

The LTQ XL linear ion trap mass spectrometer delivers more structural information faster and with more confidence.

LTQ XL™

More Structural Information with MSⁿ



- **Electron Transfer Dissociation (ETD) enabled**
- **Multiple dissociation techniques including PQD**
- **Extensive coverage for predicted and unpredicted metabolites**
- **Fast polarity switching for high-sensitivity analysis of unknowns**
- **Intelligent Data Dependent™ acquisition**
- **Platform for hybrid MSⁿ high resolution, accurate mass**

The LTQ XL extends the MSⁿ performance of the LTQ linear ion trap with powerful new tools to generate extensive structural information for the most demanding proteomics and metabolism applications. With unparalleled sensitivity and ultra-fast cycle time, the LTQ XL delivers more information from less sample in less time. The unmatched high quality spectra of the LTQ XL in combination with powerful new software packages deliver complete solutions for your structural elucidation questions.

The advanced Xcalibur™ Data Dependent software suite, which includes the MS³ neutral loss experiment, enables rapid identification of post-translational modifications and metabolites. This feature greatly reduces the amount of time needed to analyze and interpret the data. Powerful software control and data processing in addition to innovative technology provide superior coverage for protein and metabolite analysis.

Hardware Features

Ion Max™ API Source

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

Transfer Ion Optics

- Advanced ion guides
- High stability and ion transmission efficiency

2D Linear Quadrupole Ion Trap Mass Spectrometer

- Optimized analyzer dimensions
- Regulated helium flow for stable performance
- Automatic system calibration
- High-efficiency radial ion ejection

Vacuum System

- Differentially-pumped vacuum system to 10^{-5} Torr
- Split-flow turbomolecular pump controlling vacuum in three regions
- Dual rotary vacuum pump configuration
- High-vacuum aluminum analyzer chamber

Detection System

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

Integrated Divert Valve

- Fully-automated data system control enables user to divert the solvent front, gradient end point and any other portion of the HPLC run to waste
- User-definable default state of the valve, either "to waste" or "to source"

Integrated Syringe Pump

- Syringe Pump allows automated infusion under data system control

Options

- ESI probe compatible with liquid flow rates of <1 $\mu\text{L}/\text{min}$ to 1 mL/min , without splitting
- APCI source compatible with liquid flow rates of 50 $\mu\text{L}/\text{min}$ to 2 mL/min , without splitting
- APCI/APPI source compatible with liquid flow rates of 50 $\mu\text{L}/\text{min}$ to 2 mL/min , without splitting
- Electron Transfer Dissociation (ETD) enabled
- vMALDI™ ion source combines the speed of MALDI with the sensitivity and selectivity of MS/MS
- Nanospray source supports static packed tip and dynamic nanospray experiments, compatible with liquid flow rates of 50 nL/min^* to 2 $\mu\text{L}/\text{min}$
- Metal needle option for high- and low-flow analyses

*Lower limit is dependent on gauge of needle used

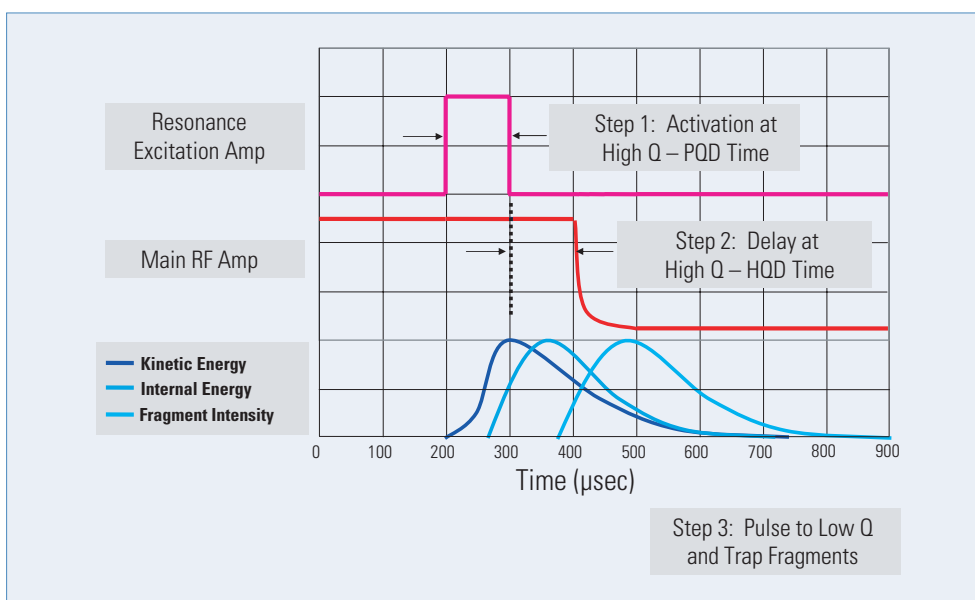
Software Features

Data System

- Xcalibur processing and instrument control software
- LCQUAN™ 2.5 quantification package
- Microsoft® Office XP software package
- Microsoft Windows® XP operating system
- High-performance PC with Intel® Pentium® microprocessor
- High-resolution LCD color monitor

Scan Functions

- Full-scan mass spectra for sensitive analyses and rapid screening of unknown compounds
- Selected Ion Monitoring (SIM) for selected ions for target compound analysis
- Full-scan product ion spectra at sensitivities higher than any ion trap mass spectrometer
- Selected Reaction Monitoring (SRM) for a traditional LC/MS/MS quantitative analytical experiment
- MSⁿ for multi-stage MS experiments to probe the structure of ions
- ZoomScan™, a high-resolution, full-range scan to resolve isotopic envelopes often used for charge state determination of peptides and ionization state determination of organometallics
- Ultra ZoomScan for ultimate resolution
- TurboScan™, an ultra-fast scan to improve signal-to-noise and sampling rate



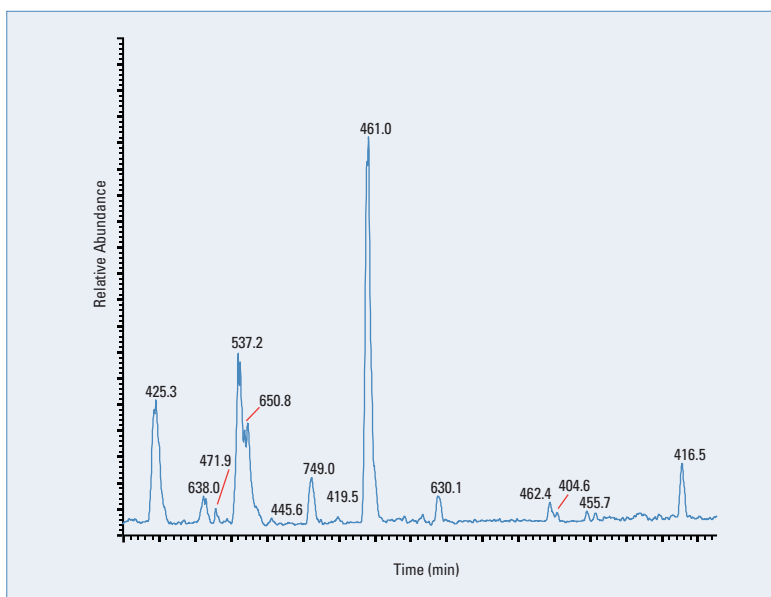
Schematic of Pulsed Q Collision Induced Dissociation Process

Exclusive Technologies

- Pulsed Q Collision Induced Dissociation (PQD) enables trapping of low mass fragment ions
- Electron Transfer Dissociation (ETD) enabled capability delivers peptide sequence information not available from conventional methods
- High Resolution Isolation (HRI) allows for the separation of an isobaric interfering species down to 0.3 Da or for isolation of a thermally labile compound
- 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 MSⁿ spectra from lower intensity ion species
- WideBand Activation™ generates more structurally informative spectra
- Normalized Collision Energy™ compensates for the mass-dependent energy deposition characteristics of ion trap mass spectrometers in MS/MS experiments, providing reproducible data from instrument to instrument
- Stepped Normalized Collision Energy allows for the variation of the collision energies in an experiment
- Multistage Activation generates combination 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
- Triple Play determines the charge state and MS/MS scan range of a multiply charged ion



LC/MS analysis of an enzymatic digest of 4 fmol of myoglobin.

- Nth Order Triple Play allows the number of ions undergoing a Triple Play to be defined
- Data Dependent Neutral Loss (NL) MS³ triggers MS³ scan only on the MS/MS product ions with the pre-defined neutral loss to identify and characterize metabolites and post-translational modifications
- 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
- Data Dependent Zoom Map generates sequential MS/MS experiments using a ZoomScan for charge state determination prior to each MS/MS experiment
- MSⁿ Browser software displays data generated by Data Dependent Ion Tree and Ion Mapping experiments

Optional Application-Specific Software

- MetWorks™ – automated metabolite identification using spectral trees
- Mass Frontier™ – spectral interpretation and classification software to identify unknowns
- BioWorks™ – protein identification and quantitation featuring SEQUEST®
- PEAKS – powerful, easy *de novo* sequencing
- ProMass™ Deconvolution – intact protein analysis
- SIEVE™ – automated label-free differential expression of proteins and peptides
- ProSight PC™ – top-down protein identification

System Specifications

MS/MS Sensitivity

Electrospray Ionization (ESI) – A loop injection of 2 μL of a 125 fg/ μL solution of reserpine (250 femtograms total sample) at a flow of 400 $\mu\text{L}/\text{min}$ of 50% isopropyl alcohol/50% water 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, 397 and 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.

Atmospheric Pressure Chemical Ionization (APCI)

– A loop injection of 2 μL of a 125 fg/ μL solution of reserpine (250 femtograms total sample) at a flow of 400 $\mu\text{L}/\text{min}$ of 50% isopropyl alcohol/50% water 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, 397 and 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.

MSⁿ Sensitivity

Electrospray Ionization (ESI)

A loop injection of 2 μL of a 125 fg/ μL solution of reserpine (250 femtograms total sample) at a flow of 400 $\mu\text{L}/\text{min}$ of 50% isopropanol/50% water will produce a minimum signal-to-noise ratio of 25:1, for the transition of the unit isolated protonated molecular ion at m/z 609 to the product ion at m/z 397 which is further fragmented to the product ion at m/z 365, 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.

Installation Requirements

Power

- One 230 Vac \pm 10.0%, 15 Amps, 50/60 Hz, single phase, with earth ground dedicated to the instrument
- 120 or 230 Vac single phase, with earth ground for the data system

Gas

- One high-purity (99% pure, flow rate 15 L/min) nitrogen gas supply for the API source
- One ultra high-purity helium gas supply (99.998% pure) with less than 1 ppm each of water, oxygen, and total hydrocarbons for the mass analyzer

Environment

- System averages 2300 W (8000 Btu/h) output when considering air conditioning needs
- Operating environment must be 15-27 °C (59-80 °F) and relative humidity must be 40-80% with no condensation
- Optimum operating temperature is 18-21 °C (65-70 °F)

Dimensions/Weight

- MS: 56 x 79 x 59 cm (h x w x d)
- MS: ~120 kg
- Two roughing pumps: 38.6 kg each

Performance Specifications

Mass Range

- m/z 15 – 200
- m/z 50 – 2000
- m/z 200 – 4000

Resolution

- Down to 0.05 FWHM (full width half maximum) with Ultra ZoomScan

Polarity Switching

- 100 msec between positive and negative

MS Scan Power

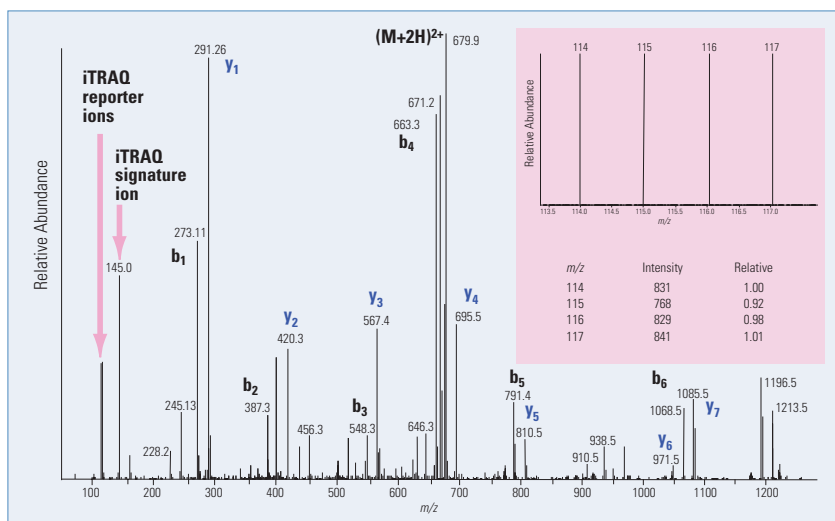
- MSⁿ, for n = 1 through 15

Contact Closure

- Start In/Out
- Start Out is programmable

Analog Inputs

- One (1) analog Input (0-1 V)
- One (1) analog Input (0-10 V)



PQD spectrum for QNCDQFEK in BSA digest derivatized with the four iTRAQ[®] reagents mixed together at a ratio of 1:1:1:1

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