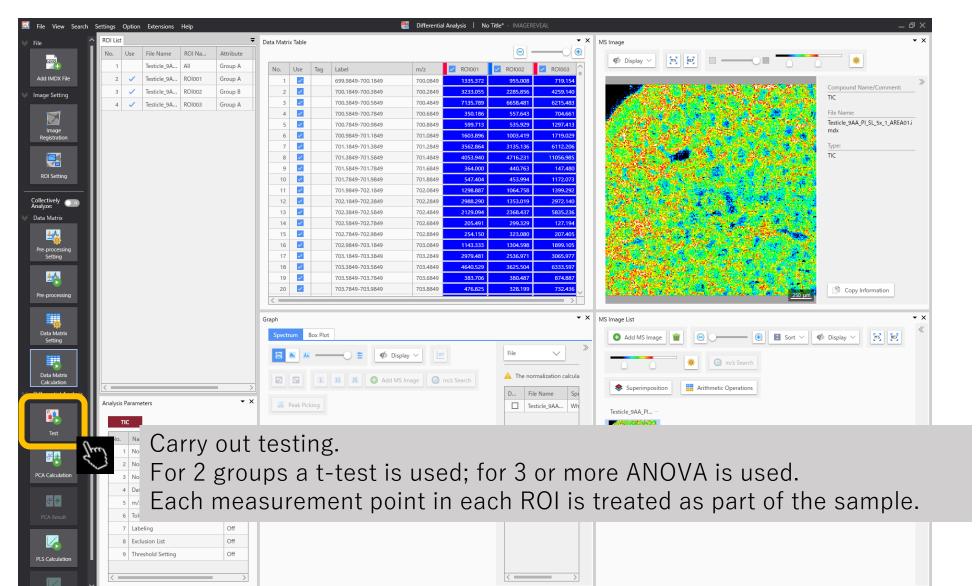
2.7 Data matrix calculations are complete



Steps

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

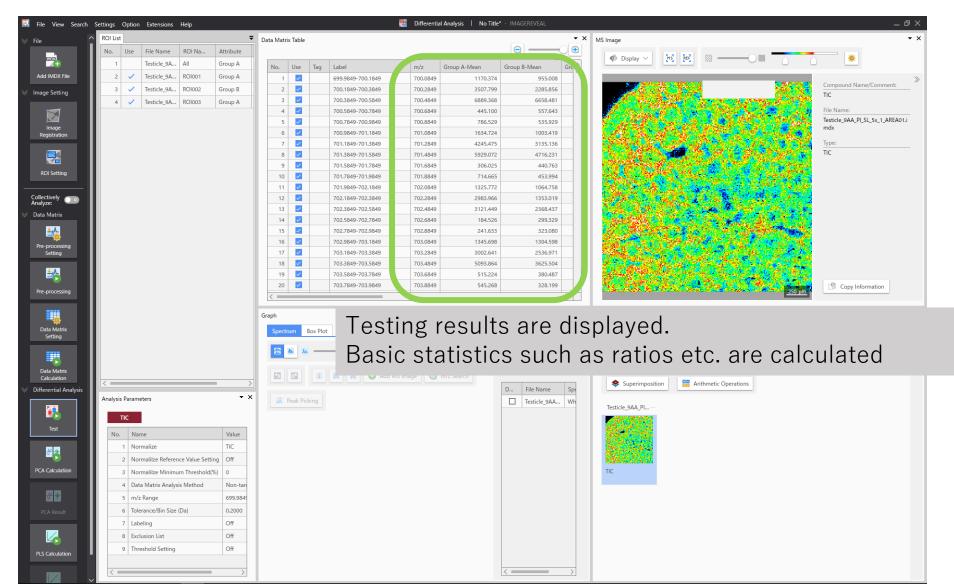
3.1 Testing



3.2 Dialogue window during calculations



3.3 Testing results



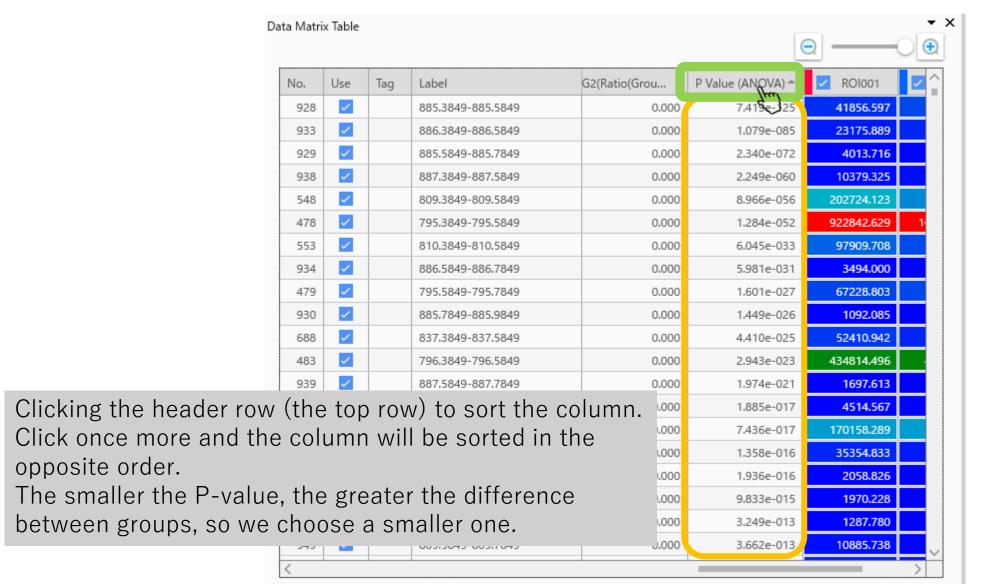
3.4 Testing results

No.	Use	Tag	Label	G2(Ratio(Grou	P Value (ANOVA) ^	✓ ROI001	✓ ^
928	~		885.3849-885.5849	0.000	7.419e-125	41856.597	
933	~		886.3849-886.5849	0.000	1.079e-085	23175.889	
929	~		885.5849-885.7849	0.000	2.340e-072	4013.716	
938	~		887.3849-887.5849	0.000	2.249e-060	10379.325	
548	~		809.3849-809.5849	0.000	8.966e-056	202724.123	
478	~		795.3849-795.5849	0.000	1.284e-052	922842.629	1
553	~		810.3849-810.5849	0.000	6.045e-033	97909.708	
934	~		886.5849-886.7849	0.000	5.981e-031	3494.000	
479	~		795.5849-795.7849	0.000	1.601e-027	67228.803	
930	~		885.7849-885.9849	0.000	1.449e-026	1092.085	
688	~		837.3849-837.5849	0.000	4.410e-025	52410.942	
483	~		796.3849-796.5849	0.000	2.943e-023	434814.496	
939	~		887.5849-887.7849	0.000	1.974e-021	1697.613	
67	~		713.1849-713.3849	0.000	1.885e-017	4514.567	
488	~		797.3849-797.5849	0.000	7.436e-017	170158.289	
908	~		881.3849-881.5849	0.000	1.358e-016	35354.833	
024			005 0040 005 4040	0.000	1030-010	2050.025	

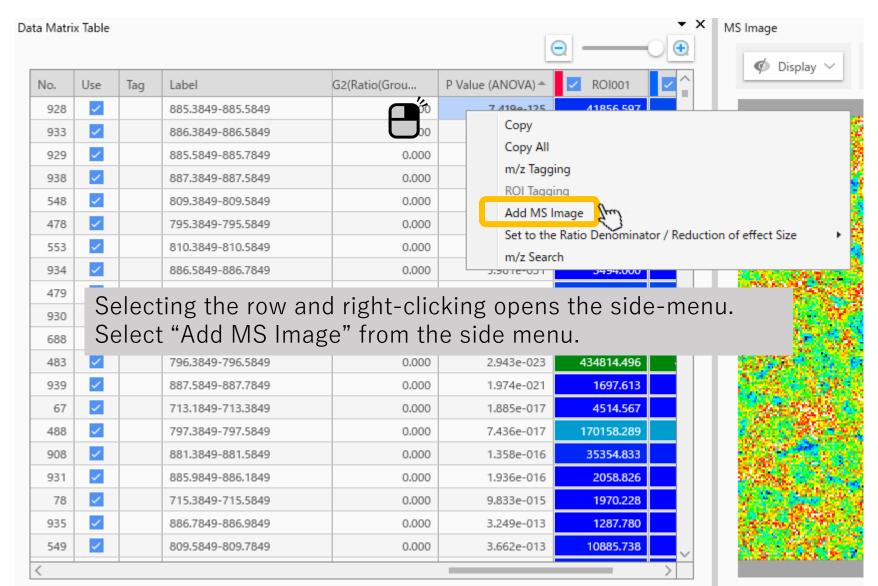
Slide the scroll bar to the right to view the P-values amongst the testing results.

935	~	886.7849-886.9849	0.000	3.249e-013	1287.780
549	~	809.5849-809.7849	0.000	0,000.000	V
<				gru)	>

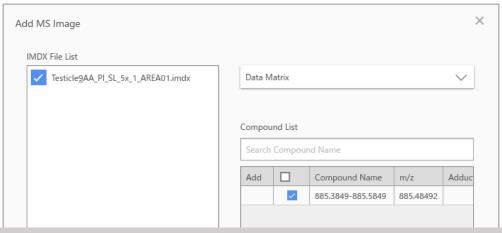
3.5 Testing results



3.6 Right-click→ "Add MS Image"

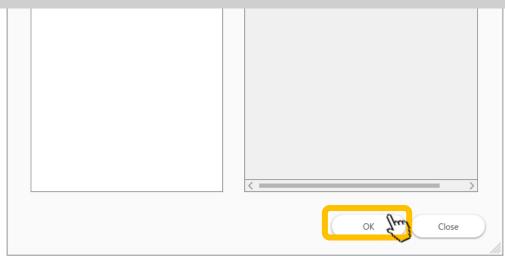


3.7 Select the data file and click "OK"

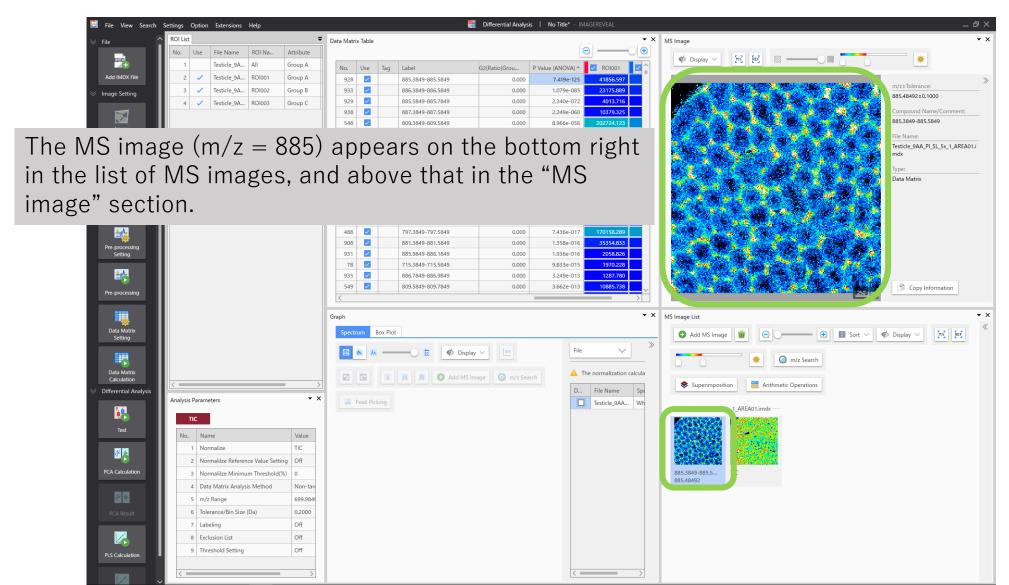


The "Add MS Image" dialogue window opens.

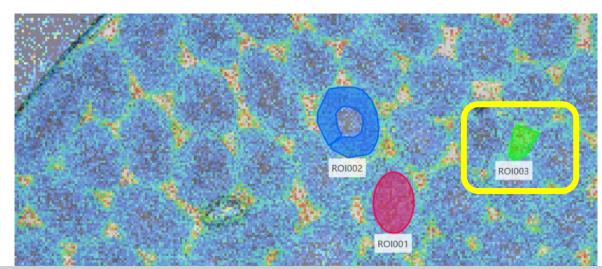
If multiple data files are read in, select here which data files images should be added. (In this example, there is only one imdx file.)



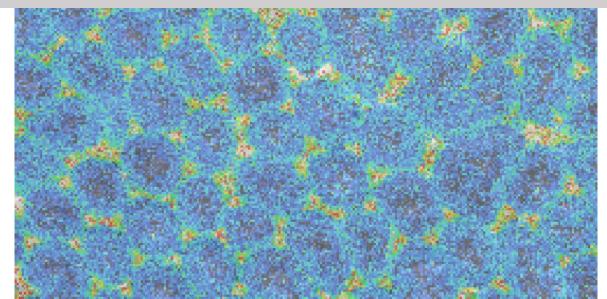
3.8 The MS image is added



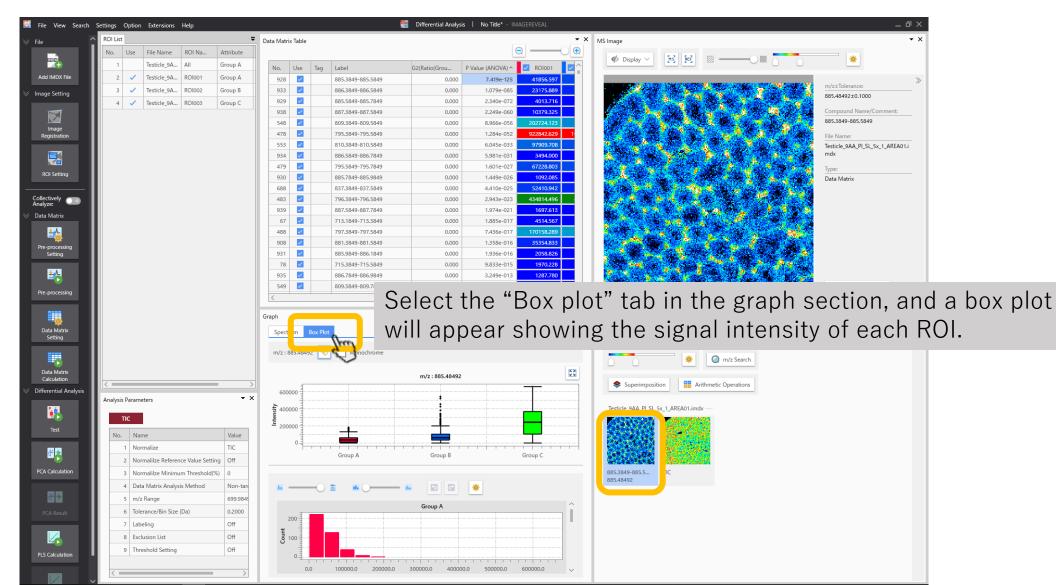
3.9 Distinctiveness of ROI3



Overlaying the ROIs, we see that ROI3 (in green) is a distinctive region.



3.10 Displaying a box plot



3.11 Histogram Adjustment

