

LIFE SCIENCE MASS SPECTROMETRY

SCiLS™ Lab 2023b – What's New?

T-ReX feature finding for TIMS, QTOF, and MRMS data

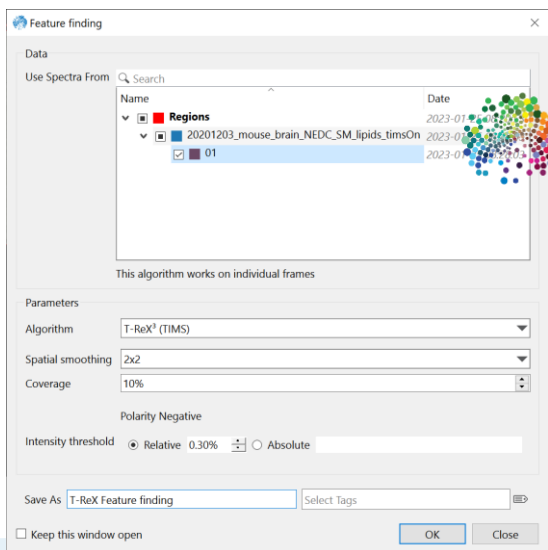
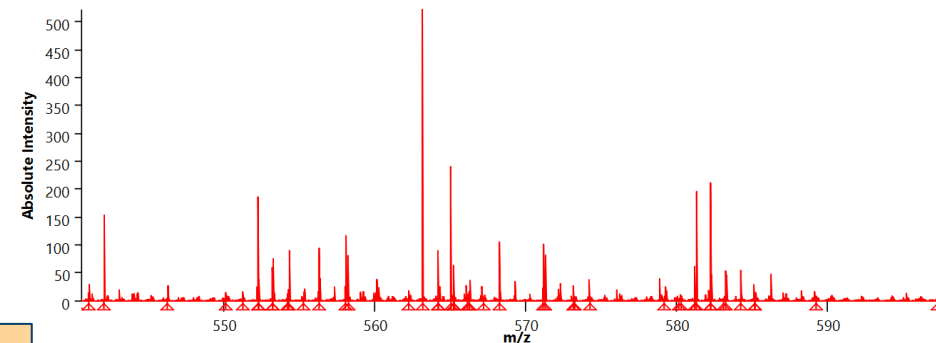
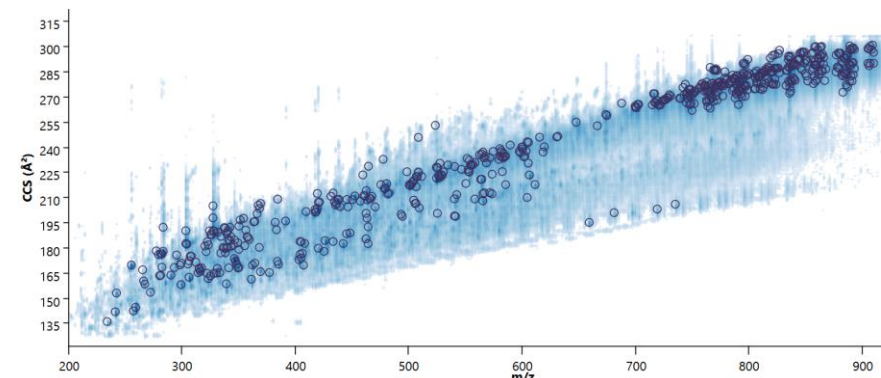


TIMS
QTOF

MRMS

4D Feature Finding
T-ReX³

3D Feature Finding
T-ReX²

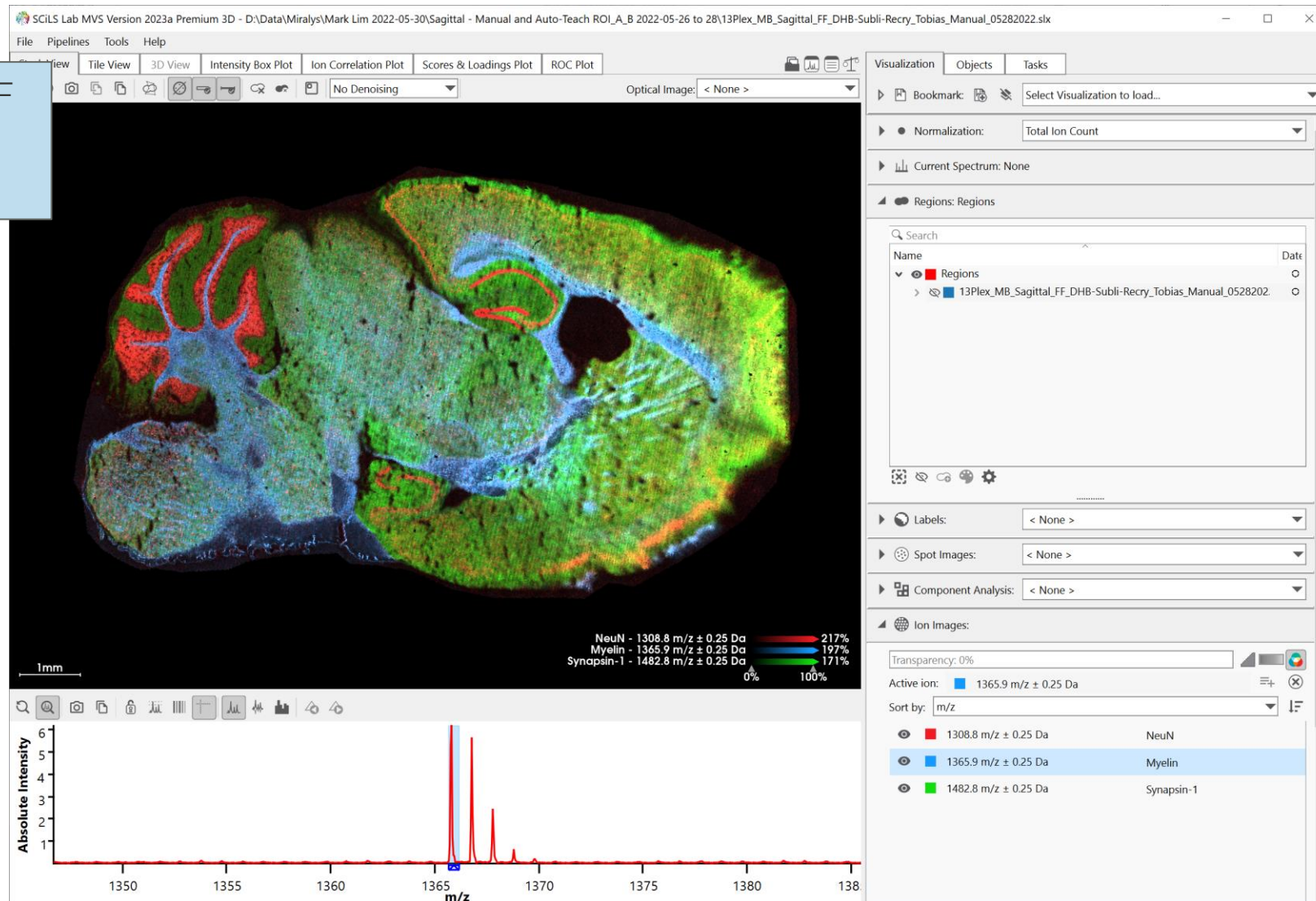


SCiLS

- 3D/4D feature finding integrated into SCiLS Lab 2023b
- Algorithm and default parameterization optimized for MALDI imaging data
- Simple, unified UI gives access to different available algorithms

Export feature images as OME-TIFF – Not only for MALDI Hplex IHC

- Export SCiLS Lab ion images to OME-TIFF
- Including feature names and colors
- Spatial resolution preserved



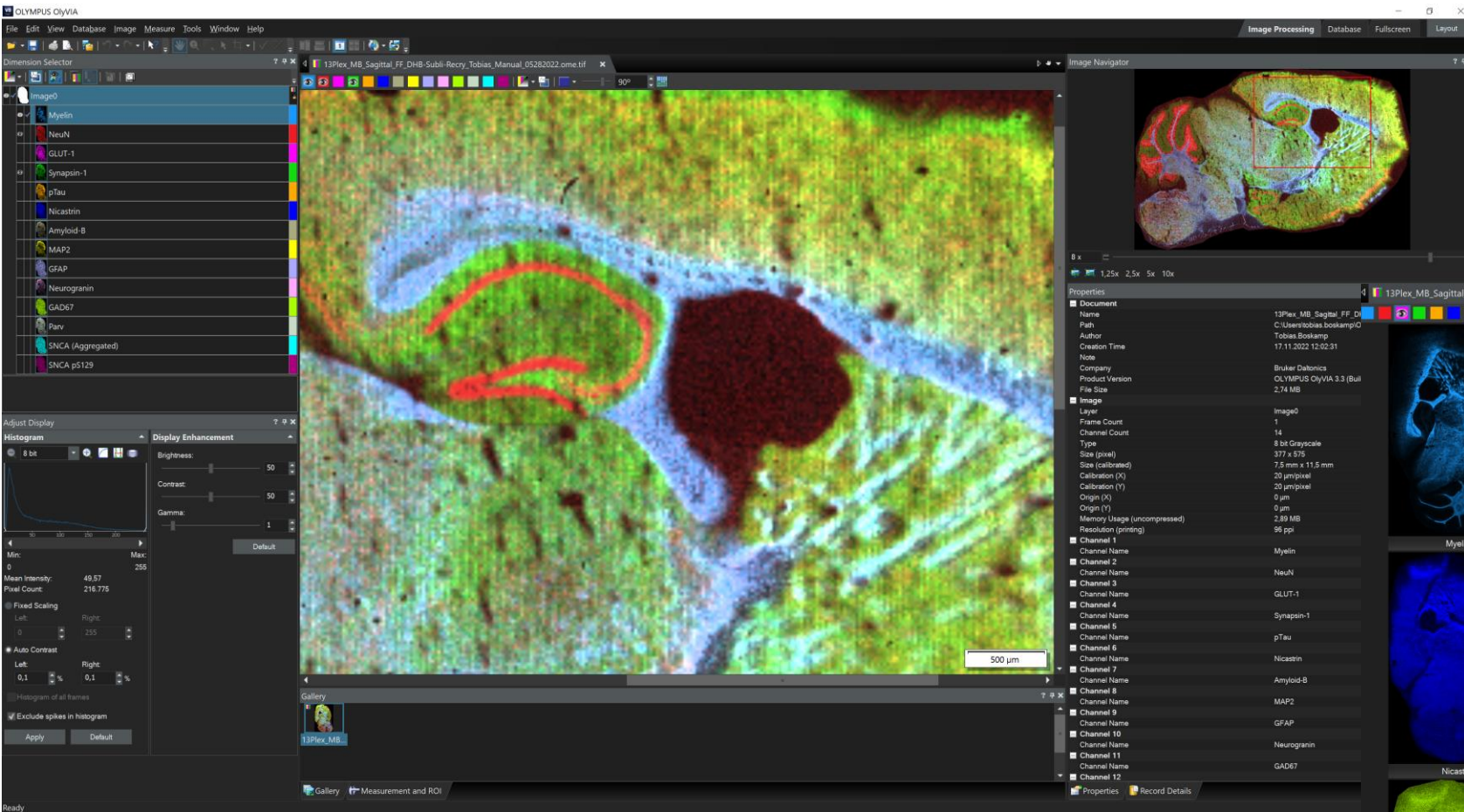
Feature Table

Feature list 2022-05-28 Manual Brain Panel (14)

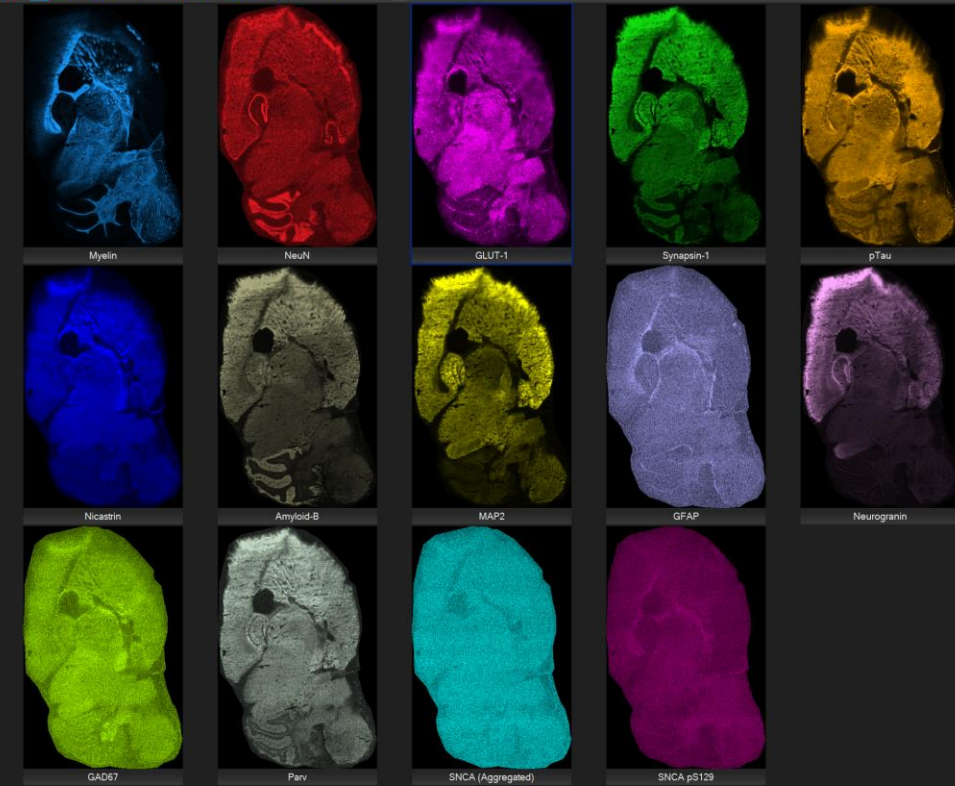
m/z	Name
856.6 m/z ± 0.25 Da	GLUT-1
1027.7 m/z ± 0.25 Da	SNCA (Aggregated)
1057.7 m/z ± 0.25 Da	GAD67
1144.7 m/z ± 0.25 Da	Nicastrin
1201.7 m/z ± 0.25 Da	pTau
1308.8 m/z ± 0.25 Da	NeuN
1365.9 m/z ± 0.25 Da	Myelin
1377.8 m/z ± 0.25 Da	GFAP
1395.8 m/z ± 0.25 Da	Neurogranin
1432.8 m/z ± 0.25 Da	SNCA pS129
1482.8 m/z ± 0.25 Da	Synapsin-1
1539.8 m/z ± 0.25 Da	Parv
1570 m/z ± 0.25 Da	MAP2
1770.9 m/z ± 0.25 Da	Amyloid-B



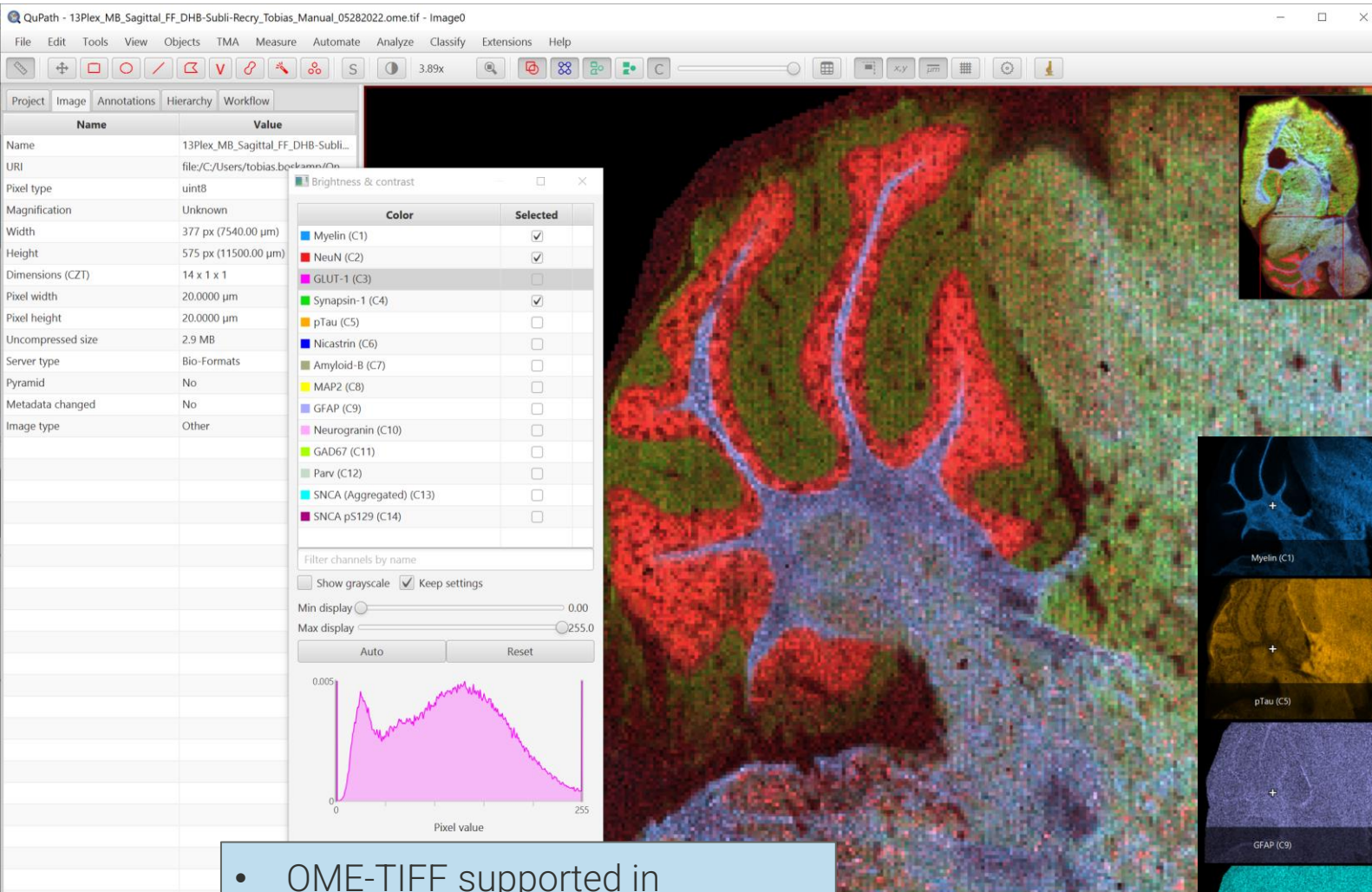
MALDI Hiplex IHC data in digital microscopy software



- OME-TIFF supported by major digital microscopy vendors



MALDI Hplex IHC data in open bioimage analysis software

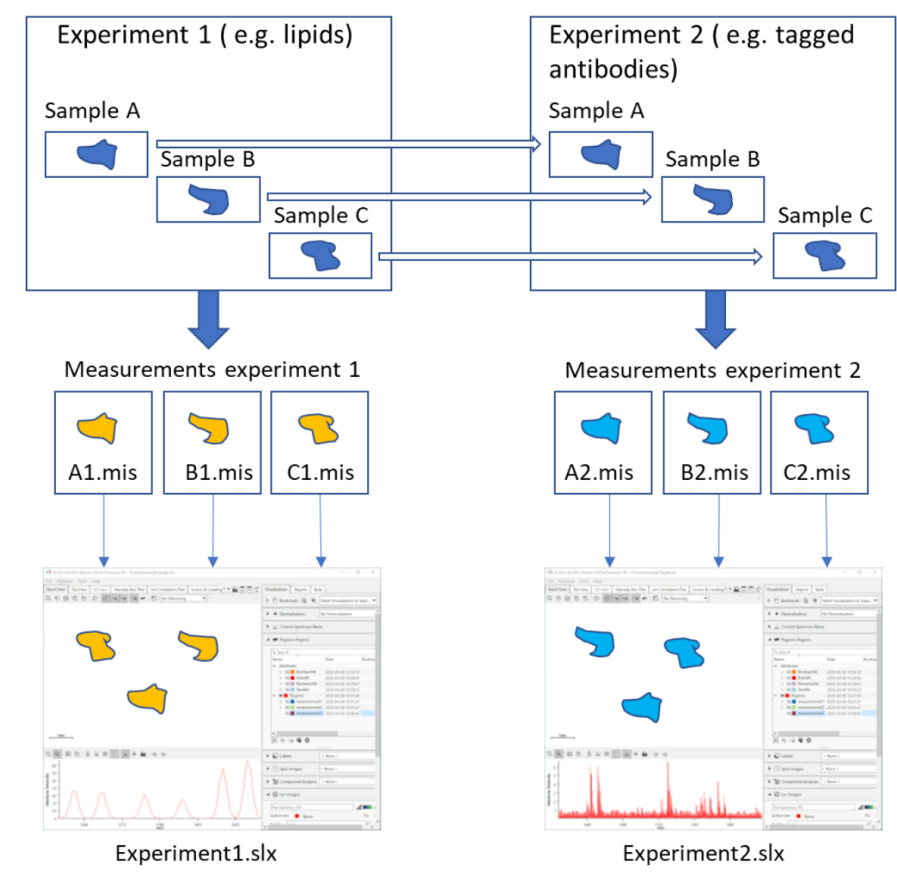
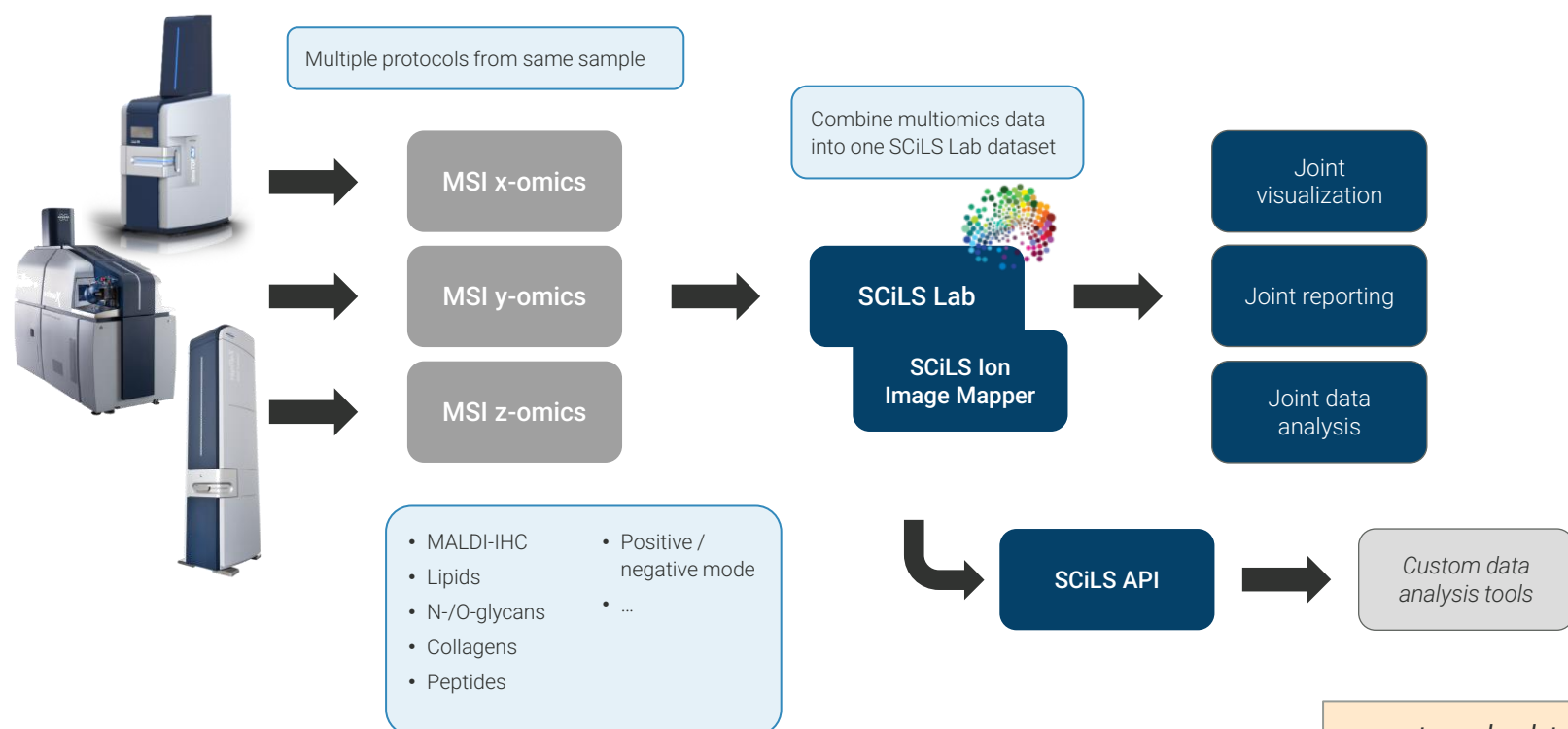


QuPath
Open Software for Bioimage Analysis
<https://qupath.github.io/>

- OME-TIFF supported in numerous open source projects

Multimomics MSI – Support for multi-sample studies

Multimomics workflow established with SCiLS Lab 2023a ...



... extended to support multiple samples in SCiLS Lab 2023b

**SCiLS Ion Image Mapper
Transfer feature intensities**



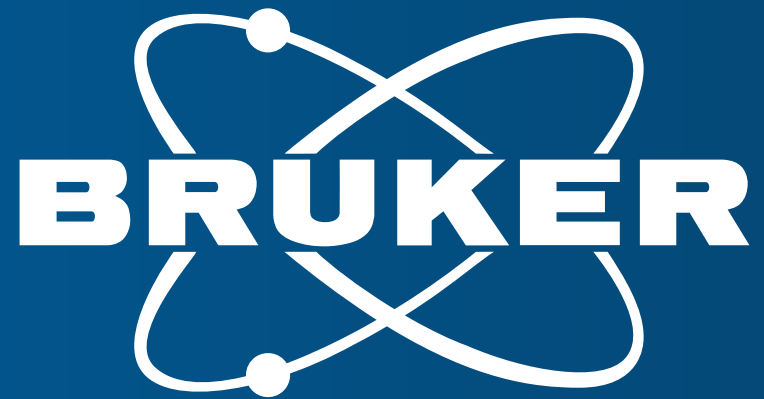
SCiLS Lab Software – Changelog

SCiLS Lab 2023b 11.01.14623 (2023-02-22):

- New 3D and 4D feature finding for Bruker QTOF, TIMS and MRMS data
 - Feature finding for TIMS data based on the T-ReX³ algorithm
 - Feature finding for Bruker QTOF and MRMS data based on the T-ReX² algorithm
- Importer improvements and automation
 - Running the importer no longer blocks the main SCiLS Lab application
 - Increase importer performance by storing temporary data in a dedicated location / local SSD
 - Polarity mode is automatically determined during import
 - New command line importer enables automatic data import after acquisition
 - Improved handling of I/O errors during import
- CCS enabled imaging
 - Support mass-mobility features in computing classification models (LDA)
 - Create custom normalizations to reference mass-mobility features
 - Default mobility width can now be configured in File Properties
- Multiomics workflow, SCiLS Ion Image Mapper (prototype)
 - Support source and target data sets with multiple samples or measurement areas
 - Support mass-mobility features in multiomics workflow
 - Generate automatic names for unnamed features transferred to a target data set
- Multiple feature enhancements
 - Export feature list ion images as standard OME-TIFF files
 - Manage list of original data sources from which a SCiLS Lab file was created
 - Custom normalizations can now be deleted in the Objects tab
 - Automatic closing of data sets opened from a network location can now be configured
- SCiLS API improvements
 - New API function to write custom normalizations
 - New API function to retrieve filename and UUID of current file
 - Added binary package for Python 3.11. Python 3.7 is deprecated, will be removed in the next release.
 - Removed binary package for R4.0
- Multiple bug fixes
 - When importing centroided data (e.g., MRMS, TIMS, QTOF) and reducing the m/z range for import, TIC and RMS normalizations are now computed on the reduced range instead of the full m/z range
 - Fixed a bug in the feature navigator where the mass-mobility heatmap was not rendered correctly on close zoom-in
 - Improved layout on high dpi monitors with Windows screen scaling enabled
 - Fixed a bug where very large optical images (more than 4 billion pixels) were not rendered correctly
 - Fixed a bug where network locations with very long folder names were not supported
 - Improved path handling with Unicode characters
 - Fixed a bug where non-latin encodings in .mir exports and imports were not handled correctly

SCiLS Lab 2023a 11.00.14179 (2022-09-09):

- Fixed a bug on multiscreen setups where the file menu and tooltips would appear on the wrong screen
- Update Wibu CodeMeter License service to 7.50



Innovation with Integrity