

LIFE SCIENCE MASS SPECTROMETRY

# SCiLS™ Lab 2025b – What's New?

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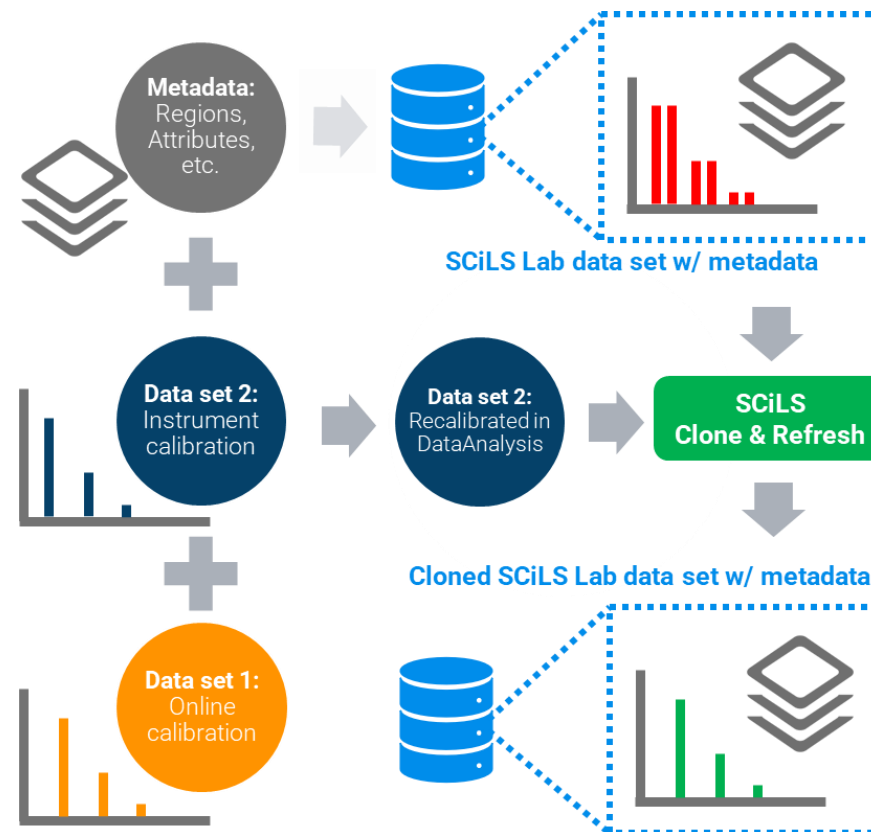
# SCiLS™ Lab 2025b – What’s New?

**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

# 01

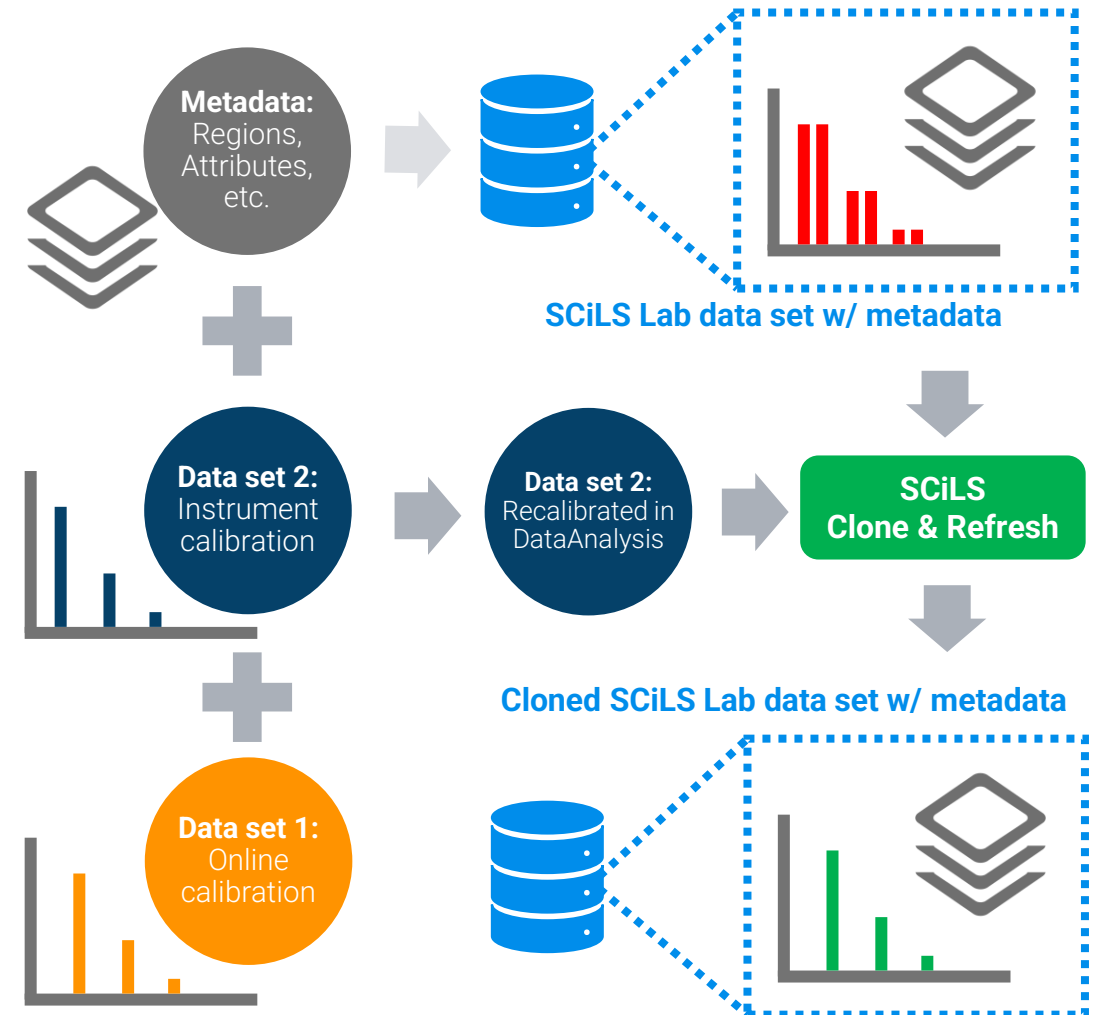
## Clone & Refresh

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## 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



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

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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	✗

## SCiLS Clone & Refresh:

# A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

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## 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:*

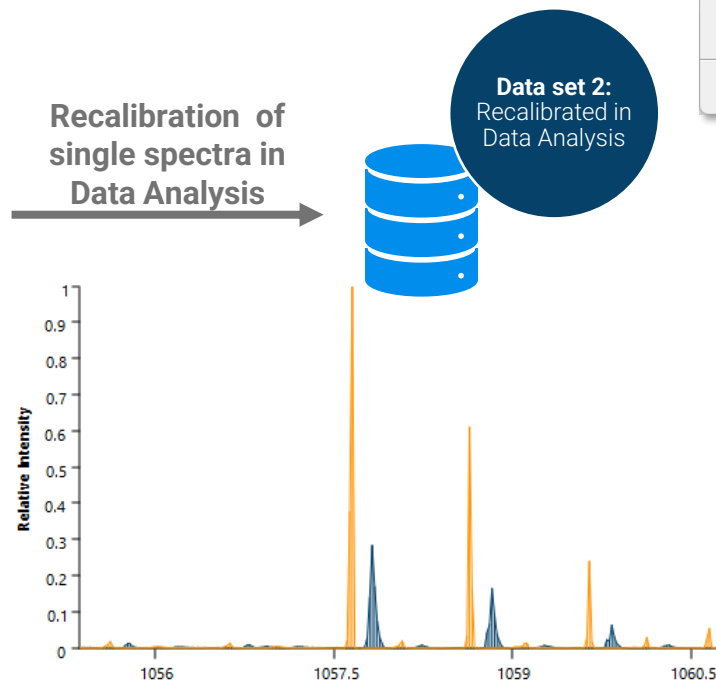
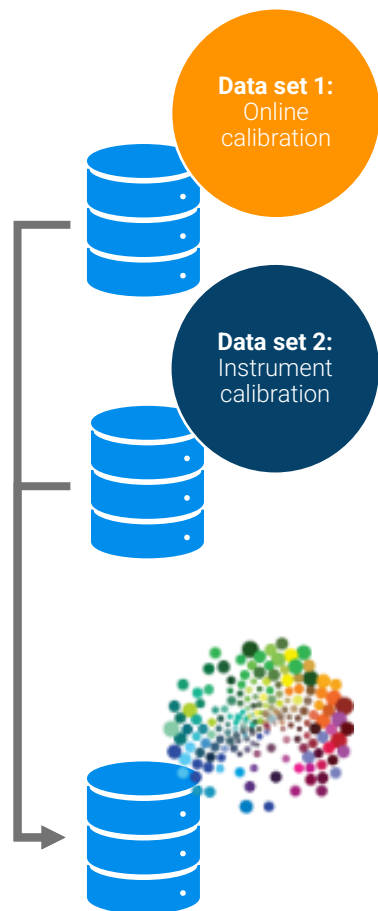
Perform a mass recalibration in Data Analysis, and create a fresh SCiLS Lab import using the recalibrated source data set. Import the optical images in the new SCiLS Lab data set, and import the regions of interest using the .sef file format. All region attributes have to be recreated manually.

### *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.

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

## Recreate SCiLS Lab data set after recalibration of source data



Clone and refresh : Axial TOF Project

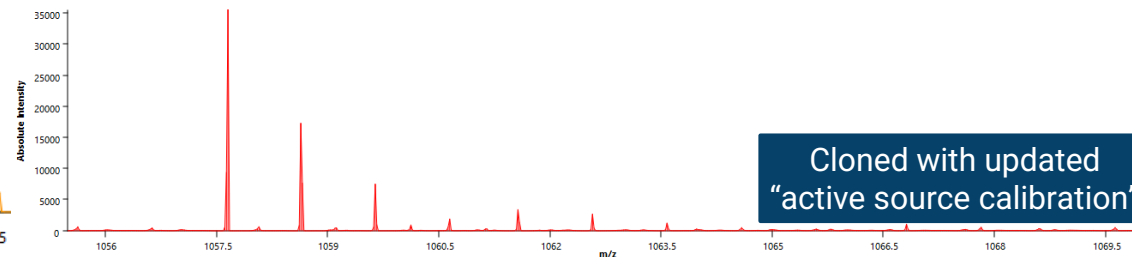
Create a clone of the current SCiLS Lab data set and re-import all spectral data

- By default, all sources will be reimported using the active source calibration.
- To keep current calibration, enable checkbox.

	Source path	Keep current calibration	Active source calibration	Selected clone calibration
1	D:\TEMP\20240415_LungAden...no_Demo_DHB_sub_NeoFlex.d	<input type="checkbox"/>	Unchanged	Created on 2024-04-15T13:56:59.003+02:00
2	D:\TEMP\20240415_LungAden...no_Demo_DHB_sub_NeoFlex.d	<input type="checkbox"/>	Newer	Created on 2024-04-15T13:56:59.003+02:00

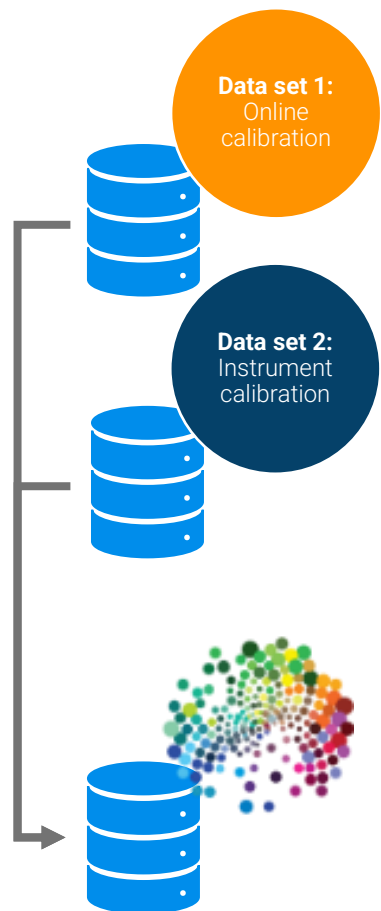
Next > Cancel

Recalibration updates "Active source calibration"

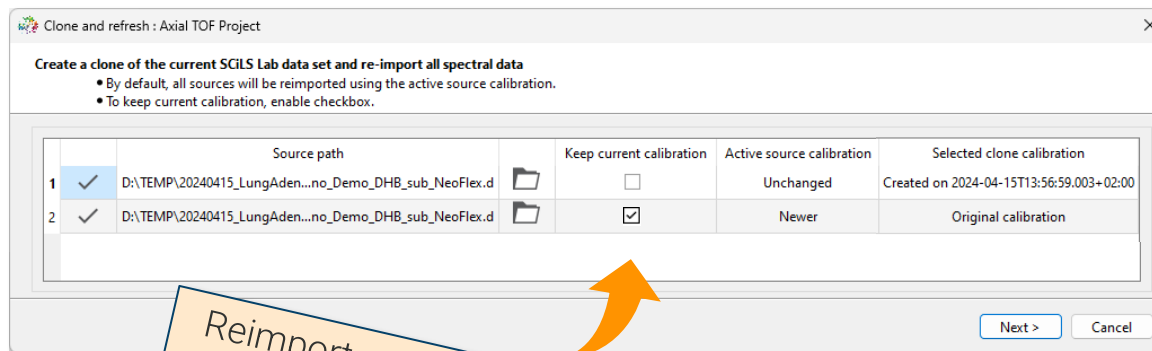
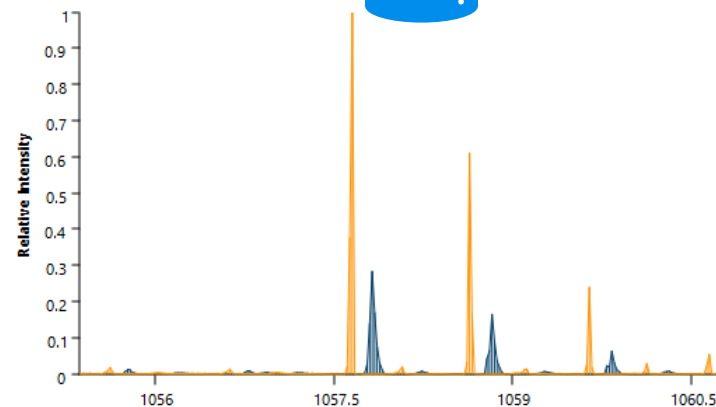


# Clone & Refresh: A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

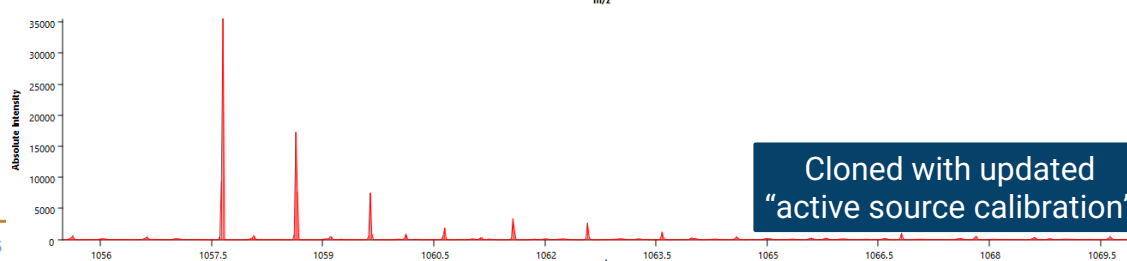
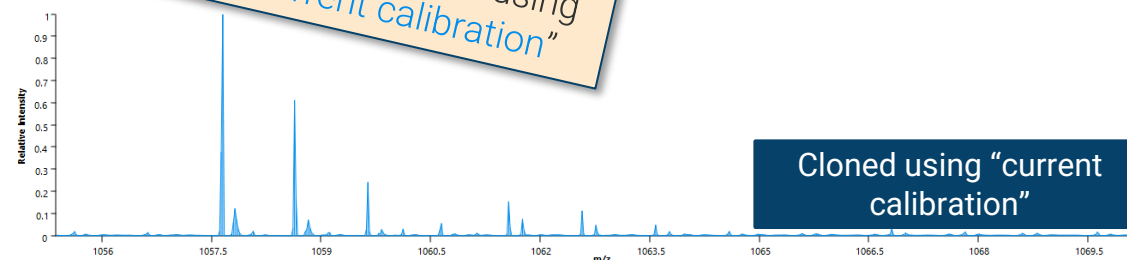
## Recreate SCiLS Lab data set after recalibration of source data



Recalibration of single spectra in Data Analysis



Reimports the data using the "current calibration"





## SCiLS Clone & Refresh:

# A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

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## 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:*

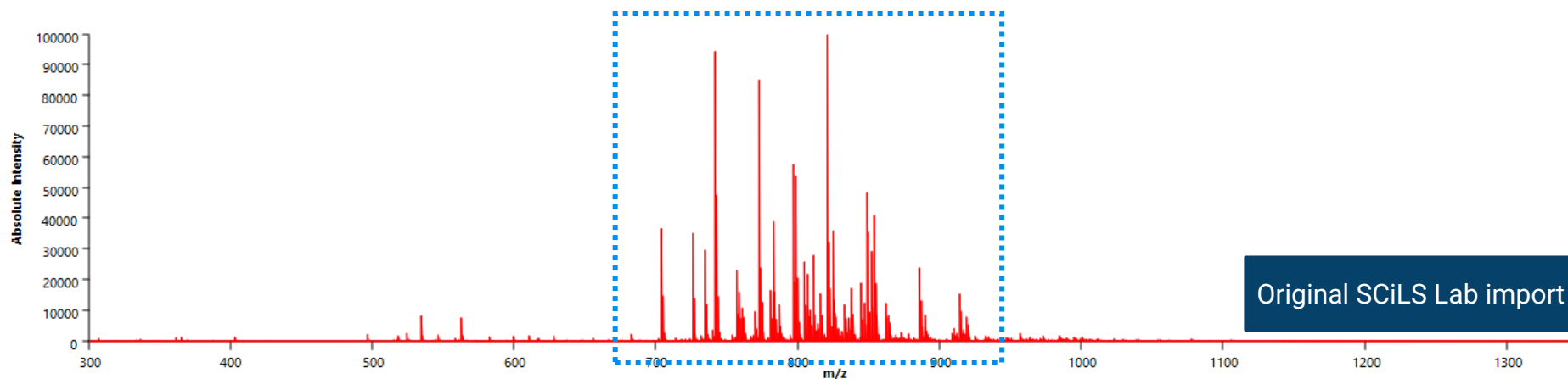
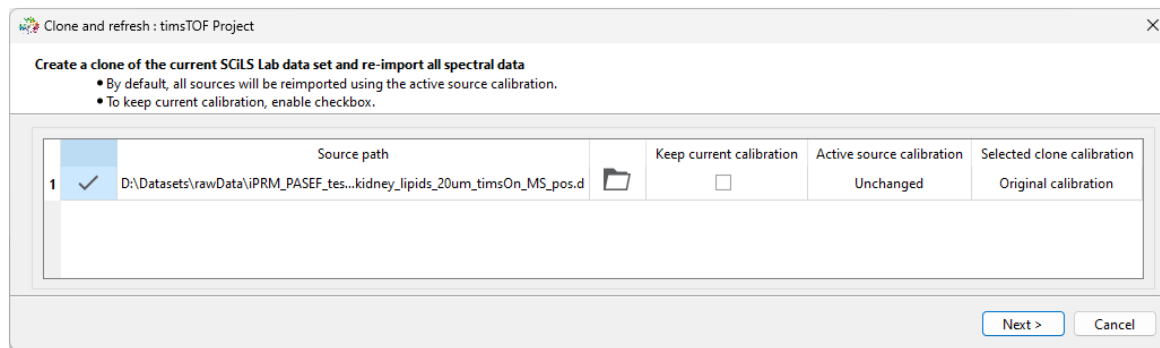
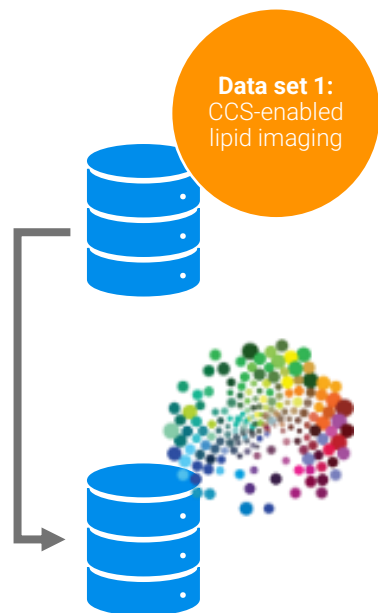
Either create a new SCiLS Lab data set by re-importing the source data, or importing the .slx file, and subsequently re-import and recreate the metadata.

### *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.

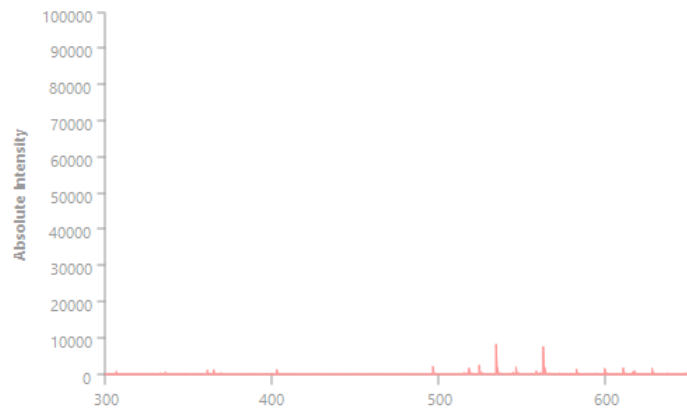
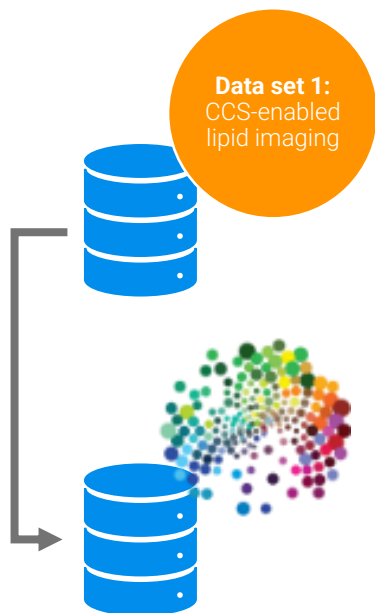
# Clone & Refresh: A new workflow to recreate SCiLS™ Lab data sets maintaining metadata

## Reprocess mass axis of a SCiLS Lab data set



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

## Reprocess mass axis of a SCiLS Lab data set



Clone and refresh : timsTOF Project

**Mass axis settings**  
Specify the mass axis of your imported data set

m/z Range

Automatic range

Min m/z:

Max m/z:

Axis Parameters

Automatic axis

Type:

Bin size:

at m/z:

Number of bins: 61078

Bin size at min m/z: 3.5 mDa

Bin size at max m/z: 4.75 mDa

**Data set**

Resulting Common Mass Axis (Number of bins 61078)

rat\_kidney\_lipids\_20um\_timsOn\_MS\_pos\_Orig\_fullmz (Number of bins 300816)

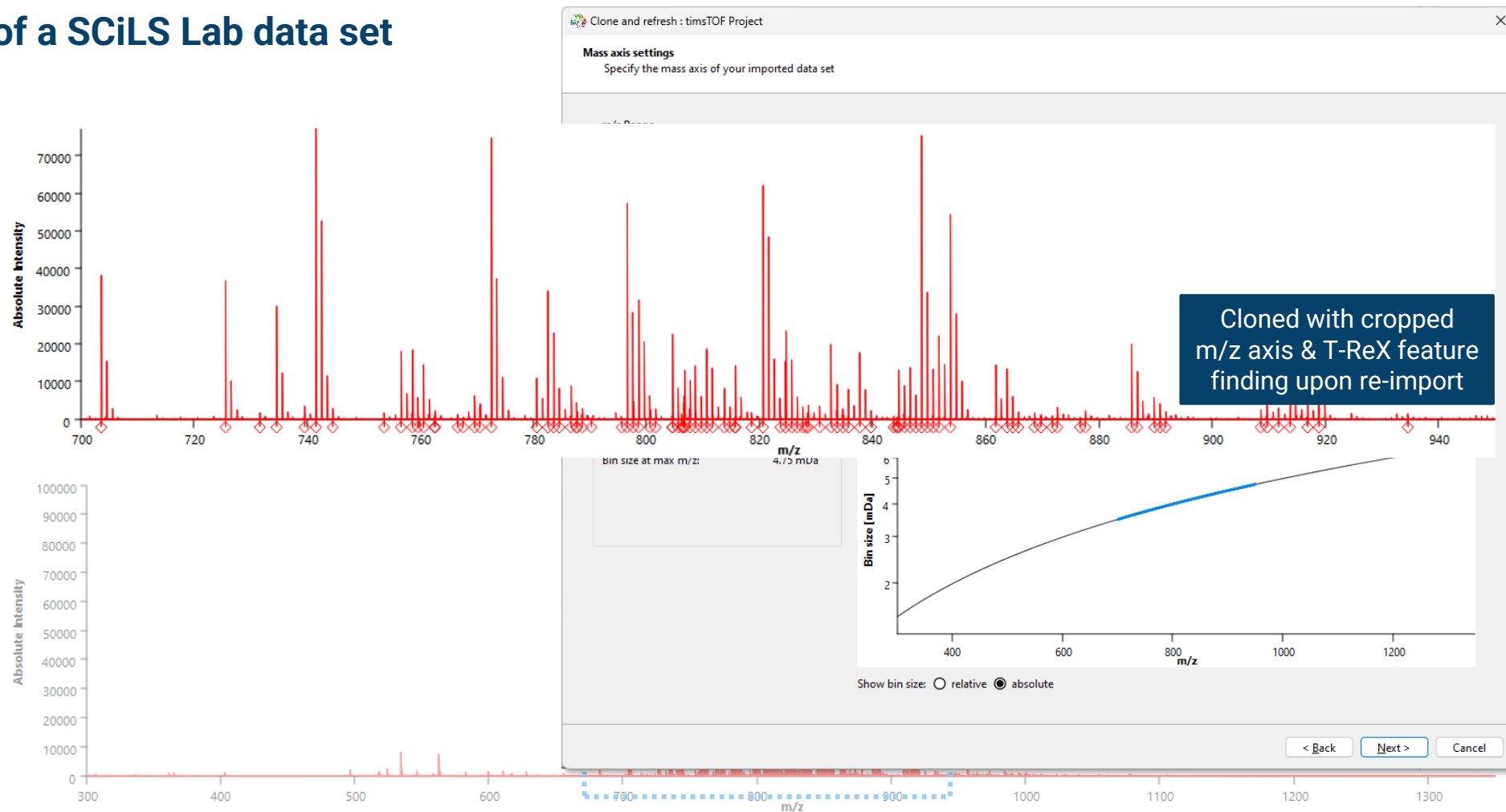
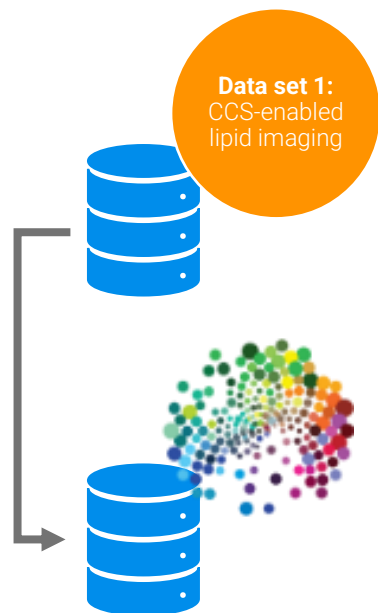
Bin size [mDa]

m/z

Show bin size:  relative  absolute

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

## Reprocess mass axis of a SCiLS Lab data set



# 02

## iprm-PASEF

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# *iprm-PASEF* A reminder...

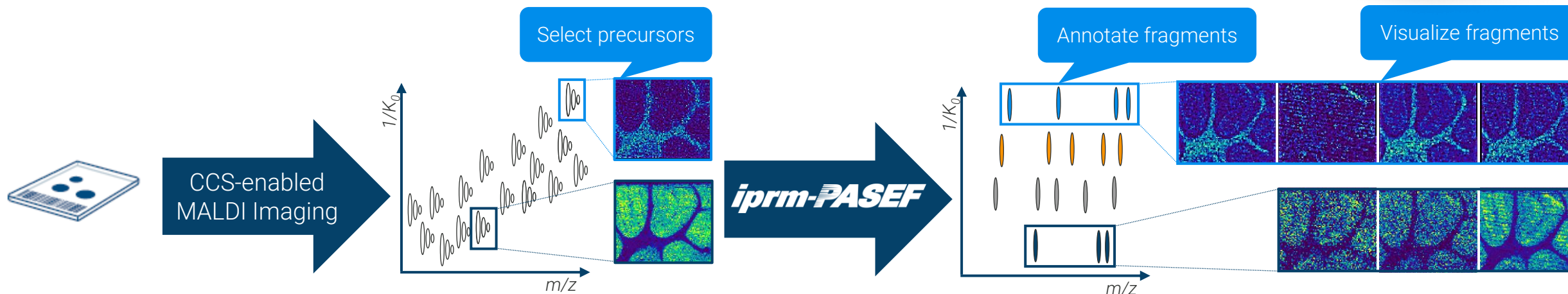


## timsTOF fleX-based targeted fragmentation with spatial fidelity

- 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**

## *iprm-PASEF*

Powered by 4D-Multiomics



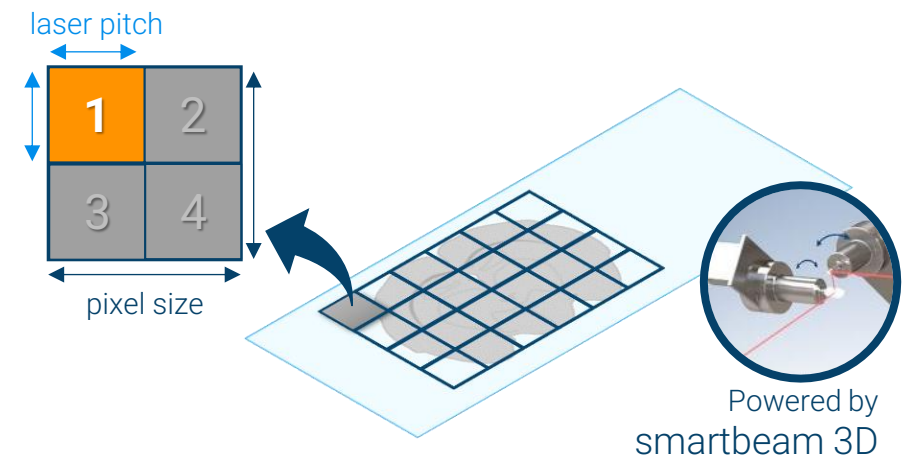
# *iprm-PASEF* A reminder...

- 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



***iprm-PASEF***

Powered by 4D-Multiomics



Powered by  
smartbeam 3D

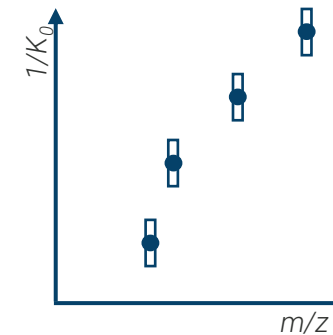
# *iprm-PASEF*®

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

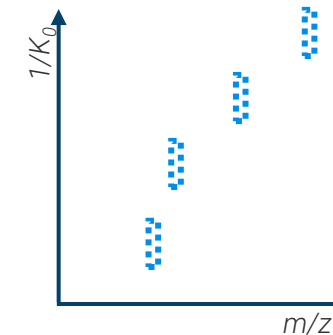
- Combine **iprm-PASEF data sets** based on the **same precursor list** into a single SCiLS Lab data set.
- When the precursor list is identical between multiple iprm-PASEF data sets, one can combine data sets obtained...
  - from different measurement regions
  - using different m/z isolation widths
  - 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

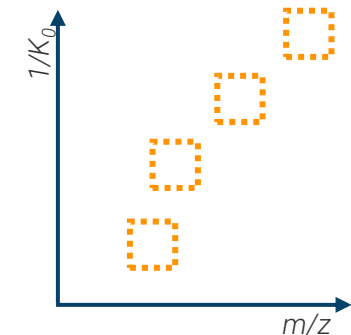
### CCS-enabled MALDI Imaging



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



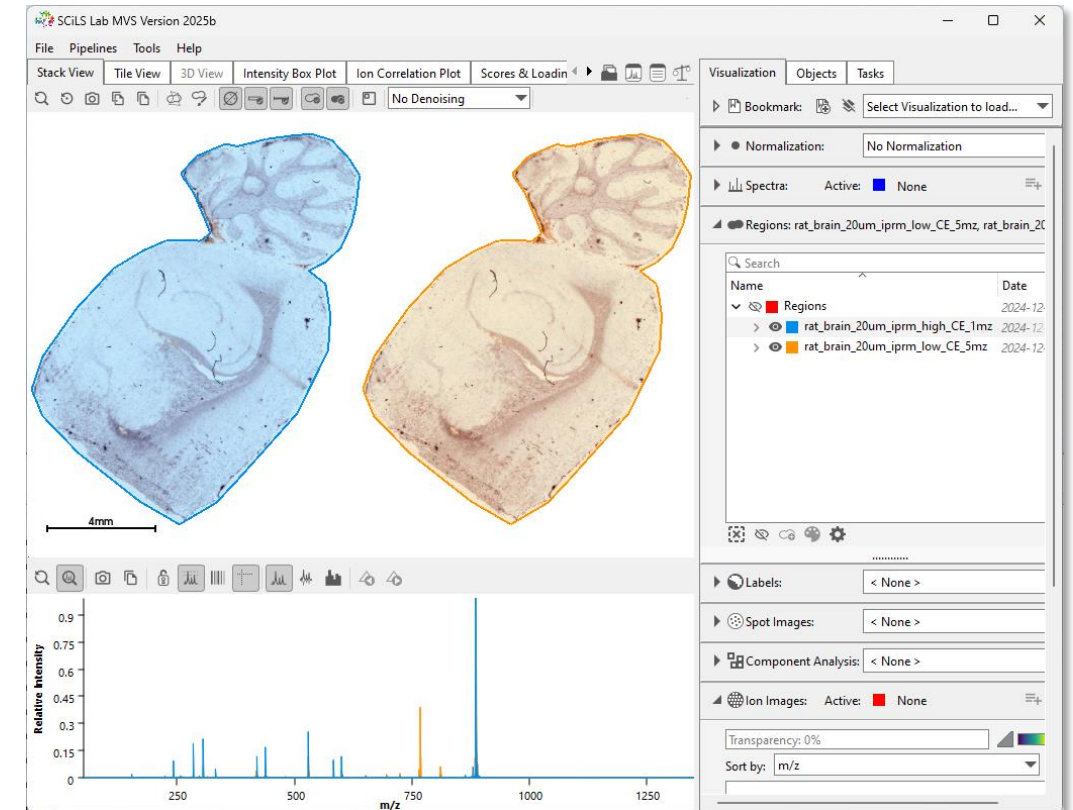
**iprm-PASEF data set 2:**  
 Precursor list 1  
 Isolation width: 5 m/z  
 Collision energy: low



# *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

# 03

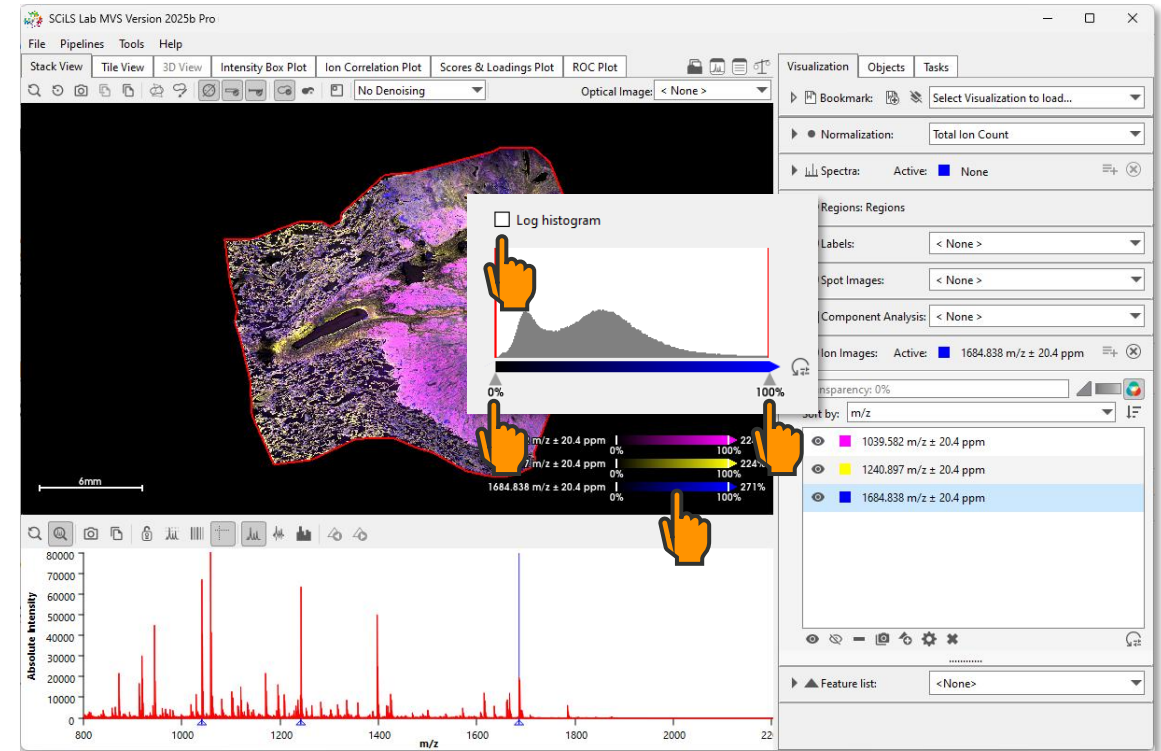
## Multiple feature enhancements

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# *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





# 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

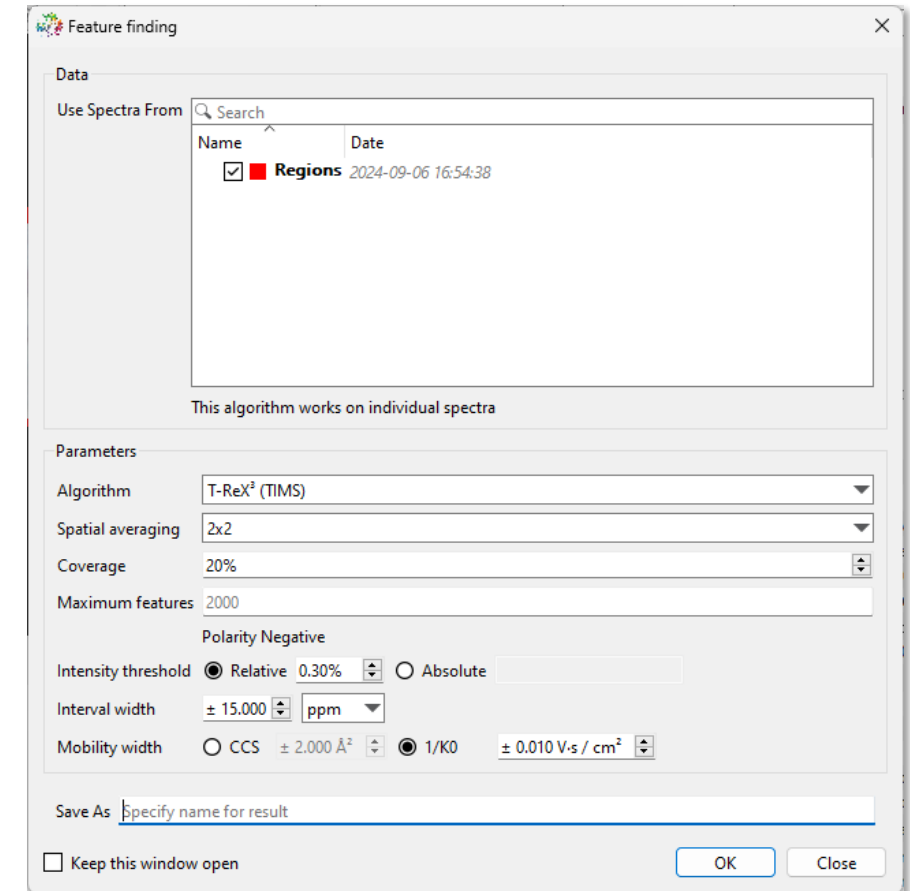
The screenshot shows the Feature Table interface with a list of features. The columns are: m/z, n/z width [z mDa], 1/ΔV [V/cm], Name, and Intensity [Regions]. The Intensity [Regions] column is highlighted in blue. The table contains various chemical species and their corresponding intensities.

m/z	n/z width [z mDa]	1/ΔV [V/cm]	Name	Intensity [Regions]
904.6180	6 1.4936	0.0098	(1-sulfoglucosyl)-Ces(18:1/24:1152)(20H)	32547.9375
417.2367	6 0.9673	0.0097	19-dimethylsilyl-nonadecanoic acid	16343.7993
794.5176	6 1.4376	0.0098	PSIP-16:0(22:47Z,10Z,13Z,16Z)	11995.7939
772.5135	6 1.3680	0.0098	PS(13:0/22:11Z,16Z)	2645.19024
821.5353	6 1.4261	0.0098	PG(18:2/6Z,12Z)/22:47Z,10Z,13Z,16Z)	5853.95966
891.6320	6 1.4959	0.0098	PIP-20:0(18:0)	21121.8242
816.5544	6 1.4318	0.0098	PE(20:3/6Z,11Z,14Z)/22:47Z,10Z,13Z,16Z)	567.99238
835.5470	6 1.4326	0.0098	PG(19:0/22:6Z,7Z,10Z,13Z,16Z,19Z)	175.228974
768.5221	6 1.4140	0.0098	PS(O-16:0(20:4)3Z,6Z,11Z,14Z)	8316.34473
887.5305	6 1.3101	0.0098	PAIP-18:0(18:0)	718.347107
740.5132	6 1.3466	0.0098	PA(22:4/7Z,10Z,13Z,16Z)/18:1(9Z)	5248.92408
888.6172	6 1.4855	0.0098	(1-sulfoglucosyl)-Ces(18:1/24:115Z)	78223.2422
747.4815	6 1.3371	0.0098	Adthromycin	121654.445
878.5965	6 1.4758	0.0098	(1-sulfoglucosyl)-Ces(18:1/22:0)(20H)	28889.0391
806.5386	6 1.4124	0.0098	(1-sulfoglucosyl)-Ces(18:1/18:0)	27945.2676
862.6075	6 1.4673	0.0098	PI-Ces(18:1/22:0)	9964.64355
834.5899	6 1.4426	0.0098	(1-sulfoglucosyl)-Ces(18:1/20:0)	7031.69873
729.5372	6 1.3409	0.0098	PE(8:0/18:1)(9Z)	4220.41553
809.2778	6 0.8755	0.0096	Pentylpentadec-11-enoate	4912.87768
727.5434	6 1.3359	0.0098	CesPE(14:2(4E,4E)/24:1(15Z)(20H)	5337.58789
822.5347	6 1.4215	0.0098	(1-sulfoglucosyl)-Ces(18:1/18:0)(20H)	7765.64453
831.2612	6 0.9023	0.0096	10-[3]-ladderane-decanoic acid	10295.1396
888.6111	6 1.4876	0.0098	PIP-20:0(18:0)(2)	8814.48039
802.5870	6 1.4873	0.0098	Am-PE(16:0/20:3)(Z,11Z,14Z)	1700.84216
701.5055	6 1.3057	0.0098	PA(17:0/18:1)(9Z)	4092.1406
774.5364	6 1.3757	0.0098	PS(17:0/18:1)(9Z)	23096.0664
803.2302	6 0.8646	0.0096	4,10,14,18-tetrastatetraenoic acid	3072.709
899.4804	6 1.2958	0.0098	PA(22:1/12Z,16Z)/14:0	20963.7773
794.5631	6 1.3918	0.0098	PC(22:4/7Z,10Z,13Z,16Z)/13:0	24110.9688
786.5184	6 1.3920	0.0098	PS(16:0/20:2)(11Z,14Z)	9849.30664
327.2298	6 0.9052	0.0096	LMF601031176	28327.5957
673.4764	6 1.2739	0.0098	PA(12:0/22:1(11Z))	20482.791
838.5505	6 1.4402	0.0098	PS(20:4/3Z,6Z,11Z,14Z)/20:0	15108.96
742.5304	6 1.3373	0.0098	PC(20:2)(11Z,14Z)/13:0	12491.8834
771.5199	6 1.3489	0.0098	PA(22:4/7Z,10Z,13Z,16Z)/18:0	11244.2129
727.5237	6 1.3307	0.0098	PA(18:1)(6Z/18:1)(9Z)	3363.5376
850.5649	6 1.4489	0.0098	PS(18:1)(6Z/22:47Z,10Z,13Z,16Z)	4676.34239
748.5207	6 1.3487	0.0098	PS(17:0/16:0)	9484.43309

# 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<sup>3</sup>-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<sup>2</sup>-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



# 04

## Bug fixes

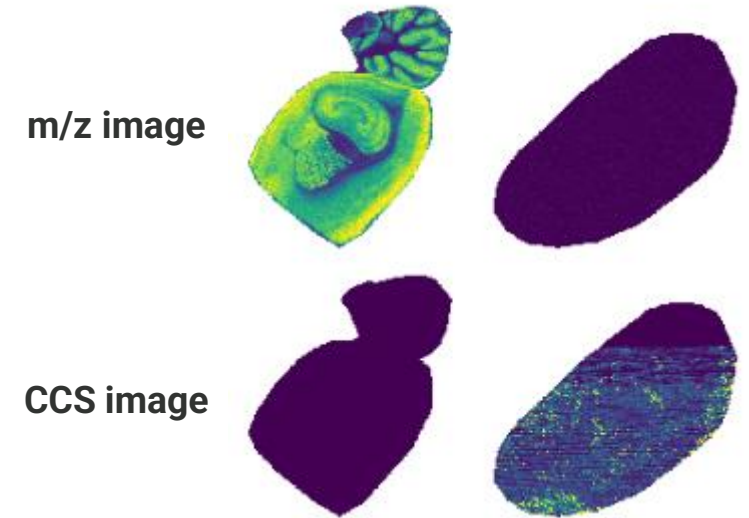
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# Bug fixes

## 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



## 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.



# 05

## SCiLS API improvements

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# SCiLS™ API improvements

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

🏠 SCiLS Lab API Documentation

**CONTENTS:**

- Installation and package documentation
- Workflow example - Python
- Workflow example - R
- Display image in SCiLS Lab layout - Python
- Display image in SCiLS Lab layout - R
- UMAP with CCS images - Python
- UMAP with CCS images - R
- Multimodal Analysis - Python
- Multimodal Analysis - R
- Attribute dataframe - Python
- Attribute dataframe - R
- Mean peak intensities per region - Python
- Regions, indices and transformations
- Using an API Client with a Remote Server
- Exchanging Regional Information with External Modalities - SEF Files
- Interval Processing Modes

🏠 / Welcome to the SCiLS Lab API Documentation! [View page source](#)

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## Welcome to the SCiLS Lab API Documentation!

This is the main documentation of the SCiLS Lab API. The SCiLS REST API is intended to give SCiLS Lab users the full flexibility in working with their mass spectrometry imaging data. It enables to access the most important characteristics of an imaging experiment loaded in SCiLS Lab. The list of features includes:

- Access to the region tree information (name, ID, spot list, attributes and polygons).
- Access single or multiple spectra by their spot ID.
- Access mean spectra of regions.
- Access ion images and the internal raster transformation.
- Access ion intensities for a given m/z interval.
- Feature lists can be accessed and written.
- M/Z features, ion mobility features and external features can be accessed and written.
- Labels can be accessed and written.
- Various types of spot images can be accessed and written to allow visualizing externally calculated spatial information in SCiLS Lab.
- Optical images and their respective spatial transformations can be accessed and written.

# 06

## Deprecated SCiLS Lab features

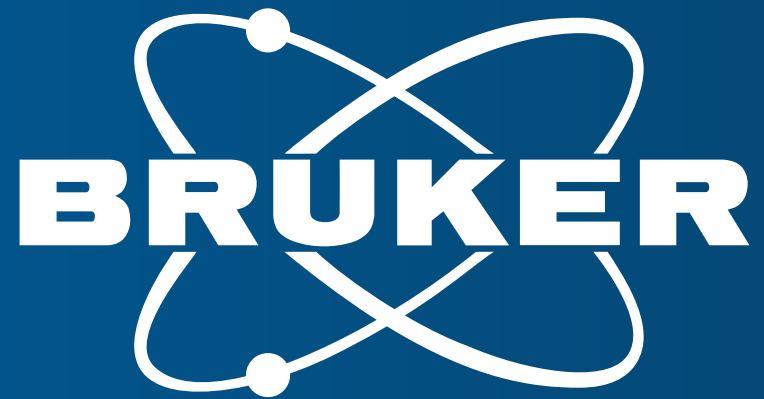
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## Deprecated SCiLS™ Lab features

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



Innovation with Integrity