LIFE SCIENCES MASS SPECTROMETRY

SCiLS™ Lab 2027a – What's New?

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SCiLS™ Lab 2027a – What's New?

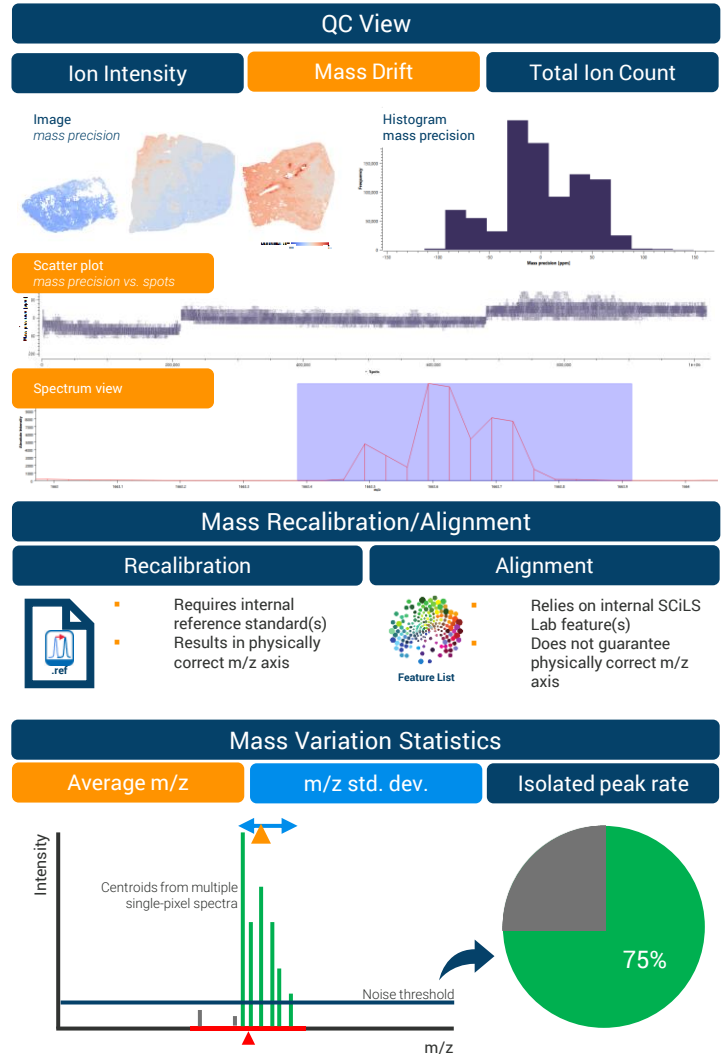
01 **QC View**
Monitor data quality

02 **Mass Variation Statistics**
Quantify performance

03 **Mass Recalibration / Alignment**
Ensure reproducibility

04 **timsMRMS compatibility**
Import, recalibrate, analyze timsMRMS data

05 **Multiple feature enhancements**
Improved mass axis binning, interval widths & many more…



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01

QC View

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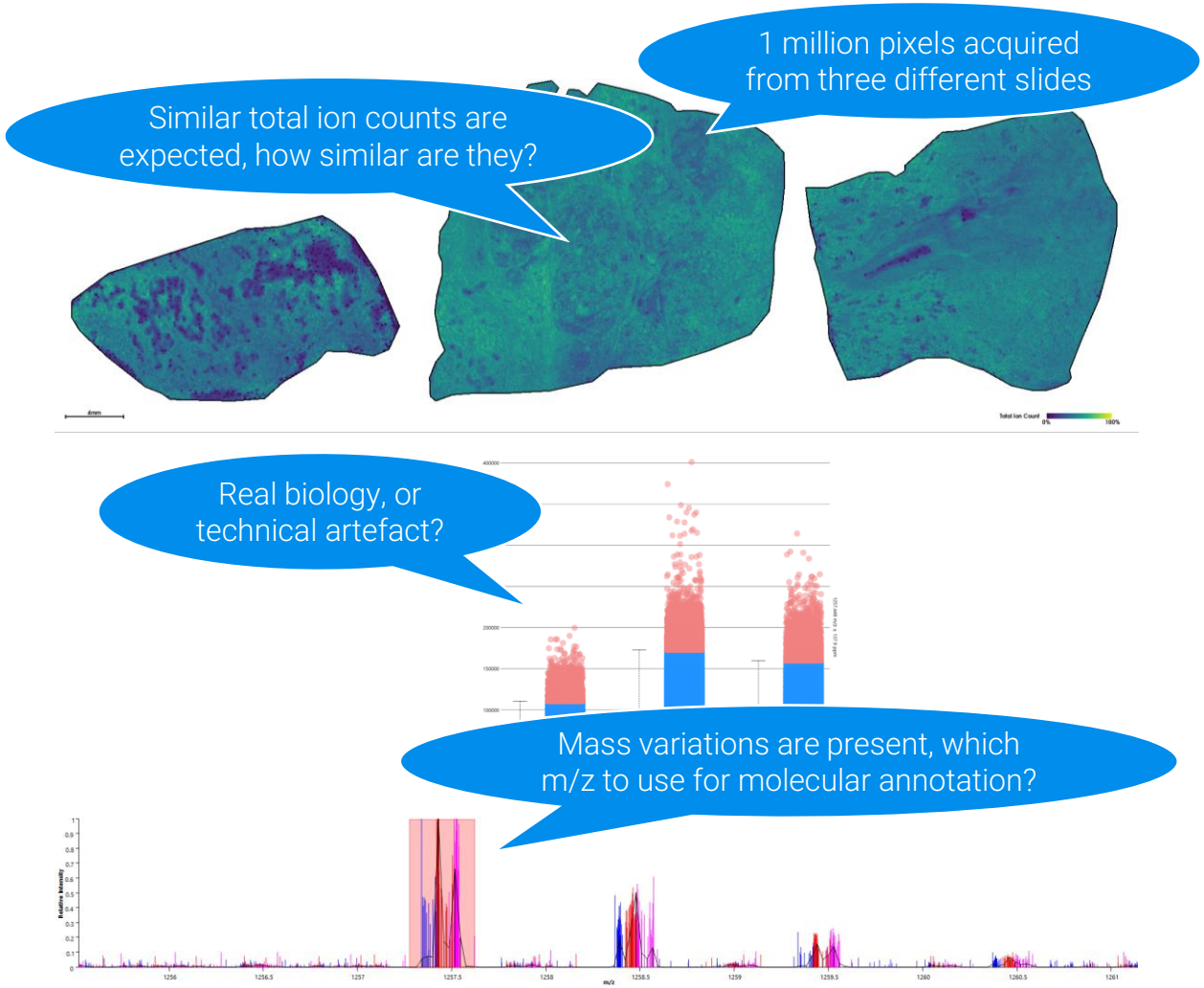
QC View

Easy-to-use tools to monitor data quality

- Trustworthy scientific **insights** require high **data quality**
  - In large, multi-acquisition data sets, **batch effects** easily go unnoticed, but can become a dominant source of variation
  - **Mass variations** accumulate over longer and/or multiple experiments and lead to incomparable data sets and incorrect molecular annotations

- **QC View** offers easy-to-use **data quality monitoring** and inspires **confidence** before analyzing data



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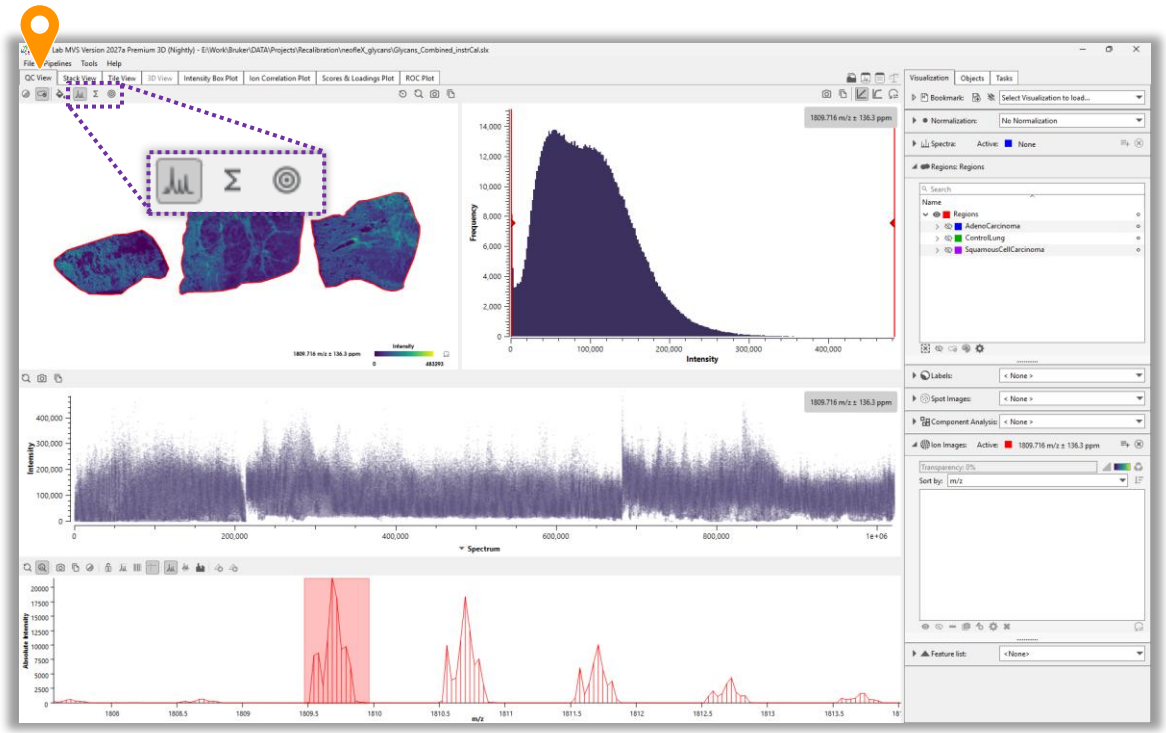
QC View

Easy-to-use tools to monitor data quality

- **QC View** offers a quick insight into:
  - Absolute ion **intensity** distributions
  - **Total ion count** distributions
  - Ion **mass variation** distributions



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QC View
Easy-to-use tools to monitor data quality

- **QC View** offers a quick insight into:
  - Absolute ion **intensity** distributions
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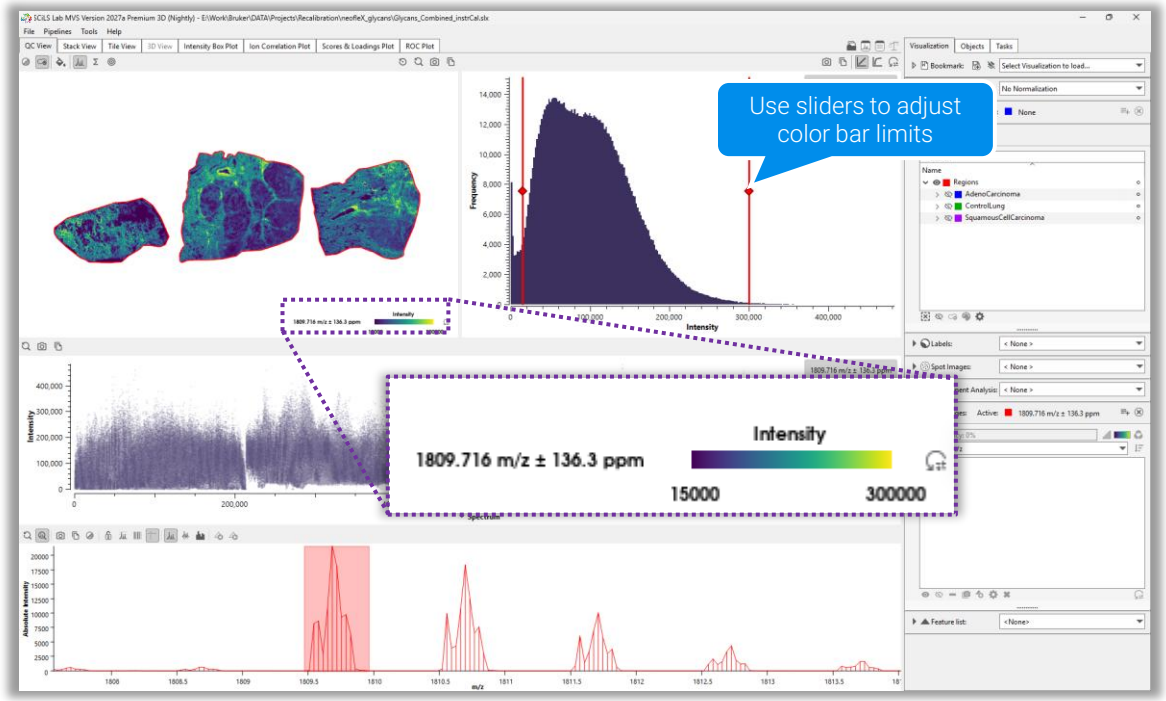
- Adjust the **color bar limits** using the sliders in the histogram
  - Click and drag the sliders
  - Double-click on the diamond to enter a numerical value



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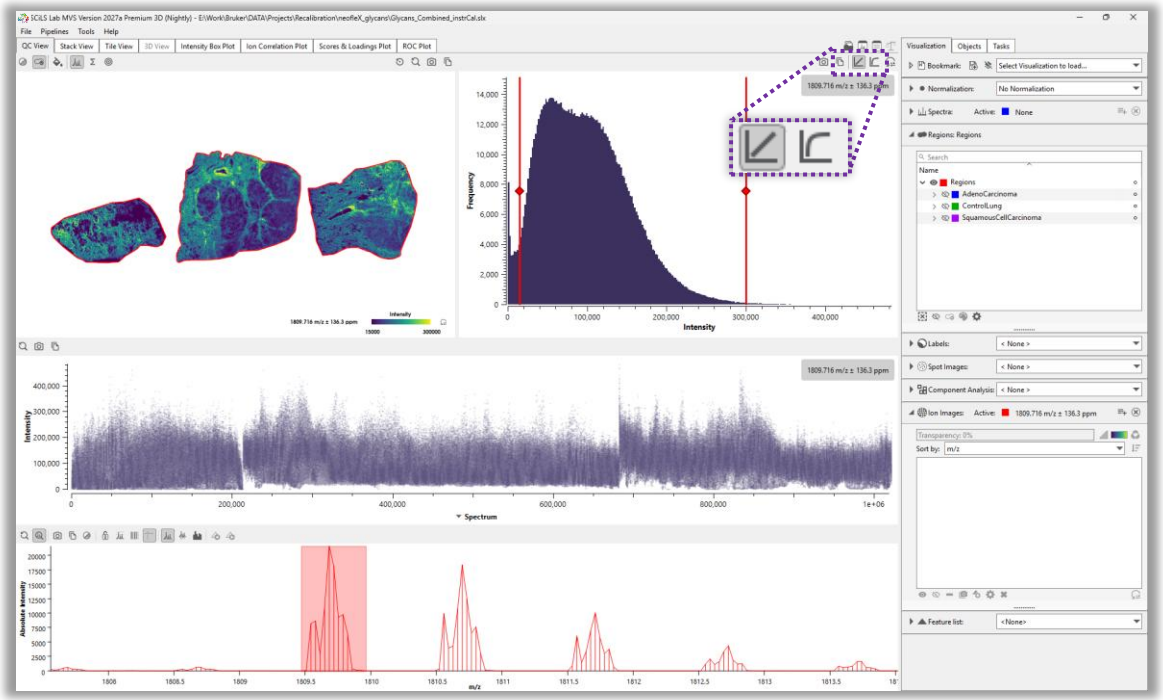
- Change the **scale** of the histogram frequency axis from linear to logarithmic



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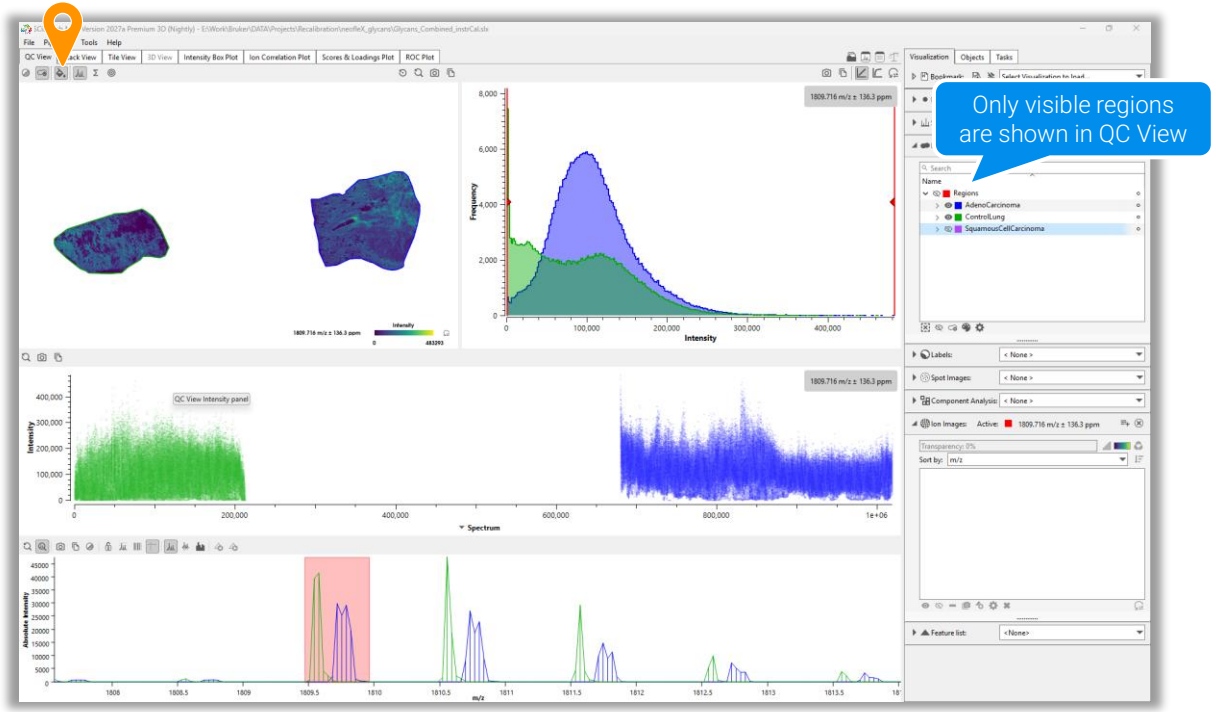
  - Double-click on the diamond to enter a numerical value
- Change the **scale** of the histogram frequency axis from linear to logarithmic
- **Filter** and **color** the QC View content by selecting regions of interest in the Regions widget



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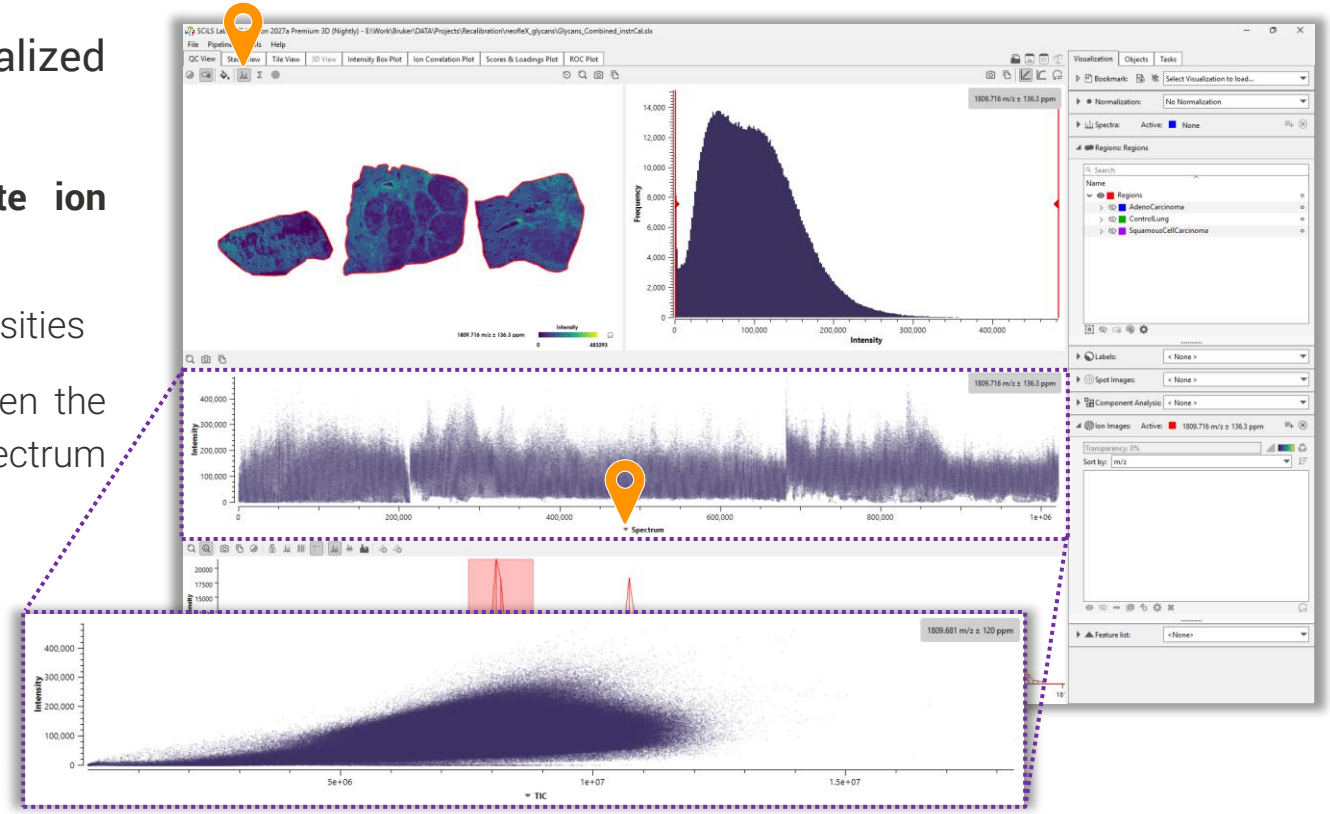
QC View
Intensity panel

- The **Intensity panel** provides insight into the normalized absolute intensity distributions of the active ion
  - The **image display** shows the **color-coded absolute ion intensity distribution without hotspot removal**
  - The **histogram** generates insight into distribution of intensities
  - The **scatter plot** can be used to study relations between the absolute ion intensity and the total ion count, or the spectrum index



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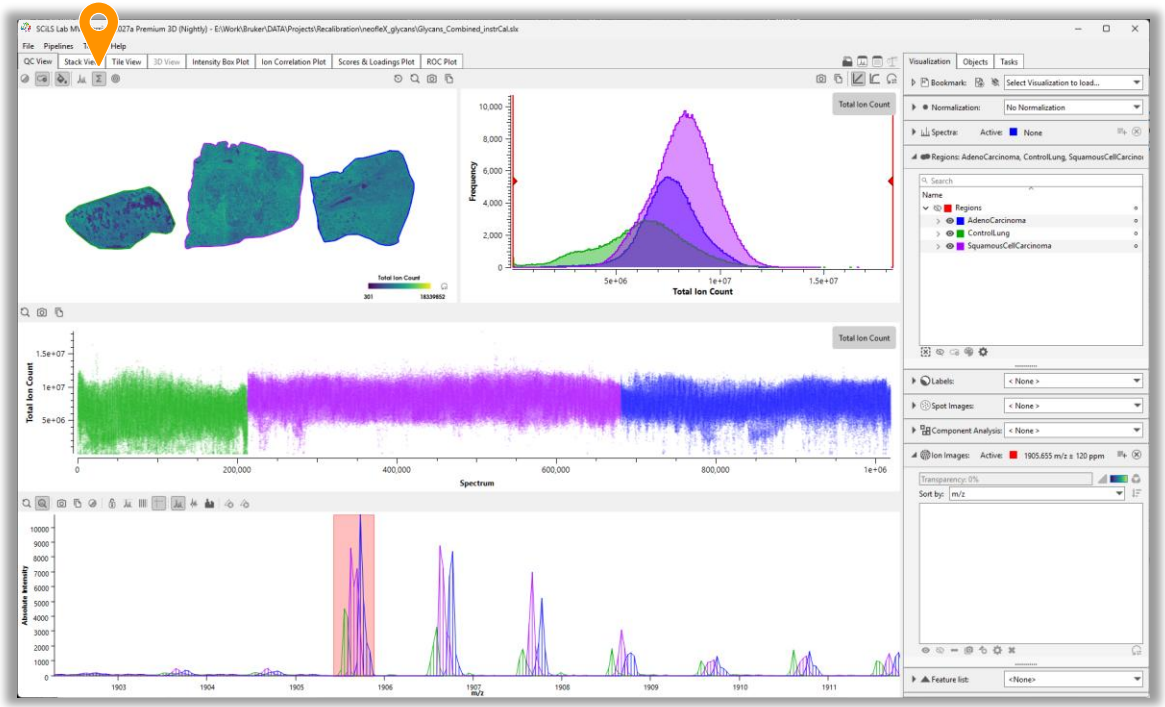
QC View
Total ion count panel

- The **Total ion count panel** displays the total ion count of each spectrum, displayed as absolute values and regardless of the active ion or selected normalization
  - The **image display** shows the color-coded total ion count distribution from the minimum to maximum value
  - The **histogram** generates insight into distribution of total ion counts of selected regions
  - The **scatter plot** can be used to study relations between the total ion count and the spectrum index



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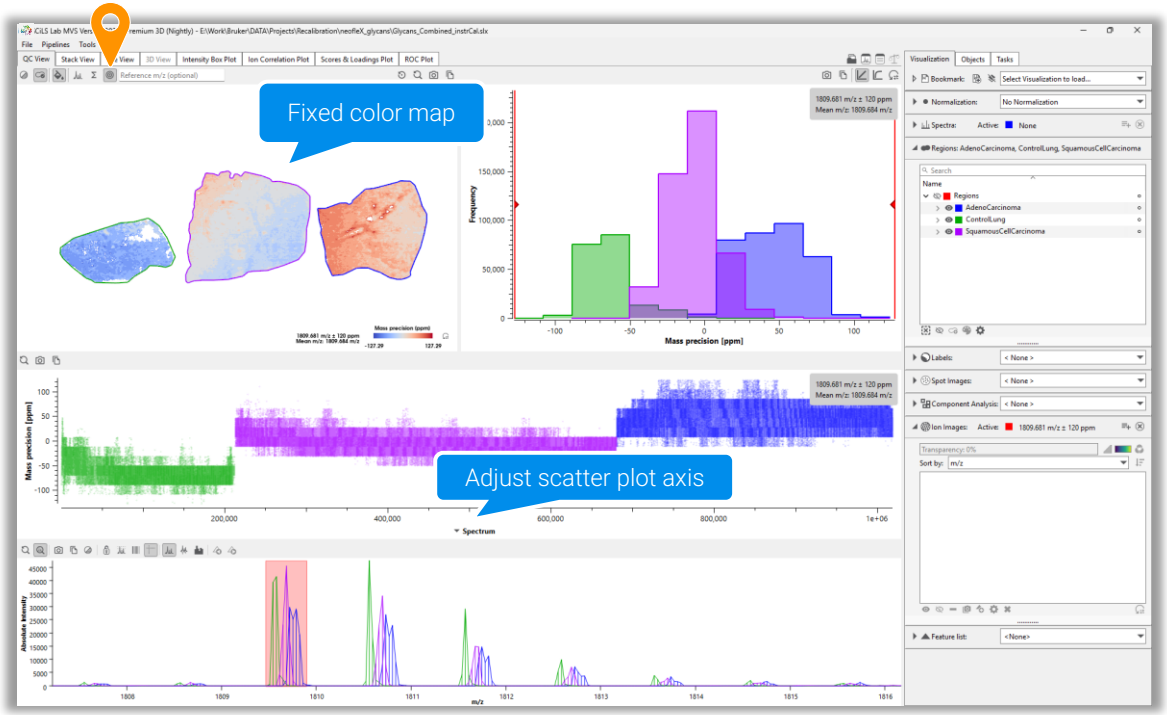
QC View
Mass variation panel

- The **Mass variation panel** displays the variation of the m/z apex position of the active ion across all spectra
  - The Image display uses a fixed **blue-to-red color map**, such that by default values close to zero are colored **light gray**
  - The horizontal axis of the scatter plot can be adjusted to display the spectrum indices, active ion intensity or total ion count



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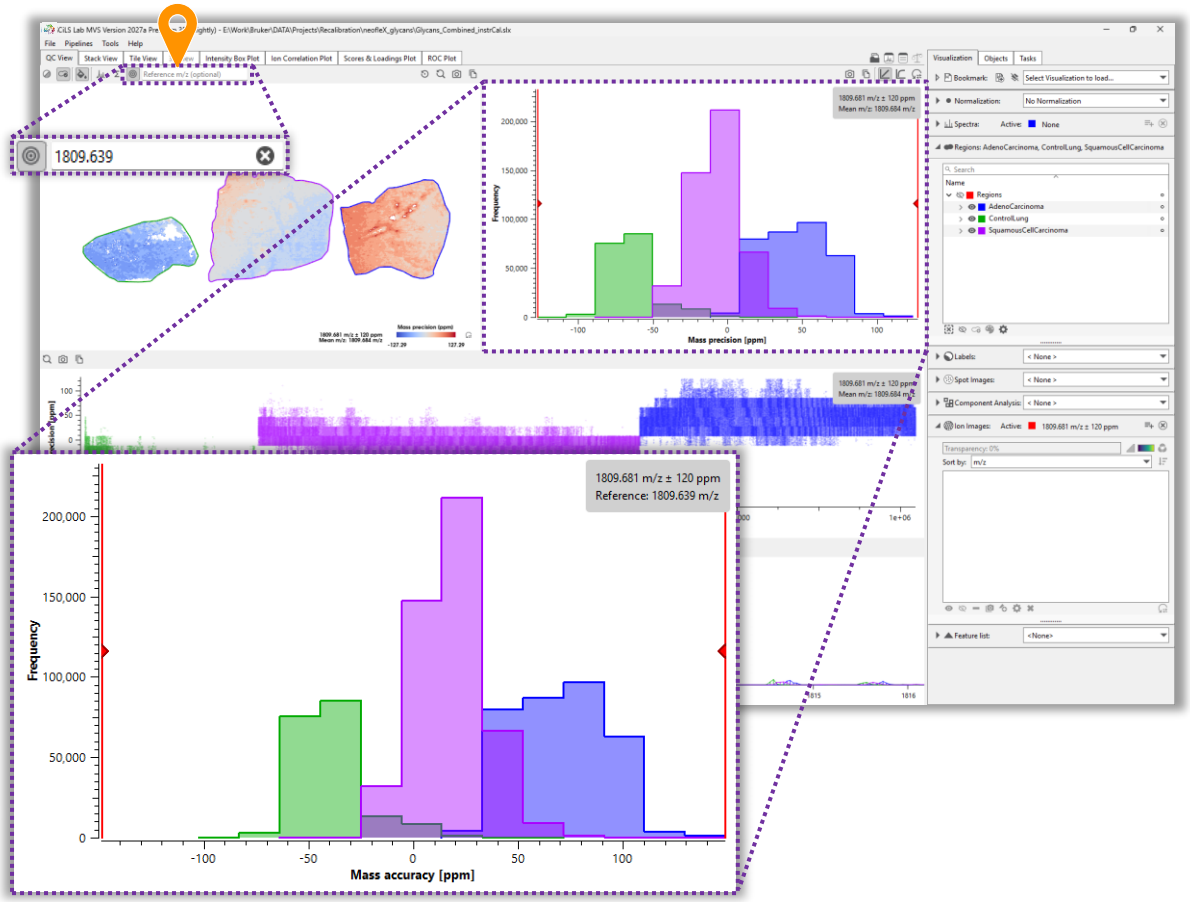
  - The Image display uses a fixed **blue-to-red color map**, such that by default values close to zero are colored **light gray**
  - The horizontal axis of the scatter plot can be adjusted to display the spectrum indices, active ion intensity or total ion count
  - By default, the **relative mass precision** compared to the average peak apex position across all spectra is displayed
  - Enter an explicit reference m/z to display the **absolute mass accuracy** with respect to the reference



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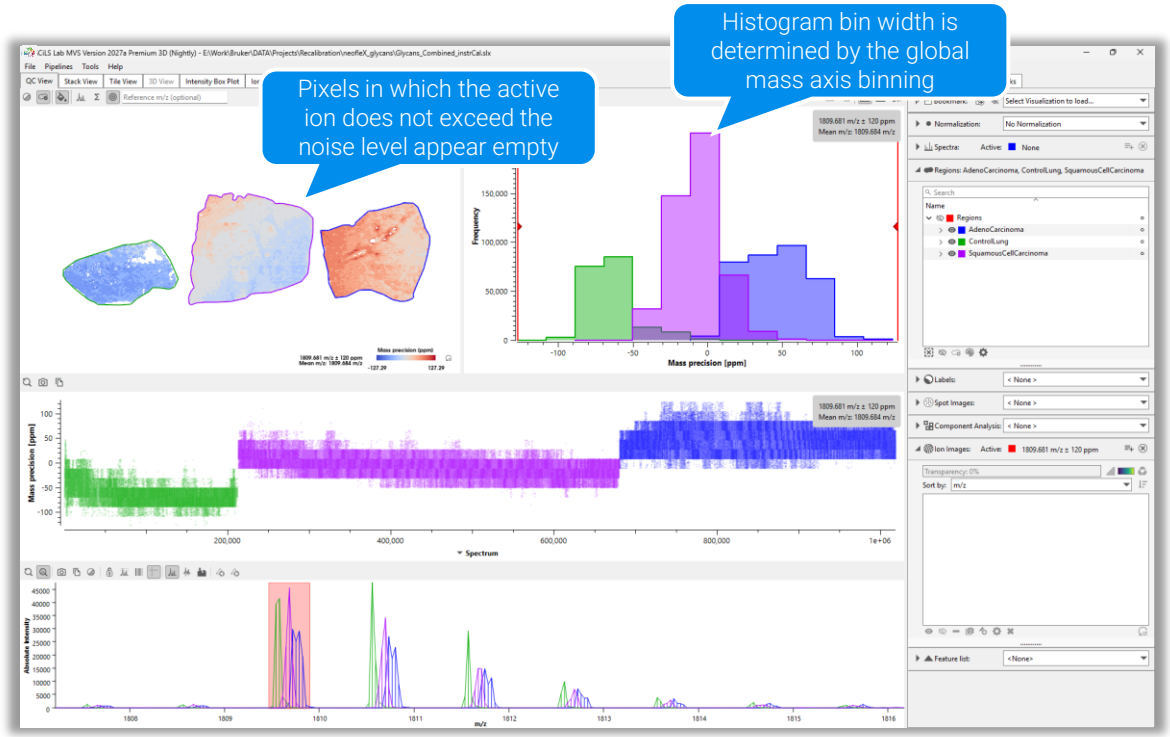
QC View
Mass variation panel

- **NOTE:**
  - For computing the mass variation, a noise level for the active ion's m/z interval is estimated. All intensities below the noise level are ignored, and thus, the number of spots shown in the scatter plot and contributing to the histogram may depend on the active ion
  - For performance reasons, the accuracy of the mass precision and accuracy values is limited by the binning of the global mass axis. The binning is reflected by the width of the bars in the histogram, as well as by the height of the horizontal clusters in the scatter plot
  - Mass variations can only be computed for m/z features. If the currently selected feature is a CCS-feature or an external feature, no data is displayed in the mass variation panel



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02

Mass Variation Statistics

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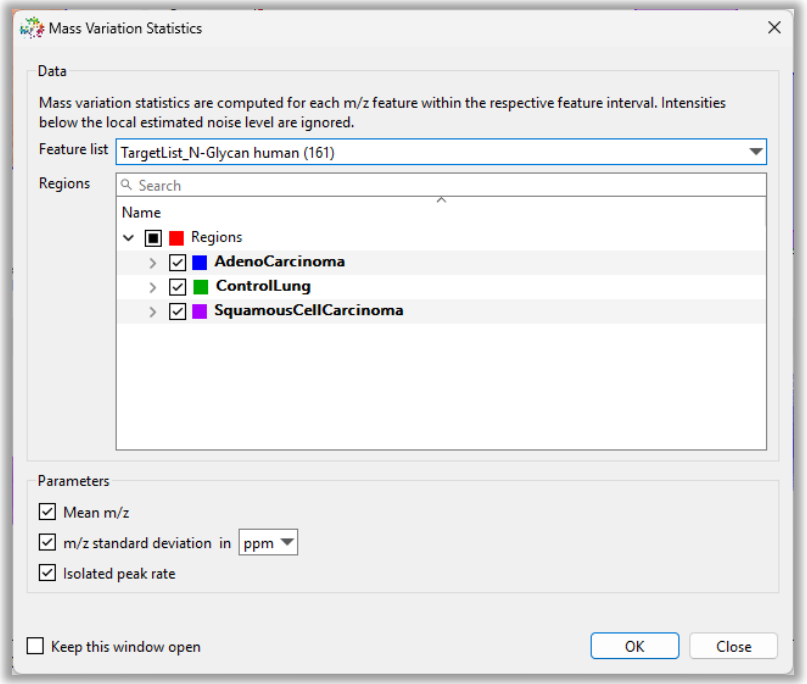
Mass Variation Statistics
Quantify quality and performance

- Use the **Mass Variation Statistics** tool to calculate key performance metrics for feature lists and regions:
  - **Mean m/z** for a given feature interval
  - **m/z standard deviation** for a given feature interval
    - **NOTE:** Because of performance considerations, the accuracy of the Mass Variation Statistics tool results is higher compared to the results shown in the Mass Variations panel of the QC View. Unlike the QC View, the tool calculations are not restricted by the overall mass axis binning of the data set.
  - **Isolated Peak Rate**
    - The relative number of pixels in a region in which a given feature interval contains only a single centroid above the estimated noise level
    - A high value for the Isolated Peak Rate indicates that a feature could serve as a recalibration/alignment reference



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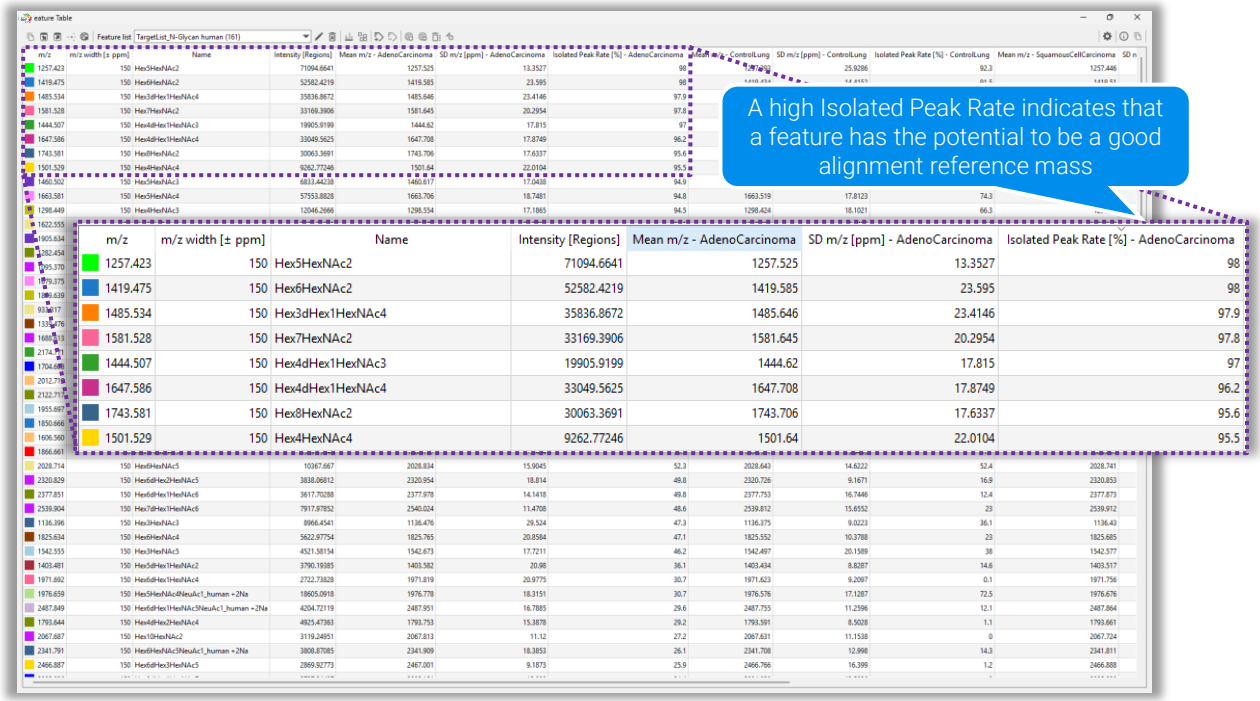
    - The relative number of pixels in a region in which a given feature interval contains only a single centroid above the estimated noise level
    - A high value for the Isolated Peak Rate indicates that a feature could serve as a recalibration/alignment reference
  - The tool results are added in new **Feature Table columns**



m/z	m/z width [± ppm]	Name	Intensity [Regions]	Mean m/z - AdenoCarcinoma	SD m/z [ppm] - AdenoCarcinoma	Isolated Peak Rate [%] - AdenoCarcinoma
1257.423	150	Hex5HexNAc2	71094.6641	1257.525	13.3527	98
1419.475	150	Hex6HexNAc2	52582.4219	1419.585	23.595	98
1485.534	150	Hex3dHex1HexNAc4	35836.8672	1485.646	23.4146	97.9
1581.528	150	Hex7HexNAc2	33169.3906	1581.645	20.2954	97.8
1444.507	150	Hex4dHex1HexNAc3	19905.9199	1444.62	17.815	97
1647.586	150	Hex4dHex1HexNAc4	33049.5625	1647.708	17.8749	96.2
1743.581	150	Hex8HexNAc2	30063.3691	1743.706	17.6337	95.6
1501.529	150	Hex4HexNAc4	9262.77246	1501.64	22.0104	95.5

03

Mass Recalibration / Alignment

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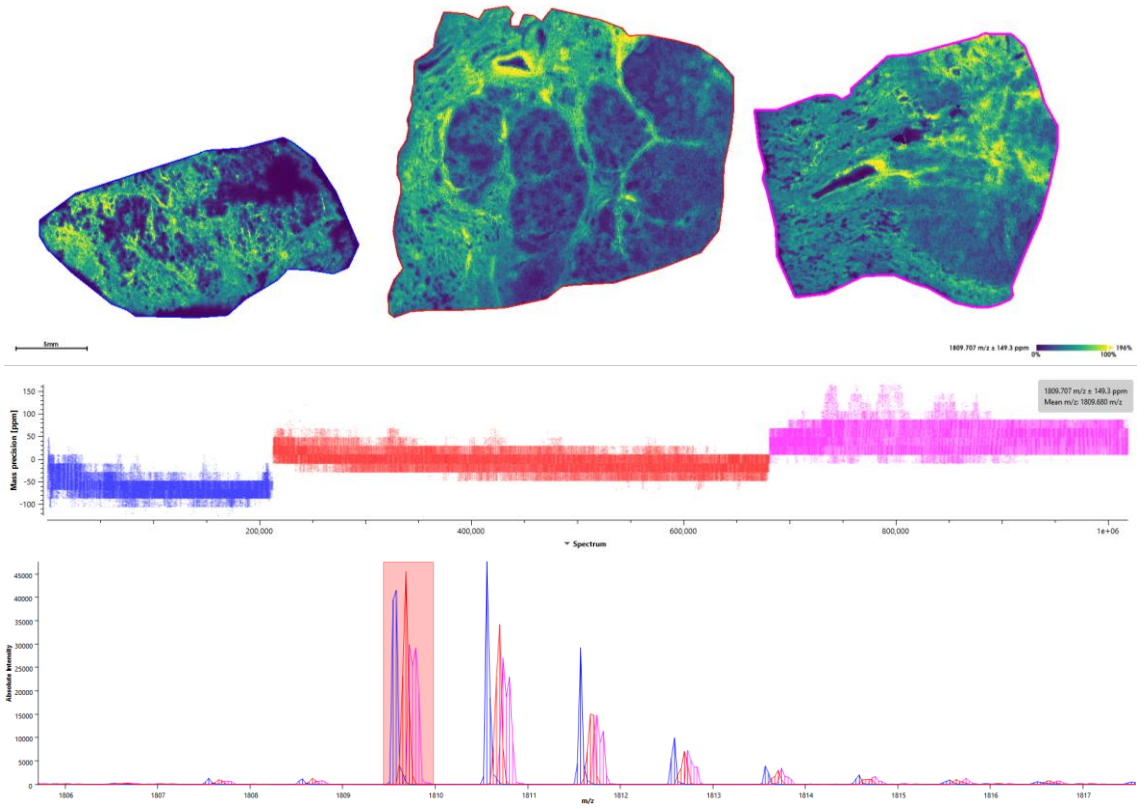
Mass Recalibration / Alignment

Recalibrate or align every single spectrum in your data set

- Deviations in **mass precision** and **mass accuracy** are amongst the most common **batch effects** in MALDI Imaging data sets
- Mass variations can have a variety of causes:
  - Sample geometry – height, thickness, topography
  - Ion generation – matrix heterogeneity, sample conductivity
  - Instrumental effects – temperature drift, system instability
  - Calibration model effects – external vs. internal, poor reference
- Mass variations have a large impact on:
  - Comparability of spectra and images across large data sets
  - Feature finding algorithms
  - Confidence in molecular annotation results
  - Quantitative results



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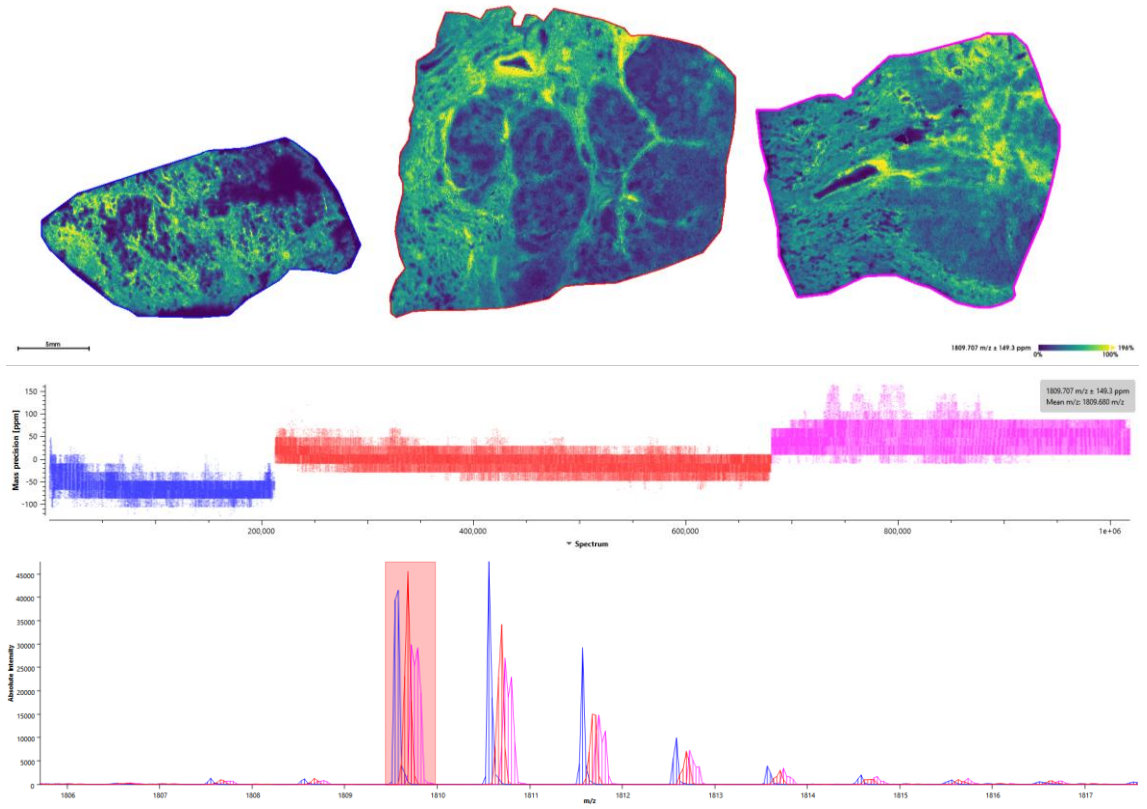
Mass Recalibration / Alignment

Ensure comparable spectra within and across experiments

- The new **Mass Recalibration/Alignment** workflow enables **correction of mass variation artefacts** in any SCiLS Lab data set to improve comparability across spectra
  - The workflow makes use of an **m/z-proportional, linear correction** method, which works both for reference lists containing:
    - A single reference mass (i.e., lock mass calibration)
      - Results in a simple local correction of m/z shifts
      - Residual mass errors increases away from the lock mass
    - Multiple reference masses
      - Results in a robust global correction of m/z shifts
      - Residual mass error is distributed over the recalibrated m/z range



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Mass Recalibration / Alignment

Ensure comparable spectra within and across experiments

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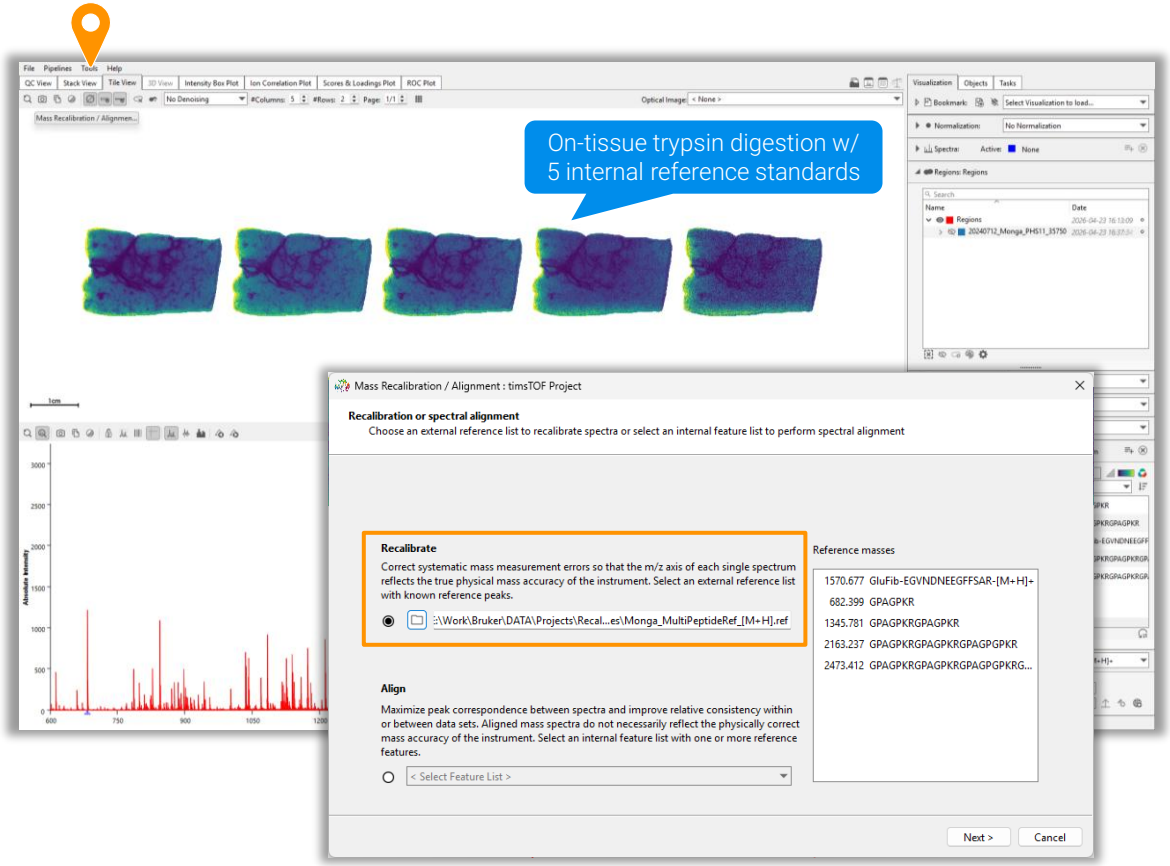
  - **Tools > Mass Recalibration / Alignment**

- **Recalibrate** – improves mass precision & accuracy
  - Adjustment of the m/z axis using known internal reference standards to restore a physically correct m/z axis
  - Requires the use of an external reference mass list
    - Supported formats: .ref, .mcl, .tlst, .sef



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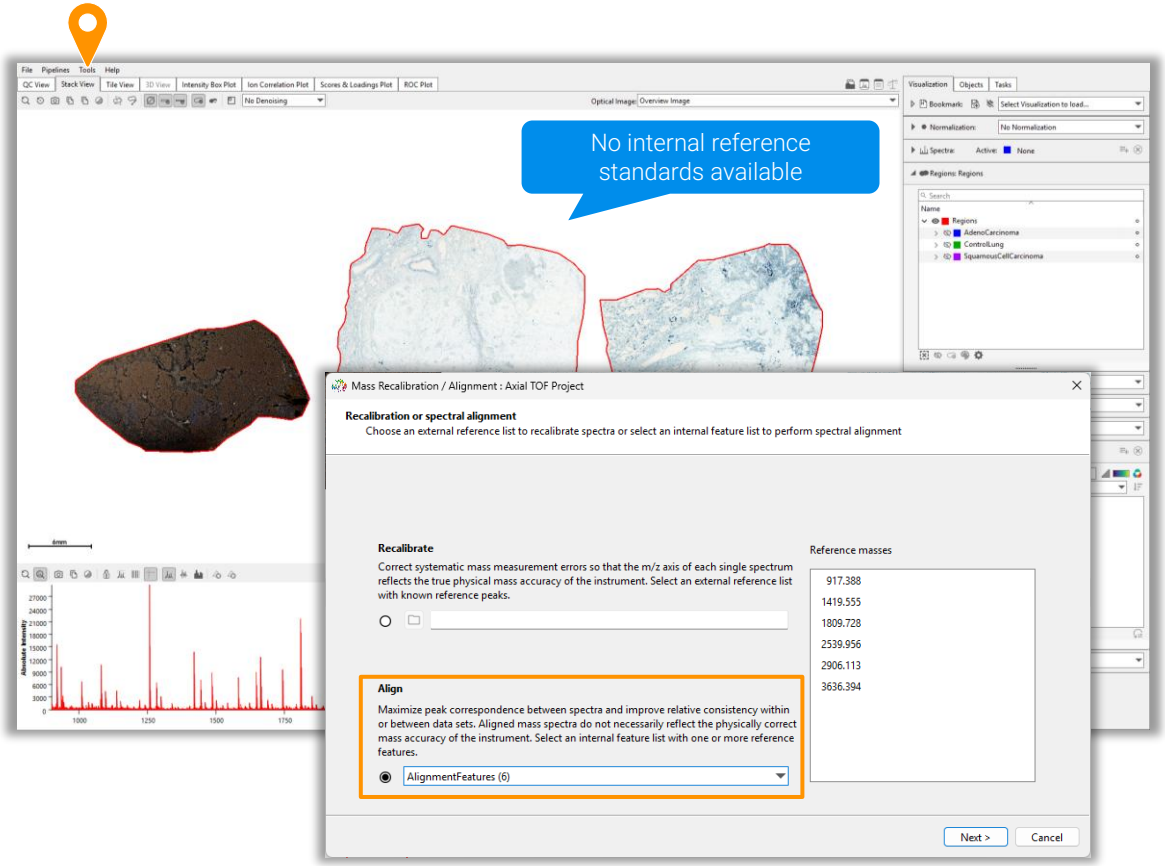
  - **Tools > Mass Recalibration / Alignment**

- **Align** – improves mass precision
  - Adjustment of m/z axes relative to each other using intrinsic features so that corresponding peaks coincide
    - **Note:** alignment does not guarantee a physically correct m/z axis
  - Requires the use of an internal SCiLS Lab feature list



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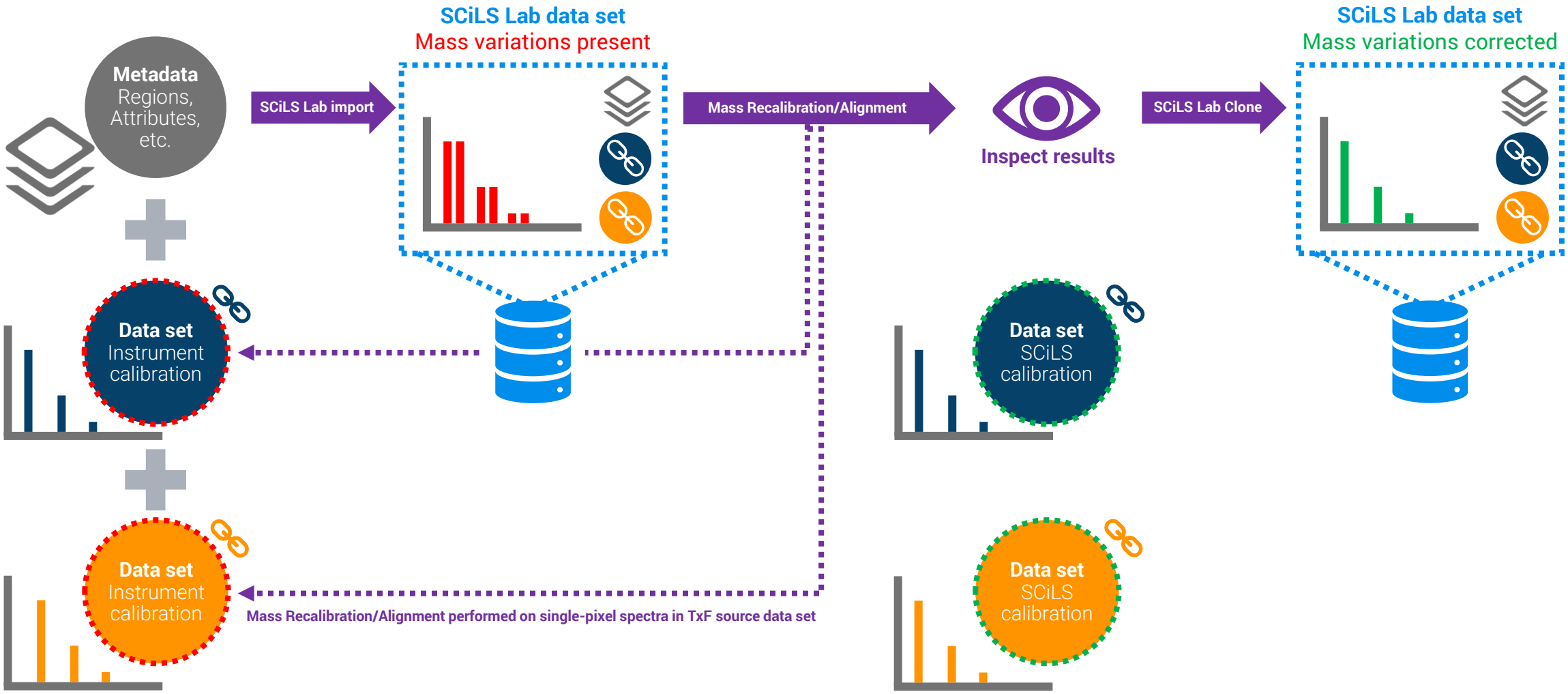
Mass Recalibration / Alignment

Workflow for SCiLS Lab files based on sources in TxF data format



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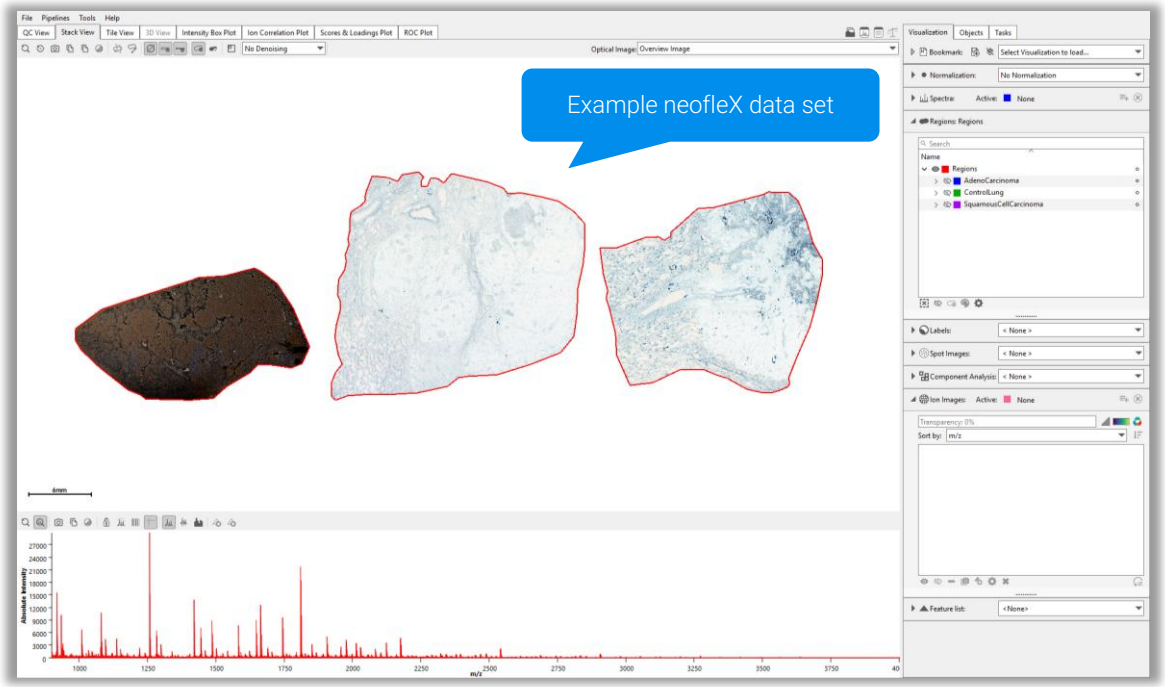
Mass Recalibration / Alignment

SCiLS Lab data sets based on TxF source data sets

- The **timsTOF fleX**, **neofleX** and **timsMRMS** platforms write data into the **TxF data format**. When a SCiLS Lab data set is based on TxF source data sets exclusively, the Mass Recalibration/Alignment workflow operates on the spectra in the source data sets
  - Recalibration/alignment results are stored with the source data and can be interpreted by other Bruker software solutions like Data Analysis and the TDF-SDK.
    - **NOTE:** The recalibration procedure does not alter the raw spectra. There is no need duplicate source data to revert the calibration results
  - When importing a recalibrated TxF source data set into a SCiLS Lab project, the recalibrated spectra will be imported by default
  - Using the SCiLS Clone&Refresh workflow, a SCiLS Lab data set can be cloned using any of the available calibrations in the TxF source data set (see **Updates to SCiLS Clone&Refresh**)



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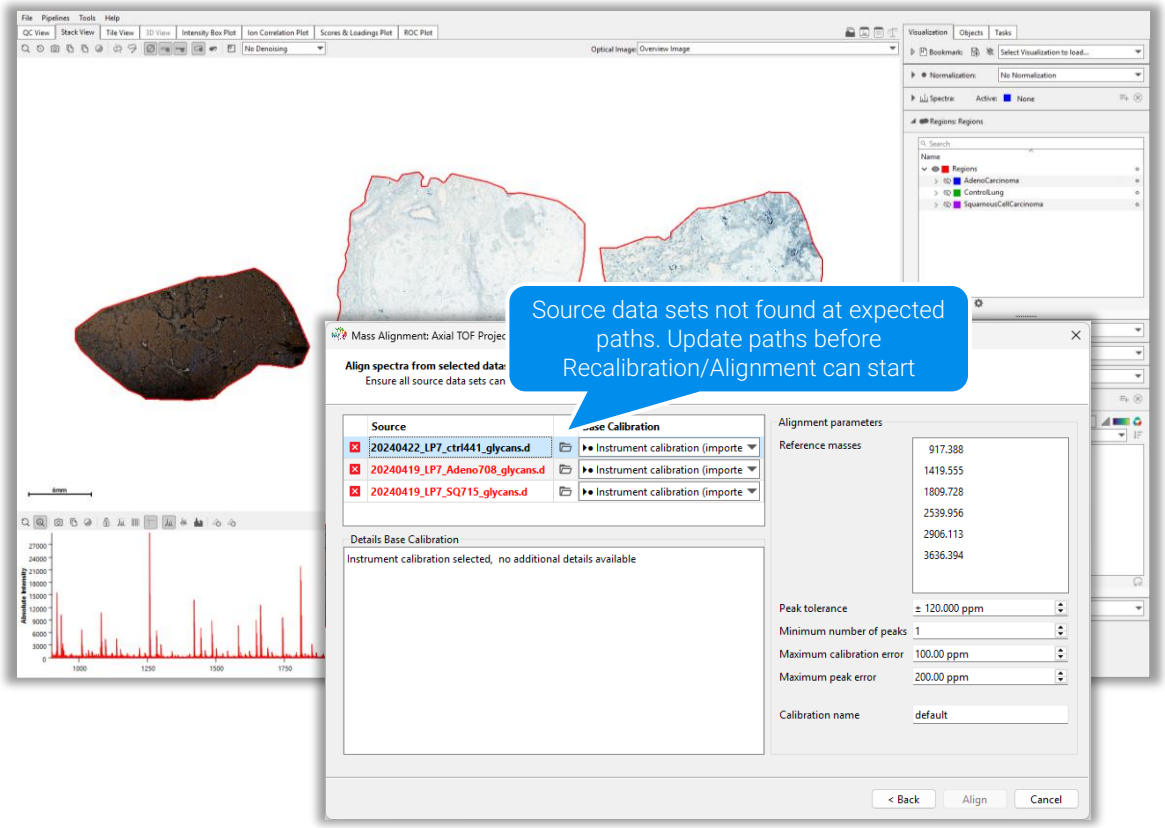
Mass Recalibration / Alignment

SCiLS Lab data sets based on TxF source data sets

- In order to recalibrate the TxF source data sets, SCiLS Lab needs to **link to the path** where the source data sets are stored
  - Updating the links to the source data paths can be achieved in the **Sources table on page 2 of Mass Recalibration/Alignment wizard**, or by navigating to the **Sources** section in the **Objects** tab before the Mass Recalibration/Alignment wizard is started



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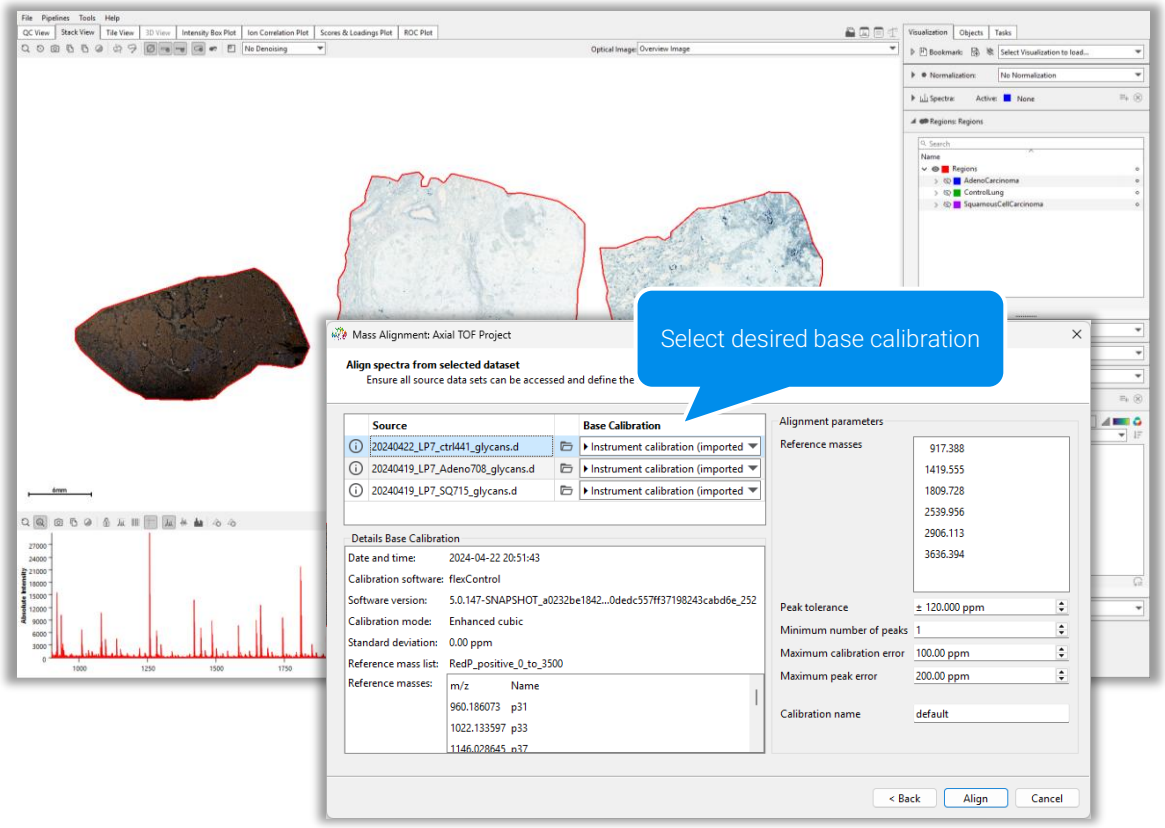
Mass Recalibration / Alignment

SCiLS Lab data sets based on TxF source data sets

- Before starting a new recalibration/alignment, a **base calibration** needs to be selected for each source
  - The base calibration is the set of **calibration coefficients to be corrected** in the upcoming recalibration/alignment procedure
  - The calibration used to import the source data set in the active SCiLS Lab file is selected as the default base calibration
- Use-case example
  - Online calibration is used to apply a lock mass calibration during MALDI Imaging acquisition. Upon loading data in SCiLS Lab the recalibration results appear unsatisfactory. A recalibration in SCiLS Lab can be performed to:
    - **Correct the lock mass calibration** results using the flexControl/timsControl recalibration as base calibration
    - **Perform a new recalibration** using the Instrument Calibration as base calibration.



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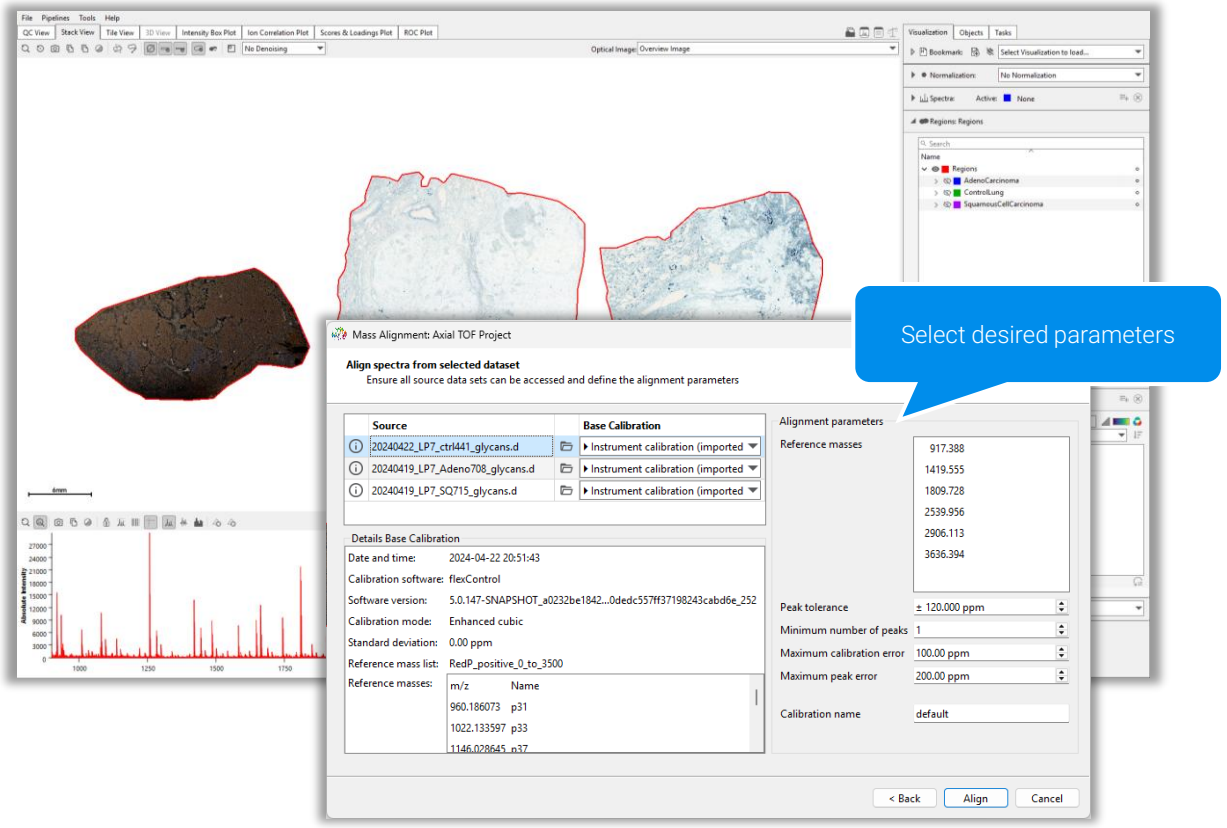
Mass Recalibration / Alignment

Setting the recalibration / alignment parameters

- Before starting the recalibration/ alignment, check the default parameters and adapt where needed
  - **Peak tolerance** – the maximum allowed distance between measured peak and reference mass
    - By default, equal to the default m/z interval width set in File Properties
  - **Minimum number of peaks** – the minimum number of measured peaks in a spectrum that needs to be assigned to a reference masses
  - **Maximum calibration error** – the maximum allowed root mean square error between measured peaks and corresponding reference masses in a spectrum after recalibration/alignment
  - **Maximum peak error** – the maximum allowed error between a single measured peak and its corresponding reference mass after recalibration/alignment



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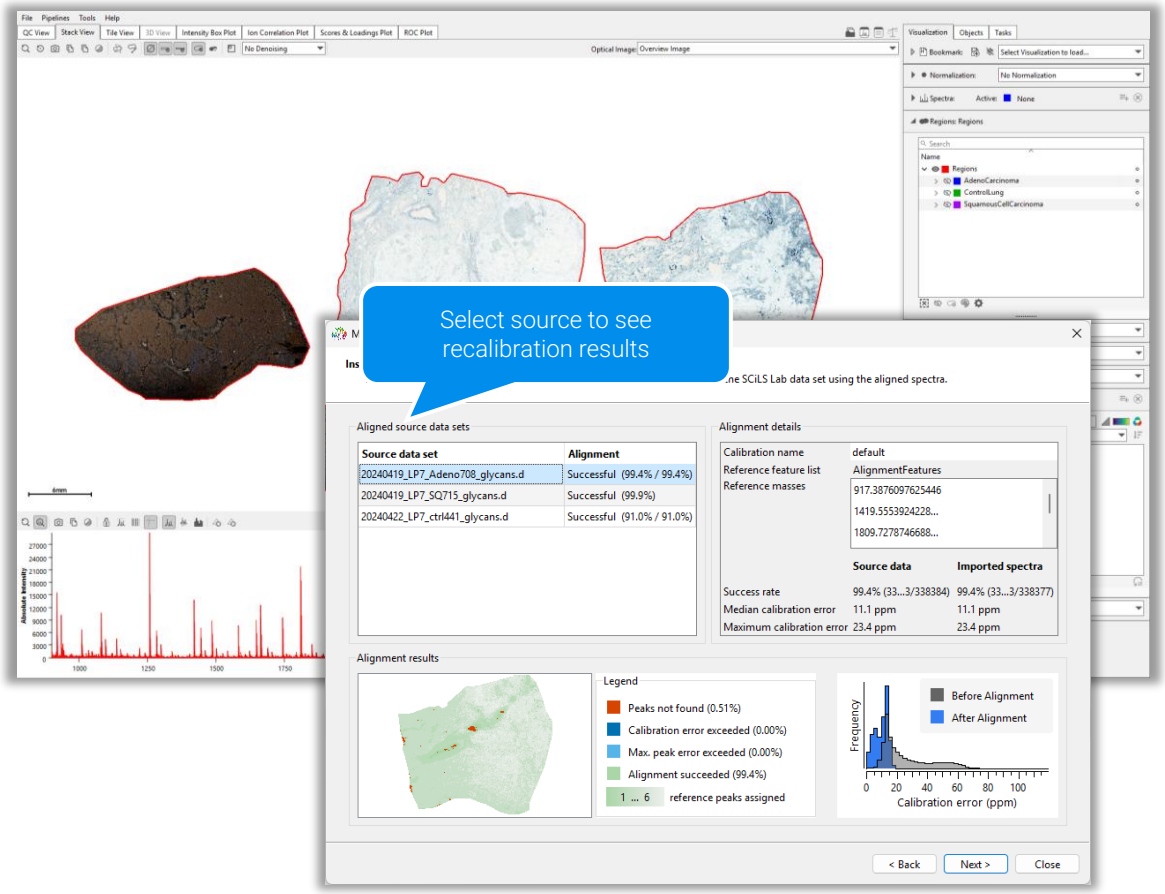
Mass Recalibration / Alignment

Review recalibration/alignment results before creating the clone

- After recalibration/alignment is done, the results are displayed on the **Recalibration/Alignment Results** page
  - Find out where:
    - **Recalibration/alignment succeeded** and how many reference masses were used to recalibrate/align the spectrum
    - **Recalibration/alignment failed** and why:
      - No peak(s) found in tolerance window(s)
      - Calibration error exceeded
      - Maximum peak error exceeded
    - **NOTE:** In case recalibration/alignment fails for a given spectrum, it inherits the calibration coefficients of the last successfully processed spectrum
  - Go back to the parameter page to discard the recalibration/alignment result, or close the wizard and keep/discard the recalibration/alignment result



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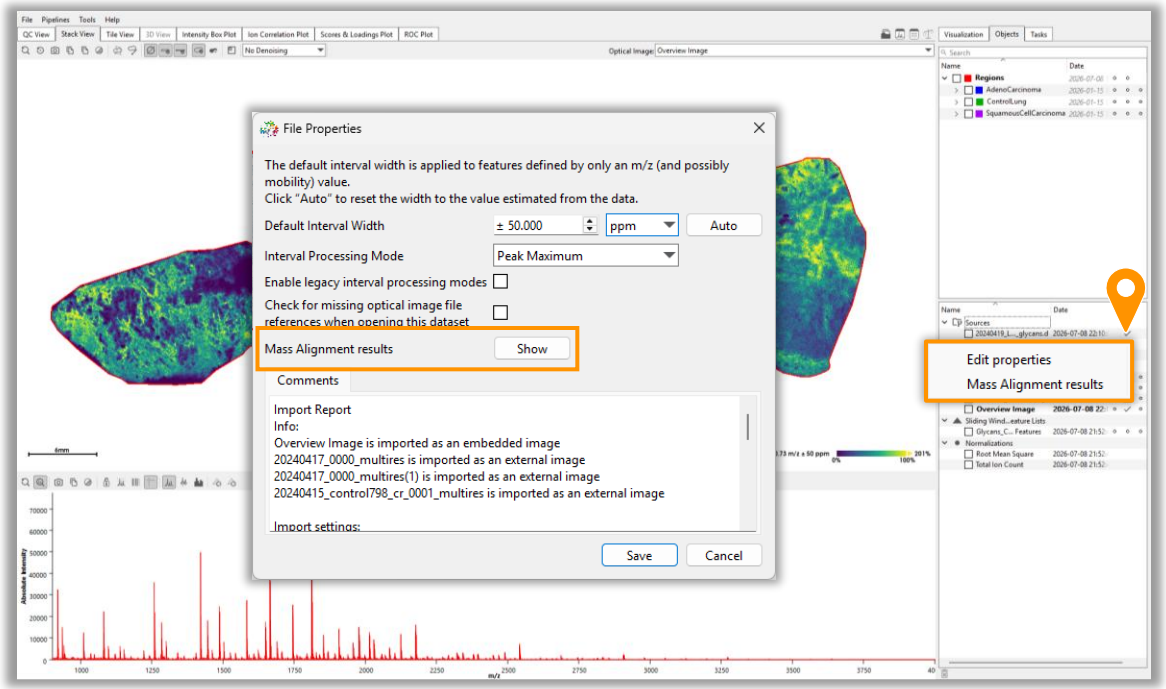
Mass Recalibration / Alignment

Creating a clone using recalibrated/aligned spectra

- The final step in the Mass Recalibration/Alignment wizard is creating a clone of the active SCiLS Lab file with a fresh import of the recalibrated spectra
  - When the data set is cloned using the Mass Recalibration/ Alignment wizard, the Recalibration/Alignment Results page can be recalled in the recalibrated clone through:
    - **File Properties > Mass Recalibration/Alignment results**
    - **Objects tab > Sources > Mass Recalibration/Alignment results**



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Mass Recalibration / Alignment

Workflow for SCiLS Lab files based on any other source data format

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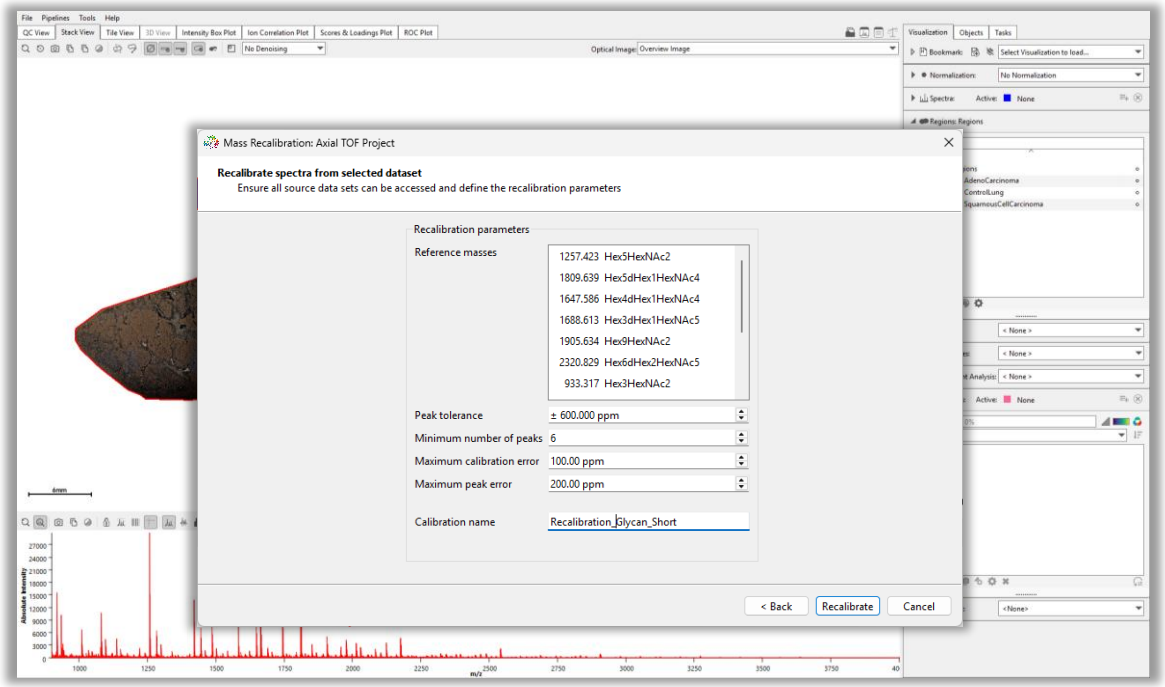
Mass Recalibration / Alignment

SCiLS Lab files not based TxF source data

- **Recalibrate/align any SCiLS Lab file**
  (e.g., rapifleX, solariX/scimaX, MVS data sets)
  - For any SCiLS Lab file, not based on TxF source data sets, recalibration/alignment is performed on spectra stored in the SCiLS Lab data set, not on the source data files
  - Calibration results cannot be interpreted by other Bruker software solutions
  - Recalibrated/aligned spectra can be exported from SCiLS Lab to CSV or imzML format (Bruker data only), or they can be accessed using the SCiLS API



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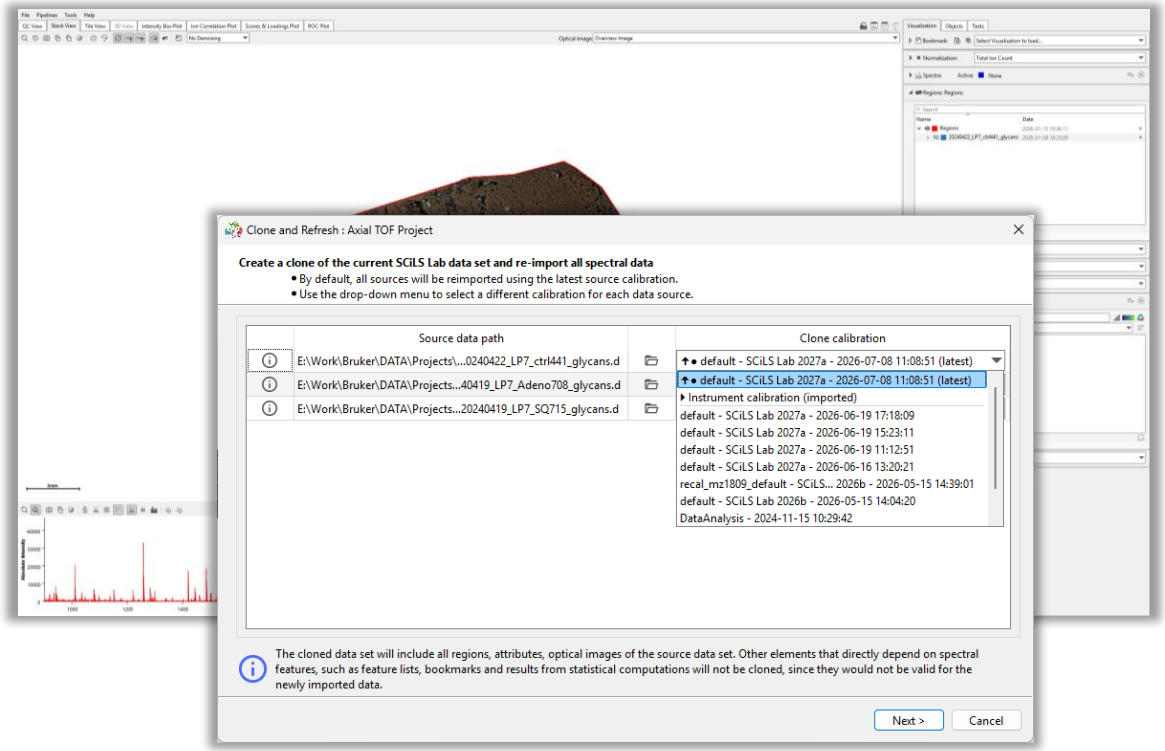
Mass Recalibration / Alignment

Updates to SCiLS Clone&Refresh

- **SCiLS Clone & Refresh** is an operation that creates a **copy of a data set** with a **fresh re-import of all spectra**
  - **File > Clone and Refresh**
  - Available for:
    - Bruker timsTOF fleX
      - TDF – TIMS-mode
      - TSF – QTOF-mode
    - Bruker neofleX
      - TSF (centroid and profile)
    - Bruker MRMS
      - TSF (centroid and profile)
      - peaks.sqlite
  - For data sets in **TxF format** it is now possible to select any of the available calibrations as Clone calibration



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04

timsMRMS compatibility

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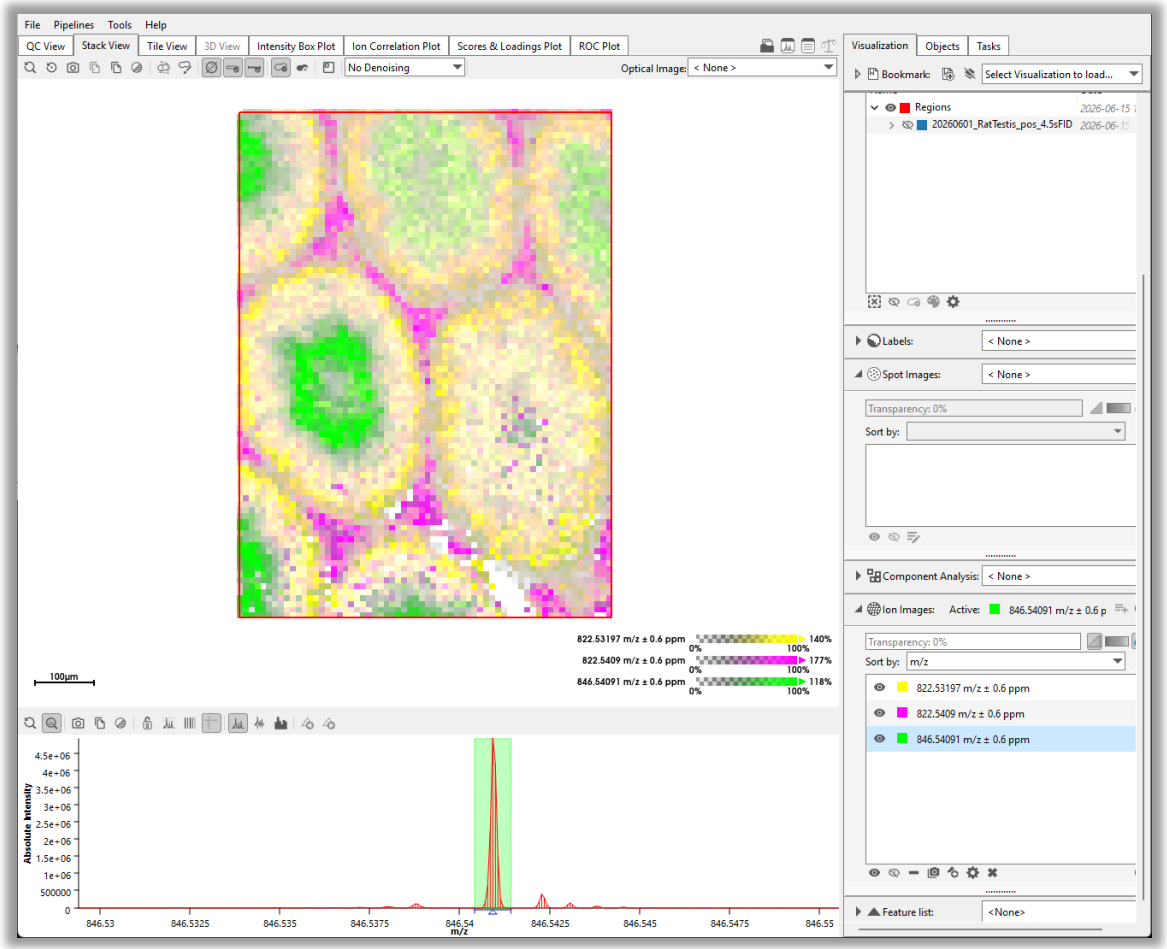
timsMRMS compatibility

Load, process and analyze timsMRMS data

- The all new **timsMRMS** instrument is capable of acquiring data at **both high spatial resolution** and **high mass resolution**, producing extremely rich data sets
  - timsMRMS writes **centroid and/or profile** data in the TSF data format



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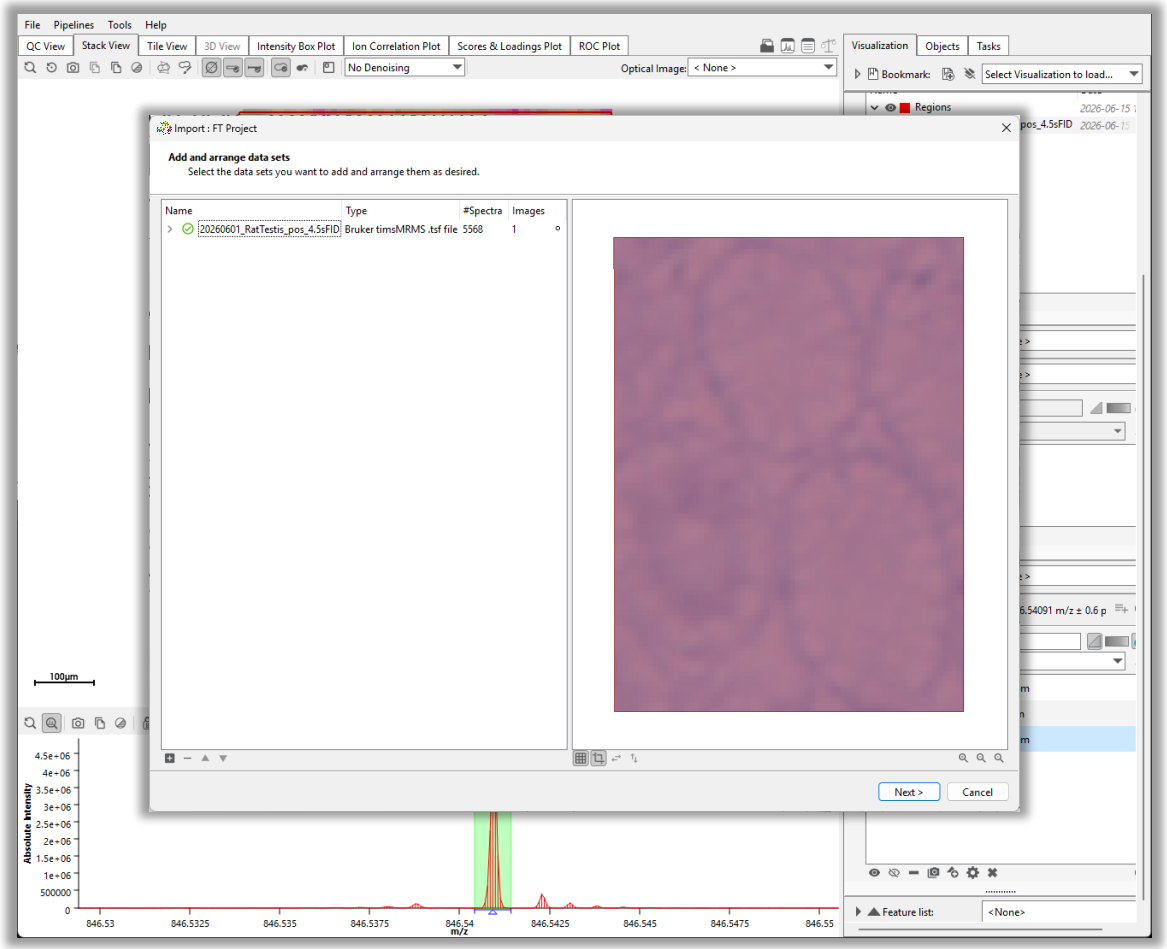

timsMRMS compatibility

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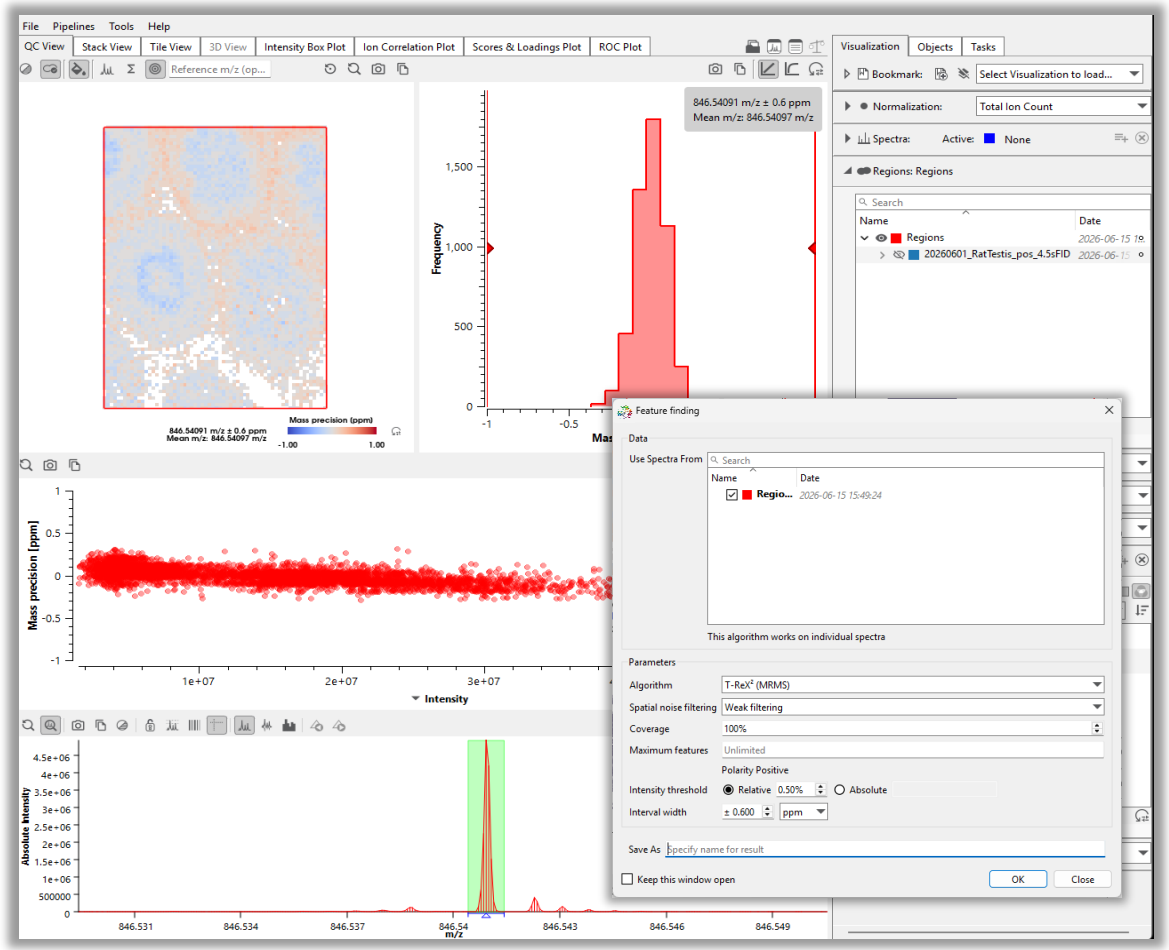
  - timsMRMS writes **centroid and/or profile** data in the TSF data format
  - **Import** timsMRMS centroid or profile data sets directly into SCiLS Lab
  - The all-new **QC View**, **Mass Recalibration/Alignment**, and **Mass Variations Statistics**, as well as **T-ReX² Feature Finding** and **Clone&Refresh** workflows are all available for timsMRMS data sets



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05

Multiple feature enhancements

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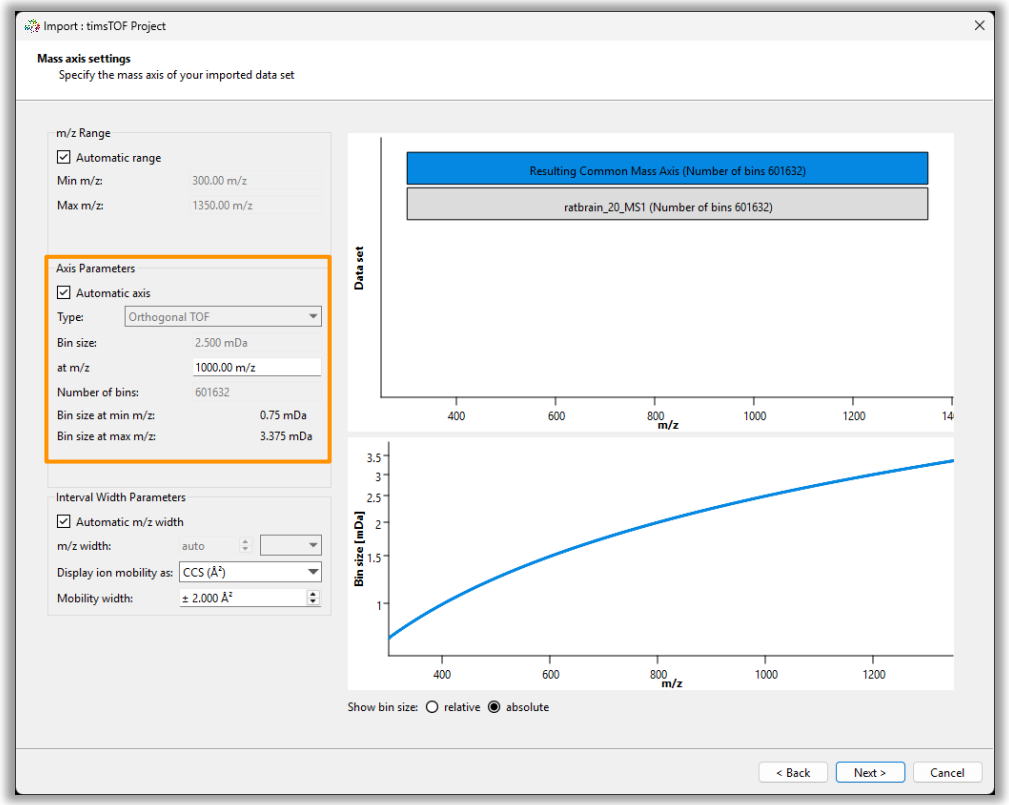
Multiple feature enhancements

Improved mass axis binning and interval width parameters

- The **mass axis settings page** and its underlying algorithms in the SCiLS Lab importer have been improved:
  - **Default bin size** for **timsTOF fleX** and **neofleX** data sets has been decreased to better reflect the mass resolution of the data acquired by the instrument
    - **NOTE:** expect longer import times (~30-50%) and increased .sbd file sizes (<5%)



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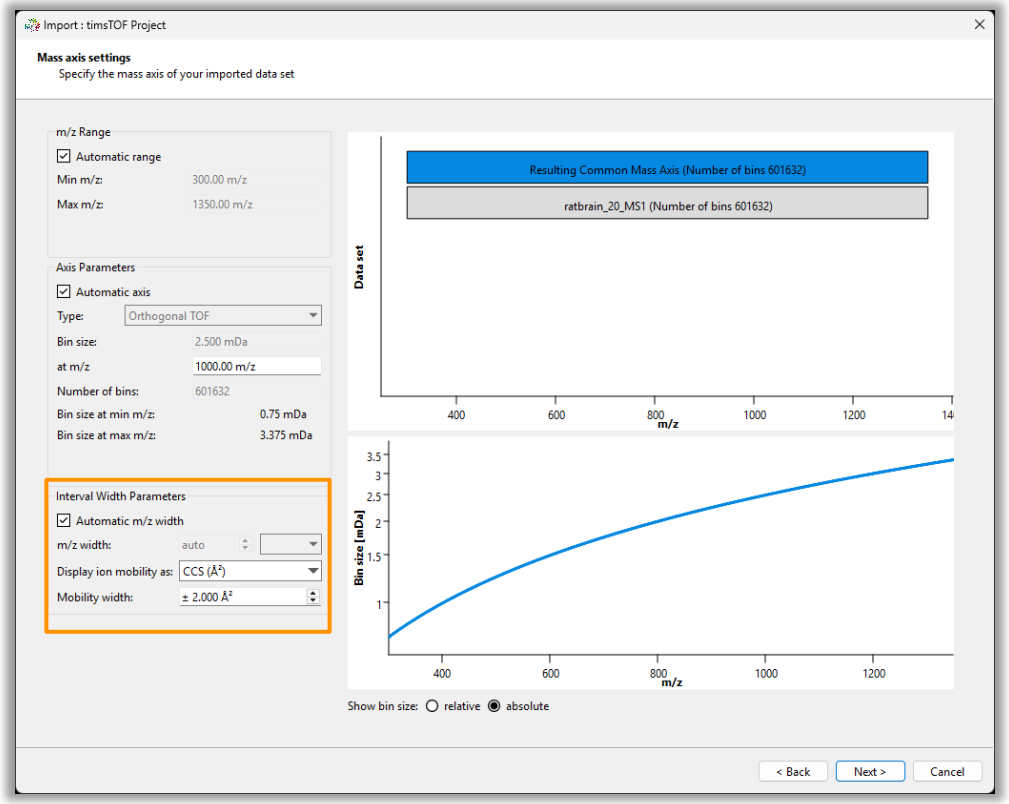
Multiple feature enhancements

Improved mass axis binning and interval width parameters

- The **mass axis settings page** and its underlying algorithms in the SCiLS Lab importer have been improved:
  - **Interval Width Parameters** have been moved to the mass axis settings page for all project types.
    - Consequently, they have been removed from the page to set up Feature Finding during import (for timsTOF, iprm-PASEF and MRMS projects)



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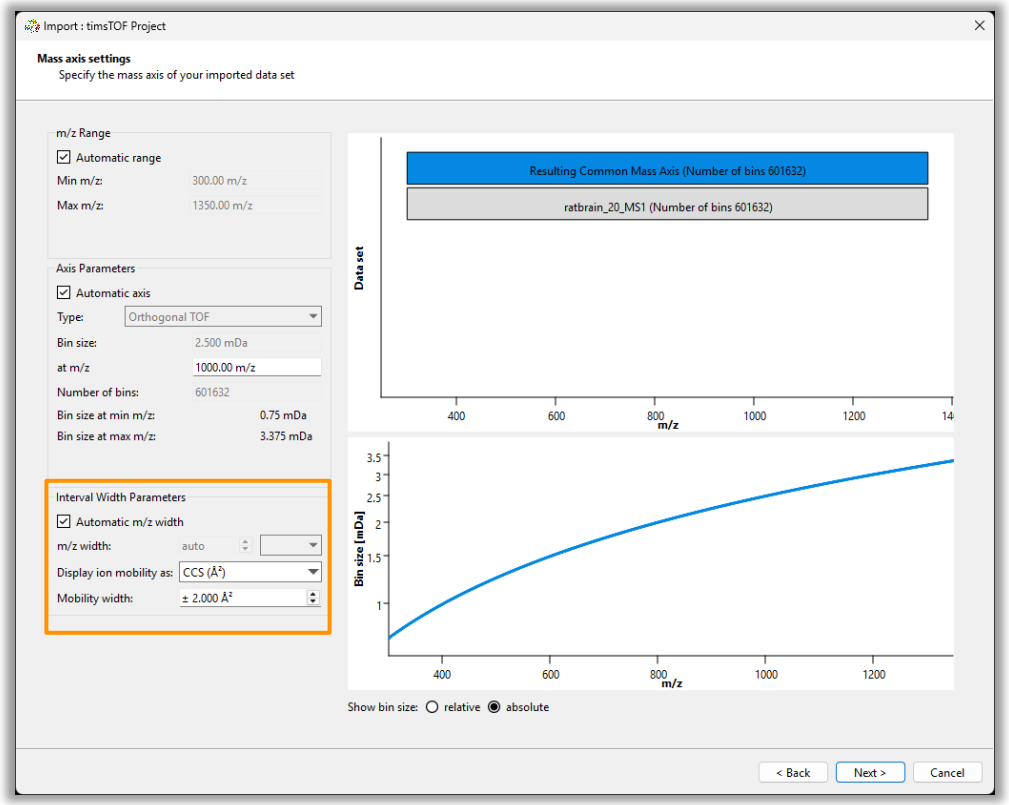
Multiple feature enhancements

Improved mass axis binning and interval width parameters

- The **mass axis settings page** and its underlying algorithms in the SCiLS Lab importer have been improved:
  - **Automatic m/z interval width**
    - Captures the full peak width
    - Returns a meaningful interval width
      - (e.g., ±15 ppm in stead of ±14,89 ppm)
    - **NOTE:** when using the "auto" setting, the default m/z interval width is calculated during the import procedure. The default settings can be changed in the File Properties (**File > File Properties**). Using the "Auto" button on the File Properties page will set the default m/z interval width to the value calculated during the original import of the SCiLS Lab file.



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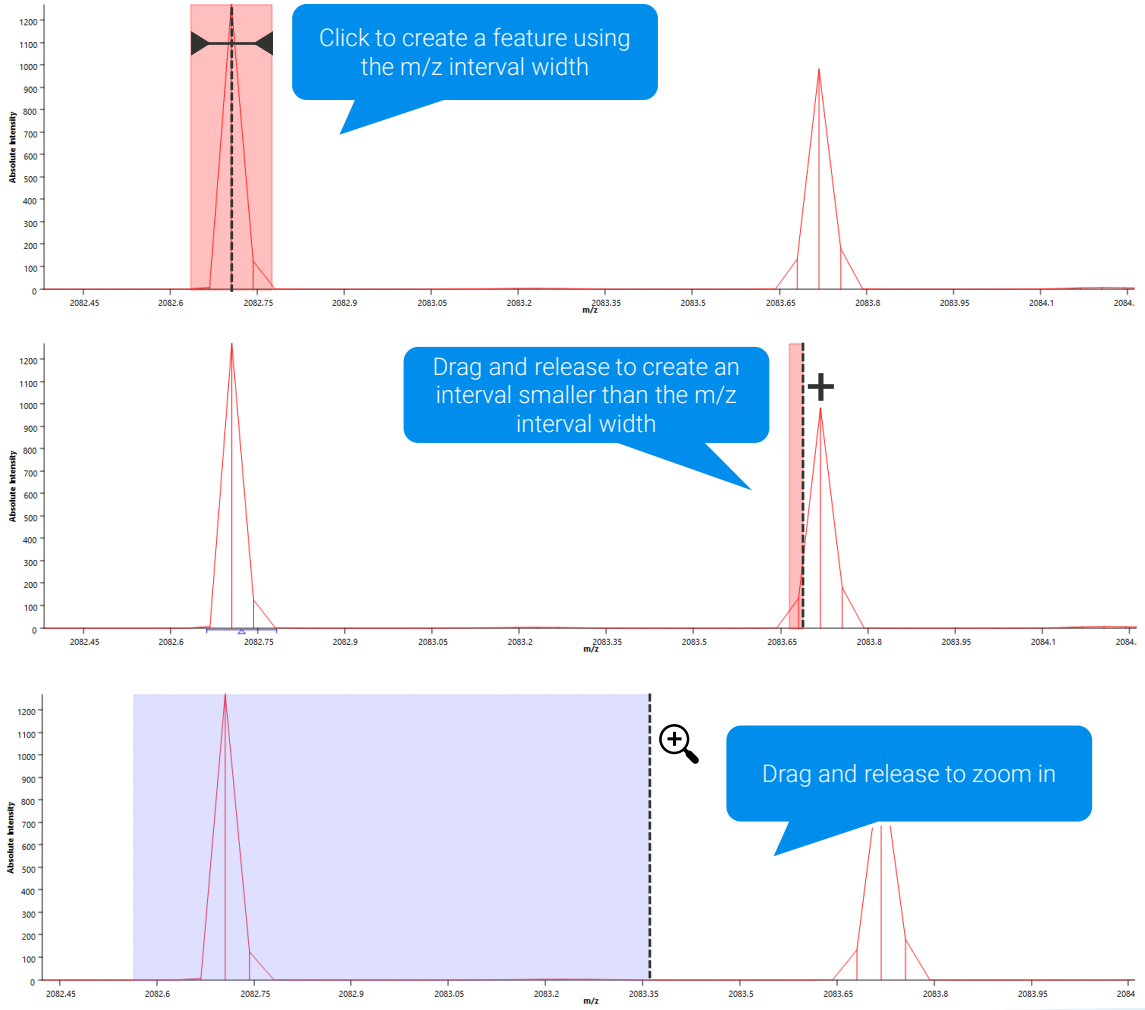
Multiple feature enhancements

Minimum m/z interval width has been removed from Spectrum View

- The **m/z interval width no longer acts as a minimum value for m/z interval selection** in the Spectrum View, making it more convenient to select m/z intervals smaller than the m/z interval width
  - **Click** in the spectrum plotter to select an interval using the m/z interval width
  - **Drag and release** to zoom-in or select an interval with any width



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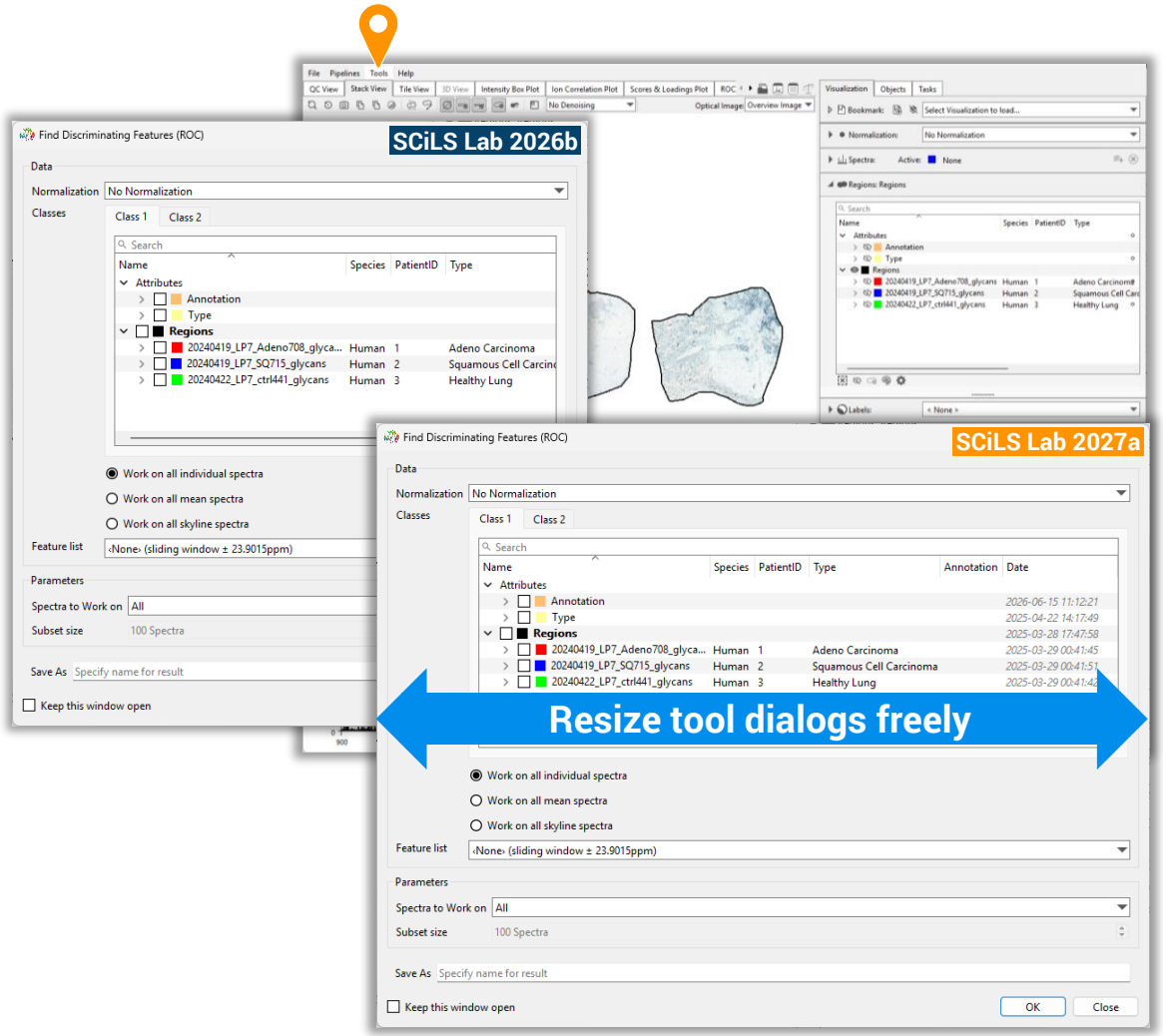
Multiple feature enhancements

Resizing Tool dialogs

- **Tool dialogs** now have an **unrestricted maximum width**, so that key information for Region selection can be made visible



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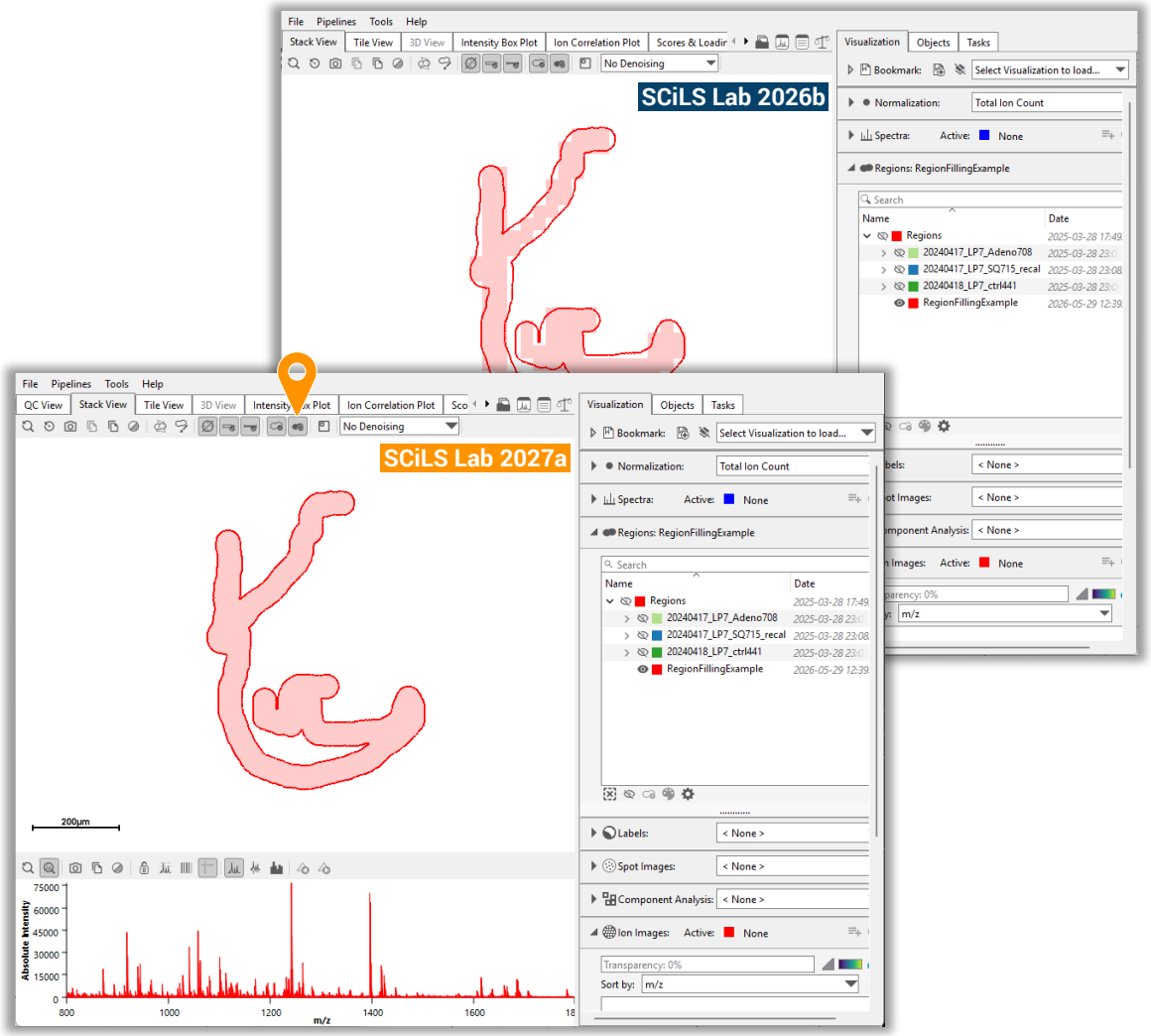
Multiple feature enhancements

Improved region filling in Stack View

- **Region filling** makes it easier to see exactly which pixels belong to a region especially for large, complex and/or overlapping regions
  - **Performance** and **aesthetics** have been improved



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Multiple feature enhancements

Compatibility notes

- **QuPathToSCiLS export plugin v1.5** is compatible with the latest **QuPath 0.7.0** version released last March.

- CCS-enabled MALDI Imaging data recorded using the **Enhanced Linear Mobility calibration** (available with timsControl 8.0/Compass timsTOF 2027) can now be processed by SCiLS Lab

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06

API improvements

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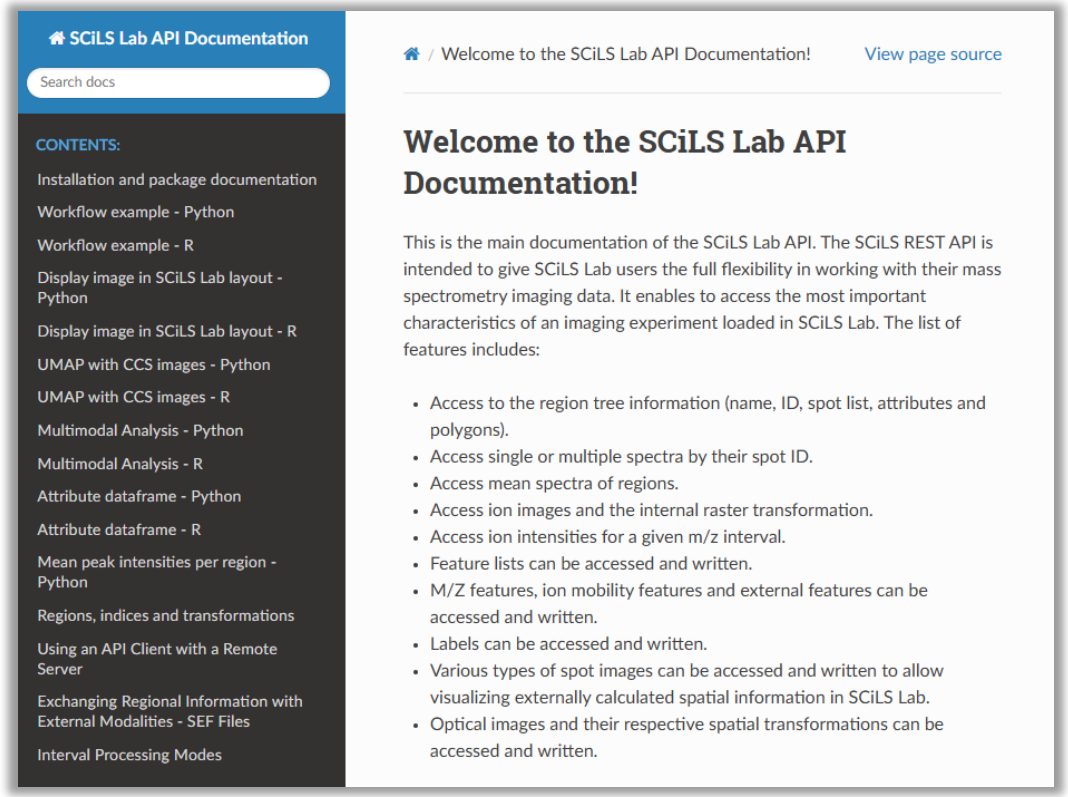
SCiLS™ API improvements

- SCiLS API maintenance
  - Updated R dependencies
  - Marked R 4.4 as deprecated
  - Marked Python 3.10 binary package as deprecated

- New SCiLS API functionalities
  - The **Region Variance** and the **Region Skyline spectrum** can now be retrieved with new function calls
    - Python:
      - `DatasetProxy.get_skyline_spectrum([region_id, normalization_id])`
      - `DatasetProxy.get_variance_spectrum([region_id, normalization_id])`
    - R:
      - `getSkylineSpectrum(con, regionId, normId = "")`
      - `getVarianceSpectrum(con, regionId, normId = "")`
  - Function calls that require a **Region identifier** *(see examples above)*
    - The fully qualified name of a region can now be used
    - The UUID of a region can still be used
    - Valid for both R and Python API



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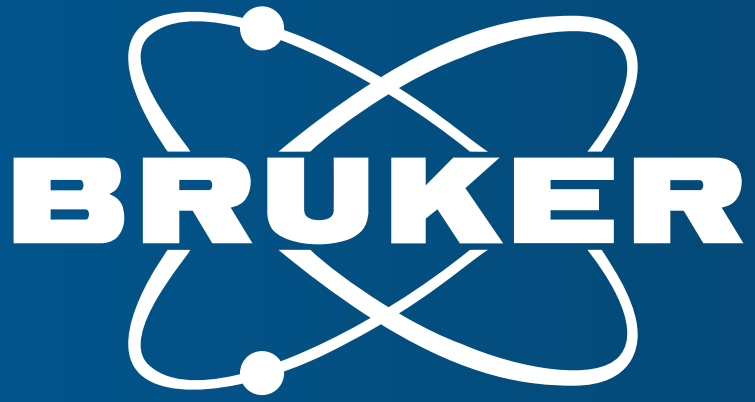

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