

A QUATERNARY HYBRID INSTRUMENT FOR STATE-OF-THE-ART FT-ICR MASS SPECTROMETRY AT 14.5 AND 21 TESLA

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The quaternary hybrid instrument configuration of the 14.5 and 21 T permits unprecedented flexibility for tandem MS experiments, allowing for data acquisition within the FT-ICR, Orbitrap, and linear RF ion trap simultaneously. Parallel acquisition of MS², MS³, or higher order MSⁿ occurs simultaneously with data acquisition in the ICR cell. The inherent value of high-resolution accurate mass analysis in the MS¹ has been broadly demonstrated via assignment of unknown molecular species for small molecules and large biomolecules alike. In many cases, MS¹ analysis alone cannot properly distinguish between analytes or provide the analytical information desired; therefore, MSⁿ data is often required. In the previous version of this instrument, which employed a Velos Pro dual linear trap, MSⁿ acquisition was possible but not fully parallelized, resulting in a low MSⁿ duty cycle.

Thermo Fisher Orbitrap™ Eclipse™ Tribrid™ mass spectrometers are coupled to the MagLab 14.5 and 21 T FT-ICR systems. A quadrupole ion guide transports ions from the Eclipse dual linear ion trap to the MagLab quadrupole ion trap and finally the ICR cell. Custom hardware and software enable synchronous control of ICR ion transfer and data acquisition by the Eclipse computer for seamless parallel operation of four mass analyzers. Data can be stored in .raw (Thermo) and .dat (MagLab) formats, which optimally supports Thermo, MagLab, and third-party data analysis software. Electrospray, APPI, APCI, and MALDI are supported ionization techniques. Collisional, electron transfer, proton transfer, and photodissociation are available for structural characterization.

Systems integration of MagLab ICR hardware with the commercial Eclipse instrument permits method-based operation of the instrument directly from within Thermo Fisher Xcalibur™ and Tune. This integration paves the way for automation of both direct-infusion and LC-MS workflows. Here we demonstrate method-based tandem MS with FT-ICR MS¹ survey acquisitions while using the Orbitrap and linear RF ion trap for both data-dependent and targeted tandem MS. These scanning modes include FT-ICR MS¹-Orbitrap MS², FT-ICR MS¹-Ion trap MS², FT-ICR MS¹-Orbitrap MS²-Ion trap MS², and FT-ICR MS¹-Orbitrap MS²-Ion Trap MS³. Simultaneous acquisition of Thermo Fisher .raw file format and unprocessed transient .dat (FT-ICR only) files is possible without duty cycle impact.

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