Advanced Data Acquisition and Processing in FTMS: Applications

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FTMS mass analyzers

Data processing (mass spectra)

Data acquisition (phased transients)

Figure 1. Advanced data acquisition and data processing for leveraging FTMS applications. A high-performance data acquisition system (FTMS Booster) enables acquisition of time-domain data (transients) from any FTMS instrument, including Orbitraps. Transients (i) are acquired during the whole time ions induce signals, (ii) contain signals from all ions in the mass analyzer, and (iii) can be recorded in parallel with ion accumulation and fragmentation events (overheads). Uniquely, the obtained transients are phased (for both ICR and Orbitrap FTMS) and thus may directly provide absorption mode FT (aFT) mass spectra. Data processing is enabled by Peak-by-Peak for the following workflows: metabolomics, shotgun lipidomics, imaging, petroleomics, top-down MS, & TMT quantitation.

Figure 2. Structure and simulated isotopic fine structure of a small molecule drug, amiodarone (1 million resolution).

Figure 3. Amiodarone isotopic fine structure analysis on a benchtop Q Exactive HF Orbitrap FTMS with an FTMS Booster. Absorption mode FT (aFT) is via AutoVectis.

Figure 4. Abundance ratio accuracy can be improved via conditional co-adding of transients (Peak-by-Peak).

Figure 5. Bottom-up proteomics of a HeLa tryptic digest using LC-MS/MS with ETD on a Fusion Lumos. Shown are the total ion current and transient periods.

Figure 6. ETD MS/MS data. Expanded views into product ions: black for the original centroid data (.RAW); red for the FTMS Booster acquired transient data processed with aFT.

Figure 7. Improved product ion sensitivity and confidence doubles the number of proteins identified in parallel.

Figure 8. Multiplexed LC/GC/CE MS or MS/MS workflow. Acquisition of 2-10 technical replicates is followed by transient or spectral summation across the multiple LC/GC/CE runs. The increase in S/N is proportional to the $\sqrt{N}$ where $N$ is the number of runs.

Figure 9. Metabolite mixture analysis using LC-MS on a Q Exactive Orbitrap FTMS (total ion current). Two chromatograms are aligned (Peak-by-Peak). Expanded view shows a targeted peak in a given elution time window. N1 and N2 are scan numbers.

Figure 10. Spectral (reduced profile eFT,.RAW, shown in black) versus transient (full profile mFT,.H5, shown in red) summation demonstrates increase in sensitivity, thus more confident isotopic structure analysis of metabolites using transients.

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