LIFE SCIENCE MASS SPECTROMETRY

SCiLS™ Lab 2025b – What's New?

© 2024 Bruker

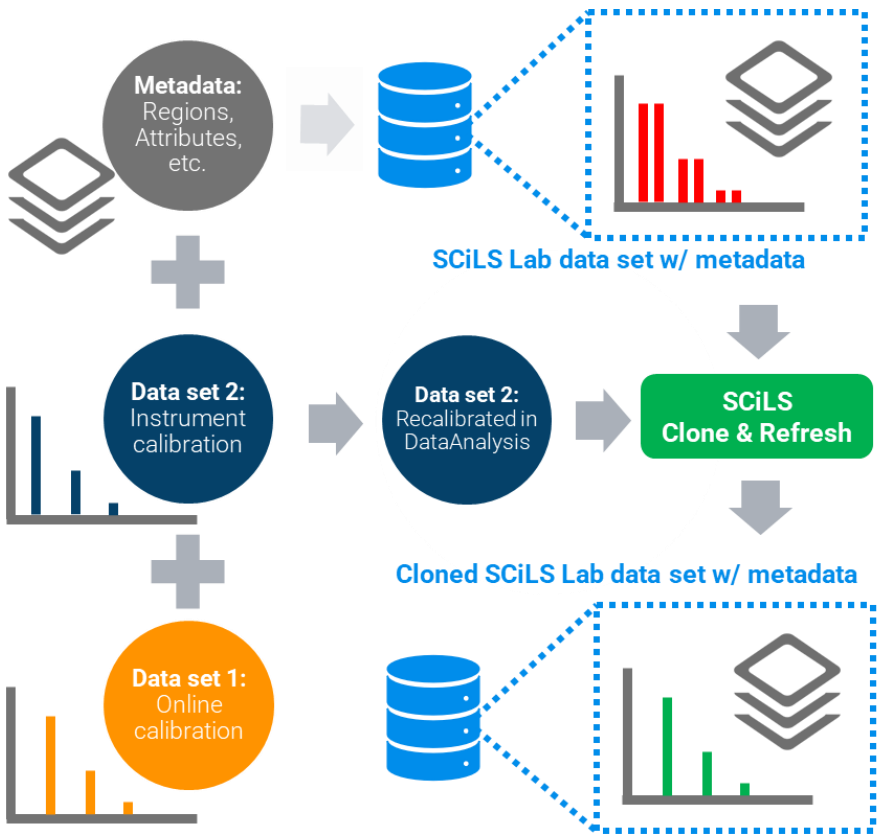
SCiLS™ Lab 2025b – What's New?

01 *Clone & Refresh:*
Recreate a data set with recalibrated data

02 *iprm-PASEF:*
Combining multiple iprm-PASEF data sets

03 *Multiple feature enhancements:*
Various improvements and changes

04 *Bug fixes:*



Available for customers since December 12, 2024

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

01

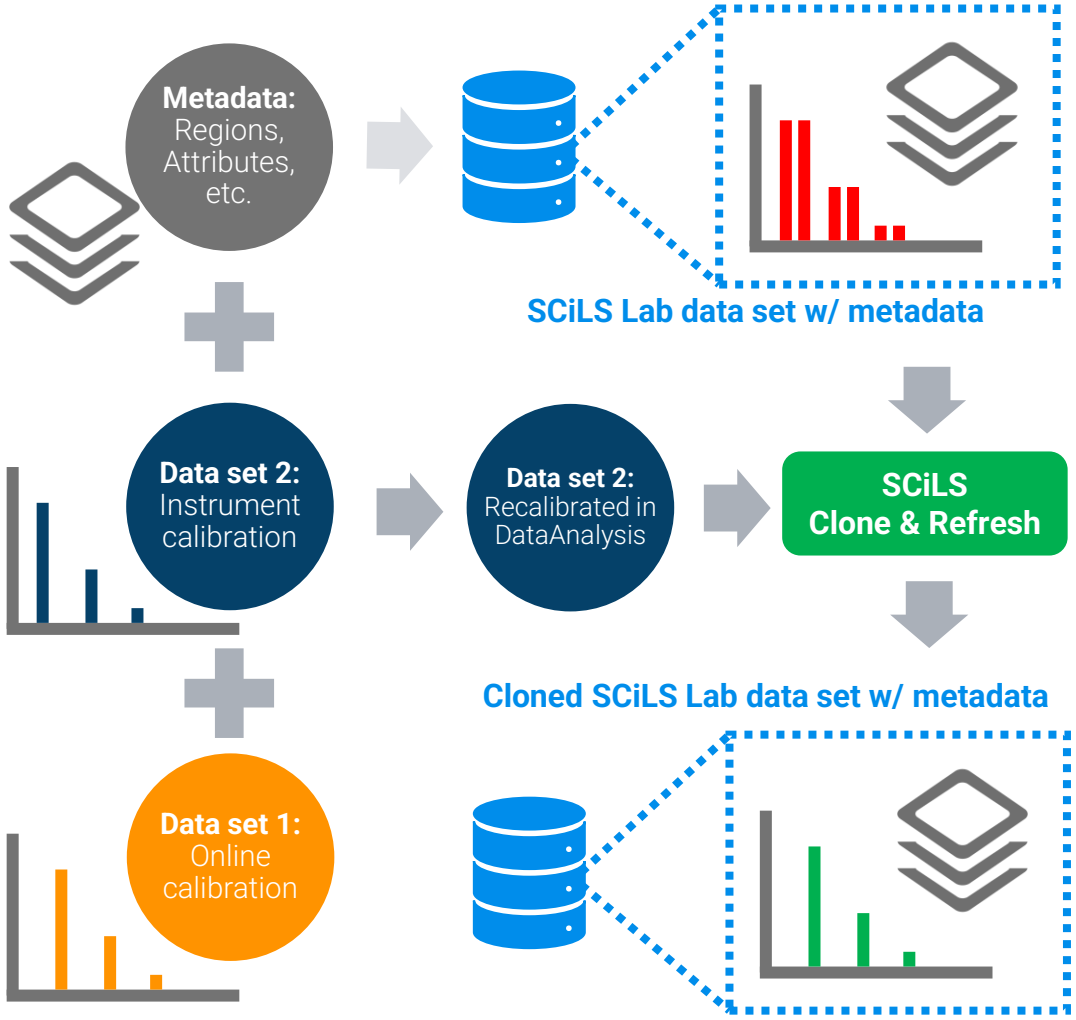
Clone & Refresh

© 2024 Bruker

For Research Use Only. Not for use in clinical diagnostic procedures.

SCiLS Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

- **Calibration errors** can severely hamper data analysis and molecular annotation
- Recreating a data set using recalibrated source data is time-consuming, mainly due to a **loss of metadata**
- SCiLS **Clone & Refresh** offers a new workflow to recreate an existing data set based on recalibrated source data and maintain (most) metadata
- **File > Clone & Refresh**
- **Centroid data** acquired with Bruker timsTOF fleX in both QTOF and TIMS mode, MRMS and neofleX instruments, as well as neofleX profile data are supported



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

SCiLS Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

- **Calibration errors** can severely hamper data analysis and molecular annotation
- Recreating a data set using recalibrated source data is time-consuming, mainly due to a **loss of metadata**
- SCiLS **Clone & Refresh** offers a new workflow to recreate an existing data set based on recalibrated source data and maintain (most) metadata
- ***File > Clone & Refresh***
- **Centroid data** acquired with Bruker timsTOF fleX in both QTOF and TIMS mode, MRMS and neofleX instruments, as well as neofleX profile data are supported

Metadata	Maintained after Clone & Refresh
Attributes	✓
External features	✓
iprm-PASEF isolation windows	✓
Labels	✓
Layout	✓
Optical images	✓
Regions	✓
Spot images	✓
Bookmarks	✗
CCS features	✗
Classification results	✗
Component analysis results	✗
Custom normalizations	✗
Hypothesis test results	✗
m/z features	✗
Segmentation results	✗

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

SCiLS Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Recreate SCiLS Lab data set after recalibration of source data

Use case:
A mass calibration error becomes apparent in a SCiLS Lab data set after spending substantial effort in adding metadata to the data set, for example, by importing optical images, drawing regions of interest, and grouping these regions using region attributes.

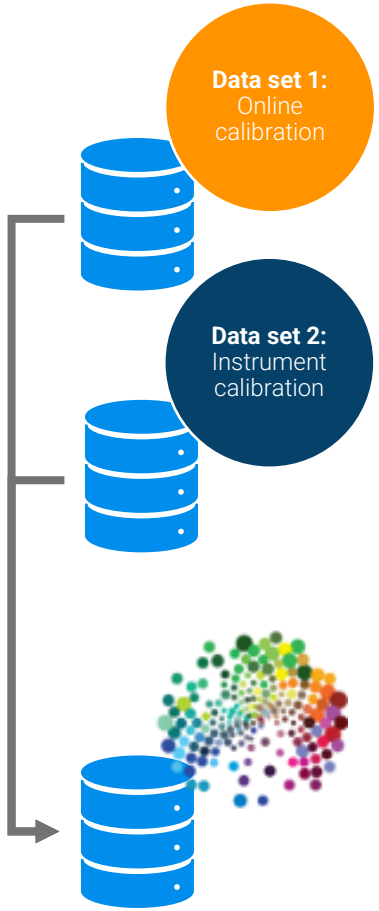
Current work-around:
Perform a mass recalibration in Data Analysis, and create a fresh SCiLS Lab import using the recalibrated source data set. Import the optical images in the new SCiLS Lab data set, and import the regions of interest using the .sef file format. All region attributes have to be recreated manually.

SCiLS Clone & Refresh:
Perform a mass recalibration in Data Analysis, and use SCILS Clone & Refresh to create a clone of the original SCiLS Lab file with a fresh re-import of all spectral data. Note that there will be no need to re-import optical images, and regions, and re-create region attributes, as these have been cloned from the original data set.

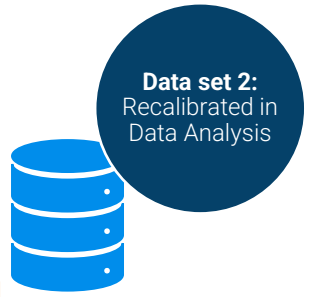
© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

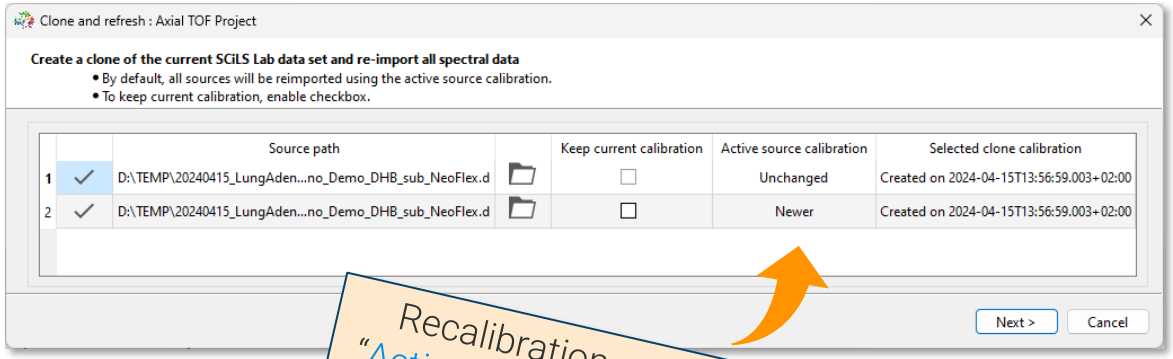
Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Recreate SCiLS Lab data set after recalibration of source data

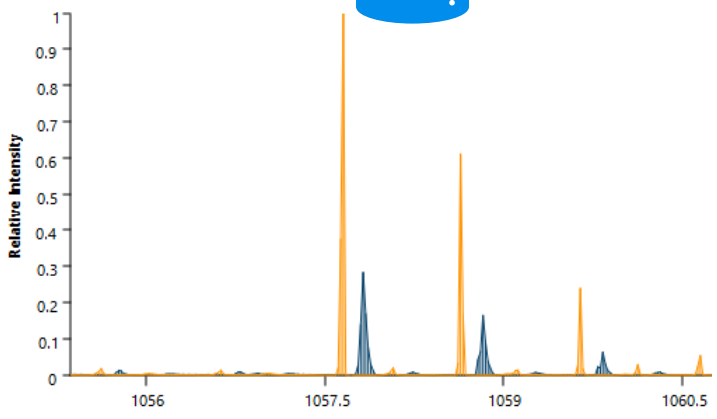


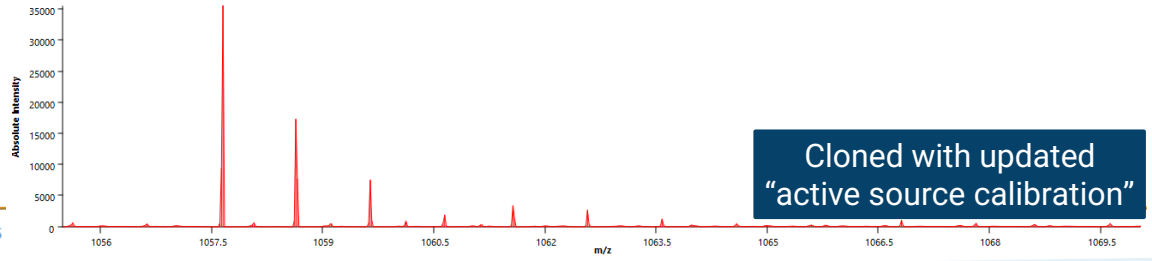
Recalibration of single spectra in Data Analysis





Recalibration updates "Active source calibration"



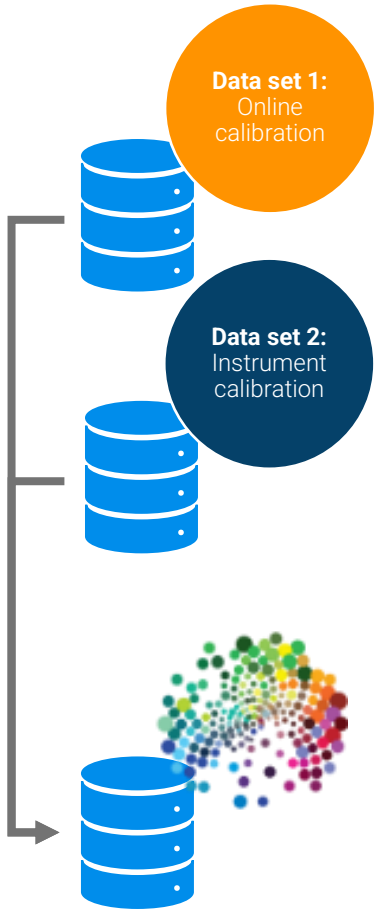


Cloned with updated "active source calibration"

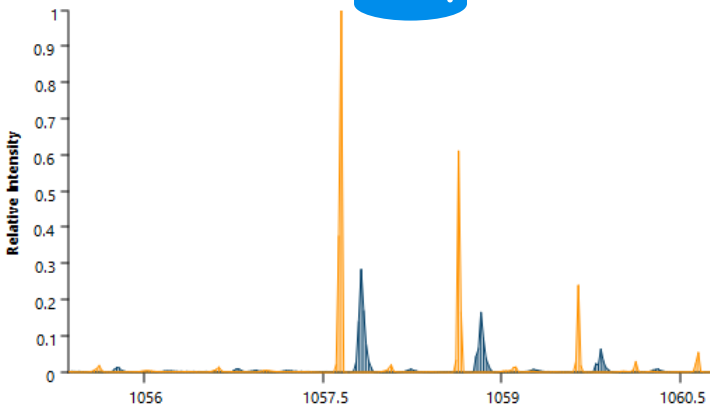
© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

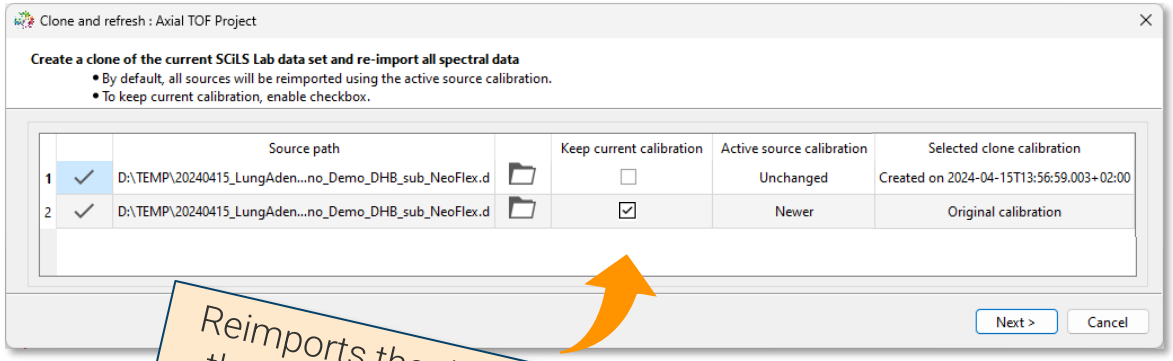
Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Recreate SCiLS Lab data set after recalibration of source data

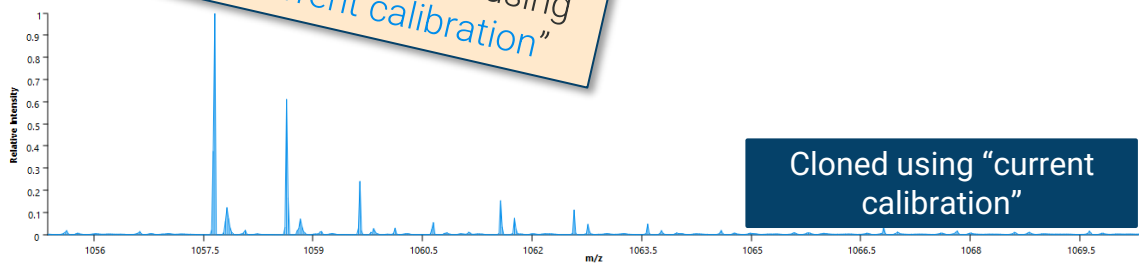


Recalibration of single spectra in Data Analysis

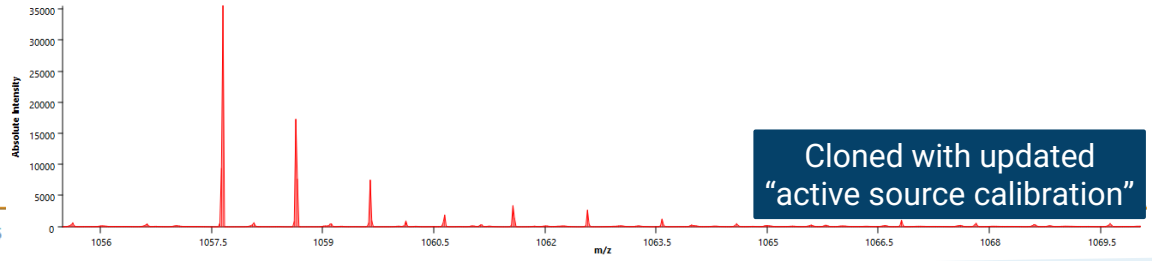




Reimports the data using the "current calibration"



Cloned using "current calibration"



Cloned with updated "active source calibration"

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

SCiLS Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Reprocess mass axis of a SCiLS Lab data set

Use case:
A SCiLS Lab data set has been created using the default m/z range and mass axis parameters, and substantial effort has been put in adding metadata. Later, the default parameters used during import turn out to be undesirable (e.g., m/z range too wide, mass axis binning too wide).

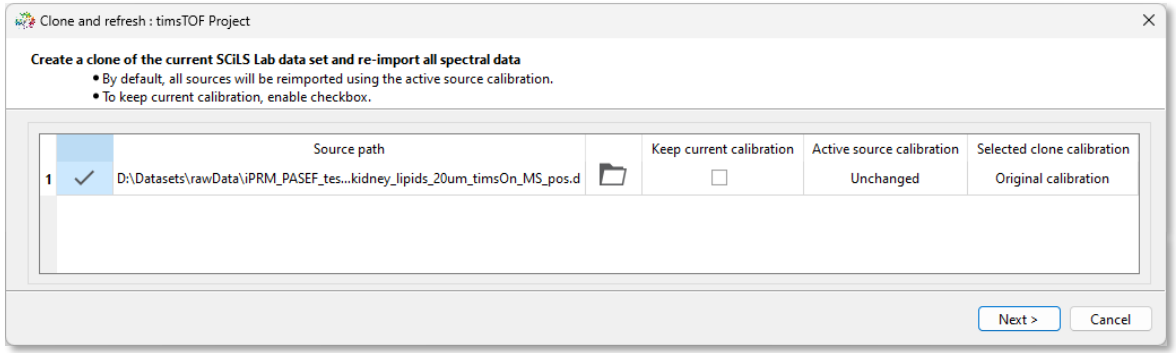
Current work-around:
Either create a new SCiLS Lab data set by re-importing the source data, or importing the .slx file, and subsequently re-import and recreate the metadata.

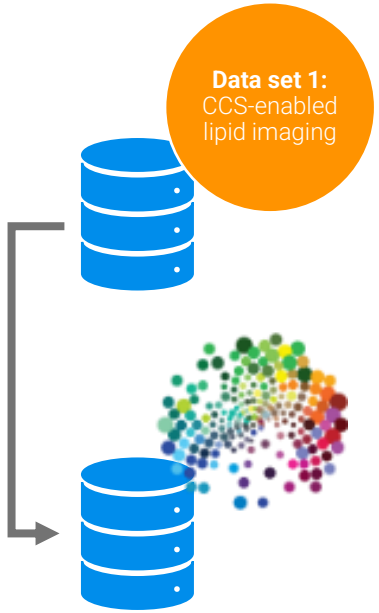
SCiLS Clone & Refresh:
Create a clone of the original SCiLS Lab data set, and adjust the m/z range and mass axis parameters to desired values. Note that there will be no need to recreate or re-import the metadata.

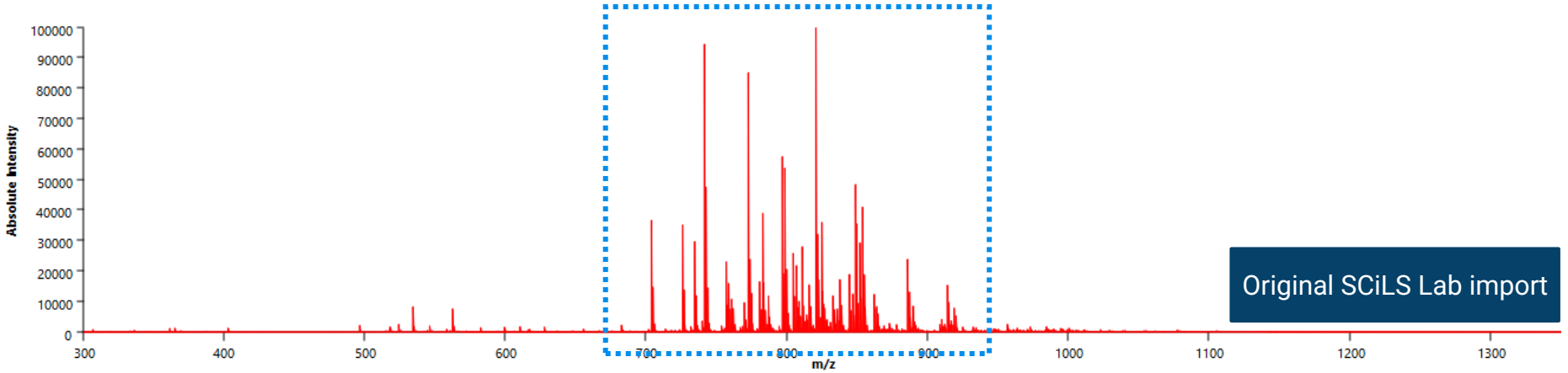
© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Reprocess mass axis of a SCiLS Lab data set



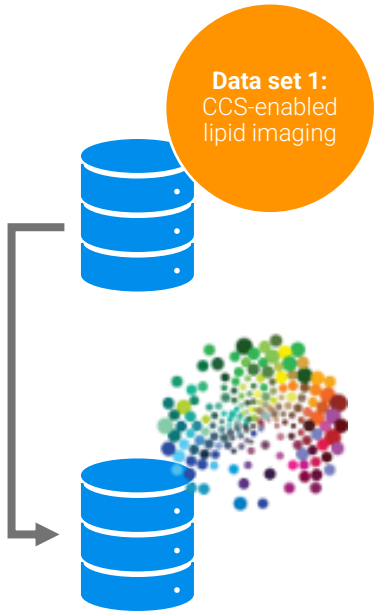


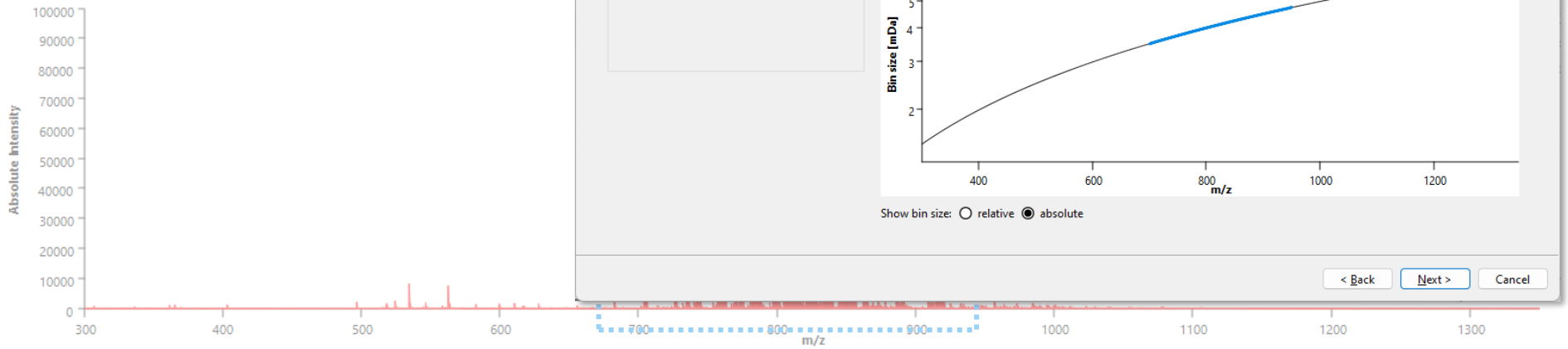


© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Reprocess mass axis of a SCiLS Lab data set

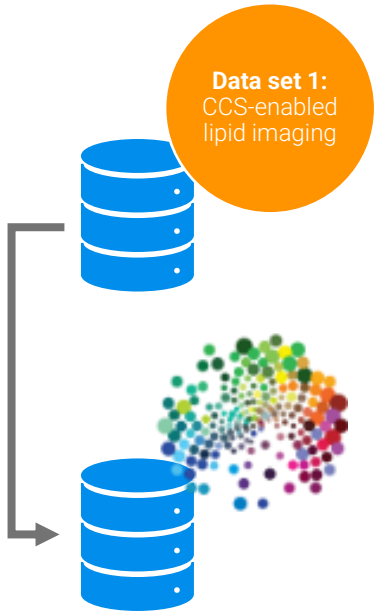


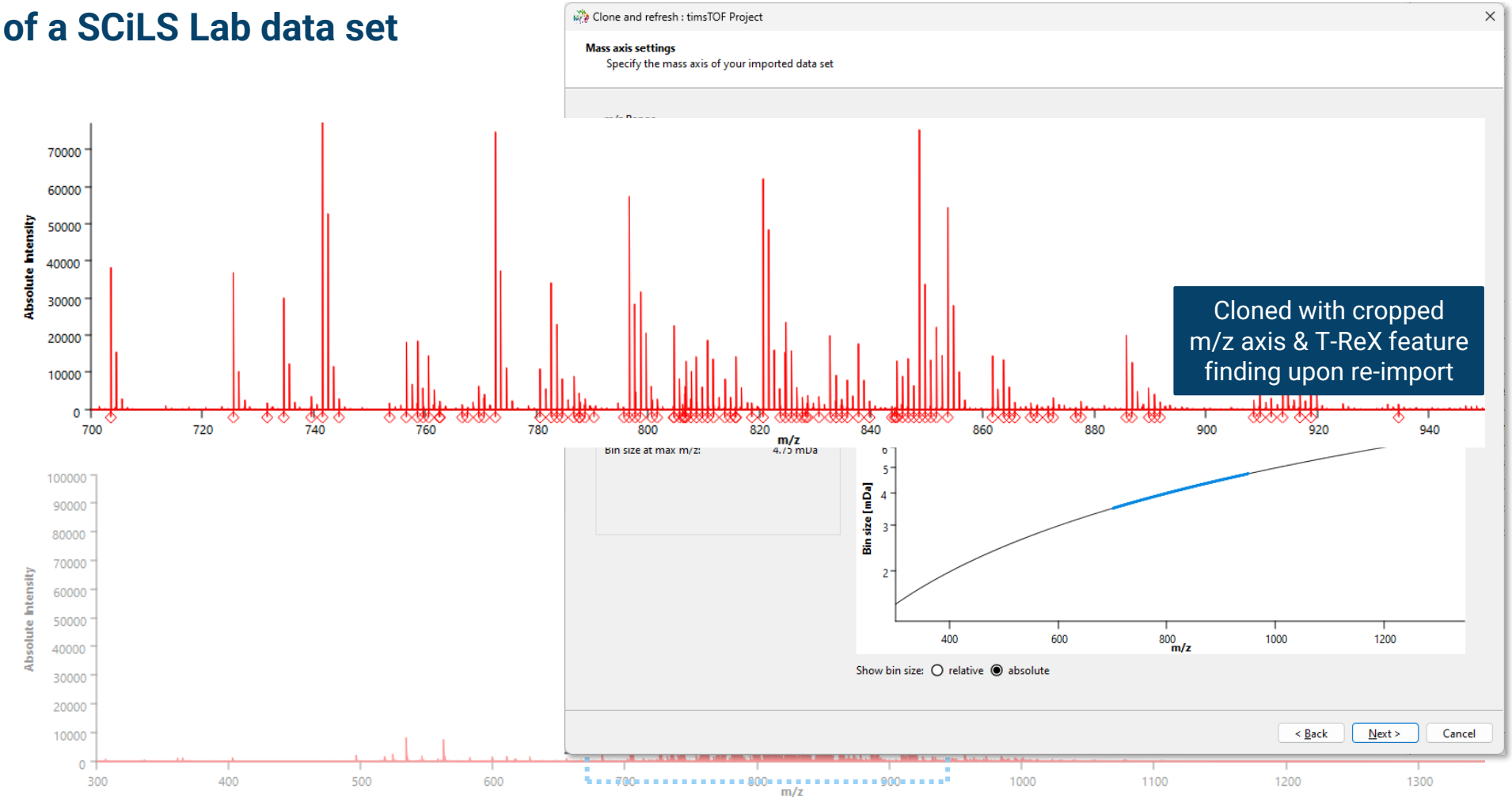


© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Clone & Refresh:
A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

Reprocess mass axis of a SCiLS Lab data set





© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

02

iprm-PASEF

© 2024 Bruker

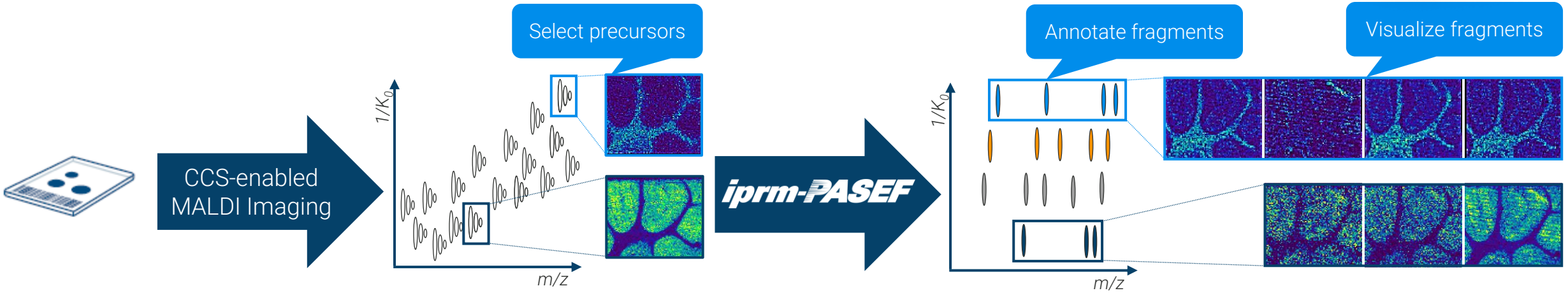
For Research Use Only. Not for use in clinical diagnostic procedures.

iprm-PASEF
A reminder…

timsTOF fleX-based targeted fragmentation with spatial fidelity

- Targeted and CCS-enabled precursor isolation and fragmentation with spatial fidelity for up to 25 precursors in a single acquisition

- The first **fully integrated** commercial imaging solution for fragmentation-based Molecular Annotation – **Acquire, Analyze, Annotate**

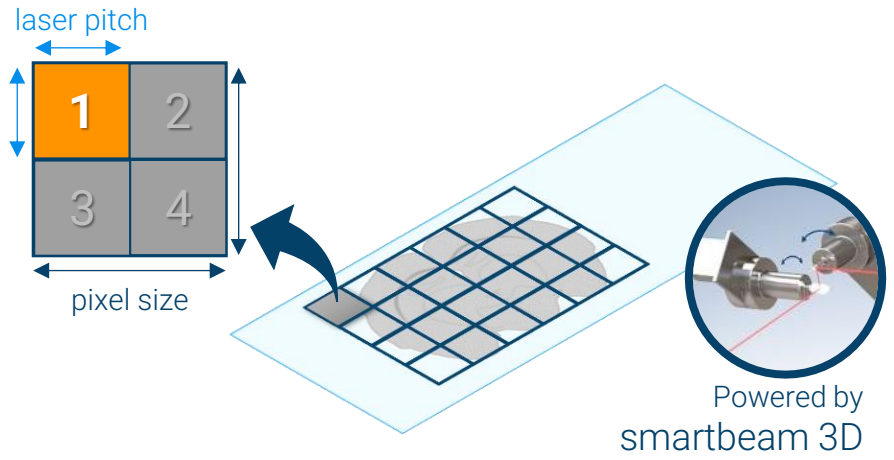


© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

iprm-PASEF
A reminder…

- Use the smartbeam 3D laser to generate complementary iprm-PASEF data sets from a single tissue.

- For example:
  - Multiple precursor lists with complementary precursors
  - The same precursor list analyzed with different collision energy regimes
  - The same precursor list analyzed with different m/z isolation widths



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

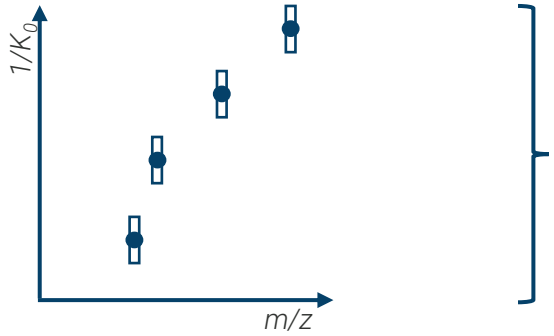
iprm-PASEF®
Combining multiple iprm-PASEF data sets in SCiLS™ Lab

- **Combine iprm-PASEF data sets** based on the **same precursor list** into a single SCiLS Lab data set.

- When the precursor list is identical between multiple iprm-PASEF data sets, one can combine data sets obtained…
  - from different measurement regions
  - using different m/z isolation widths
  - using different collision energy settings

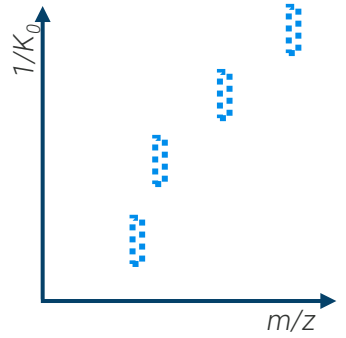
NOTE: Precursor lists are considered identical when they are consistent with respect to m/z windows, and have the same mobility windows up to calibration tolerance

CCS-enabled MALDI Imaging

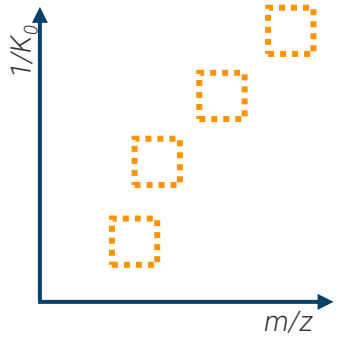


Precursor list 1

m/z centroid	1/K0 begin	1/K0 end
Precursor 1	…	…
Precursor 2	…	…
Precursor 3	…	…
Precursor 4	…	…



iprm-PASEF data set 1:
Precursor list 1
Isolation width: 1 m/z
Collision energy: high



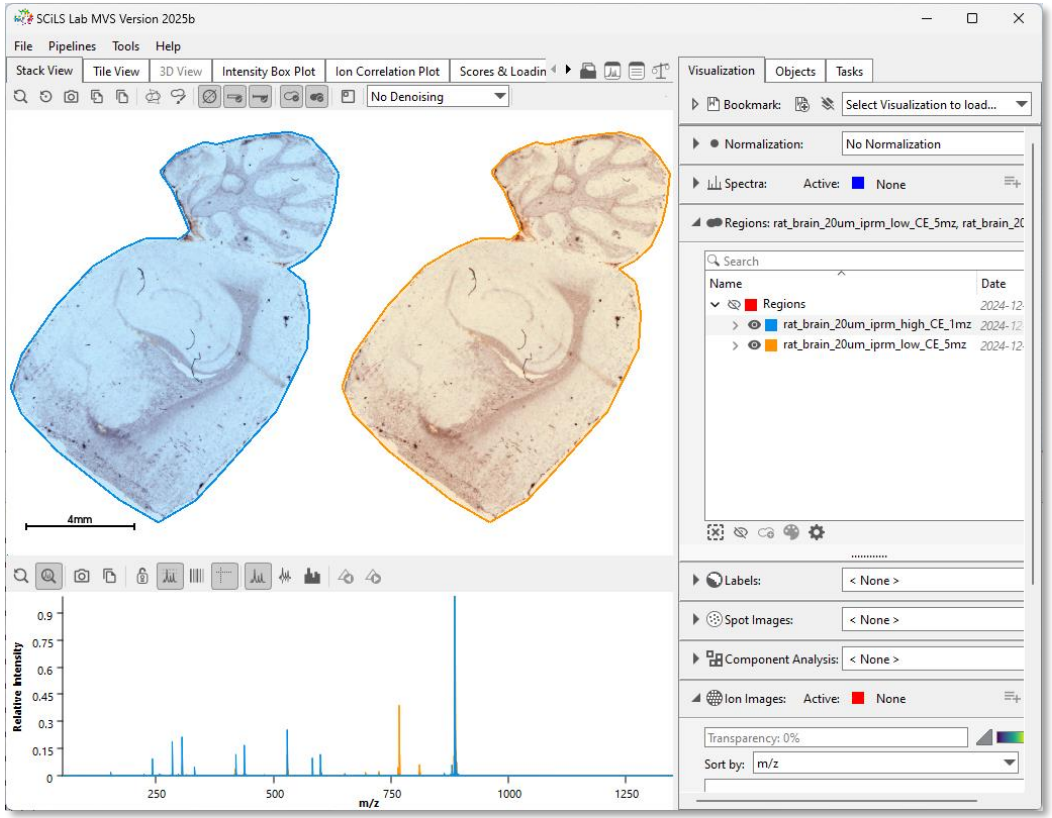
iprm-PASEF data set 2:
Precursor list 1
Isolation width: 5 m/z
Collision energy: low

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

iprm-PASEF®
Combining multiple iprm-PASEF data sets in SCiLS™ Lab

- **Combine iprm-PASEF data sets** based on the **same precursor list** into a single SCiLS Lab data set.

- When the precursor list is identical between multiple iprm-PASEF data sets, one can combine data sets obtained…
  - from different measurement regions
  - using different m/z isolation widths
  - using different collision energy settings



iprm-PASEF data set 1:
Precursor list 1
Isolation width: 1 m/z
Collision energy: high

iprm-PASEF data set 2:
Precursor list 1
Isolation width: 5 m/z
Collision energy: low

NOTE: Precursor lists are considered identical when they are consistent with respect to m/z windows, and have the same mobility windows up to calibration tolerance

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

03
Multiple feature enhancements

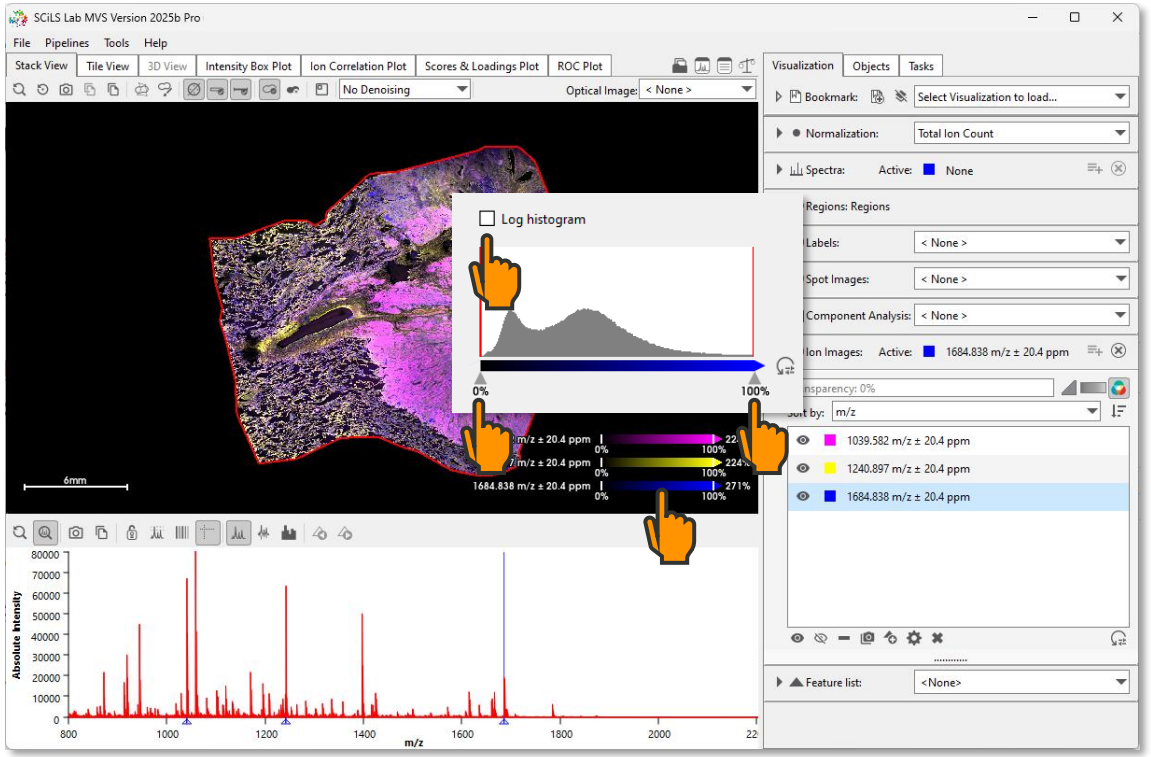
© 2024 Bruker

For Research Use Only. Not for use in clinical diagnostic procedures.

Ion image colorbar adjustment

Feature intensity-guided colorbar adjustment for ion images

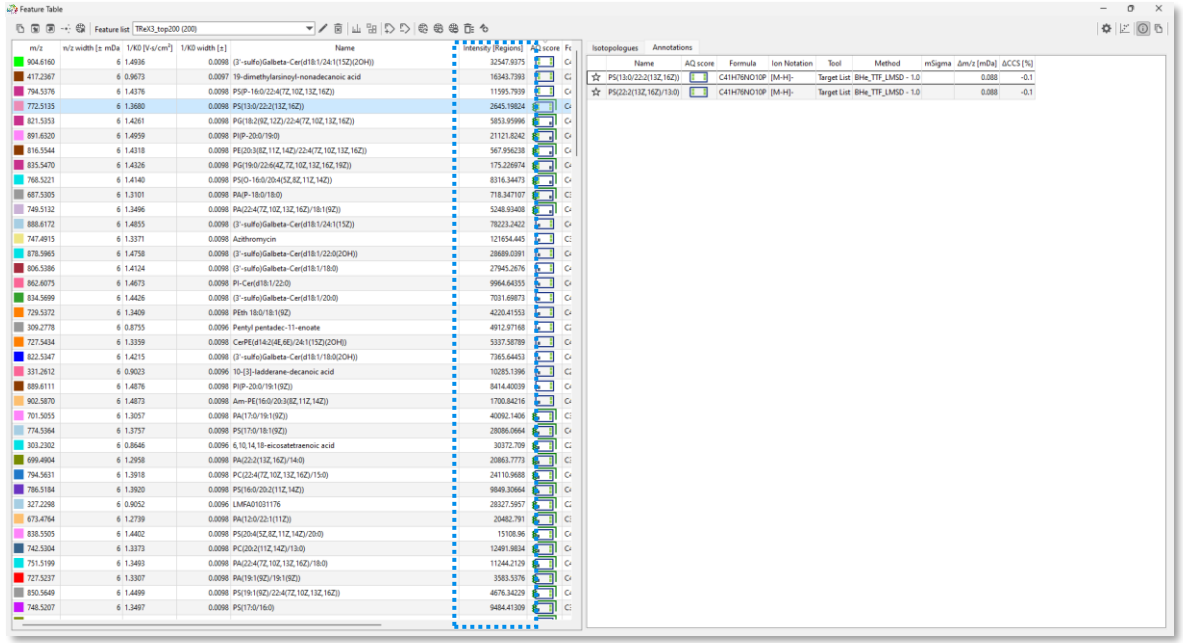
- **Adjust the colorbar using the intensity histogram** of a feature in Stack View, Tile View and 3D View
- **Click on the colorbar** to display the intensity histogram of its feature
- **Adjust the slider positions** to update the colorbar
- **Double-click and type new values** to update values
- Display **log-scaled histogram values**
- Click on another colorbar to open its histogram
- Click and drag to move the histogram dialog
- Click outside the histogram dialog to close



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Multiple feature enhancements
Feature Table – Intensity [Regions] column

- The Feature Table includes the default **"Intensity [Regions]"** column which always displays the **non-normalized average root region ("Regions") intensity**
- For mass-mobility features these intensities are only available after extracting the CCS ion images
- The "Intensity [Regions]" column cannot be deleted, but can be hidden from the Feature Table
- Automatically computed for Legacy data sets and External feature added through Ion Image Mapper or the SCiLS API



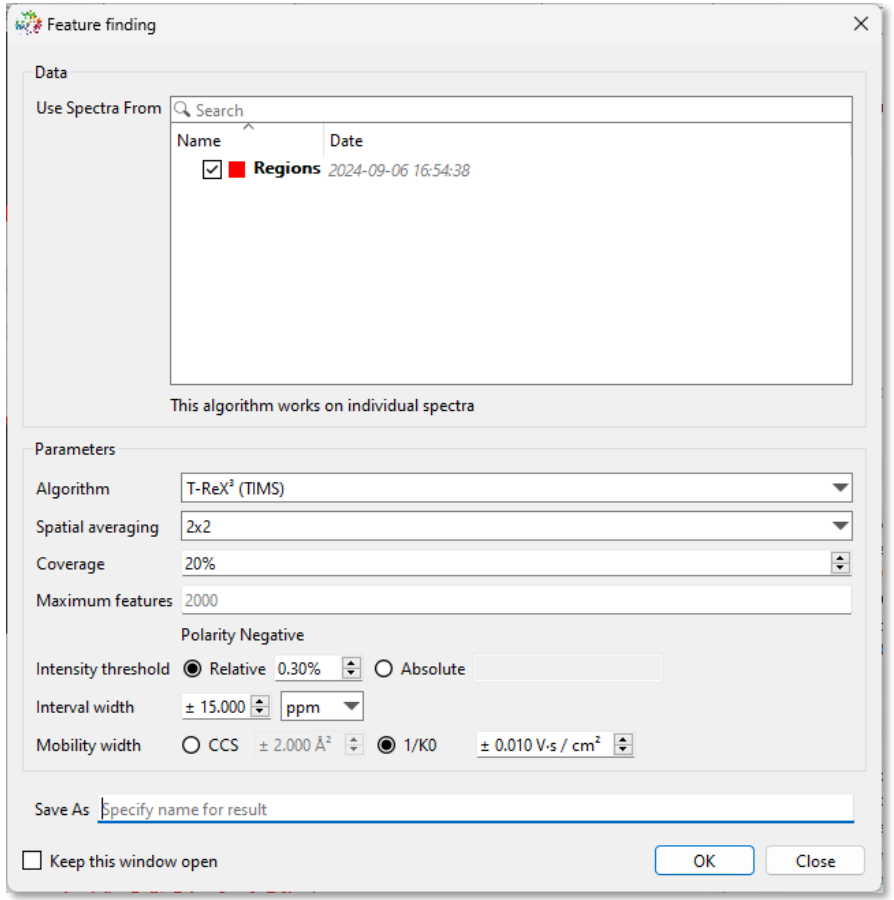
© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Multiple feature enhancements
T-ReX feature finding dialog improvements

- **Set desired interval widths** for the feature finding result in the feature finding dialog.

- T-ReX^3-specific changes:
  - The "Spatial smoothing" parameter has been renamed to "**Spatial averaging**" and the tooltip has been updated to describe its functionality
  - Spatial averaging sets the number of mass-mobility spectra that are averaged before feature finding

- T-ReX^2-specific changes:
  - Updated the tooltip for "**Spatial noise filtering**" to better describe its functionality
  - Spatial noise filtering removes features with sparse ion images, as they most likely result from noise peaks



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

04

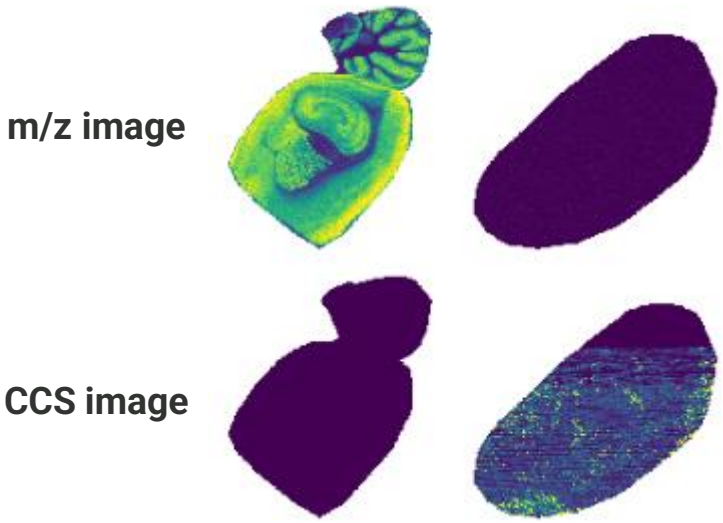
Bug fixes

© 2024 Bruker

For Research Use Only. Not for use in clinical diagnostic procedures.

Bug fixes
CCS image extraction

- A bug in CCS image extraction in SCiLS™ Lab files created from multiple .tdf data sources would produce CCS images with artefacts. The bug was introduced in SCiLS 2025a and is now fixed. We recommend the following procedure:
  - Open the affected data set with 2025b
  - Export the feature list with CCS features to .sef
  - Delete the existing CCS features from the feature table
  - Run the "Optimize file size" tool
  - Import the .sef file and extract the CCS images



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

Bug fixes
Importing high-resolving power MRMS data

- SCiLS™ Lab is limited to importing spectra with a maximum of 10 million bins. In case of high-resolving power MRMS data (e.g., data obtained using 8M or 16M transients and/or with a small lower m/z bound), the likelihood of exceeding this limit increases. In previous versions. SCiLS Lab would often crash when it would encounter such a data set.

- Now, SCiLS Lab shows appropriate warning and error messages, and will guide the user to adjust the mass axis parameters in such a way that the data can still be imported.

- To reduce the number of imported bins, either
  - decrease the imported m/z range (increasing the low m/z is most effective), or
  - increase the bin width

- In case the command line importer encounters such a data set, an error message is generated, suggesting a manual import of the data set.

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

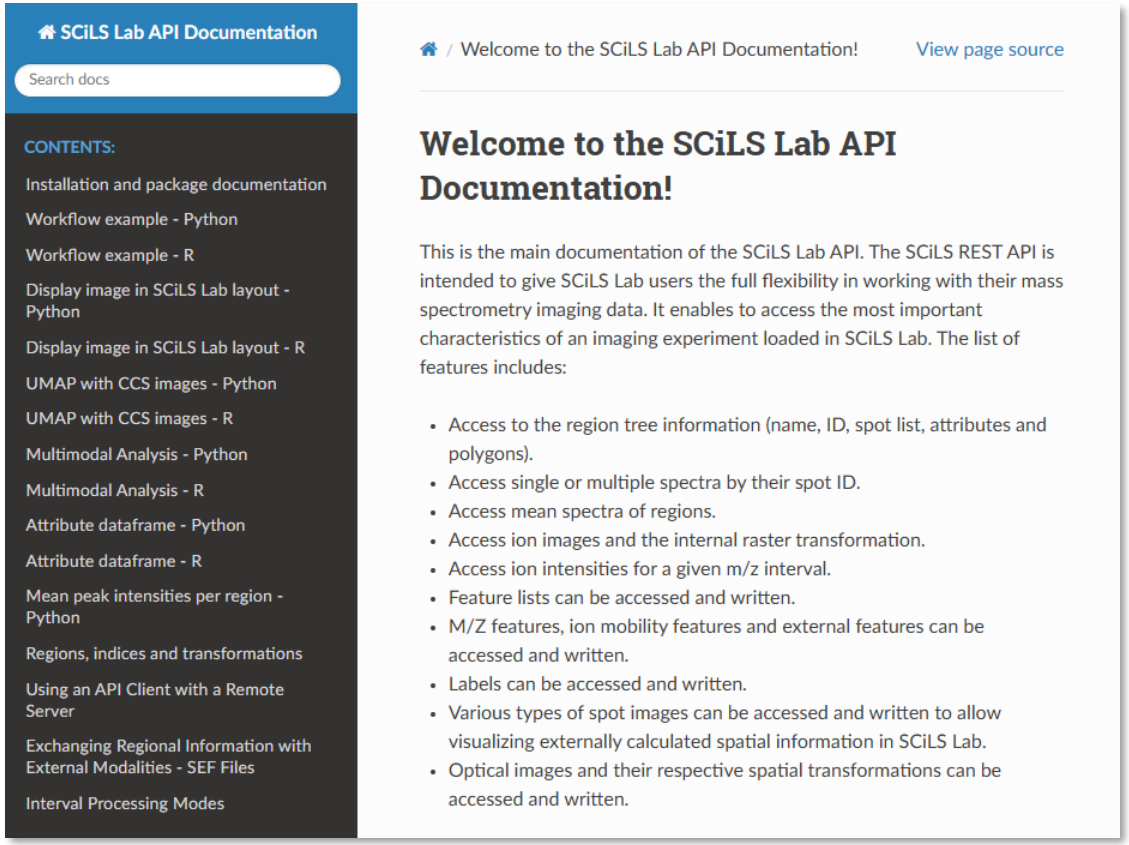
05
SCiLS API improvements

© 2024 Bruker

For Research Use Only. Not for use in clinical diagnostic procedures.

SCiLS™ API improvements

- Added binary package for Python 3.13
- Removed binary package for Python 3.8



© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.

06

Deprecated SCiLS Lab features

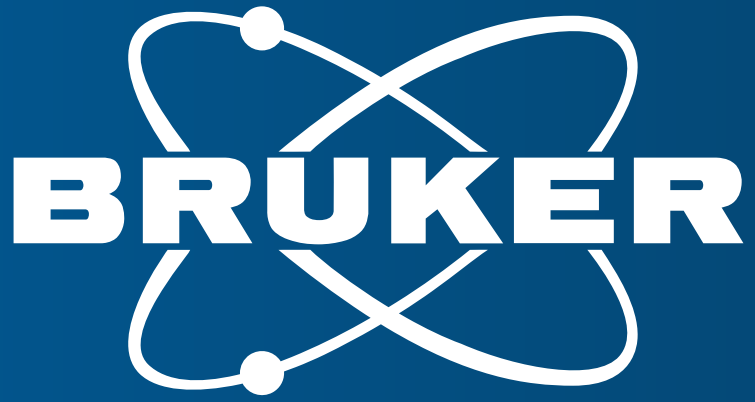
© 2024 Bruker

For Research Use Only. Not for use in clinical diagnostic procedures.

Deprecated SCiLS™ Lab features

- The functionalities to define **Tags and Filters** have been removed from SCiLS Lab
- The **Batch importer** functionality has been removed, as it was outdated

© 2024 Bruker For Research Use Only. Not for use in clinical diagnostic procedures.



Innovation with Integrity