

EMPOWER YOUR MASS SPECTROMETRY IMAGING RESEARCH

Process, Analyze, & Visualize MSI Data – No Matter the File Size or the MSI Platform



MALDI MSI with a Spectroglyph Inc. Ion Source

Mozaic peak annotation capabilities applied to mouse brain tissue imaging (50 um spatial resolution), acquired on an Orbitrap Elite[™] (Thermo Fisher Scientific) equipped with a MALDI injector from Spectroglyph. They showcase a **targeted** approach leveraging isotopologues analysis (top) and an **untargeted** approach based on **isotopic chain** analysis to reveal user-specified mass differences (bottom).





Ultrahigh-Mass Resolution Mass Spectrometry Imaging with an Orbitrap Externally Coupled to a High-Performance Data Acquisition System, Grgic et al., Anal. Chem. 2024, 96, 2, 794–801

External Data Systems Enable Enhanced (and Sustainable) Fourier Transform Mass Spectrometry Imaging for Legacy Hybrid Linear Ion Trap – Orbitrap Platforms, Leach et al., JASMS, 2024, 35, 2690-2698

MALDI MSI with a MassTech Inc. Ion Source



Traumatic brain injury (TBI) tissue sample analyzed using an Exploris 480TM Orbitrap mass spectrometer (Thermo Fisher Scientific) equipped with a MALDI ion source from MassTech (25 um spatial resolution). Data courtesy of Dr. Hua Tian (University of Pittsburgh) and Dr. Gilles Frache (Luxembourg Institute of Science and Technology).



The Mozaic screenshot illustrates a complete data analysis cycle of a DESI MSI dataset of a rat kidney (50 um spatial resolution), acquired using a high-resolution TOF MS (**SELECT SERIES MRT** from Waters). Data courtesy of Dr. Marco Giampà (Laboratory of Applied Mass Spectrometry (LAMaS)/ VIB Metabolomics core Leuven).

Imaging and Direct Sampling Capabilities of Nanospray Desorption Electrospray Ionization with Absorption-Mode 21 T FT-ICR MS, Anderton et al., Anal. Chem. 2022, 94, 8, 3629–3636

Imaging of Triglycerides in Tissues Using Nanospray Desorption Electrospray Ionization (Nano-DESI) Mass Spectrometry, Laskin et al., Int. J. Mass Spectrom., 2020, 448, 116269

Key Features: Data Processing

- A full cycle of MSI data processing, also for the unreduced data of any size
- MALDI, DESI, & MALDESI ion sources, including from MassTech, TransMIT, & Spectroglyph
- Forms an integrated hardware-solution to access and process **transients** in FTMS-based MSI
- High speed of calculations: python, HDF file structure, & multi-threading
- Mass spectra re-calibration and data validation via mass accuracy evaluation
- No m/z scale binning: avoiding artifacts & increasing processing speed
- Accurate simulations of isotopic envelopes: avoiding artifacts (instrument-specific!)
- Peak annotation & clustering: spectral matching of experimental and simulated data
- Sensitivity & quantitation: running average of MSI data from adjacent pixels
- Resolution & throughput: super-resolution signal processing (least-squares fitting)

Key Features: 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, clustering, and further data analysis: embedded and external workflows, e.g., via imzML upload to third-party software tools. For example, Mozaic performs centroiding and re-calibration of DESI (MR)TOF MS (Waters) data and generates imzML files compatible with Metaspace.





Enhanced MSI via Unreduced Data Acquisition and 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 high-performance data acquisition system providing access to the time-domain transients from Orbitrap and Ion Cyclotron Resonance (ICR) FTMS instruments, see https://spectroswiss.ch/hardware/





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