

LIFE SCIENCE MASS SPECTROMETRY

# SCiLS™ Lab 2025a – What's New?

---

# 01

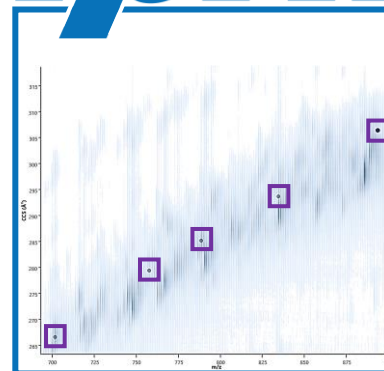
## Multiple feature enhancements

---

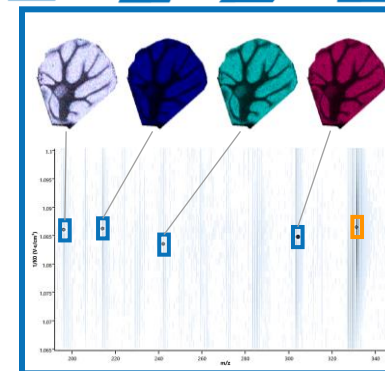
## SCiLS™ Lab 2025a – What's New?

- 01 *Multiple feature enhancements:*  
Various improvements and changes
- 02 *iprm-PASEF:*  
Fragmentation-based molecular annotation
- 03 *T-ReX<sup>®</sup> feature finding:*  
Visualize T-ReX deisotoping results
- 04 *SCiLS API improvements:*
- 05 *neofleX support:*

# iprm-PASEF




Export precursors



Analyze fragments

- m/z
- Isotope pattern
- Mobility
- MS/MS



Identify precursors

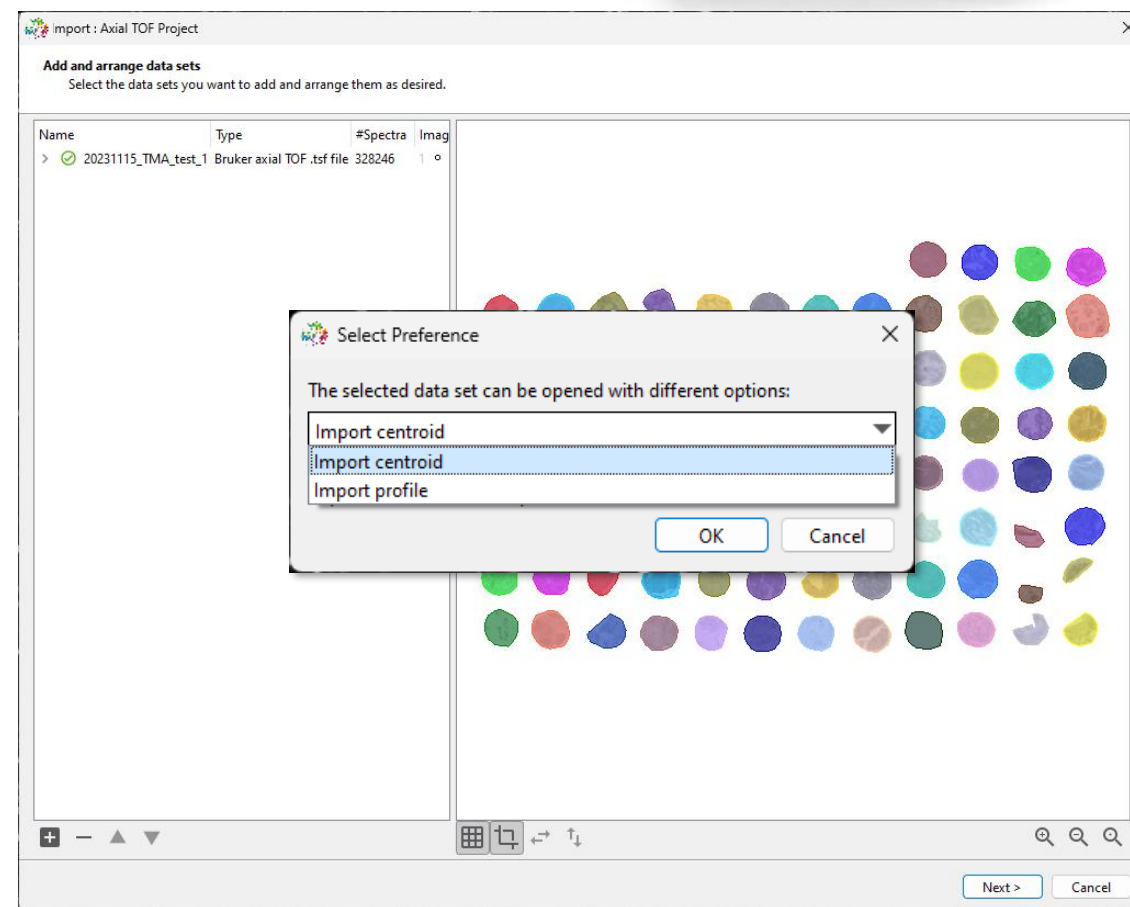


Available for  
Customers since  
October 1st, 2024

# Multiple feature enhancements

## Importing neofleX data into SCiLS™ Lab

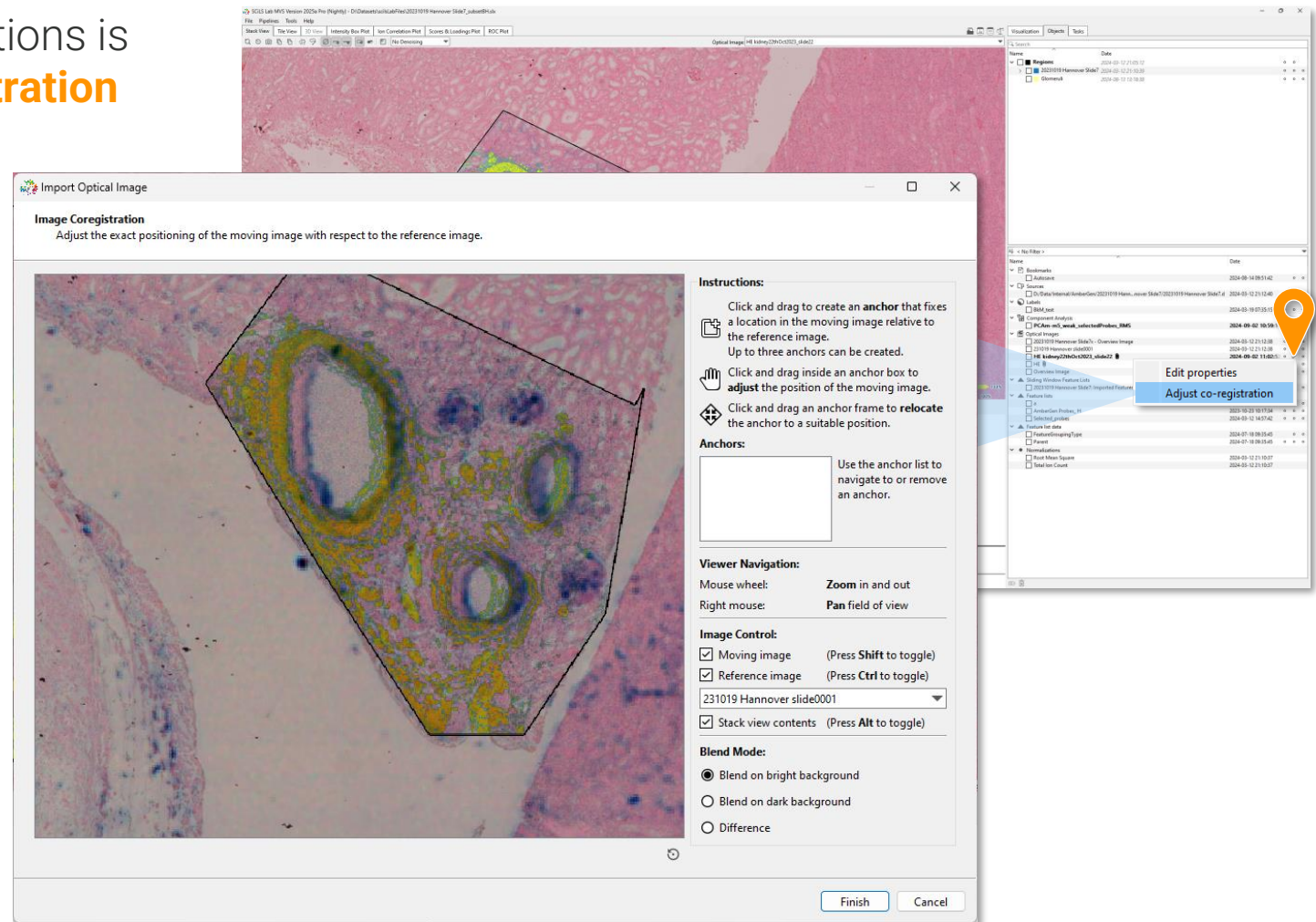
- SCiLS Lab 2025a can read .d/tsf data acquired by the all-new **neofleX** axial TOF instrument
- Import **centroid** or **profile** neofleX data into a SCiLS Lab “Axial TOF project”
- neofleX profile data can be combined with rapifleX profile data (.d container format)
- Combining centroid and profile axial TOF data is not supported
- T-ReX® Feature Finding is not enabled for neofleX data sets



# Multiple feature enhancements




## Adjust registration for previously imported optical images

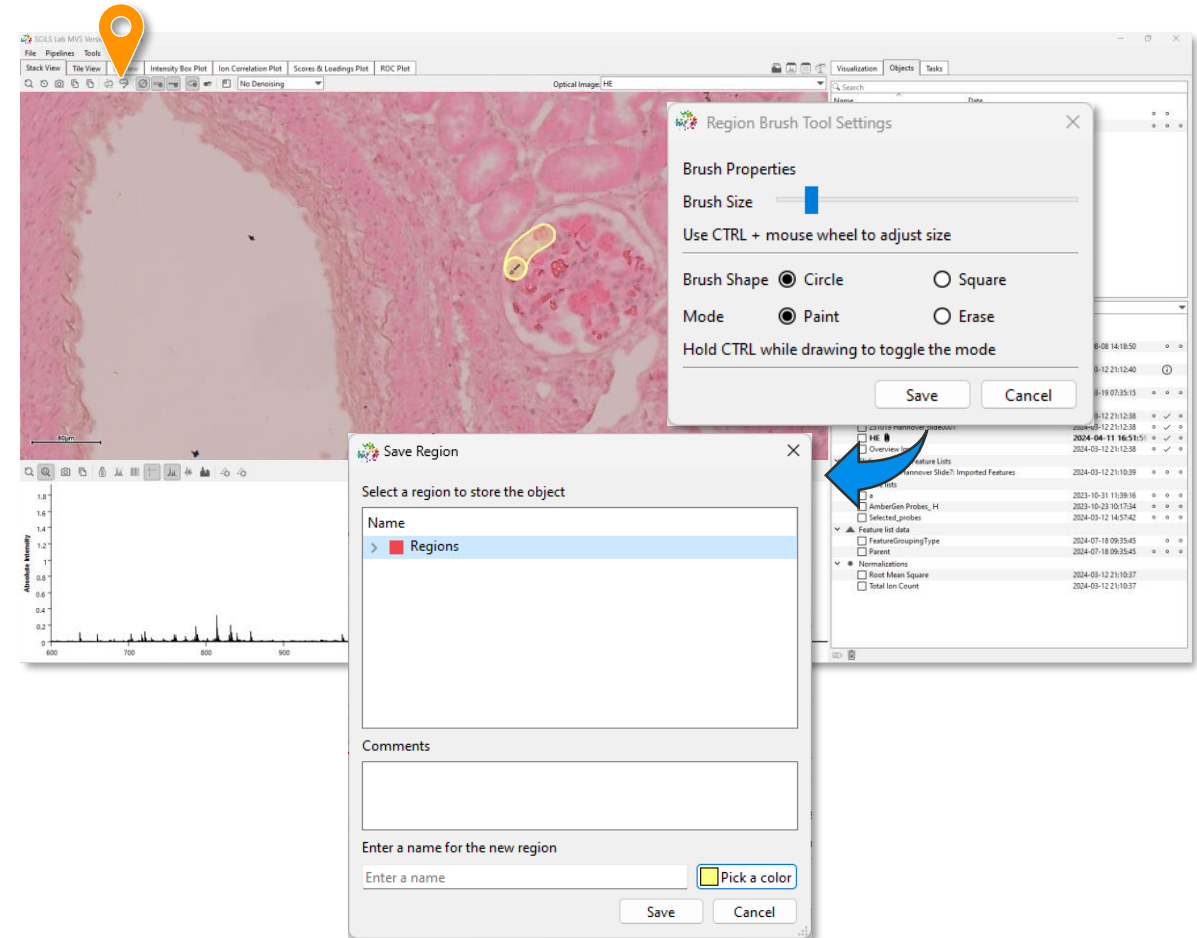
- In case any of the optical image registrations is unsatisfactory, one can **Adjust co-registration**
  - No image orientation required
  - Detailed registration identical to optical image import
  - Allows changing the reference image
  - New registration overwrites previous
  - Cancelling restores original registration



# Multiple feature enhancements

## Brush tool for region of interest definition

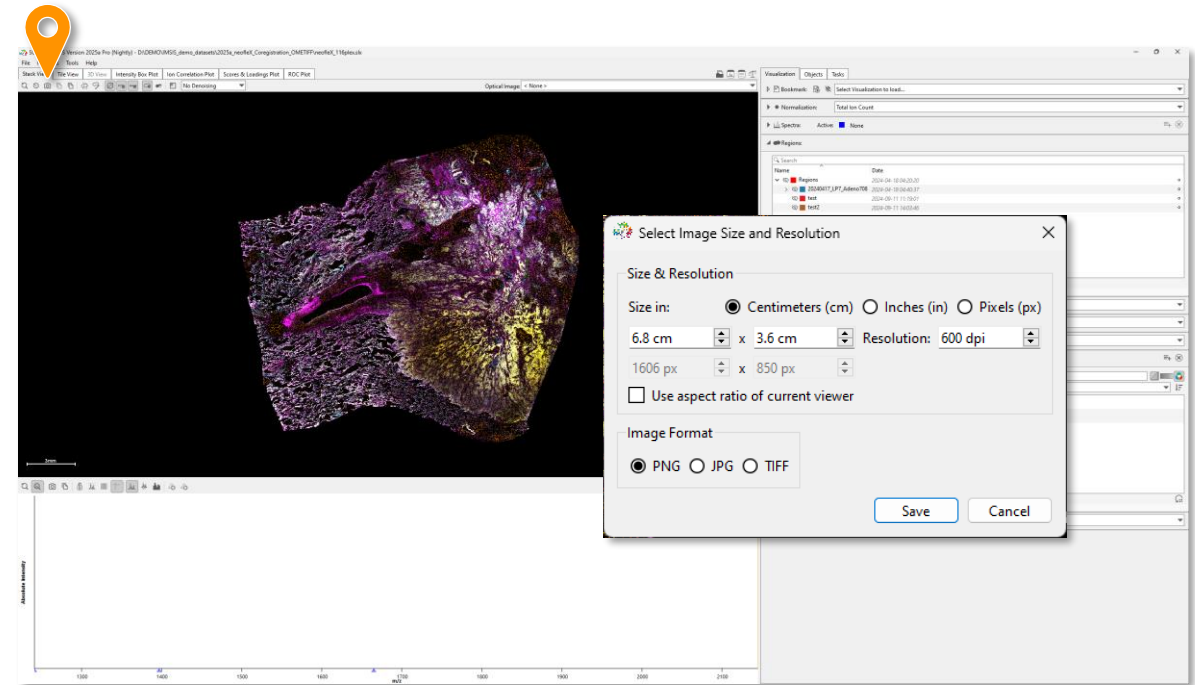
- SCiLS™ Lab 2025a now includes a **brush tool** to define regions of interest: 
- Switch between **Painting**  and **Erasing** 
- Switch between **Circular** and **Square** brush shape
- Fluently **change brush size** while painting
- Allows to **create disjointed regions**



# Multiple feature enhancements



## Improved screenshot export

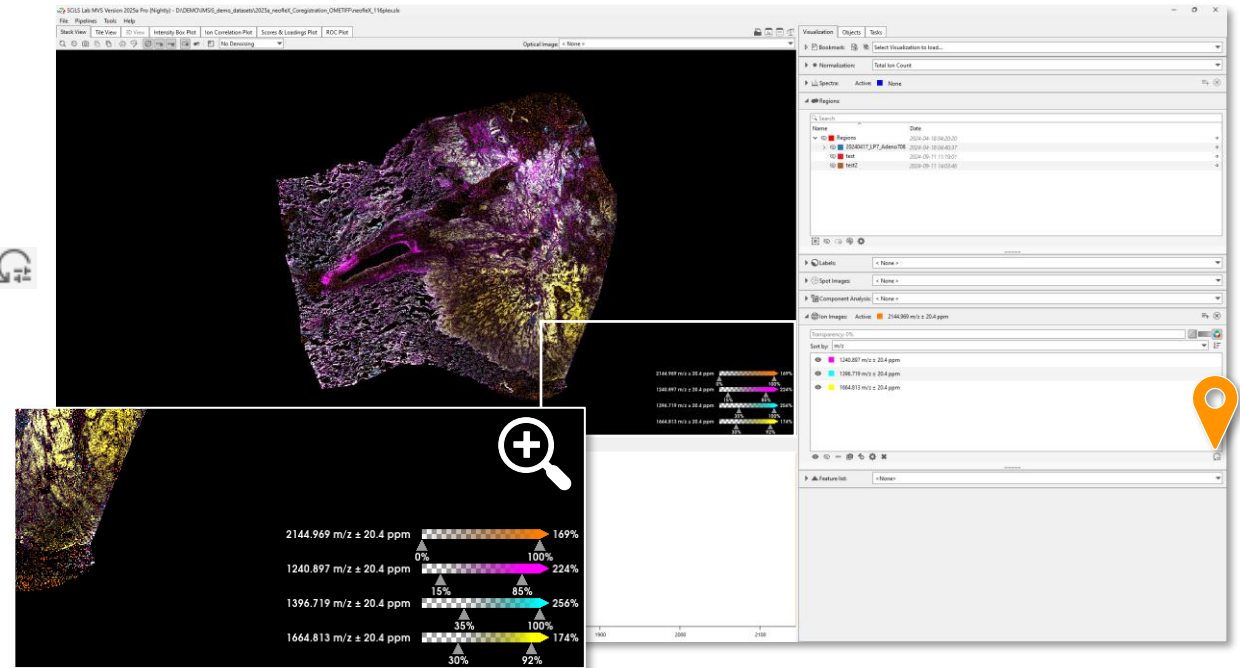
- Different usage of images often come with specific **size and image resolution requirements**.
- Set the dimensions and image resolution when using **Save screenshot**: 📷



# Multiple feature enhancements

## Individual colorbar scaling in Stack View

- Set color bars for individual images independently when in **image blend mode**: 
- Reinstate the default 0% and 100% positions for all images simultaneously using **Reset all color bars**: 





# Multiple feature enhancements

## Feature Table update

- SCiLS™ **Feature Table** has been updated
- Functionality-based grouping** of tools
- m/z and mobility intervals** now have their own Feature Table columns (*hidden by default*)

m/z	m/z interval [%]	1/K0 [V-s/cm <sup>2</sup> ]	1/K0 interval [V-s/cm <sup>2</sup> ]	CCS [Å <sup>2</sup> ]	CCS interval [Å <sup>2</sup> ]	Name
741.5274	0.0 1.4186	0.0196	289.3905	4.0000		
810.5960	0.0 1.4598	0.0196	297.3329	4.0000		
848.5529	0.0 1.4739	0.0197	299.9818	4.0000		
798.5358	0.0 1.4458	0.0196	294.5583	4.0000		
820.5218	0.0 1.4436	0.0196	293.9827	4.0000		

Feature list: <All Features> (1189)

- Copy-to-clipboard
- Import feature list
- Export feature list
- Export ppm-PASEF parameters
- Export feature images (OME-TIFF)

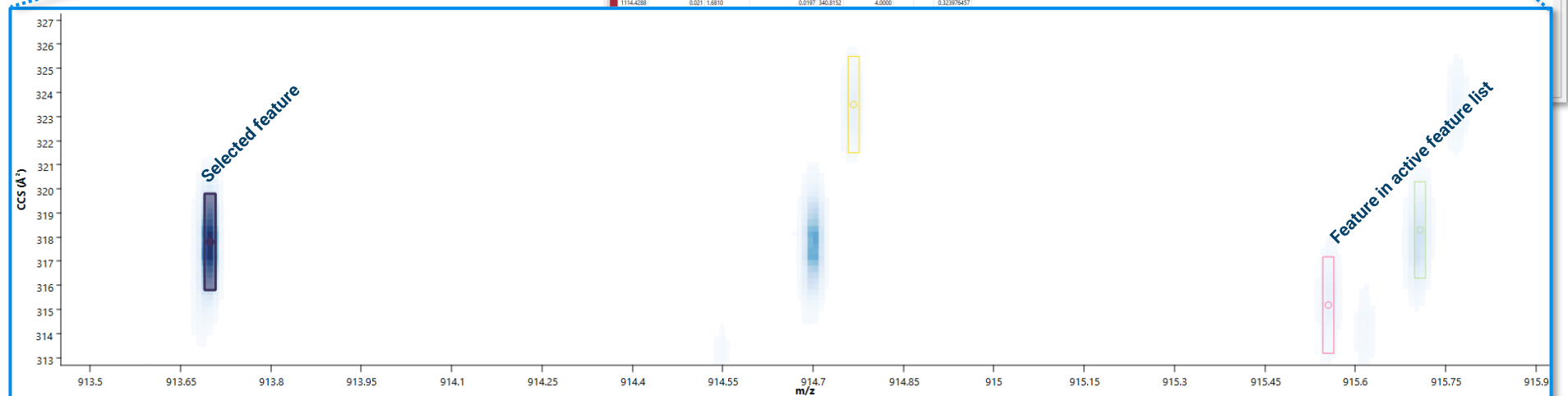
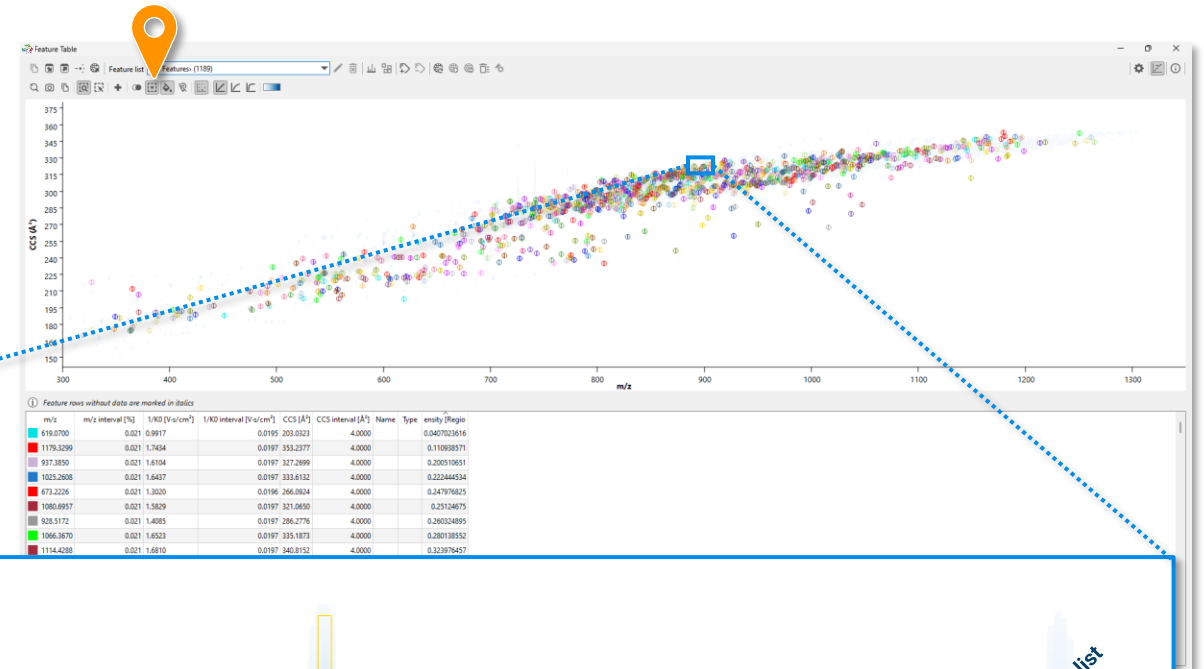
- Select feature list
- Edit name
- Delete current feature list
- Add intensity column(s)
- Add "Component Analysis loadings" column
- Create molecular annotations
- Delete annotations for selected features
- Extract missing CCS images
- Create ion images from selection
- Remove selected ion images
- Remove selected rows from feature table
- Create new feature list from selected rows

- Manage columns
- Show feature navigator
- Show detailed feature information
- Copy-to-clipboard (detailed feature info)

# Multiple feature enhancements

## Feature Navigator improvement

- **CCS feature outline** can be displayed in the Feature Navigator:
- Indicates actual feature m/z and mobility interval
- Original marker indicates m/z and mobility centroid



# Multiple feature enhancements

## Feature Table detailed information tabs



- Specific feature details are now shown in the **Detailed Information** panel of the Feature Table
- Sub-panels for different sets of information:
  - Isotopologues**
    - Only for data sets compatible with T-ReX<sup>®</sup> feature finding
  - Annotations**
    - Available for all data sets, only used when performing MetaboScape-powered Molecular Annotation
  - Fragments**
    - Only available in iprm-PASEF data sets
- Contents of the Detailed Information sub-panels can be exported using the dedicated **copy-to-clipboard** button

The screenshot displays the 'Feature Table' window with a list of features and a 'Detailed Information' panel. The feature list includes columns for m/z, width, intensity, and name. The detailed panel shows information for a selected feature, including its name, AG score, formula, ion notation, and method.

m/z	width [s.mDa]	1/KD [1/s.cm <sup>2</sup> ]	1/KD width [s]	Name	Intensity [Regions]	AG score
904.6160	6	1.4936	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/24:1/15Z)(2OH)	32547.9375	
417.2367	6	0.9673	0.0097	19-dimethylsilynyl-nonadecanoic acid	16343.7393	
794.5376	6	1.4376	0.0098	PS(9-16:0/22:4/7Z,10Z,13Z,16Z)	11595.7939	
772.5135	6	1.3680	0.0098	PS(13:0/22:2/13Z,16Z)	2645.19824	
821.5353	6	1.4261	0.0098	PG(18:2(6Z,12Z)/22:4/7Z,10Z,13Z,16Z)	5853.95996	
891.6320	6	1.4959	0.0098	PIP-20:0/19:0	2121.8242	
816.5544	6	1.4318	0.0098	PE(20:3(6Z,11Z,14Z)/22:4/7Z,10Z,13Z,16Z)	567.956238	
835.5470	6	1.4326	0.0098	PG(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)	175.228874	
795.5221	6	1.4140	0.0098	PS(9-16:0/20:4/3Z,6Z,11Z,14Z)	8316.34473	
867.5055	6	1.3101	0.0098	PIP-18:0/19:0	718.347197	
745.5132	6	1.3466	0.0098	PA(23:4/7Z,10Z,13Z,16Z/18:1/9Z)	5248.05408	
888.6172	6	1.4855	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/24:1/15Z)	7822.24622	
747.4913	6	1.3371	0.0098	Azithromycin	121654.445	
876.5965	6	1.4758	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/22:0/2OH)	28689.0391	
806.5386	6	1.4124	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/18:0)	27945.2676	
862.6073	6	1.4673	0.0098	PI-Cer(18:1/22:0)	9964.64335	
834.5699	6	1.4426	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/20:0)	7031.69873	
726.5372	6	1.3409	0.0098	PEm 18:0/18:1/9Z)	4220.41553	
306.2778	6	0.8755	0.0098	Pentyl pentadec-11-enoate	4912.97168	
727.5434	6	1.3359	0.0098	CerPE(14:2(4E,6E)/24:1/15Z)(2OH)	5337.58789	
822.5347	6	1.4215	0.0098	( <sup>3</sup> -sulfo)GalBeta-Cer(18:1/18:0/2OH)	7365.64453	
331.2812	6	0.9203	0.0098	10-[3]-ladderane-decanoic acid	10285.1396	
889.6111	6	1.4676	0.0098	PIP-20:0/19:1/9Z)	8414.40039	
902.5970	6	1.4673	0.0098	Am-PE(16:0/20:3(6Z,11Z,14Z)	1700.84216	
701.5053	6	1.3057	0.0098	PA(17:0/19:1/9Z)	40082.1406	
774.5364	6	1.3797	0.0098	PS(17:0/18:1/9Z)	28096.0664	
303.2302	6	0.8646	0.0098	6,10,14,18-tetracosatetraenoic acid	30372.709	
699.4904	6	1.2958	0.0098	PA(22:2/13Z,16Z)/14:0)	20863.7773	
794.5631	6	1.3918	0.0098	PC(22:4/7Z,10Z,13Z,16Z)/15:0)	24110.9688	
786.5184	6	1.3920	0.0098	PS(16:0/20:2/11Z,14Z)	9849.30684	
327.2298	6	0.9052	0.0098	LMFA0103176	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)	13108.96	
742.5304	6	1.3373	0.0098	PC(20:2/11Z,14Z)/19:0)	12491.9834	
751.5199	6	1.3469	0.0098	PA(22:4/7Z,10Z,13Z,16Z)/18:0)	11244.2129	
721.5237	6	1.3207	0.0098	PA(19:1(6Z)/19:1(6Z))	3583.5376	
856.5649	6	1.4409	0.0098	PS(19:1(6Z)/22:4/7Z,10Z,13Z,16Z)	4676.34229	
748.5207	6	1.3407	0.0098	PS(17:0/16:0)	9484.41309	

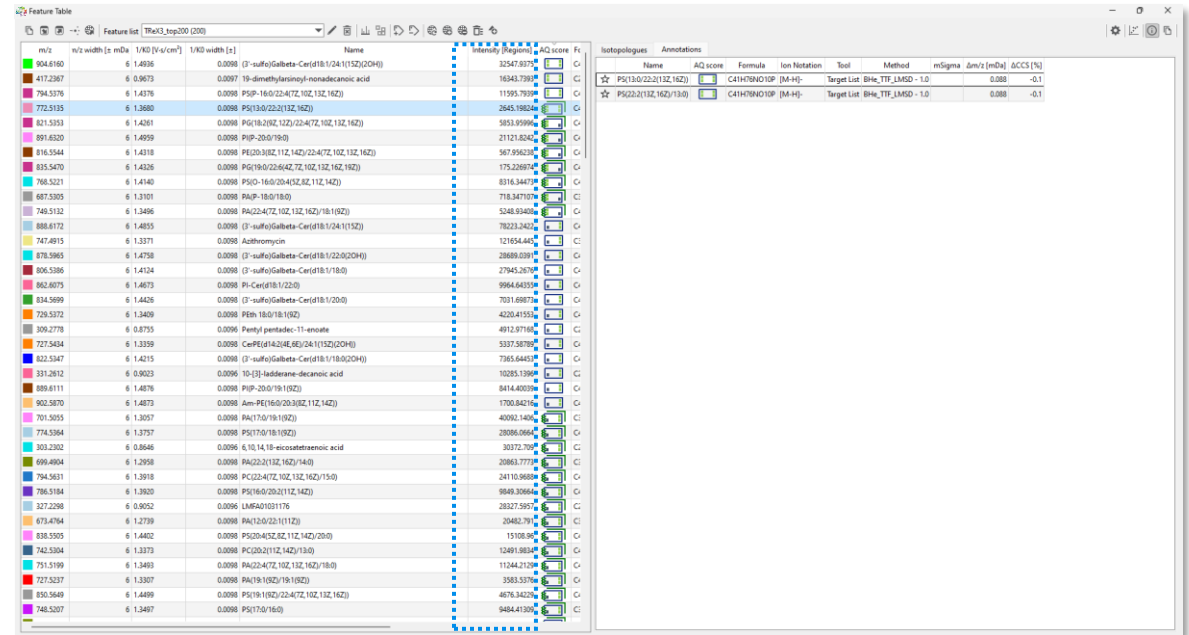
The detailed information panel shows the following data for the selected feature (PS(13:0/22:2/13Z,16Z)):

Name	AG score	Formula	Ion Notation	Tool	Method	mSigma	Am/z [mDa]	ACC [%]
PS(13:0/22:2/13Z,16Z)		C41H78NO10P	[M+H] <sup>+</sup>	Target List	BHe_TIF_LMSD - 1.0	0.088	-0.1	
PS(22:2/13Z,16Z)/13:0		C41H78NO10P	[M+H] <sup>+</sup>	Target List	BHe_TIF_LMSD - 1.0	0.088	-0.1	

# Multiple feature enhancements

## Feature Table – Intensity [Regions] column

- Previously, the Feature Table did not contain a default intensity column, and the user had to manually create one if they wanted to sort a feature list based on intensities.
- Now, 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

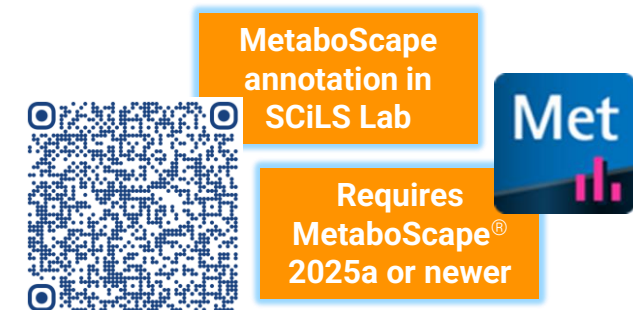
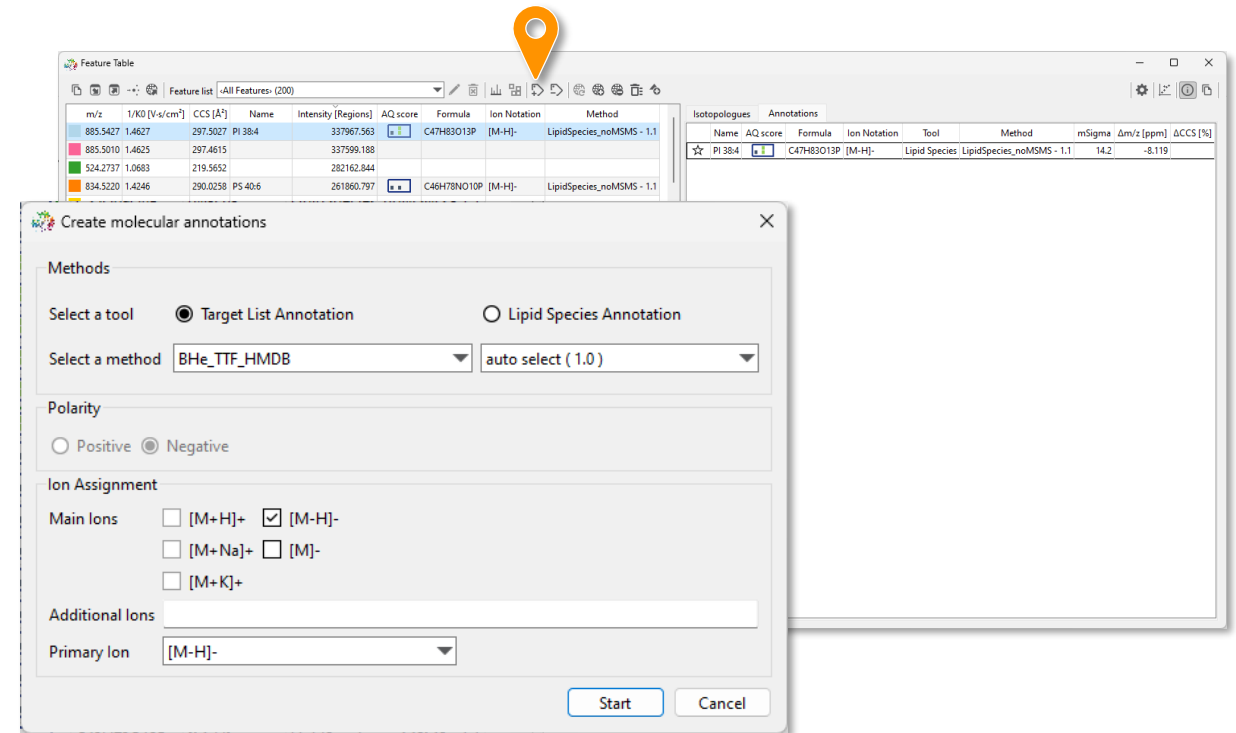


m/z	n/z width [s.mDa]	1/KD [1/s.cm <sup>2</sup> ]	1/KD width [s]	Name	Intensity [Regions]	AG score	Fr.
904.6160	6	1.4636	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/24:1/15:2)(O4H)	32547.8738		
417.2367	6	0.9673	0.0097	19-dimethylarsinoyl-nonadecanoic acid	16343.7399		
794.5376	6	1.4376	0.0098	PS19-16:0/22:4/7:2,10:2,13:2,16:2)	11595.7939		
772.5135	6	1.3680	0.0098	PS13:0/22:2/13:2,16:2)	2645.9824		
821.5353	6	1.4261	0.0098	PG18:2(8:2,12:2)/23:4/7:2,10:2,13:2,16:2)	5853.9596		
891.6320	6	1.4959	0.0098	PIP-20:0/19:0)	2121.8242		
816.5544	6	1.4318	0.0098	PE20:3(8:2,11:2,14:2)/22:4/7:2,10:2,13:2,16:2)	567.95623		
835.5470	6	1.4326	0.0098	PG19:0/22:6(4:2,7:2,10:2,13:2,16:2,19:2)	175.228874		
765.5221	6	1.4140	0.0098	PS5:0-16:0/20:4/3:2,6:2,11:2,14:2)	8316.34479		
887.5055	6	1.3101	0.0098	PA9:0-18:0/19:0)	718.34719		
748.5132	6	1.3466	0.0098	PA23:4/7:2,10:2,13:2,16:2/18:1/9:2)	5248.0540		
888.6172	6	1.4855	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/24:1/15:2)	7822.3242		
747.4915	6	1.3171	0.0098	Azithromycin	121654.44		
878.5965	6	1.4758	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/22:0/20H)	28889.0391		
806.5386	6	1.4124	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/19:0)	27945.2670		
862.6073	6	1.4673	0.0098	PI-Cer(18:1/22:0)	9964.64339		
834.5699	6	1.4426	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/20:0)	7031.69879		
726.5372	6	1.3409	0.0098	PEm 18:0/18:1/9:2)	4220.41551		
306.2778	6	0.8755	0.0096	Pentyl pentadec-11-enoate	4912.9716		
727.5434	6	1.3339	0.0098	CerPE(14:2(4E,6E)/24:1/15:2)(20H)	5337.5870		
822.5347	6	1.4215	0.0098	( <sup>3</sup> -sulfo)Galbata-Cer(18:1/18:0/20H)	7365.6443		
331.2812	6	0.9203	0.0096	10-[3]-ladderane-decanoic acid	10285.1396		
888.6111	6	1.4876	0.0098	PIP-20:0/19:1/9:2)	8414.4009		
902.5970	6	1.4673	0.0098	Am-PE(16:0/20:3(8:2,11:2,14:2))	1700.84216		
701.5053	6	1.3057	0.0098	PA(17:0/19:1/9:2)	40082.744		
774.5364	6	1.3797	0.0098	PS(17:0/18:1/9:2)	28086.0664		
303.2302	6	0.8646	0.0096	6,10,14,18-tetrasatetraenoic acid	30372.709		
699.4904	6	1.2958	0.0098	PA(22:2/13:2,16:2)/14:0)	20863.7777		
794.5631	6	1.3918	0.0098	PC(22:4/7:2,10:2,13:2,16:2)/15:0)	24110.9688		
786.5184	6	1.3920	0.0098	PS(16:0/20:2/11:2,14:2)	9849.30644		
327.2298	6	0.9052	0.0096	LMFA01031176	28327.5951		
678.4784	6	1.2739	0.0098	PA(12:0/22:1/11:2)	20482.70		
838.5505	6	1.4402	0.0098	PS(20:4/32:8:2,11:2,14:2)/20:0)	13108.86		
742.5304	6	1.3173	0.0098	PC(20:2/11:2,14:2)/19:0)	12491.9814		
751.5199	6	1.3460	0.0098	PA(22:4/7:2,10:2,13:2,16:2)/18:0)	11244.2109		
721.5237	6	1.3307	0.0098	PA(19:1/8:2/19:1/9:2)	3583.5396		
850.5649	6	1.4409	0.0098	PS(19:1/9:2)/22:4/7:2,10:2,13:2,16:2)	4876.3421		
745.5207	6	1.3487	0.0098	PS(17:0/16:0)	9484.4130		

# Multiple feature enhancements

## MetaboScape®-powered rule-based Lipid Species annotation

- An additional tool for MetaboScape–powered Molecular Annotation available
- Methods list filtered on active tool selection
- Rule-based **Lipid Species** annotation
  - m/z accuracy
  - Isotope pattern
  - Mobility (if available)
  - MS/MS (can be disabled in MetaboScape)
- In case of MS1 data, only returns species level annotations, which avoids over-interpretation of the lipid identity
  - **NOTE:** by default, Lipid Species annotation methods require MS/MS information. This parameter can be turned off in MetaboScape.



# 02

## iprm-PASEF

---

# *iprm-PASEF*

## A workflow to identify your images with confidence

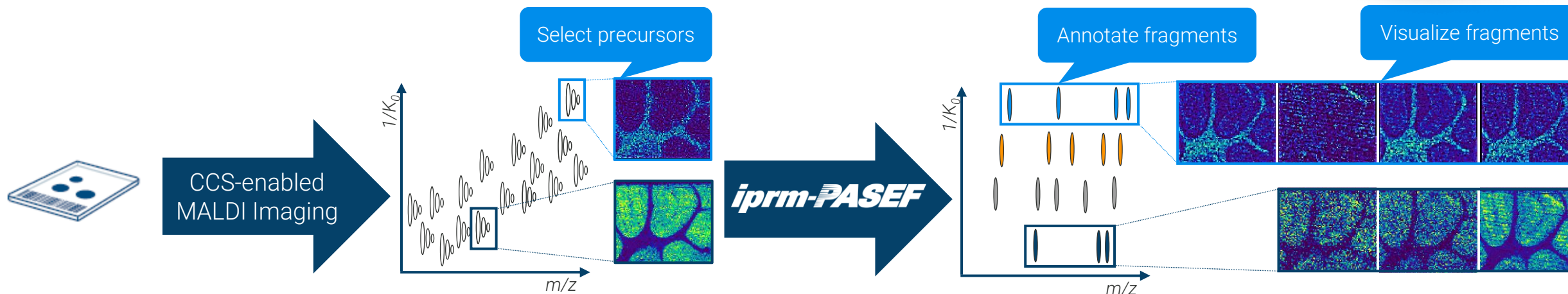
### timsTOF fleX-based targeted fragmentation with spatial fidelity

- Targeted and CCS-enabled precursor isolation and fragmentation with spatial fidelity
- The first **fully integrated** commercial imaging solution for fragmentation-based Molecular Annotation – **Acquire, Analyze, Annotate**



### *iprm-PASEF*









Powered by 4D-Multiomics





# iprm-PASEF

## Create target precursor list in SCiLS™ Lab

- New “**Export iprm-PASEF parameters**” option in CCS-enabled MALDI Imaging datasets
  - Feature table:     
  - Objects tab:  Export feature list (flexImaging, SCiLS Exchange Format, CSV)  Export feature images (OME-TIFF)  Export iprm-PASEF parameters
- **prm-PASEF setting** in timsControl determines maximum Precursor list length
  - **NOTE:** *does not alter setting in timsControl*
  - **Warning** shown when maximum feature list length is exceeded, this disables export
- Define **export format**
  - SCiLS iprm-PASEF parameter file (.spp)
    - Can include feature AND regions
    - Read by timsControl & flexImaging
  - Comma-separated values (.csv)
    - Only includes features
    - Read by timsControl

Export iprm-PASEF parameters

Select iprm-PASEF precursor features  
Select the prm-PASEF setting of your timsTOF fleX fragmentation method to select the correct (maximum) number of precursors.

**prm-PASEF setting**

Mobility-based isolation and fragmentation settings (max. 25 precursors)


m/z-based isolation and fragmentation settings (max. 15 precursors)

	<input type="checkbox"/>	m/z	CCS (Å <sup>2</sup> )	1/K0 (V-s/cm <sup>2</sup> )	1/K0 begin	1/K0 end
1	<input type="checkbox"/>	306.0752	160.3779	0.7666	0.7570	0.7761
2	<input type="checkbox"/>	346.0530	171.2776	0.8227	0.8131	0.8323
3	<input type="checkbox"/>	303.2302	180.9485	0.8646	0.8550	0.8741
4	<input type="checkbox"/>	426.0181	182.9623	0.8850	0.8754	0.8947
5	<input type="checkbox"/>	331.2612	188.1738	0.9023	0.8927	0.9119
6	<input type="checkbox"/>	327.2298	188.8679	0.9052	0.8956	0.9148
7	<input type="checkbox"/>	391.2217	195.0346	0.9409	0.9312	0.9505
8	<input type="checkbox"/>	417.2367	200.0991	0.9673	0.9576	0.9770
9	<input type="checkbox"/>	419.2527	202.2823	0.9780	0.9683	0.9877
10	<input type="checkbox"/>	437.2616	207.5131	1.0046	0.9949	1.0143
11	<input type="checkbox"/>	463.2213	207.6406	1.0069	0.9972	1.0166
12	<input type="checkbox"/>	462.2942	213.4961	1.0352	1.0256	1.0449
13	<input type="checkbox"/>	478.2880	214.3523	1.0404	1.0307	1.0501
14	<input type="checkbox"/>	500.2740	216.5045	1.0521	1.0424	1.0618
...	<input type="checkbox"/>	...	...	...	...	...

Export to SCiLS iprm-PASEF parameter file (.spp) Auto-resolve

Export to .csv

**Information**

 The current number of features exceeds the maximum for the selected prm-PASEF setting.

Export Add regions Cancel





# iprm-PASEF

## Create target precursor list in SCiLS™ Lab

- Table contains features in **current feature list**
- Precursor list **restrictions**
  - Precursor list length
    - determined by prm-PASEF setting
  - Only non-overlapping 1/K0 windows allowed
    - $1/K0_{end \rightarrow begin} \geq 0.01$
- Resolve overlapping 1/K<sub>0</sub> windows** by:
  - Manual adjust of 1/K0 begin and/or 1/K0 end values
    - Double-click on value and change
  - Uncheck conflicting features
  - Auto-resolve conflicting 1/K0 windows
    - Only enabled when number of features does not exceed maximum precursor list length
    - Adjusts 1/K0 begin and 1/K0 end values of features with overlapping 1/K0 windows
    - Always includes 1/K0 centroids of both original features
  - Export disabled until all overlapping 1/K0 are resolved

Export iprm-PASEF parameters

Select iprm-PASEF precursor features  
Select the prm-PASEF setting of your timsTOF fileX fragmentation method to select the correct (maximum) number of precursors.

prm-PASEF setting

Mobility-based isolation and fragmentation settings (max. 25 precursors)

m/z-based isolation and fragmentation settings (max. 15 precursors)

	<input type="checkbox"/>	m/z	CCS (Å <sup>2</sup> )	1/K0 (V-s/cm <sup>2</sup> )	1/K0 begin	1/K0 end
1	<input checked="" type="checkbox"/>	306.0752	160.3779	0.7666	0.7570	0.7761
2	<input checked="" type="checkbox"/>	346.0530	171.2776	0.8227	0.8131	0.8323
3	<input type="checkbox"/>	303.2302	180.9485	0.8646	0.8550	0.8741
4	<input checked="" type="checkbox"/>	426.0181	182.9623	0.8850	0.8754	0.8947
5	<input type="checkbox"/>	331.2612	188.1738	0.9023	0.8927	0.9119
6	<input type="checkbox"/>	327.2298	188.8679	0.9052	0.8956	0.9148
7	<input checked="" type="checkbox"/>	391.2217	195.0346	0.9409	0.9312	0.9505
8	<input type="checkbox"/>	417.2367	200.0991	0.9673	0.9576	0.9770
9	<input checked="" type="checkbox"/>	419.2527	202.2823	0.9780	0.9683	0.9877
10	<input type="checkbox"/>	437.2616	207.5131	1.0046	0.9949	1.0143
11	<input checked="" type="checkbox"/>	463.2213	207.6406	1.0069	0.9977	1.0166
12	<input type="checkbox"/>	462.2942	213.4961	1.0352	1.0256	1.0449
13	<input type="checkbox"/>	478.2880	214.3523	1.0404	1.0307	1.0501
14	<input checked="" type="checkbox"/>	500.2740	216.5045	1.0521	1.0424	1.0618
...	<input type="checkbox"/>	...	...	...	...	...

Export to SCiLS iprm-PASEF parameter file (.spp) Auto-resolve

Export to .csv

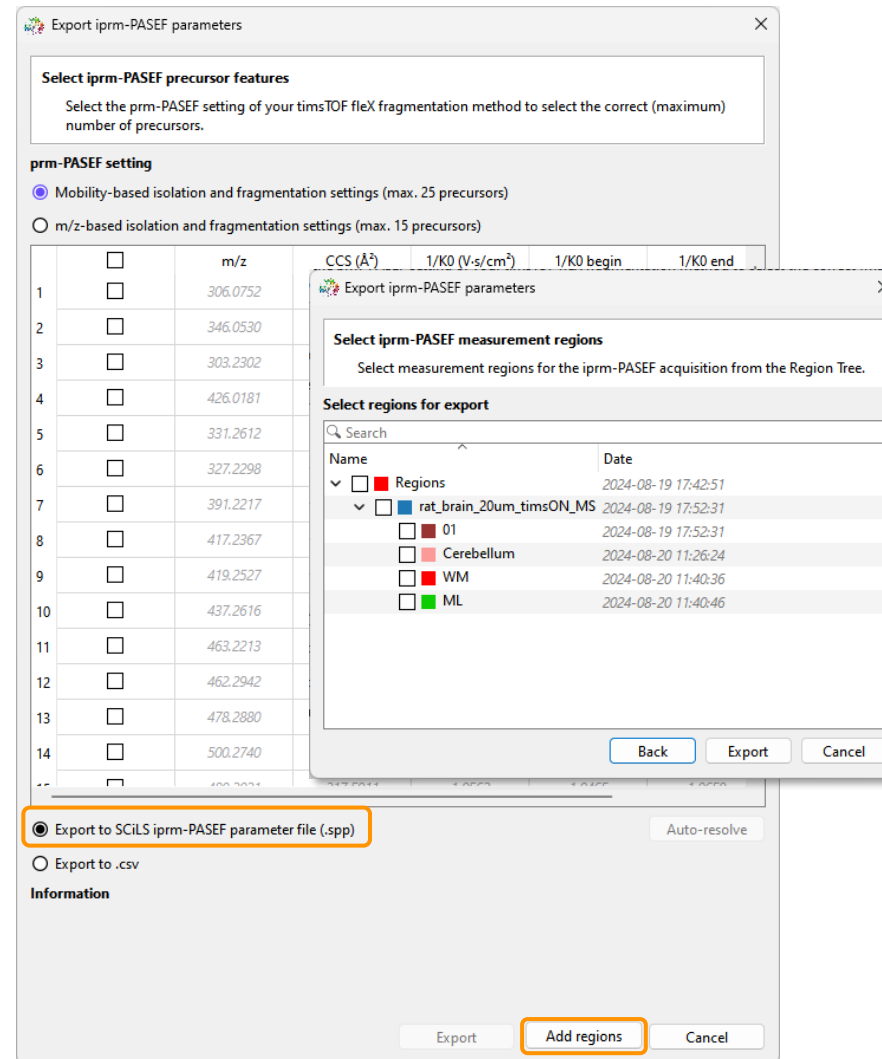
Information

Export Add regions Cancel

# iprm-PASEF

## Create target precursor list in SCiLS™ Lab

- **Add regions** to import and define measurement regions in flexImaging
  - Regions cannot overlap as flexImaging does not support overlapping measurement regions
  - Disjoined regions appear as individual measurement regions in flexImaging



**Export iprm-PASEF parameters**

Select iprm-PASEF precursor features  
Select the prrm-PASEF setting of your timsTOF fleX fragmentation method to select the correct (maximum) number of precursors.

**prrm-PASEF setting**

Mobility-based isolation and fragmentation settings (max. 25 precursors)

m/z-based isolation and fragmentation settings (max. 15 precursors)

	<input type="checkbox"/>	m/z	CCS (Å <sup>3</sup> )	1/K0 (V-s/cm <sup>2</sup> )	1/K0 begin	1/K0 end
1	<input type="checkbox"/>	306.0752				
2	<input type="checkbox"/>	346.0530				
3	<input type="checkbox"/>	303.2302				
4	<input type="checkbox"/>	426.0181				
5	<input type="checkbox"/>	331.2612				
6	<input type="checkbox"/>	327.2298				
7	<input type="checkbox"/>	391.2217				
8	<input type="checkbox"/>	417.2367				
9	<input type="checkbox"/>	419.2527				
10	<input type="checkbox"/>	437.2616				
11	<input type="checkbox"/>	463.2213				
12	<input type="checkbox"/>	462.2942				
13	<input type="checkbox"/>	478.2880				
14	<input type="checkbox"/>	500.2740				

**Export iprm-PASEF parameters**

Select iprm-PASEF measurement regions  
Select measurement regions for the iprm-PASEF acquisition from the Region Tree.

**Select regions for export**

Search

Name	Date
<input type="checkbox"/> Regions	2024-08-19 17:42:51
<input checked="" type="checkbox"/> rat_brain_20um_timsON_MS	2024-08-19 17:52:31
<input type="checkbox"/> 01	2024-08-19 17:52:31
<input type="checkbox"/> Cerebellum	2024-08-20 11:26:24
<input type="checkbox"/> WM	2024-08-20 11:40:36
<input type="checkbox"/> ML	2024-08-20 11:40:46

Export to SCiLS iprm-PASEF parameter file (.spp) Auto-resolve

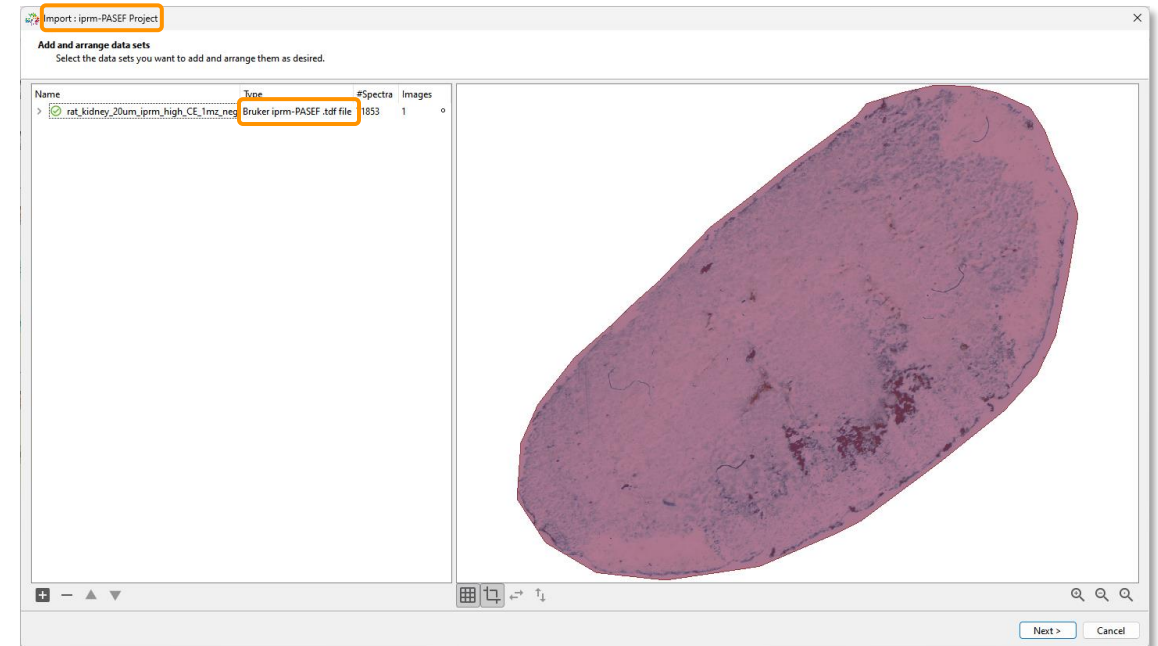
Export to .csv

**Information**

Export **Add regions** Cancel

# *iprm-PASEF* Import iprm-PASEF data into SCiLS™ Lab

- iprm-PASEF source data sets will be imported into SCiLS Lab as an **“iprm-PASEF project”**
- iprm-PASEF data cannot be mixed with other data types (e.g. “regular” .tdf timsTOF fleX data)
- T-ReX® feature finding can be performed upon manual import of iprm-PASEF projects
  - Only returns features found within the mobility boundaries of the precursor isolation windows
  - Default settings and internal parameters have been optimized for iprm-PASEF data

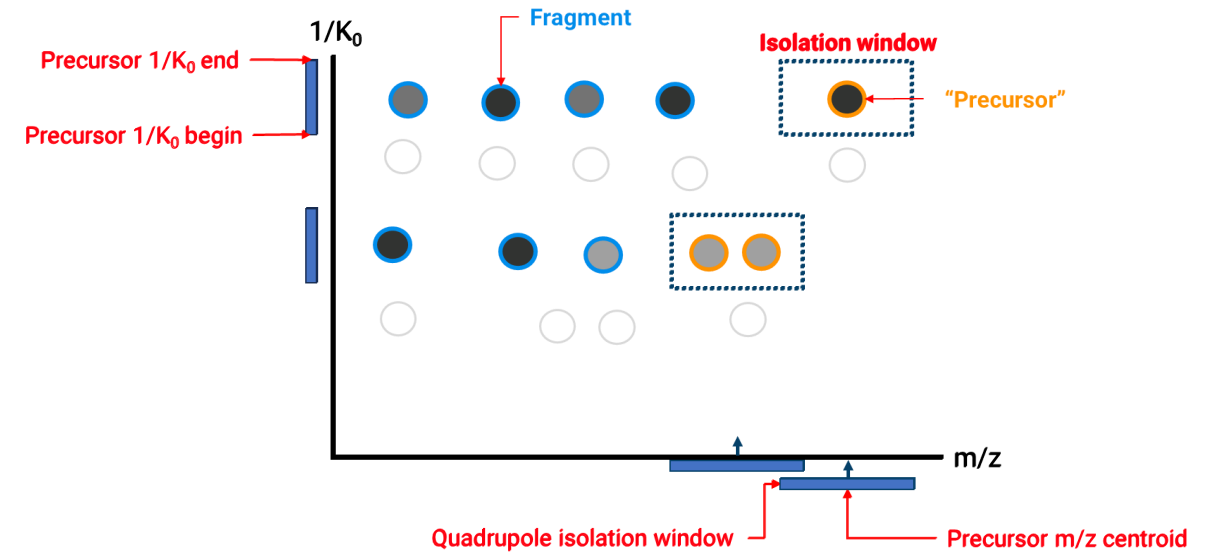




## *iprm-PASEF*

# Feature relations in iprm-PASEF data sets

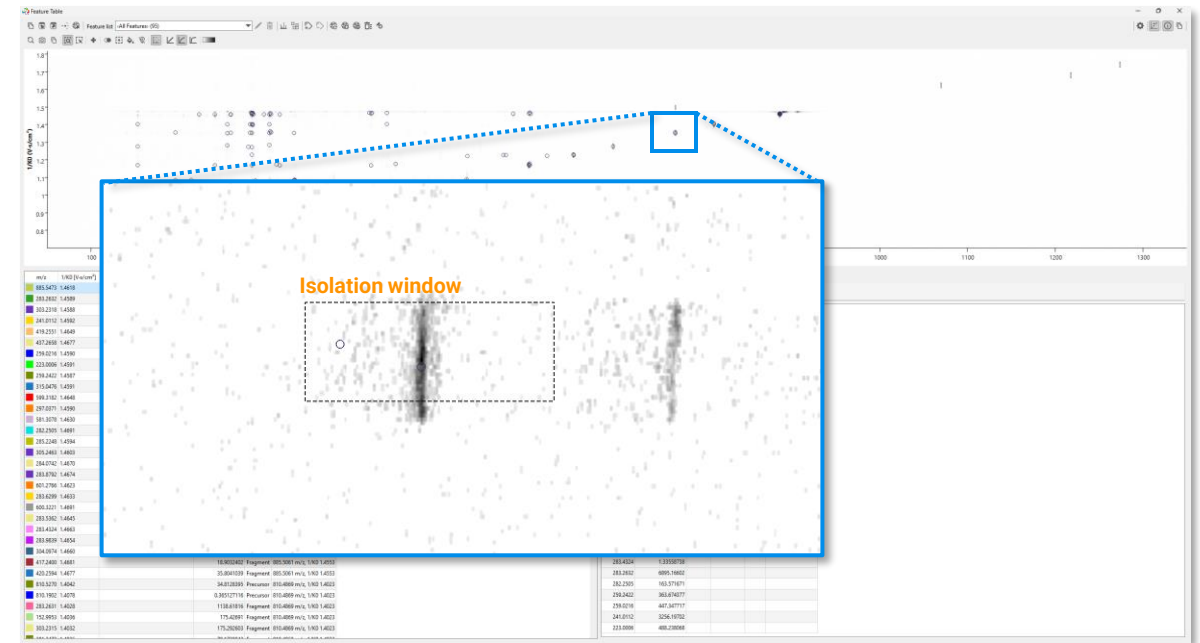
- Features are grouped by the **Isolation Windows**
- Features are split into three different types:
  - Precursors**
    - All features within quadrupole isolation window and mobility window
  - Fragments**
    - All other features within mobility windows
  - None**
    - All feature outside the isolation window
    - Are not detected by T-ReX® feature finding
- Features are automatically grouped and characterized in the Feature Table



# *iprm-PASEF*

## Feature relations in *iprm-PASEF* data sets

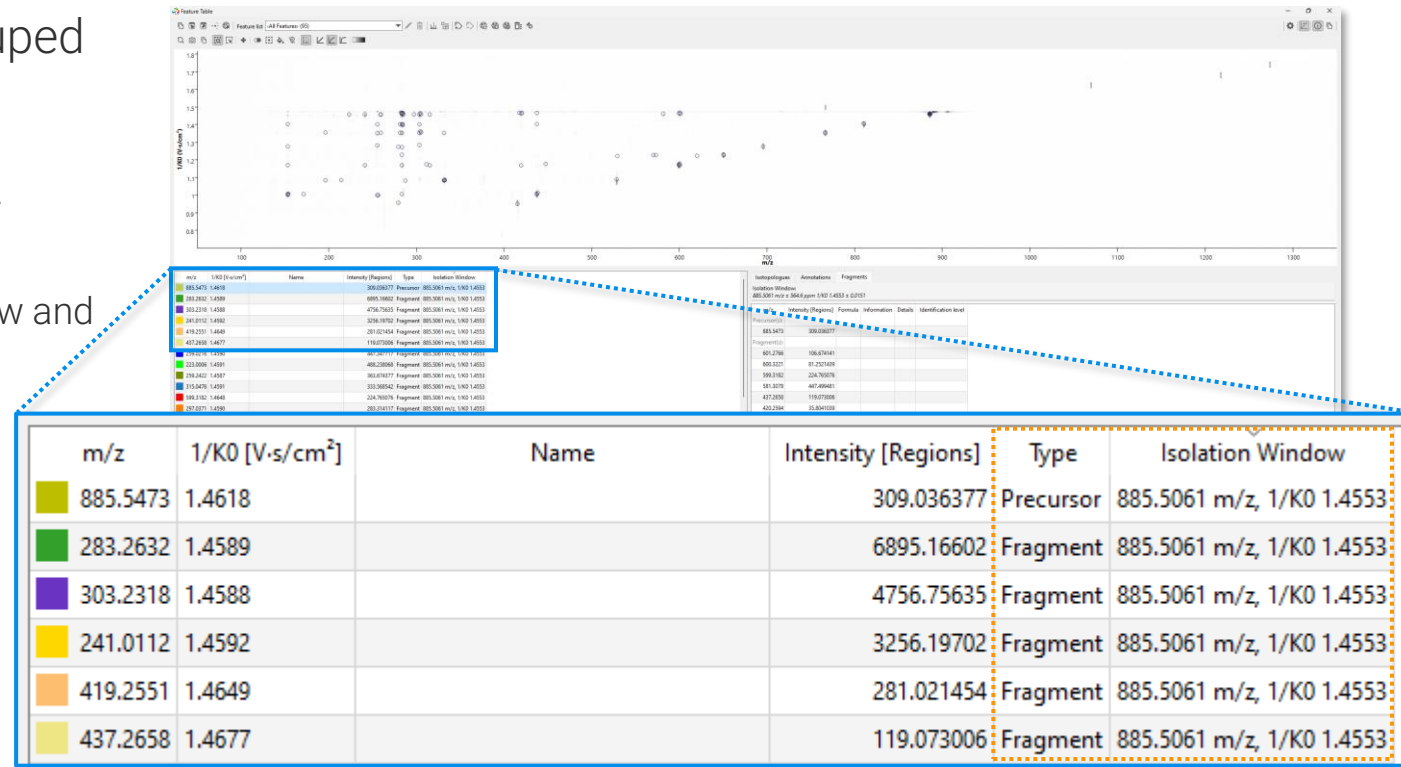
- Features are detected within and can be grouped by the **Isolation Windows**
- Features can be split into two different types:
  - Precursors**
    - All features within quadrupole isolation window and mobility window
  - Fragments**
    - All other features within mobility windows
  - None**
    - All feature outside the isolation window
    - Are not detected by T-ReX® feature finding
- Features are automatically grouped and characterized in the Feature Table



# iprm-PASEF

## Feature relations in iprm-PASEF data sets

- Features are detected within and can be grouped by the **Isolation Windows**
- Features can be split into two different types:
  - Precursors**
    - All features within quadrupole isolation window and mobility window
  - Fragments**
    - All other features within mobility windows
  - None**
    - All feature outside the isolation window
    - Are not detected by T-ReX® feature finding
- Features are automatically grouped and characterized in the Feature Table



# iprm-PASEF

## Feature relations in iprm-PASEF data sets

- Fragments sub-panel in the detailed feature information panel shows all precursors and fragments associated to the active feature and present in the active feature list

The screenshot displays the 'Isotopologues' sub-panel with a table of data. A vertical orange dashed box highlights a portion of the table, and a vertical orange text label 'Centroided & deisotoped MS/MS spectrum' is placed next to it. A zoomed-in view of the 'Fragments' sub-panel is shown to the right, mirroring the highlighted data.

m/z	Intensity [Regions]	Formula	Information	Details	Identification level
Precursor(s):					
885.5473	309.036377				
Fragment(s):					
601.2766	106.674141				
600.3221	81.2521439				
599.3182	224.765076				
581.3078	447.499481				
437.2658	119.073006				
420.2594	35.8041039				
419.2551	281.021454				
417.2400	18.9032402				
315.0476	333.568542				
305.2463	11.3184233				
304.0974	1.25566554				
303.2318	4756.75635				
297.0371	283.314117				
285.2248	47.1849403				
284.0742	1.84743583				
283.9839	1.70866454				
283.8792	1.39700389				
283.6299	1.86090302				
283.5362	1.75935328				
283.4324	1.33558738				
283.2632	6895.16602				
282.2505	163.571671				
259.2422	363.674377				
259.0216	447.347717				
241.0112	3256.19702				
223.0006	488.238068				

# MetaboScape-powered molecular annotation for iprm-PASEF



- Following MetaboScape®-powered Molecular Annotation, **precursor features are annotated** based on:

- Precursor mass error
- Precursor isotope pattern quality
- Precursor mobility error
- MS/MS spectrum

- Annotation options including MS/MS information:

- Rule-based Lipid Species annotation**
  - Requires MetaboScape 2025a or newer
  - Provides fragment annotations
- Target list w/ associated Spectral Library**
  - Requires MetaboScape 2023b or newer
  - Identifications restricted to Target list entries

m/z	Intensity [Relative]	Name	Intensity [Relative]	Type	Substance Information	Formula	Ionization	Scan	All ions
885.5473	1.4419	P1 188_204	308.08277	Precursor	885.5067 m/z, 1.80 L4033	C24H40O13P	[M+H]	Lipid Species	4/21
402.2761	1.4423	188 (acyl chain fragment neutral loss)	186.87416	Fragment	885.5067 m/z, 1.80 L4033	PC24H40O13			
880.3201	1.4481		87.251439	Fragment	885.5067 m/z, 1.80 L4033				
339.3162	1.4448		224.767076	Fragment	885.5067 m/z, 1.80 L4033				
181.8978	1.4480	204 (acyl chain fragment neutral loss)	487.688481	Fragment	885.5067 m/z, 1.80 L4033	PC27H40O13			
402.2658	1.4477		119.073006	Fragment	885.5067 m/z, 1.80 L4033				
419.2551	1.4449		19.849109	Fragment	885.5067 m/z, 1.80 L4033				
417.2463	1.4481		281.621454	Fragment	885.5067 m/z, 1.80 L4033				
115.0490	1.4481		16.8022402	Fragment	885.5067 m/z, 1.80 L4033				
355.5483	1.4480		333.982642	Fragment	885.5067 m/z, 1.80 L4033				
348.5478	1.4480		11.318423	Fragment	885.5067 m/z, 1.80 L4033				
333.2124	1.4338	204 (acyl chain fragment)	2.2988574	Fragment	885.5067 m/z, 1.80 L4033				
332.2028	1.4374		479.7655	Fragment	885.5067 m/z, 1.80 L4033	CD41O2			
342.6242	1.4420		283.214177	Fragment	885.5067 m/z, 1.80 L4033				
348.8838	1.4454		47.348483	Fragment	885.5067 m/z, 1.80 L4033				
334.792	1.4474		1.8070389	Fragment	885.5067 m/z, 1.80 L4033				
333.6201	1.4483		1.8682082	Fragment	885.5067 m/z, 1.80 L4033				
335.5482	1.4443		1.7955328	Fragment	885.5067 m/z, 1.80 L4033				
334.624	1.4460		1.3318738	Fragment	885.5067 m/z, 1.80 L4033				
332.6242	1.4489	188 (acyl chain fragment)	6895.1662	Fragment	885.5067 m/z, 1.80 L4033	C18H30O2			
332.2028	1.4481		182.217871	Fragment	885.5067 m/z, 1.80 L4033				
338.4422	1.4487		364.617277	Fragment	885.5067 m/z, 1.80 L4033				
336.2028	1.4490	head group fragment	447.847777	Fragment	885.5067 m/z, 1.80 L4033				
34.4915	1.4482		3386.1762	Fragment	885.5067 m/z, 1.80 L4033	CD41O2			
233.0006	1.4391		488.238806	Fragment	885.5067 m/z, 1.80 L4033				
181.8978	1.4478	P1 188_204	348.018395	Precursor	810.4888 m/z, 1.80 L4023	C48H78O13P	[M+H]	Lipid Species	6/21
437.2463	1.4239		27.3308	Fragment	810.4888 m/z, 1.80 L4023				
332.2028	1.4432	204 (acyl chain fragment)	173.202803	Fragment	810.4888 m/z, 1.80 L4023	C28H30O2			
342.6242	1.4438		54.262979	Fragment	810.4888 m/z, 1.80 L4023				
344.624	1.4434		0.47361168	Fragment	810.4888 m/z, 1.80 L4023				
332.2028	1.4428	188 (acyl chain fragment)	118.81878	Fragment	810.4888 m/z, 1.80 L4023	C18H30O2			
331.2027	1.4428		76.175842	Fragment	810.4888 m/z, 1.80 L4023				
332.2028	1.4432		54.458879	Fragment	810.4888 m/z, 1.80 L4023				
152.893	1.4238	head group fragment	175.42391	Fragment	810.4888 m/z, 1.80 L4023	C18H30O2			
338.4717	1.3211		26.848138	Precursor	786.5047 m/z, 1.80 L2336				
786.5048	1.3278		0.26899119	Precursor	786.5047 m/z, 1.80 L2336				
331.2638	1.3338		107.758198	Fragment	786.5047 m/z, 1.80 L2336				
332.4439	1.3275		34.471447	Fragment	786.5047 m/z, 1.80 L2336				
334.2219	1.3481		49.907711	Fragment	786.5047 m/z, 1.80 L2336				
332.2027	1.3338		1488.8006	Fragment	786.5047 m/z, 1.80 L2336				
332.6242	1.3346		3028.7881	Fragment	786.5047 m/z, 1.80 L2336				
334.2638	1.3353		47.848734	Fragment	786.5047 m/z, 1.80 L2336				
338.4422	1.3254		115.184621	Fragment	786.5047 m/z, 1.80 L2336				
332.2021	1.3221		423.141359	Fragment	786.5047 m/z, 1.80 L2336				
336.6253	1.3284		21.254546	Fragment	786.5047 m/z, 1.80 L2336				
349.9461	1.2712		16.781702	Precursor	885.4514 m/z, 1.80 L2775				
332.2024	1.2832		76.071495	Fragment	885.4514 m/z, 1.80 L2775				
332.8214	1.2733		9.182481	Fragment	885.4514 m/z, 1.80 L2775				
279.2523	1.2752		24.988044	Fragment	885.4514 m/z, 1.80 L2775				
335.2020	1.2831		35.168240	Fragment	885.4514 m/z, 1.80 L2775				
332.896	1.2770		31.775826	Fragment	885.4514 m/z, 1.80 L2775				



Acquire Bruker Spectral Libraries here:

MetaboScape annotation in SCiLS Lab





# iprm-PASEF

## MetaboScape-powered molecular annotation for iprm-PASEF

- Annotations sub-panel** of the detailed feature information displays all annotations associated to the Isolation Window of the active feature.
  - Annotations are sorted by AQ score
  - The highest-ranking annotation is active by default
  - Only one active annotation per isolation window
- Fragments sub-panel** of the detailed feature information shows the annotations of the fragments that “explain” the active annotation
  - Fragment annotations are also added to the Name column of the Feature Table

The screenshot displays the MetaboScape software interface. The top panel shows a list of features with columns for Name, Intensity [Regions], Type, Isolation Window, Formula, Ion Notation, Tool, and AQ score. The middle panel, titled 'Annotations', shows an 'Isolation Window' of 885.5061 m/z ± 564.6 ppm 1/K0 1.4553 ± 0.0151. Below this, a table lists annotations with columns for Name, Precursor m/z, AQ score, Formula, Ion Notation, Tool, Method, and mSigma. The bottom panel, titled 'Fragments', shows a table with columns for m/z, Intensity [Regions], Formula, Information, Details, and Identification level. The interface includes navigation icons like a magnifying glass and a plus sign.

Name	Precursor m/z	AQ score	Formula	Ion Notation	Tool	Method	mSigma
PI 18:0_20:4	885.5473	309.036377	C47H83O13P [M-H]-		Lipid Species	LipidSpecies_MSMS - 1.5	1000.0
PI 38:4	885.5473	309.036377	C47H83O13P [M-H]-		Lipid Species	LipidSpecies_MSMS - 1.5	1000.0

m/z	Intensity [Regions]	Formula	Information	Details	Identification level
885.5473	309.036377	C47H83O13P	PI 18:0_20:4		
601.2766	106.674141	PC29H46O11^1-	acyl chain fragment neutral loss 18:0		molecular species level
600.3221	81.2521439				
599.3182	224.765076				
581.3078	447.499481	PC27H50O11^1-	acyl chain fragment neutral loss 20:4		molecular species level
437.2658	119.073006				
420.2594	35.8041039				
419.2551	281.021454				
417.2400	18.9032402				
315.0476	333.568542				
305.2463	11.3184233				
304.0974	1.25566554				
303.2318	4756.75635	C20H31O2^1-	acyl chain fragment	20:4	molecular species level
297.0371	283.314117				
285.2248	47.1849403				
284.0742	1.84743583				
283.9839	1.70866454				
283.8792	1.39700389				
283.6299	1.86090302				
283.5362	1.75935328				
283.4324	1.33558738				
283.2632	6895.16602	C18H35O2^1-	acyl chain fragment	18:0	molecular species level
282.2505	163.571671				
259.2422	363.674377				
259.0216	447.347717				
241.0112	3256.19702	CGH10O8P^1-	head group fragment		species level
223.0006	488.238068				

# *iprm-PASEF* Display fragment ion images

The screenshot displays the SCILS Lab MVS software interface. The main window shows a 3D visualization of a leaf structure, with a blue callout bubble pointing to it that says "Fragment ion images". Below the 3D view is a mass spectrum plot with "Absolute Intensity" on the y-axis and "m/z" on the x-axis. A blue callout bubble points to the mass spectrum with the text "Fragment annotations". On the right side, there is a control panel with various settings. A blue callout bubble points to the "Sort by" dropdown menu, which is set to "m/z", with the text "Sort by name, isolation window, etc.". The control panel also shows a table of regions and a list of ion images.

Name	Date
Regions	2024-09-06 16:54:00
ratrain_20_iprm-PASEF	2024-09-06 16:58:01

m/z	Intensity	Label
241.0112	15 ppm	1/K0 1.4592 ± 0.01 head group fragment
283.2632	15 ppm	1/K0 1.4589 ± 0.01 18:0 (acyl chain fragment)
303.2318	15 ppm	1/K0 1.4588 ± 0.01 20:4 (acyl chain fragment)
581.3078	15 ppm	1/K0 1.463 ± 0.01 20:4 (acyl chain fragment neutral loss)
601.2766	15 ppm	1/K0 1.4623 ± 0.01 18:0 (acyl chain fragment neutral loss)
885.5473	15 ppm	1/K0 1.4618 ± 0.01 PI 18:0_20:4

# 03

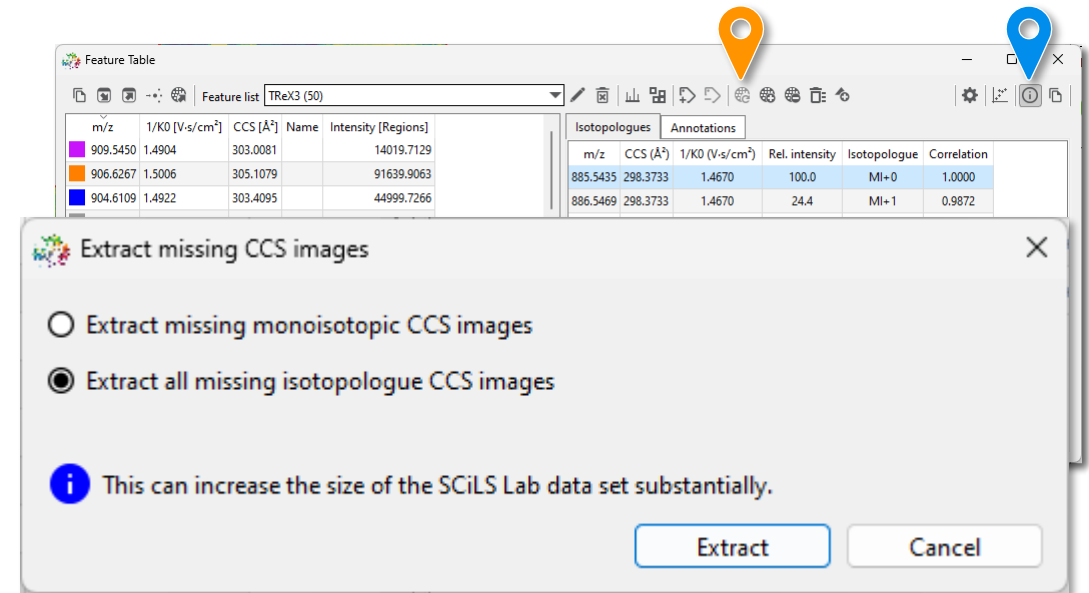
## T-ReX<sup>®</sup> feature finding

---

# T-ReX feature finding

## Display T-ReX® isotopologues in SCiLS™ Lab

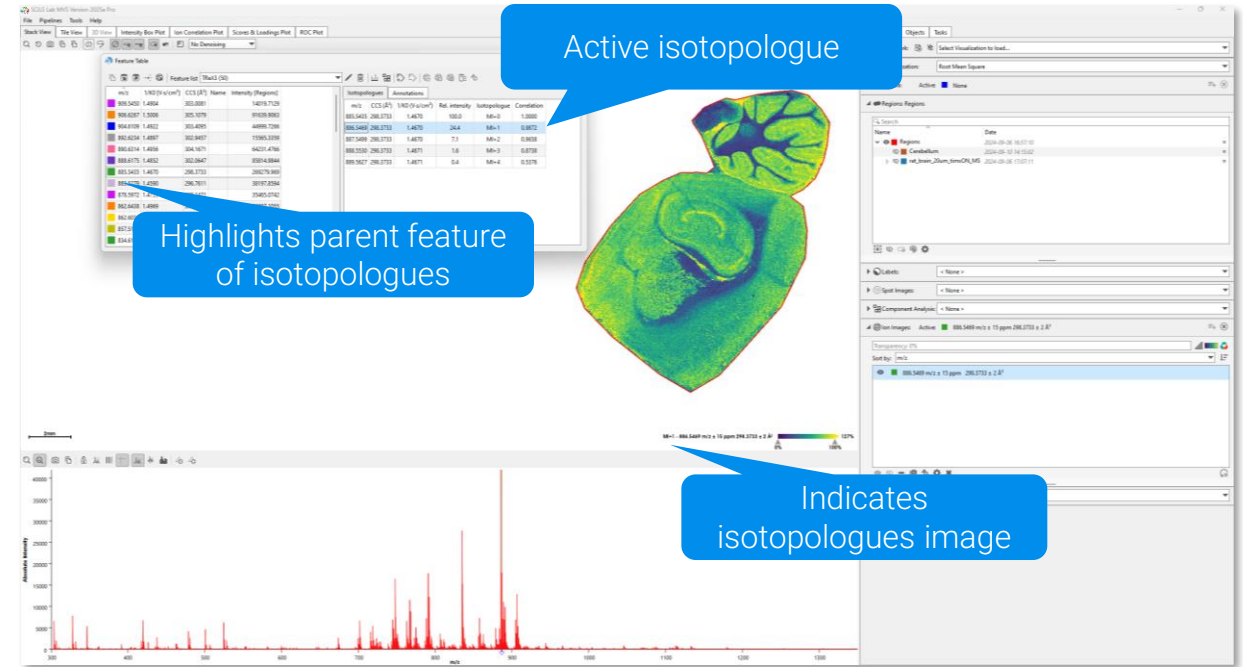
- T-ReX feature finding algorithm performs **deisotoping**, and stores the isotopologue details with its features
- The **isotopologues** sub-panel of the detailed feature information shows the isotopologues detected by T-ReX feature finding
- For CCS-enabled images, isotopologues ion images can be extracted separately
- Relative isotopologue intensities are extracted by the T-ReX feature finding algorithm.
- Correlation column shows Pearson correlation between the isotopologue and the monoisotope



# T-ReX feature finding

## Display T-ReX® isotopologues in SCiLS™ Lab

- Isotopologue features can be added to the Ion Image list and shown in various plots:
  - Correlation plots
  - Correlation table
  - Box plots
  - ROC plots



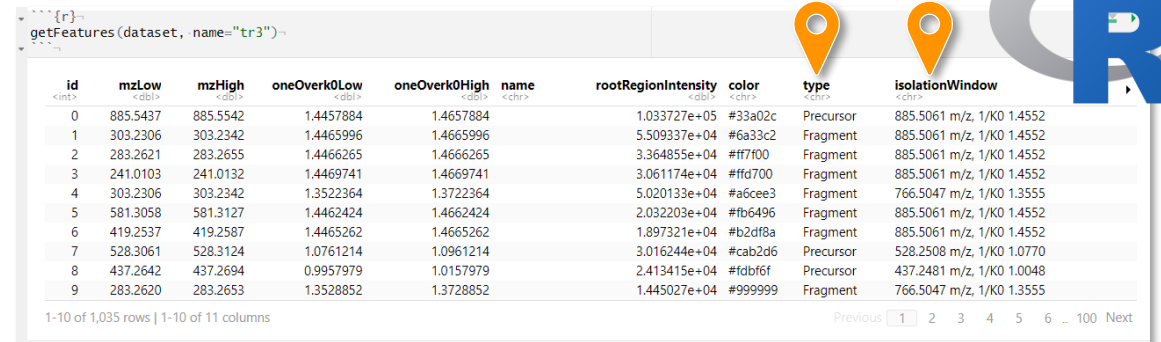
# 04

## SCiLS API improvements

---

# SCiLS API improvements

- Added support for R 4.4, binary package for R 4.2 removed
- Normalizations** can now be called via **Name**, rather than their uuid's
- For **iprm-PASEF** data sets, the Fragment and Precursor types, as well as their relation to the Isolation Windows is maintained, and shown in the Feature table.
  - This allows **easy reconstruction of MS/MS spectra** for auxiliary database searches.



```
[r]-
getFeatures(dataset, name="tr3")
```

id	mzLow	mzHigh	oneOverkLow	oneOverkHigh	name	rootRegionIntensity	color	type	isolationWindow
0	885.5437	885.5542	1.4457884	1.4657884		1.033727e+05	#33a02c	Precursor	885.5061 m/z, 1/K0 1.4552
1	303.2306	303.2342	1.4465996	1.4665996		5.509337e+04	#6a33c2	Fragment	885.5061 m/z, 1/K0 1.4552
2	283.2621	283.2655	1.4466265	1.4666265		3.364855e+04	#ff7f00	Fragment	885.5061 m/z, 1/K0 1.4552
3	241.0103	241.0132	1.4469741	1.4669741		3.061174e+04	#ffd700	Fragment	885.5061 m/z, 1/K0 1.4552
4	303.2306	303.2342	1.3522364	1.3722364		5.020133e+04	#a6cee3	Fragment	766.5047 m/z, 1/K0 1.3555
5	581.3058	581.3127	1.4462424	1.4662424		2.032203e+04	#fb6496	Fragment	885.5061 m/z, 1/K0 1.4552
6	419.2537	419.2587	1.4465262	1.4665262		1.897321e+04	#b2df8a	Fragment	885.5061 m/z, 1/K0 1.4552
7	528.3061	528.3124	1.0761214	1.0961214		3.016244e+04	#cab2d6	Precursor	528.2508 m/z, 1/K0 1.0770
8	437.2642	437.2694	0.9957979	1.0157979		2.413415e+04	#fdbf6f	Precursor	437.2481 m/z, 1/K0 1.0048
9	283.2620	283.2653	1.3528852	1.3728852		1.445027e+04	#999999	Fragment	766.5047 m/z, 1/K0 1.3555

1-10 of 1,035 rows | 1-10 of 11 columns

# 05

## neofleX support

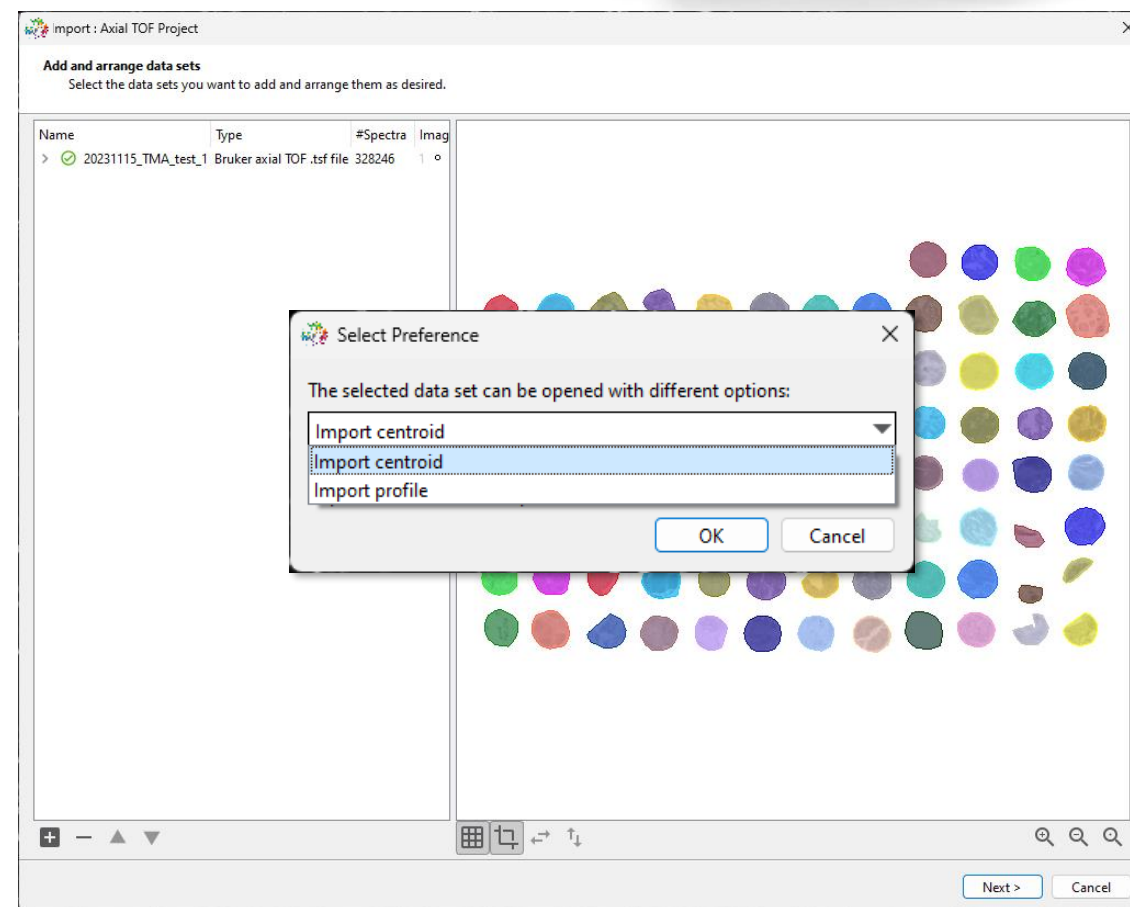
---



*neofleX* support

## Importing neofleX data into SCiLS™ Lab

- SCiLS Lab 2025a can read .d/tsf data acquired by the all-new **neofleX** axial TOF instrument
- Import **centroid** or **profile** neofleX data into a SCiLS Lab “Axial TOF project”
- neofleX profile data can be combined with rapifleX profile data (.d container format)
- Combining centroid and profile axial TOF data is not supported
- T-ReX® Feature Finding is not enabled for neofleX data sets



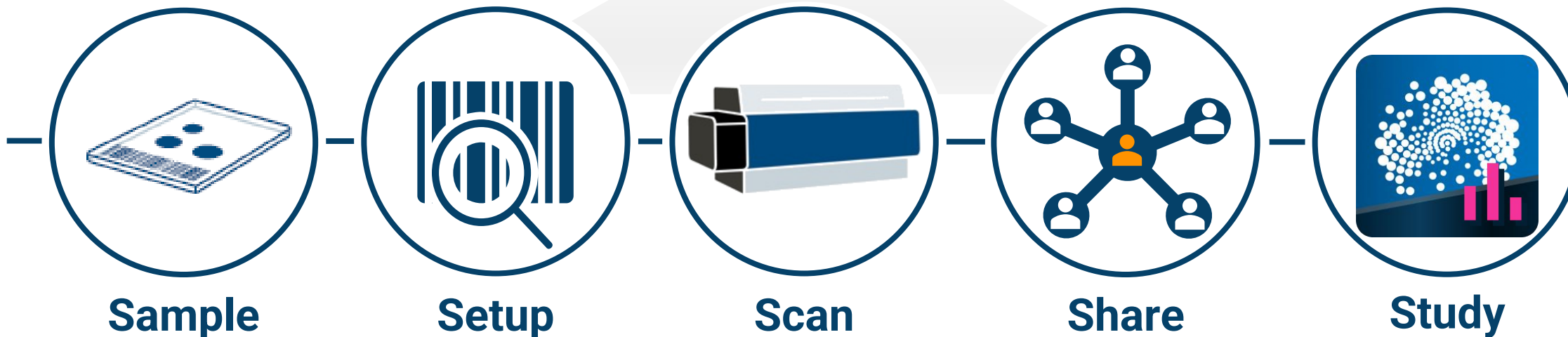


neofleX support

# SCiLS™ autopilot – smoothly from sample to images

Powered by

## SCiLS autopilot



**Automated acquisition setup for neofleX, timsTOF fleX & rapifleX**

**Automated SCiLS™ Lab data import and pre-processing**

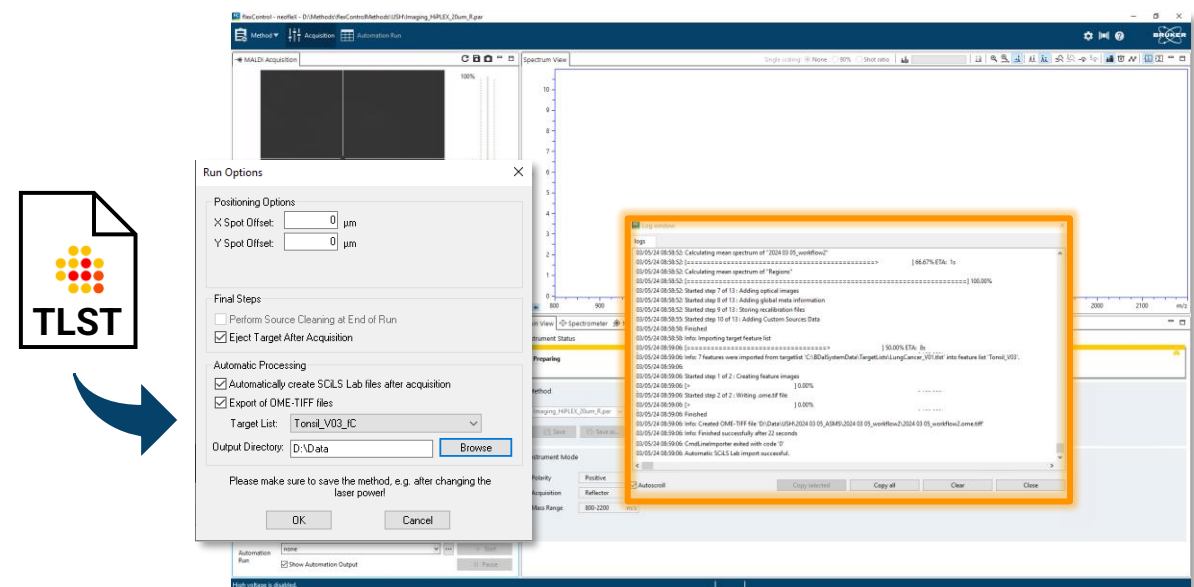
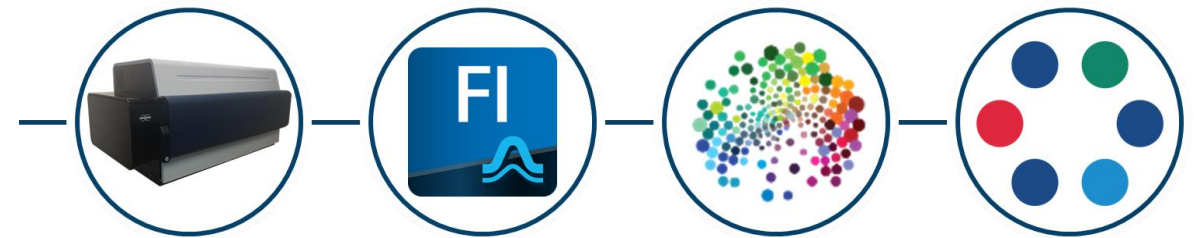
**Automated image extraction and OME-TIFF export**



# Multiple feature enhancements

## Auto-convert to OME-TIFF

- **SCiLS autopilot** can now automatically generate a SCiLS Lab file, and export the features specified in a Target List (.tlst) file to **OME-TIFF format**
- Acquisition PC needs access to an **active SCiLS Lab license** (no seat consumed), or the **SCiLS autopilot converter license**
- Requires the following software versions:
  - flexControl 5.0
  - flexImaging 7.5
  - SCiLS Lab 2024b

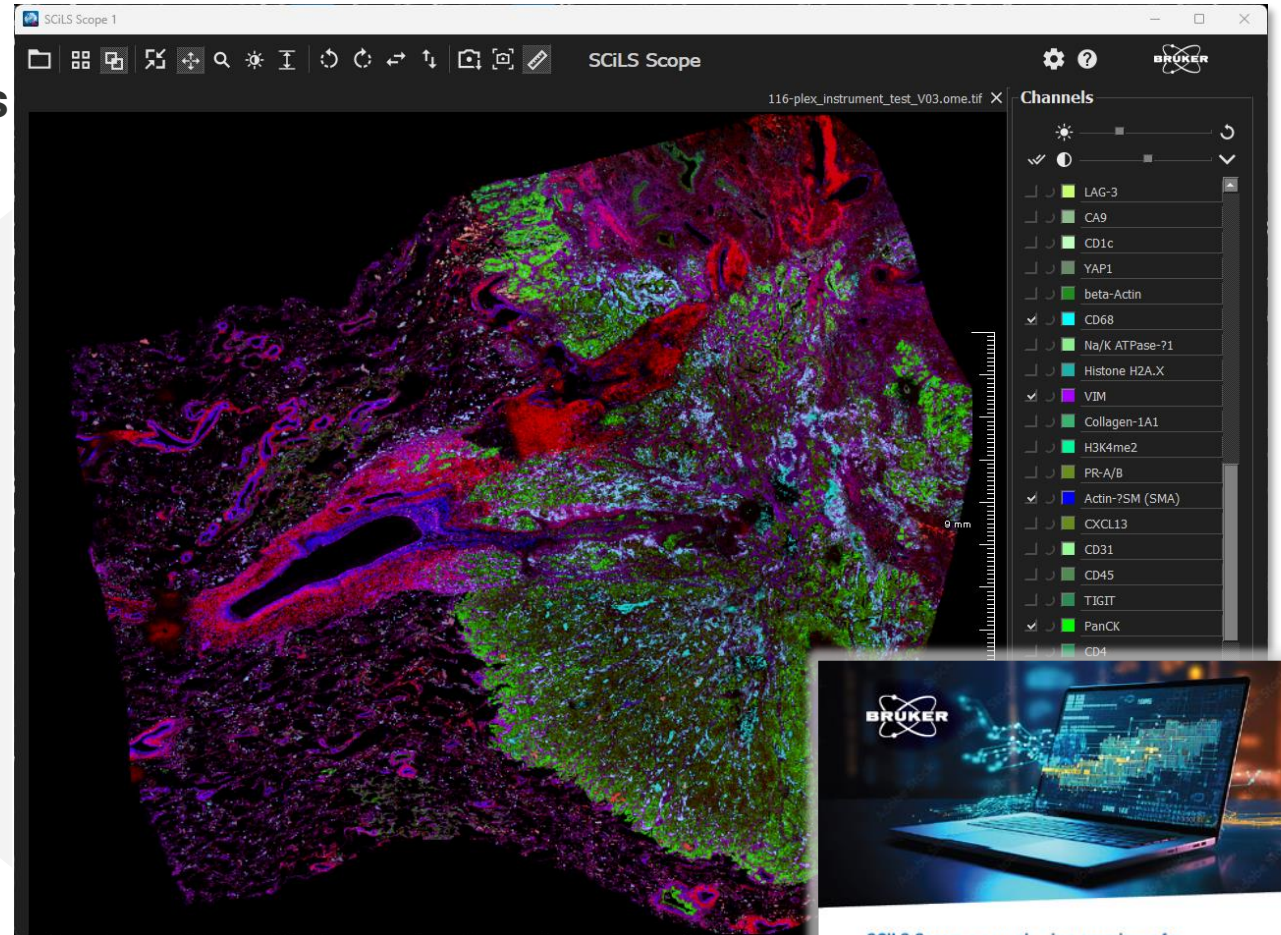
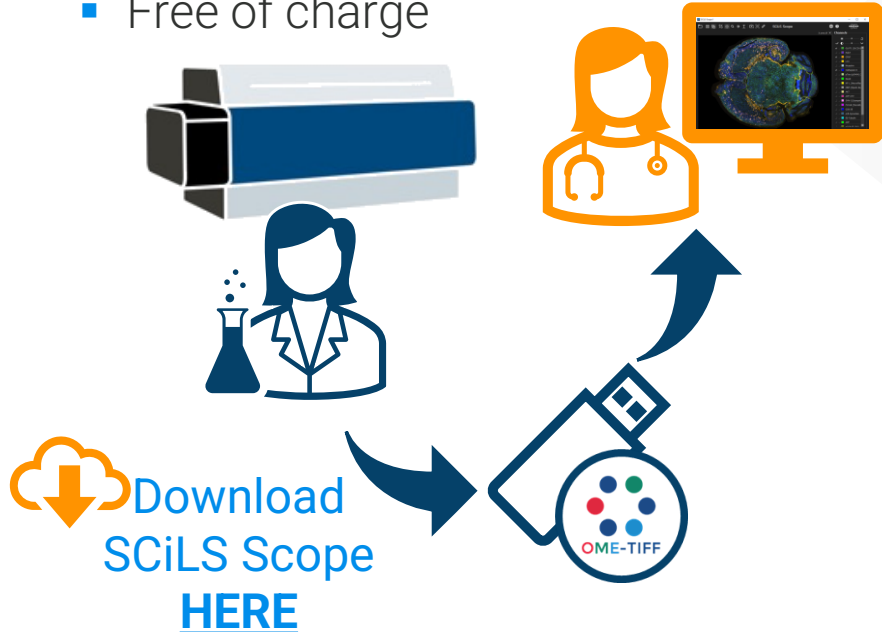




# SCiLS™ Scope – access images in an instant

## Easy-to-use viewer for MALDI HiPLEX-IHC images

- Share results efficiently in OME-TIFF format
- Select and adjust your images of interest
- Measure distances between relevant structures
- Free of charge



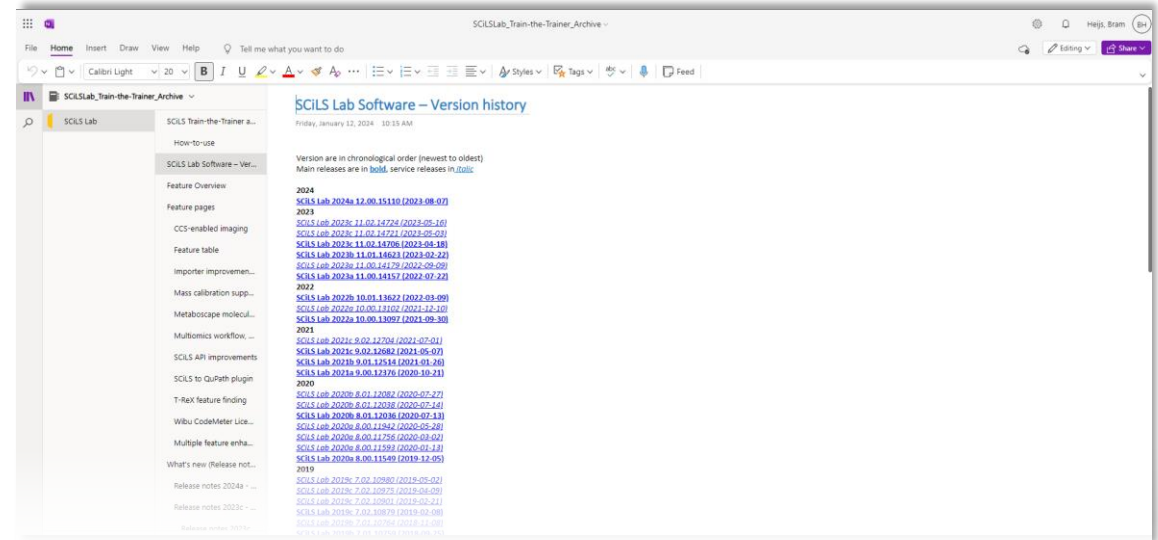


# SCiLS™ Lab Train-the-trainer Archive

---

# SCiLS™ Lab Train-the-trainer Archive

- What does it contain?
  - SCiLS Lab change log
  - Feature development history
  - Links to available Train-the-Trainer slides
  
- What's it for?
  - Knowledge transfer
  - Consolidating SCiLS Lab training material
  - Easy access to SCiLS Lab training material
  
- Where to find it?
  - MS TEAMS > TEAMS > IMM > SCiLSLab
    - Files > Release Notes & What's New
      - [SCiLSLab\\_Train-the-Trainer\\_Archive](#)



Release notes



Feature overview



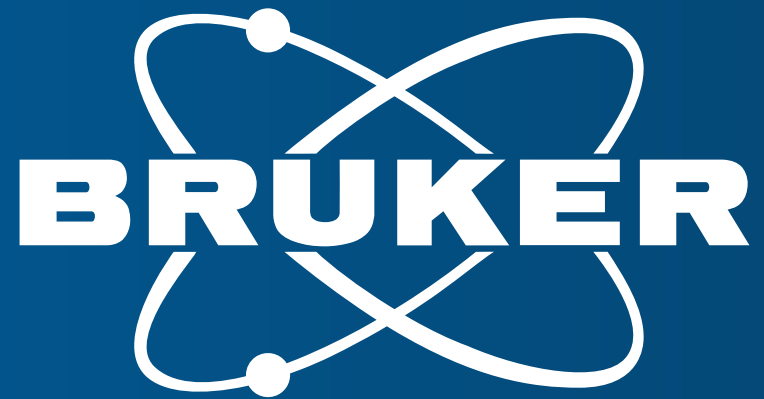
Train-the-Trainer slides

# Thank you!

**Bram Heijs, PhD**

Product Owner R&D, SCiLS Lab

[bram.heijs@bruker.com](mailto:bram.heijs@bruker.com)



Innovation with Integrity