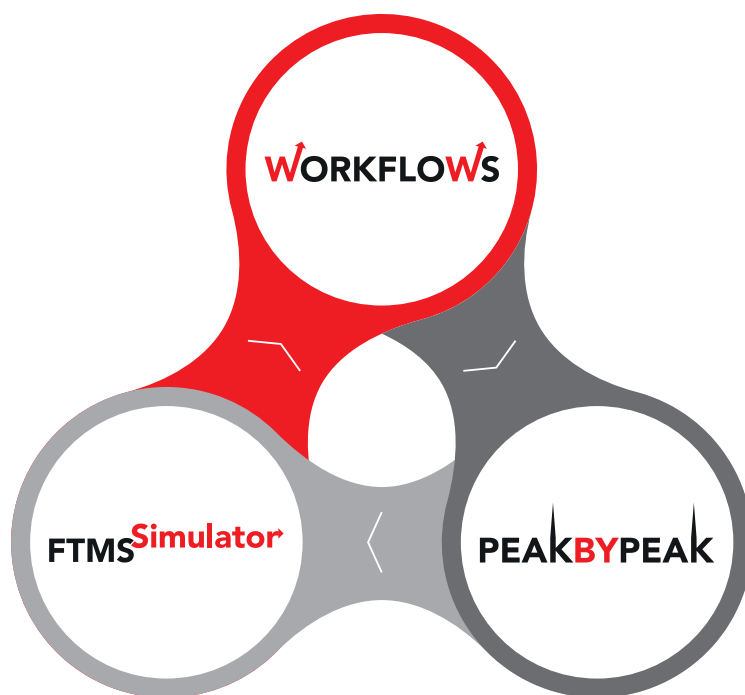


SOFTWARE FOR MASS SPECTROMETRY DATA PROCESSING AND ANALYSIS



MS Imaging, Breath Analysis, Process Analysis, Glycoproteomics, Metabolomics, Affinity-Selection, Stable Isotopic Labeling, Complex Mixtures, Isotopic Ratios, BioPharma, CDMS, Super-Resolution, Cyclic Peptides, & FTMS Simulator

Spectro+swiss

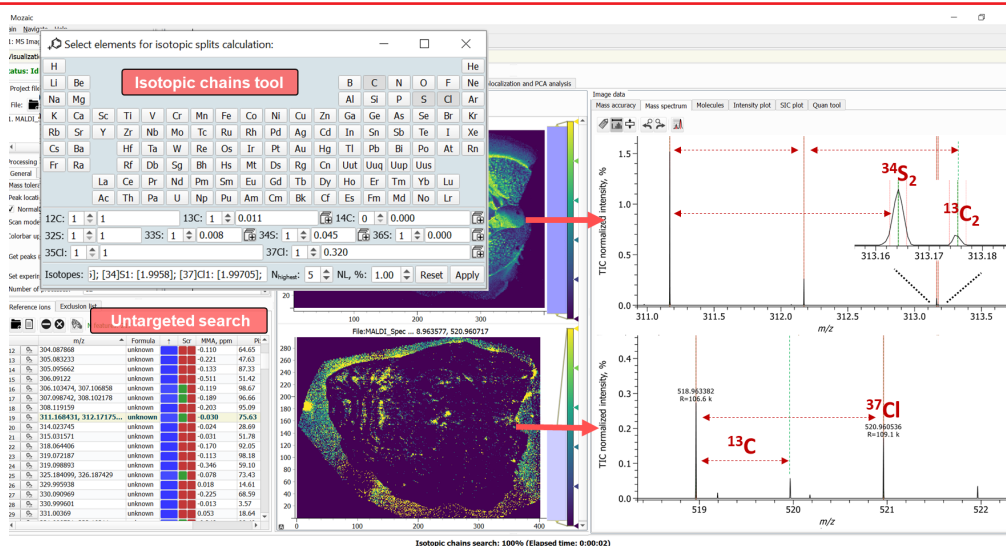
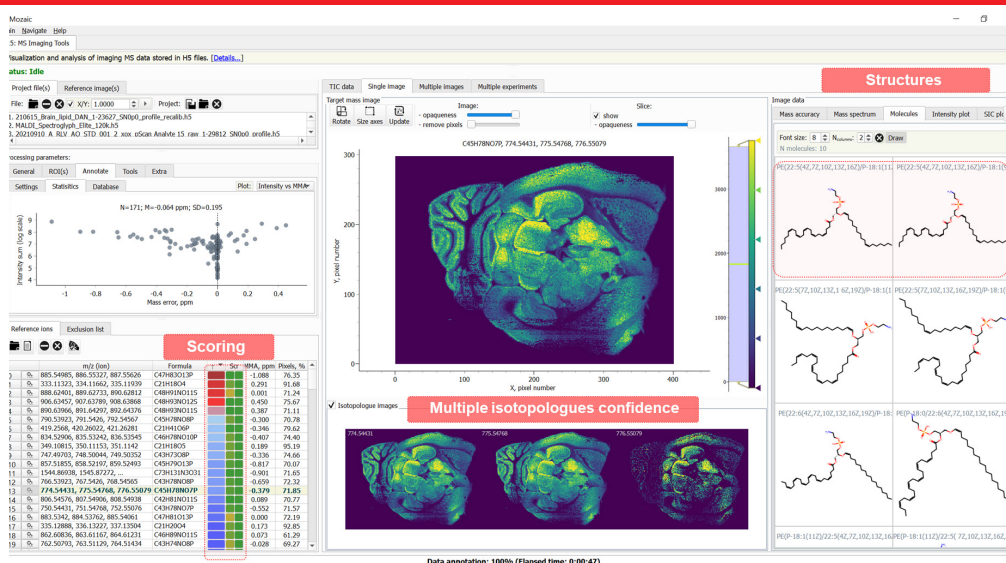
Imaging: Mosaic

Process, analyze, and visualize MSI data - no matter the file size or the MS platform.



- A full cycle of MSI data processing, also for the unreduced data of **any size**
- MALDI, DESI, & MALDESI ion sources, including from MassTech, TransMIT, & Spectrograph
- 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 accurately simulated data
- Sensitivity & quantitation: **running average** of MSI data from adjacent pixels
- Resolution & throughput: **super-resolution** signal processing (least-squares fitting)

Data Processing

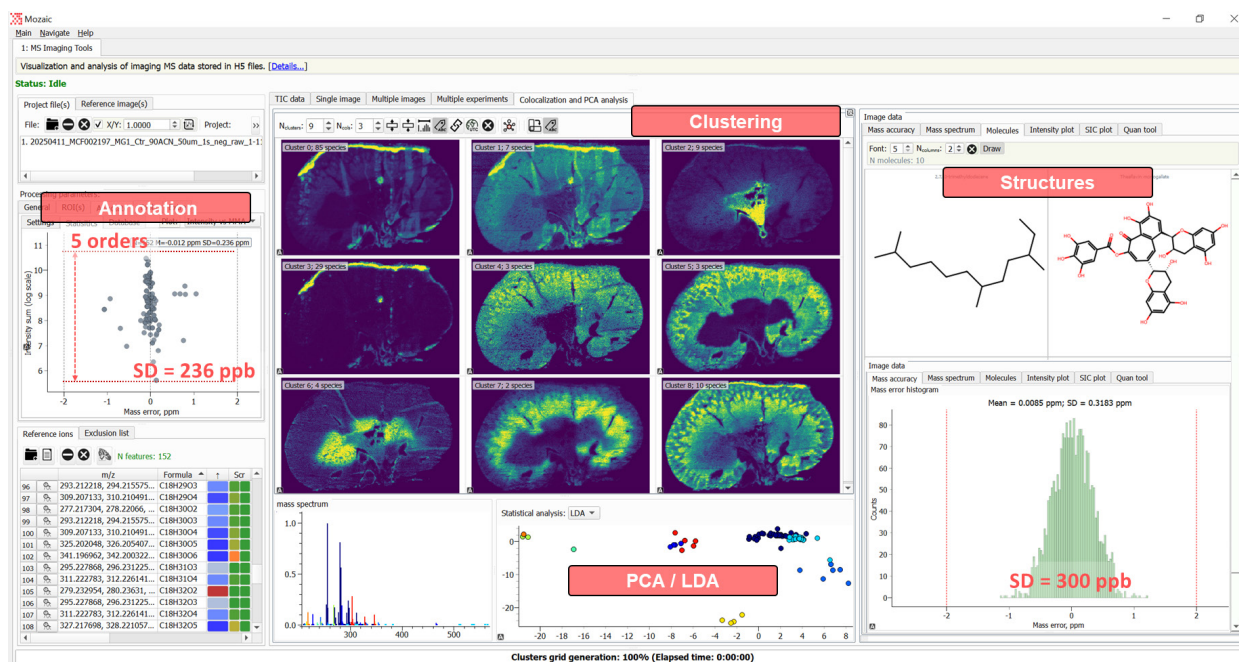
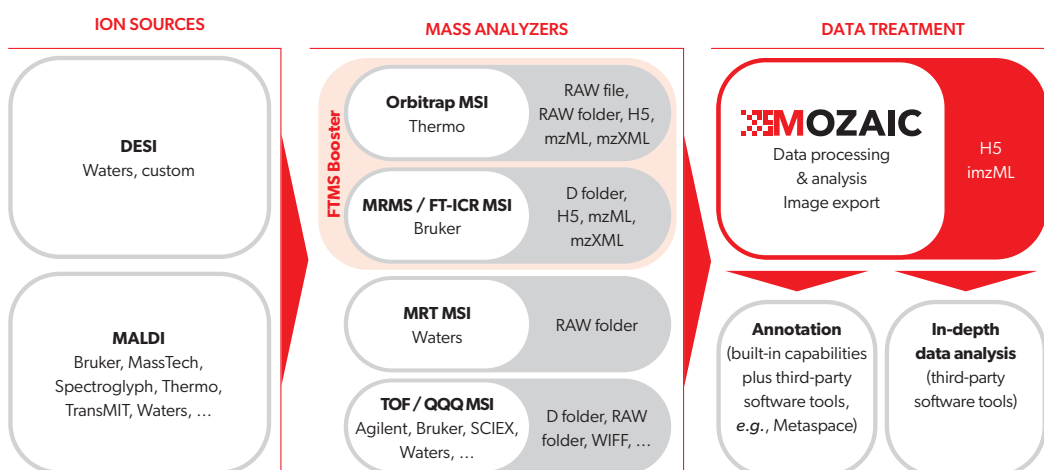


These Mozaic screenshots illustrate peak annotation capabilities applied to mouse brain tissue imaging (50 μm spatial resolution), acquired on an Orbitrap Elite™ (Thermo Fisher Scientific) equipped with a MALDI injector from Spectrograph. They showcase a **targeted** approach (top) and an **untargeted** approach based on **isotopic chain** analysis for revealing user-specified mass differences (bottom).

High throughput stable isotope feature extraction for xenobiotic metabolite identification, Chris Brown et al., TOH pm (4:10 PM), 74th ASMS, San Diego, CA, 31 May – 4 June 2026

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 Metaspacer, see below.



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 Laboratory of Applied Mass Spectrometry (LAMaS)/ VIB Metabolomics core Leuven.

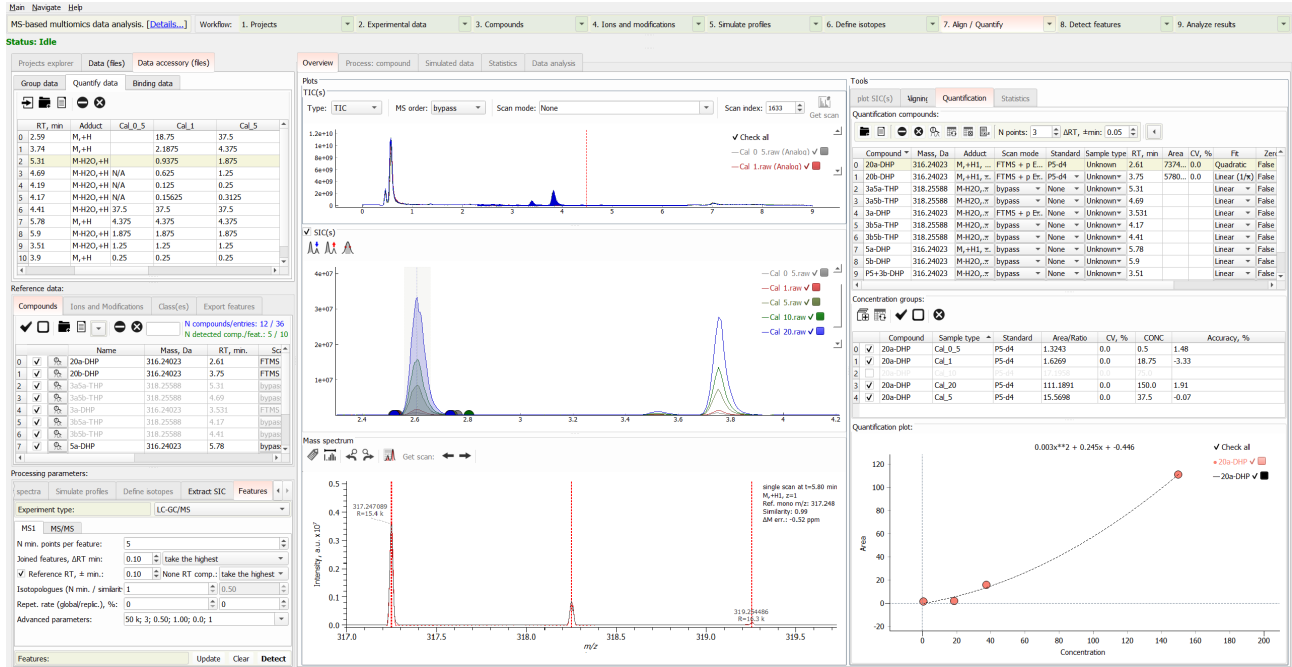
Enhancing the sensitivity of mass spectrometry imaging through spatial signal averaging, Yury Desyaterik et al., J. Am. Soc. Mass Spectrom., in print

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

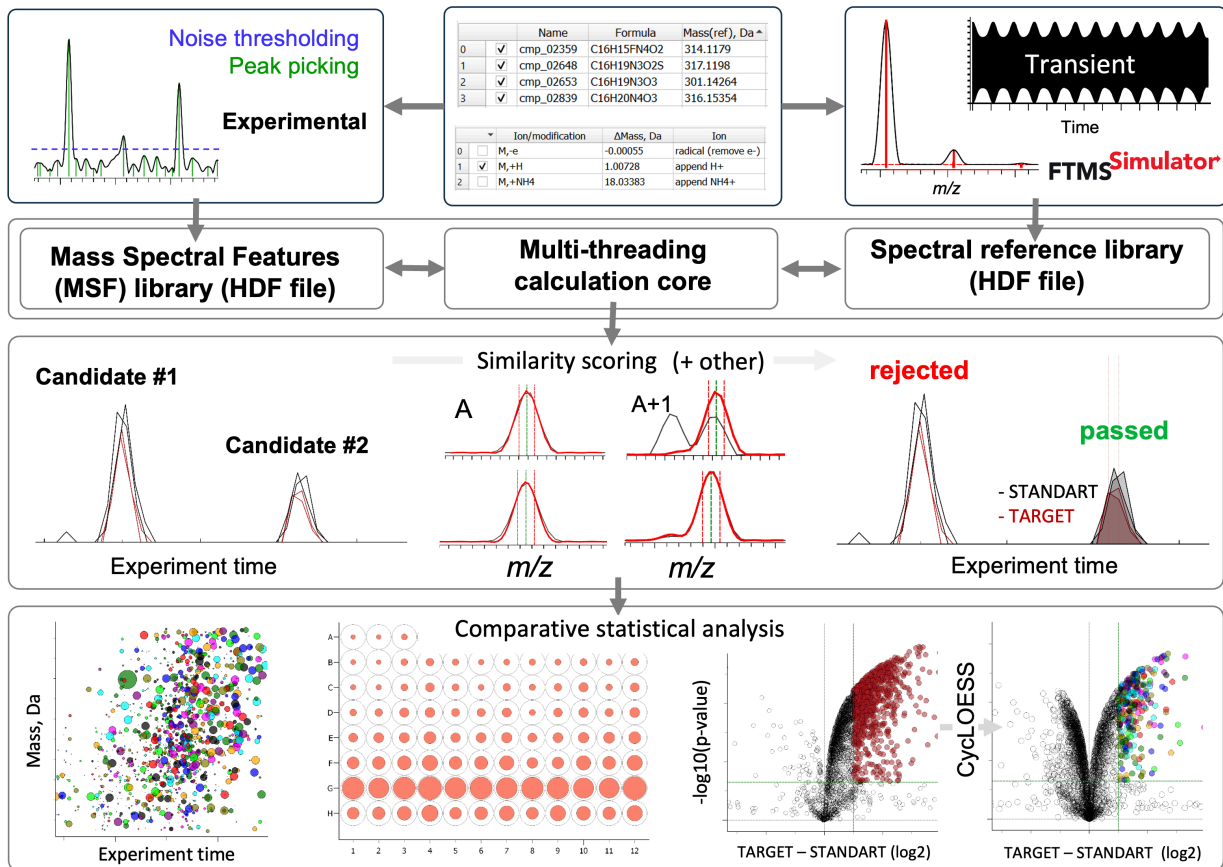
Metabolomics & Affinity-Selection Mass Spectrometry

Our targeted deconvolution (spectral matching) approach, based on the accurate simulation of the isotopic envelope profiles, enhances the feature extraction performance and visual control of small molecule analysis workflows, including:

- **Metabolomics and lipidomics:** Feature extraction and quantitation workflows.
- **Affinity-selection mass spectrometry (AS-MS):** Screening and binding workflows for ligand analysis.



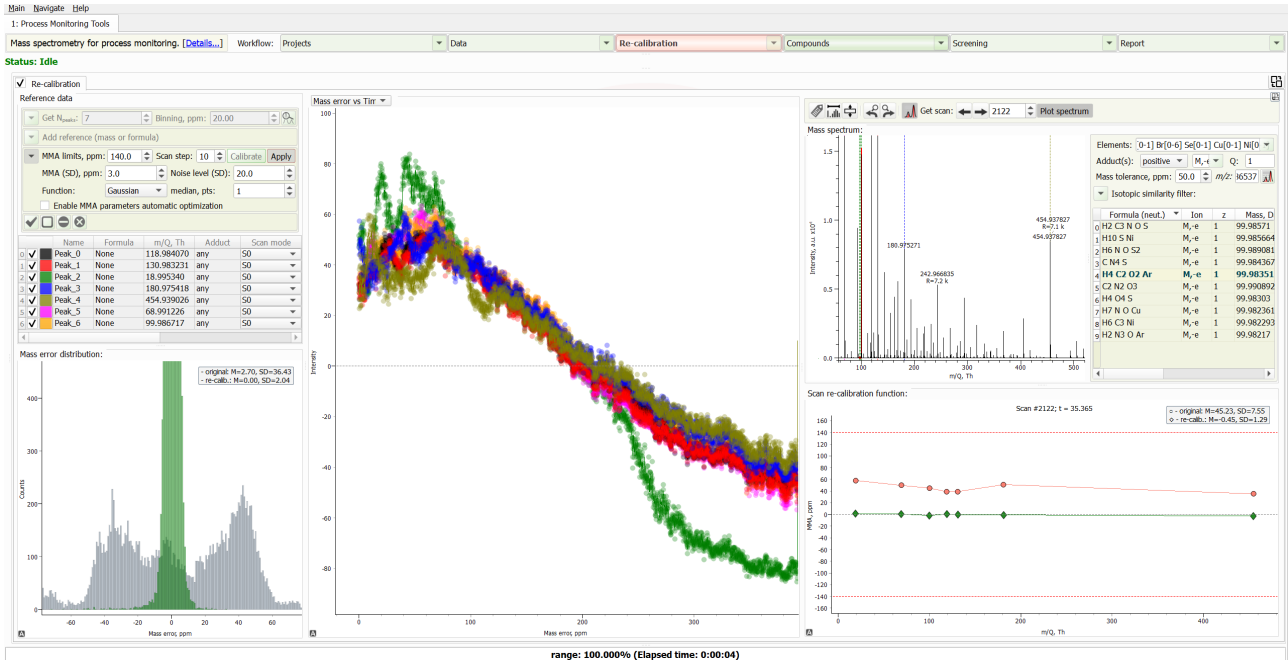
Targeted Deconvolution and Feature Extraction Workflow



High-throughput protein-ligand analysis and targeted deconvolution enables identification of binders to intractable membrane proteins, Nagornov et al., MOH am 9:10, ASMS, Anaheim, CA, June 2024

Process Monitoring for Real-Time MS: GC-MS, EI-MS, & Breath Analysis

Supporting process and environmental monitoring applications using real-time mass spectrometry over extended acquisition periods. These include direct sample introduction in EI-MS workflows with TOF-MS instruments (e.g., from Tofwerk) and high-resolution GC-TOF MS platforms (e.g., from LECO). The workflow accommodates both targeted and untargeted molecular analyses, supported by efficient recalibration procedures and scalable data handling for datasets of any size.



Supporting **breath analysis** applications using SESI-MS ion sources (Fossil Ion Technologies) coupled to Orbitraps and other types of mass spectrometers. These analyses are marked by rapid fluctuations in analyte composition during exhalation, requiring robust data handling. Our workflow enables efficient spectral recalibration, accurate alignment of exhalation profiles, and streamlined untargeted molecular identification.

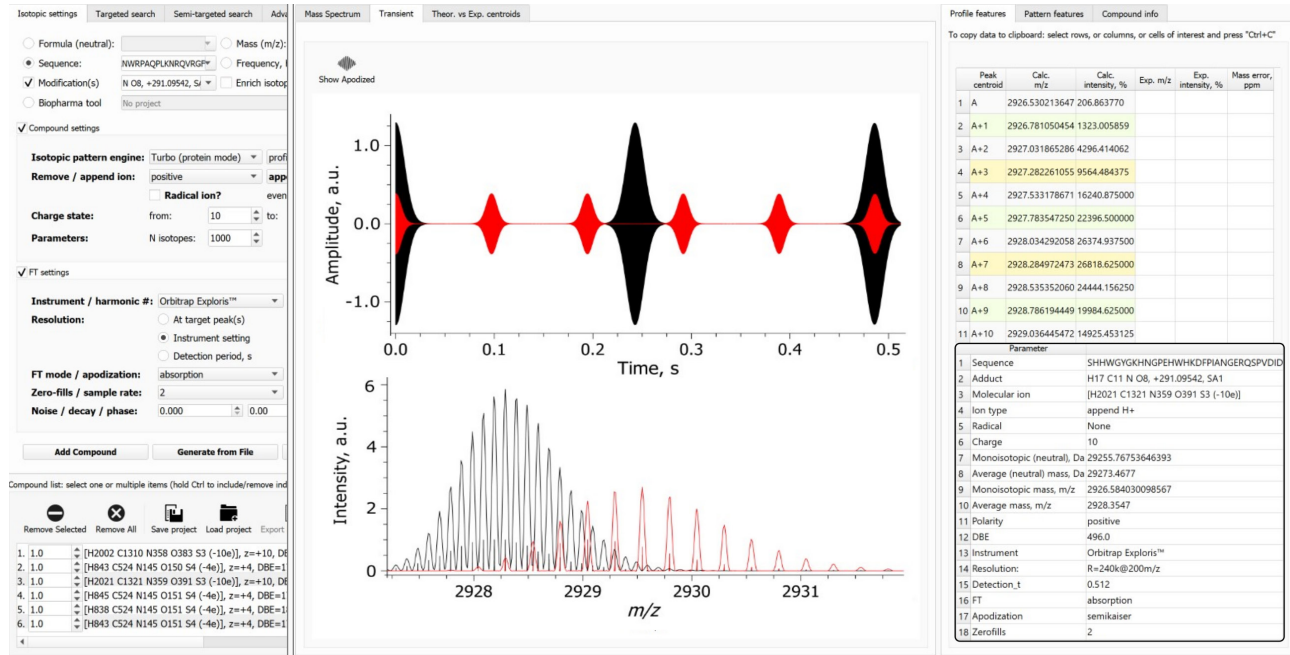


High-speed adaptive re-calibration of mass spectra for process monitoring, Nagornov et al., MOC pm 15:10, 73rd ASMS, Baltimore, MD, 2 June 2025

FTMS Simulator

A software tool to accurately simulate FTMS isotopic envelopes and mass spectra:

- to generate “gold-standard” datasets for the development and validation of data analysis software tools across diverse FTMS applications, e.g., top-down proteomics & complex mixture analysis
- to visually validate and verify the experimental results and hypotheses, perform data quality control
- to teach the FTMS subject by demonstrating realistic transients and corresponding mass spectra
- to search the experimental data with a like-for-like simulated data using similarity score ranking
- to design FTMS experiments by selecting optimum settings and FT data processing parameters



Key Features

- Applicable to (almost) any size molecules – from metabolites to monoclonal antibodies and viruses
- Applicable to (almost) any complexity mass spectra – from isotopic envelopes to full scale top-down data
- Analyte parameters selection: elemental composition, amino acid sequence, charge carrier, modifications, isotopic enrichment/depletion, number of charge states, and number of isotopologues
- FTMS experiment parameters: FTMS instrument selection (models of Orbitrap™ & ICR), resolution setting (@ m/z), add noise, set signal intensity thresholds, set initial phase, sampling rate, and decay rate
- Data processing parameters: absorption or magnitude FT, unapodized or apodization function, number of zero-fills, full or reduced profile mass spectra, centroids
- Visualize transients with and without apodization, visualize frequency spectra
- Use mass spectra: manually or automatically set peak intensities, visualize isotopic envelopes, plot multiple isotopic envelopes for a broadband view, extract high quality figures or data points for analysis
- Results output: use simulated data to search experimental data, rank search results by the similarity score (m/z , intensity), save project for future use, create report as a PDF file

FTMS Simulator

Transient-Mediated Simulations of FTMS Isotopic Distributions and Mass Spectra to Guide Experiment Design and Data Analysis. Konstantin O. Nagornov, Anton N. Kozhinov, Natalia Gasilova, Laure Menin, and Yury O. Tsybin. *JASMS*, 2020, 31, 9, 1927–1942

Characterization of the Time-domain Isotopic Beat Patterns of Monoclonal Antibodies in Fourier Transform Mass Spectrometry. Konstantin O. Nagornov, Anton N. Kozhinov, Natalia Gasilova, Laure Menin, and Yury O. Tsybin. *JASMS*, 2022, 33, 7, 1113–1125

Web-App FTMS Simulator with In-Browser Capabilities: www.peakbypeak.com

- **Real-time, in-browser FTMS simulations:** From isotopic envelopes to high-accuracy FT mass spectra – no software installation required.
- **Hybrid local/server architecture:** Fast local calculations combined with high-fidelity server-side transient and FTMS data-heavy processing.
- **Interactive and educational:** Tailored for teaching, workshops, and remote learning in mass spectrometry.
- **Secure by design:** Protein sequences and elemental compositions remain local – ideal for confidential biotherapeutics work.

https://www.peakbypeak.com

No compounds
Please add or select a compound.

Welcome to the FTMS Isotopic Simulator!
Powered by your FTMS innovators for the global community

Spectros+swiss ZAKODIUM

Isotopic settings

Instrument: Orbitrap QEx Harmonic #: 1

Resolution: 10000

Instrument setting: 17.5k@200m/z

Detection period, s: 0.1

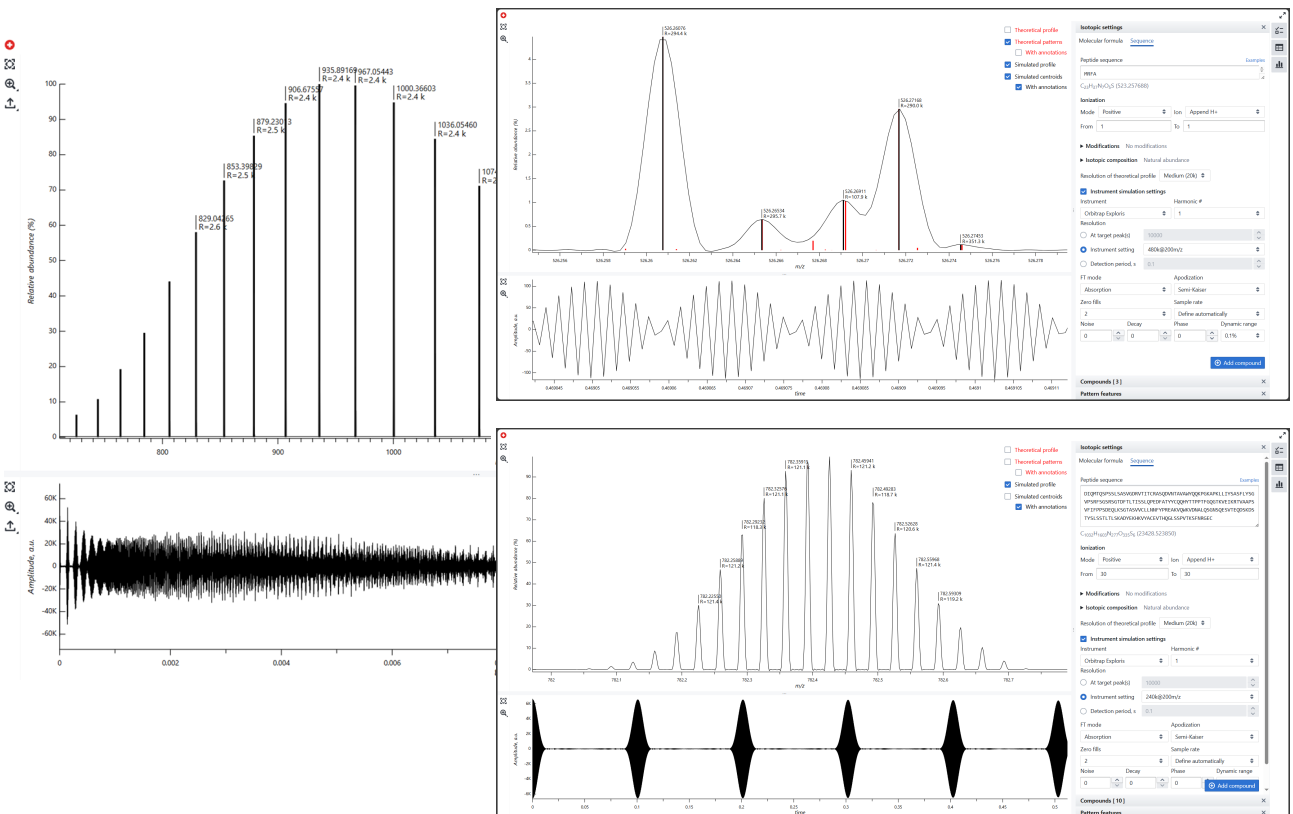
FT mode: Apodization

Absorption: Absorption Semi-Kaiser

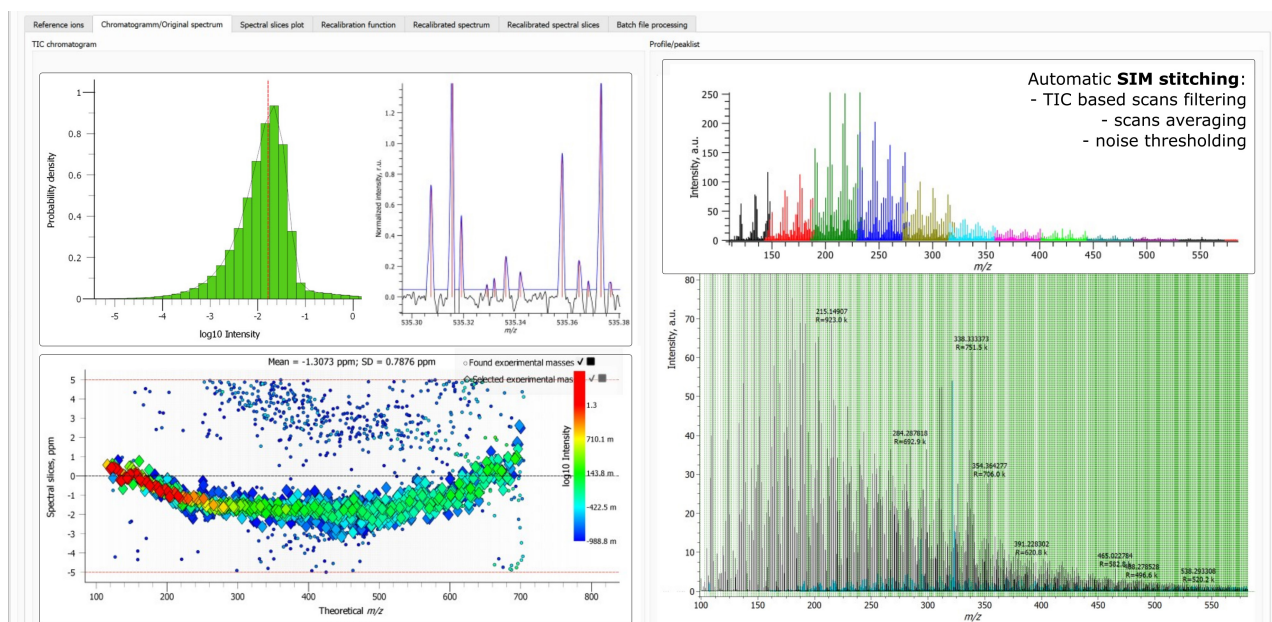
Zero fills: 2 Sample rate: Define automatically

Noise: 0 Decay: 0 Phase: 0

Compounds [0]

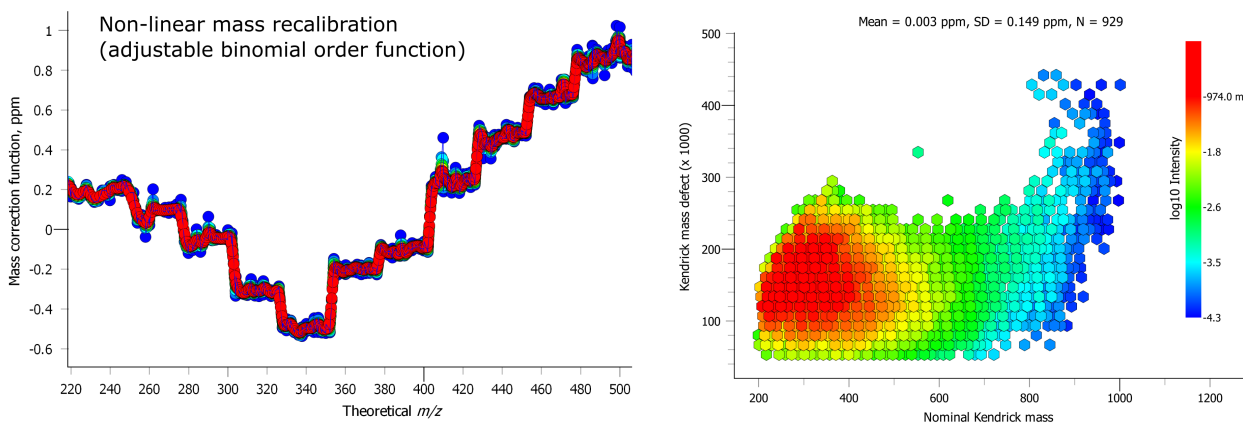


Advanced processing and analysis of (very) complex mixtures mass spectrometry data



Key Features

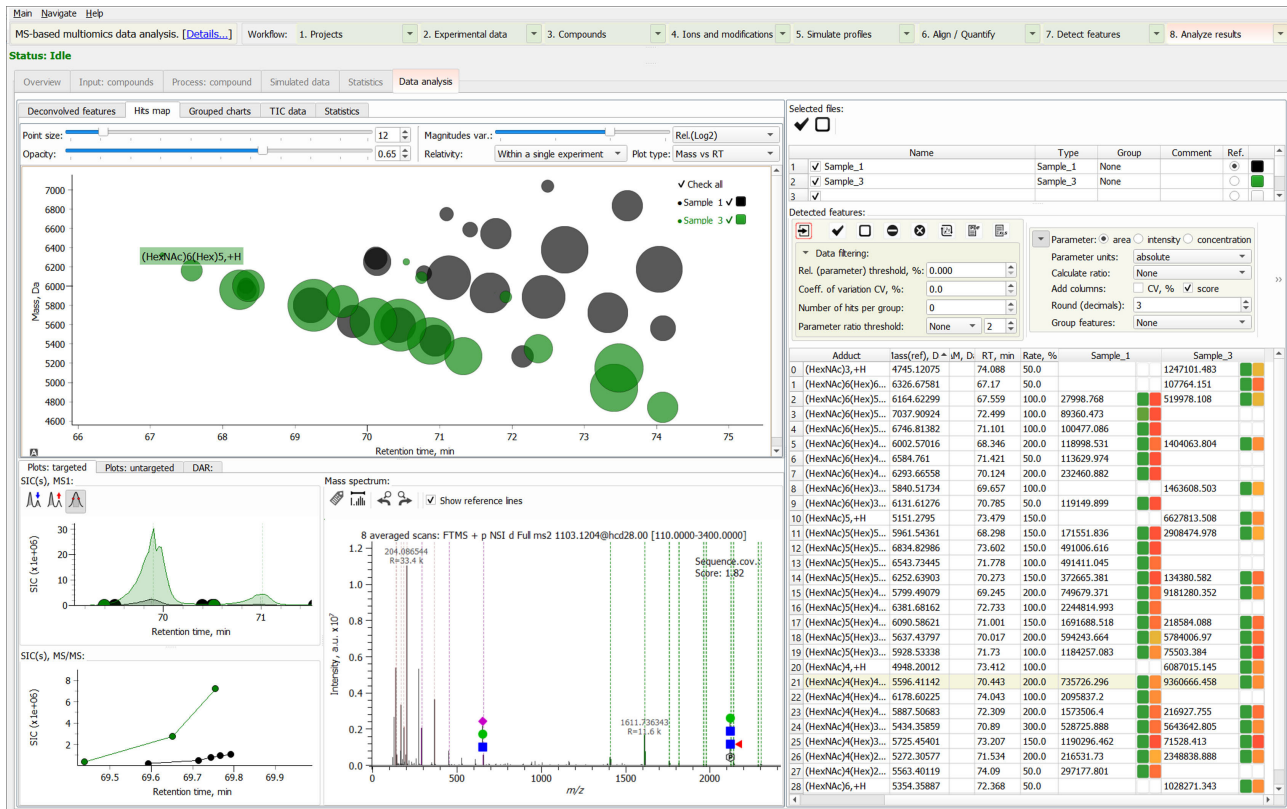
- Integration and processing of practically any size .RAW, .d folders, and .H5 files
- Open file formats for transients & mass spectra: H5, DAT, MGF, mzXML, and mzML
- Time-domain transient processing: advanced FT with pre- and post-processing, including apodization, zero-filling, magnitude and absorption mode FT
- Visualization of time-domain transients and mass spectra
- Visual comparison of mass spectra from separate data sets
- Spectral and time-domain transient averaging for high sensitivity and dynamic range
- Processing of LC-MS data for petroleomics and biofuels applications
- Data averaging across MS and LC-MS multiple technical replicates
- Narrow m/z window (SIM) stitching of the unreduced data for enhanced performance
- Advanced peak picking and efficient baseline correction
- Noise thresholding, reduced-profile mode mass spectra representation
- Mass scale calibration equations, including iterative re-calibration for complex mixtures



Iterative Method for Mass Spectra Recalibration via Empirical Estimation of the Mass Calibration Function for Fourier Transform Mass Spectrometry-Based Petroleomics. Anton N. Kozhinov, Konstantin O. Zhurov, and Yury O. Tsybin. *Anal. Chem.* 2013, 85, 13, 6437–6445

Quantitative Bottom-Up Proteomics for PTMs Analysis

Supports comparative analysis and reporting of extracted and annotated features via a dynamic global result matrix with a **quick access** to the experimental data: multiparameter filtering (CV, intensity, repetition rate, etc.), selectable experiments, compounds, groups and parameter table, original and deconvolved mass spectra in MS and MS/MS modes, bubble plot, hits map, bar-chart (grouped and stacked), statistical analysis output.

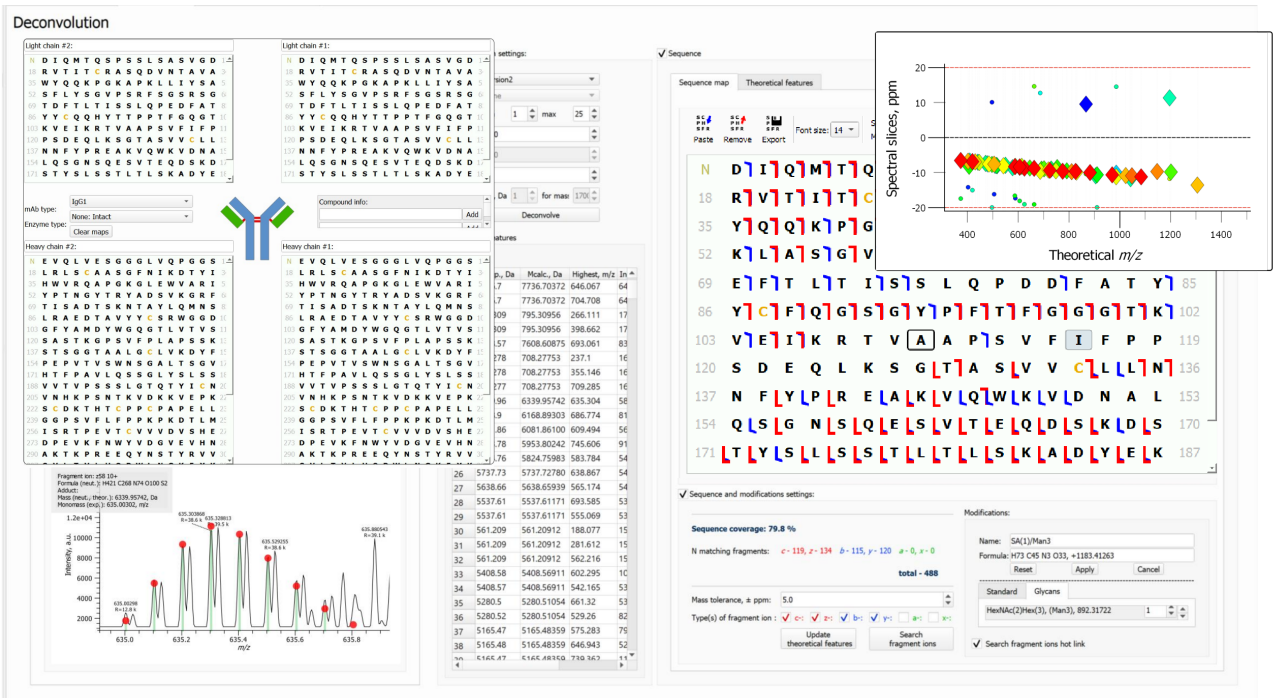
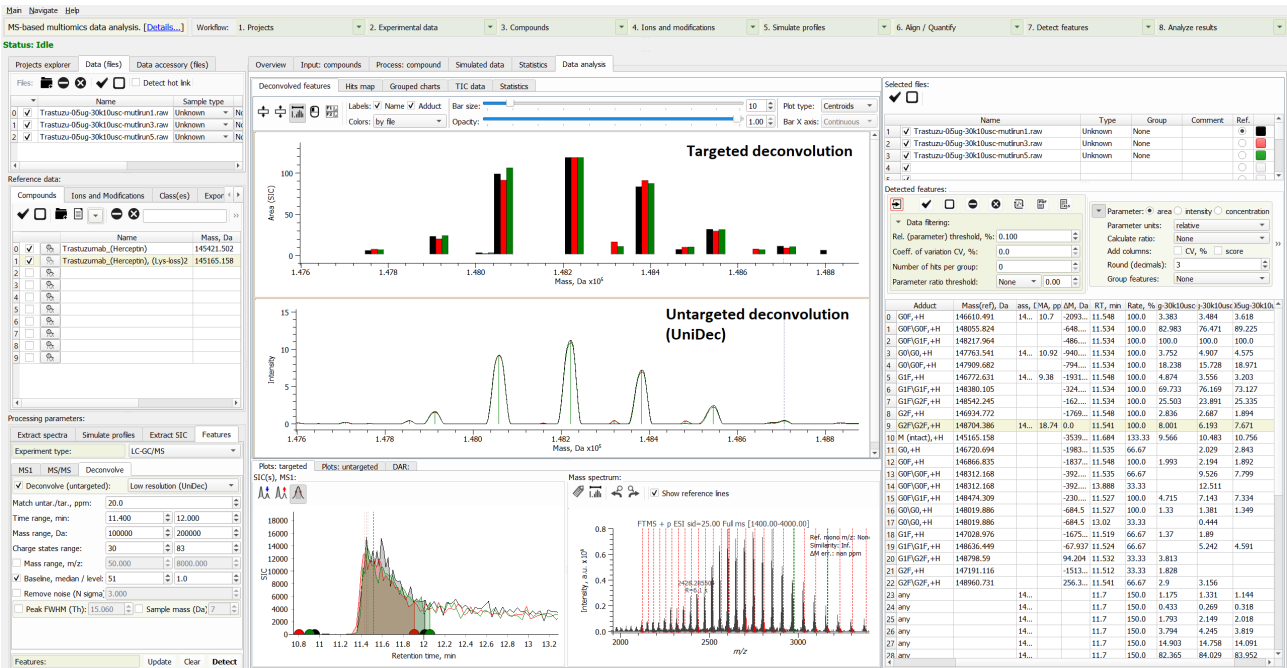
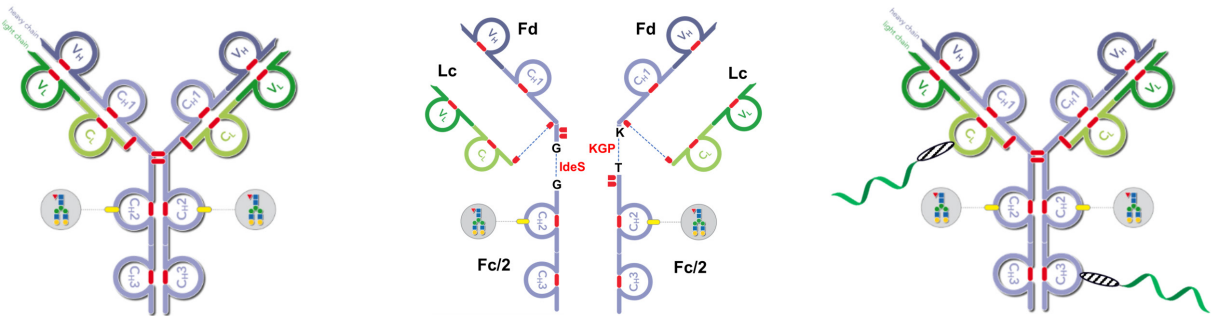


Key Features

- Rapid switching between projects from diverse omics applications, & automated batch file processing
- **Multi-vendor** support, featuring a direct data import of major vendor and open-source file types
- Automatic recognition of meta-information (e.g., instrument model and experimental settings), and
- Support of multiple acquisition modes (MS, MS/MS, SIM, etc.)
- Processes reduced and unreduced **data of any size**, including full profile mass spectra and transients
- Empowered by **FTMS Simulator** enabling accurate simulation of isotopic envelopes & full mass spectra
- Targeted MS and MS/MS experimental data search and annotation with simulated isotopic envelopes
- Targeted & untargeted low-resolution & high-resolution deconvolution, own & third-party approaches
- Multiple parameters for feature extraction and filtering: number of data points in the elution peak,
- Experimental vs. simulated profile similarity, repetition rate, number of adducts, etc.
- User-defined isotopic grouping: averaged isotopologues or isotopic fine structure (IFS) level
- Elemental formula assignment by accurate mass, with a similarity score ranking vs the simulated data
- Data validation through mass accuracy evaluation and mass spectra re-calibration via linear (on-the-fly, lock mass) and non-linear approaches; mass spectral peak alignment
- Quantification of compounds and classes of compounds (via area under the curve in LC/GC-MS): absolute quantification, semi-quantification, and standard addition (external calibration)
- Advanced & routine data processing and data analysis capabilities, user-defined results **reporting** formats
- User-defined selection of parameters output for further data analysis with third party tools

Protein Analysis & BioPharma: Intact Mass, Middle-Up, & Top/Middle-Down

- In-depth processing and quantitative analysis of MS and MS/MS protein analysis data
- BioPharma applications: support for the analysis of mAbs, ADCs, and other (glyco)proteins



Charge Detection Mass Spectrometry (CDMS)

- Supports time-domain transient processing for CDMS workflows;
- Forms an integrated solution with proprietary data acquisition systems to enable implementation of the CDMS approach on practically any FTMS & CDMS instrument.



Key Features

- A complete support of the Peak-by-Peak Multiomics infrastructure for project management
- A dedicated workflow with a graphic user interface for CDMS applications with a frequency-intensity variance segmented (FIVS) algorithm

Integrated hardware-software solution

- Complements FTMS Booster X2T to enable CDMS workflows on high-mass range Orbitrap™ platforms, including a Q Exactive UHMR™ and a Q Exactive HF BioPharma™, and on CDMS instruments with a single detector;
- Complements FTMS Booster X3T to enable CDMS workflows on FT-ICR MS and CDMS instruments with two (and more) detectors

Analyses of Individual Singly Charged Ions Using a High-Field Orbitrap Analyzer, Heck et al., Anal. Chem. (2026) 98, 20, 15250–15258

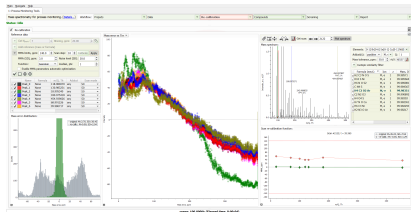
Prolonged Trapping of Adeno-Associated Virus Capsids Reveals that Genome Packaging Affects Single-Ion Mass Spectrometry Measurements, Heck et al., J. Am. Chem. Soc. (2025) 147, 13, 10925–10934

Ultra-Long Transients Enhance Sensitivity and Resolution in Orbitrap-Based Single-Ion Mass Spectrometry, Heck et al., Nature Methods (2024) 21, 619–622

Software tools for data processing and analysis

Spectroswiss software solutions represent a transformative advance in MS data quality and processing performance. Engineered for multi-vendor compatibility and optimized for computational efficiency, our tools seamlessly handle datasets of any size and from any type of mass spectrometer. The software enables application-specific workflows through intuitive, step-by-step routines for streamlined data processing and in-depth analysis.

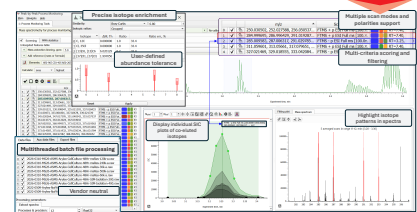
Peak-by-Peak application-specific workflows



Real-time process monitoring
(GC-MS, EI-MS, etc.)



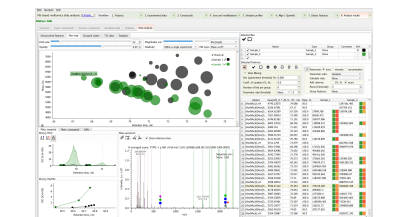
Volatiles: breath, nose-space, and headspace analysis



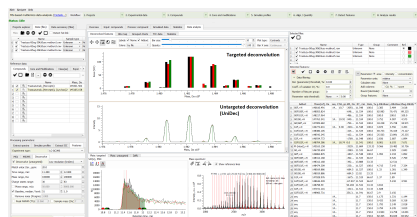
Isotopic analysis: stable isotopic labeling, isotopic ratios



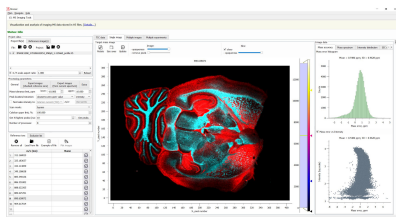
Metabolomics, lipidomics, protein-ligand interactions



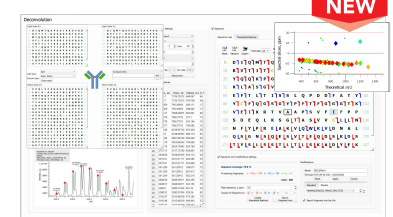
Quantitative bottom-up proteomics, glycoproteomics, PTMs analysis



Proteins & proteoforms: intact mass & quantitation



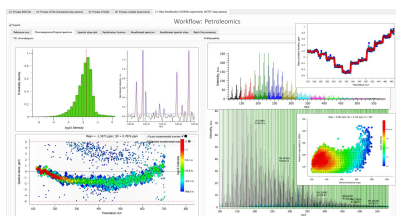
MS Imaging: MALDI & DESI



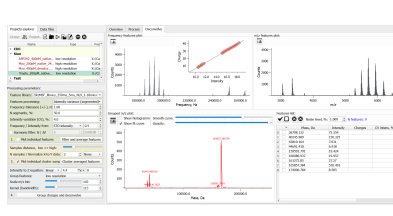
Proteoforms sequencing: Waterfall-powered top-down analysis



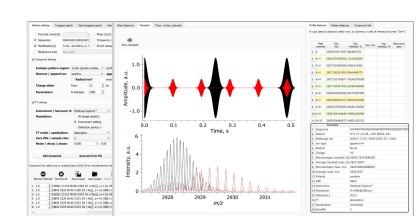
Custom workflows, e.g., Cyclic peptide analysis & Super-resolution MS



Complex mixture analysis
(direct infusion & LC-MS)



Charge detection mass spectrometry (CDMS)



FTMS Simulator: desktop and web-app versions, www.peakbypeak.com

Software Information and Distribution

To learn more about our software tools or to get your free evaluation license, you are most welcome to visit <https://spectroswiss.ch/software/> and to contact us at info@spectroswiss.ch

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FTMS Simulator

WORKFLOWS



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