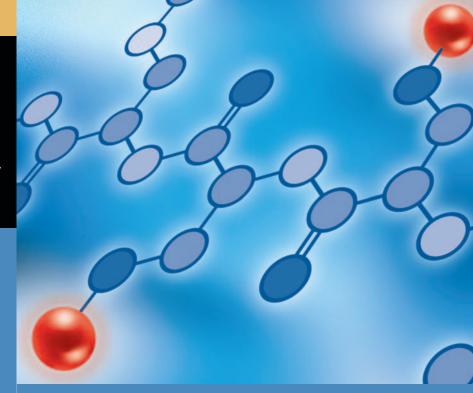
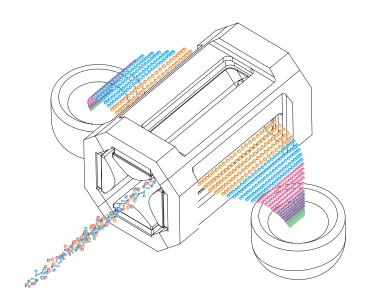
LTQ XL™ Linear Ion Trap Mass Spectrometer



More Structural Information with MS<sup>n</sup>

## SUPERIOR ION TRAP TECHNOLOGY

From the leader in Ion Trap Mass Spectrometry, the LTQ XL Linear Ion Trap delivers ultimate sensitivity at breakthrough speed.



## Proteomics:

- Maximum protein coverage resulting from superior cycle times and sensitivity
- Automated MS" triggered Data Dependent™ neutral loss scan
- Flexibility of ionization modes, inlets, and chromatographic solutions

## Metabolite Identification:

- Superior MS" spectral quality and full-scan acquisition
- Structural information on low level metabolites without knowing MRM transitions
- Data Dependent and Dynamic Exclusion™ acquisition for maximum information in complex samples

## Discovery Quantitation:

- Excellent ion statistics for robust quantitation
- Optimum efficiency with Normalized Collision Energy™
- Simultaneous identification and quantitation for the regulated laboratory environment

# Forensic and Clinical Analysis:

- Outstanding robustness for reliable quantitation in complex matrices
- Simultaneous quantitation and confirmation in both positive and negative ionization modes
- Ease of use for the production laboratory



With the Accela™ High Speed LC System, the LTQ XL is the perfect tool for high throughout applications.



sing multiple dissolution techniques, including Pulsed-Q Dissociation (PQD) and Electron Transfer Dissociation (ETD), the LTQ XL generates extensive structural information for the most demanding proteomics samples.

> The LTQ XL Linear Ion Trap— Technology You Can Trust



## METABOLITE IDENTIFICATION AND CONFIRMATION

Automatically find all the metabolites the first time, even the ones that you didn't predict...

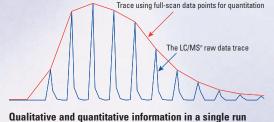
Metabolic studies are performed both in vivo and in vitro necessitating the analysis of target compounds in complex matrices. These biological matrices contain the parent drug, all of its metabolites in a wide range of concentrations, and additional endogenous metabolic materials. Furthermore, it is not possible to predict, in advance, all of the metabolites for a potentially new drug compound.

### Intelligent precursor ion selection

Automated Data Dependent MS<sup>n</sup> acquisition gives you information on not only the predicted metabolites (parent list), but also on the unpredicted metabolites. In addition, classes of metabolites can be detected using the automated Data Dependent Constant Neutral Loss (CNL) triggered MS3 feature. Data analysis can be facilitated using MetWorks™ and Mass Frontier™ software that enhances the screening and characterization of metabolites in complex matrices.

## Metabolite Identification

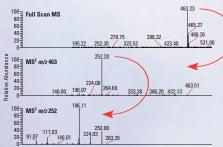
- Analog signal-triggered Data Dependent MS<sup>n</sup> acquisitions
- Constant Neutral Loss Data Dependent MS<sup>n</sup> acquisitions
- MetWorks software
- Mass Frontier software



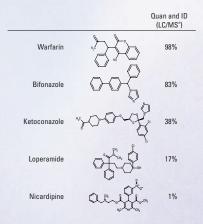
## 100 -90 80-70 Relative Abundance 50 20 10

Reconstructed ion chromatograms for 13 identified drugs and metabolites in less than three minutes.

## Simultaneous Metabolite Identification and Quantitation for Metabolic Stability



Data Dependent MS<sup>n</sup> metabolite identification



Quantitation for metabolic stability

# ELECTRON TRANSFER DISSOCIATION (ETD) FOR PROTEOMICS AND BIOMARKER APPLICATIONS



Available for the LTQ and LTQ XL mass spectrometers, ETD offers ECD-like fragmentation in a linear ion trap, producing abundant peptide fragmentation while preserving labile

PTMs, such as phosphorylation. ETD, combined with the high ion storage capacity of Thermo Scientific linear ion traps, creates a powerful new tool for protein and peptide analysis.

## ETD Makes the LTQ XL Even More Powerful for Proteomics

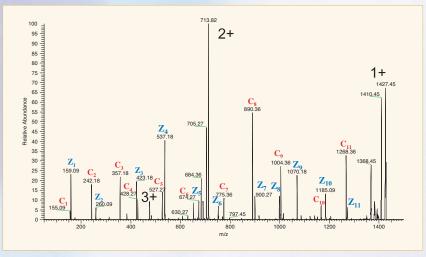
- Complementary with CID— Improves protein coverage
- Preserves labile PTMs, simplifying their analysis
- Automated CID and ETD in a single injection

## Electron Transfer Dissociation (ETD)

$$[M + 3H]^{3+} + A^{-} \longrightarrow [M + 3H]^{2+} + A$$

$$[M+3H]^{2+} \longrightarrow \underbrace{[C+2H]^{1+}}_{C} + \underbrace{[Z+H]^{1+}}_{Z}$$

ETD ion/ion chemistry. The LTQ XL ion trap is the ideally suited device to exploit this technique.



ETD MS/MS spectrum of VIP 1-12 m/z 476.3 (3+) showing rich production of c and z ion series

### Detected by CID or ETD or Both

### $\underline{100~fmol}$ OVALBUMIN (P01012):

MGSIGAASMEFCFDVFKELKVHHANENIFYCPIAIMSALAMVYLGAKDSTRTQINKVVRFDKLPGFGDSIEAQCGTSVNVHSSLRDILNQITKPNDVYSFSLASRLYAEERYPILPEYLQCVKELYRGGLEPINFQTAADQARELINSWVESQTNGIIRNVLQPSSVDSQTAMVLVNAIVFKGLWEKAFKDEDTQAMPFRVTEQESKPVQMMYQIGLFRVASMASEKMKILELPFASGTMSMLVLLPDEVSGLEQLESIINFEKLTEWTSSNVMEERKIKYYLPRMKMEEKYNLTSVLMAMGITDVFSSSANLSGISSAESLKISQAVHAAHAEINEAGREVVGSAEAGVDAASVSEEFRADHPFLFCIKHIATNAVLFFGRCVSP

### 40 fmol ALBUMIN (P02769):

MKWVTFISLLLLFSSAYSRGVFRRDTHKSEIAHRFKDLGEEQFKGLVLIAFSQYLQQCPFDEHVKLV NELTEFAKTCVADESHAGCEKSLHTLFGDELCKVASLRETYGDMADCCEKQEPERNECFLSHKDDS PDLPKLKPDPNTLCDEFKADEKKFWGKYLYEIARRHPYFYAPELLYYANKYNGVVFQDCCQAEDKG ACLLPKIETMREKVLASSARQRLRCASIQKFGERALKAWSVARLSQKFPKAEFVEVTKLVTDLTKV HKECCHGDLLECADDRADLAKYICDNQDTISSKLKECCDKPLLEKSHCIAEVEKDAIPENLPPLTAD FAEDKDVCKNYQEAKDAFLGSFLYEYSRRHPEYAVSVLLRLAKEYEATLEECCAKDDPHACYSTVF DKLKHLVDEPQNLIKQNCDQFEKLGEYGFQNALIVRYTRKVPQVSTPTLVEVSRSLGKVGTRCCTK PESERMPCTEDYLSLILNRLCVLHEKTPVSEKVTKCCTESLVNRRPCFSALTPDETYVPKAFDEKLFT FHADICTLPDTEKQIKKQTALVELLKHKPKATEEQLKTVMENFVAFVDKCCAADDKEACFAVEGPK LVVSTQTALA

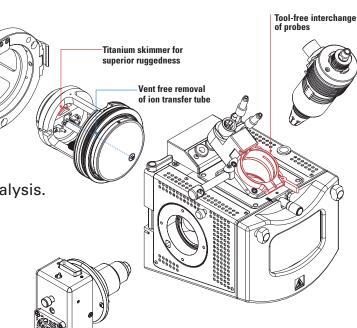
### Improved sequence coverage with ETD; complementary to other methods

### **Comparison of Detection Methods**

	CID	ETD	CID and ETD Combined	Increase in Coverage with CID and ETD Combined
Ovalbumin	137	129	184	15%
Albumin	239	248	345	18%

# MULTIPLE IONIZATION MODES

A variety of ionization techniques are available on the LTQ XL that allow for maximum flexibility in sample analysis.



### Ion Max™ source

ESI, APCI, and APPI probes are based on the revolutionary Ion Max source design. It imparts superior performance and features simple, tool-free switching of ESI and APCI probes. Full probe adjustment in the x, y, and z directions allows optimized positioning for maximum sensitivity and robustness in both low and high flow applications. The 60° angle dramatically improves performance by reducing chemical noise. Maintenance of API sources, as well as switching between various probes, is vent-free. Automatic source recognition adds to ease of use.

## Nanospray source

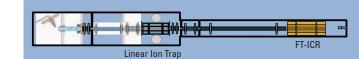
The new Nanospray ion source features easy coupling with low dead volume and interchangeable probes for static, dynamic, and packed tip nanospray. The liquid junction provides excellent spray stability even when spraying 100% aqueous mobile phase. The versatile Nanospray source accommodates uncoated and packed tip needle designs to support low- and high-flow applications.

## Source Configurations for Every Need

- Electrospray ionization (ESI)
- Atmospheric pressure chemical ionization (APCI)
- Atmospheric pressure photoionization (APPI)
- Electron transfer dissociation (ETD)
- Nanospray ionization (NSI)



# A PLATFORM FOR HIGH RESOLUTION AND HIGH MASS ACCURACY



The LTQ XL hybrid mass spectrometers have established themselves as the new analytical standard for research in Proteomics and Drug Discovery.

## LTQ Orbitrap™

...Breakthrough Technology
Combining patented Orbitrap technology with the LTQ XL linear ion trap, the LTQ Orbitrap offers fast, sensitive, reliable detection and identification of compounds in complex mixtures. Its outstanding mass accuracy, mass resolution and reliable, high sensitivity MS<sup>n</sup> performance make it a clear alternative to existing hybrid time-of-flight systems.

### LTQ FT Ultra™

... Ultimate Performance

The LTQ FT Ultra combines the most advanced Ion Trap and Fourier Transform Ion Cyclotron Resonance (FT-ICR) technologies into a single instrument, with unprecedented analytical power and versatility. Ultra-high resolution and sensitivity, coupled with sub ppm mass accuracy and accuracy, enable routine analysis of even the most complex samples. ECD and

IRMPD are available for top down

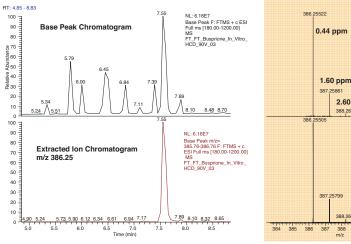
protein analysis.

# Accurate Mass on a Chromatographic Time Scale

- Robust and reliable high mass accuracy
- Simultaneous high mass resolution, mass accuracy, and sensitivity
- Fast data acquisition rate with ultra high mass resolution







Accurate mass determination of an in vitro buspirone sample analyzed on the LTQ Orbitrap

Experimental

Theoretical

2.60 ppm

## **Laboratory Solutions Backed by Worldwide Service and Support**

Tap our expertise throughout the life of your instrument. Thermo Scientific Services extends its support throughout our worldwide network of highly trained and certified engineers who are experts in laboratory technologies and applications. Put our team of experts to work for you in a range of disciplines – from system installation, training and technical support, to complete asset management and regulatory compliance consulting. Improve your productivity and lower the cost of instrument ownership through our product support services. Maximize uptime while eliminating the uncontrollable cost of unplanned maintenance and repairs. When it's time to enhance your system, we also offer certified parts and a range of accessories and consumables suited to your application.

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