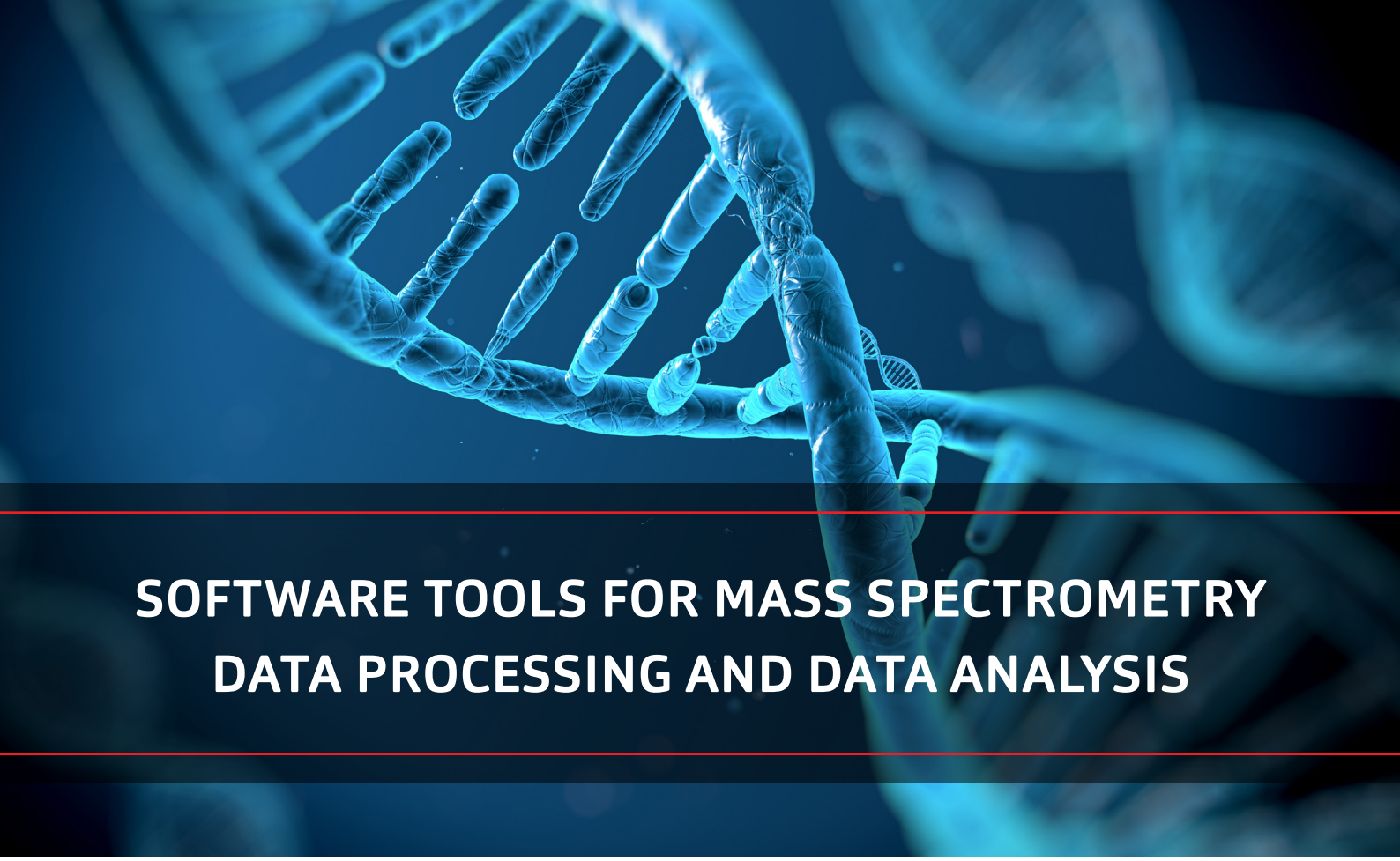
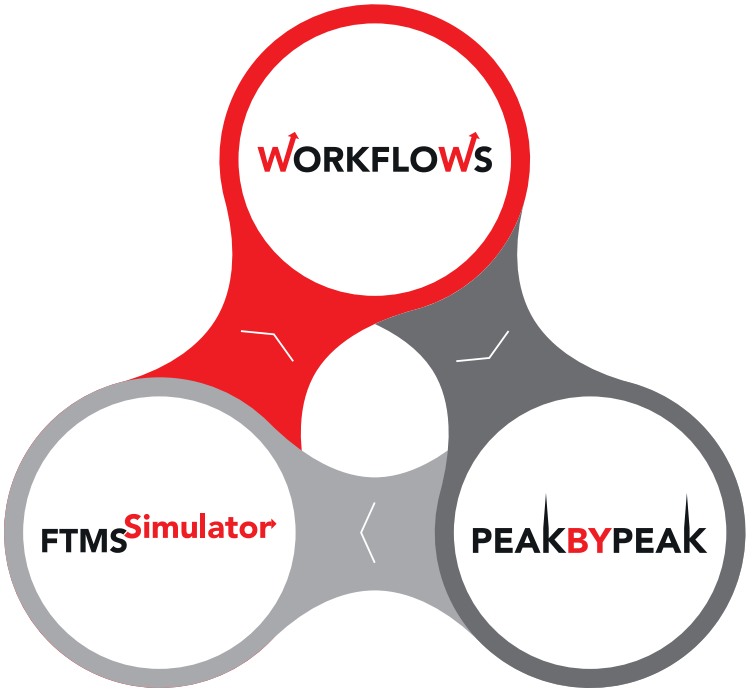


SOFTWARE TOOLS FOR MASS SPECTROMETRY DATA PROCESSING AND DATA ANALYSIS



Spectroswiss

Data processing and data analysis software tools

Spectroswiss software solutions provide a step-change in mass spectrometry data quality and processing sophistication, helping you to take on the most complex and challenging applications.

PEAKBYPEAK

The **Peak-by-Peak** framework is a foundation for our software solutions. It comprises a set of computational modules with a graphic user interface to process mass spectra or FTMS time-domain transients giving you the tools to powerfully investigate your samples. Chose from our Base or Expert Editions.

Software	Base edition	Expert edition
Simulation of FTMS data (The FTMS Isotopic Simulator)	⊕	⊕
RAW file statistics (data distributions: scan time, IT, charge state) and metadata overview	⊕	⊕
Mass spectra processing: baseline correction, noise thresholding and peak-picking	⊕	⊕
Plot multiple mass spectra: experimental and/or simulated data comparison	⊕	⊕
Mass spectra re-calibration: single mass spectra	⊕	⊕
Mass spectra re-calibration: LC-MS/GC-MS (1D datasets)	–	⊕
Mass spectra re-calibration: imaging (2D datasets)	–	⊕
Process multiple FTMS experiments:		
plot TICs and SICs for each input file	⊕	⊕
plot single and/or average mass spectra	⊕	⊕
align LC-MS or LC-MS/MS chromatograms	–	⊕
average data between any files (including between technical replicates)	–	⊕
SIM-window stitching from spectral or time-domain data	–	⊕
SIM-window averaging and stitching	–	⊕
Deconvolution of low-resolution data	–	⊕
Deconvolution of high-resolution data	⊕	⊕
Data visualization and output: high quality images and/or mass spectra in open file formats	⊕	⊕

FTMS Simulator

FTMS Simulator allows to in-silico accurately represent isotopic envelopes and full range mass spectra of any complexity for Orbitrap™ & ICR FTMS platforms.

WORKFLOWS

Together, Peak-by-Peak and FTMS Simulator power the application-specific **Workflows** that enable step-by-step advanced data processing and data analysis for FTMS and other MS platforms.

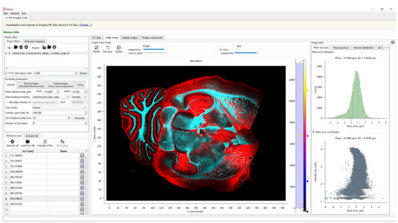
Key features

- step-by-step workflows for mass spectrometry data processing and data analysis
- vendor-neutral approach, featuring a direct data import of major vendor file types
- support of reduced and unreduced data, including full profile mass spectra and time-domain transients
- baseline correction, noise thresholding, peak picking, aligning, normalization, mass re-calibration
- simulation of isotopic envelopes and mass spectra: stand-alone and workflow-embedded
- experimental data search and annotation with simulated centroid and profile isotopic envelopes
- parallel computing on multiple CPU-cores and GPUs for fast data processing
- powerful and memory-efficient handling of (very) large datasets

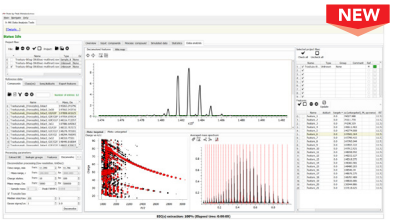
Workflows

Customer-centered, computationally-efficient, ergonomic, and flexible workflows for your most challenging mass spectrometry applications – to handle (practically) any size dataset from any type of a mass spectrometer.

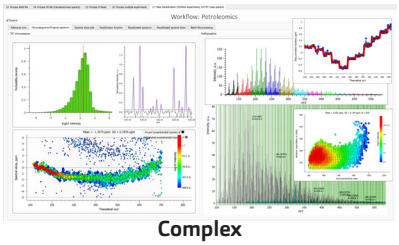
Quantitative Metabolomics & Lipidomics



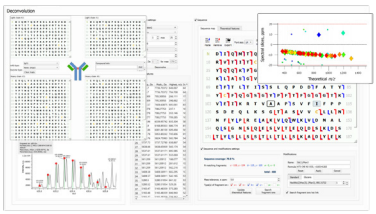
MALDI & DESI Imaging



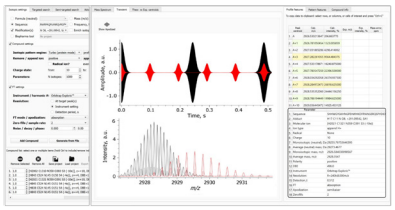
Protein Analysis (BioPharma)



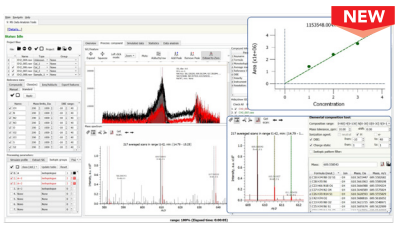
Complex Mixture Analysis



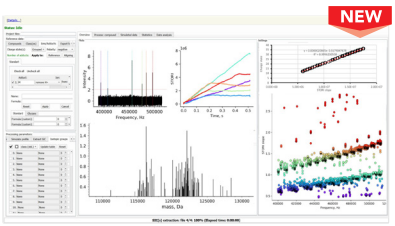
Top-Down & Middle-Down Analysis



FTMS Simulator (Protein-grade!)



Quantitative LC/GC-MS analysis of Compound Classes



Charge Detection Mass Spectrometry (CDMS): Individual (Single) Ion Counting

Custom Workflows

Graphical User Interface and Powerful Custom Workflows

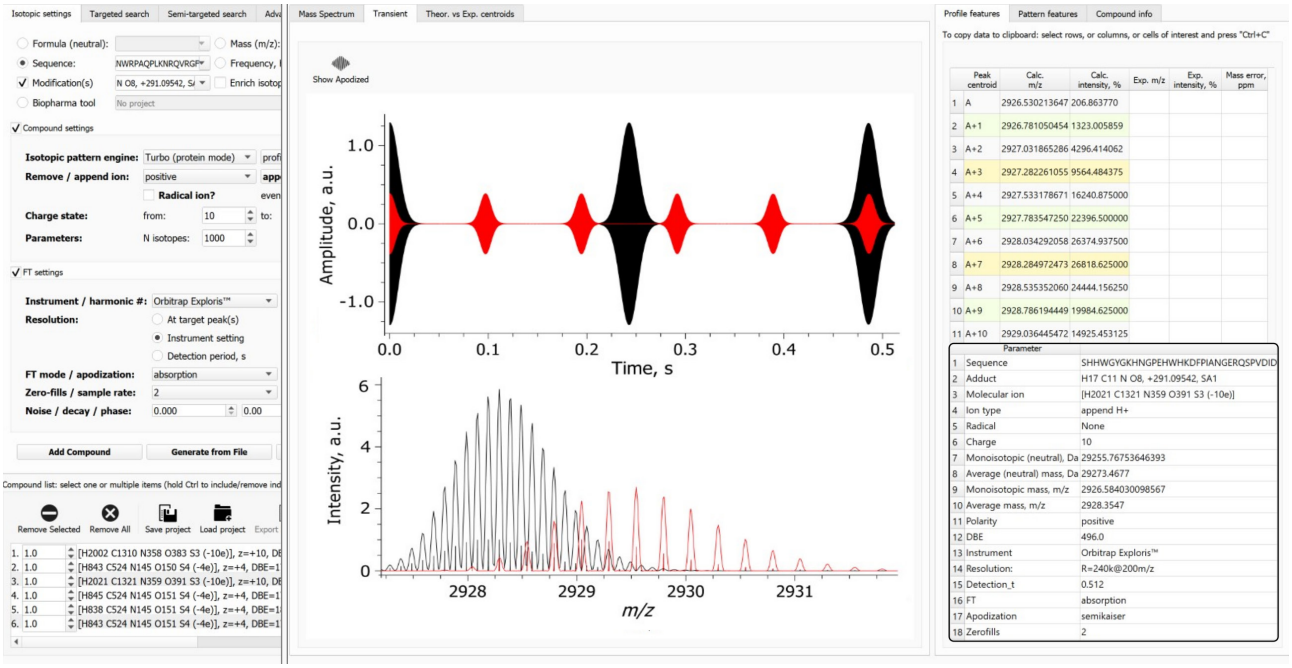
Our powerful computational algorithms and flexible graphical user interface (GUI) templates can be configured to match your needs and offer computationally-efficient, fast, and accurate data processing and analysis solutions.

WORKFLOWS

FTMS Simulator

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

- 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

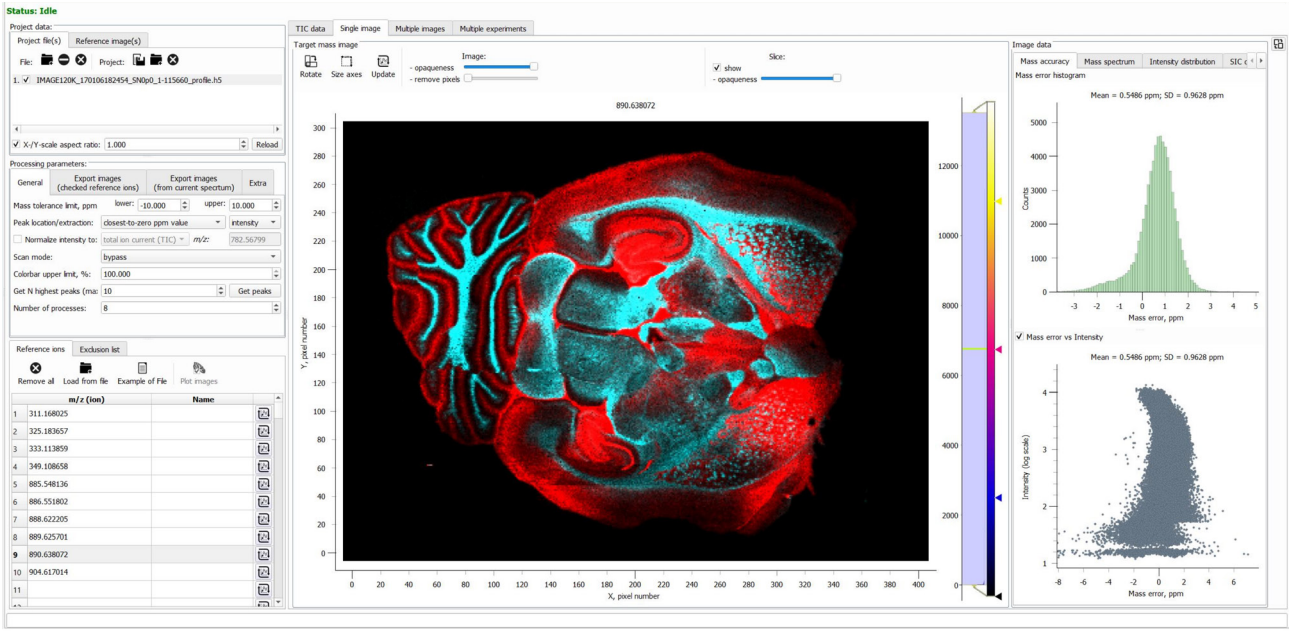
FTMS Simulator

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, DOI 10.1021/jasms.1c00336

Imaging

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



The presented dataset (mouse brain tissue imaging, 50 x 50 µm pixel size) was acquired on an LTQ Orbitrap Elite™ FTMS instrument (Thermo Fisher Scientific) equipped with a MALDI Injector (Spectroglyph). Panels in the right column show mass error distributions as a function of (top) spectral counts and (bottom) peak intensities.

Key features

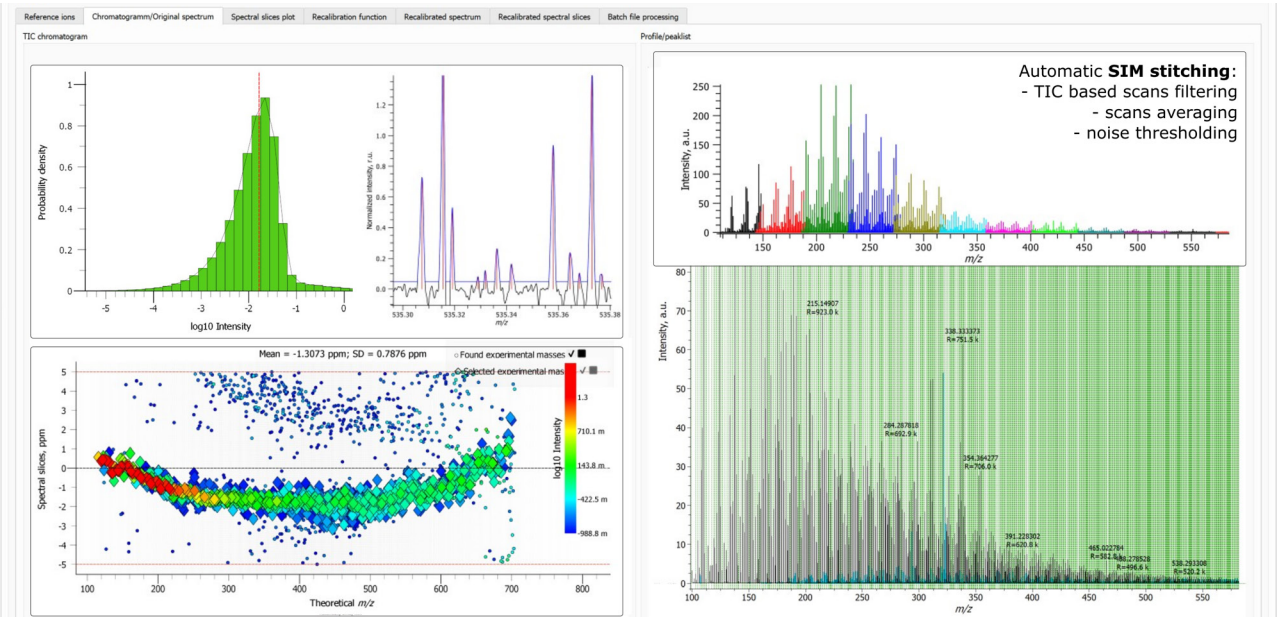
- A vendor-neutral platform for MSI data processing and analysis from diverse MS instruments, including Orbitrap™ FTMS, FT-ICR MS or MRMS, MRT MS, TOF MS, and QQQ MS
- A direct data import of major vendor file types, including Agilent, Bruker, Thermo Fisher Scientific, and Waters; accompanied by import of MSI data in the **imzML** file format
- Support for both MALDI and DESI ion sources, including those from niche manufacturers, e.g., MassTech, Spectroglyph, and TransMIT
- Automatic recognition of acquisition modes (MS, MS/MS, SIM, etc.), ion sources, and ion polarity
- Data validation and correction through mass accuracy evaluation
- Time-domain transient processing: super-resolution data processing (e.g., with least squares fitting)
- Mass spectra processing: user-defined parameters (e.g., noise thresholding, data averaging)
- Image processing: normalization, noise reduction, hotspot removal, etc.
- Instant visualization of mass spectra and images (click and see)
- Regions of interest (ROI) definition, analysis and geometry handling
- Comparative analysis of (averaged) mass spectra from multiple ROIs for the same or different data sets
- Co-localization and overlay of (multi-mode) images
- Pixels/rows aligning by the time stamps when scan times are not fixed (e.g., when AGC is enabled)
- Image weighted transparency, add color function, customizable and adjustable color maps

MOZAIC

Imaging and Direct Sampling Capabilities of Nanospray Desorption Electrospray Ionization with Absorption-Mode 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. Gregory W. Vandergrift, *et al.,. Anal. Chem.* 2022, 94, 8, 3629–3636

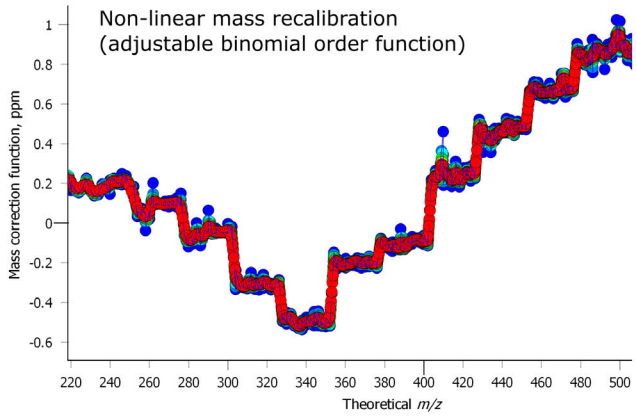
Complex mixture analysis, petroleomics & bio-fuels

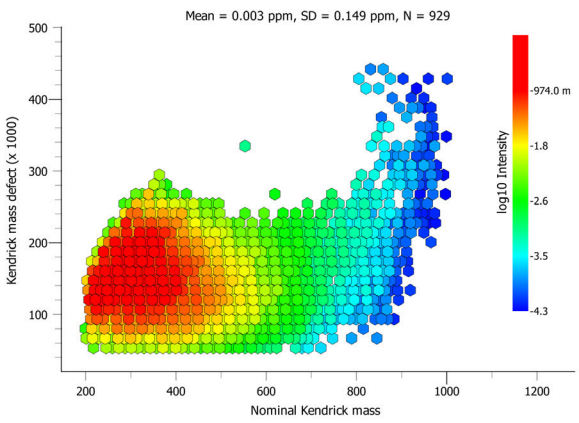
Advanced processing and analysis of (very) complex mixtures mass spectrometry data



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

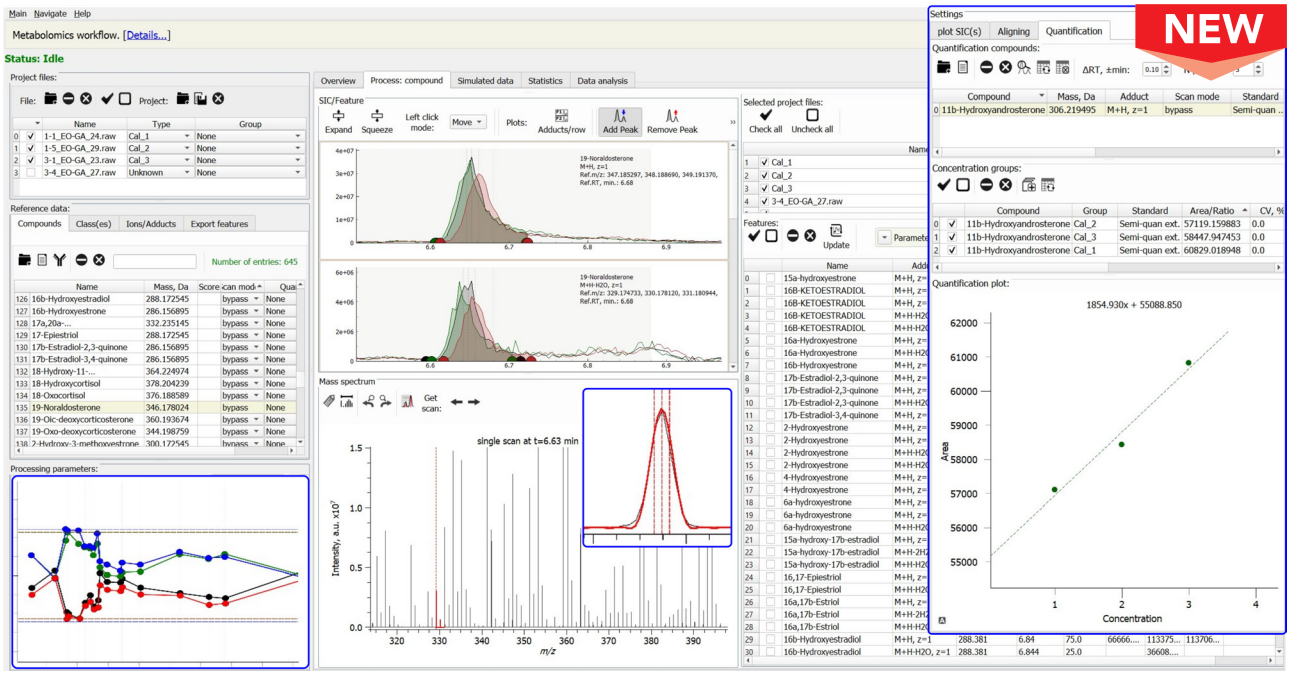




Iterative Method for Mass Spectra Recalibration via Empirical Estimation of the Mass Calibration Function for Fourier Transform Mass Spectrometry-Based Petroleomics. Anton N. Kozhinov, Konstantin O. Zhurov, and Yury O. Tsybin. *Anal. Chem.* 2013, 85, 13, 6437–6445

Metabolomics

In-depth processing and quantitative analysis of mass spectrometry metabolomics and lipidomics data

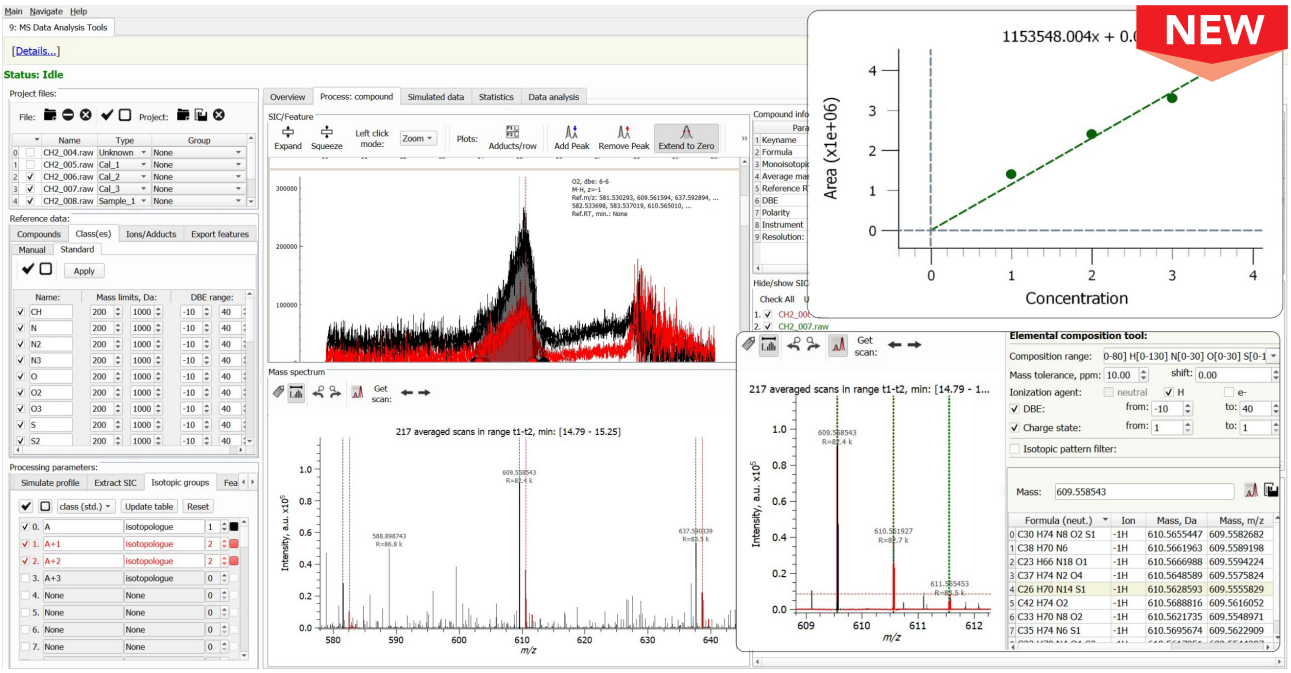


Key features

- Common interface: a vendor-neutral platform for metabolomics data processing and analysis from diverse mass spectrometers, supporting both LC-MS and GC-MS
- Automatic recognition of meta-information (e.g., instrument model and experimental settings), and support of multiple acquisition modes (MS, MS/MS, SIM, etc.)
- Input of target and semi-target databases of individual compounds of interest; charge state grouping;
- **Aligning** of LC-MS experiments with or without extracted feature lists:
  - targeted (user-selected mass values from mass spectra, or reference compounds)
  - untargeted (parameter-dependent feature extraction, without annotation)
- **Quantification** of compounds (via area under the curve in LC/GC-MS):
  - absolute quantification (labelled compounds as internal standards, ratio of analyte compound signal to the internal standard compound)
  - semi-quantification (internal standards provide quantitative information, expressed as areas under the curve; information used for other compounds)
  - semi-quantification, standard addition (external calibration)
- Accurate and reliable peak picking with the adjustable mass spectra parameters
- 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
- Elemental formula assignment by accurate mass, with a similarity score ranking vs the simulated data
- Experimental data matching with the simulated isotopic envelopes. User-defined analyte parameters for simulations: elemental composition, amino acid sequence, charge carrier, adduct, modifications, isotopic enrichment/depletion, number of charge states and isotopologues
- 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
- Support for batch file processing of large data sets: practically any number of LC-MS data sets
- User-defined selection of parameters output for further data analysis with third party tools
- Comparative analysis of extracted features via a dynamic global result matrix (deconvolved mass spectrum, hits map, selectable parameter table, and a quick access to the experimental data)
- Wide range of time-domain data processing parameters: absorption/magnitude FT, apodization function, number of zero-fills, full or reduced profile mass spectra, centroids, visualize transients

Compound classes analysis: LC/GC-MS complex mixture analysis

In-depth processing and quantitative analysis of mass spectrometry **compound classes** data

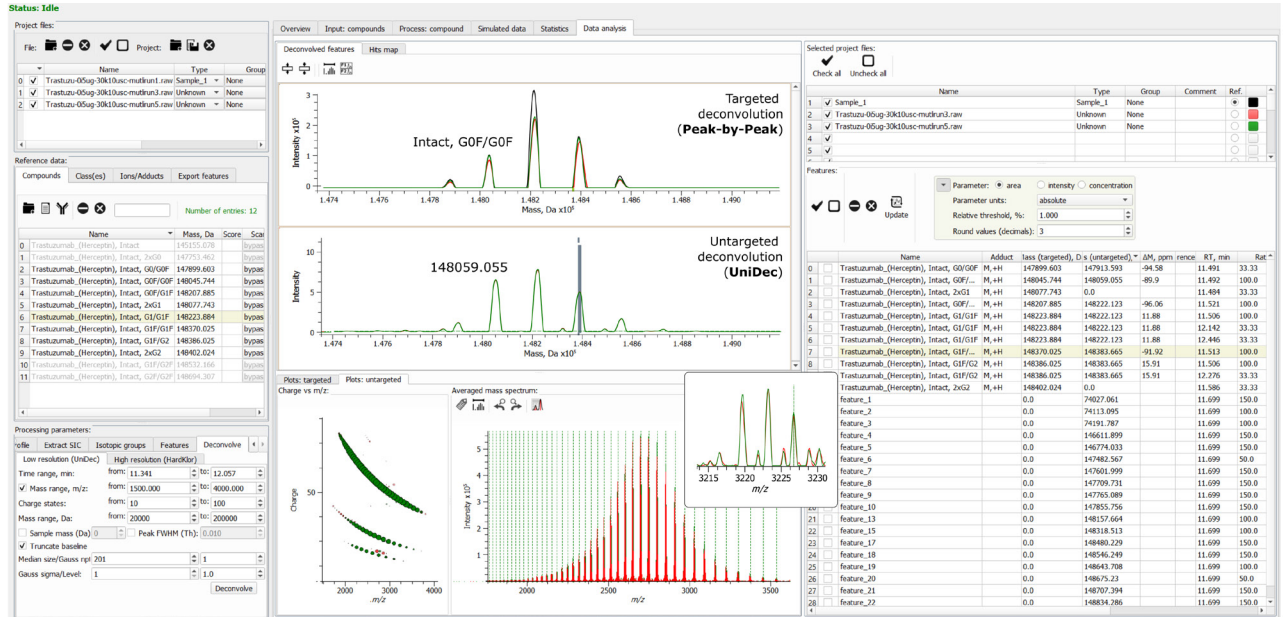


Key features

- Input of target and semi-target databases of pre-set and user-defined classes of compounds of interest
- Common interface: a vendor-neutral platform for complex mixture analysis data processing and analysis from diverse mass spectrometers, supporting both LC-MS and GC-MS
- Automatic recognition of meta-information (e.g., instrument model and experimental settings)
- **Quantification of classes of compounds** (via area under the curve in LC/GC-MS):
  - absolute quantification (labelled compound classes as internal standards, ratio of analyte compound classes signal to the internal standard compound classes)
  - semi-quantification (internal standards provide quantitative information, expressed as areas under the curve; information used for other compound classes)
  - semi-quantification, standard addition (external calibration)
- Accurate and reliable peak picking with the adjustable mass spectra parameters
- 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
- Elemental formula assignment by accurate mass, with a similarity score ranking vs the simulated data
- Experimental data matching with the simulated isotopic envelopes. User-defined analyte parameters for simulations: elemental composition, amino acid sequence, charge carrier, adduct, modifications, isotopic enrichment/depletion, number of charge states and isotopologues
- 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
- Support for batch file processing of large data sets: practically any number of LC-MS data sets
- User-defined selection of parameters output for further data analysis with third party tools
- Comparative analysis of extracted features via a dynamic global result matrix (deconvolved mass spectrum, hits map, selectable parameter table, and a quick access to the experimental data)
- Wide range of time-domain data processing parameters: absorption/magnitude FT, apodization function, number of zero-fills, full or reduced profile mass spectra, centroids, visualize transients

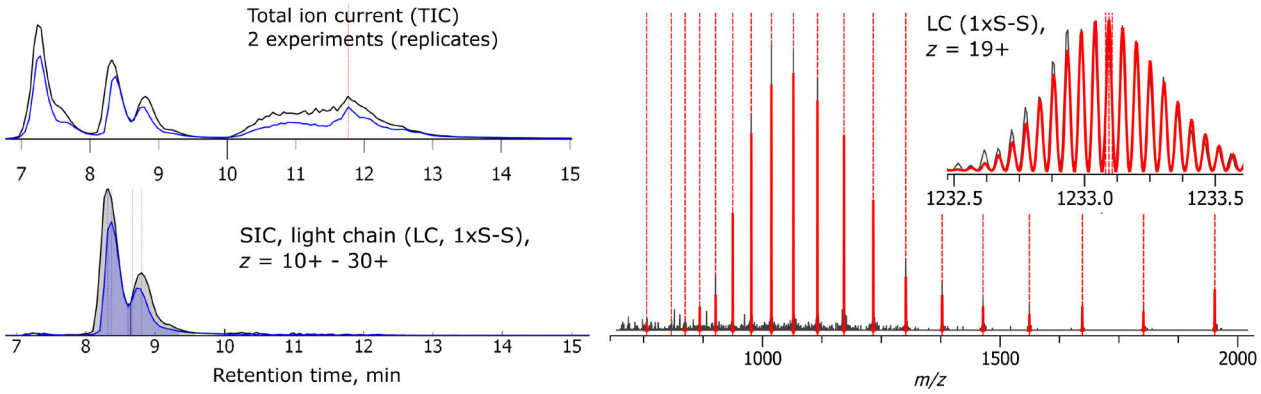
Protein Analysis - BioPharma

In-depth processing and quantitative analysis of mass spectrometry protein analysis data



Key features

- Advanced and proprietary mass spectrometry solutions for mAb analysis, including complex ADCs/AOCs
- Automatic recognition of meta-information (e.g., instrument model and experimental settings)
- Input of target and semi-target databases of individual proteoforms of interest; charge state grouping;
- **Deconvolution** of low-resolution and high-resolution mass spectra with **targeted** (see Figure below) and untargeted approaches. Perhaps a unique commercial implementation of **UniDec** for deconvolution

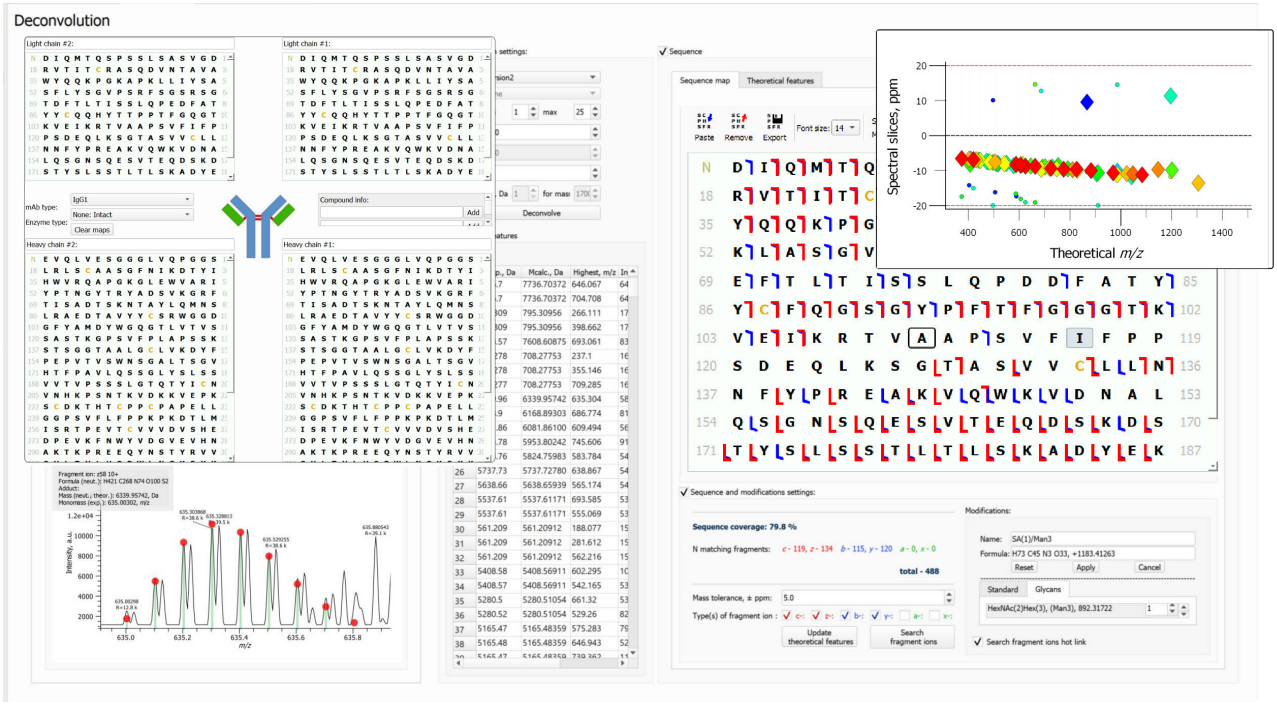


- Data validation through mass accuracy evaluation and mass spectra re-calibration via linear (on-the-fly, lock mass) and non-linear approaches; mass spectral peak alignment
- Experimental data matching with the simulated isotopic envelopes. User-defined analyte parameters for simulations: amino acid sequence, charge carrier, adduct, modifications, isotopic enrichment/depletion, number of charge states and isotopologues
- Support for batch file processing of large data sets: practically any number of LC-MS data sets
- Advanced time-domain transient processing: matching the mass spectral resolution to the sample characterization needs – from high-resolution to ultra-low resolution for enabling proteoform peak integration approach

Drug-to-Antibody Ratio Estimation via Proteoform Peak Integration in the Analysis of Antibody–Oligonucleotide Conjugates with Orbitrap Fourier Transform Mass Spectrometry. Konstantin O. Nagornov, Natalia Gasilova, Anton N. Kozhinov, Pasi Virta, Patrik Holm, Laure Menin, Victor J. Nesatyy, and Yury O. Tsybin. *Anal. Chem.* 2021, 93, 38, 12930–12937

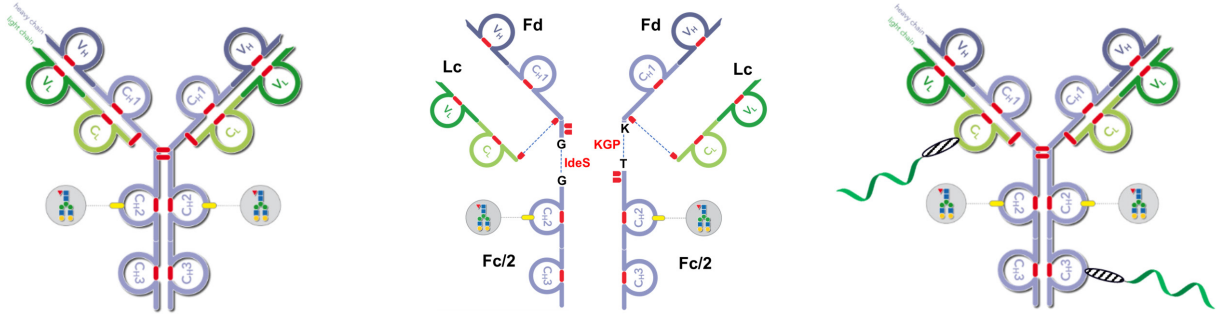
Protein Analysis via Top-Down and Middle-Down Approaches

Advanced processing and analysis of intact, middle-down, and top-down data



Key features

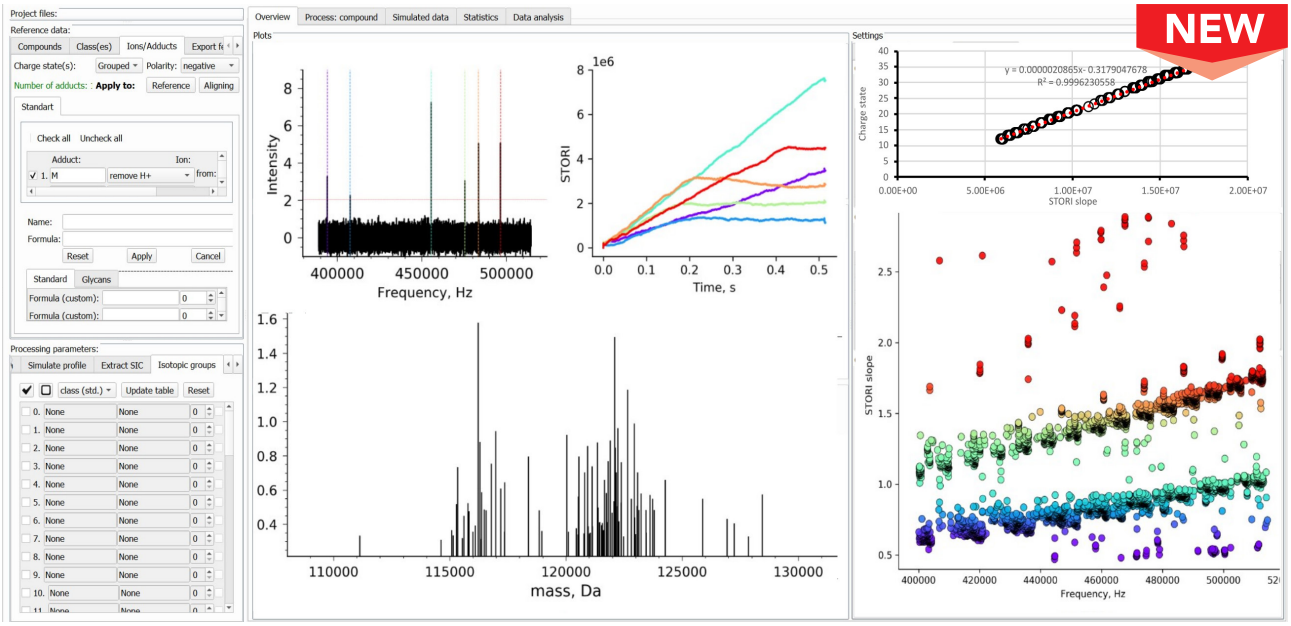
- Advanced and proprietary mass spectrometry solutions for mAb analysis, including complex ADCs/AOCs
- Superior quality data owing to proprietary methods and techniques for Orbitrap FTMS
- Integration of intact mass, middle-up, middle-down, top-down, and bottom-up mass spectrometry data
- Data averaging of LC-MS/MS and MS/MS data from multiple experiments (technical replicates)
- Recalibration of intact (MS data) and middle/top-down (MS/MS data) mass spectra
- Embedded database of common monoclonal antibodies with sequences and modifications
- Accurate simulation of mass spectra based on proteoform sequence and modifications
- Comparison of experimental and simulated isotopic envelopes and mass spectra
- High-resolution and low-resolution deconvolution, charge state grouping, quantitation
- Intact mass and product ion assignment to the deconvolved data
- Interactive graphical representation of sequence maps (add proteoforms, remove assignments, etc.)
- Graphical output (images), mass spectral data and peak lists



Structural Analysis of Monoclonal Antibodies with Top-down and Middle-down Electron Transfer Dissociation Mass Spectrometry: The First Decade. Luca Fornelli, Daniel Ayoub, Kristina Srzentić, Konstantin Nagornov, Anton Kozhinov, Natalia Gasilova, Laure Menin, Alain Beck, and Yury Tsybin. CHIMIA, 2022, 76, 114-126

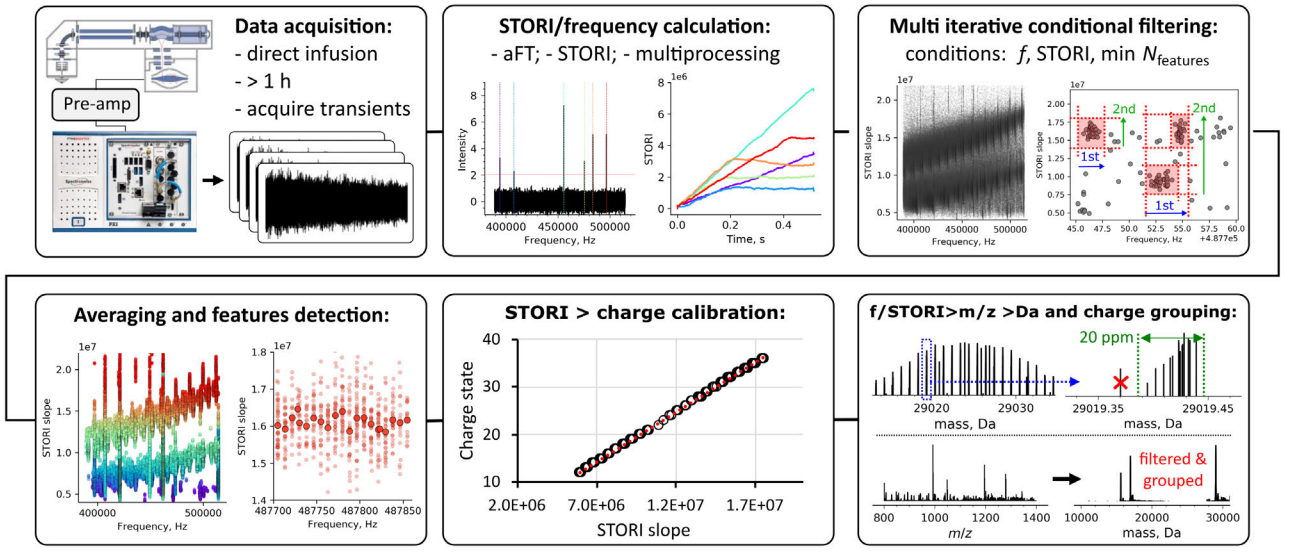
Charge Detection Mass Spectrometry (CDMS)

An integrated solution enabling individual (single) ion counting approach on Orbitrap™ and ICR FTMS

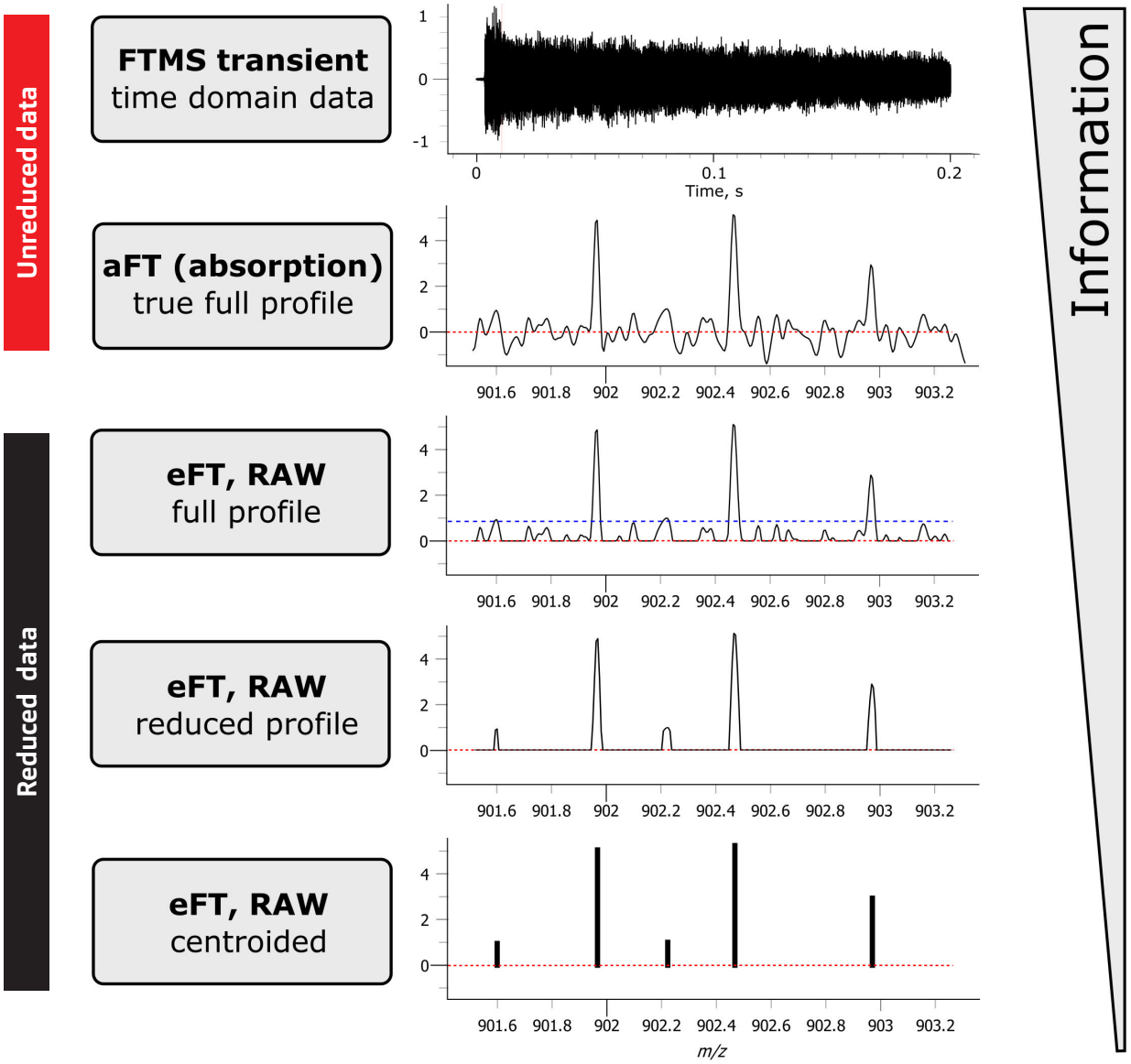


Individual (Single) Ion Counting Workflow

- Access to the **time-domain transients** from Orbitrap™ and ICR FTMS instruments via our proprietary add-on high-performance data acquisition systems – FTMS Boosters
- Wide range of time-domain data processing parameters: absorption/magnitude FT, apodization function, number of zero-fills, full or reduced profile mass spectra, centroids, visualize transients
- Advanced time-domain data processing, including STORI (selective temporal overview of resonant ions) approach
- User-controllable multi-iterative conditional filtering, averaging, and feature detection
- Charge calibration and charge grouping procedures
- Results comparison with conventional approaches for time-domain transient analysis



FTMS Didactics: Unreduced and Reduced Data



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

PEAKBYPEAK FTMSSimulator WORKFLOWS

Spectroswiss

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