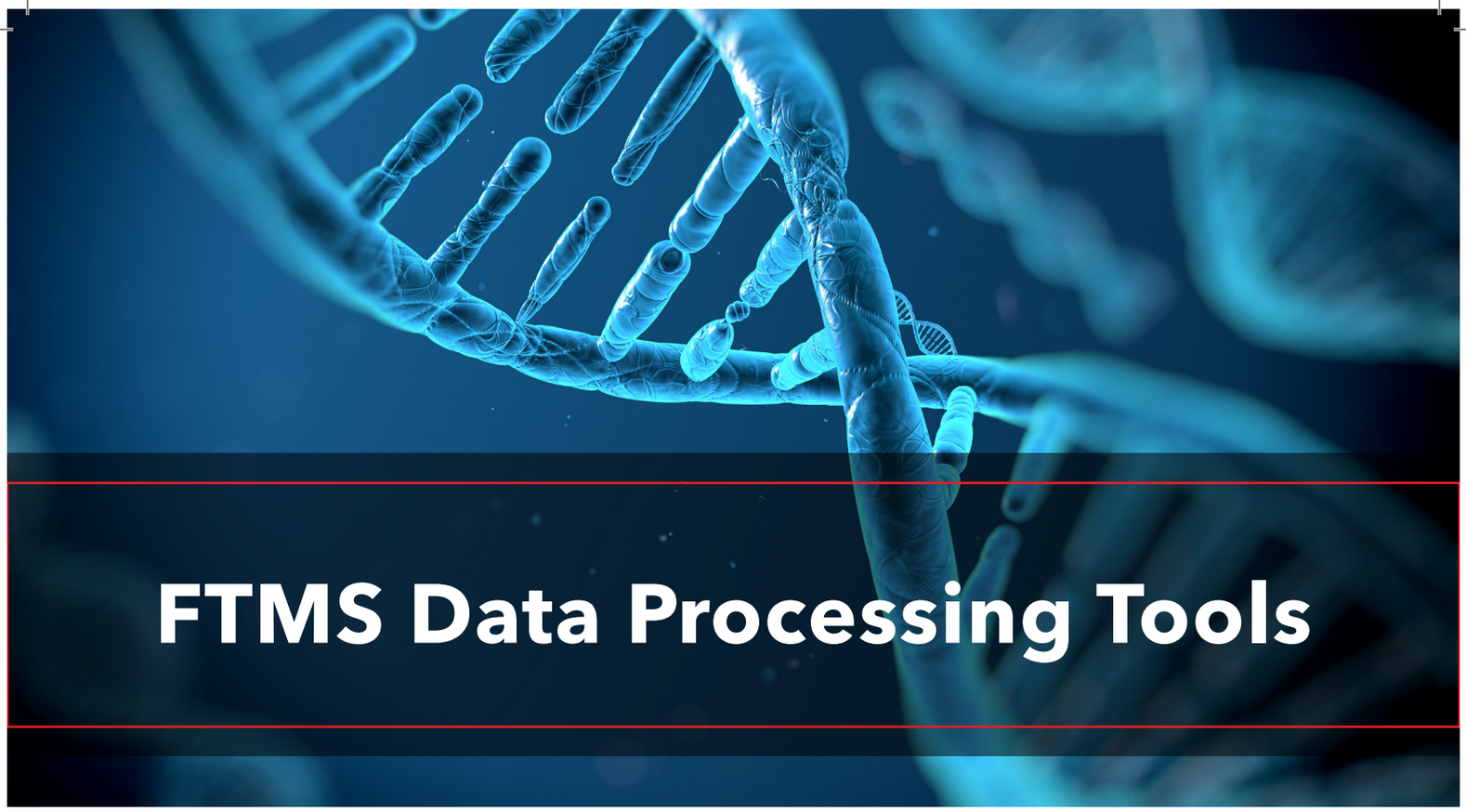
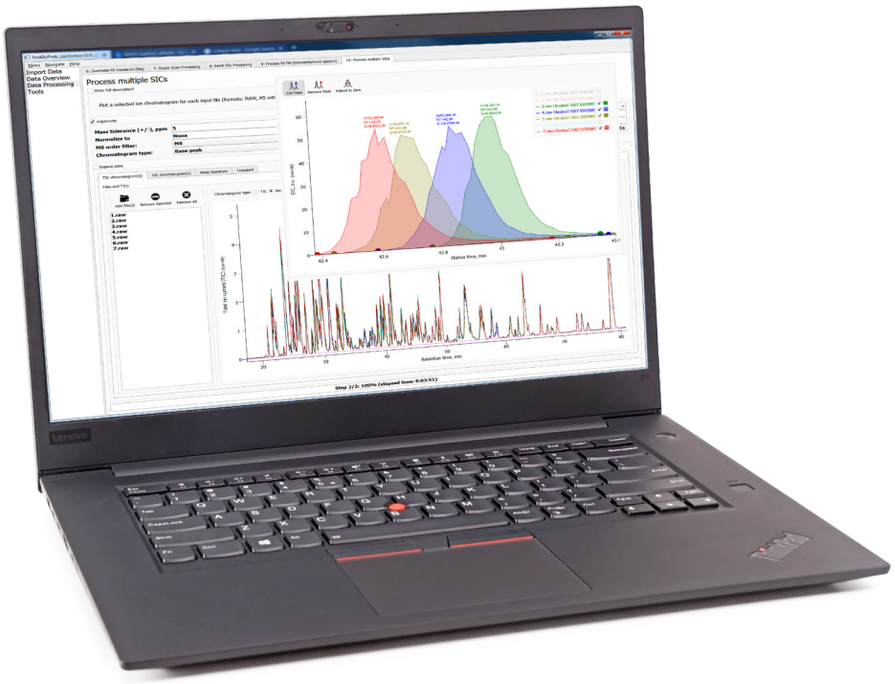


FTMS Data Processing Tools

peakbypeak

FTMS DATA ANALYSIS

by spectroswiss



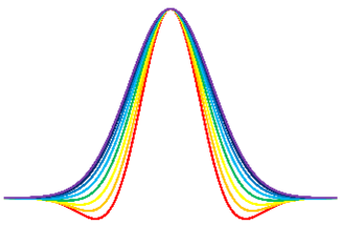
Spectroswiss

FTMS Data Processing Tools

Most FTMS instruments provide only processed and noise-reduced data (reduced profile or centroided mass spectra). The availability of the unprocessed (full profile) mass spectra and true raw data (FTMS transients) allows for the most efficient data processing including powerful time-frequency conversion using Fourier transform and super-resolution algorithms (e.g., least-squares fitting).

The Spectroswiss software solutions (**Peak-by-Peak** and **AutoVectis**), alone or empowered by our high-performance data acquisition system (**FTMS Booster**), provide a step change in FTMS data quality and processing sophistication, helping you to take on the most complex and challenging applications. Our solutions are capable of processing both, FTMS transients and mass spectra, represented in either full profile, reduced profile, or centroided modes.

peakbypeak
FTMS DATA ANALYSIS
by spectroswiss



Workflows

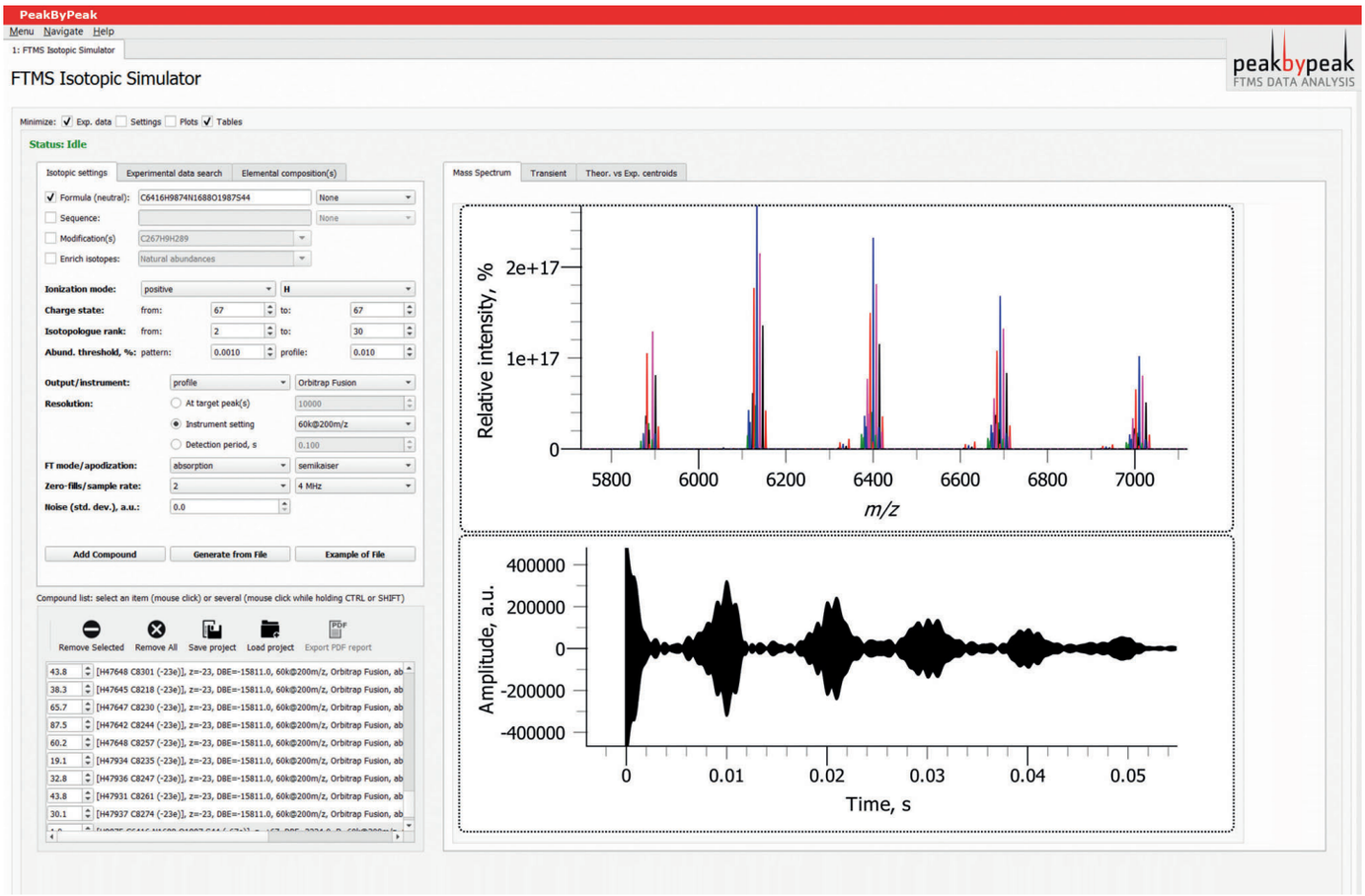
- Metabolomics
- Petroleomics
- GC applications
- Lipidomics
- Top-down MS
- Spectroscopy
- Imaging
- Proteomics
- On demand

Key features

- step-by-step workflows for FTMS data processing
- processing of .RAW files, .d folders, .H5 files
- powerful handling of (very) large datasets
- baseline correction, noise thresholding, peak picking, calibration
- FTMS-specific simulation of isotopic envelopes and mass spectra
- experimental data search with simulated centroid and profile isotopic envelopes
- parallel computing on multiple CPU-cores and GPUs for fast data processing
- GPU-driven least-squares fitting (LSF) for targeted applications
- output file formats: H5, TXT, MGF, mzXML, mzML, imzML

FTMS Data Simulator

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



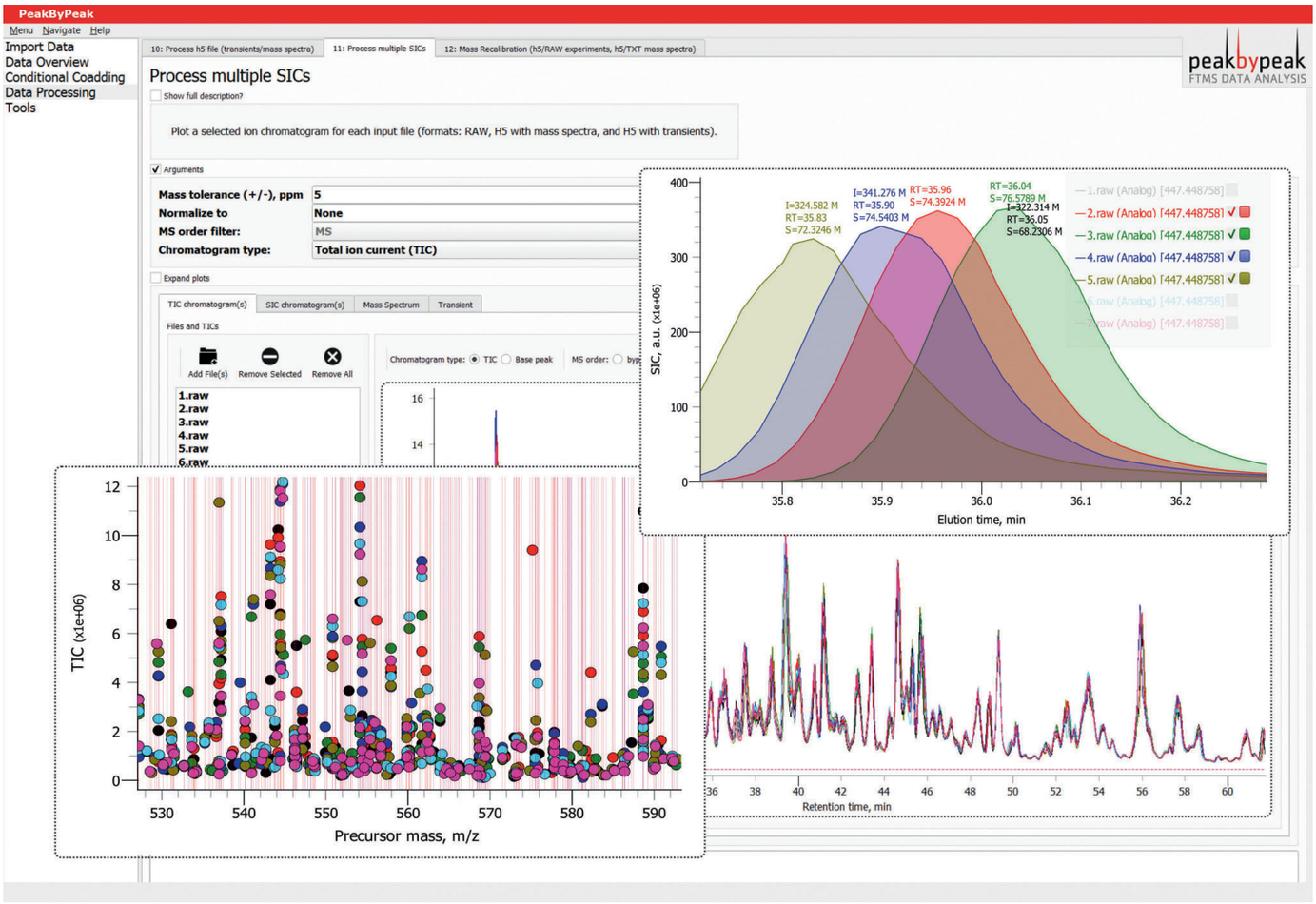
Key features

- design FTMS experiments by defining your molecules, selecting appropriate FTMS parameters for the major commercial FTMS instruments and data processing parameters;
- search the experimental data with a like-for-like theoretical data using similarity score;
- teach the FTMS subject by demonstrating both transient and mass spectra;
- analyte parameters: elemental composition, amino acid sequence, charge carrier, modifications, isotopic enrichment/depletion, number of charge states and isotopologues
- FTMS experiment parameters: FTMS instrument selection (models of Orbitrap™ & ICR), resolution setting (@ *m/z*), transient sampling rate, add noise, set thresholds
- data processing parameters: absorption/magnitude FT, apodization function, number of zero-fills, full or reduced profile mass spectra, centroids, visualize transients
- use mass spectra: set ratios of intensities, visualize isotopic envelopes, plot multiple envelopes, extract high quality figures, extract data points for analysis
- results output: search experimental data, rank search results by the similarity score (*m/z*, intensity), save project for future use, create report as a PDF file

Nagornov, et al., Overcoming the sensitivity versus resolution trade-off in gas chromatography Orbitrap mass spectrometry by multiplexed digital processing, Submitted

Metabolomics & Proteomics

Advanced data processing improves LC/GC FTMS performance



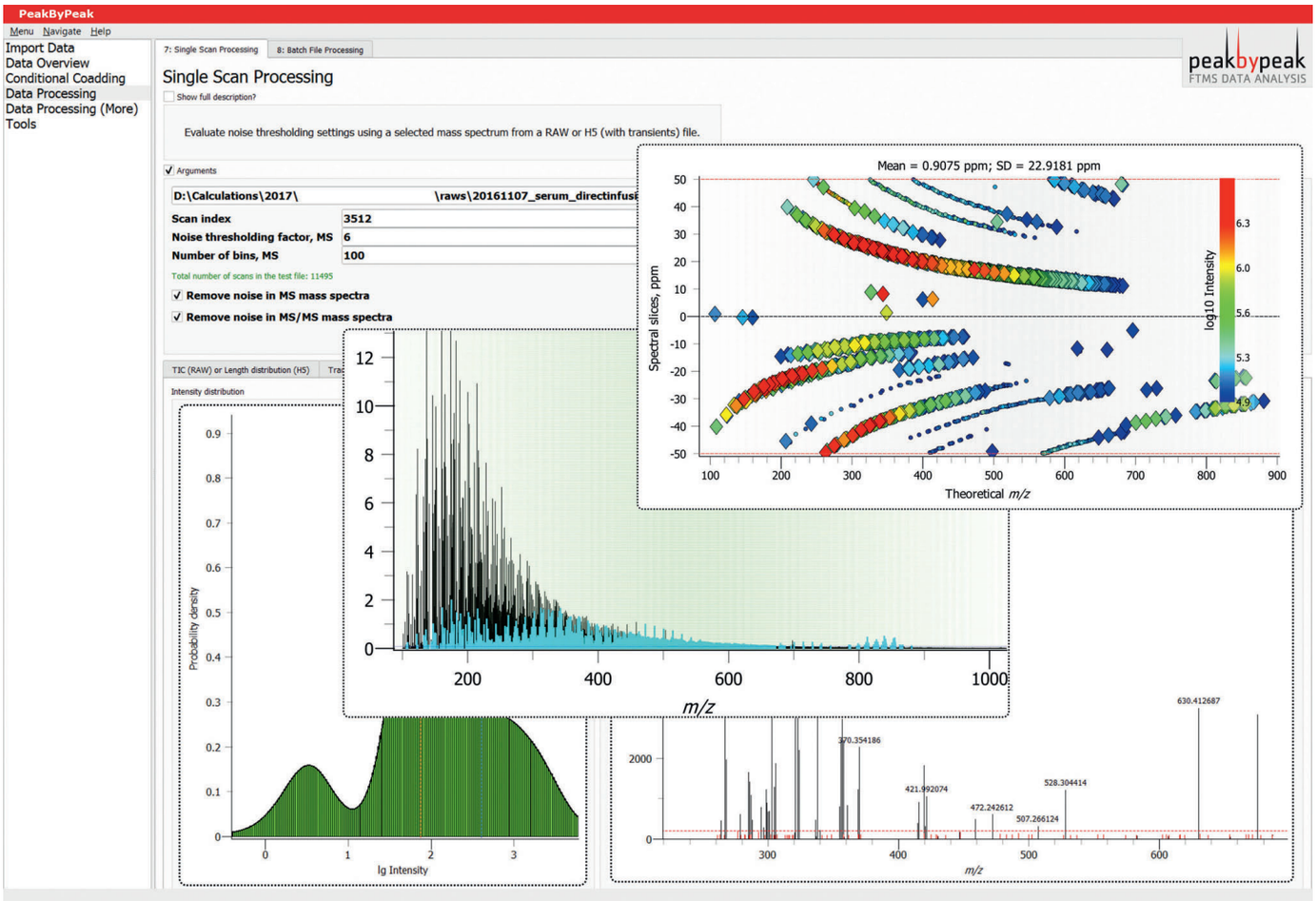
Key features

- workflows based on full profile mass spectra & transients acquired with FTMS Booster.
- scan co-indexing between .RAW and transient datasets for every LC/GC-MS run.
- visualization and processing of practically any size LC/GC-MS datasets (.RAW).
- absorption mode FT of phased transients matches the performance of eFT processing.
- data summation across a number of LC/GC-MS runs, including chromatogram alignment.
- capabilities of data (mass spectra and transients) averaging within a single and across a number of DDA and DIA proteomics experiments.
- supporting quantitation workflows via selected ion chromatograms and area calculations.
- recalibration of mass spectra to improve mass accuracy.
- super-resolution signal processing for targeted quantitative proteomics applications.
- advanced control of processing parameters, including noise analysis.
- automated batch analysis of LC/GC-MS datasets.
- output file formats enable further analysis with commercial and open source tools.

Srzentić, et al., Multiplexed middle-down mass spectrometry as a method for revealing light and heavy chain connectivity in a monoclonal antibody. Analytical Chemistry, (2018) 90, 12527−12535

Petroleomics & Lipidomics

Advanced processing of FTMS data for analysis of (very) complex mixtures



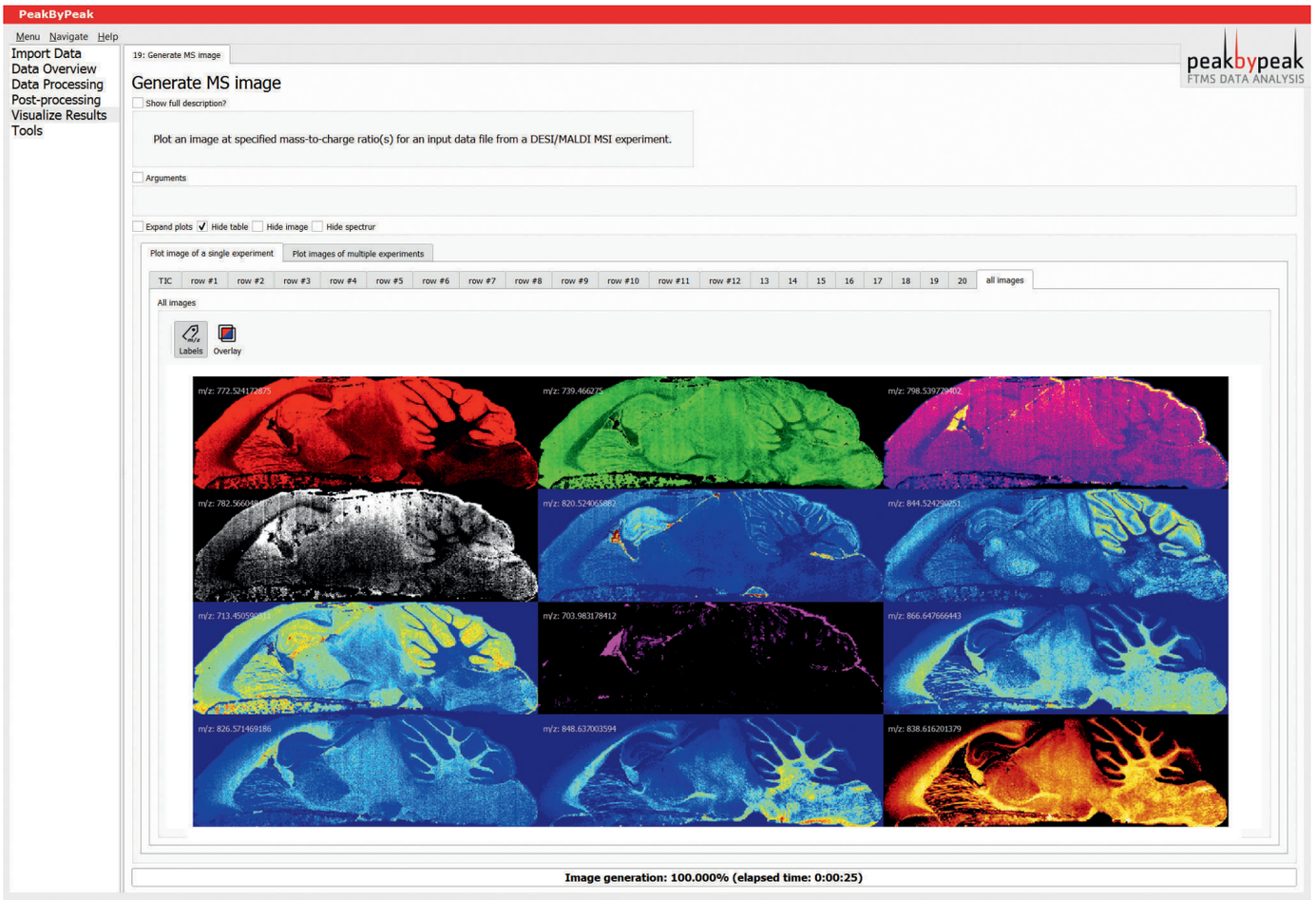
Key features

- integration and processing of practically any size .RAW files, .d folders and .H5 files.
- open file formats for transients & mass spectra : H5, MGF, mzXML, mzML, imzXML.
- visualization of transients and mass spectra, visual comparison from separate data sets.
- spectral and transient averaging for high sensitivity and dynamic range.
- processing of LC-MS data for petroleomics/biofuels/lipidomics applications.
- basic discrete FT with parallel, multi-CPU computing.
- advanced FT with pre- and post-processing, including apodization, zero-filling, magnitude and absorption mode FT.
- noise thresholding, reduced-profile mode mass spectra representation.
- peak picking with N-points interpolation and efficient baseline correction.
- mass scale calibration equations, including iterative re-calibration for complex mixtures.

Krajewski, et al., Characterization of Biocrude Oils with an Orbitrap Fusion Mass Spectrometer with Increased Resolution and Dynamic Range, Submitted

Imaging Mass Spectrometry

Advanced processing of FTMS data for imaging with Orbitrap™ and FT-ICR MS maximizes FTMS data quality for further data analysis with statistical tools

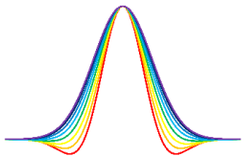


Key features

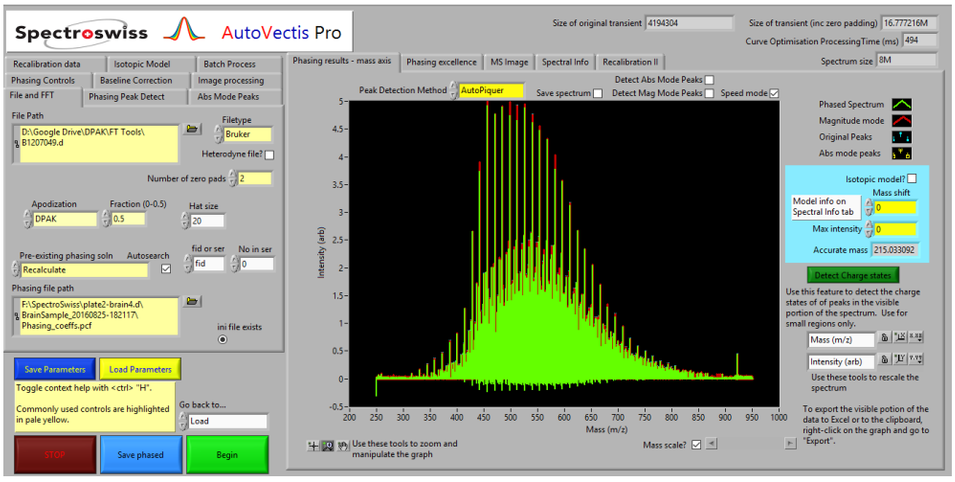
- workflows based on transients acquired with FTMS Booster or provided by manufacturer.
- data processing of large (e.g., 0.1-1.0 TB) imaging mass spectra datasets (RAW, d. folder).
- post-processing of large transient datasets increases FTMS imaging throughput.
- efficient visualization and processing of practically any size imaging datasets.
- imaging-grade and scale absorption mode FT (aFT) of phased transients.
- data averaging over selected areas of images, including via transients, to up sensitivity.
- recalibration of mass spectra to improve mass accuracy over entire images.
- super-resolution signal processing for targeted applications : drug profiling.
- advanced control of processing parameters, including noise analysis.
- output file formats, imzML, enable further analysis with commercial and open source tools.

Kooijman, et al., Increased throughput and ultrahigh mass resolution in DESI FT-ICR MS imaging through new-generation external data acquisition system and advanced data processing approaches, Scientific Reports (2019) 9 :8

AutoVectis : aFT & FTMS Data Analysis

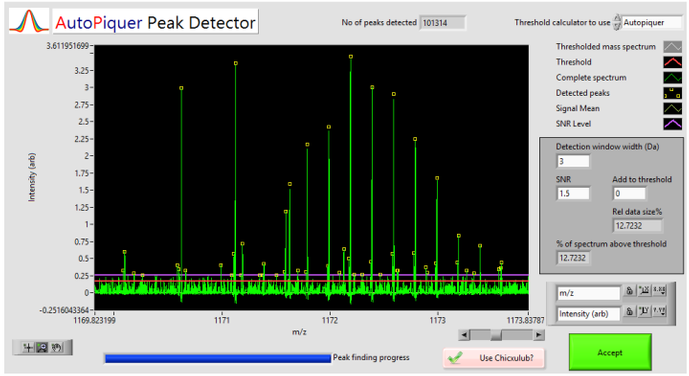


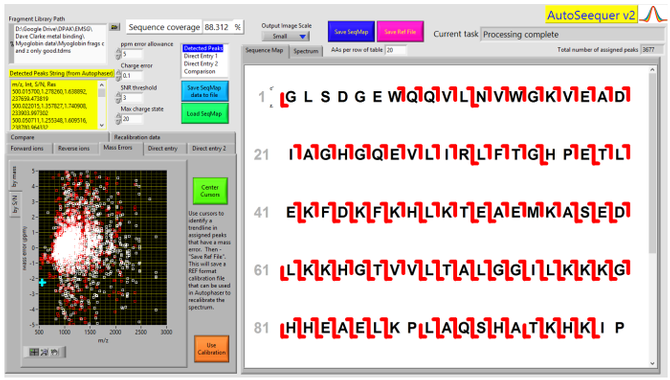
FTMS data representation in **absorption mode**, instead of the normal magnitude mode, lets you detect more peaks and gives you improved mass accuracy. Or it lets you record spectra up to twice as fast. As a data post-processing technique, it does not require any changes to the instrument. Using powerful algorithms, AutoVectis automates the steps required to produce absorption mode FT (aFT) mass spectra so the benefits can be easily enjoyed by everyone.



- A graphical user interface and built-in help system lead users through FTMS aFT data processing.

- Built-in tools include advanced peak detection (AutoPiquer) and top-down protein sequencing (AutoSeequer).





Key features

- easy to learn, absorption mode Fourier transform signal processing for FTMS ;
- advanced capabilities and powerful algorithms, but simple to use ;
- support for single mass spectra and also LCMS data and FTMS images ;
- support for data formats of common FTMS instruments and software ;
- configured for petroleomic, proteomic or any high mass accuracy application ;
- is compatible with Peak-by-Peak for easy integration and data co-processing ;
- developed in collaboration with Dr. David Kilgour – www.kilgourlab.com

van der Burgt, et al., Structural analysis of monoclonal antibodies by ultrahigh resolution MALDI in-source decay FT-ICR mass spectrometry, Analytical Chemistry (2019) 91, 2079-2085

How to get FTMS Data Simulator, Peak-by-Peak and AutoVectis software tools

If you are interested to learn more about FTMS data processing tools from Spectroswiss or want to get your free evaluation license, you are most welcome to contact us at info@spectroswiss.ch.

We would be pleased to support you in evaluating and improving your FTMS workflows, including developing customized solutions.

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FTMS Science and Technology

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