Combining the next generation Thermo Scientific Velos Pro ion trap with the new high-field Orbitrap technology, the Thermo Scientific Orbitrap Elite hybrid MS provides the ultimate level of versatility and performance for your research.

# Product Specifications

# Thermo Scientific Orbitrap Elite

High-Field Orbitrap Hybrid Mass Spectrometer





- Novel high-field Orbitrap analyzer
- Resolving power > 240,000 FWHM
- Advanced signal processing
- Multiple fragmentation techniques: CID, HCD and optionally ETD
- Parallel MS and MS<sup>n</sup> analysis
- Velos Pro ion trap generation II ion optics with neutral blocking technology increase robustness

The Thermo Scientific Orbitrap Elite MS is the industry-leading high performance hybrid mass spectrometer combining the novel high-field Orbitrap<sup>™</sup> analyzer with the latest dual-pressure linear ion trap, the Thermo Scientific Velos Pro.

The high-field Orbitrap analyzer increases speed, sensitivity and dynamic range to dig deeper into your samples.

The ultrahigh resolution provides certainty in analytical results by enabling molecular weight determination for intact proteins and in-depth analysis of isobaric species. The unsurpassed resolution of the system is especially useful when dealing with complex and low abundance samples, in applications such as proteomics, metabolomics and lipidomics.

The Orbitrap Elite hybrid MS can perform a wide variety of experiments from in-depth discovery based experiments to comprehensive qual/quan experiments. The availability of multiple fragmentation techniques (CID, HCD and optional ETD) offers a new level of versatility and performance for the most challenging research applications.



# Hardware Specifications

# Velos Pro Dual-Pressure Linear Trap

# lon Max™ API Source

- Enhanced sensitivity and ruggedness
- Sweep Gas<sup>™</sup> reduces chemical noise
- 60° interchangeable ion probe orientation
   Removable metal ion transfer tube
- Removable metal ion transfer tube provides vent-free maintenance

# S-Lens

- A progressively spaced stacked ring ion guide (S-lens)
- The S-lens is a radio frequency (RF) device that captures and efficiently focuses the ions in a tight beam
- Large variable spacing between electrodes allows for better pumping efficiency and improves ruggedness
- Automatic tuning program for optimizing transmission

# **Transfer Ion Optics**

- Generation II ion optics with neutral blocking technology for improved robustness
- High stability and ion transmission efficiency dual-pressure linear ion trap
- High-pressure cell for improved precursor ion trapping, isolation and fragmentation efficiency
- Low-pressure cell for improved scan speed, resolving power and mass accuracy

## Vacuum System

- Differentially pumped vacuum system to 10<sup>-5</sup> Torr
- Split-flow turbomolecular pump controlling vacuum in three regions
- Dual rotary vacuum pump configuration
- Aluminum high-vacuum analyzer chambers
- Novel electron multipliers with higher linear dynamic range for improved quantitation capabilities
- Digital electronic noise discrimination

# **Orbitrap Mass Analyzer**

- Gas-free multipole ion transfer optics
- Gas (nitrogen) filled C-Trap
- High-transmission ion transfer optics
- Straight multipole collision cell with axial field for HCD
- Next generation high-field Orbitrap analyzer
- Active temperature control using a Peltier element
- Differentially pumped vacuum system with:
  - Rotary vane pumps as fore-vacuum pumps, three water-cooled 60 L turbomolecular pumps, and one water-cooled 210 L turbomolecular pump
  - Final vacuum under operating conditions < 2 x 10<sup>-10</sup> Torr
  - Vacuum control by active Pirani gauge and cold ion gauge
- New low noise detect amplifier
- 14-bit signal digitization
- Ultra-fast real-time data acquisition and instrument control system
- Automatic calibration of all ion transfer and Orbitrap parameters via instrument control software

## Options

- H-ESI II Heated Electrospray Ionization Source for enhanced ionization efficiency with flow rates of 1  $\mu$ L/min up to < 2,000  $\mu$ L/min (required)
- $\bullet$  ESI probe compatible with liquid flow rates of <1  $\mu L/min$  to 1 mL/min without splitting
- New NanoSpray Flex Ion Source supports static packed tip and dynamic nanospray experiments, compatible with liquid flow rates of 50 nL/min to 2 µL/min. Lower limit is dependent on gauge of needle used
- APCI/APPI source compatible with liquid flow rates of 50  $\mu L/min$  to 2 mL/min without splitting
- Metal needle option for high- and low-flow analyses

# **Performance Characteristics**

Mass Range	<i>m/z</i> 50 - 2,000, <i>m/z</i> 200 - 4,000
Resolution (FWHM)	60,000 at <i>m/z</i> 400 at a scan rate of 4 Hz, minimum resolution 15,000, maximum resolution > 240,000 at <i>m/z</i> 400
Mass Accuracy	< 3 ppm RMS with external calibration < 1 ppm RMS using internal calibration
MS/MS Sensitivity of Ion Trap	Electrospray lonization (ESI): 2 $\mu$ L of a 50 fg/ $\mu$ L solution of reserpine (100 femtograms total) injected at a flow of 500 $\mu$ L/min will produce a minimum signal-to-noise ratio of 100:1 for the transition of the isolated protonated molecular ions at <i>m</i> /z 609 to the largest two product ions, <i>m</i> /z 397 and <i>m</i> /z 448, when the mass spectrometer is operated at unit resolution in the full scan MS/MS mode, scanning the product ion spectrum from <i>m</i> /z 165-615. <sup>[1]</sup>
Dynamic Range	> 5,000 within a single scan guaranteeing specified mass accuracy
MS Scan Power	$MS^n$ , for n = 1 through 10
ETD Option	3 µL/min infusion of a 1 pmol/µL solution of Angiotensin I will produce an electron transfer dissociation fragmentation efficiency of > 15%

<sup>[1]</sup> Requires H-ESI II





# Software Features

#### **Data System**

- High performance PC with Intel<sup>®</sup> microprocessor
- High resolution LCD color monitor
- Microsoft Windows<sup>®</sup> 7 operating system
- Microsoft Office 2010 software package
- Thermo Scientific Xcalibur processing and instrument control software
- FT-Programs software tools: Protein Calculator and Recalibrate Offline

# **Operation Modes**

- Data Dependent Decision Tree Automatic selection of the optimal fragmentation technique based on peptide properties (charge state, m/z) for highest fragmentation efficiency
- High resolution accurate mass scans at high repetition rates
- Precursor ion isolation and fragmentation in the linear ion trap (CID) with high resolution accurate mass MS/MS and MS<sup>n</sup> data acquisition in the Orbitrap mass analyzer
- Higher collision energy dissociation (HCD) for triple-quadrupole like fragmentation
- Data Dependent<sup>™</sup> scans using both the linear ion trap and the Orbitrap mass analyzer
- Data Dependent MS/MS with parallel acquisition of multiple MS<sup>n</sup> scans in the linear ion trap while acquiring a high resolution full scan MS spectrum in the Orbitrap analyzer
- Ion Mapping, Neutral Loss Ion Mapping, Parent Ion Mapping, user selectable Dynamic Exclusion<sup>™</sup>, Nth order Triple Play experiment, Data Dependent Ion Tree experiment, Total Ion Map experiment

# Optional Application-Specific Software

- Thermo Scientific Proteome Discoverer

   Mass informatics platform for protein scientists
- ProSightPC<sup>™</sup> Top-down identification and characterization of proteins including PTMs
- Thermo Scientific MetWorks automated metabolite identification using spectral trees and accurate mass data
- Mass Frontier<sup>™</sup> predictive fragmentation software for spectral interpretation and classification software to identify unknowns
- PEAKS<sup>™</sup> powerful, easy *de novo* sequencing
- Thermo Scientific SIEVE automated differential expression analysis in proteomics or metabolomics applications
- ProMass<sup>™</sup> Deconvolution intact protein analysis

# **Exclusive Technologies**

- Precursor ion selection in the linear ion trap and fragmentation in the new collision cell (HCD) with high resolution accurate mass detection in the Orbitrap mass analyzer
- Pulsed-Q Collision Induced Dissociation (PQD) enables trapping of low mass fragment ions
- Unique, patented\* Automatic Gain Control (AGC<sup>™</sup>) ensures that the ion trap is always filled with the optimum number of ions for any scan type
- Dynamic Exclusion allows acquisition of MS/MS and MS<sup>n</sup> spectra from lower intensity ion species
- WideBand Activation<sup>™</sup> generates more structurally informative spectra
- Normalized Collision Energy<sup>™</sup> for both CID and HCD fragmentation techniques providing reproducible data from instrument to instrument
- Stepped Normalized Collision Energy (CID and HCD) allows for the variation of the collision energies in MS/MS experiments
- Multistage Activation (MSA) generates combination of MS/MS spectra and MS<sup>3</sup> spectra based on a user defined neutral loss

## Advanced Data Dependent Experiments

- Data Dependent features trigger acquisition of MS<sup>n</sup> spectra only when a compound of interest is detected
- Isotopic Data Dependent scanning software triggers MS/MS scanning only when a specified isotopic pattern is detected
- Ion Mapping automatically generates a three-dimensional MS/MS map, yielding product ions, precursor ions, and neutral loss information
- Ion Mapping Browser software displays data generated by Ion Mapping experiments
- Data Dependent Ion Tree performs MS<sup>n</sup> experiments on up to 25 species
- MS<sup>n</sup> Browser software displays data generated by Data Dependent Ion Tree and Ion Mapping experiments
- Monoisotopic precursor selection for Data Dependent MS/MS experiments
- Data Dependent (accurate) Neutral Loss
   Trigger MS<sup>3</sup> scans on only the MS/MS product ions with a pre-defined neutral loss

46642.586

100-



Analysis of intact Yeast Enolase (46.64 kDA), zoom in on charge state 47<sup>+</sup> ions (left) and deconvoluted spectrum of yeast enolase (monoisotopic mass 46642.214 Da) (right).

# Installation Requirements

#### **Orbitrap Elite Hybrid MS**

#### Power

- 230 V<sub>ac</sub> ± 10% 3 phase, 15 Ampere, 50/60 Hz, with earth ground for the instrument
- 120 or 230  $\rm V_{ac}$  single phase with earth ground for the data system
- 120 or 230 V<sub>ac</sub> single phase, 15 Ampere, with earth ground for the water chiller

#### Gas

#### Helium

Ultra-high purity (99.999%) with less than 1 ppm each of water, oxygen and total hydrocarbons

#### Nitrogen

High purity (99.5% pure, flow rate 15 L/min) nitrogen gas supply for the API source and the C-Trap

#### Environment

- System averages 2,800 W (10,000 Btu/hr) output when considering air conditioning needs
- Operating environment must be 16 - 26 °C (59 - 78 °F) and relative humidity must be 50 - 80% with no condensation
- Optimum operating temperature is 18 - 21 °C (65 - 70 °F)

#### Weight

MS: ~ 620 kg

#### Water Cooler

Provided with the instrument

## Dimensions

MS with ETD: (h x w x d) 142 cm x 87 cm x 171 cm 55.9 in x 34.3 in x 67.3 in

MS without ETD: 142 cm x 87 cm x 142 cm 55.9 in x 34.3 in x 55.9 in

#### **ETD Option**

#### Gas

Nitrogen supply for ETD option: Ultra-high purity nitrogen (UHP, 99.999%) with less than one ppm each water and oxygen

#### Access

At least 94 cm access required at the rear of the instrument

#### Environment

System averages with ETD 3,500 W (12,000 Btu/hr) output when considering air conditioning needs



#### www.thermofsiher.com/OrbitrapElite

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