



**Thermo Scientific Orbitrap Elite**  
Hybrid Mass Spectrometer



## High-Field Orbitrap

# Creating new possibilities

Ultrahigh resolution • Faster scanning  
Higher sensitivity • Complementary fragmentation

**Thermo**  
SCIENTIFIC

# The highest resolution, most versatile Orbitrap instrument ever

The Thermo Scientific Orbitrap Elite hybrid mass spectrometer raises the bar for MS and MS<sup>n</sup> performance and versatility by combining our premier dual-pressure linear ion trap mass spectrometer with a novel high-field Orbitrap™ mass analyzer. The system delivers greater than 240,000 resolution (FWHM), increased sensitivity, high scan speeds and a larger dynamic range.

## High field Orbitrap mass analyzer for ultrahigh resolution

The high-field Orbitrap mass analyzer geometry and advanced signal processing technologies enable resolution of >240,000 FWHM, a 4x increase over previous technology. This ultrahigh resolution is especially useful when analyzing samples of high complexity and targeting analytes of low abundances in applications such as proteomics, metabolomics and lipidomics.

## Faster scanning for UHPLC compatibility

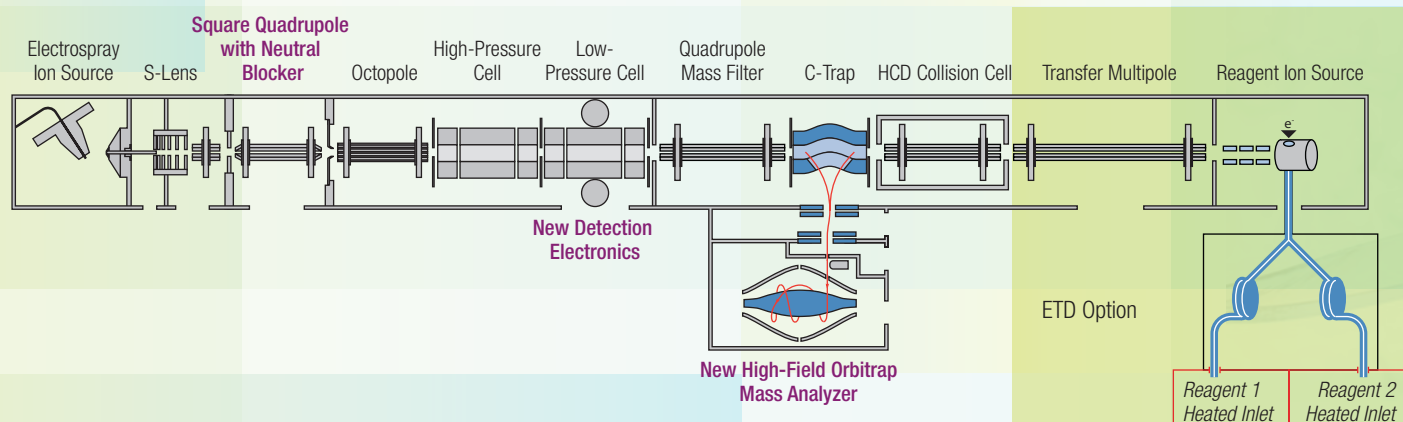
The high-field Orbitrap geometry and advanced signal processing also provide an up to 4x improvement in scan speed, making the Orbitrap Elite system more compatible with narrow chromatographic peaks from UHPLC separations.

## Higher sensitivity for complex samples

Innovations in the pre-amplifier electronics improve sensitivity. Paired with the ultrahigh resolution, they provide more comprehensive data and a deeper look into complex samples.

## Fragmentation options increase versatility

In addition to traditional collision-induced dissociation (CID), the Orbitrap Elite mass spectrometer features higher-energy collisional dissociation (HCD) that provides superior fragmentation and higher-quality MS/MS spectra for many types of samples. Optional electron transfer dissociation (ETD) preserves labile post-translational modifications of proteins. Intelligent data-dependent decision tree (DDT) logic can combine multiple fragmentation techniques in a single analysis to significantly improve proteome coverage.



The Orbitrap Elite mass spectrometer can analyze complex samples at a greater depth than ever before, helping scientists meet the most demanding challenges in proteomics, metabolomics, lipidomics and metabolism.

### A Quantum leap in Orbitrap MS performance:

#### Key features of the Orbitrap Elite system:

- High-field Orbitrap mass analyzer for higher mass resolution and higher scan speed
- Advanced signal processing for higher resolution
- Improved ion optics for efficient ion injection into the Orbitrap
- New Orbitrap image current pre-amplifier for higher sensitivity
- Velos Pro linear ion trap generation II ion optics with neutral blocking technology for increased robustness



# A new standard of performance

## for comprehensive proteomics

Orbitrap-based mass spectrometers are an essential tool in many proteomics labs. The enhanced power of the Orbitrap Elite instrument enables new standards of performance for multiple proteomics applications.

### Top-down analysis

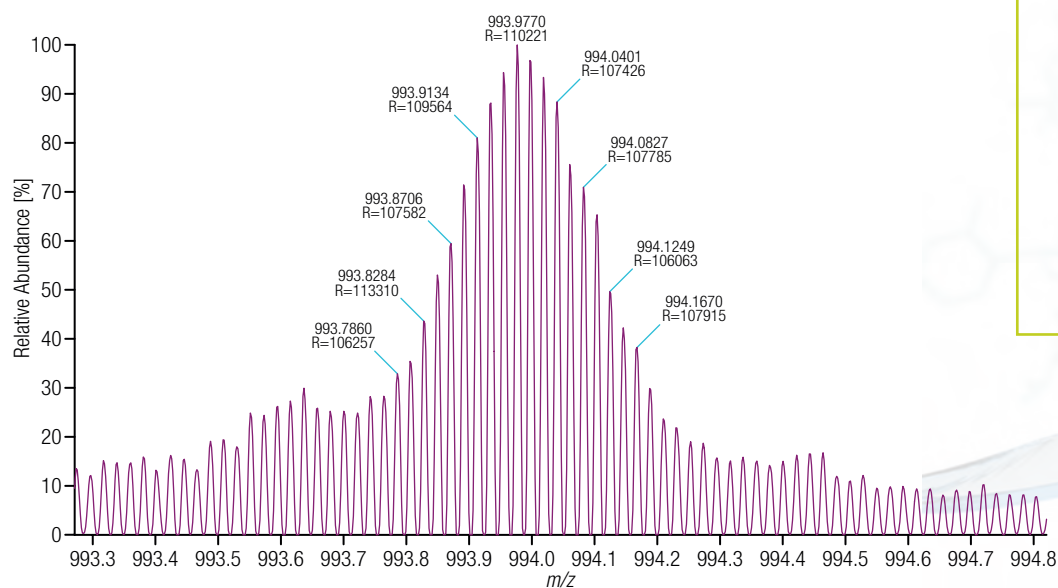
Maximum resolution of >240,000 FWHM and complementary fragmentation modes facilitate better top-down protein identification and characterization.

### PTM analysis

Available electron transfer dissociation (ETD) preserves labile side chains while creating fragmentation throughout the peptide backbone for better analysis of post-translational modifications (PTMs).

### Intact protein analysis

47+ Charge state of yeast enolase showing resolution of >100,000 FWHM at  $m/z$  1,000



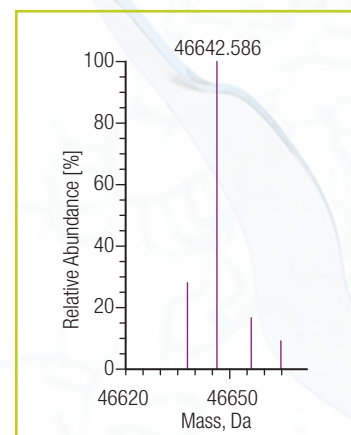
Analysis of intact yeast enolase (46.64 kDa) on the Orbitrap Elite hybrid MS demonstrates the superior resolution that makes it the new standard for proteomics applications.

### Protein ID

Faster scanning for more data points across a peak, combined with high resolution and superior spectral quality, yields more protein identifications in a single analysis.

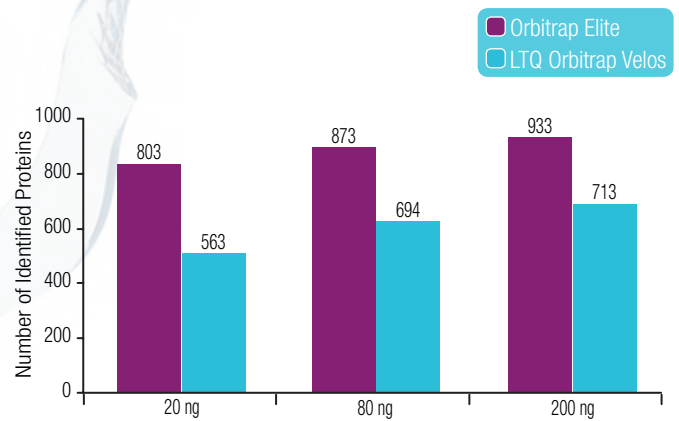
### Quantitative proteomics

Superior resolution and selectivity of the Orbitrap mass analyzer for both full-scan MS and MS<sup>n</sup> enhance relative quantitation analyses such as those using stable isotope labeling or isobaric mass tags.

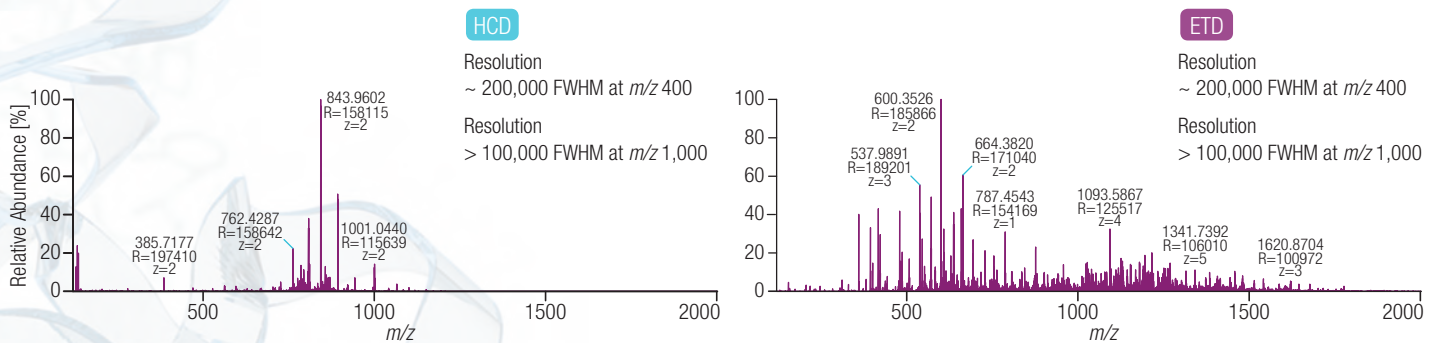
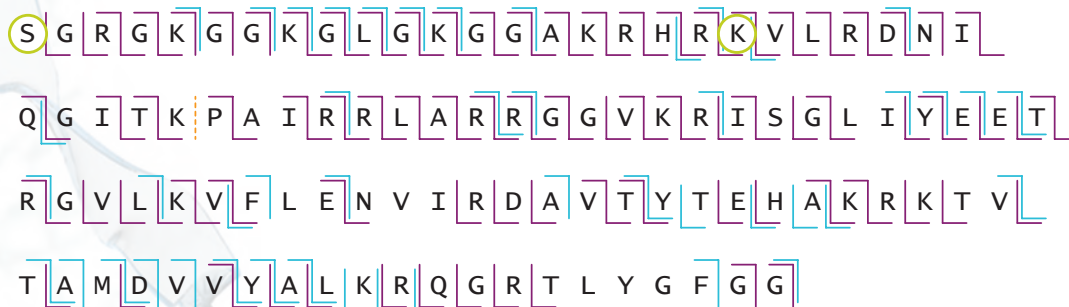


Deconvoluted spectrum of yeast enolase (monoisotopic mass 46642.214 Da).

The superior resolution and spectral quality, as well as higher scan speed of the Orbitrap Elite instrument, increase proteome coverage in complex samples even with very low sample amounts. Here, analysis of the *E. coli* proteome labeled with Thermo Scientific Pierce Tandem Mass Tags demonstrates significant improvement over the already outstanding performance of the previous generation Thermo Scientific LTQ Orbitrap Velos hybrid MS.



### Top-down analysis



Analysis of histone H4 demonstrates the complementary nature of the HCD and ETD fragmentation techniques in the Orbitrap Elite instrument. Analysis using HCD and ETD in a single run significantly improved sequence coverage over each of the techniques used separately.

# A total solution

## for metabolism and metabolomics research

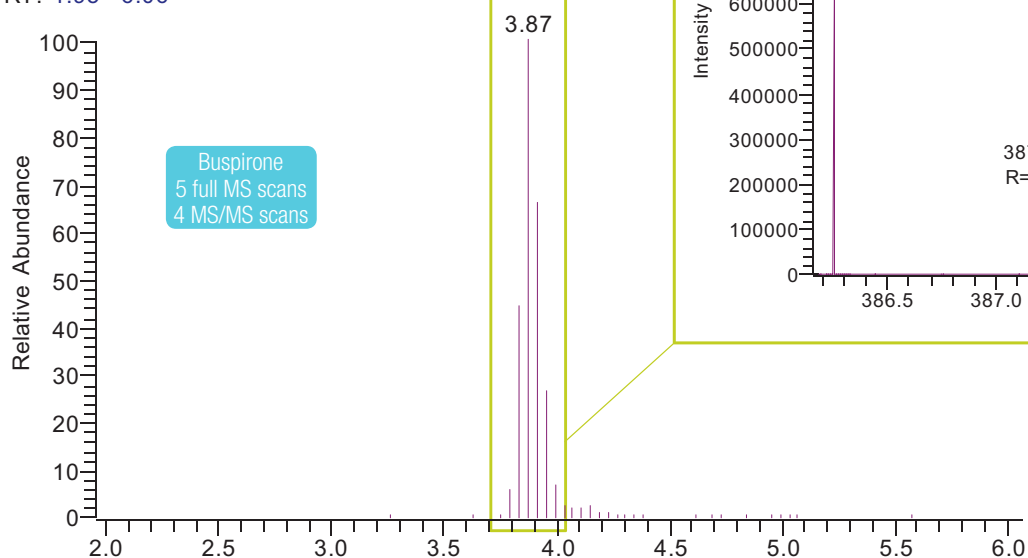
The Orbitrap Elite system offers a higher maximum resolution of >240,000 FWHM that allows complete visibility into the sample components and distinguishes them from complex matrix components. Improved sensitivity ensures detection of more metabolites in biological samples. High-quality MS<sup>n</sup> spectral trees provide extensive structure information for metabolite identification and location of modification sites. Improved robustness enables true 24/7 operation.

### Uncompromised performance

The Orbitrap Elite system delivers ultrahigh resolution analysis at high sensitivity without compromising speed or MS<sup>n</sup> performance.

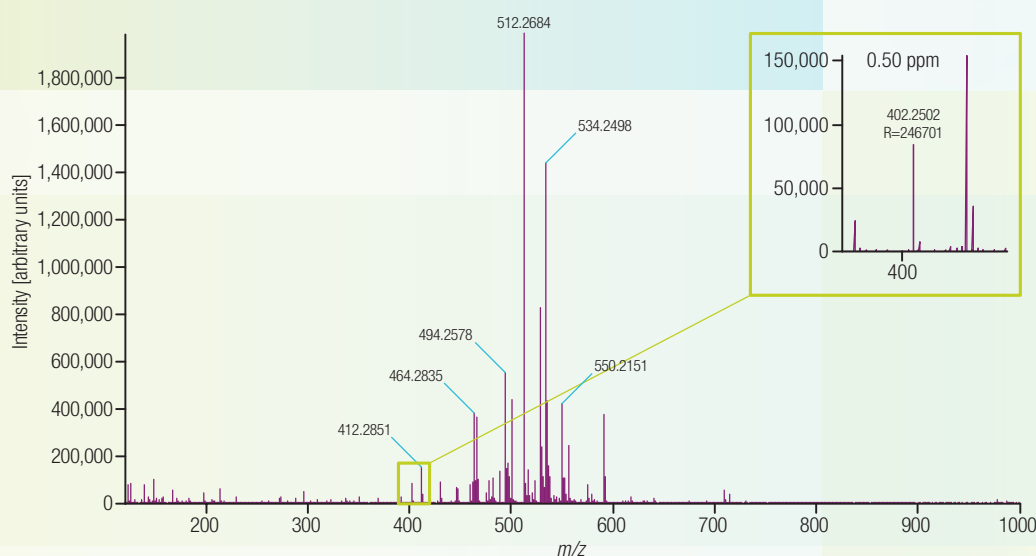
- Resolve isobaric species and isotope fine structures for isotope tracing experiments
- Fast scan speed and high resolution improve precision and confidence for quantitation experiments
- MS<sup>n</sup> *de novo* structural elucidation for identification of novel metabolites on a UHPLC time scale
- Lower maintenance, higher productivity when analyzing low-level lipids and metabolites in complex biological matrixes

RT: 1.95 - 6.06



Even when acquiring MS and MS/MS data, the increased scan speed of the Orbitrap Elite system provides excellent coverage over narrow LC peaks. This analysis of buspirone demonstrates acquisition of full-scan data at a quarter of a million resolution at one Hz. In total nine scans were acquired during the elution of the peak, five full MS scans, four MS/MS scans.

## High-resolution, accurate-mass full-scan MS spectrum of an oxidative metabolite of buspirone



The Orbitrap Elite system provides accurate mass determination even in complex bile matrices. Here, an oxidative metabolite of buspirone eluting in the window of several bile matrix components was still detected with an absolute mass deviation of 0.5 ppm.

## Total solution for Metabolism and Metabolomics

### Metabolism

Thermo Scientific MetWorks and Thermo Scientific Mass Frontier software can utilize the ultrahigh-resolution accurate-mass data from the Orbitrap Elite system for streamlined xenobiotic metabolite profiling and identification. The MetWorks™ software integrates acquisition, processing and reporting for metabolite identification from LC/MS<sup>n</sup> analyses and offers in-depth data mining tools for expected and unexpected metabolites. The Mass Frontier™ software provides chemically intelligent annotation of MS<sup>n</sup> spectral trees with automated fragment prediction. Fragment Ion Search (FISH) in Mass Frontier software allows for automated localization of biotransformations.

### Metabolomics

Thermo Scientific SIEVE and Mass Frontier software utilize the ultrahigh-resolution accurate-mass data from the Orbitrap Elite for comprehensive analysis of endogenous metabolites. The SIEVE™ software finds components that have reproducible differences across multiple sample groups. Optimized component detection dramatically decreases false positive identifications caused by chemical background and redundant signals. The SIEVE software searches local and web-based databases for putative identification. Mass Frontier software provides confirmation of known compounds through interpretation of MS<sup>n</sup> spectra, as well as *de novo* structural elucidation for unknown compounds.

# Application-specific software

turning data into information

## Thermo Scientific Xcalibur Data System

### Stable operating platform

Xcalibur™ software is the versatile, easy-to-use data system that controls all Thermo Scientific MS systems. The home page of the Xcalibur software offers easy navigation through the process of instrument setup, sequence setup, and data acquisition.

### Xtract

Xtract software deconvolutes isotopically resolved data for intact protein analyses and complex MS/MS spectra acquired in top-down analyses.

## Thermo Scientific Proteome Discoverer Software

### Mass informatics platform for protein scientists

Proteome Discoverer™ software is a workflow-based proteomics data processing software for in-depth data mining of complex LC-MS<sup>n</sup> data sets. With the ability to exploit data from different dissociation techniques (CID, HCD, ETD, IRMPD and ECD), Proteome Discoverer software provides extra certainty for peptide and protein identifications. Optional inclusion of multiple search algorithms increases analytical flexibility, and results can now be merged into a single report for easier interpretation.

## Thermo Scientific ProSightPC Software

ProSightPC™ software was developed to address the specific requirements of a top-down and middle-down proteomics strategy. The fragmentation spectra of multiply charged, intact proteins are exceedingly complicated. The software processes high-resolution, accurate-mass data from the Orbitrap Elite MS to produce a list of neutral fragment masses and performs comparisons to proteome databases to identify and characterize proteins.

## Thermo Scientific ProteinCenter Software

### Revealing meaningful biological information

ProteinCenter™ software is a web-based data interpretation tool that enables scientists to compare and interpret proteomic data sets and extract meaningful biological information quickly and easily. It provides access to a single database consolidated from more than 20 public databases, including all historical data.

## Thermo Scientific Pinpoint Software

### Facilitating quantitative proteomics

Pinpoint™ software facilitates the transition from early-stage biomarker discovery to larger-scale, quantitative verification of putative biomarkers and general quantitative proteomics. Pinpoint software simplifies the creation of targeted quantitative assays. It allows researchers to leverage previously acquired data from discovery experiments. Pinpoint software largely automates the development of preliminary methods. It enables acquisition and analysis of preliminary data, which is in turn used to optimize the method.

## SimGlycan™ Software

### Predicting glycan and glycopeptide structure

SimGlycan software analyzes mass spectrometric data to predict the structure of glycans and glycopeptides. It compares experimental MS/MS data against its own database of theoretical fragments and generates a list of probable candidate structures. Each candidate structure is scored to reflect how closely it matches the experimental data. The software also provides additional biological information for probable glycans and identified glycopeptides.

## Thermo Scientific MetWorks

### Drug Metabolism Software

#### Simplify the interpretation of complex metabolism data

MetWorks software simultaneously searches multiple modifications of one or more parent drugs and interprets simple to complex isotope patterns, or unexpected or low-abundance metabolites.

## Thermo Scientific Mass Frontier Spectral Interpretation Software

### Confident path from spectra to structure

Mass Frontier software allows confident structural elucidation through chemically intelligent spectral annotation, state-of-the-art fragmentation prediction, and unparalleled spectral and fragmentation mechanism knowledge management.

## Thermo Scientific SIEVE Differential Expression Software

### Analysis of differential expression based on comparison of LC-MS datasets

SIEVE software provides label-free, semi-quantitative differential analysis of proteins, peptides, or metabolites from the comparison of multiple LC-MS data sets. It is a statistically rigorous tool for analyzing data from metabolism or biomarker discovery experiments.

[www.thermoscientific.com/OrbitrapElite](http://www.thermoscientific.com/OrbitrapElite)

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