

LIFE SCIENCE MASS SPECTROMETRY

SCiLS™ Lab 2024a – What's New?

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- 01** *MetaboScape molecular annotation:*
New integrated annotation workflow
- 02** *Multionomics imaging:*
Improved fusion of multionomics imaging data into one dataset
- 03** *Improved timsTOF fleX TIMS data import:*
Higher accuracy for low intensity features
- 04** *Calibration information stored with timsTOF fleX data:*
More transparent and reliable compatibility with re-calibration workflows

Integrated MetaboScape molecular annotation workflow

User manual, Section 3.1.5

Feature Table

m/z	CCS [Å²]	Name
419.2793 m/z ± 0.013 Da	211.6069 ± 2	
453.1949 m/z ± 0.013 Da	210.6931 ± 2	
465.2478 m/z ± 0.013 Da	204.2788 ± 2	
469.1612 m/z ± 0.013 Da	211.735 ± 2	
496.3441 m/z ± 0.013 Da	229.4164 ± 2	

Create molecular annotations

Methods
 Select a method: Lipid Maps Structure Database | auto select (1.0)

Polarity
 Positive Negative

Ion Assignment
 Main Ions: [M+H]⁺ [M-H]⁻
 [M+Na]⁺ [M]⁻
 [M+K]⁺

Additional Ions:

Primary Ion: [M+H]⁺

Start Cancel

1. Launch molecular annotation tool from SCiLS Lab feature table
2. Specify annotation method and ion assignment parameters
3. Metaboscape background engine creates molecular annotations

Feature Table

m/z	CCS [Å²]	Name	AQ score	MA	Formula	Ion Notation	Tool	Method
419.2793 m/z ± 0.013 Da	211.6069 ± 2	Oblatone D		TL	C25H38O5	[M+H] ⁺	Target List	Lipid Maps Structure Database
453.1949 m/z ± 0.013 Da	210.6931 ± 2	Heteroartoinin A		TL	C26H28O7	[M+H] ⁺	Target List	Lipid Maps Structure Database
465.2478 m/z ± 0.013 Da	204.2788 ± 2	Testosterone glucuronide		TL	C25H36O8	[M+H] ⁺	Target List	Lipid Maps Structure Database
469.1612 m/z ± 0.013 Da	211.735 ± 2	Dichamanetin		TL	C29H24O6	[M+H] ⁺	Target List	Lipid Maps Structure Database
496.3441 m/z ± 0.013 Da	229.4164 ± 2	PE(19:0/0:0)			C24H50NO7P	[M+H] ⁺	Target List	Lipid Maps Structure Database



4. Use MetaboScape AQ scores to rank features in SCiLS Lab feature table
5. Compare multiple candidate assignments in SCiLS Lab annotation detail view

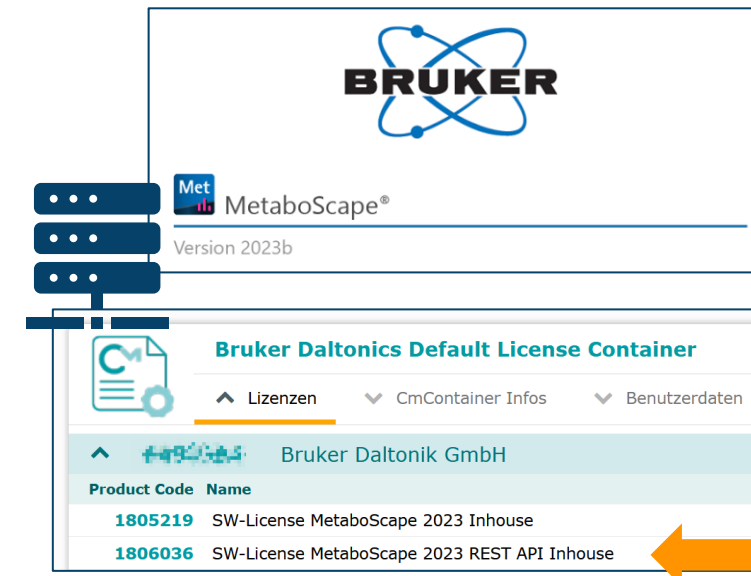
Feature Table

Name	AQ score	Name	AQ score	Formula	Ion Notation	Tool	Method	mSigma	Δm/z [Da]	ΔCCS [%]
PA(P-16:0/21:0)		PA(P-16:0/21:0)		C40H79O7P	[M+H] ⁺	Target List	Lipid Maps Structure Database - 1.0	20.2	0.002	0.9
PG(15:0/16:0)		PA(P-20:0/17:0)		C40H79O7P	[M+H] ⁺	Target List	Lipid Maps Structure Database - 1.0	20.2	0.002	1.1
PE(20:5(5Z,8Z,11Z,14Z,17Z)/...)		PA(P-18:0/19:0)		C40H79O7P	[M+H] ⁺	Target List	Lipid Maps Structure Database - 1.0	20.2	0.002	1.2
PG(20:5(5Z,8Z,11Z,14Z,17Z)/...)		PA(O-20:0/17:1(9Z))		C40H79O7P	[M+H] ⁺	Target List	Lipid Maps Structure Database - 1.0	20.2	0.002	1.6
PA(P-16:0/22:0)		PA(O-18:0/19:1(9Z))		C40H79O7P	[M+H] ⁺	Target List	Lipid Maps Structure Database - 1.0	20.2	0.002	1.7
PC(P-16:0/16:0)										

Molecular annotation – MetaboScape requirements and setup

Requirements:

- MetaboScape 2023b or later
- Separate MetaboScape REST API license item
- MetaboScape API server addressable from SCiLS Lab workstation
 - May be a local server on same workstation

BRUKER

MetaboScape®
Version 2023b

Brucker Daltonics Default License Container

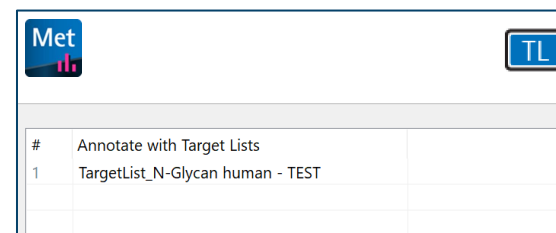
Lizenzen CmContainer Infos Benutzerdaten

Brucker Daltonik GmbH

Product Code	Name
1805219	SW-License MetaboScape 2023 Inhouse
1806036	SW-License MetaboScape 2023 REST API Inhouse

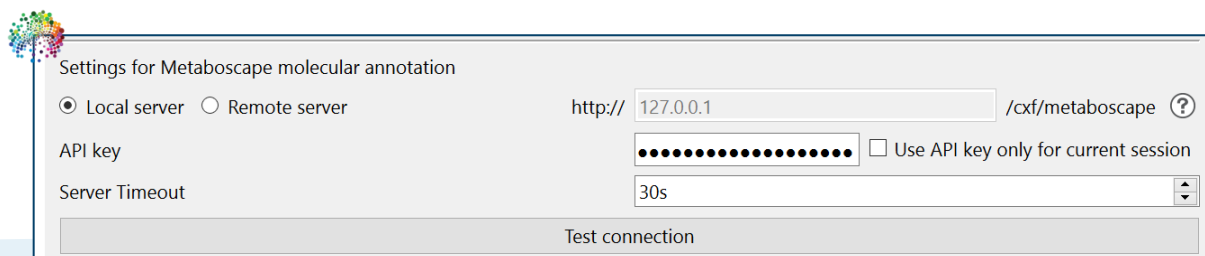
Setup:

- Configure MetaboScape annotation methods
 - Only target list annotation tool currently supported
- Create API key for MetaboScape user
- Configure MetaboScape server access in SCiLS Lab Settings



#	Annotation Method
1	TargetList_N-Glycan human - TEST

User manual,
Section 6.1



Settings for Metaboscape molecular annotation

Local server Remote server

http:// 127.0.0.1 /cxf/metaboscape ?

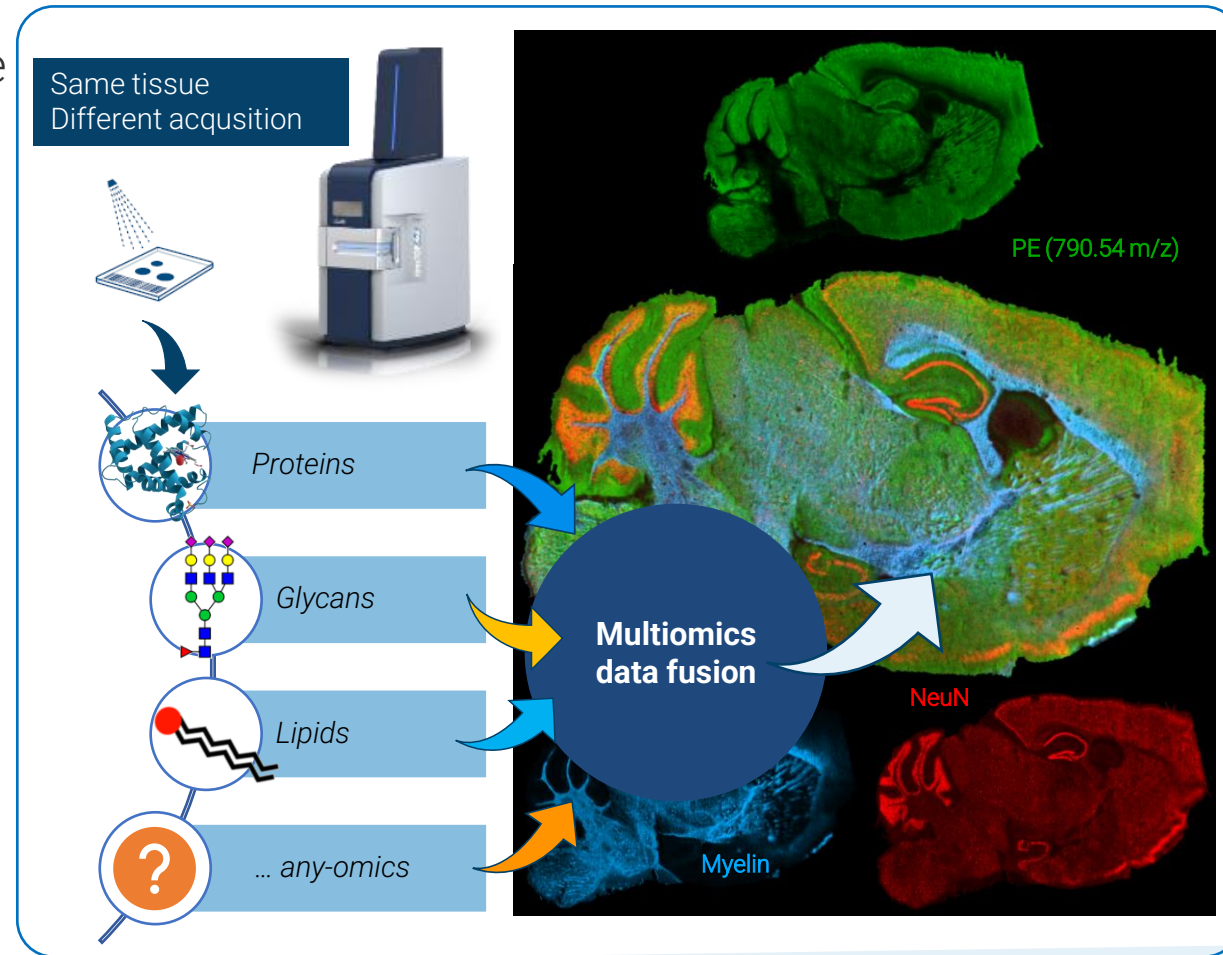
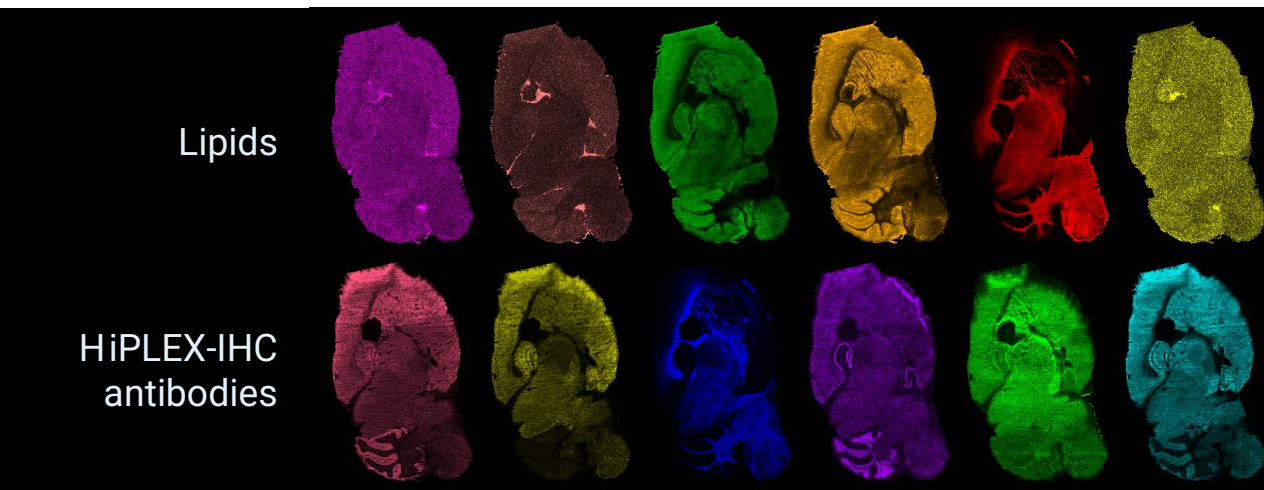
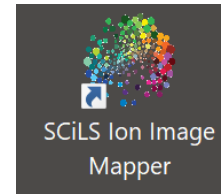
API key Use API key only for current session

Server Timeout 30s

Test connection

Multomics imaging workflow

- Use **SCiLS Ion Image Mapper** for multomics data fusion
 - Ion images from multiple acquisitions from the same tissue sample are combined into one dataset
- SCiLS Ion Image Mapper installed as separate software tool
 - See Quickstart documentation from **Help** menu



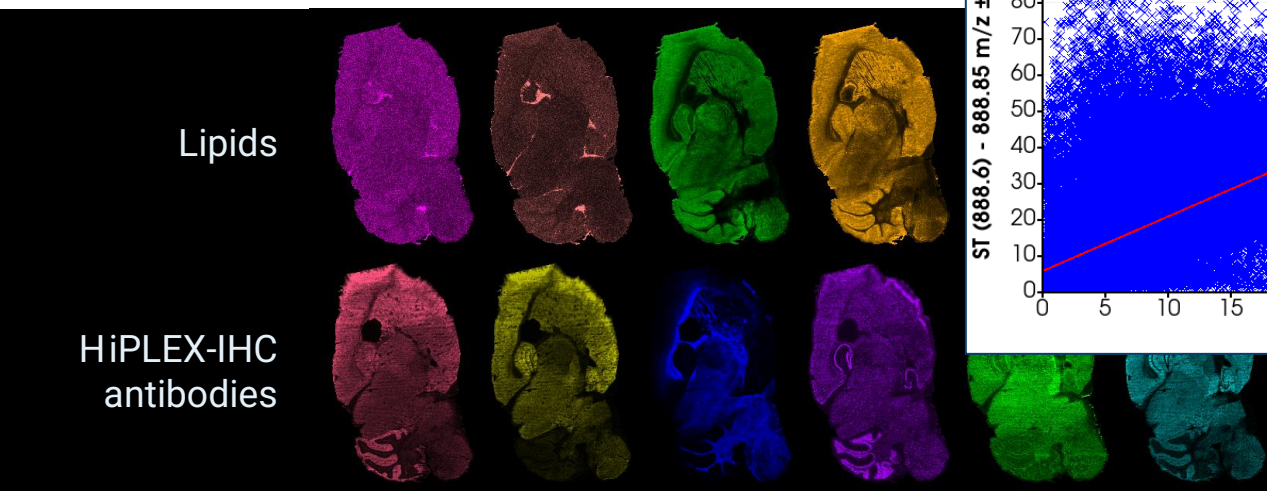
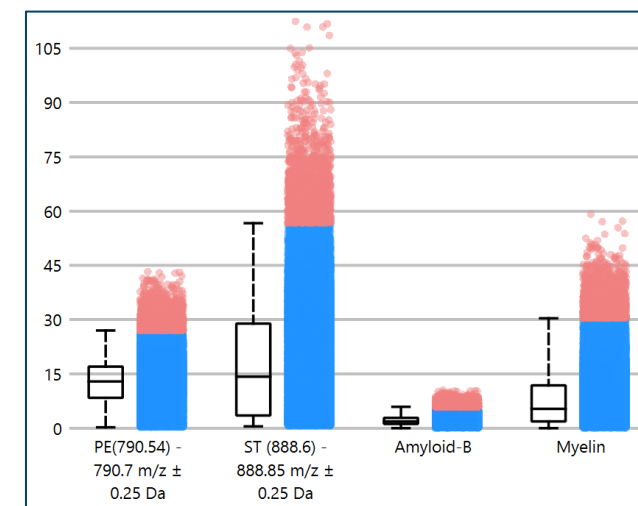
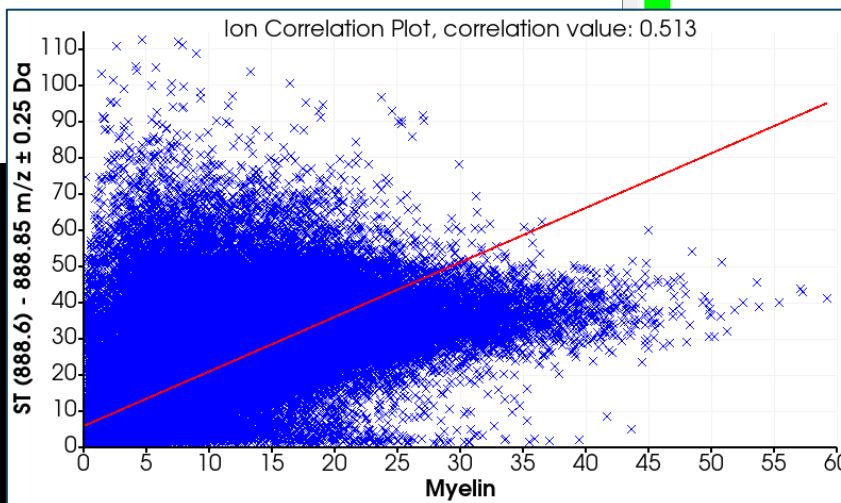
Multionomics imaging workflow

- Ion images transferred from source dataset now represented as **external features** in destination dataset
 - No m/z value, identified by name
 - Independent of normalization
 - Supported by most data plots and computational tools

Feature Table

Feature list: Selected mixed native / external (12)

m/z	Name	Source	Co-loc to Myelin
616.7 m/z ± 0.25 Da	LPE		-0.231391255
687.8 m/z ± 0.25 Da	Crasseride 2		-0.220387917
790.7 m/z ± 0.25 Da	PE(790.54)		-0.607734527
885.8 m/z ± 0.25 Da	TG(17:1(9Z)/17:2(9Z,12Z)/20:0)[iso6]		-0.637249283
888.85 m/z ± 0.25 Da	ST (888.6)		0.715979567
1235.9 m/z ± 0.25 Da	GM3 (1235.79)		-0.224688944
	Amyloid-B	Selected antibodies	-0.225298406
	MAP2	Selected antibodies	-0.239451331
	Myelin	Selected antibodies	1
	NeuN	Selected antibodies	0.0340874562
	Nicastrin	Selected antibodies	0.143326763
	Synapsin-1	Selected antibodies	-0.249192853

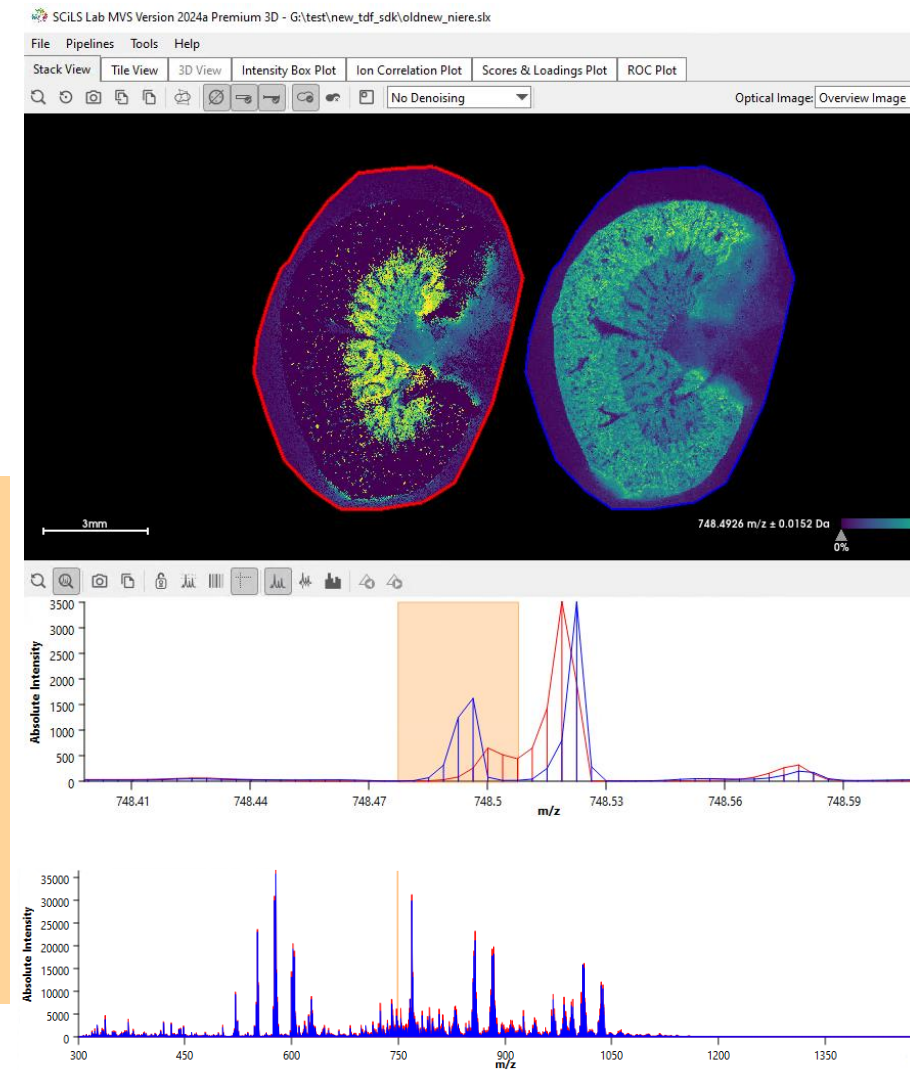


Improved timsTOF fleX TIMS data import

- New version of TDF library for timsTOF fleX data import integrated
- More accurate representation of spectral features in TIMS mode data, in particular for low intensity features

■ Note:

- It is not recommended to combine TIMS mode data imported with the new TDF library with TIMS data that has been imported with an earlier version of SCiLS Lab.
- If you need to combine multiple timsTOF fleX TIMS datasets, please consider re-importing the data using the latest SCiLS Lab version.

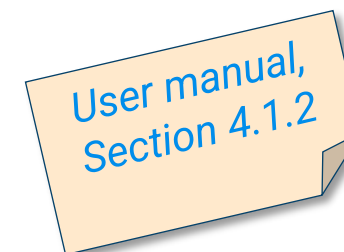
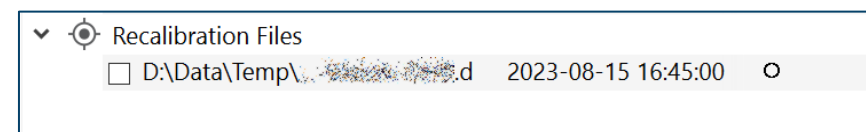


Calibration information stored with timsTOF fleX data

- timsTOF fleX data format (TDF/TSF) supports flexible mass recalibration workflows
 - Example: Online calibration during acquisition, followed by subsequent recalibration using a reference mass list in DataAnalysis
- SCiLS Lab maintains a reference to the calibration that was active during data import


```
285 [15.08.2023 [...] [TimsDataSource] [info]:
Recalibration status for dataset D:\Data\Temp\demo_data.d
286 [15.08.2023 [...] [TimsDataSource] [info]:
Saved recalibration id 4753d250-d25a-4411-9d07-df769d50293b
```

 - This ensures that all SCiLS Lab analysis results are consistent with the originally imported data
 - Particularly relevant for operations on TIMS mode data that require access to the original raw data:
 - CCS-enabled T-ReX³ feature finding
 - Extraction of CCS images
- In rare cases, it may be necessary to restore the original calibration state
 - Can be recovered from the data stored with the SCiLS Lab file



SCiLS Lab 2024a Changelog

Open changelog in SCiLS Lab:

- [Help > What's New](#), or
- **Ctrl + B**

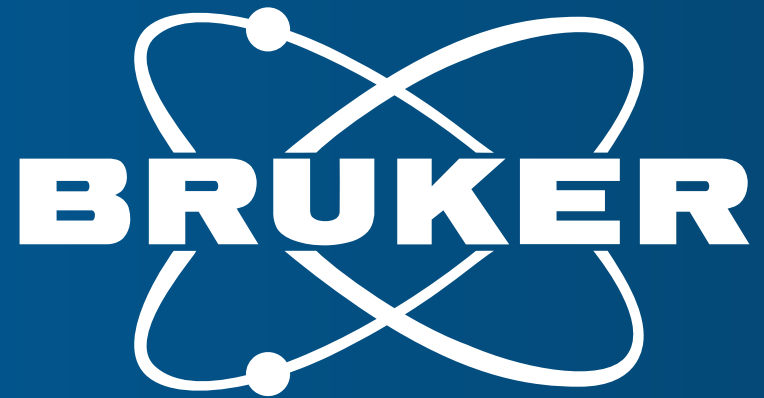
What's New? (Release Notes)

SCiLS Lab Software – Changelog

SCiLS Lab 2024a 12.00.15110 (2023-08-07):

- Metaboscape molecular annotation
 - Metaboscape molecular annotation is now directly accessible from the SCiLS Lab feature table
 - Target list annotation methods configured in Metaboscape can be selected to provide molecular annotations to a SCiLS Lab feature list
 - Multiple annotation candidates can be reviewed and managed in the new feature table annotation details view
 - Isotope patterns are extracted by the T-ReX feature finding and are used to provide more accurate annotations
 - Access to Metaboscape server is configured through the SCiLS Lab Settings dialog
 - Target list library "TargetList_N-Glycan human" has been updated to be compatible with the Metaboscape molecular annotation workflow
 - **Notes:** Requires Metaboscape 2023b or later. Separate Metaboscape and Metaboscape REST API licenses required. Molecular annotations currently limited to the Metaboscape "Target list" annotation tool
- Multiomics imaging
 - Ion images transferred using the SCiLS Ion Image Mapper are now represented in the destination dataset as a new type of features, external intensity features
 - External intensity features don't carry explicit m/z or mobility information, but are identified by their names
 - Normalization is not applied to such external intensity features
 - External intensity features can be used in most tools and plots, including box, ROC, and correlation plots, as well as co-localization tool, segmentation, and component analysis
 - External intensity features are supported in exports to CSV and OME-TIFF
 - An application shortcut to the SCiLS Ion Image Mapper is now directly available from the user's desktop
- Improved import of timsTOF fleX TIMS mode data
 - The TDF library for accessing timsTOF fleX raw data was updated to a new version, allowing to import TIMS mode data at a higher accuracy, in particular with respect to low intensity signals
 - **Note:** It is not recommended to combine TIMS mode data imported with the new TDF library with TIMS data that has been imported with an earlier version of SCiLS Lab. If you need to combine multiple timsTOF fleX TIMS datasets, please consider re-importing the data using the latest SCiLS Lab version.
- Improved support for timsTOF fleX calibration information
 - SCiLS Lab now maintains the information on the active mass calibration at the time of import and makes sure consistent data is used when later accessing the timsTOF fleX raw data to perform feature finding, extract CCS images or re-generate the CCS heatmap
 - The calibration source file that was current at the time of importing the timsTOF fleX data is now stored with the SCiLS Lab dataset and can be re-created by exporting it from the Objects tab
- Further improvements and bug fixes
 - Successful execution of background tasks and certain other events are no longer signaled by notification pop-ups
 - Adding intensity columns to the feature table is now performed in a background task, thus allowing to continue working even in extreme cases where this operation may take more than a few seconds
 - Added a context menu command to delete name entries for a selection of multiple features in the feature table.
 - Fixed a bug where references to original Bruker raw spectra may have been incorrect in special cases where a new, secondary SCiLS Lab dataset was created from a subregion of an existing SCiLS Lab dataset that was created from a measurement including multiple measurement regions with different raster width settings.
 - **Note:** It is recommended to recreate the secondary SCiLS Lab dataset in such cases.
 - Polarity information now stored correctly when importing from another SCiLS Lab dataset or from non-Bruker data (requires MVS license)
 - Arrow up and down keys are now handled correctly in the ion image list
 - The intensity box plot now supports Copy to clipboard on systems with screen scaling other than 100%
- SCiLS API
 - Deprecated binary package for Python 3.7 was removed.
 - Added binary package for R 4.3. R 4.1 is now deprecated, will be removed in the next release.

Close



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