FTMS Data Acquisition & Processing Systems

NEW

Charge Detection Mass Spectrometry (CDMS)

Spectroswiss

FTMS Data Acquisition and Processing

Most Fourier transform mass spectrometers (FTMS) provide only processed and noise reduced data (mass spectra). Having access to the true raw data (FTMS time-domain transients) permits the most informative and efficient data processing possible. Our **FTMS Boosters**, compatible with all FTMS instruments on the market, enable time-domain transient acquisition and access to high quality unreduced data. Combine them with our **Peak-by-Peak** software for advanced data processing and data analysis to take full advantage of your FTMS platforms!

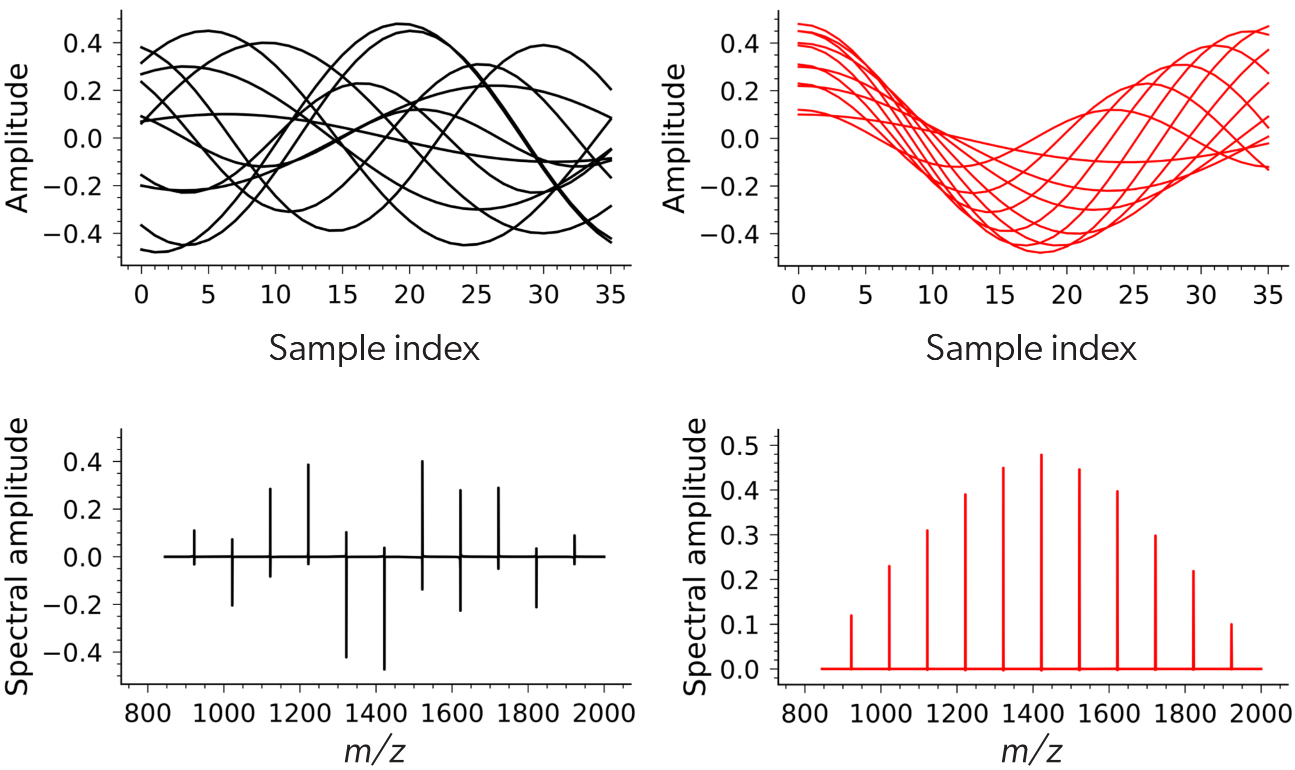
In-hardware phased transients and aFT mass spectra

Ion signals in FTMS are recorded in the time-domain as **transients**, where each ion signal is defined by its frequency, amplitude, and phase. The **absorption mode FT** (aFT) mass spectra preserve all the information contained in the transients, providing equal information.

The unreduced (full profile) aFT mass spectra maximize the FTMS performance, including resolution and sensitivity, and thus the information output.

The **in-hardware phased transients**, where all ion signals have the same initial phase, as provided by the firmware of the FTMS Boosters, greatly facilitate access to the aFT mass spectra.

REGULAR TRANSIENTS | **PHASED TRANSIENTS**



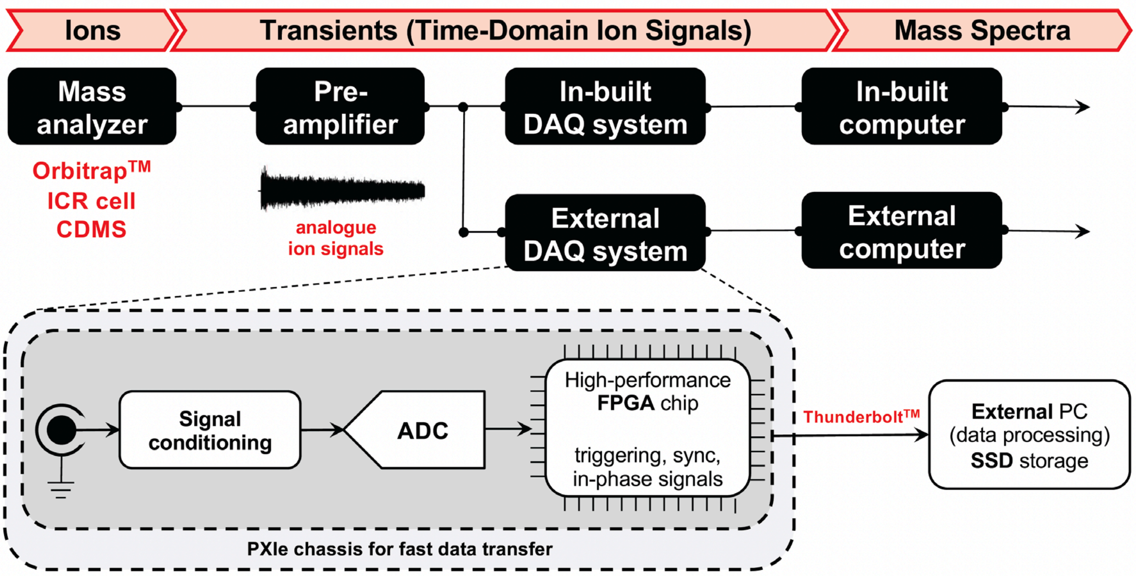
Transients vs. aFT: Fourier transform (FT) of a regular FTMS transient whose components have diverse phases (left, top) yields a mixed-mode mass spectrum (left, bottom) that requires post-processing for it to be represented in absorption mode (aFT). Right panels: FT of transients with in-phase ion signals (right, top) generates mass spectra directly in absorption mode (right, bottom).

Heck et al., Ultralong transients enhance sensitivity and resolution in Orbitrap-based single-ion mass spectrometry. *Nature Methods (2024) 21, 619-622*

Marcus et al., Improved uranium isotope ratio analysis in LS-AP glow discharge / Orbitrap FTMS coupling through the use of an external data acquisition system. *JASMS (2021) 32, 5, 1224–1236*

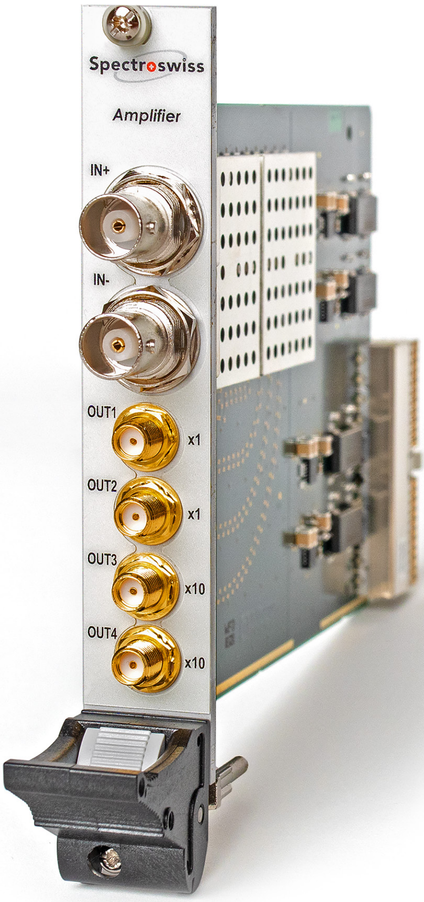
Bleiner et al., Trace-level persistent organic pollutant analysis with GC Orbitrap MS - enhanced performance by complementary acquisition and processing of time-domain data. *JASMS (2020) 31, 2, 257–266*

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

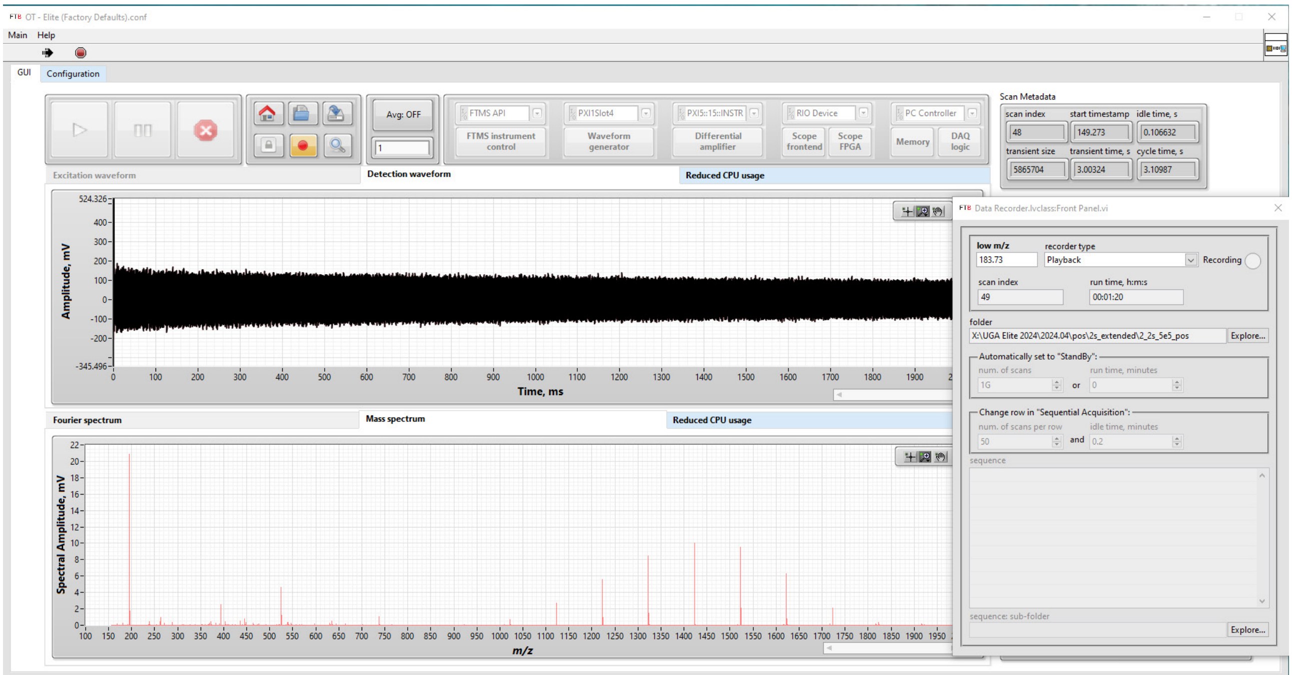
Acquisition of a single waveform, e.g. detect transient in FTMS & CDMS

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

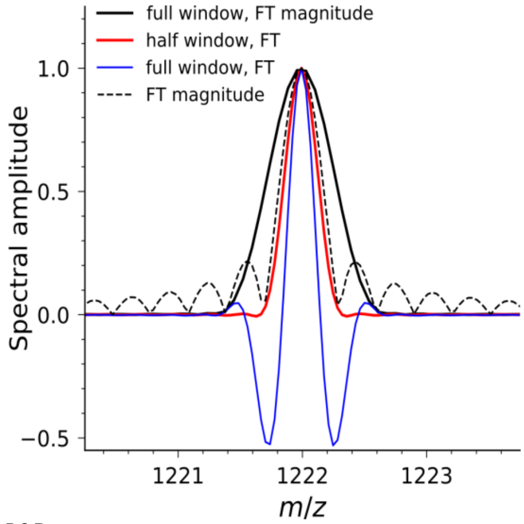


Implemented on

LTQ Orbitrap™	Q Exactive™	Exploris 480™
LTQ Orbitrap XL™	Q Exactive Focus™	Fusion™
LTQ Orbitrap Velos™	Q Exactive Plus™	Fusion Lumos™
LTQ Orbitrap Elite™	Q Exactive HF™	
Exactive EMR™	Q Exactive GC™	
	Q Exactive UHMR™	*(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
- [NEW] Calibrated signal amplitudes to provide complementary data (e.g. ion charges for CDMS applications, ion transmission tuning)
- [NEW] Data visualization modes: single scan and transient averaging (micro-scans average, moving average, cumulative average)
- [NEW] Acquisition of an arbitrary long signal (continuous data stream) for R&D set-ups
- [NEW] Auxiliary real-time high-dynamic range digital filters for R&D set-ups
- Option: a stand-alone powerful **data analysis workstation**



Ultra-High Resolution Capability via Extended Length Transients Acquisition

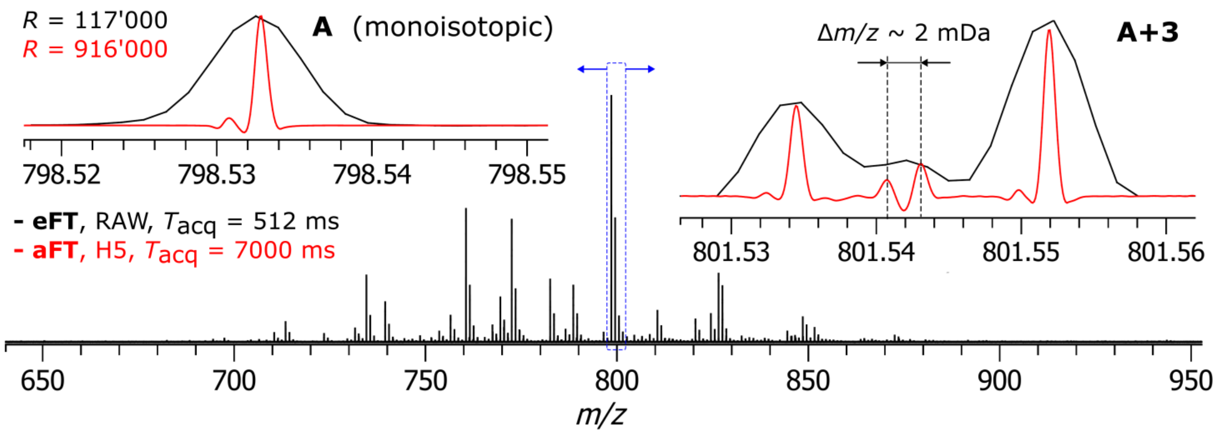
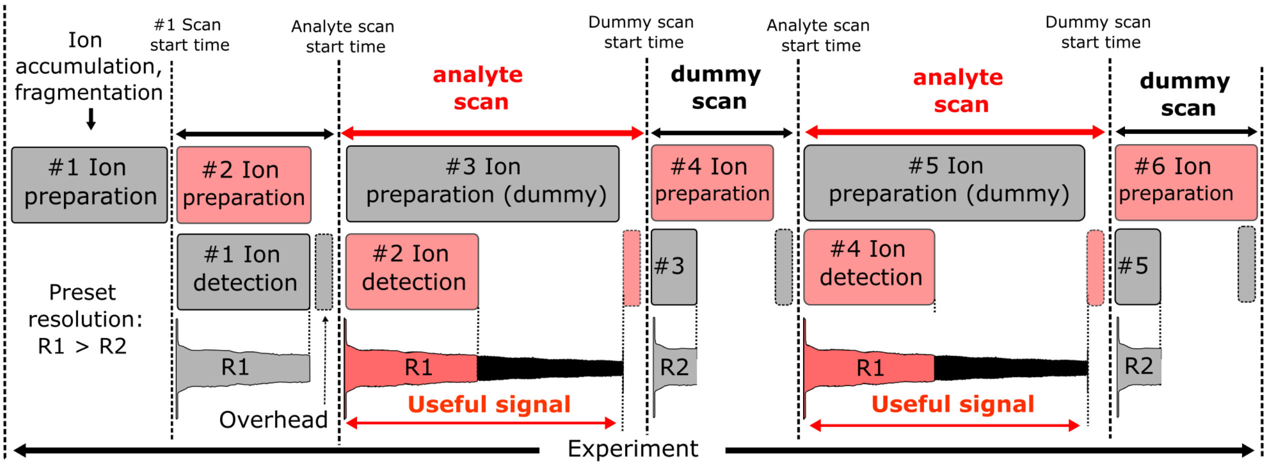


Figure above shows MALDI imaging MS analysis of a mouse brain tissue section performed using a Q Exactive HF (50 scans, RAW, eFT, 240k @ *m/z* 200, black trace) equipped with an FTMS Booster X2 (50 scans, aFT, 7 seconds transients, red trace).* Transients with the extended length were acquired in parallel 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.



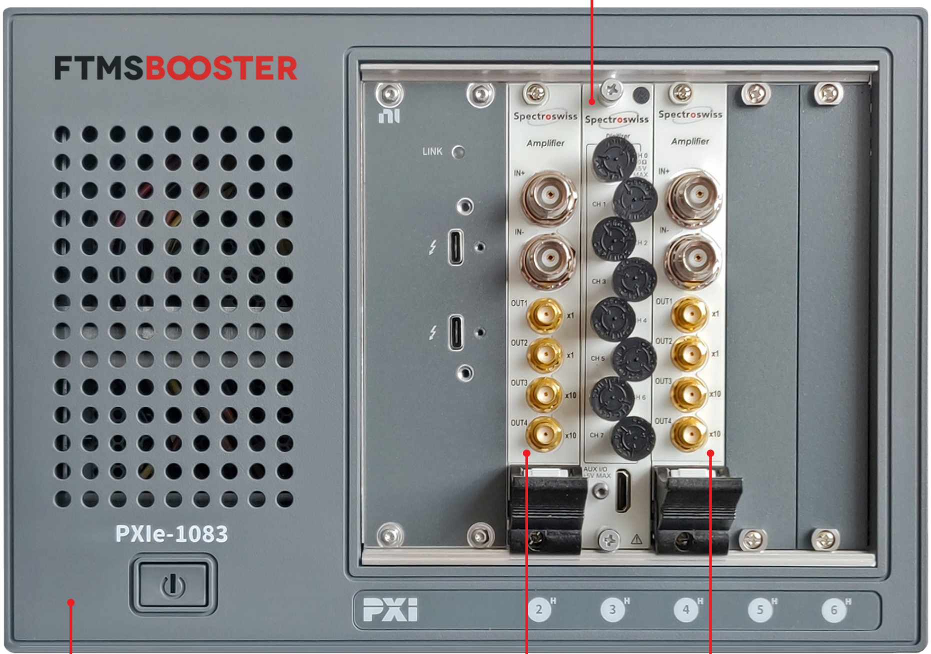
* Ellis et al., Ultrahigh-Mass Resolution Mass Spectrometry Imaging with an Orbitrap Externally Coupled to a High-Performance Data Acquisition System, Analytical Chemistry (2024) 96, 794-801

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

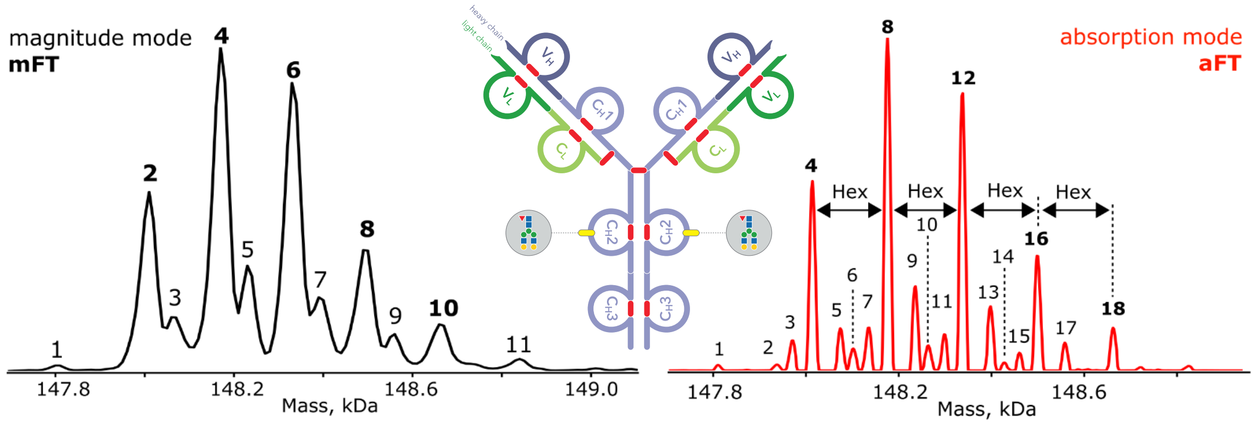
- Easy add-on to any FT-ICR MS, as well as any Orbitrap™ FTMS
- **Thunderbolt™** technology for remote control and rapid data transfer
- Acquisition of both excite and detect waveforms in FT-ICR MS
- All capabilities of the FTMS Booster X2T
- Two reserved slots for hardware extension modules
- Option: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

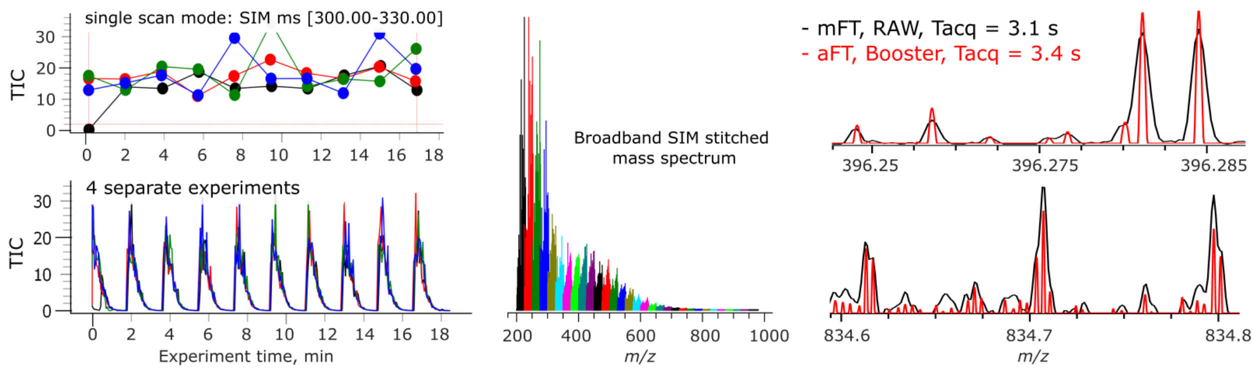
Intact and Top-Down Protein Analysis on a 15 T FT-ICR MS: aFT vs. mFT



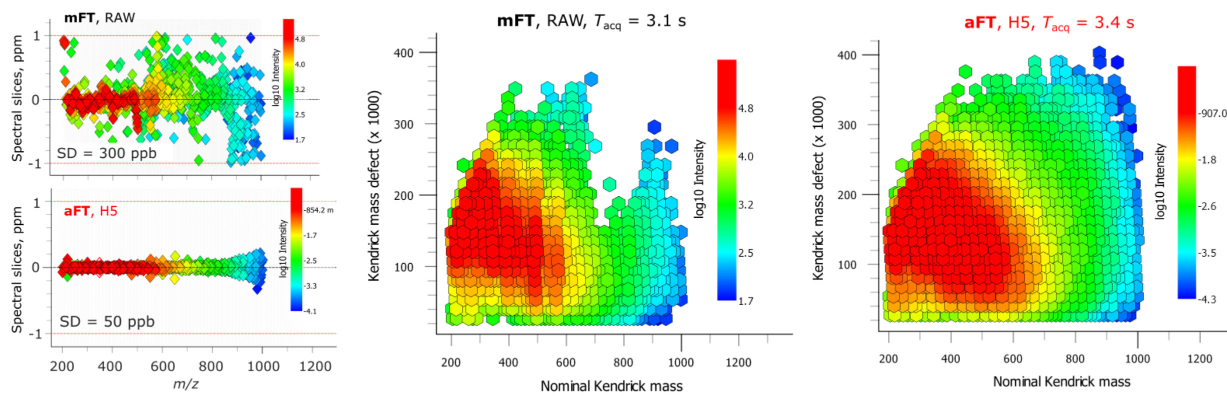
The benefits of the absorption mode FT (aFT) in comparison to the magnitude mode FT (mFT) mass spectral representation are shown for native MS analysis of an intact mAb (NIST) on a 15 T SolariX FT-ICR MS (Infinity cell, Bruker Daltonics). Data were acquired in parallel using (black) the instrument's 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.

Selected references

FTMS instrument	Reference
Q Exactive GC Orbitrap™	Trace-level persistent organic pollutant analysis with GC Orbitrap MS -enhanced performance by complementary acquisition and processing of time-domain data, *Bleiner et al., JASMS 2020, 31, 2, 257–266*
Q Exactive Focus Orbitrap™	Improved uranium isotope ratio analysis in LS-AP glow discharge / Orbitrap FTMS coupling through the use of an external data acquisition system, *Marcus et al., JASMS 2021, 32, 5, 1224–1236*
Q Exactive Plus Orbitrap™	Image-wide adjacent-pixel data averaging increases sensitivity toward dosed drugs of abuse and antiretrovirals in Q Exactive mass spectrometry imaging, *Desyaterik et al., ASMS 2023, TP337*
Q Exactive HF Orbitrap™	Ultrahigh-mass resolution mass spectrometry imaging with an Orbitrap externally coupled to a high-performance data acquisition system, *Ellis et al., Anal. Chem. 2024, 16, 794*
Q Exactive UHMR Orbitrap™	Ultralong transients enhance sensitivity and resolution in Orbitrap-based single-ion mass spectrometry, *Heck et al., Nature Methods, 2024, 21, 619*
Exploris 480 Orbitrap™	Omnitrap-Orbitrap performance enhancement via unreduced data processing, *Kozhinov et al. ASMS 2023, WOA am 08:30*
Fusion Lumos Orbitrap™	Super-resolution MS enables rapid, accurate, and highly multiplexed proteomics at the MS2 level, *Kozhinov et al., Anal. Chem. 2023, 7, 3712*
LTQ Orbitrap XL™	High mass range Orbitrap FTMS imaging of glycomic profiles in a Syrian golden hamster model of SARS-CoV-2 variant infections, *Leach et al., ASMS 2024, MP035*
7 T LTQ FT-ICR MS	Increased throughput and ultra-high mass resolution in DESI FT-ICR MS imaging through new-generation external data acquisition system and advanced data processing approaches, *Ellis et al., Sci Rep 9, 8 (2019)*
21 T LTQ FT-ICR MS	Imaging and direct sampling capabilities of nanoDESI with absorption-mode 21 T FT-ICR MS, *Anderton et al., Anal. Chem. 2022, 8, 3629–3636*
12 T & 15 T SolariX XR™ FT-ICR MS	Integration of tandem high resolution ion mobility and mass spectrometry for complex mixture analysis, *Forero et al., ASMS 2024, ThP406*
7 T scimaX™ FT-ICR MS	Optimizing 7 Tesla FT-ICR MS equipped with frequency multiple detection and absorption mode processing for high throughput organic matter analysis, *Kew et al. ASMS 2023, WP 319*

Spectroswiss

Spectroswiss Inc. | 245 First Street | Riverview II | Cambridge, MA 02142 | USA
Spectroswiss Sàrl | EPFL Innovation Park | 1015 Lausanne | Switzerland
Spectrotech SAS | 132 rue Bossuet | 69006 Lyon | France
www.spectroswiss.ch