

LTQ Orbitrap – A Breakthrough Mass Spectrometer for Accurate Mass, High Resolution MS and MSⁿ Analysis on a LC Time Scale

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Identifying modifications or structural changes of molecules is of increasing importance in most all fields, including drug discovery, metabolomics, and proteomics. Since these species are often present in minor concentration, the requirements for more powerful mass spectrometers are demanding. There is a clear need for accurate mass determination combined with MS/MS capabilities and highest possible dynamic range as a standard detection tool for on-line chromatography. The knowledge of the accurate mass of a precursor ion and its product ions allows for significantly higher confidence and reliability of identification. The combination of high dynamic range with accurate mass and low detection limit in an instrument is a key to success.

The LTQ Orbitrap is a newly developed mass spectrometer which is a hybrid system with two analyzers, a linear ion trap and an Orbitrap analyzer. The linear ion trap and Orbitrap are characterized by a high ion storage capacity combined with a high scan rate and high MS/MS sensitivity; while the Orbitrap achieves high mass resolution and excellent mass accuracy with external calibration in full MS and MS/MS modes of operation.

The resolution in an Orbitrap analysis is proportional to the time the transient signal is acquired. For a resolution of 7,500 (at mass 400) the transient signal is detected for about 90 ms, where as a resolution of 60,000 requires a detection time of about 750 ms. The LTQ Orbitrap is able to make use of this time productively by operating the linear ion trap fully in parallel to the Orbitrap detector acquisition. This allows, for example, the acquisition of several MS/MS scans concurrent to the acquisition of a high resolution MS spectrum - fully automated through *data dependent* scanning. If high resolution and accurate mass information of the product ions is required, the Orbitrap analyzer is operated in the 'sequential mode', with MS and MS/MS scans performed in the Orbitrap. This yields accurate mass information on the precursor and product ions in a fully data dependent manner, without the need of an internal calibrant.

This presentation gives an overview of the new LTQ Orbitrap mass spectrometer and the Orbitrap technique. Application examples will demonstrate the power of accurate mass for full MS and MSⁿ scans and its full compatibility with the LC time scale.