

Orbitrap - Fundamentals and advances

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An Orbitrap Fourier Transform Mass Spectrometer (FTMS) is a high-resolution mass spectrometry (HRMS) instrument that measures the mass-to-charge ratio (m/z) of ions with exceptional mass accuracy, resolution, and sensitivity. It is widely used in proteomics, metabolomics, lipidomics, and structural biology due to its ability to resolve complex mixtures and detect minute molecular differences.

We will explore the key concepts and parameters of Orbitrap technology, including:

- Ion excitation by injection (electrodynamic squeezing)
- Induced current ion detection: Time-domain ion signals (transients)
- Frequency- m/z -resolution relationship
- Automatic Gain Control (AGC)
- Maximum injection time (IT_{max})
- Normalized level (NL)
- Parallel ion detection, accumulation, and fragmentation
- Fourier Transform (FT) algorithms: Enhanced FT (eFT), Magnitude Mode FT (mFT), and Absorption Mode FT (aFT)
- Mass spectral representation: Full and reduced profiles, centroids
- Microscans: Transient versus spectral averaging

Understanding these principles will provide insights into optimizing the performance of Orbitrap FTMS for high-precision mass spectrometry applications. Additionally, we will provide an overview of existing resources for FTMS data simulation and discuss recent advances in Orbitrap FTMS methods and applications.