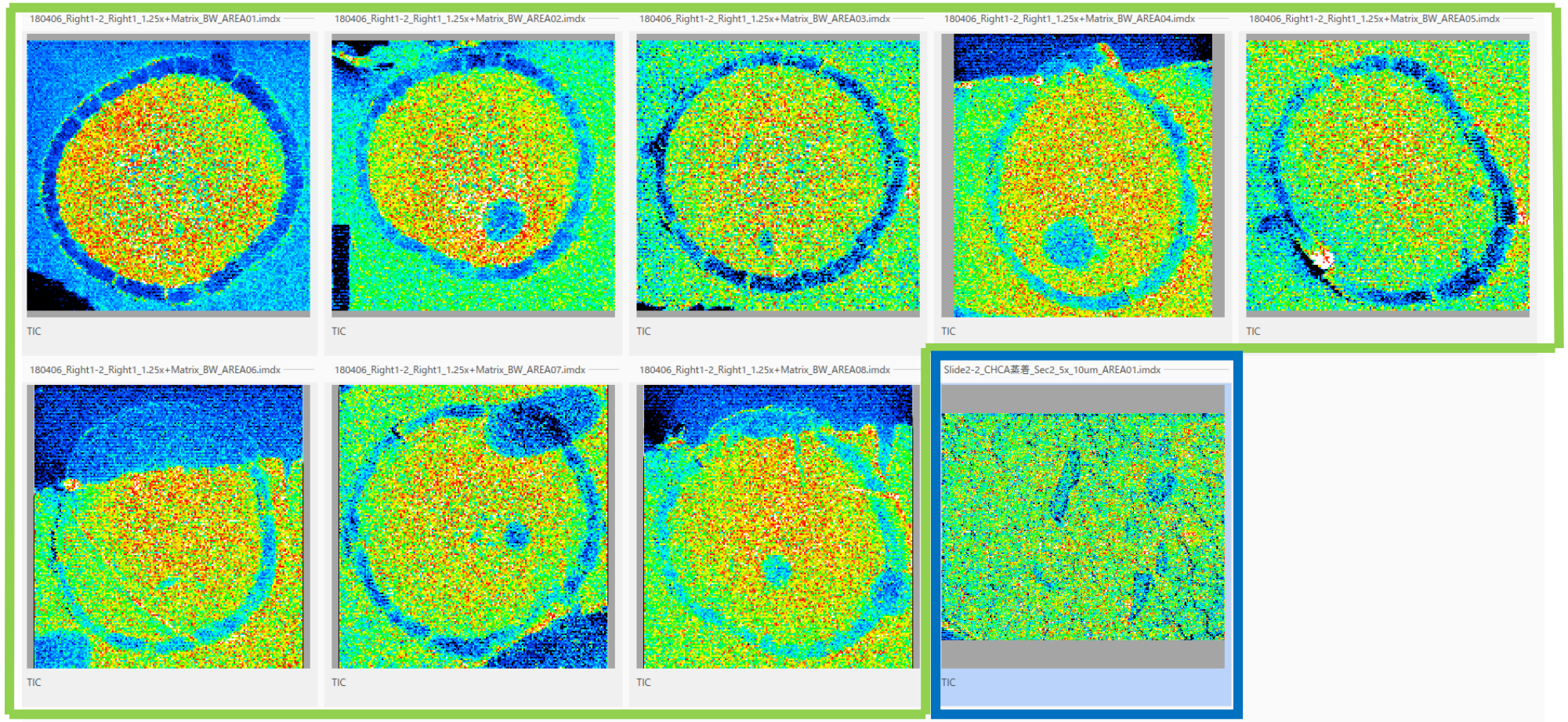
Quantitative Analysis Methods

Required data

- Calibration curve creation data and information
- Data to be quantified
- The data file can be a single file or divided into multiple files.
- Please register the target compound in advance in the compound template. (See "Compound Template Editing Method")

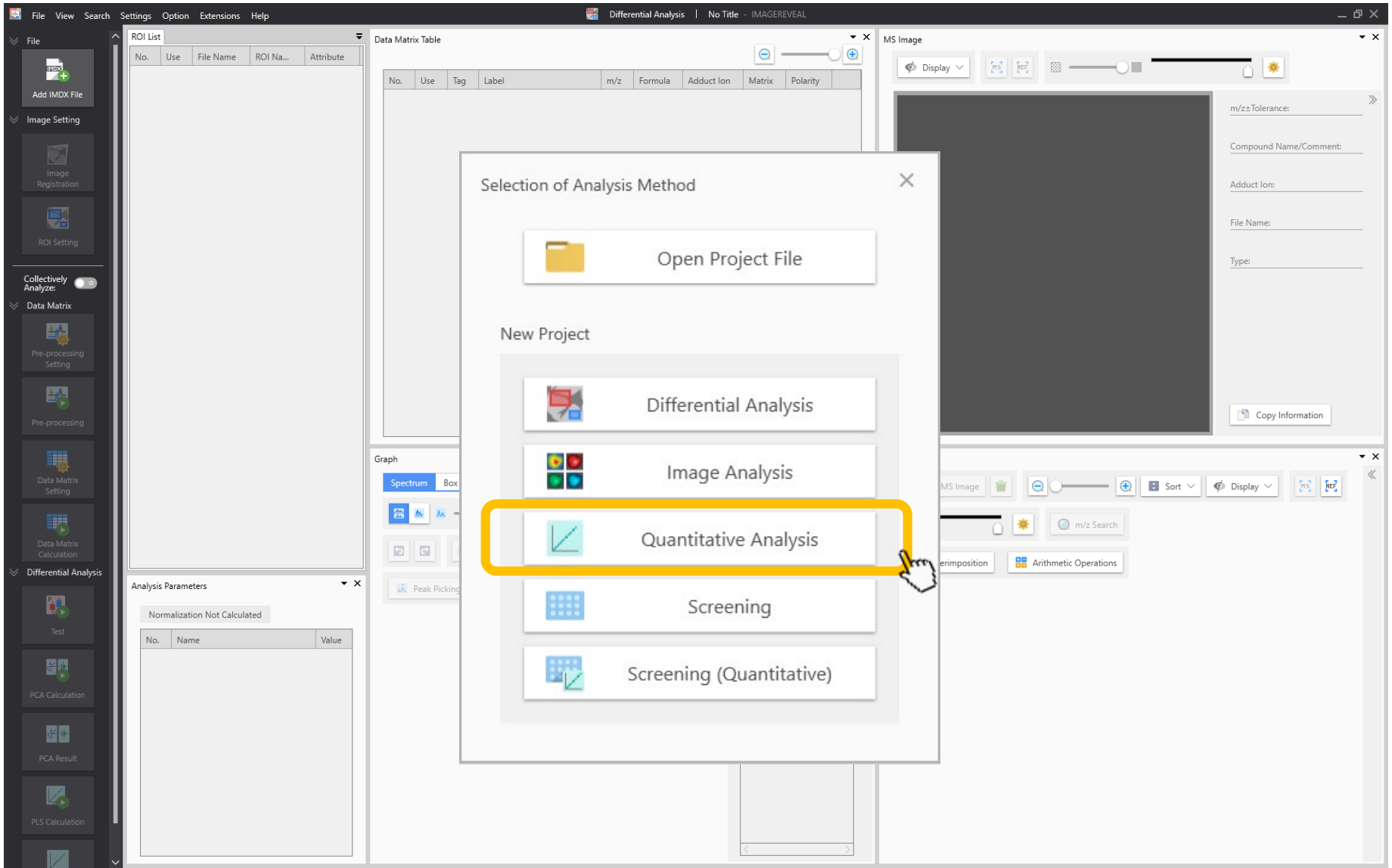
Example data: split into multiple files



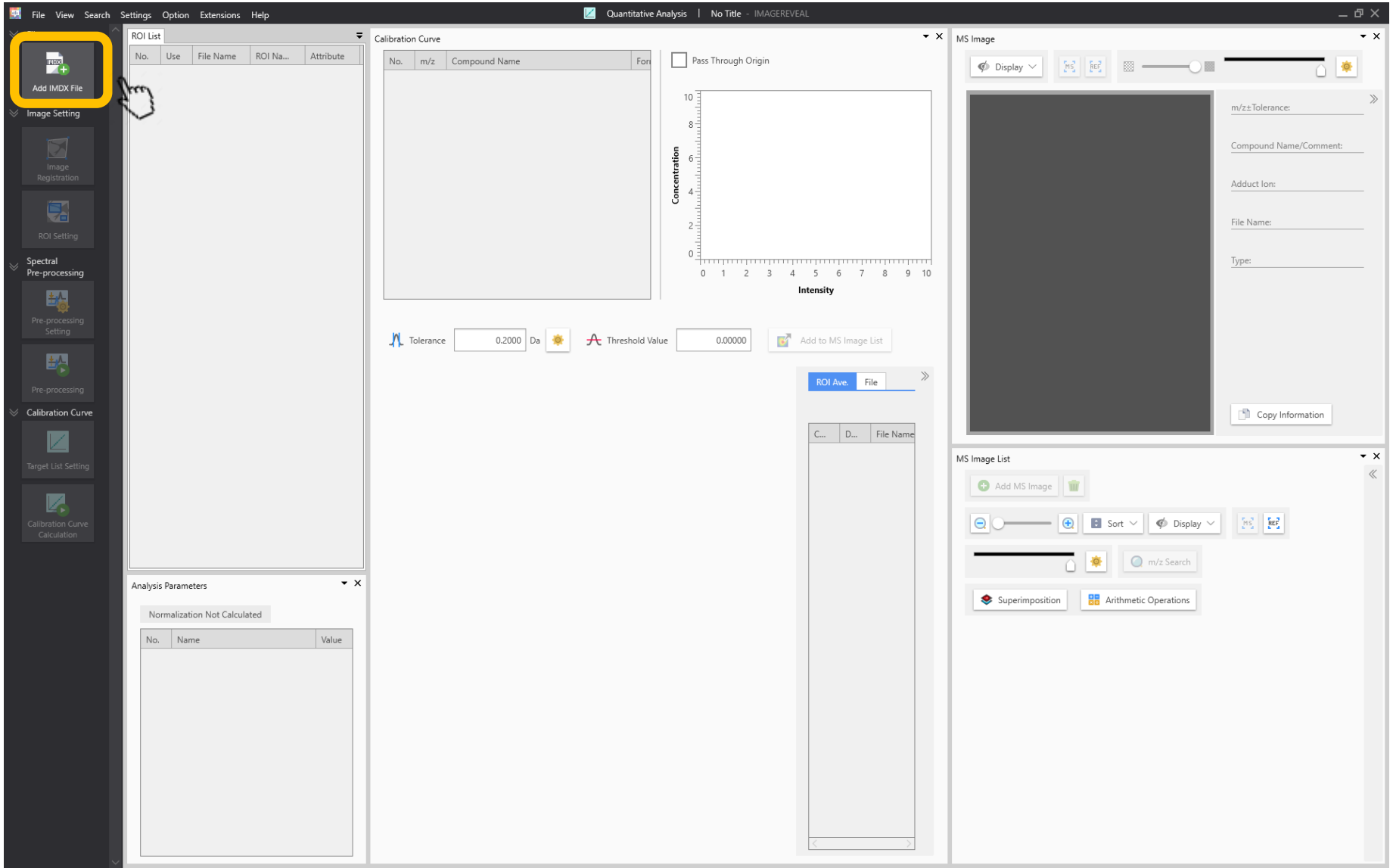
8 sets of data for calibration curves

1 set of data to be quantified

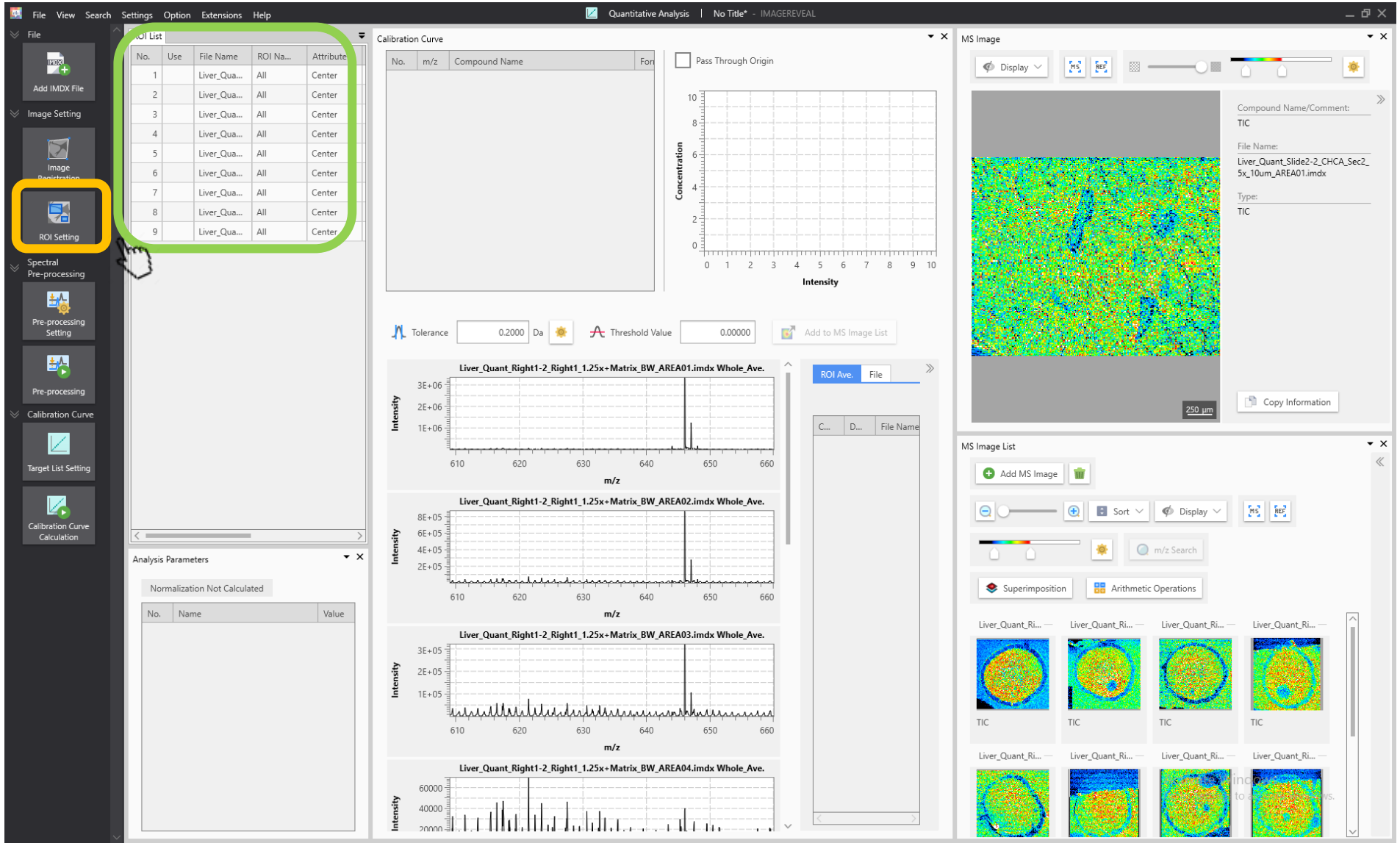
Select “Quantitative Analysis”



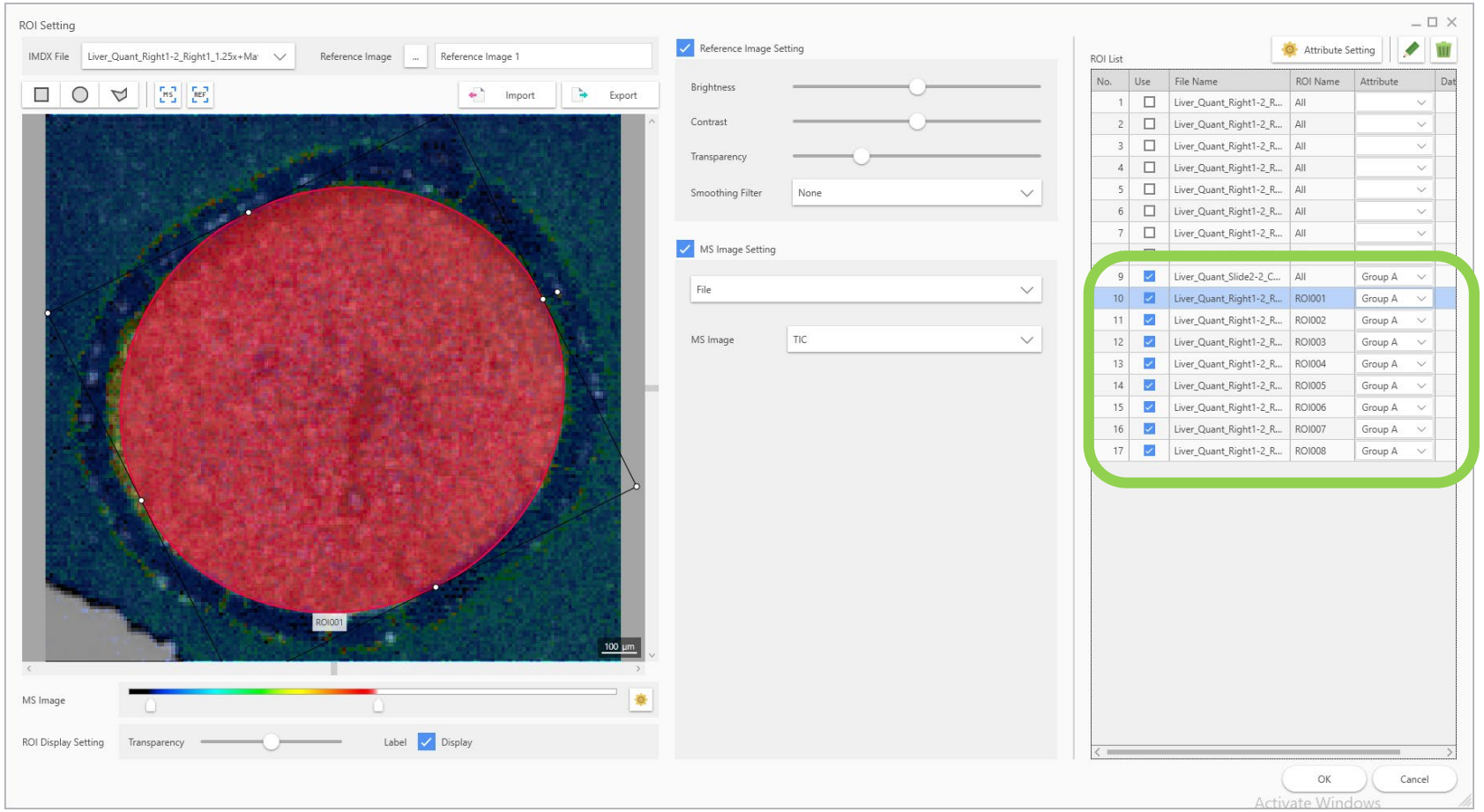
Quantitative Analysis screen: Add IMDX files



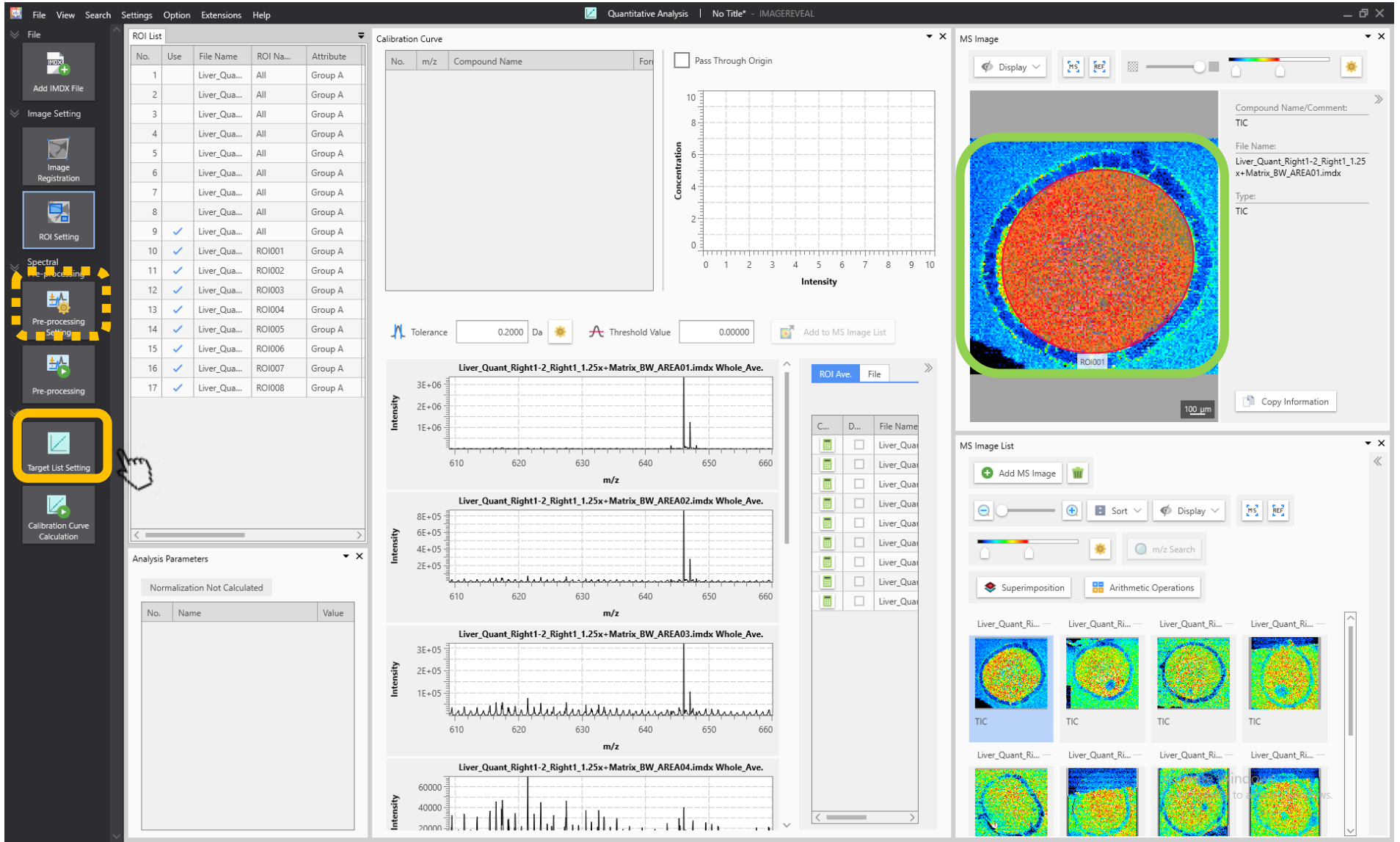
The data files are imported



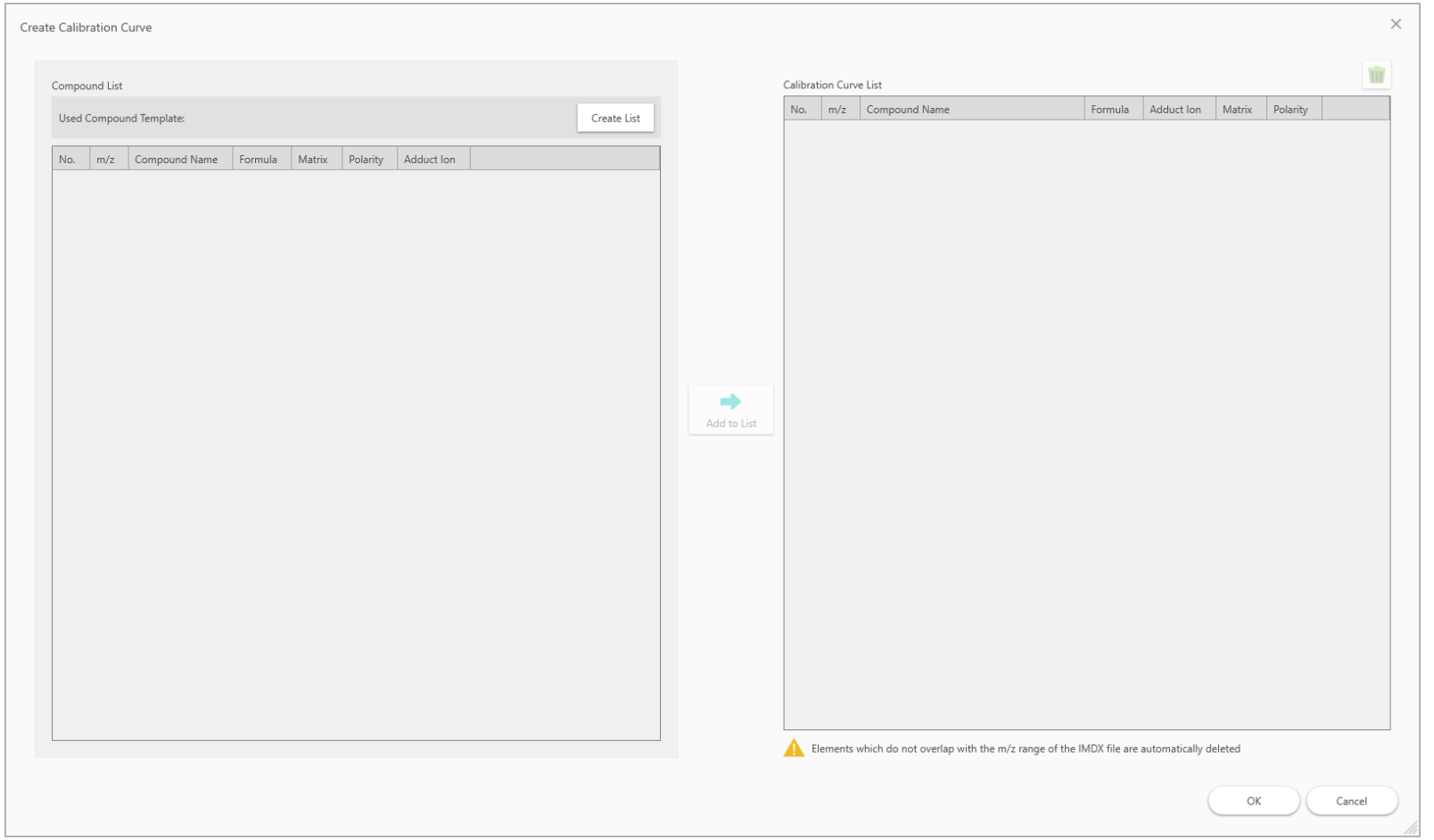
Set ROIs for each calibration curve sample



ROIs have been set

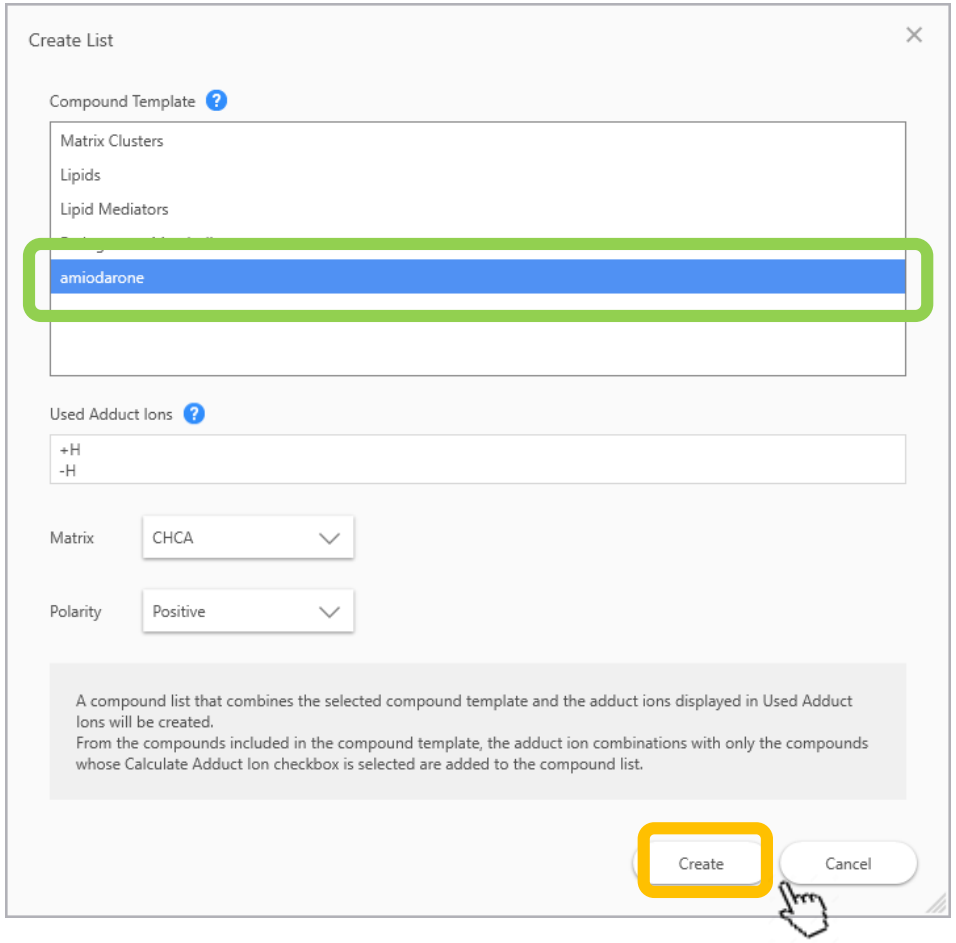


Target compound settings 1



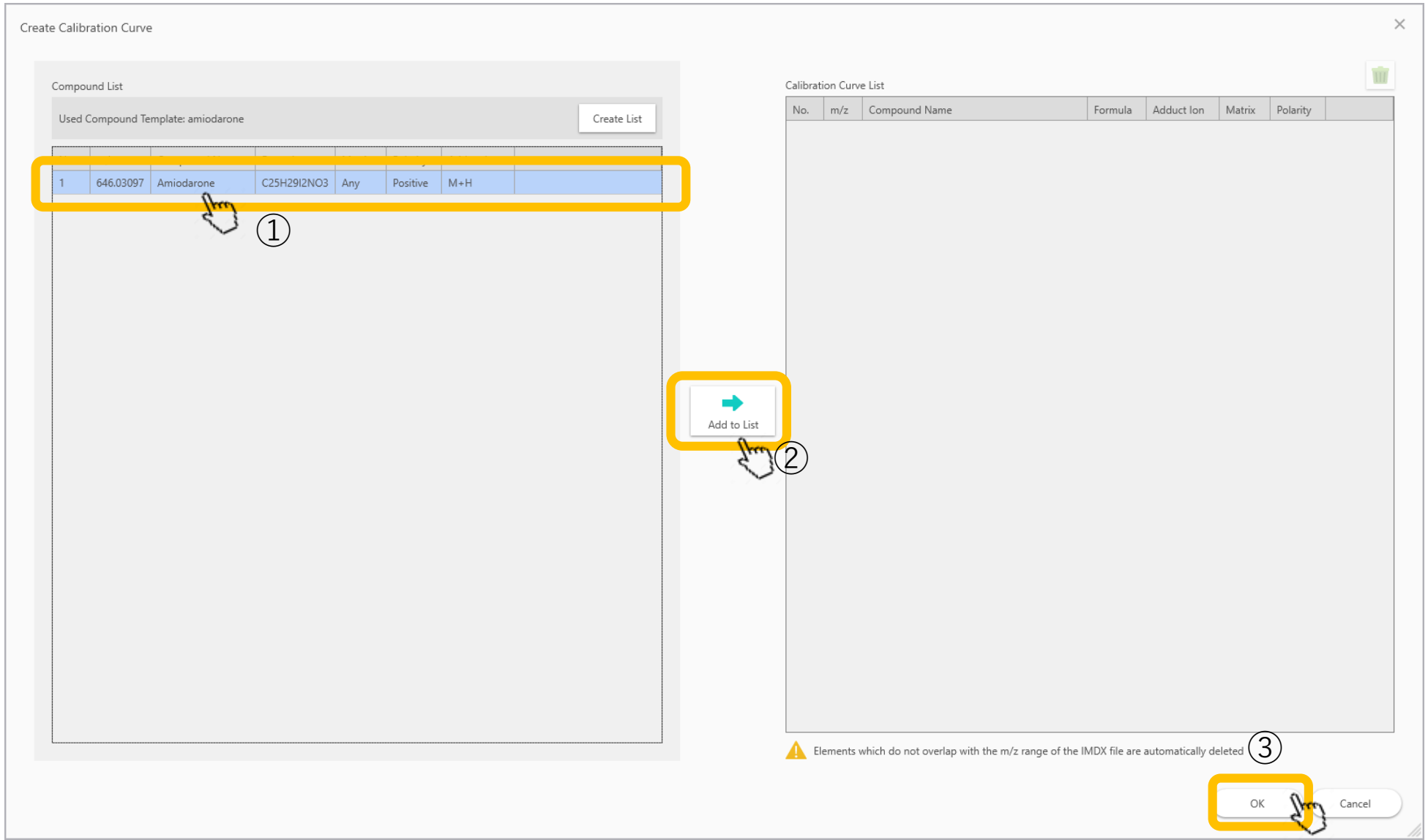
Please register target compounds and compound templates beforehand (see “How to register compound templates”)

Target compound settings 2

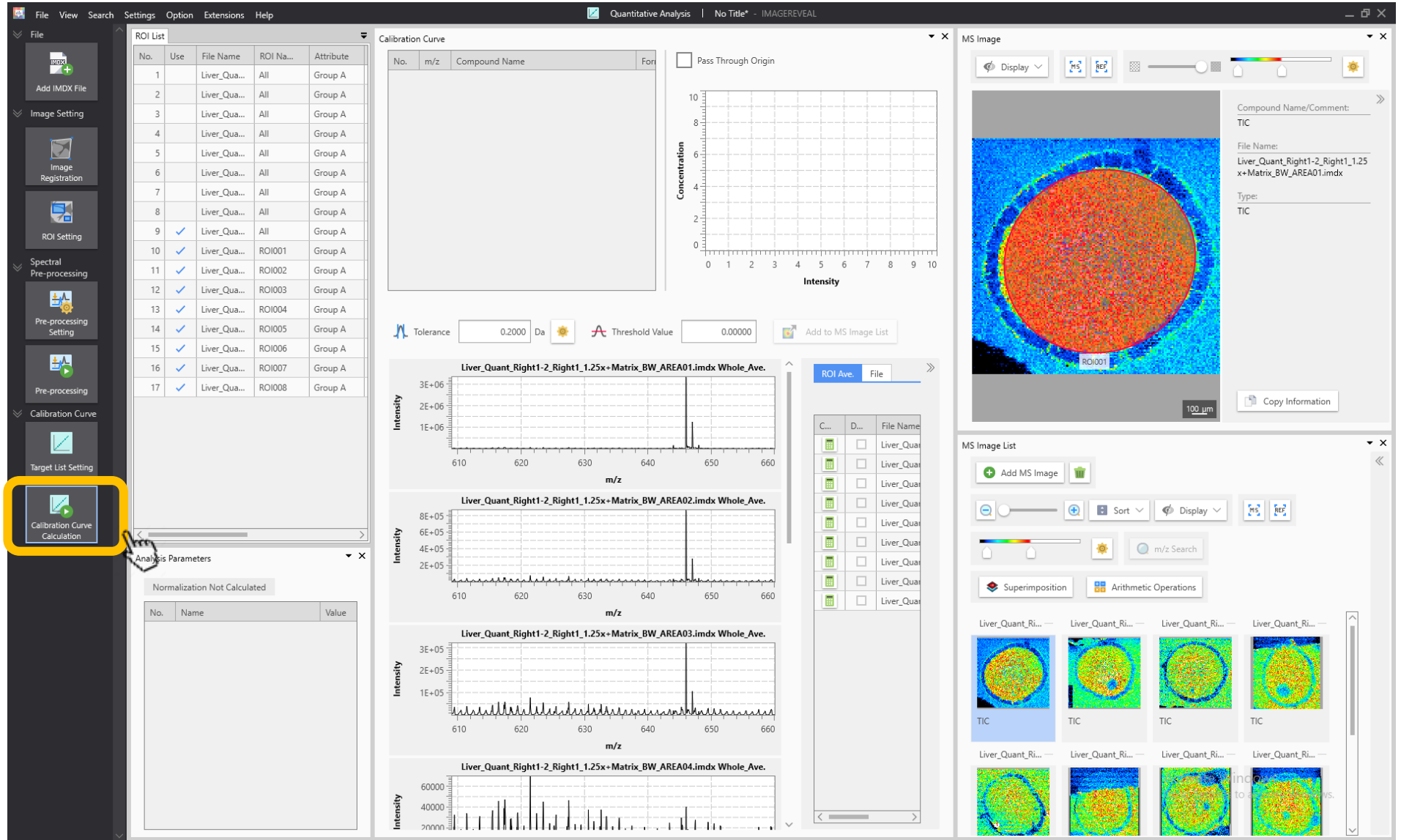


Select a previously-created compound template

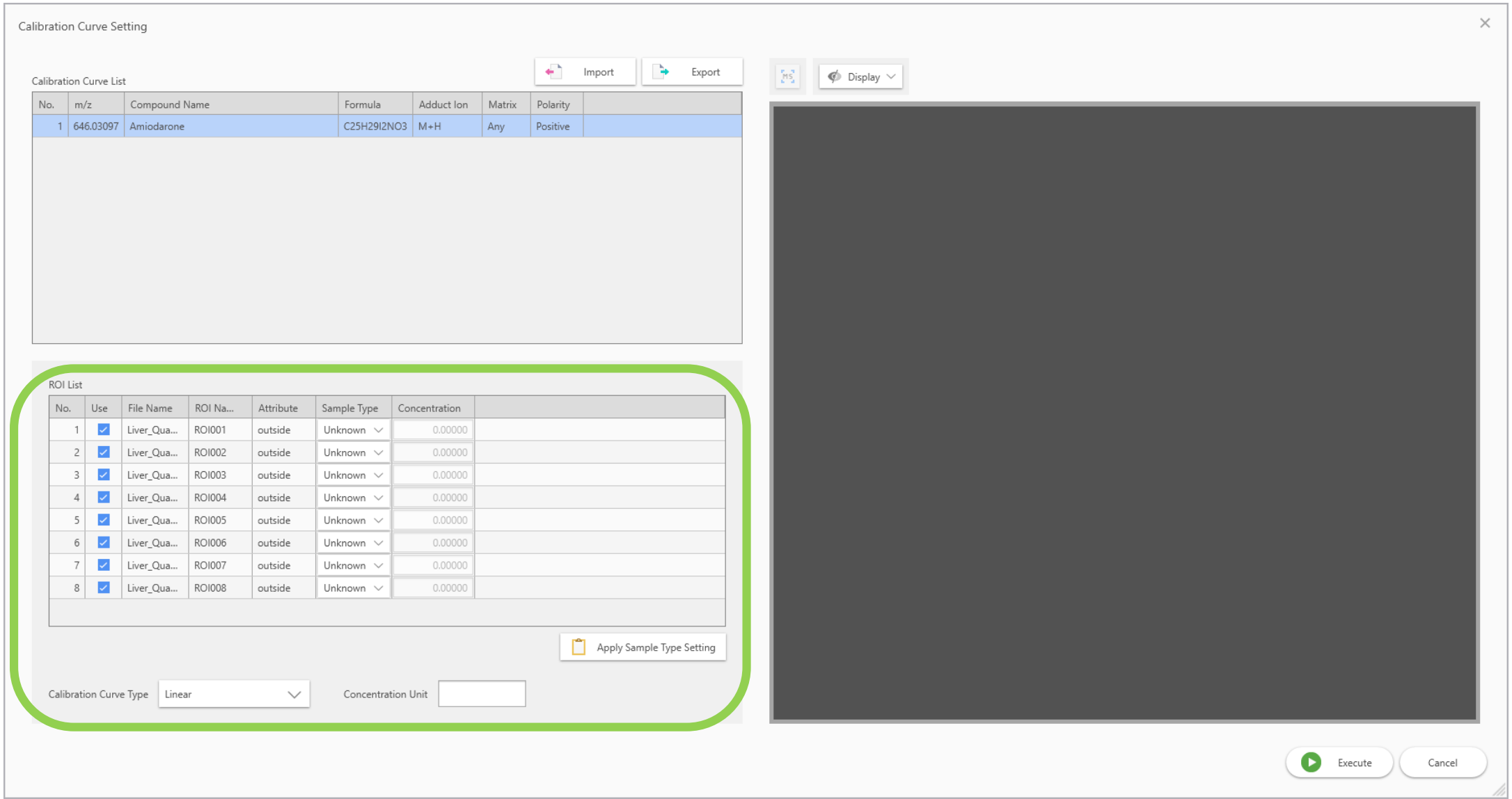
Target compound settings 3



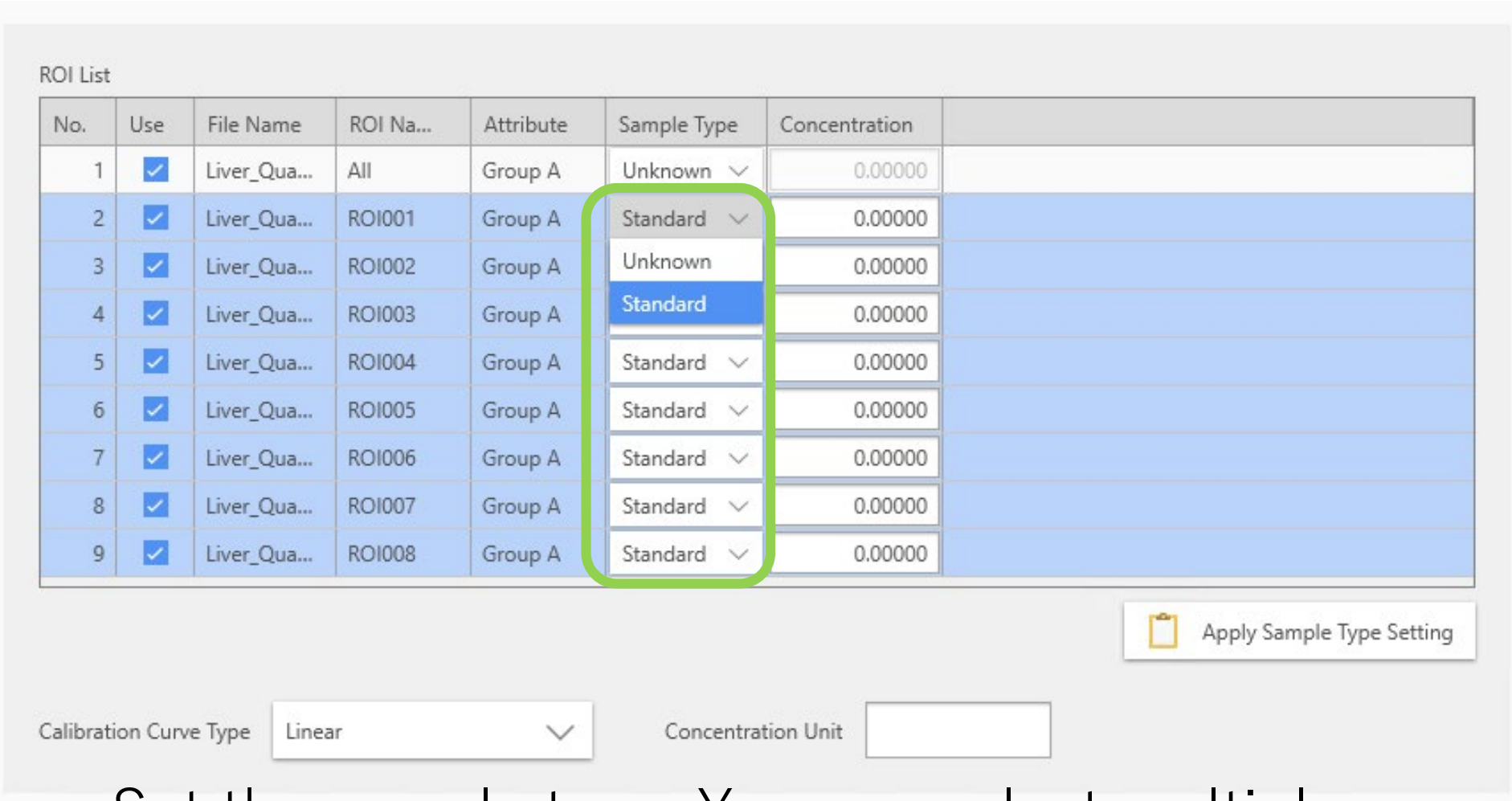
Calibration curve settings 1



Calibration curve settings 2



Calibration curve settings 3



Set the sample type. You can select multiple rows and apply a setting to all of them.

Calibration curve settings 4

ROI List

No.	Use	File Name	ROI Na...	Attribute	Sample Type	Concentration
1	☑	Liver_Quant_Slide2-...	All	Group A	Unknown	0.00000
2	☑	Liver_Quant_Right1-...	ROI001	Group A	Standard	1.13234
3	☑	Liver_Quant_Right1-...	ROI002	Group A	Standard	0.33970
4	☑	Liver_Quant_Right1-...	ROI003	Group A	Standard	0.11323
5	☑	Liver_Quant_Right1-...	ROI004	Group A	Standard	0.03397
6	☑	Liver_Quant_Right1-...	ROI005	Group A	Standard	0.01132
7	☑	Liver_Quant_Right1-...	ROI006	Group A	Standard	0.00340
8	☑	Liver_Quant_Right1-...	ROI007	Group A	Standard	0.00113
9	☑	Liver_Quant_Right1-...	ROI008	Group A	Standard	0.00000

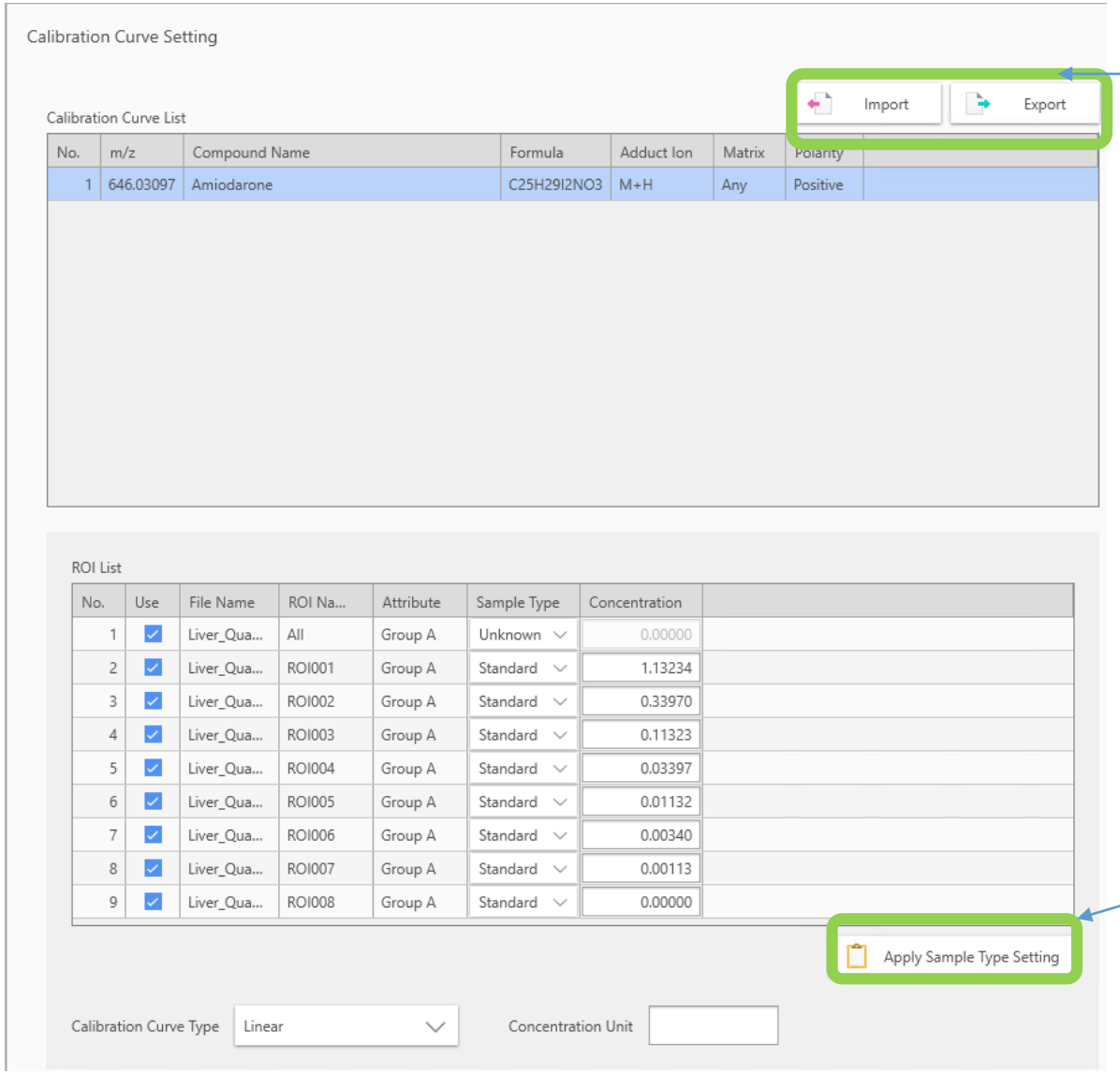
Apply Sample Type Setting

Calibration Curve Type: Linear

Concentration Unit:

Enter the concentration of the calibration curve samples

Calibration curve settings 5: Faster settings

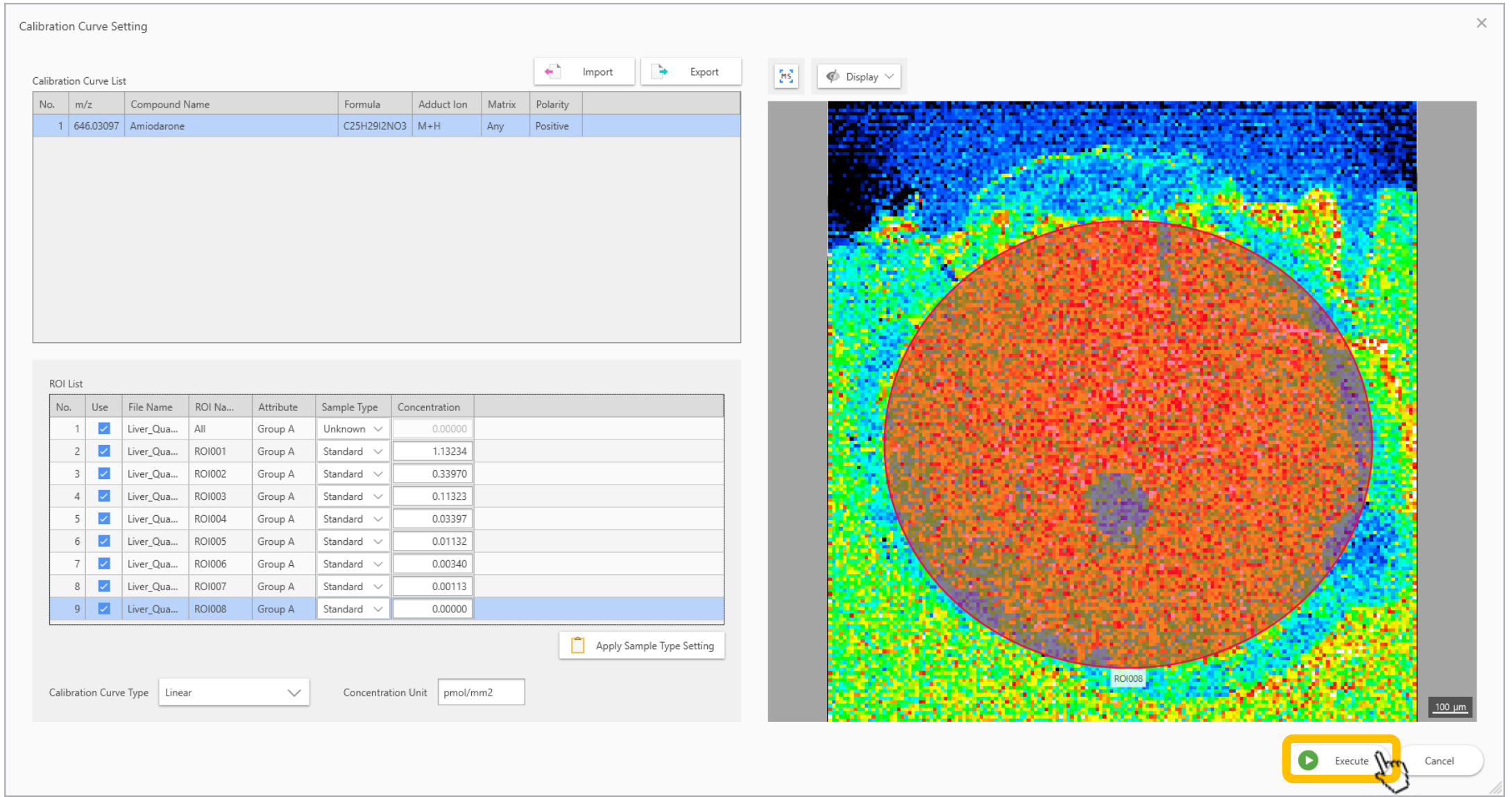


Import a CSV file to automatically enter calibration curve concentrations

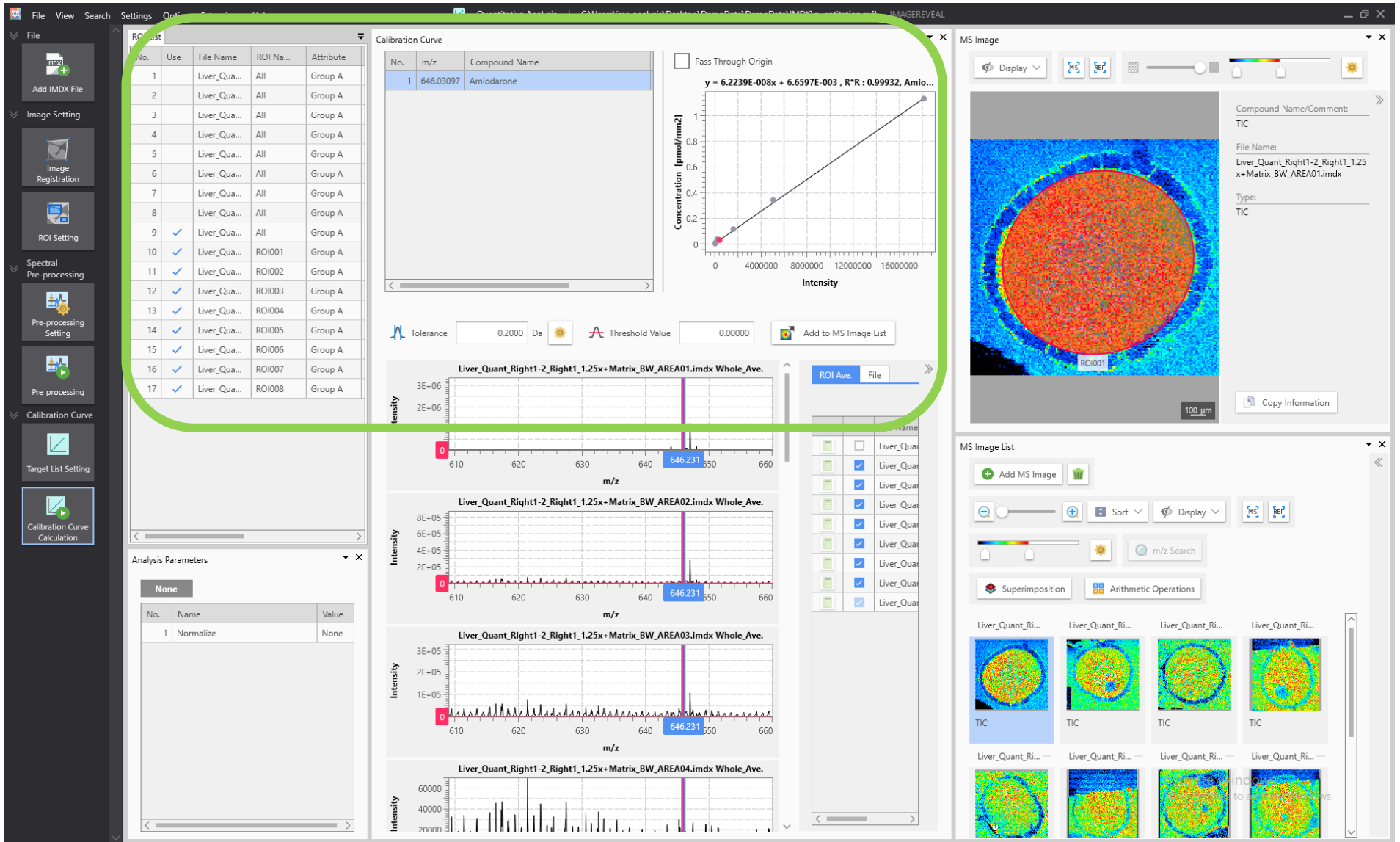
	A	B	C	D	E	F
1	646.031	Amiodarone				
2		Slide2-2_(	All	Group A	Unknown	0
3		180406_Ri	ROI001	Group A	Standard	1.13234
4		180406_Ri	ROI002	Group A	Standard	0.3397
5		180406_Ri	ROI003	Group A	Standard	0.11323
6		180406_Ri	ROI004	Group A	Standard	0.03397
7		180406_Ri	ROI005	Group A	Standard	0.01132
8		180406_Ri	ROI006	Group A	Standard	0.0034
9		180406_Ri	ROI007	Group A	Standard	0.00113
10		180406_Ri	ROI008	Group A	Standard	0
11	611.0073	610				
12		Slide2-2_(	All	Group A	Unknown	0
13		180406_Ri	ROI001	Group A	Standard	0.5

If there are multiple target compounds, you can apply a setting to them all at once.

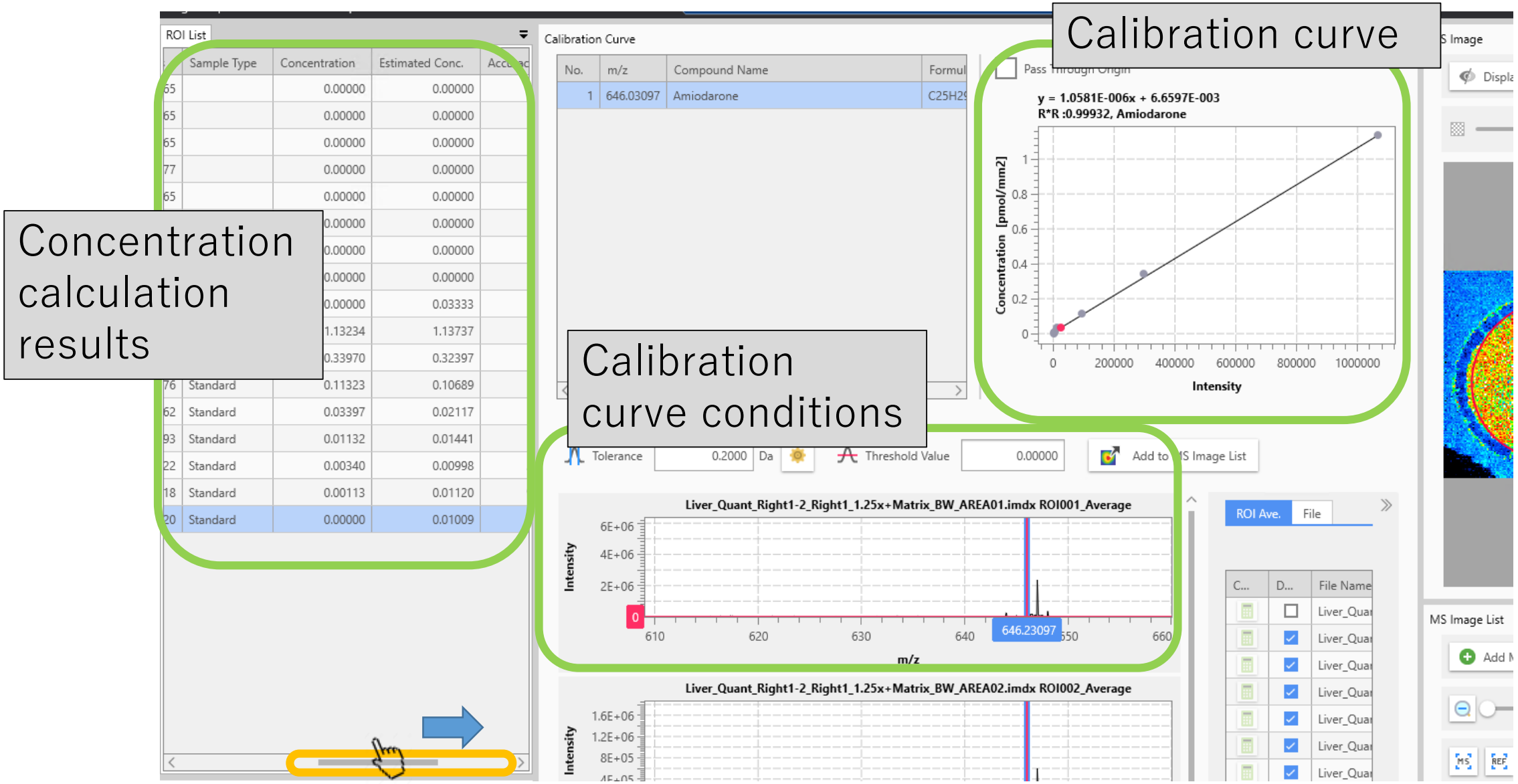
Calibration curve settings 6



Calibration curve results



Quantitation results 1



Quantitation results 2: Concentration calculations

ettings Option Extensions Help | Quantitative Analysis | C:\Users\ims-analysis

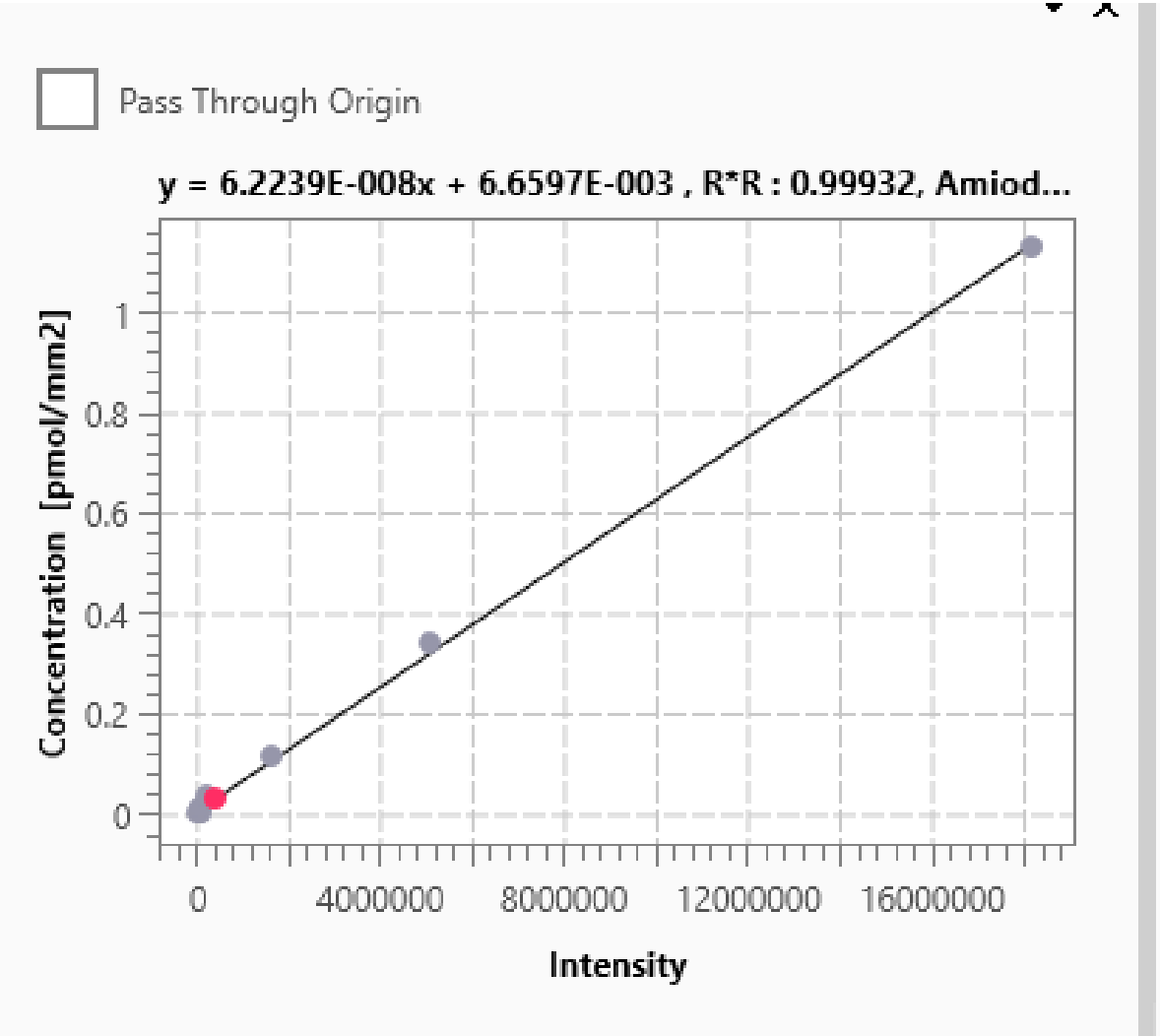
ROI List

Use	File Name	ROI Na...	Attribute	Data Points	Sample Type	Concentration	Post-normalization Intensity
	Liver_Qua...	All	Group A	25265		0.00000	0.00000
	Liver_Qua...	All	Group A	25265		0.00000	0.00000
	Liver_Qua...	All	Group A	25265		0.00000	0.00000
	Liver_Qua...	All	Group A	29177		0.00000	0.00000
	Liver_Qua...	All	Group A	25265		0.00000	0.00000
	Liver_Qua...	All	Group A	28036		0.00000	0.00000
	Liver_Qua...	All	Group A	28036		0.00000	0.00000
	Liver_Qua...	All	Group A	28036		0.00000	0.00000
✓	Liver_Qua...	All	Group A	50000	Unknown	0.03333	428550.64320
✓	Liver_Qua...	ROI001	Group A	12101	Standard	1.13234	18167298.66556
✓	Liver_Qua...	ROI002	Group A	10845	Standard	0.33970	5098337.34846
✓	Liver_Qua...	ROI003	Group A	11976	Standard	0.11323	1610431.50835
✓	Liver_Qua...	ROI004	Group A	12762	Standard	0.03397	233195.52923
✓	Liver_Qua...	ROI005	Group A	11993	Standard	0.01132	124503.96598
✓	Liver_Qua...	ROI006	Group A	10722	Standard	0.00340	53341.30796
✓	Liver_Qua...	ROI007	Group A	14618	Standard	0.00113	72990.57710
✓	Liver_Qua...	ROI008	Group A	13420	Standard	0.00000	55176.18361

Calculation results are displayed in the ROI list.

In this example, the peak concentration value in the average spectrum of the unknown sample is 0.03333

Quantitation results 3: Calibration curve



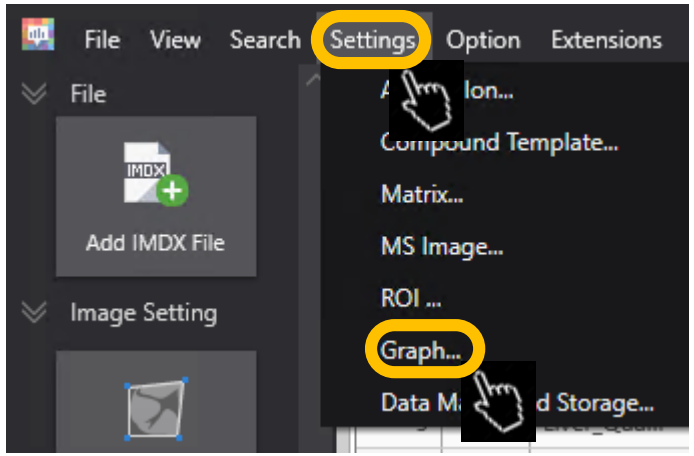
The calibration curve is shown.

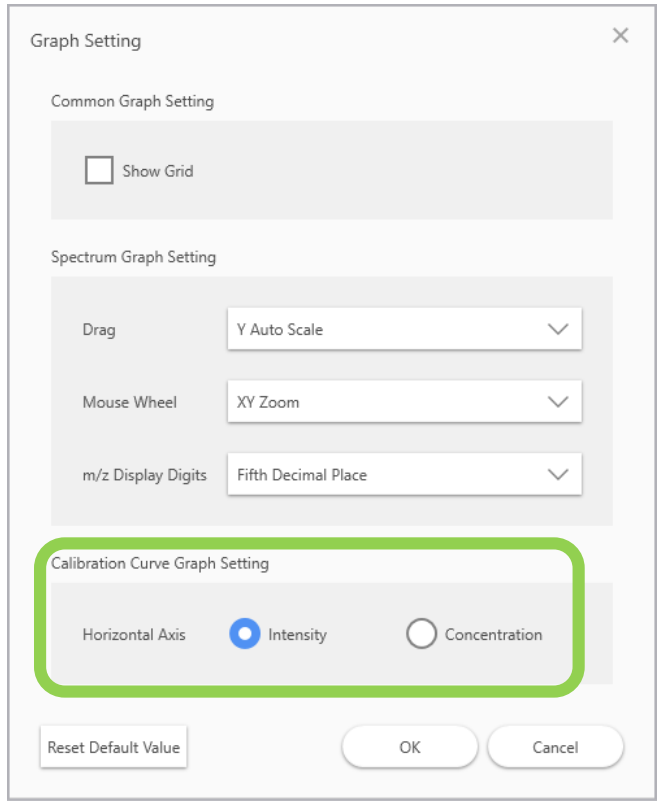
Grey points are the standards used for calibration and the red point is the unknown sample.

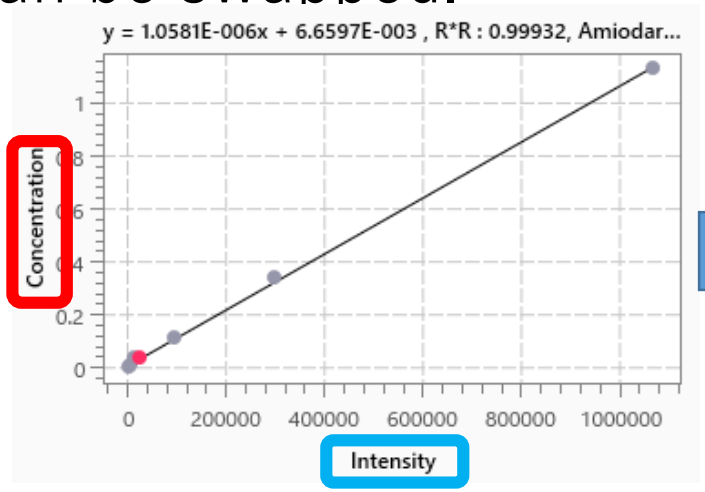
This result will change depending on the calibration curve conditions.

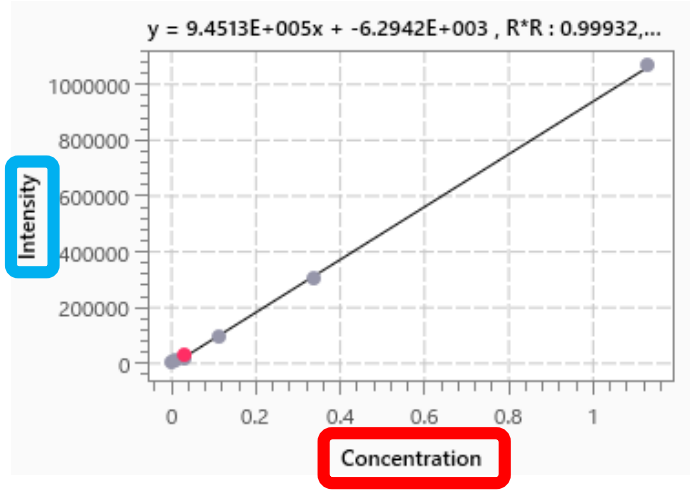
Quantitation results 3 .1: Calibration curve options

The axes of the calibration curve graph can be swapped.
Select “Settings” then “Graph”.

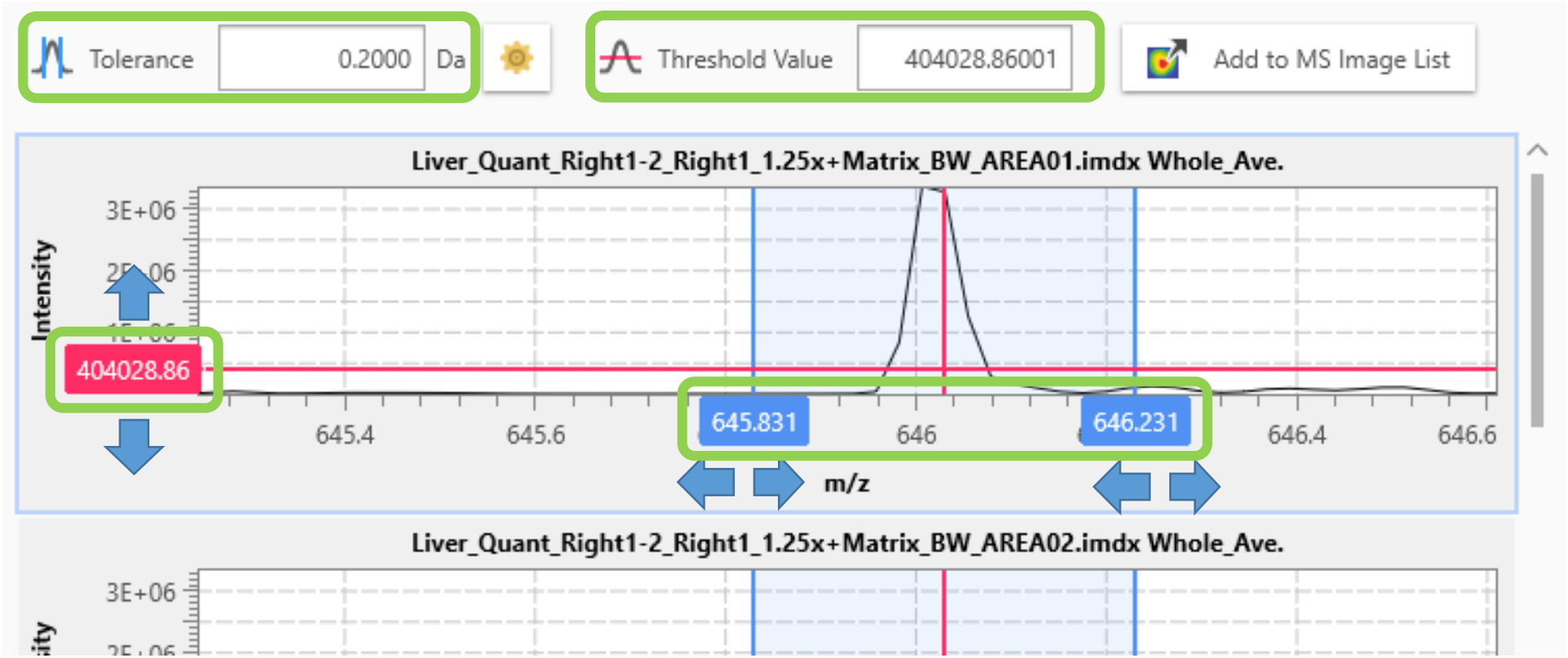








Quantitation results 4: Calibration curve conditions



When calculating the peak area, you can change the “Tolerance” and “Threshold value” shown above the spectrum. If you change the value, the calculation result will also change accordingly.

Notes

- If the operation is heavy, reduce or turn off the spectrum display.

- In the quantitative analysis mode, it is assumed that the [Sampling Interval] is the same when handling multiple data.
  - You can check the [Sampling Interval] in [Conversion Parameters] by right-clicking on the [ROI List] and selecting [Show File Parameter].