# Carrying out quantitative analysis

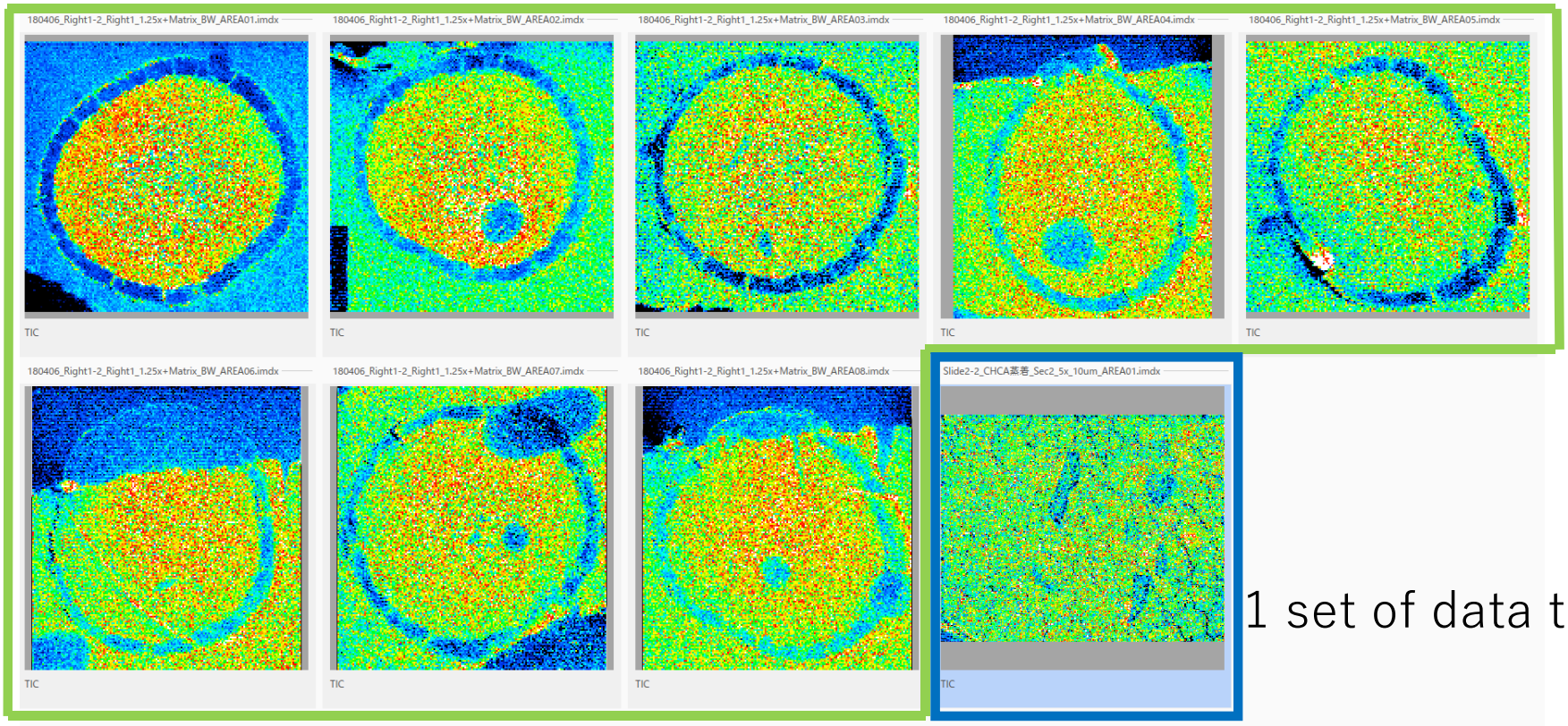
# Necessary data

- Calibration curve data and information
- Data that you want to quantify

*Data can be contained in one file or split into several

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

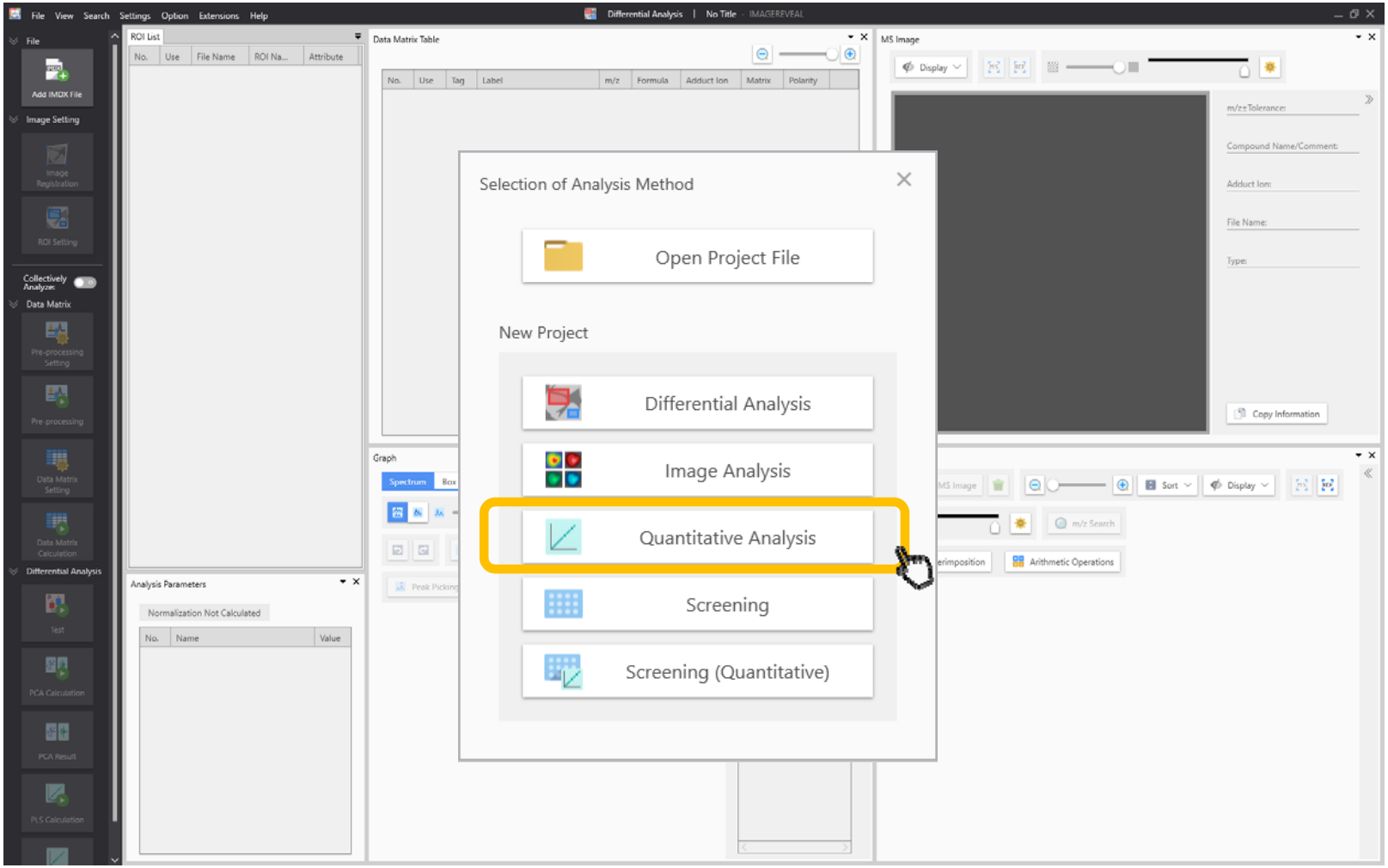
# Example data: split into multiple files



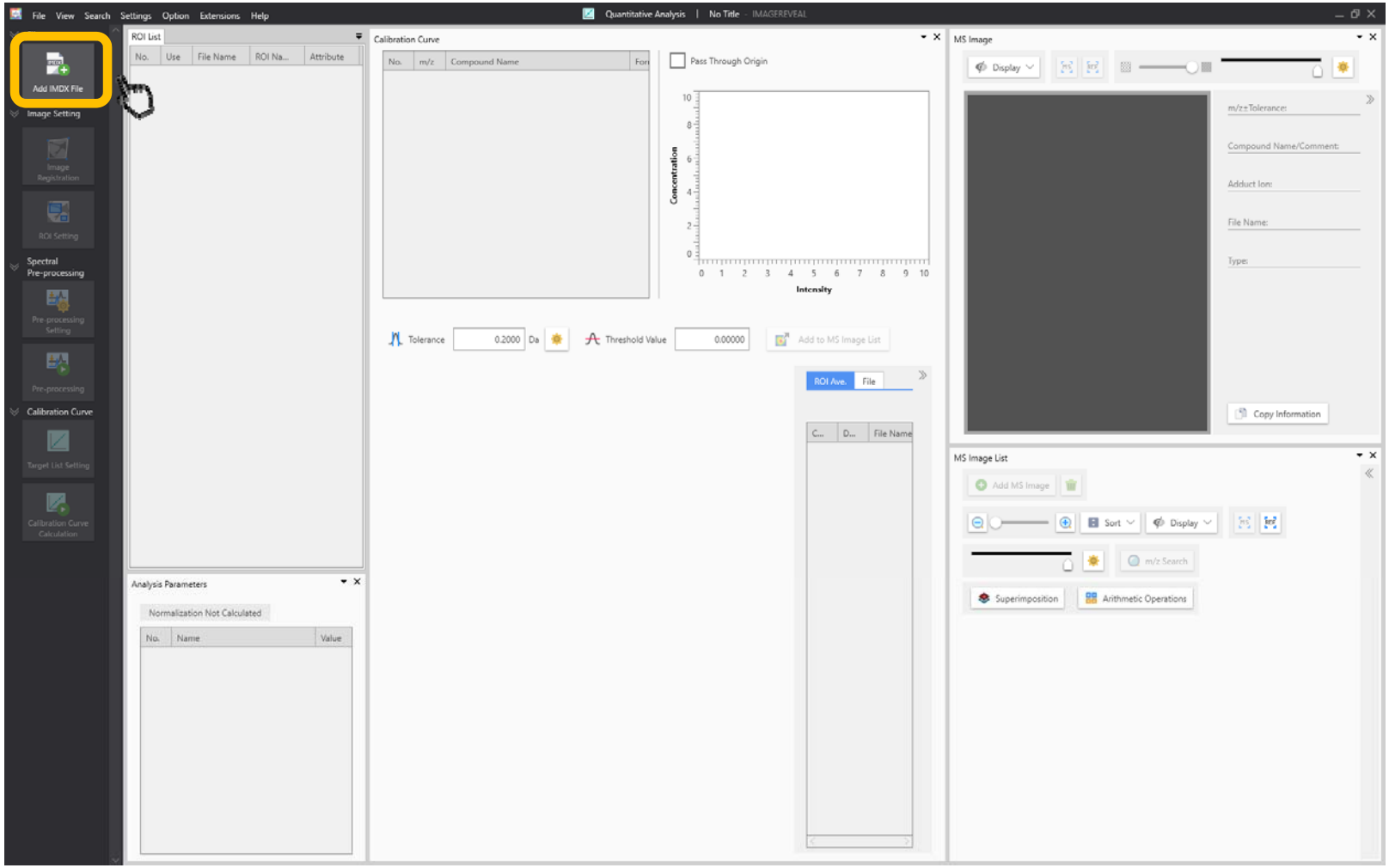

1 set of data to quantify

8 sets of data for
calibration curves

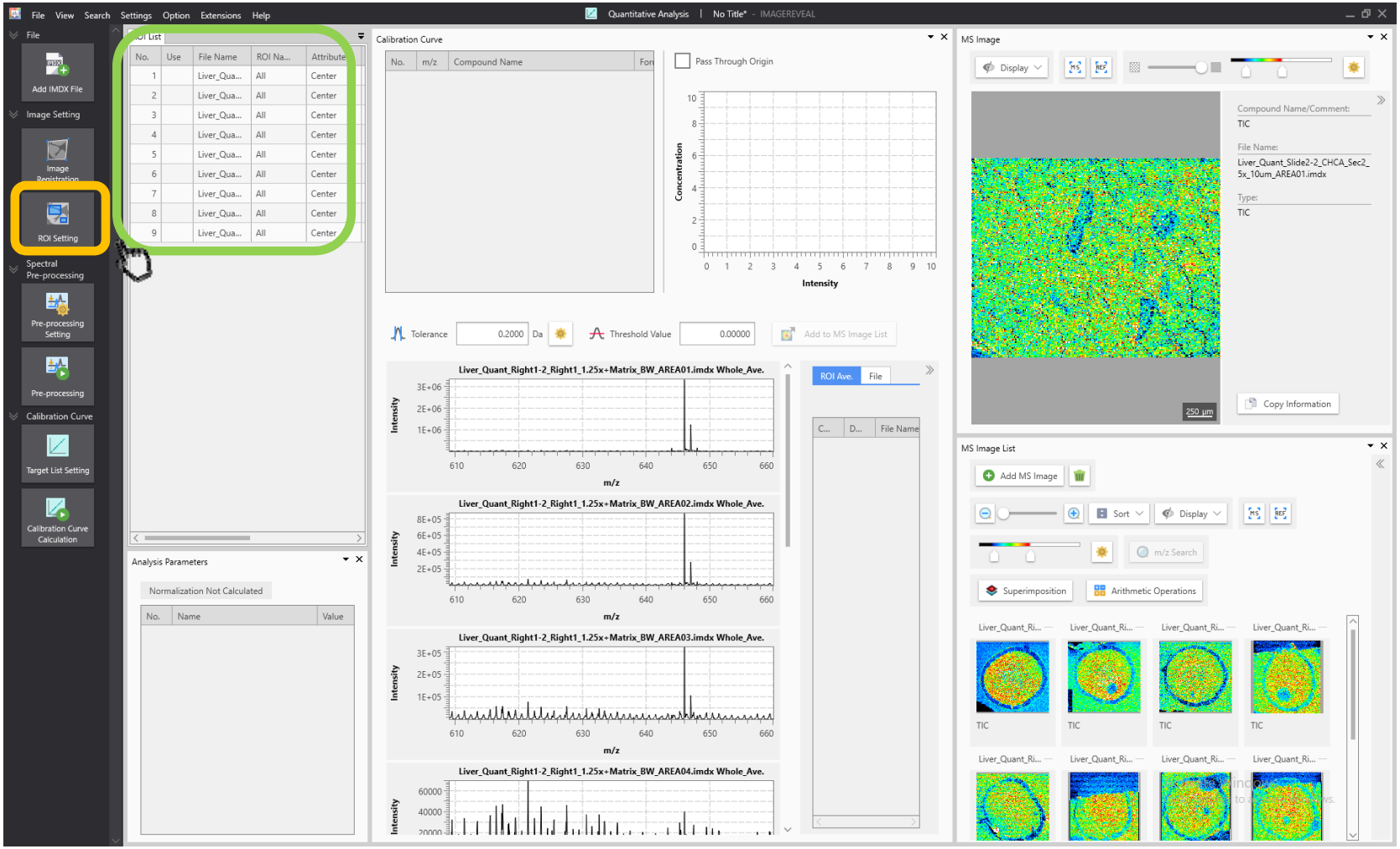
# Select “Quantitative Analysis”



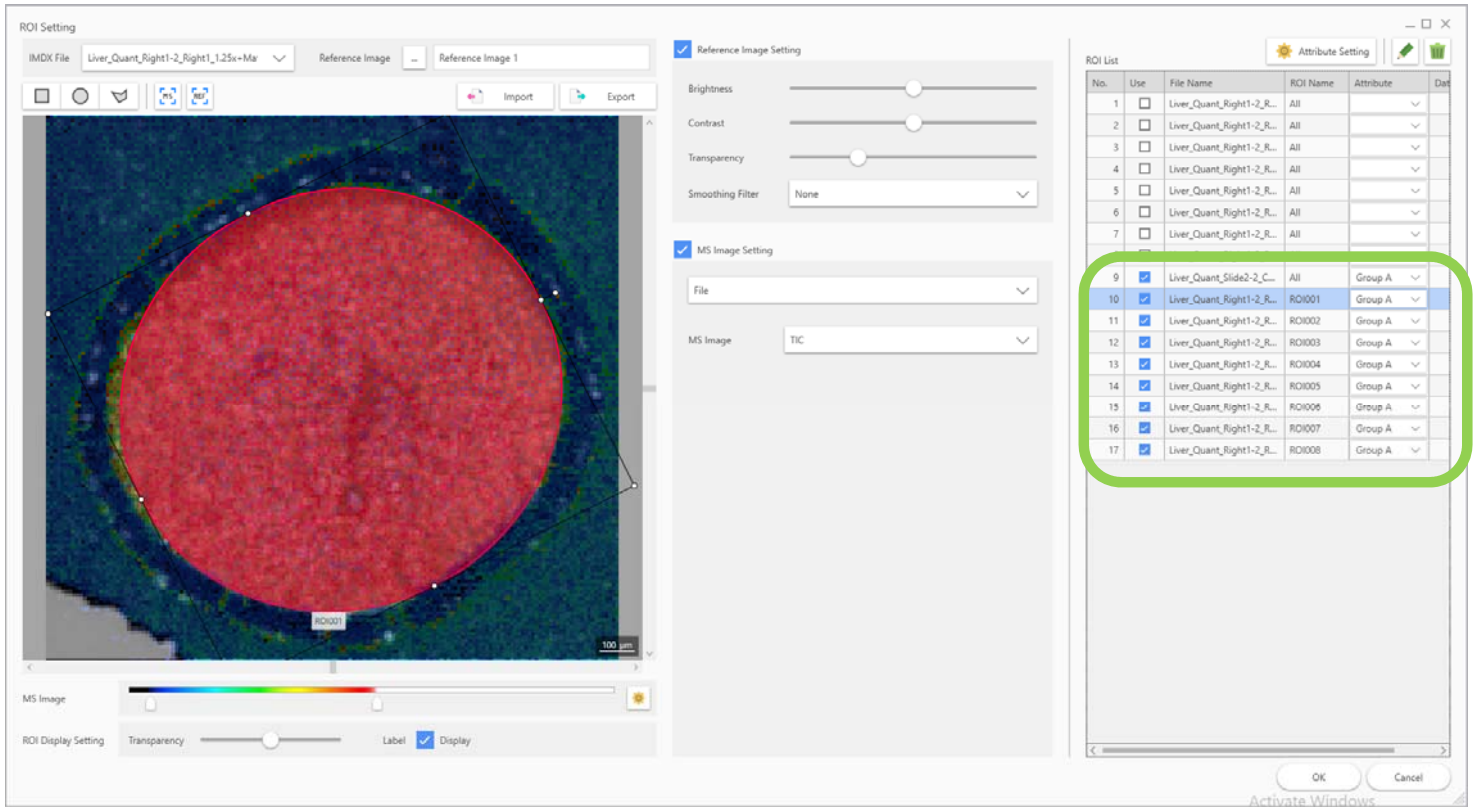
# Quantitative Analysis screen: Add IMDX files



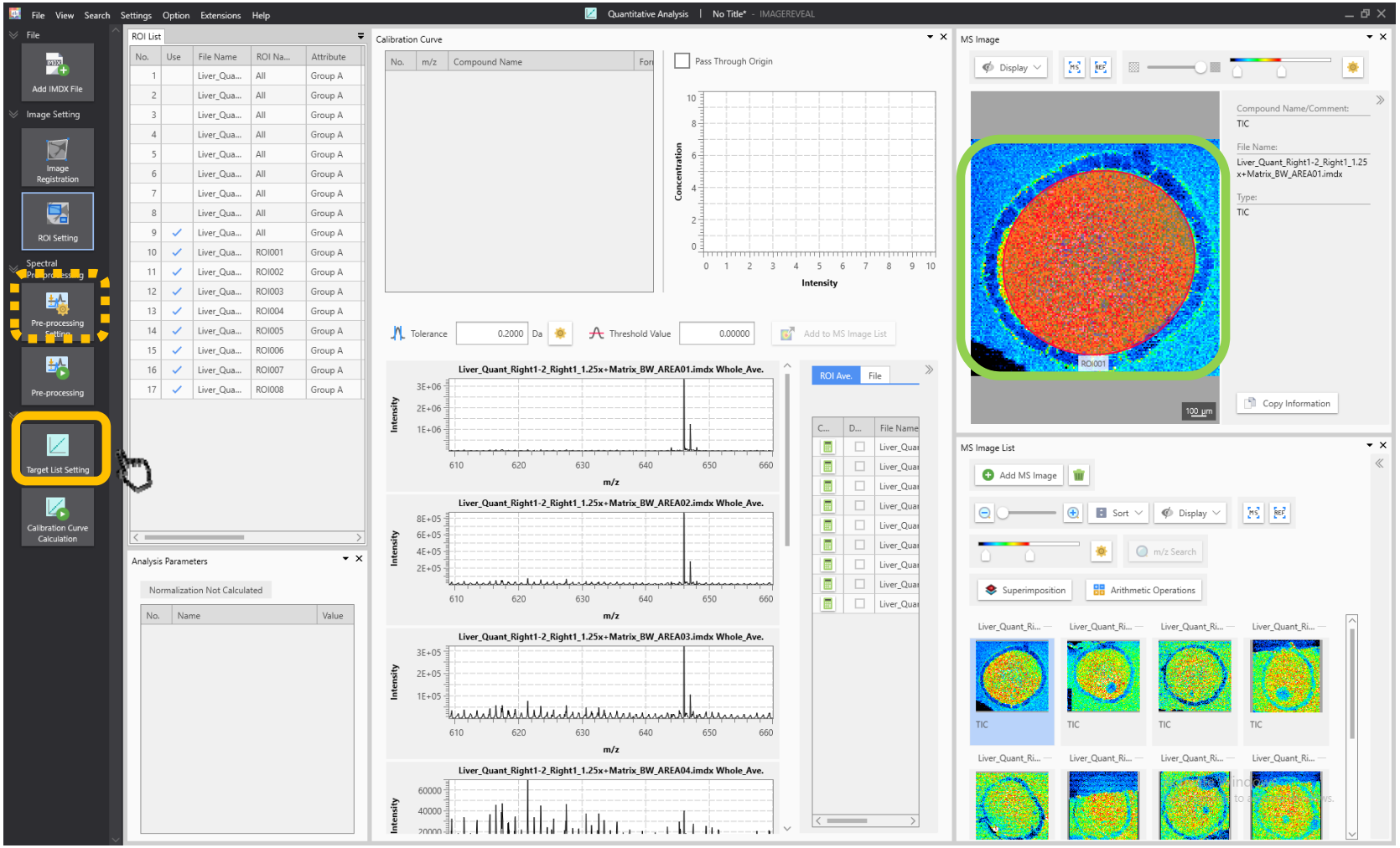
# The data files are imported



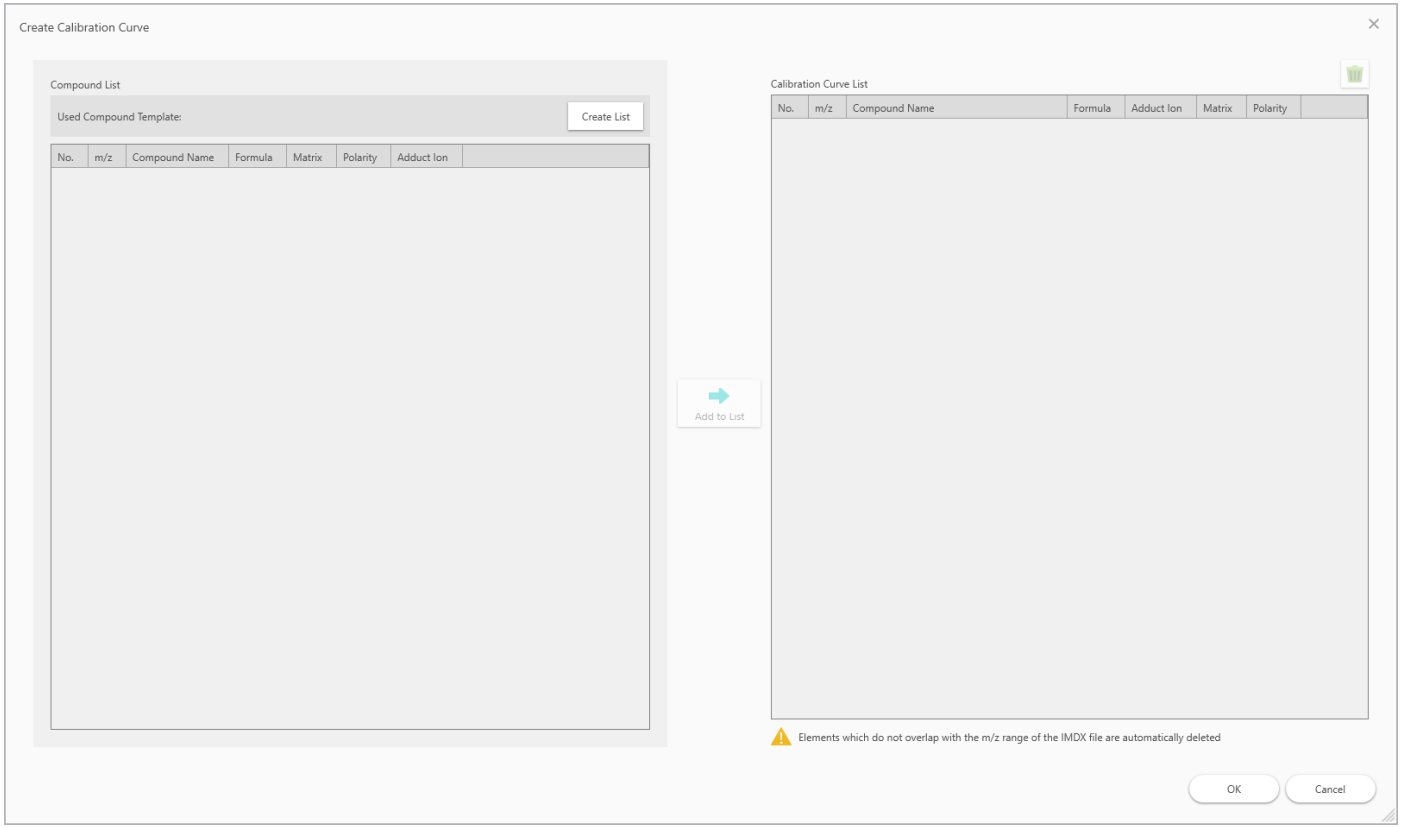
# Set ROIs for each calibration curve sample



# ROIs have been set

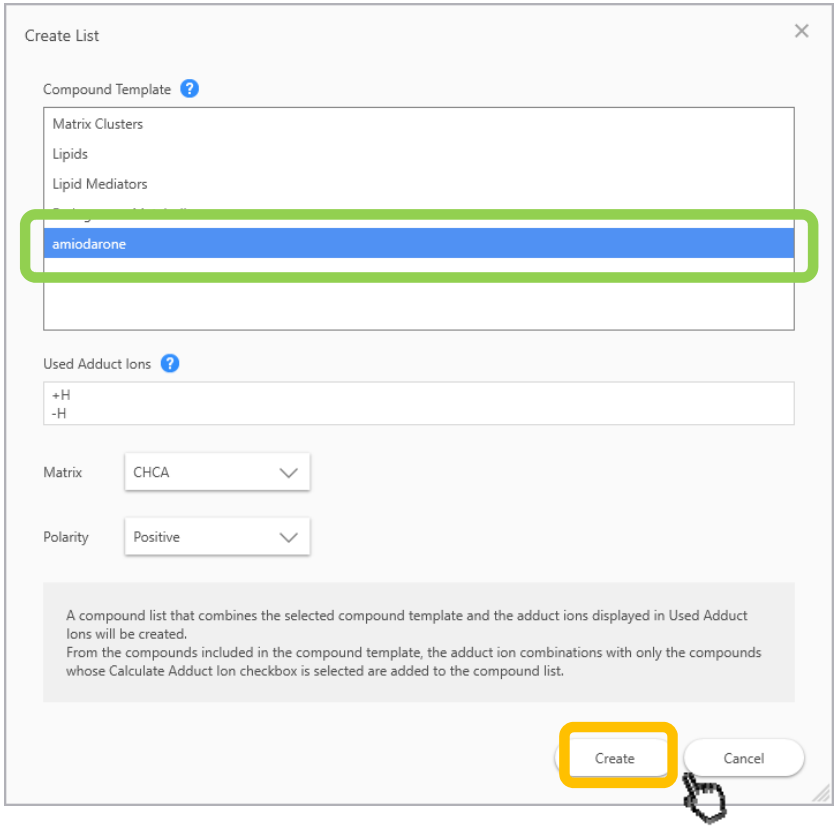


# Target compound settings 1



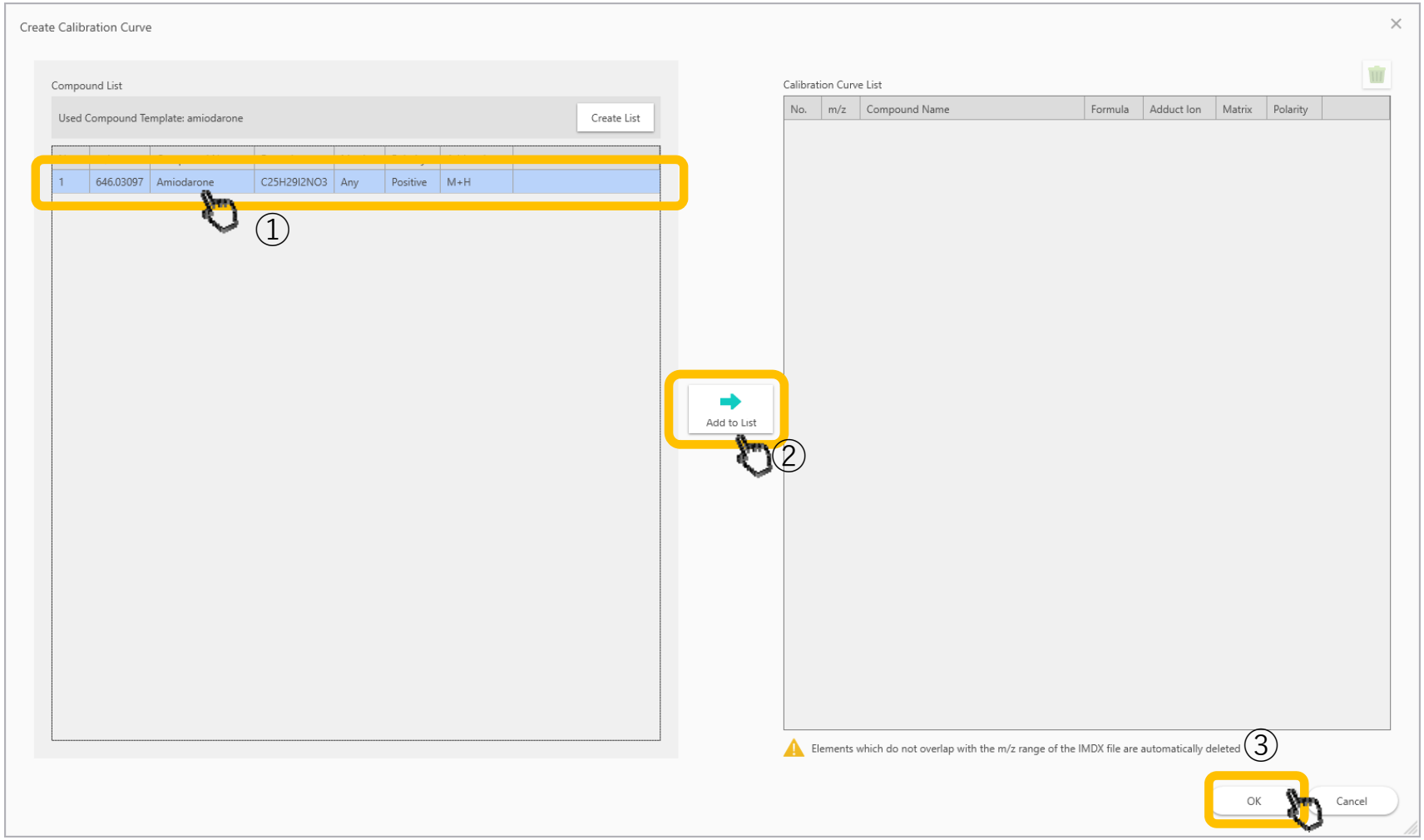

Please register target compounds and compound templates beforehand (see “How to register compound templates”)

# Target compound settings 2

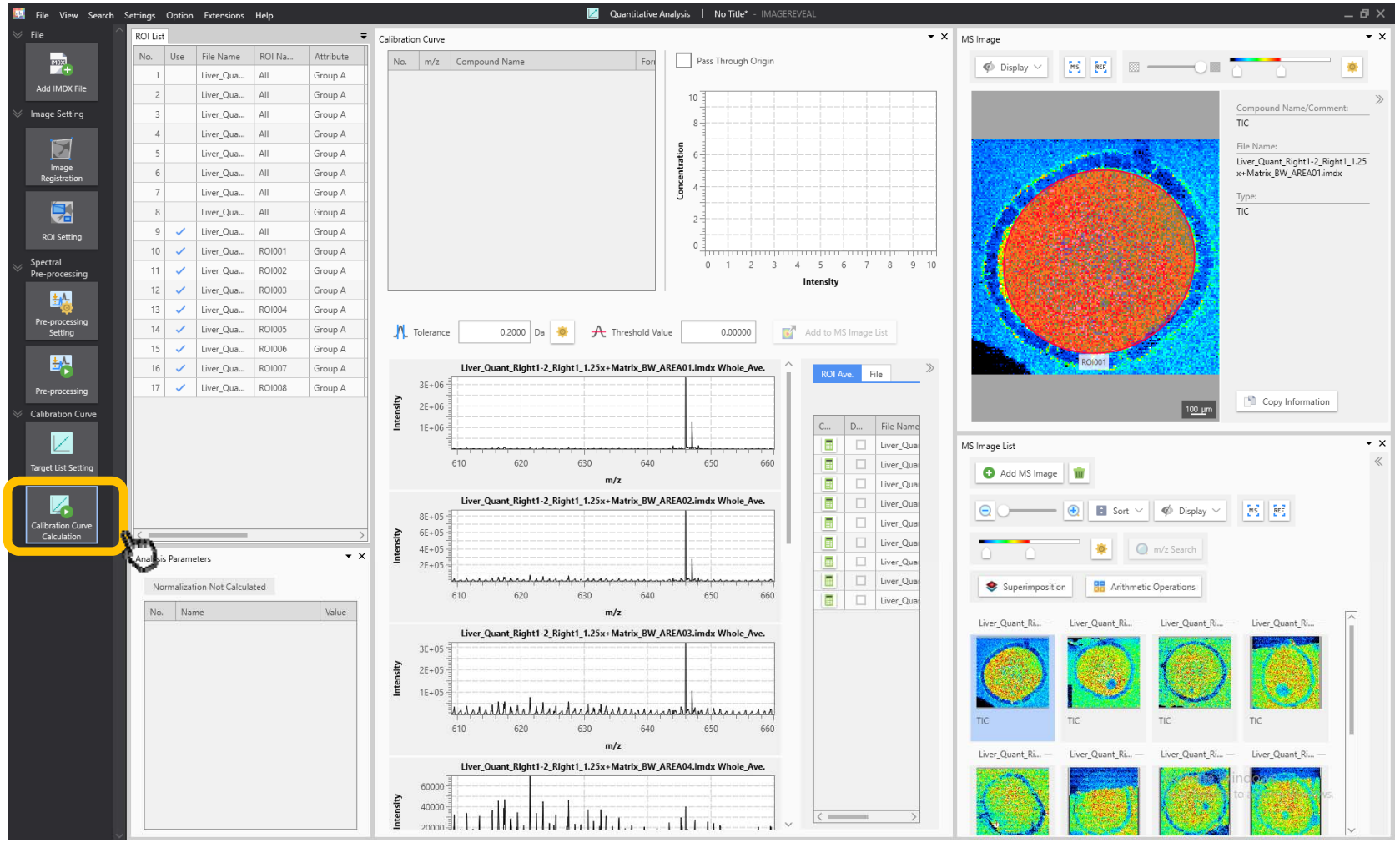



Select a previously-created compound template

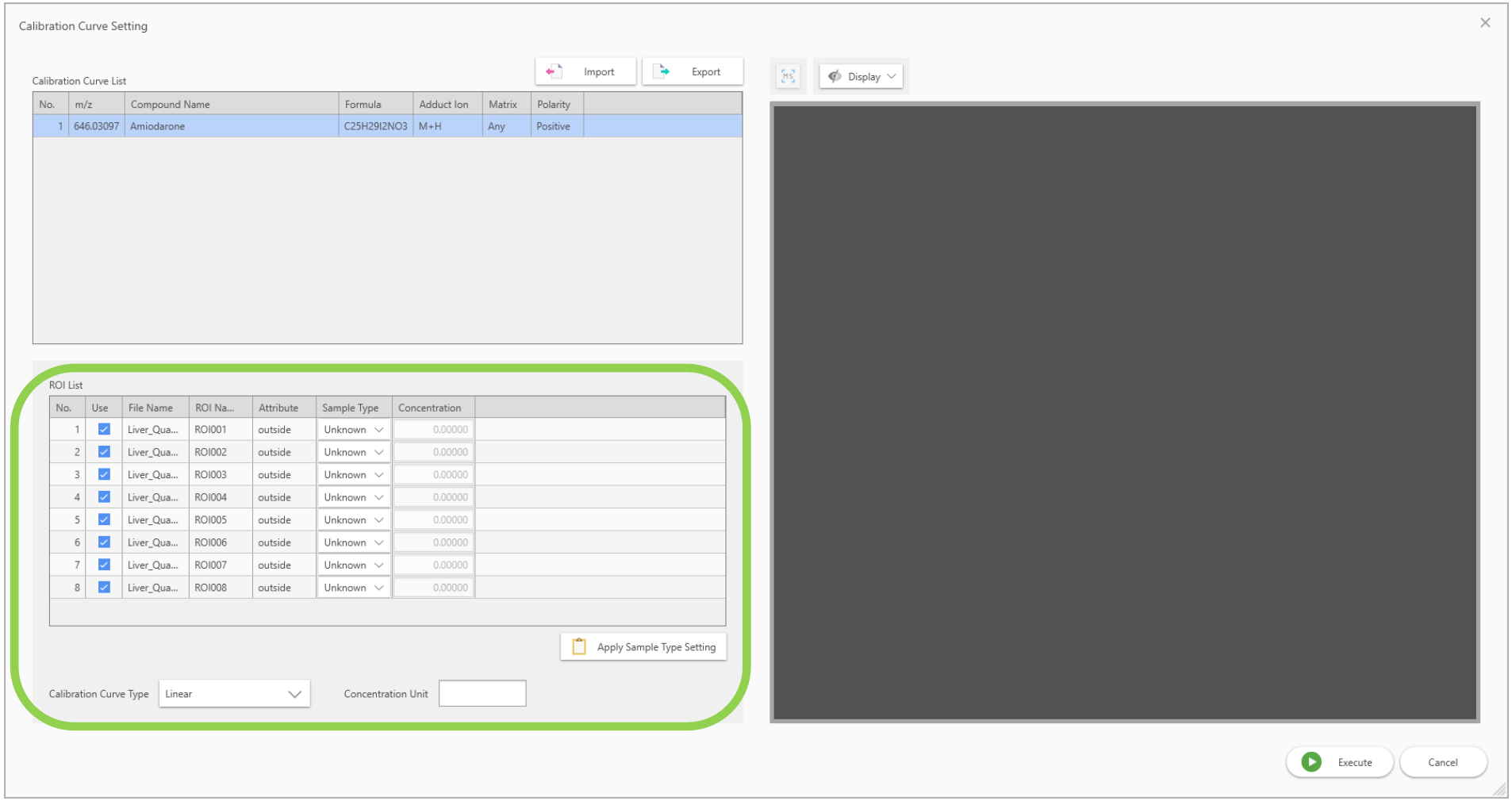
# Target compound settings 3



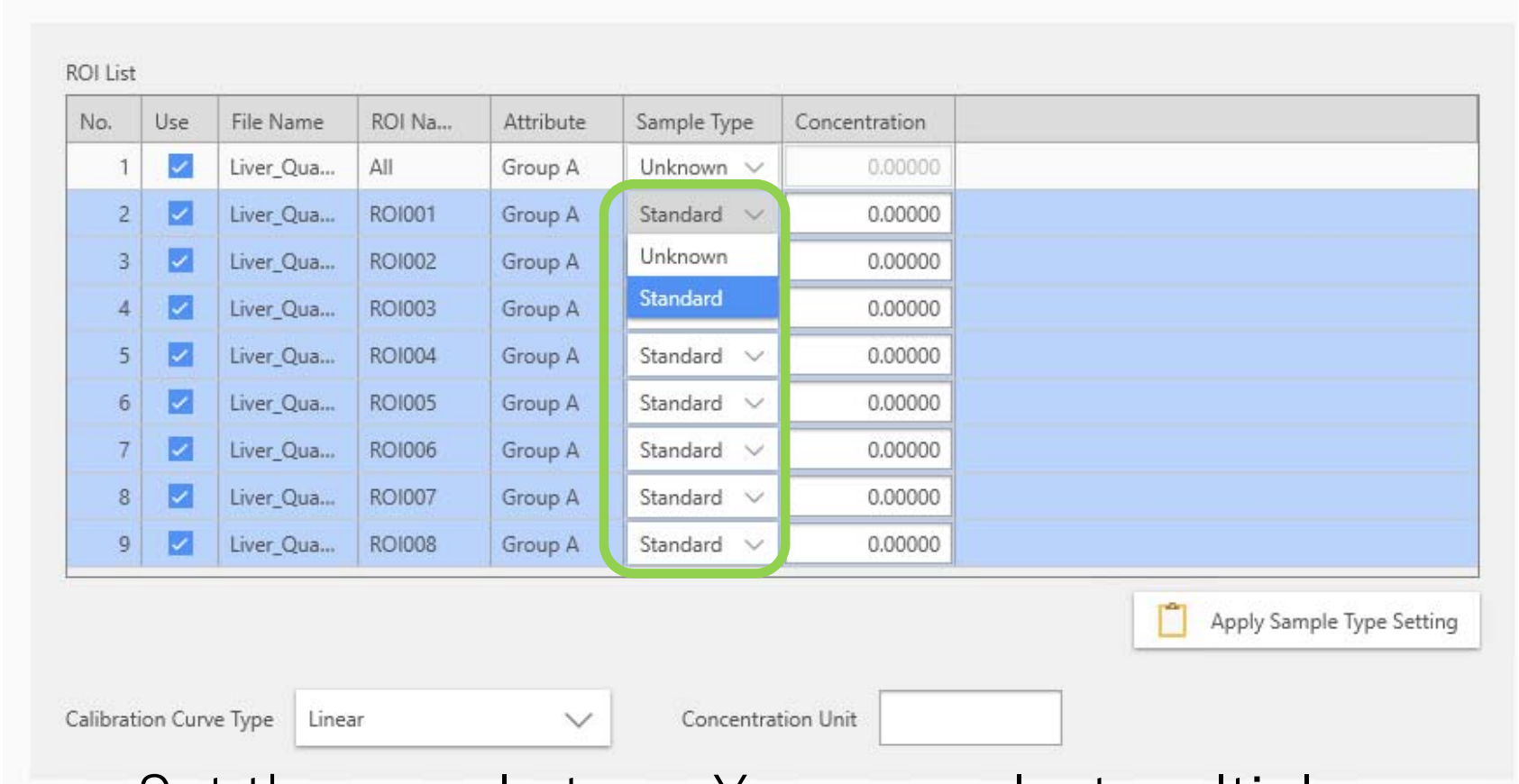
# Calibration curve settings 1



# Calibration curve settings 2

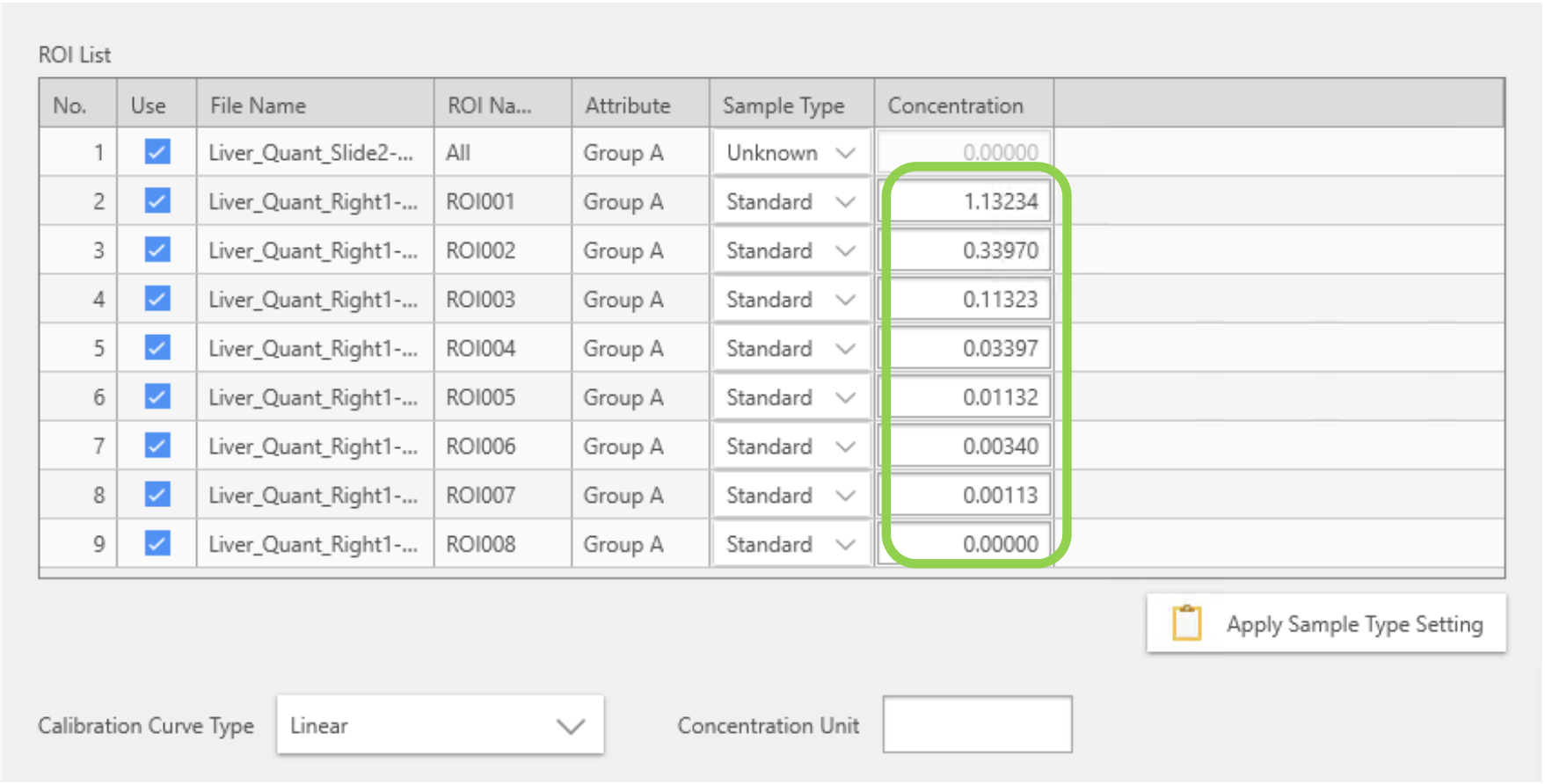


# Calibration curve settings 3



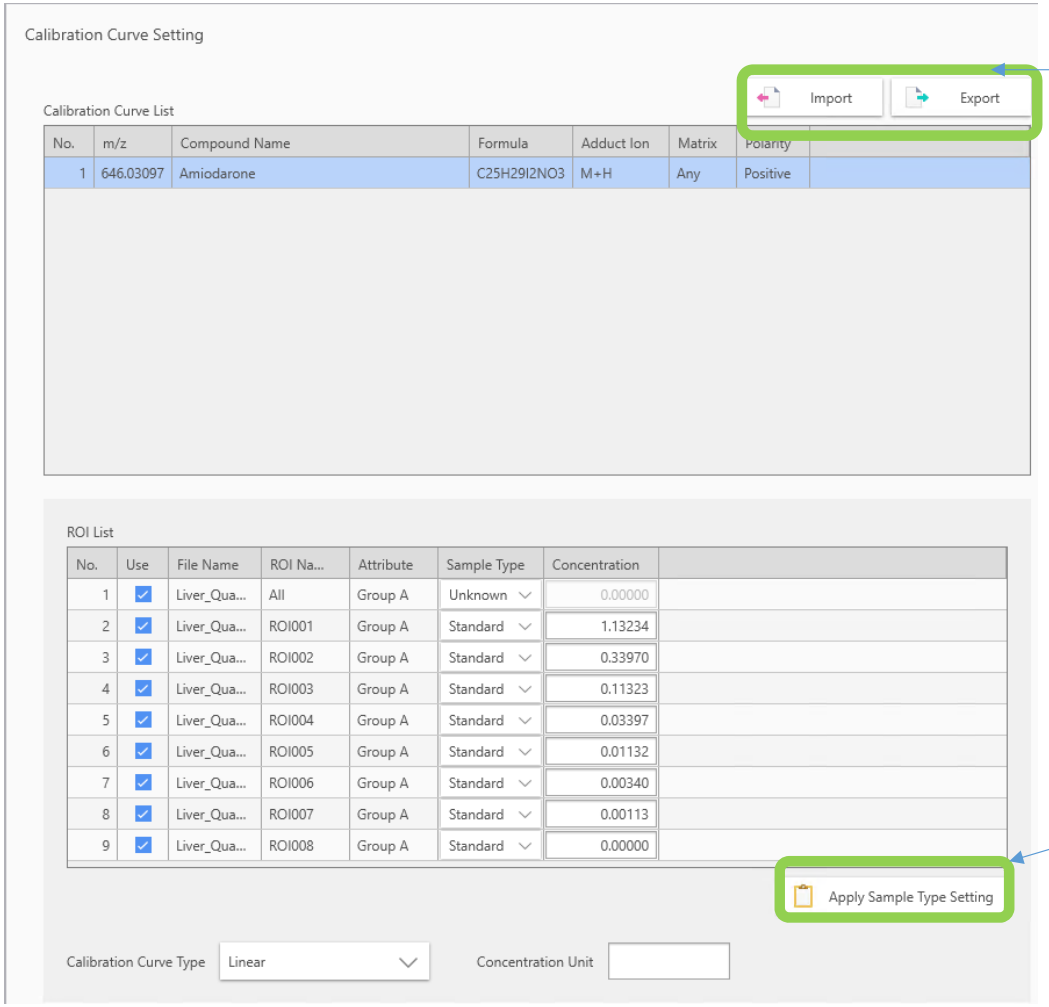

Set the sample type. You can select multiple rows and apply a setting to all of them.

# Calibration curve settings 4




Enter the concentration of the calibration curve samples

# Calibration curve settings 5: Faster settings

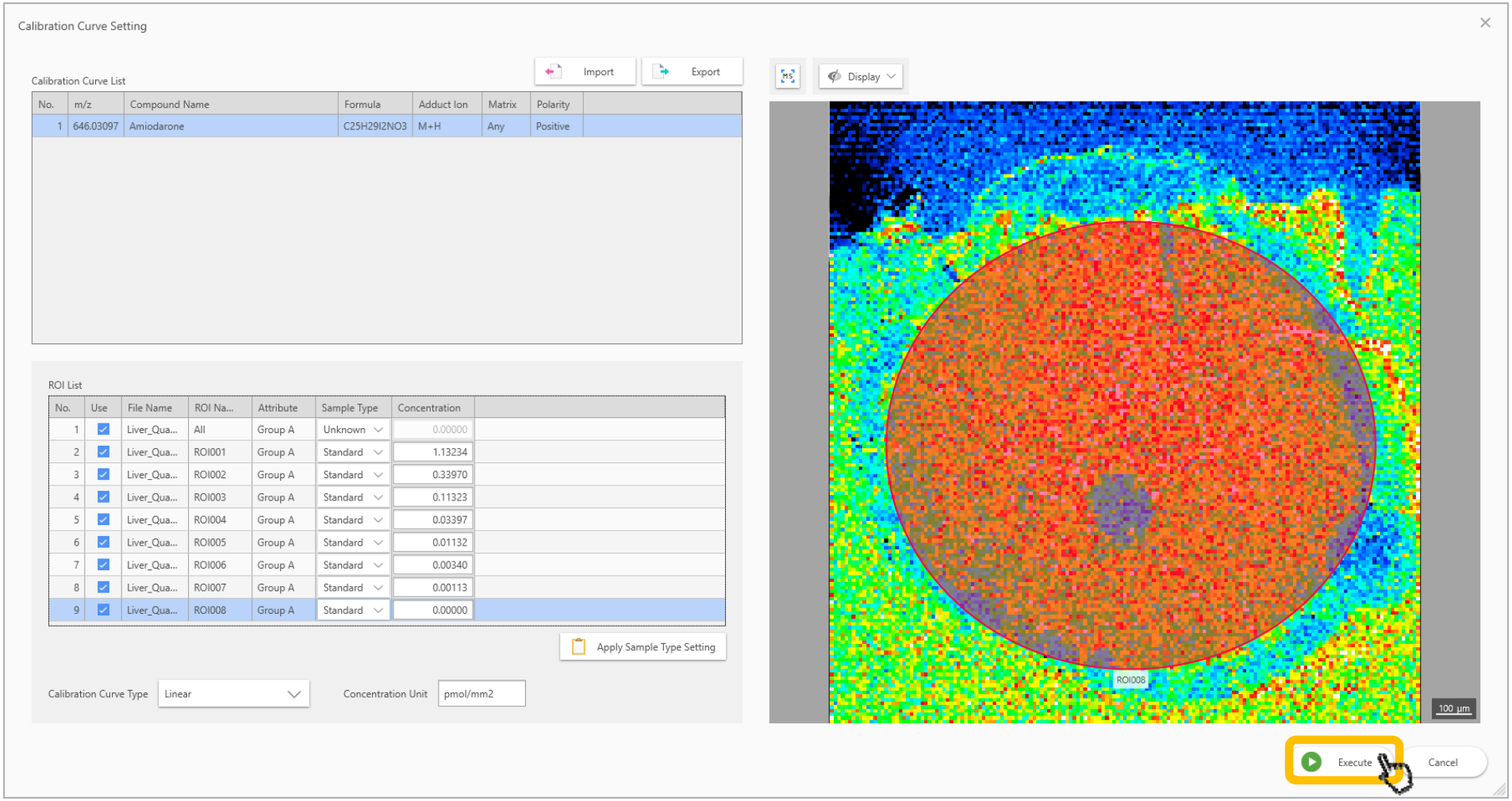



Import a CSV file to automatically enter calibration curve concentrations

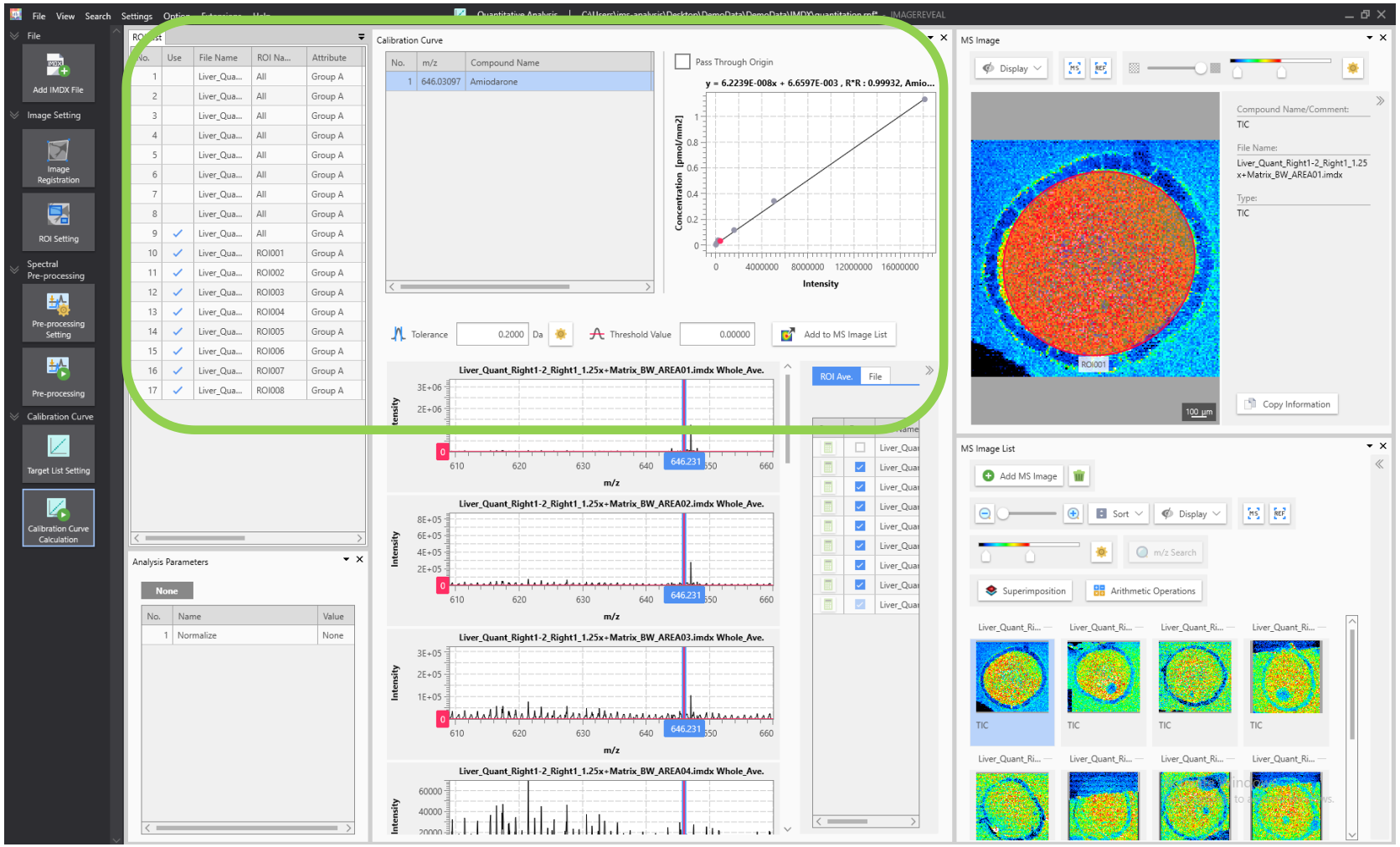
| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | 646.031 | Amiodarone | | | | |
| 2 | | Slide2-2_( | All | Group A | Unknown | 0 |
| 3 | | 180406_Ri | ROI001 | Group A | Standard | 1.13234 |
| 4 | | 180406_Ri | ROI002 | Group A | Standard | 0.3397 |
| 5 | | 180406_Ri | ROI003 | Group A | 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.

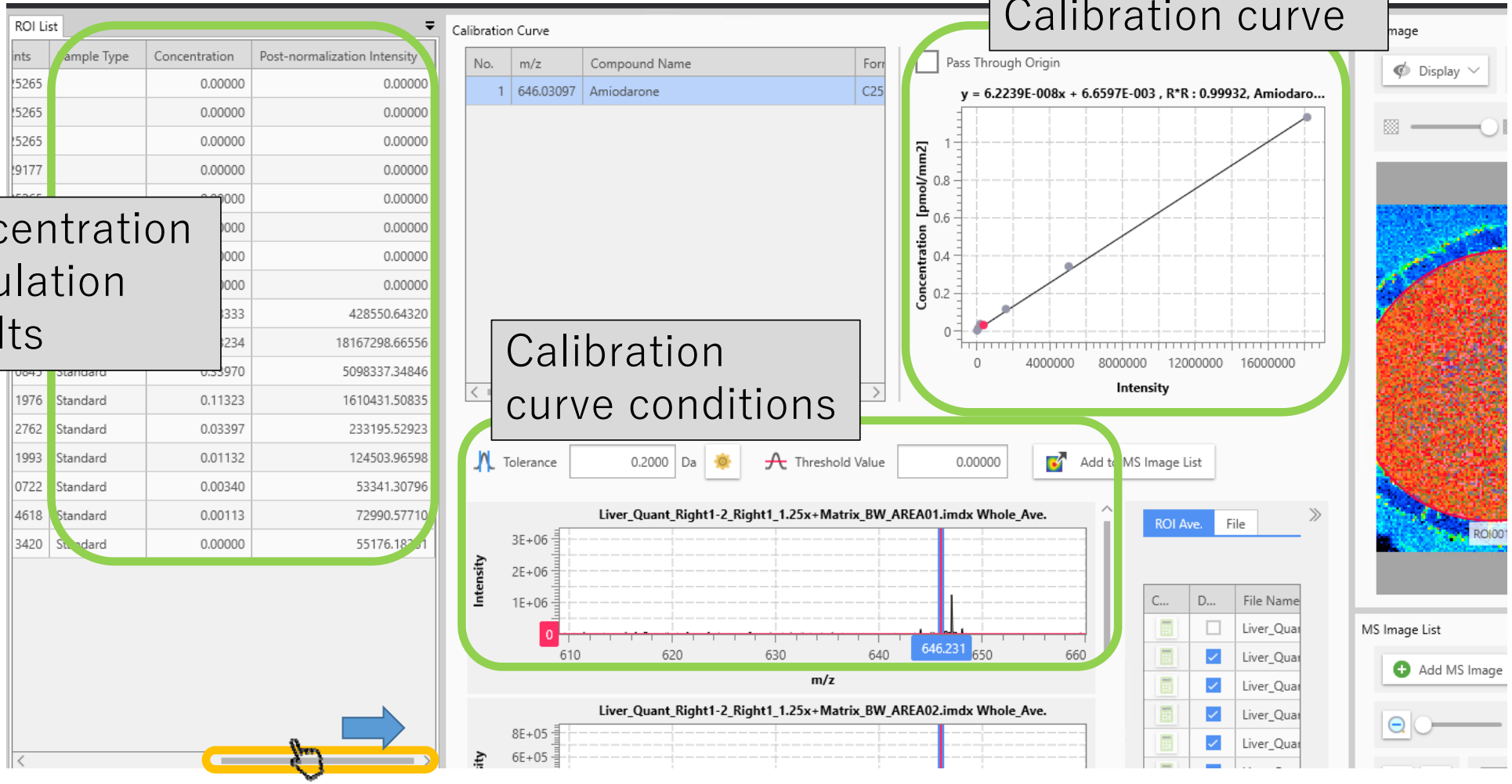
# Calibration curve settings 6



# Calibration curve results



# Quantitation results 1



# Quantitation results 2: Concentration calculations

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

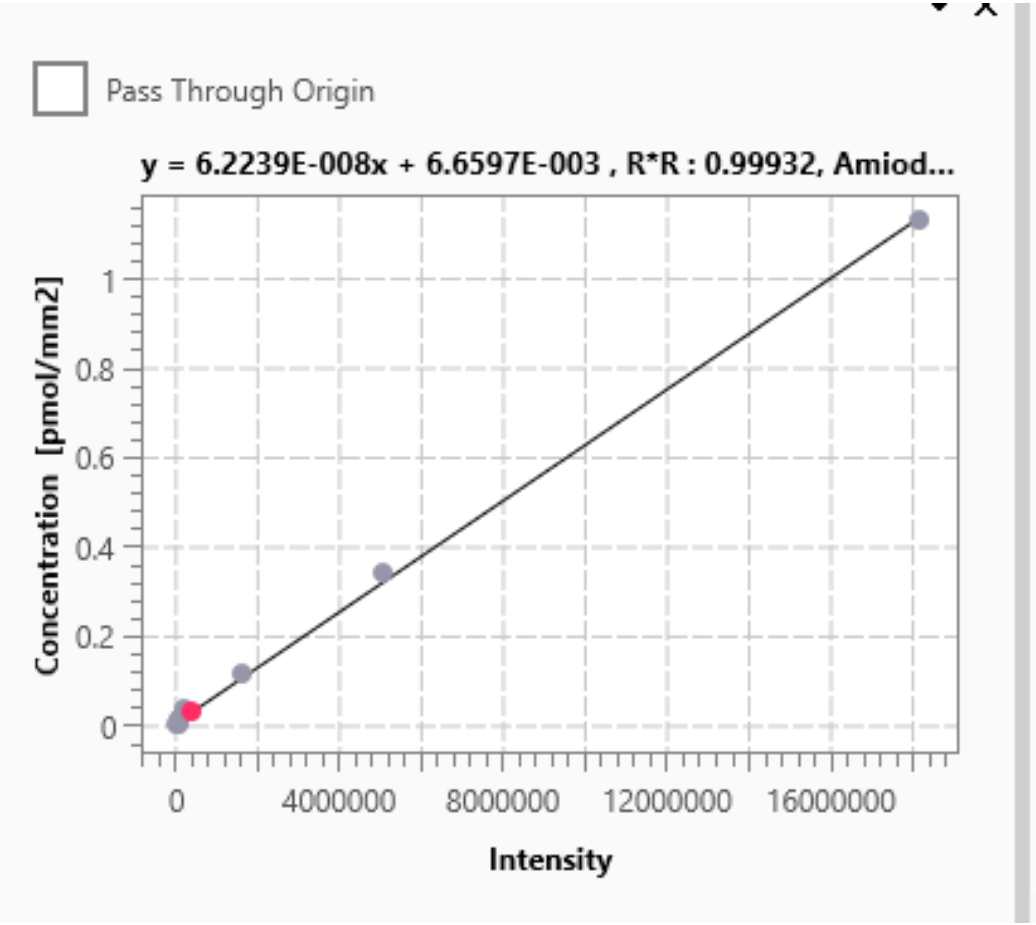
ROI List

| 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



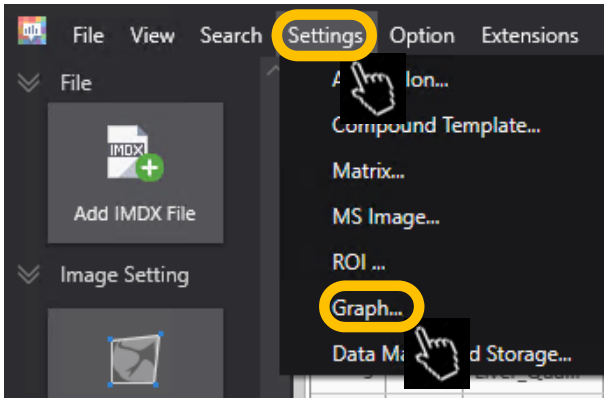

The calibration curve is shown.

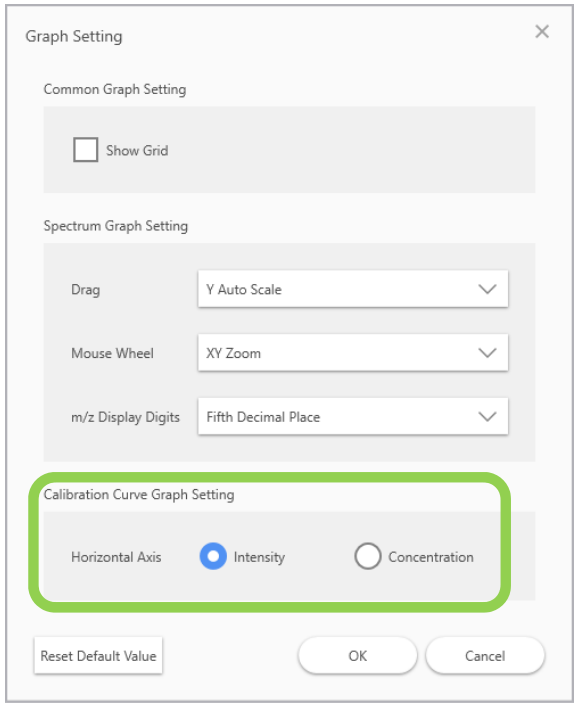
Grey points are the standards used for calibration and the red point is the unknown sample.

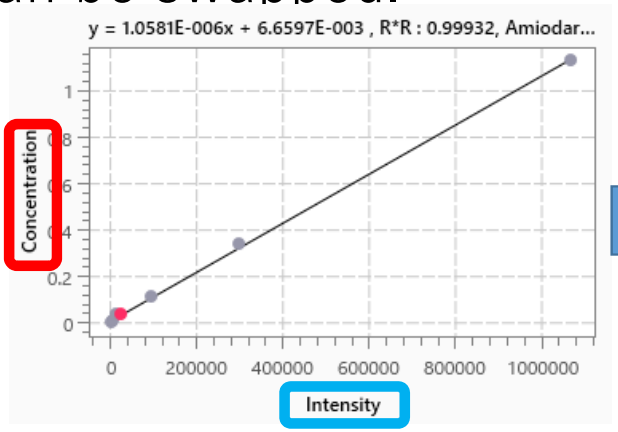
This result will change depending on the calibration curve conditions.

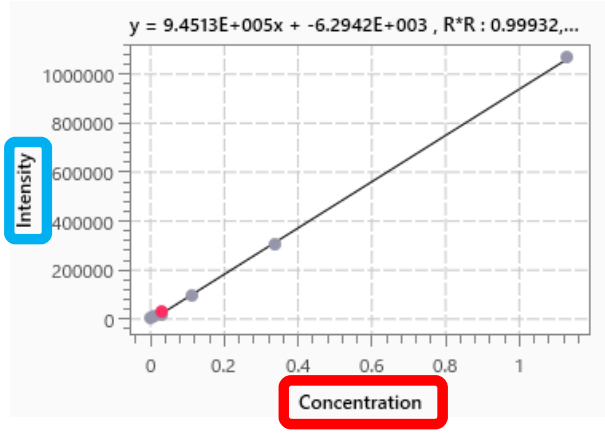
# Quantitation results 3 .1: Calibration curve options

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

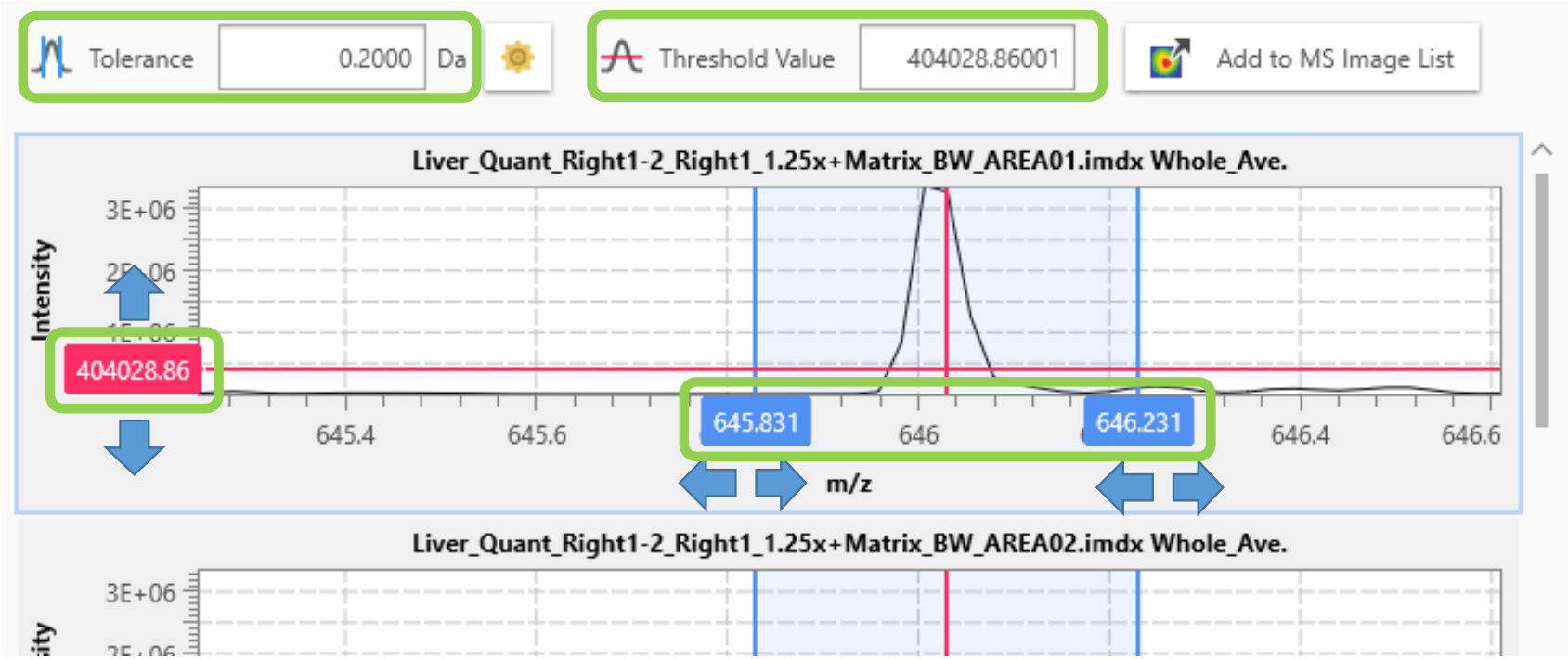


# Quantitation results 4: Calibration curve conditions




When calculating the peak area, you can change the “tolerance” and “threshold value” shown above the spectrum. This in turn changes the calculation results.

# Cautions

- When handling multiple data sets in Quantitative Analysis mode, it is assumed that the sampling interval is the same for all.
- Check the sampling interval by right-clicking on the ROI list and selecting “Show File Parameter”, then looking under “Conversion Parameter”.