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Thermo Scientífic LTQ Orbitrap Velos Hybrid FT Mass Spectrometer Performance Specifications

Performance Characteristics

- Mass Range: m/z 50-2000, m/z 200-4000
- Resolution: 60,000 at m/z 400 at a scan rate of 1 Hz, minimum resolution 7,500; maximum resolution >100,000 at m/z 400
- Mass Accuracy: < 3 ppm with external calibration, < 1 ppm using internal calibration
- MS/MS Sensitivity (Ion Trap): Electrospray Ionization (ESI) -2 µL of a 50 fg/µL solution of reserpine (100 femtograms total) injected at a flow of 500 µL/min will produce a minimum signal-to-noise ratio of 100:1, for the transition of the isolated protonated molecular ion at m/z 609 to the largest two product ions, m/z 397 and m/z 448, when the mass spectrometer is operated at unit resolution in the full-scan MS/MS mode, scanning the product ion spectrum from m/z 165 615.**
- > Dynamic Range: >5,000 within a single scan guaranteeing specified mass accuracy
- MS Scan Power MSn, for n = 1 through 10
- > ETD option: $3 \mu L/min$ infusion of a 1 pmol/ μL solution of Angiotensin I will produce an electron transfer dissociation fragmentation efficiency of >15%
- Analog Inputs: One (1) analog input (0-1 V), One (1) analog (0-10 V)

Installation Requirements

Power

- > 230 Vac \pm 10% 3 phase, 15 Amps, 50/60 Hz, with earth ground for the instrument
- > 120 or 230 Vac single phase with earth ground for the data system
- > 120 or 230 Vac single phase, 15 Amps, 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 2800 W (10,000 Btu/hr) output when considering air conditioning needs
- > Operating environment must be $16 26^{\circ}C(59 78^{\circ}F)$ and relative humidity must be 50 80% with no condensation
 - Optimum operating temperature is 18 21°C (65 70°F)

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Weight: MS: ~620 kg Dimensions: MS: (h x w x d), 141.4 cm x 87 cm x 146.3 cm Water Cooler: Provided with the instrument

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 79 cm access required at the rear of the instrument.

Environment: System averages with ETD 3500 W (12,000 Btu/hr) output when considering air conditioning needs

The Thermo Scientific LTQ Orbitrap Velos combines the proven mass accuracy and ultra-high resolution of the Orbitrap mass analyzer, with the increased sensitivity and improved cycle time of the LTQ VelosTM. The high mass accuracy of the LTQ Orbitrap Velos increases the speed and confidence of identification in complex samples by minimizing false positive identification.

The ultra-high resolution provides certainty in analytical results by enabling molecular weight determination for intact proteins and in-depth analysis of isobaric species. The new HCD cell in the LTQ Orbitrap Velos is more efficient, resulting in improved quantitation of isobarically labeled peptides, such as applications requiring Tandem Mass Tags (TMT). Electron Transfer Dissociation (ETD) generates complementary information for highly sensitive PTM analyses and *de novo* sequencing.

- New API source with new S-lens ion optics technology
- Dual-Pressure Linear Ion Trap
- > Collision cell with axial field gradient
- Resolving power of >100,000
- Mass accuracy better than 1 ppm
- Multiple fragmentation techniques: CID, HCD, and available ETD
- > Parallel MS and MS*n* analysis

Hardware Specifications LTQ Velos Dual-Pressure Linear Trap Ion Max[™] API Source

- Enhanced sensitivity and ruggedness
- > Sweep Gas[™] reduces chemical noise
- > 60° interchangeable ion probe orientation
- > 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

> Advanced ion guides • High stability and ion transmission efficiency

Dual-Pressure Linear Trap

- > High-pressure cell for improved isolation and fragmentation efficiency
- > Low-pressure cell for improved scan speed, resolving power and mass accuracy

Vacuum System

- Differential pumped vacuum system to 10-5 Torr
- Split-flow turbomolecular pump controlling vacuum in three regions
- Dual rotary vacuum pump configuration
- Aluminum high-vacuum analyzer chambers

Detection System

- Patented dual conversion dynode detector
- > Two off-axis continuous dynode electron multipliers with extended dynamic range
- > Digital electronic noise discrimination

Orbitrap Mass Analyzer

- Gas-free multipole ion transfer optics
- Improved gas (nitrogen) filled C-Trap
- High-transmission ion transfer optics
- Straight multipole collision cell with axial field for HCD
- > Orbital trap
- > Active temperature control using a Peltier element
- Differentially pumped vacuum system with:
 -Rotary vane pumps as fore vacuum pumps, one water-cooled 60 L turbomolecular pump, and two water-cooled 210 L turbomolecular pumps -Final vacuum under operating conditions: < 4 x 10-10 Torr
 - -Vacuum control by <mark>act</mark>ive Pirani gauge and cold ion gauge
- Low noise detect amplifiers
- > 14-bit signal digitization
- Ultra-fast real-time data acquisition and instrument control system
- Automatic calibration of all transfer and Orbitrap parameters via instrument control software

Options

- H-ESI II Heated Electrospray Ionization Source for enhanced ionization efficiency with flow rates of 1μL/min or to < 2000 μL/min.</p>
- \geq ESI probe compatible with liquid flow rates of < 1 μ L/min to 1 mL/min without splitting (required)
- Nanospray source supports static packed tip and dynamic nanospray experiments, compatible with liquid flow rates of 50 nL/min to 2 μL/min*
- > APCI source compatible with liquid flow rates of 50 μ L/min to 2 mL/min without splitting
- > APCI/APPI source compatible with liquid flow rates of 50 μ L/min to 2 mL/min without splitting
- Metal needle option for high- and low-flow analyses *Lower limit is dependent on gauge of needle used

Software Features

Data System

- > High performance PC with Intel® microprocessor
- High resolution LCD color monitor
- Microsoft Windows® XP operating system
- Microsoft Office XP software package
- > Thermo Scientific Xcalibur processing and instrument control software
- FT-Programs software tools: ProteinCalculator 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 MSn data acquisition in the Orbitrap mass analyzer
- \succ Data DependentTM scans using both the linear ion trap and the Orbitrap mass analyzer
- Data Dependent MS/MS with parallel acquisition of multiple MSn scan 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[™], Nth order Triple Play experiment, Data Dependent Ion Tree experiment, Total Ion Map experiment

Optional Thermo Scientific Application-Specific Software

- Proteome Discoverer Mass informatics platform for protein scientists
- Prosight PC Top down identification and characterization of proteins incl. PTMs
- \triangleright MetWorksTM automated metabolite identification using spectral trees and accurate mass data
- Mass FrontierTM predictive fragmentation software for spectral interpretation and classification software to identify unknowns
- > PEAKS[™] powerful, easy *de novo* sequencing
- SIEVETM automated differential expression analysis in proteomics or metabolomics applications
- ProMass[™] 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[™]) 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*n* spectra from lower intensity ion species
- ▶ WideBand ActivationTM generates more structurally informative spectra
- ➢ Normalized Collision Energy[™] for multiple fragmentation techniques (CID and HCD) 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 MS3 spectra based on a user defined neutral loss.

Advanced Data Dependent Experiments

- Data Dependent features trigger acquisition of MSn 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 3-dimensional MS/MS map, yielding product ion, precursor ion, and neutral loss information
- > Ion Mapping Browser software displays data generated by Ion Mapping experiments
- > Data Dependent Ion Tree performs MSn experiments on up to 25 species
- MSn 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 MS3 scans on only the MS/MS product ions with a pre-defined neutral loss





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