FTMS Data Acquisition & Processing Systems

Imaging, Charge Detection, Isotopic Ratios, Complex Mixtures, Intact Mass, Top-Down, & more

Spectroswiss

FTMS performance starts in the time domain

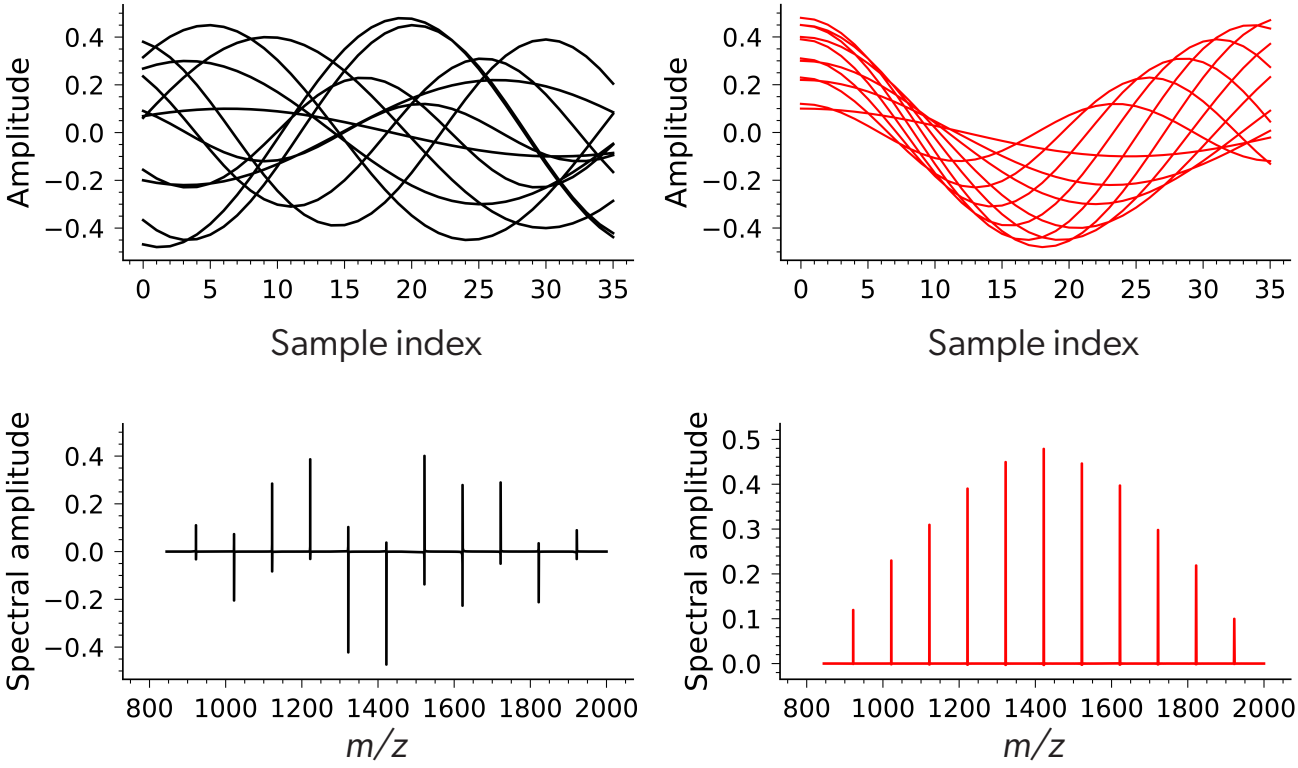
Fourier transform mass spectrometry (FTMS) records ion motion as time-domain signals, or transients. These signals contain the frequency, amplitude, and phase information that ultimately define the mass spectrum.

Most commercial FTMS workflows provide only processed spectral output. FTMS Booster systems give users access to the unreduced transient data, enabling more flexible acquisition, advanced processing, and deeper extraction of information from FTMS experiments.

In-hardware phased transients and aFT mass spectra

Absorption-mode FT processing can improve FTMS performance by using the information preserved in the transient more efficiently. FTMS Booster firmware can provide in-hardware phased transients, where ion signals share a common initial phase. This simplifies generation of absorption-mode FT mass spectra and reduces phase-related processing artifacts.

REGULAR TRANSIENTS | **PHASED TRANSIENTS**



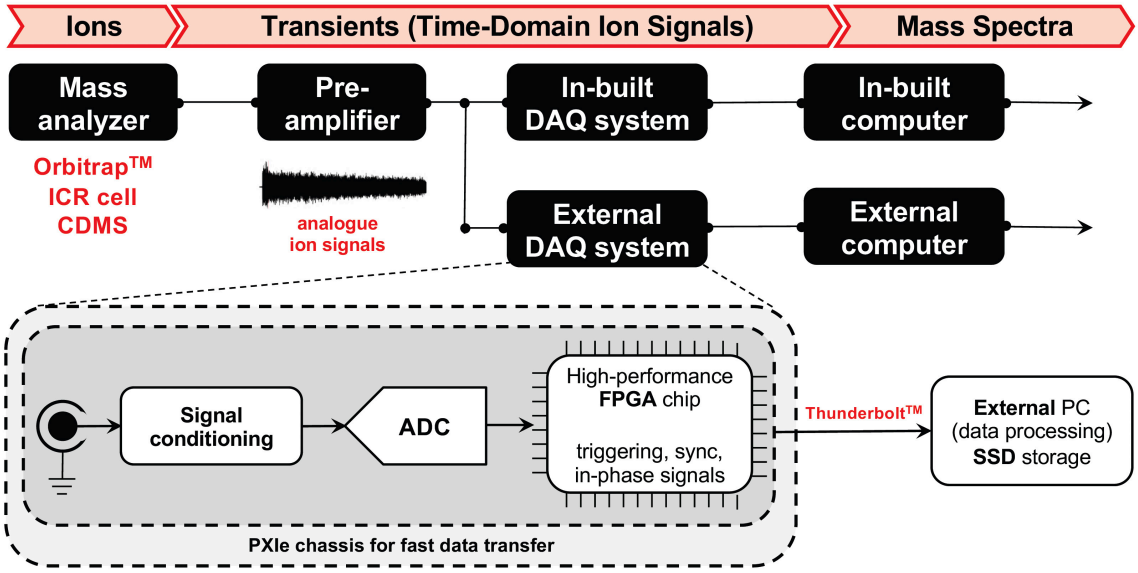
Regular vs. phased transients: Fourier transformation of regular transients with different initial phases produces mixed-mode spectra that require post-processing for absorption-mode representation. In-hardware phased transients generate spectra directly in absorption mode, simplifying data processing and improving spectral interpretability.

Kozhinov et al., High-Performance Data Acquisition for FTMS., *Chimia* (2025), 79, 77

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

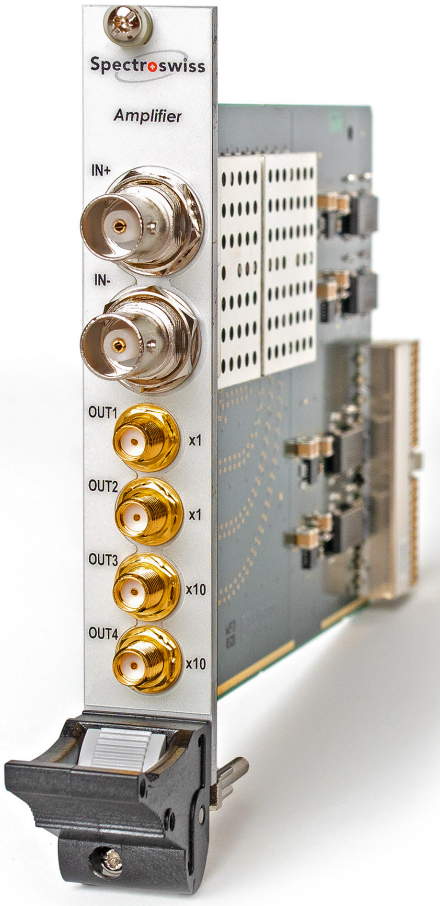
Ultra-Long Transients Enhance Sensitivity and Resolution in Orbitrap-Based Single-Ion Mass Spectrometry, Heck et al., *Nature Methods* (2024) 21, 619–622

FTMS Booster systems architecture



DAQ: data acquisition (system); ADC: analog-to-digital converter; FPGA: field programmable gate array

Key Features



PXI Amplifier

- Works in parallel with the in-built data acquisition electronics: original mass spectra (e.g., RAW) & transients are acquired in parallel without noticeable influence on each other
- Takes care of the heavy data, removing the technical challenge away from the built-in DAQ system to acquire large datasets
- Employs own patented* technology to maximize sensitivity through simultaneous acquisition of low/high gain transients via proprietary PXI amplifier (manufactured by Spectroswiss in Switzerland)
- Uniquely provides in-hardware phased transients for direct and phase artifact-free aFT mass spectra generation
- Supports advanced triggering options – recognizes both stop and start triggers, increasing experimental design flexibility and sophistication
- Allows flexible length (at the ms scale) transients – beyond the conventional two-fold increase in the data points (resolution)
- Maximizes the ion detection duty cycle, allowing extended transient recording during all the time ions ring in the mass analyzer
- Ensures full transient detection for enhanced sensitivity, duty cycle, and (ultra-high) resolution
- Detects and reports ion signals across the full *m/z* range (all ion detection)
- Removes the need for microscans in FTMS data acquisition by enabling post-processing transient averaging
- Offers transients for post-processing capabilities, including the use of advanced signal processing approaches (advanced FT and non-FT methods, such as super-resolution signal processing, e.g., least-squares fitting)
- Enables charge detection mass spectrometry (CDMS) by providing individual transients, including ultra-long transients, for post-processing

** Data acquisition apparatus and methods for mass spectrometry, by Anton Kozhinov, Yury Tsybin, and Konstantin Nagornov, Spectroswiss, Patent US 11,222,774 from January 2022*

Orbitrap™ Transients Acquisition and Processing

FTMS Booster X2T

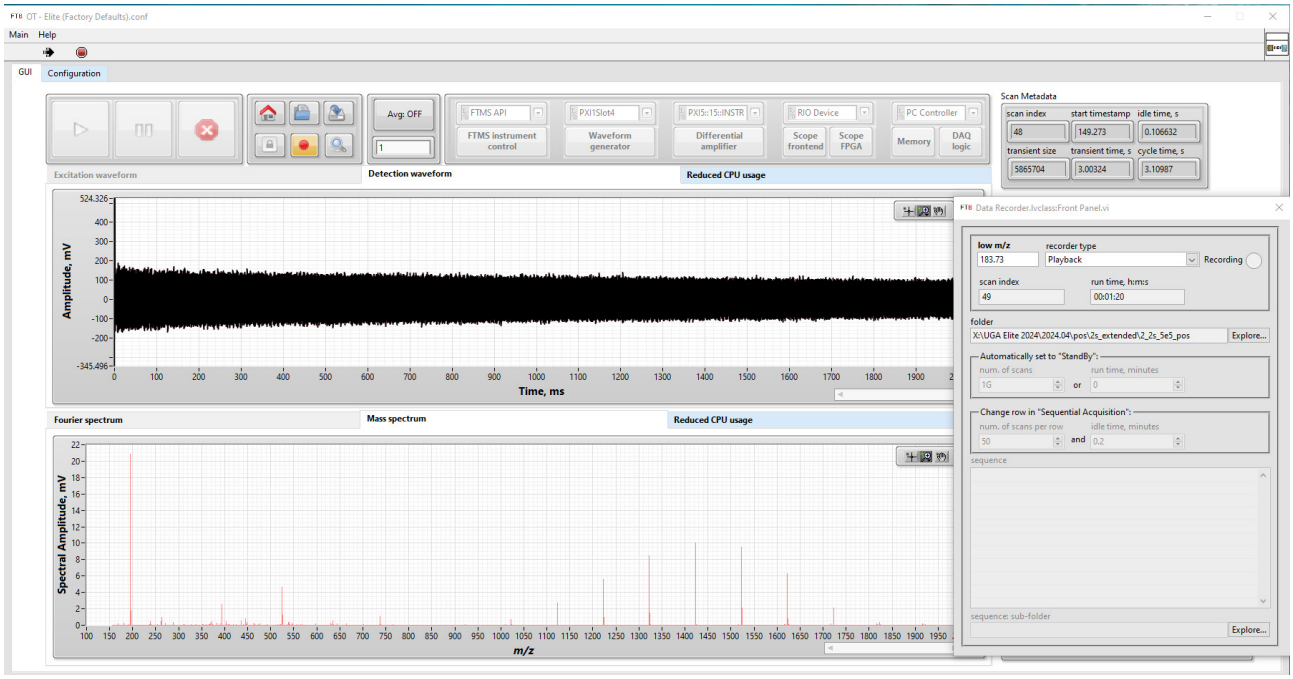
Acquisition of a single waveform, e.g. detect transient in FTMS & CDMS

High-Performance Digitizer / FPGA chip
High sample rate analog-to-digital conversion,
in-line digital signal processing and trigger decoding.

High-bandwidth Chassis
PXI Express backplane for high-speed data transfer
to/from the host PC via Thunderbolt™ interface.

Signal Amplifier
Impedance interface to FTMS.
Low noise, high bandwidth amplification with
multiple outputs (different gains).

Data Acquisition Software



Implemented on

LTQ Orbitrap™
LTQ Orbitrap XL™
LTQ Orbitrap Velos™
LTQ Orbitrap Elite™
Exactive EMR™

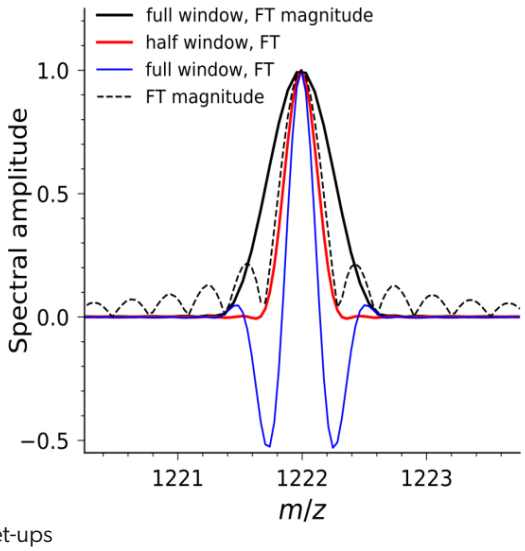
Q Exactive™
Q Exactive Focus™
Q Exactive Plus™
Q Exactive HF™
Q Exactive GC™
Q Exactive UHMR™

Exploris 480™
Exploris 240™
Fusion™
Fusion Lumos™

(all from Thermo Fisher Scientific)

Key Features

- Easy add-on to any Orbitrap™
- Works in parallel with the in-built data acquisition electronics
- **Thunderbolt™** technology for remote control and rapid data transfer
- Unlocks **absorption mode FT (aFT)** mass spectra
- Full transient detection for enhanced sensitivity, (ultra-high) resolution, and duty cycle
- Patented technology to maximize sensitivity through simultaneous acquisition of low/high gain transients via proprietary PXI amplifier
- Detection of ion signals across the full *m/z* range
- **User-defined first *m/z* value** to minimize data sizes and maximize processing speeds
- Acquires transients of any length, e.g.,> 25 s
- Takes care of the heavy data sets
- Calibrated signal amplitudes to provide complementary data (e.g. ion charges for CDMS applications, ion transmission tuning)
- Data visualization modes: single scan and transient averaging (micro-scans average, moving average, cumulative average)
- Acquisition of an arbitrary long signal (continuous data stream) for R&D set-ups
- Auxiliary real-time high-dynamic range digital filters for R&D set-ups
- Auxiliary DC-level adjustment of input signals for R&D set-ups



Ultra-High Resolution Capability via Extended Length Transients Acquisition

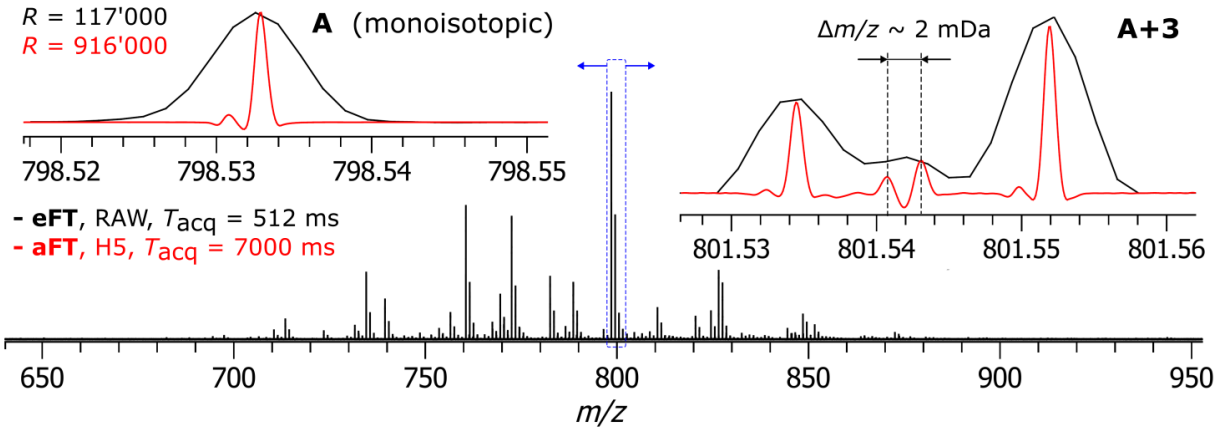
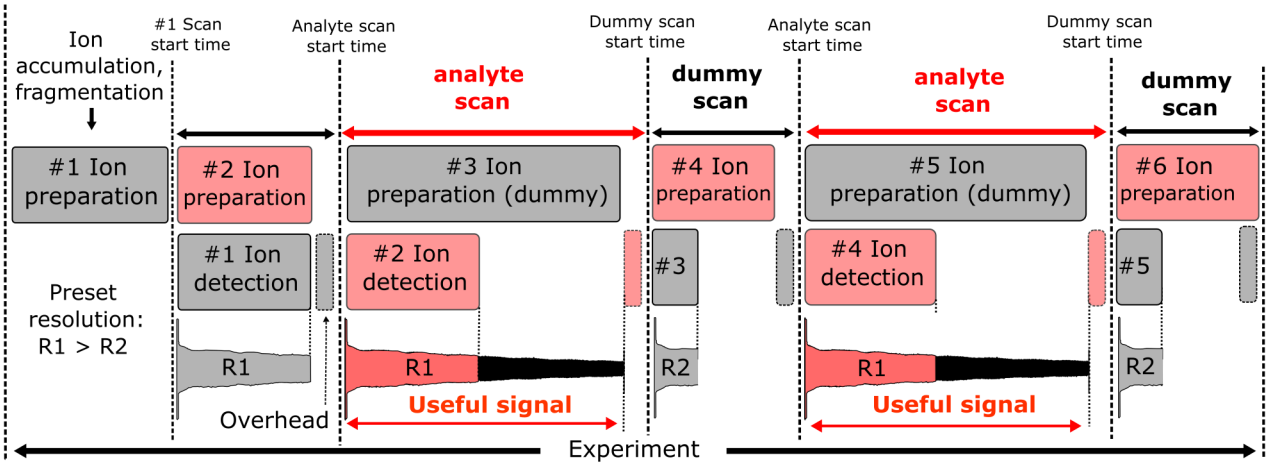


Figure above shows MALDI imaging MS analysis of a mouse brain tissue section performed using a Q Exactive HF (50 scans, RAW, eFT, 240k @ *m/z* 200, black trace) equipped with an FTMS Booster X2 (50 scans, aFT, 7 seconds transients, red trace).* Transients with the extended length were acquired in parallel with the RAW mass spectra, utilizing the FTMS Booster X2's capability to acquire data during the user-controlled overhead duration (implemented via the dummy-scan method), see below.



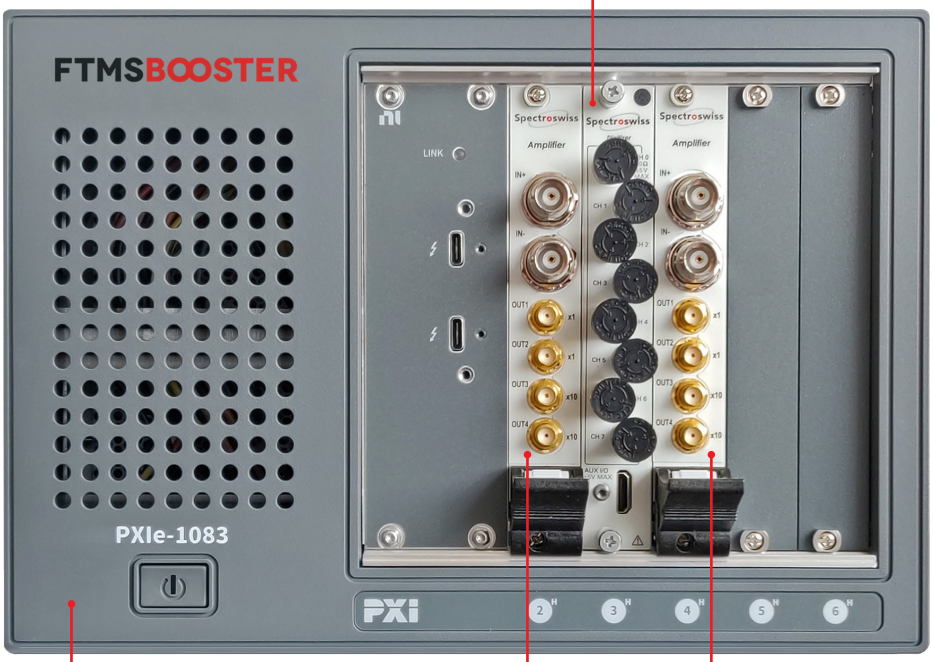
* Ellis et al., Ultrahigh-Mass Resolution Mass Spectrometry Imaging with an Orbitrap Externally Coupled to a High-Performance Data Acquisition System, Analytical Chemistry (2024) 96, 794-801

FT-ICR MS Transients Acquisition and Processing

FTMS Booster X3T

Acquisition of two waveforms, e.g. detect and excite or two detect transients in FT-ICR MS & CDMS

High-Performance Digitizer / FPGA chip
High sample rate analog-to-digital conversion,
in-line digital signal processing and trigger decoding.



High-bandwidth Chassis
PXI Express backplane for high-speed data transfer to/from the host PC via Thunderbolt™ interface.

Signal Amplifier #1: Detect Signal
Impedance interface to FTMS.
Low noise, high bandwidth amplification with multiple outputs (different gains).

Signal Amplifier #2: Excite Signal
Impedance interface to FTMS.
Low noise, high bandwidth amplification with multiple outputs (different gains).

Key Features

- Easy add-on to any FT-ICR MS, as well as any Orbitrap™ FTMS
- **Thunderbolt™** technology for remote control and rapid data transfer
- Acquisition of both excite and detect waveforms in FT-ICR MS
- All capabilities of the FTMS Booster X2T
- Two reserved slots for hardware extension modules
- Option: a stand-alone, powerful **data analysis workstation**

Implemented on

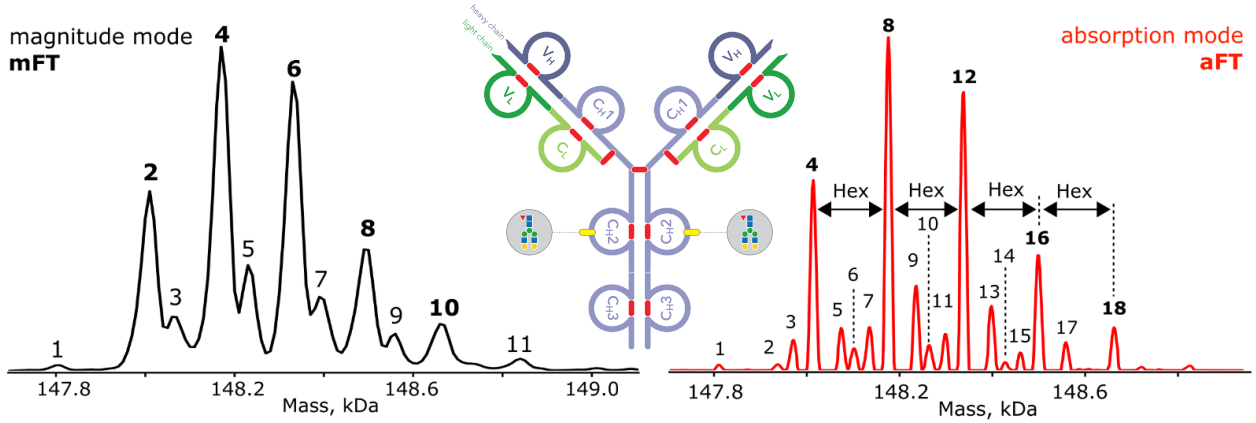
7 T LTQ FT™ (Thermo Fisher Scientific)
10 T LTQ FT™ (Thermo Fisher Scientific)
21 T LTQ FT-ICR MS (PNNL)
21 T Exploris FT-ICR MS (PNNL)

9.4 T FT-ICR MS with Infinity™ ICR cell
15 T FT-ICR MS with Infinity™ ICR cell
9.4 T SolariX XR™ FT-ICR MS
12 T SolariX XR™ FT-ICR MS
15 T SolariX XR™ FT-ICR MS
7 T scimaX™ FT-ICR MS

(from Bruker Daltonics)

Selected Applications

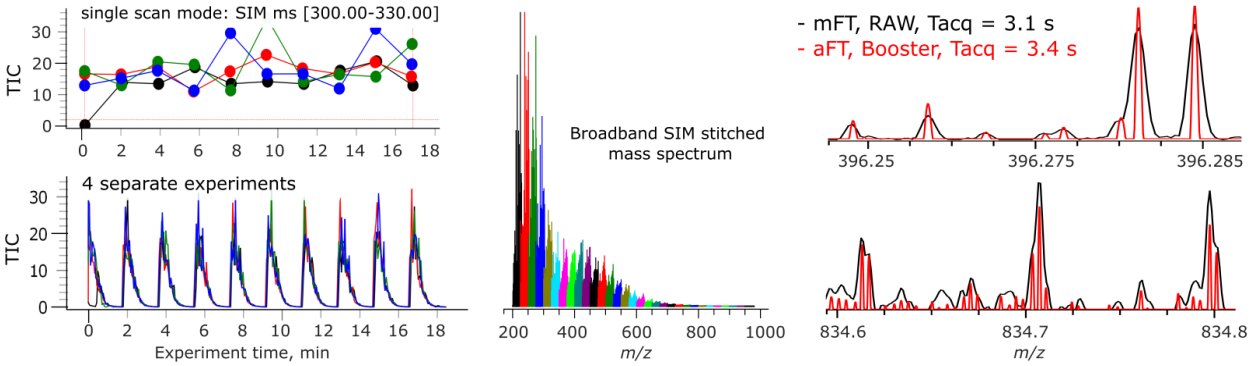
Intact and Top-Down Protein Analysis on a 15 T FT-ICR MS: aFT vs. mFT



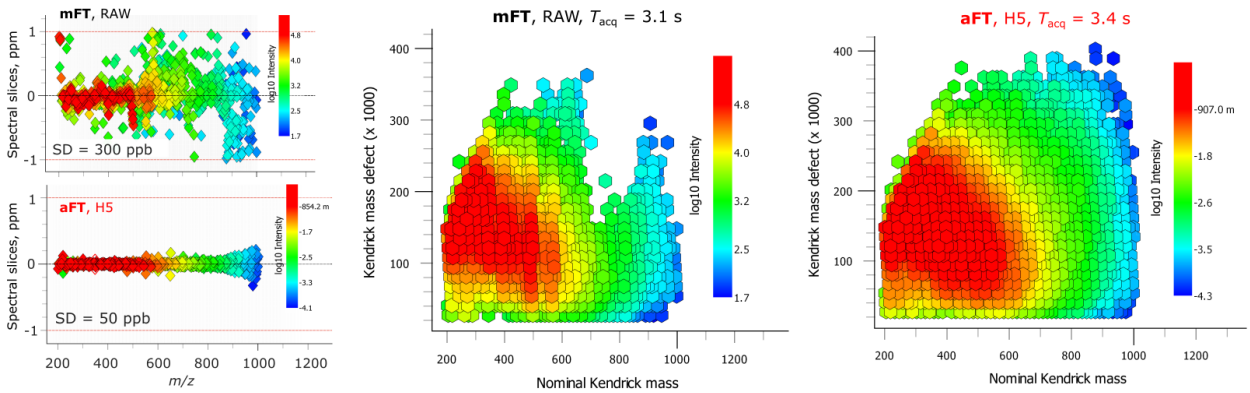
The benefits of the absorption mode FT (aFT) in comparison to the magnitude mode FT (mFT) mass spectral representation are shown for native MS analysis of an intact mAb (NIST) on a 15 T SolariX FT-ICR MS (Infinity cell, Bruker Daltonics). Data were acquired in parallel using (black) the instrument's original electronics and processed in mFT (D folder) and (red) the external data acquisition-processing system FTMS Booster X3 and processed in aFT. Data courtesy of Prof. Loo laboratory at UCLA, Los Angeles.

Complex Mixture Analysis on a 7 T FT-ICR MS

Complex mixture analysis (petroleomics) benefits from selected ion monitoring (SIM) stitching data acquisition on a 7 T LTQ FT-ICR MS (Ultra cell, Thermo Fisher Scientific). Data were acquired in parallel using (black) the instrument's original electronics and processed in mFT (RAW files) and (red) the external data acquisition-processing system FTMS Booster X3 and processed in aFT. Data courtesy of Prof. Schrader laboratory at Max-Planck-Institut für Kohlenforschung, Germany.



A feed sample was infused directly using electrospray ionization and measured using 31 narrow SIM windows of 10 Th each. Experiment was replicated 4 times. All scans of each individual SIM window were averaged, spectra (RAW) or transients (H5), within single and across separate replicates. The final mass spectra were stitched together and processed via Peak-by-Peak Multiomics (Spectroswiss).

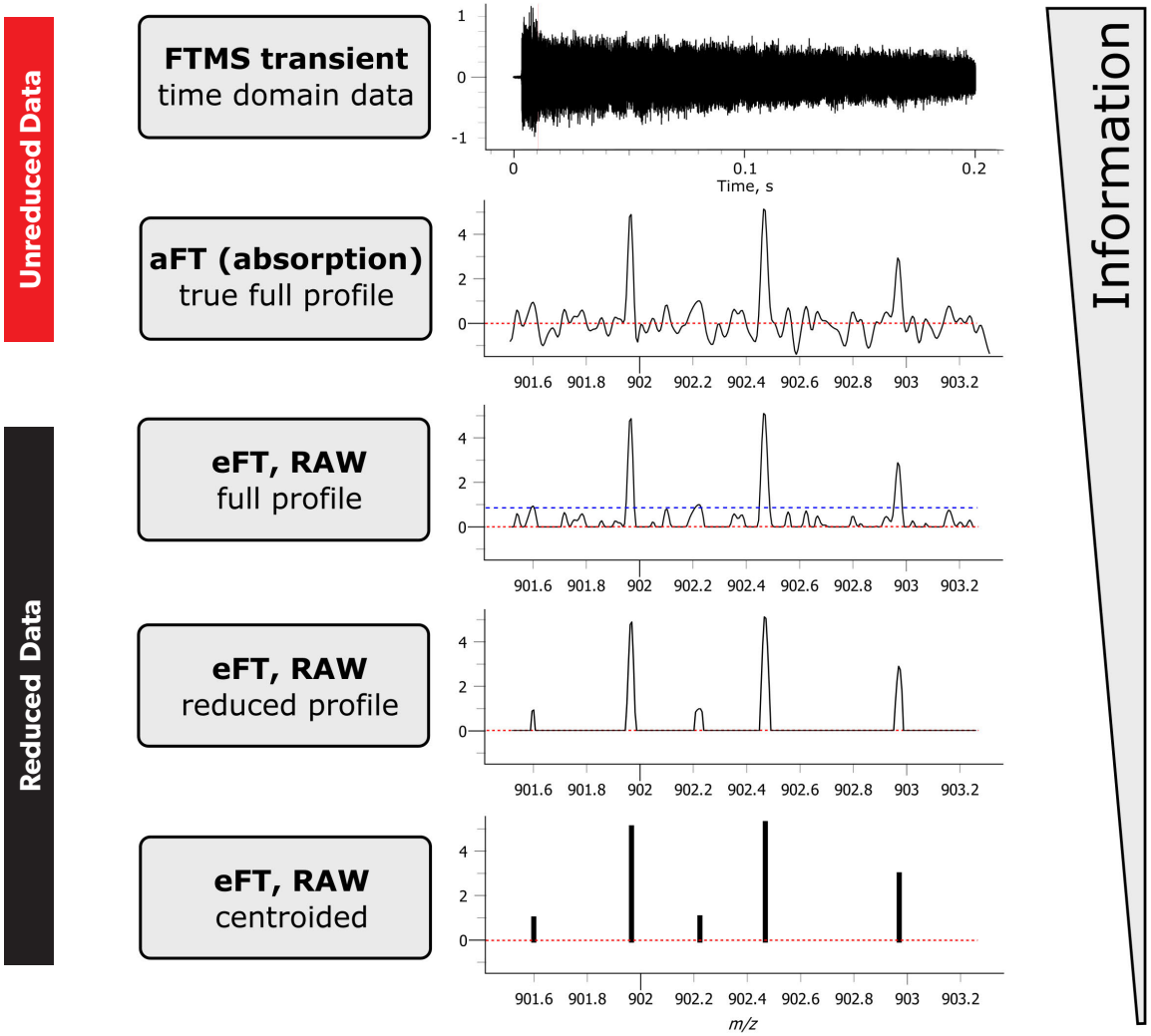


Mass error distributions and Kendrik plots for C class compounds after re-calibration identified in the mass spectra obtained via SIM stitching workflow using spectral (mFT, RAW) and transient (aFT, H5) averaging.

Choose the Data Level That Matches Your Science

- Accelerate scan speed and boost sensitivity using absorption mode FT (aFT) spectra.
- Maximize resolution and quantitation accuracy with long and ultra-long transients in FTMS, and arbitrary-length transients in CDMS.
- Increase sensitivity and dynamic range through transient and aFT spectrum averaging.
- Access complete noise statistics (e.g., standard deviations) for transparent and rigorous isotopic ratio calculations.
- Export transients for advanced post-processing, including:
  - Signal decay analysis for CDMS and collisional cross section estimation
  - Transient length optimization for accurate proteoform quantitation
  - Reduced on-line processing in fast-paced applications (e.g., MS imaging)
  - Super-resolution reconstruction (e.g., least-squares fitting)

FTMS Booster gives access to the full data hierarchy



Ready to go beyond processed FTMS spectra?

Contact Spectroswiss to discuss
FTMS Booster integration, demo data,
or application-specific workflows

Spectroswiss

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