

# Finnigan LTQ FT



Unprecedented Analytical Power

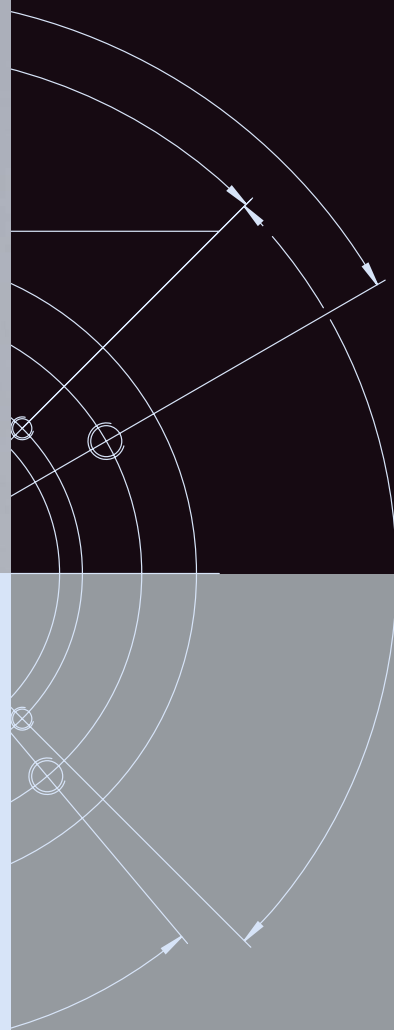
a leader in chromatography and mass spectrometry

**Thermo**  
ELECTRON CORPORATION

*The Finnigan™ LTQ FT™ combines the most advanced Ion Trap and Fourier Transform Ion Cyclotron Resonance technologies into a single instrument with unrivaled analytical power and versatility. For the first time, high resolution, accurate mass determinations, and MS<sup>n</sup> are available for routine high-throughput analysis.*

*This advanced, high-performance mass spectrometer is the right tool for your toughest analytical challenges in metabolic studies, proteome analysis, pharmaceutical discovery, and all other applications demanding rigorous structural characterization.*

**Unprecedented  
Analytical  
Power**



- **Unsurpassed LC/MS and LC/MS<sup>n</sup> performance**
- **Robust accurate mass determination**  
Mass accuracy of better than 2 ppm with external calibration
- **Very high mass resolution for mixture analysis**  
Maximum resolution of greater than 500,000 (FWHM)
- **Simultaneous high resolution, mass accuracy, and sensitivity over one mass decade (e.g. m/z 200 – m/z 2,000)**
- **Fast data acquisition rate (1 second repetition rate) with very high resolution (100,000 at m/z 400)**
- **Sub fmol on-column sensitivity (LC/MS)**

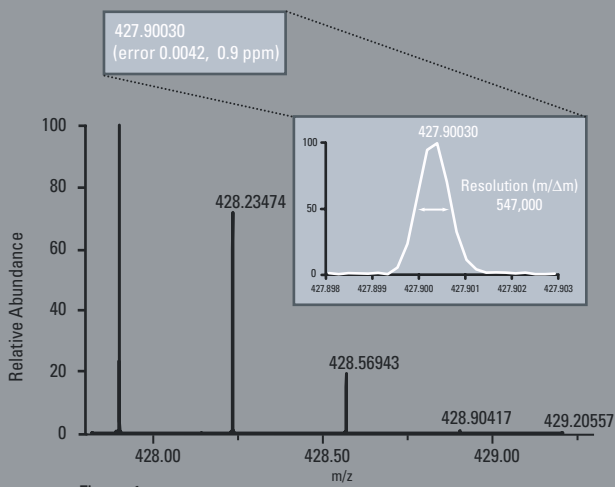


Figure 1

**Figure 1.** High resolution analysis of triply charged protonated molecular ion of angiotensin from Goosefish (NRVYVHPFHL). Mass accuracy 0.9 ppm, using external calibration.

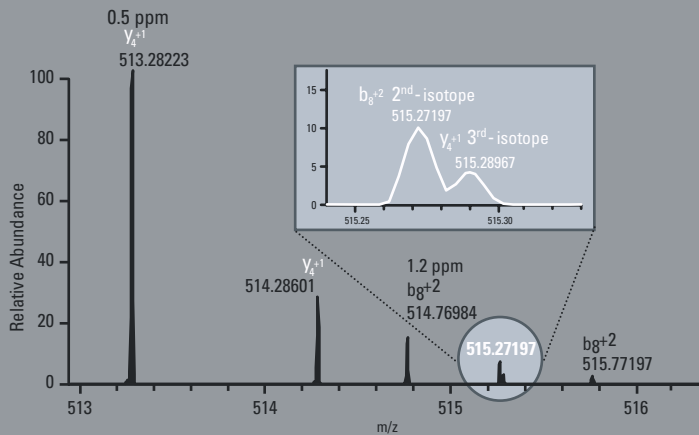


Figure 2

**Figure 2.** Accurate mass LC-MS/MS analysis of a peptide mixture with external calibration mass accuracy of first isotope,  $\approx 1$  ppm.

### High Mass Resolution Enables Analysis of Complex Mixtures

High mass resolution has long been established as the key to analysis of complex mixtures. Only by resolving individual analyte peaks which occur at the same nominal mass, can all of the components in a mixture be characterized simultaneously. The higher the mass resolution, the more complex the mixture that can be analyzed.

High mass resolution adds a powerful new dimension to experimental data – it can be used to resolve sample components, reducing demands on other separation techniques, such as chromatography. Only high mass resolution can assure accurate mass assignment, because mass determination must be based on the measurement of single ion species.

### Accurate Mass for Complete Structural Elucidation

Knowledge of the accurate mass of an ion allows (i) the unequivocal determination of the elemental composition, or (ii) determination of a very limited set of potential candidates. The analytical power of this feature becomes even more significant when the target ions are composed of known sets of atoms, such as amino acids, DNA/RNA, or carbohydrates. The accurate mass capability alone speeds up the analysis in pharmaceutical research, drug discovery, and metabolic studies enabling the user to get the right answers in record time.

### The Power of MS<sup>n</sup>

The Finnigan LTQ FT continues the MS<sup>n</sup> tradition established by the Finnigan LCQ™. It can be used to systematically unlock the structural secrets of complex molecules and can be harnessed in dedicated scan modes to selectively identify useful classes of compounds, such as post translational modifications of proteins.

### Fourier Transform Ion Cyclotron Resonance Mass Spectrometry, or FTICR-MS

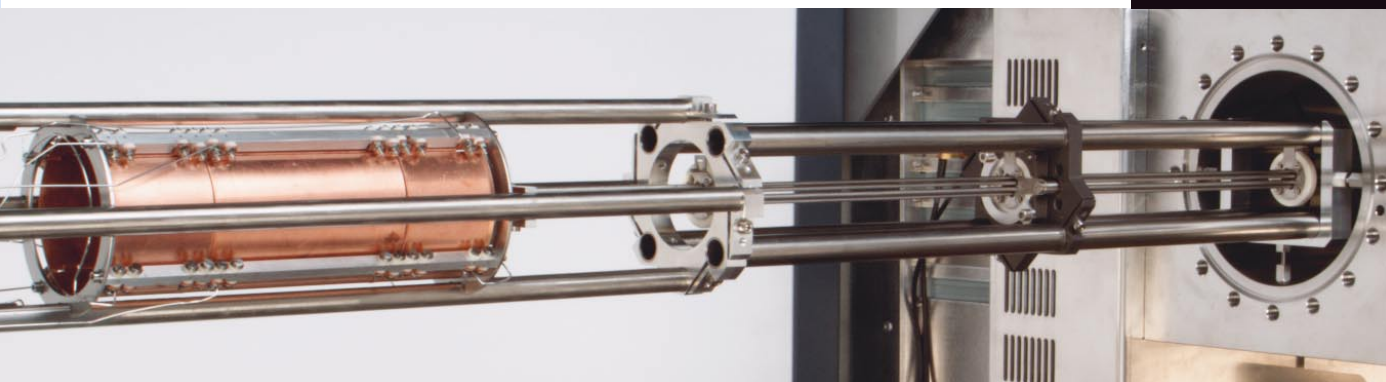
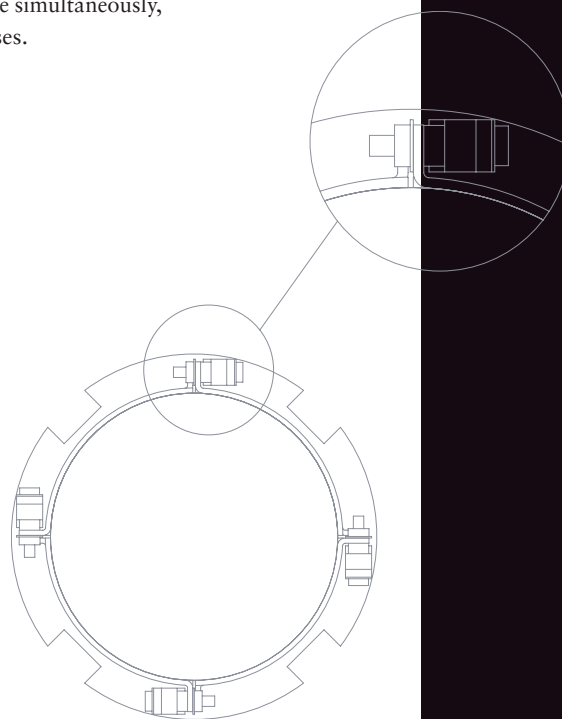
FTICR-MS is fundamentally different from other MS techniques. The heart of the system is a cylindrical cell, capable of trapping and storing gas phase ions in a very high magnetic field.

Upon excitation, trapped ions incur a radial motion away from the central axis of the cell and adopt a circular path. This excitation process is achieved by applying an RF voltage within the cell. The resulting frequency of the ion cyclotron motion is dependent on the ion's mass to charge ratio and the magnetic field strength.

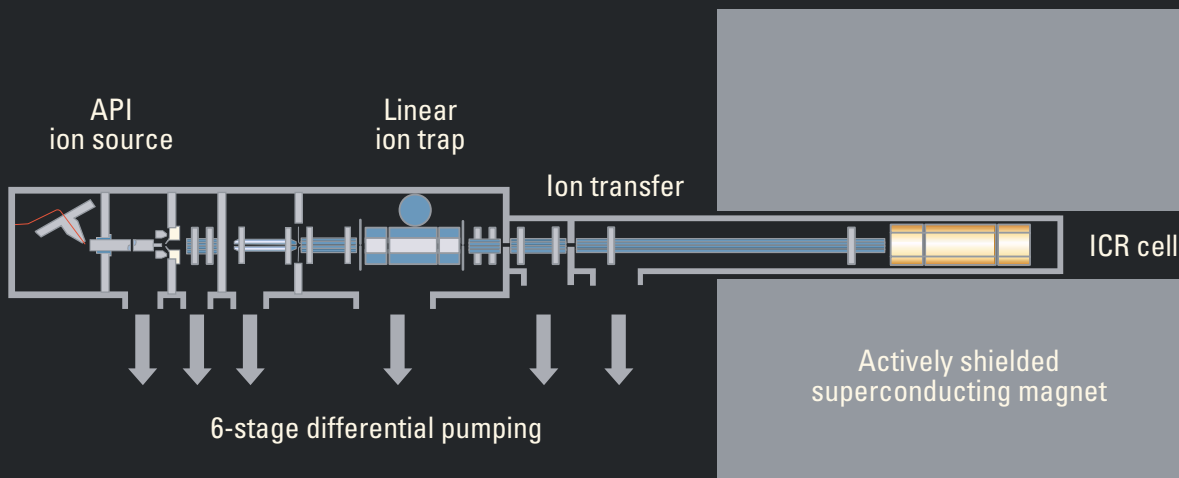
An image current of all the ions circulating in the cell is recorded. The different frequencies are extracted from the signal by Fourier Transformation and the resulting frequency spectrum is readily converted into a mass spectrum using the relationship between frequency and mass.

### What Does This Mean?

Ion detection using image current is non-destructive, meaning the ions can be stored and analyzed for an increased amount of time. Frequency is the most accurately measurable physical characteristic known, with the accuracy and precision of the measurement increasing with the duration of the acquired signal. This is the basis for the very high mass resolution capability of an FTICR-MS system. High mass resolution does not compromise sensitivity and this performance is achieved throughout the acquired mass range simultaneously, not just for a few masses.



Ion guides with ICR cell shown.



## The LTQ FT consists of three major components:

- a new generation linear ion trap mass spectrometer
- a high transmission ion guidance system
- an FTICR analyzer based on a 7 Tesla superconducting magnet



**For the first time in the history of mass spectrometry, the LTQ FT combines the ruggedness, versatility, and MS<sup>n</sup> capabilities of the most advanced ion trap mass spectrometer with the accurate mass measurement capability of a Fourier Transform Ion Cyclotron Resonance analyzer. This has been achieved without compromising the analytical capabilities of either the ion trap or the FTICR-MS.**

#### Multiple Ionization Modes

The LTQ FT can utilize a variety of ionization techniques: ESI, APCI, APPI or MALDI. Maintenance of the API source, as well as switching between AP ionization methods, is vent-free. Ions are transferred by octapole and “square” quadrupole lenses into a novel ion trap. The linear ion trap is a fully operational mass spectrometer which can store, isolate, and fragment ions and then send them either to the ICR cell via axial ion ejection for further analysis or to an off-axis SEM detector. The linear ion trap is a unique ion preparation and injection system for FTICR-MS because it has much greater ion storage capacity than conventional 3D ion trap devices.

#### Optimum FTICR Operation

Ions from the ion trap are transferred as discrete bundles into the ICR cell, via octapole ion guides. These octapole ion guides are designed to enable very efficient differential pumping between the ion trap and the ICR cell.

#### The FTICR Analyzer

The FTICR analyzer is built around an actively shielded superconducting magnet with a field strength of 7 Tesla. The ICR cell is located in the region of greatest magnetic field strength and homogeneity. Ions are trapped in the cell and excited by applying a SWIFT (Stored Waveform Inverse Fourier Transform) waveform. Ions are detected by their image currents induced at the detection electrodes. Image currents are amplified by a high sensitivity pre-amplifier with outstanding signal-to-noise characteristics.

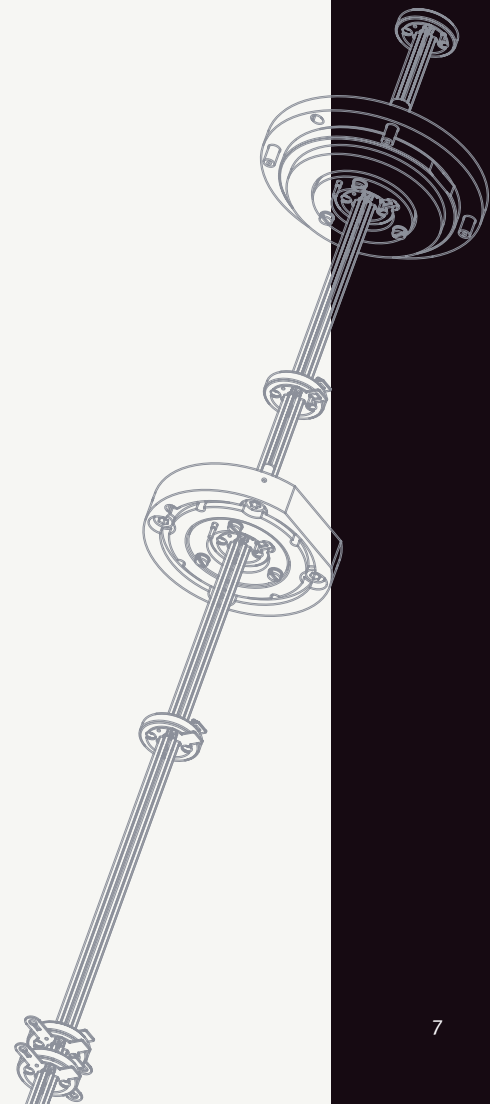
#### Rapid Data Acquisition and Processing

The amplified signal is digitized by a high-speed A/D converter and passed to a novel preprocessing system that performs the fast Fourier transformation, peak detection, and peak centroiding at unprecedented speed. This technology is capable of giving an FTICR-MS acquisition duty cycle in excess of 80%, at a scan repetition rate of 1 s. Pre-processed data are stored as centroids, peak profiles with centroids or full profiles with centroids, as selected by the user.

#### Routine Operations

The Finnigan LTQ FT is controlled by a PC, running an expanded version of the proven Xcalibur® software suite. Instrument control and operation are intuitive due to easy tuning and experiment set-up, as well as seamless integration with the Surveyor® LC system. High resolution MS, MS/MS, or MS<sup>n</sup> are fully supported by Advanced Data Dependent™ features, including Dynamic Exclusion.™

Operation of the LTQ FT is built upon the successful legacy of the LCQ Series of quadrupole ion traps. While the instrument is capable of sophisticated experimental operation, the set-up and control software ensure the user can focus on data analysis and interpretation. Using the LTQ FT is as routine as operating an LCQ, but with the additional benefits afforded by high resolution, accurate mass, and higher dynamic range.



### Nanospray Probe

The Finnigan Nanospray Ion Source supports a number of micro and nanoflow operational modes, allowing the user flexibility to select the type of experiment required for a specific analysis. Nanoflow operates in both static and dynamic flow mode.

### Dynamic/Flow Probe

The dynamic/flow nanospray probe allows connectivity to micro and nano LC columns. The flowing nanospray source allows flexibility in tip type, tip length, and diameter, and allows the installation of emitters packed with HPLC column material providing an integral separation and spray device which negates any junction issues encountered when using a discrete column and fused silica emitter.

### Static Nanospray Probe

The static nanospray probe allows analysis of low volume solutions over extended periods of time. This mode of operation allows a thorough investigation of a sample in MS and MS<sup>n</sup> modes, and allows for low-level signals to be averaged, revealing minor spectral components.

### MALDI Ionization

The MALDI ion source combines features to allow for rapid, sensitive, automated analysis of proteins and peptides. Samples, loaded on a 96- or 384- position target plate, are illuminated with a 100 Hz, 337 nm UV

laser. Intelligent data acquisition software automatically creates an optimal sampling pattern. Enhanced source technology reduces detrimental ion fragmentation and clustering. The resulting batch MS/MS spectra are automatically processed with BioWorks™ software for highly confident protein identifications and are presented graphically for easy data review. This source can be integrated with an optional robotic target plate loader for high-throughput analysis.

### APCI/APPI Ionization

The combination APCI/APPI ion source is the result of a collaboration between Thermo Electron and Syagen Technology. Building on the Finnigan APCI probe, the addition of the Syagen PhotoMate™ light source enables analysis of a wider range of compounds. The PhotoMate ion source uses a Krypton lamp which emits photons at 10.0 and 10.6 eV. Krypton was carefully selected because these photon energies, while being sufficient to ionize most analytes, are lower in energy than the ionization potentials of common reverse phase LC-MS solvents such as water, methanol, and acetonitrile. The low energy photons result in spectra with virtually no chemical noise and also ensure minimal fragmentation of the analyte allowing the protonated species or the radical cation to be identified.

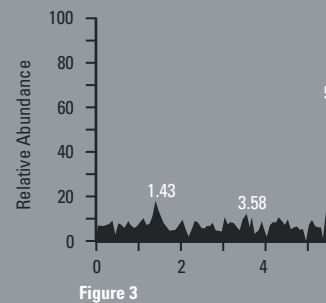


Figure 3

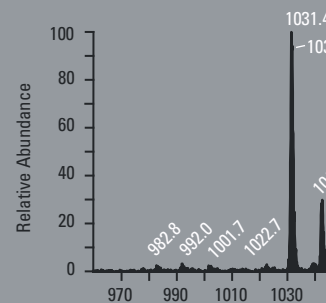


Figure 3a: LT-MS

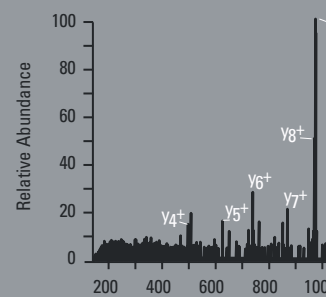
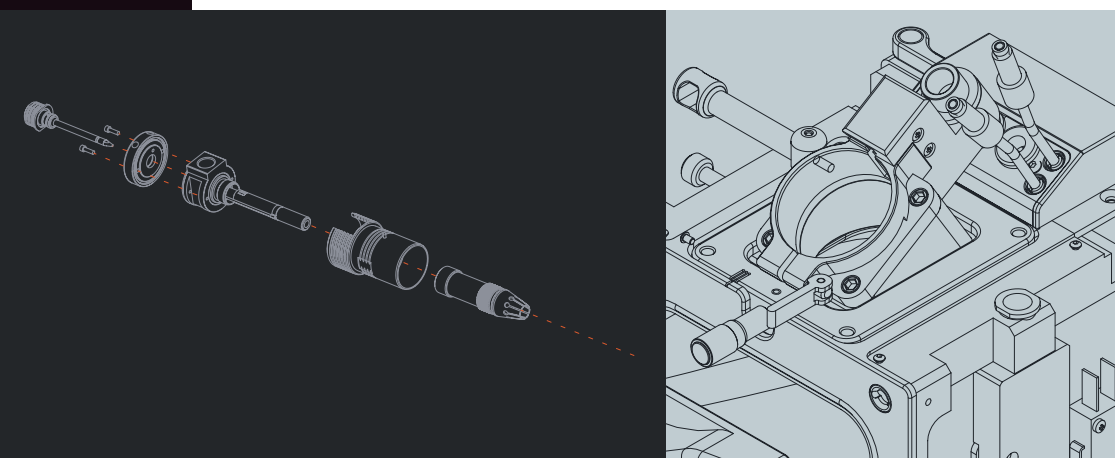


Figure 3c: FT-MSMS of m/z 1031.4





**Application-specific software is available to meet your analytical needs.**

**Solving complex analytical problems requires the extraction of key information hidden in the acquired data, comparisons, interpretation, library searches, intelligent application of mass spectrometry knowledge bases – and more. The powerful software solution package offered with the LTQ FT is your road map to results. Xcalibur, BioWorks, DeNovoX™, Mass Frontier and Metabolite ID take full advantage of the Finnigan LTQ FT's ability to acquire outstanding raw data.**

**Proteomics research is supported using new and unique database searching software, designed to exploit high mass accuracy as a key identifier.**

#### **Xcalibur Data System**

Xcalibur is the most powerful and flexible MS data handling system available on Microsoft® Windows®. The software provides fully-automated control of the LTQ FT, the Surveyor LC, and related LC devices. This comprehensive instrument control, simplified tune procedure and calibration method accelerate methods development. Xcalibur's homepage start-up screen offers easy navigation through the process of Instrument Setup, Sequence Setup, and Data Acquisition. All complementary and confirmatory data are acquired and displayed in a single file. Automated Data Dependent experiments can be routinely performed in which the instrument

acquires MS spectra in a chromatographic run and automatically switches to MS/MS mode only when a user-defined threshold has been exceeded. Thus, the maximum amount of information is generated in a single experiment. Review of results is simple with three interactive, application-specific browsers: Qual, Quan, and Library Browsers. Additional application-specific software packages provide advanced processing functions for quantitative assays, data mining complex mixtures, and proteomic analysis.

**BioWorks and DeNovoX:  
Protein/Peptide Sequencing**

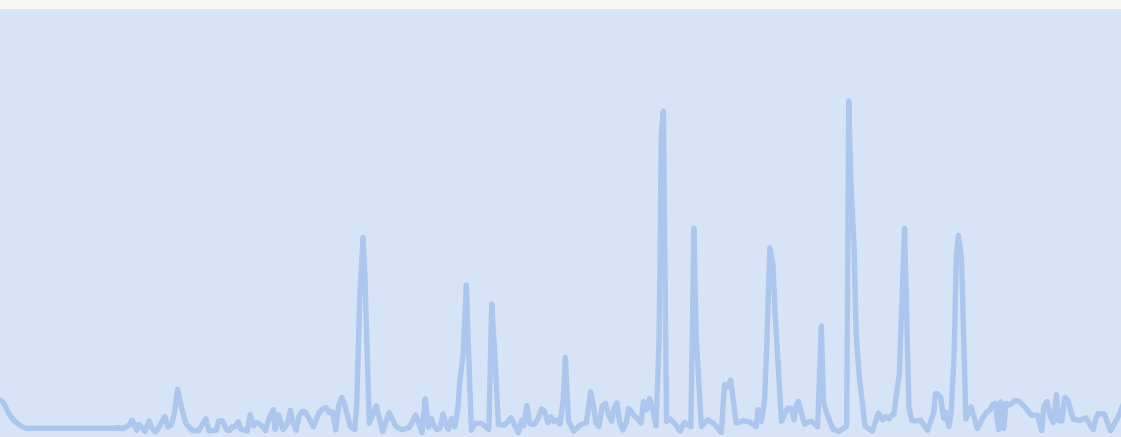
TurboSEQUENT™, part of the BioWorks software suite, uses the abundant information generated from experiments to identify proteins by correlating MS/MS spectra with predicted spectra in protein, DNA, or RNA databases. Combined with automated, intelligent data acquisition tools, such as Data Dependent scanning and Dynamic Exclusion, it is possible to identify low-abundance proteins in complex mixtures. DeNovoX is a fully-automated *de novo* sequencing software program that is capable of determining complete or partial amino acid sequences of unknown peptides by interpreting full-scan MS/MS spectra. The program has been optimized for data collected with Finnigan instruments, and is ideally suited for high-throughput analyses of peptide mixtures.

**Mass Frontier: Mass  
Spectral Interpretation  
and Management**

Mass Frontier virtually eliminates the often-tedious process of manually interpreting mass spectra for small molecule analysis. Its Fragments and Mechanisms module quickly generates “bar code” mass spectra from structures and compares theoretical fragments to actual data. The unique Spectra Classifier and Spectra Projector modules use Principle Component Analysis and Neural Networks to compare large groups of compounds to identify physical, chemical, or biological similarities. Mass spectral databases can be installed or created and subsequently searched – based on a variety of search criteria including mass spectra, molecular weight, molecular formula, and compound substructure.

**Metabolite ID: Metabolite  
Structural Identification**

Metabolite ID streamlines the review of drug metabolism LC/MS/MS samples – it rapidly increases your compound searches with an intuitive, easy-to-use interface suitable for both novice and experienced analysts. Metabolite ID simplifies the process of generating reconstructed ion chromatograms, mass spectra, and summary reports from hundreds of MS/MS scans isolated in a typical metabolic run. It includes the ability to search for both expected and unexpected metabolites, can be used in conjunction with Mass Frontier to aid first in the identification of a potential metabolite structure, as well as for a specific site or region of modification. Metabolite ID works interactively with Xcalibur to allow you to batch reprocess samples using methods created in Metabolite ID in conjunction with the power and flexibility of the Xcalibur Data System.



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AUSTRALIA  
Tel. (61) 2 9898 9000

AUSTRIA  
Tel. (43) 1 333 50340

BELGIUM  
Tel. (02) 4823030

CANADA  
Tel. (905) 712 2258  
Canada only  
Tel. (800) 721 4260

CENTRAL AND  
SOUTH AMERICA  
Tel. (01) 512 251 1530

FRANCE  
Tel. (33) 1 69 18 88 10

GERMANY  
Tel. (49) 6103 4080

ITALY  
Tel. (39) 02 950 591

JAPAN  
Tel. (81) 3 3372 3001

THE NETHERLANDS  
Tel. (31) 76 5878 722

PEOPLE'S REPUBLIC  
OF CHINA  
Tel. (86) 10 6621 0839

SPAIN  
Tel. (34) 91 657 4930

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SWITZERLAND  
Tel. (41) 61487 8400

UNITED KINGDOM  
Tel. (44) 1 442 233555

UNITED STATES  
Tel. (01) 800 532 4752