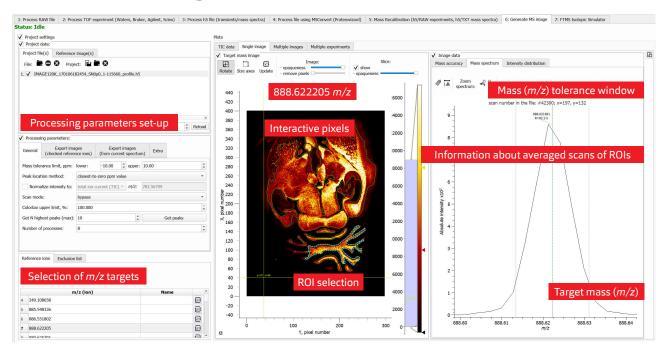


With powerful built-in tools, such as an on-the-fly mass recalibration, efficient processing without m/z scale binning, and the ability to process unreduced data formats, the **vendor-neutral Mozaic** ensures maximum information retention enabling you to gain rapid insights and deepen knowledge about your samples.

Individual m/z image



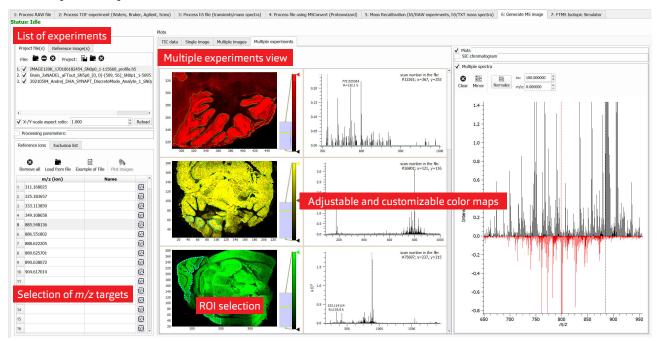
The presented dataset (mouse brain tissue imaging, 50 x 50 μ m pixel size) was acquired on a LTQ Orbitrap EliteTM FTMS instrument (Thermo Fisher Scientific) equipped with a MALDI injector from Spectroglyph.

Data processing

Step-by-step workflows built upon powerful data processing capabilities

- A vendor-neutral platform for MSI data processing and analysis from diverse MS instruments, including Orbitrap™ FTMS, FT-ICR MS, TOF MS, and QQQ MS (vendor-specific file formats and imzML datasets)
- Support for both MALDI and DESI ion sources, including from MassTech, Spectroglyph, & TransMIT
- Automatic recognition of meta information (e.g., instrument model and experimental settings), and support of multiple acquisition modes (MS, MS/MS, SIM, etc.)
- Import functionality for all types of reduced and unreduced data, including reduced and full profile enhanced FT (eFT) mass spectra, and time-domain transients from FTMS instruments
- A full cycle of FTMS data processing: unreduced (time-domain transients and absorption mode (aFT) mass spectra) and reduced (centroided, reduced, and full profile eFT and magnitude mode (mFT) mass spectra)
- Comprehensive processing of TOF and QQQ MSI data sets of practically any size
- Data validation via mass accuracy evaluation and mass spectra re-calibration using either linear (on-the-fly, single and multiple lock mass (m/z) values) or non-linear approaches
- Mass spectra processing: user-defined parameters (e.g., noise thresholding, data averaging)
- Flexible image viewers for interactive viewing and investigation from single and multiple m/z values
- Image processing: normalization, noise reduction, hotspot removal, etc.
- Super-resolution signal processing (least squares fitting) of FTMS time-domain transients to accelerate targeted MSI research

Multiple experiments

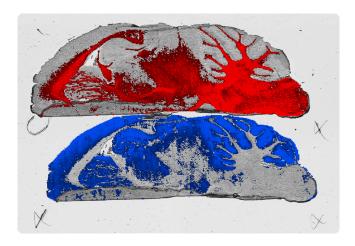


Shown are results of MALDI MSI analysis of different mouse brain tissue sections performed with: (top panel) an FT-ICR MS instrument (a 9.4 T SolariX[™] XR from Bruker Daltonics); (middle panel) a TOF MS instrument (Synapt[™] from Waters); and (bottom panel) an Orbitrap FTMS instrument (LTQ Orbitrap Elite from Thermo Fisher Scientific) equipped with a MALDI injector from Spectroglyph.

Data analysis

Memory-efficient and vendor-neutral data analysis

- Instant visualization of interactive images and mass spectra (click and see)
- · Manual and automatic definition of regions of interest (ROI), analysis and geometry handling
- · Comparative analysis of (averaged) mass spectra from multiple ROIs for the same or different data sets
- Multiple pixel interpolation approaches, image sharpening
- · Co-localization and overlay of (multi-mode) images
- Image transparency, add color function, customizable and adjustable color maps
- · Results are readily exportable in common (imzML) and advanced (H5) data formats
- High quality images are exportable in different formats: PDF, png, jpeg, tiff, svg, etc.
- · Peak annotation and further data analysis: via imzML upload to third-party software tools



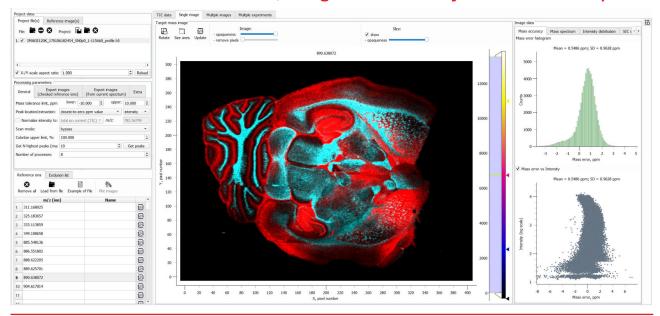
Overlay of selected MSI images of lipids with an optical image of a mouse brain (Bruker's 9.4 T SolariX XR FT-ICR MS data).

Top panel shows the spatial distribution of an 848.6376 m/z species ($[C_{48}H_{91}NO_8 + K]^+$ putatively annotated as d18:1/C24:1 glucosyl ceramide, red color).

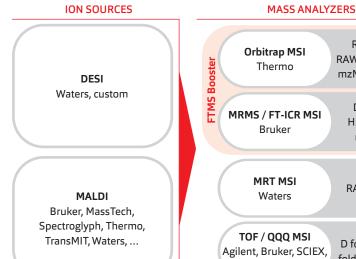
Bottom panel shows the spatial distribution of a 772.5253 m/z species ([C₄₀H₈₀NO₈P + K]⁺ putatively annotated as phosphatidylcholine 32:0, blue color).

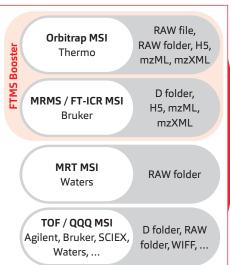
Mass accuracy evaluation and data recalibration

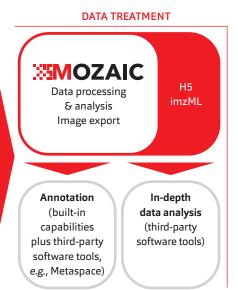
Lock-mass and iterative recalibration; histogram- and intensity-based mass errors plots



Data flow







Enhanced MSI via unreduced data processing

Integrated hardware-software solution to access and process time-domain transients



Mozaic is a stand-alone software tool. In addition, it can form an integrated solution with the Spectroswiss FTMS Booster - a highperformance data acquisition system providing access to the timedomain transients from Orbitrap and Ion Cyclotron Resonance (ICR) FTMS instruments, see spectroswiss.ch/hardware/





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