MASS SPECTROMETRY

Thermo Scientific LCQ Fleet Ion Trap LC/MS^n

Exceptional Analytical Value

Part of Thermo Fisher Scientific

Thermo SCIENTIFIC

Rapid and Reliable Detection for Every Lab

Maximize LC/MS productivity with the LCQ Fleet system

In today's fast-paced analytical laboratory, your instrument must be easy to use and deliver maximum information with minimum time and sample consumption. With these requirements in mind, we developed the Thermo Scientific LCQ Fleet ion trap mass spectrometer.

The LCQ Fleet™ system leverages the proven reputation of the award-winning LCQ™ ion trap family for excellent MS^n sensitivity, ruggedness and reliability. This cost effective ion trap mass spectrometer delivers high quality structural information for routine analysis of complex samples, on a high-throughput basis.

Continuing to set standards for rapid and reliable detection, the LCQ Fleet system is designed to meet the needs of a variety of applications, including general analytical chemistry, drug metabolism, natural product analysis and food safety. This easy-to-use ion trap LC/MS system offers exceptional analytical value while providing confident sample analysis.

With the Thermo Scientific Accela High Speed LC System, the LCQ Fleet is the perfect tool for high-throughout applications.

Confident Structural Elucidation – the power of MS^n

Your mass spectrometer provides confirmation of molecular weight – a powerful complement to any LC laboratory. But, for structural elucidation, it is essential to include the capability for sequential fragmentation by MS^n – a powerful tool available on the LCQ Fleet system. This and other automated features enable all users, from novice to expert, to easily analyze and interpret sample data.

- **Fast Positive/Negative Polarity Switching for higher throughput**
- **Normalized Collision Energy eliminates the need for tuning**
- **Data Dependent Acquisition automated analysis of unknowns**
- **Dynamic Exclusion detect low intensity ions**

Intelligent Analysis

Automated LC-MS/MS system control and data acquisition for complex sample analysis is simplified with intuitive Thermo Scientific Xcalibur software. Application-specific Thermo Scientific software aids data processing and compound identification.

- **Mass Frontier™ software for spectral interpretation and classification for the identification of unknowns**
- **MetWorks™ software automated metabolite identification using spectral trees**
- **E-Quan™ kit solution for online SPE and preconcentration of environmental samples**
- **LCQUAN™ software for acquisition and analysis package for quantitation data**

Technology You Can Trust

From the inventors of benchtop LC/MS ion trap technology, the LCQ Fleet system provides exceptional analytical value within the industry-leading portfolio of Thermo Scientific ion trap mass spectrometers.

High-Throughput Discovery Metabolite Identification

Metabolite structure elucidation and relative quantitation on a uHPLC timescale

Identification and quantitation of *in vitro* and *in vivo* metabolic products are routine analytical procedures in the pharmaceutical industry. Therefore, knowledge of toxic metabolites early in the drug discovery process can avoid costly development of non-viable lead candidates. High-throughput pharmacokinetic screening of drug candidates in early phase discovery is becoming standard. The LCQ Fleet system with fast polarity switching and high quality MS^n spectral data is an ideal tool for discovery phase metabolite identification and relative quantitation.

Results from LC-MS^n studies of in vitro metabolism of 5 uM Loperamide are shown in Figure 1. The API and 5 metabolites are chromatographically separated **in 3 minutes** and their MS^2 and MS^3 spectra were acquired. Figure 1 also shows the Expected Modification view from MetWorks software. Note: the Control Panel view is empty as there is no corresponding component in the control.

Mass Frontier software automatically deconvolutes the spectral tree and annotates the MS^n spectra which unambiguously identify all six species. This demonstrates the exceptional speed of the LCQ Fleet in uHPLC analyses. The MetReport from Metworks metabolite identification software summarizes the low intensity, coeluting component identified (Figure 2) and the proposed biotransformation pathways of Loperamide are elucidated (Figure 3).

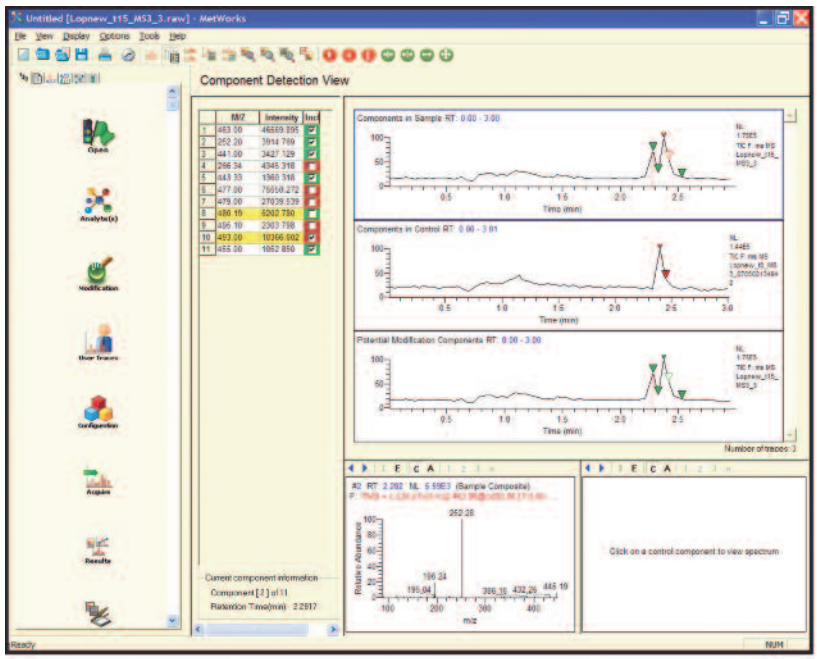


Figure 1. Loperamide Metabolism Data and Analysis Using MetWorks Component Detection

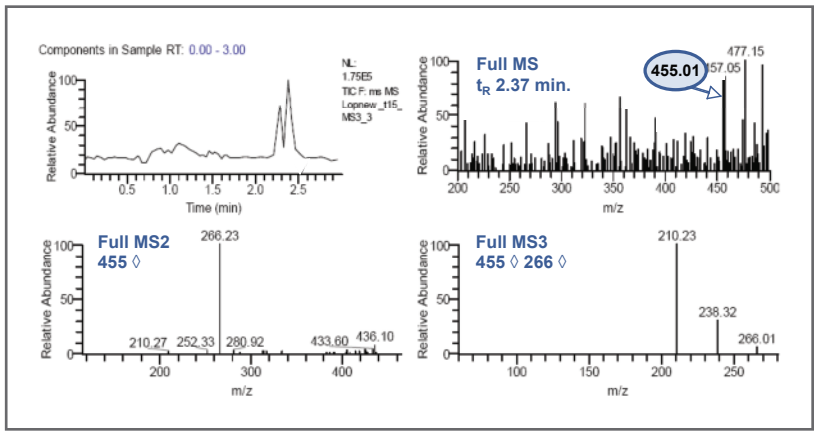


Figure 2. Loperamide Metabolism Data Analysis Using MetWorks MetReport

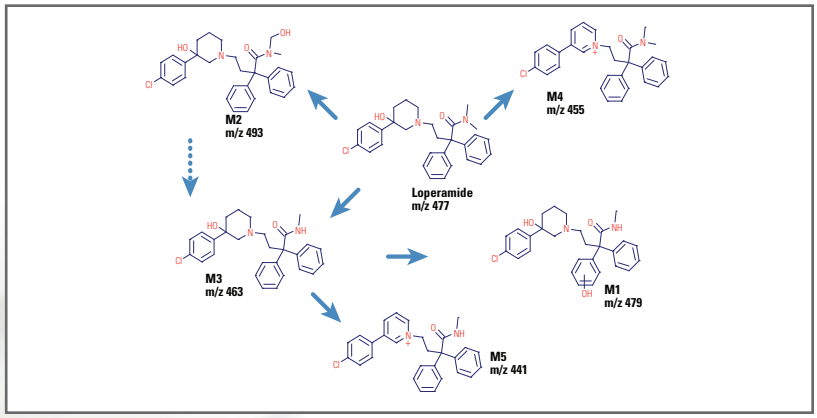


Figure 3. Proposed Biotransformation Pathways of Loperamide in Human Liver Microsomes

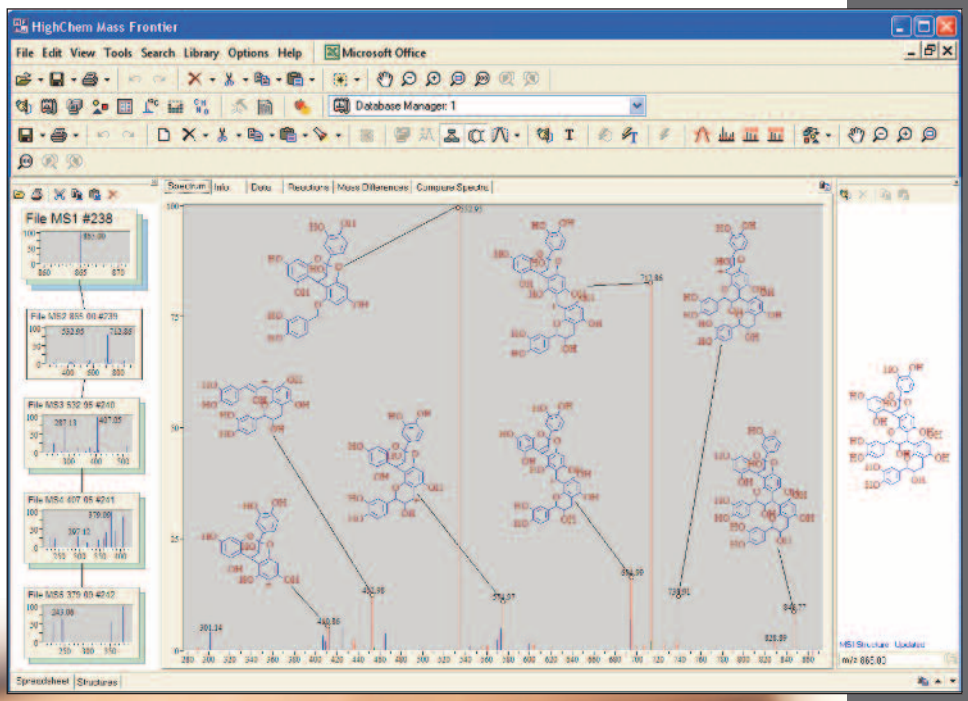
Identification of Natural Products

Robust and fast analysis provides confident structural information

Traditional approaches for the analysis of natural products have proven to be time and labor consuming. The LCQ Fleet system significantly reduces the need for a lengthy pre-purification process while delivering high quality results. It is especially suited for the routine identification of complex natural products. The benefits include:

- Reduction or elimination of time-consuming pre-purification steps with the ability to quickly analyze complex samples
- The fast cycle time of the LCQ Fleet system matches the fast LC separation of the Accela High Speed LC, enabling rapid analysis of numerous samples
- Excellent MS^n spectra quality ensures the confident structural characterization and compound identification
- The Thermo Scientific Ion Max source delivers outstanding robustness for the most demanding analytical applications
- Multiple ionization methods, including ESI, APCI, APPI provide maximum flexibility to achieve comprehensive sample information
- Data can be directly analyzed by Mass Frontier software for compound identification and data reporting

In this below example, an extract of cinnamon was studied using a fast chromatography LC-MS^n analysis. Multiple MS^n spectra (up to MS^5) were acquired in both positive and negative ionization modes to provide comprehensive structural information of the component of interest. The fragmentation spectra were analyzed using Mass Frontier software, and the corresponding substructures to all the major peaks were assigned automatically as illustrated.



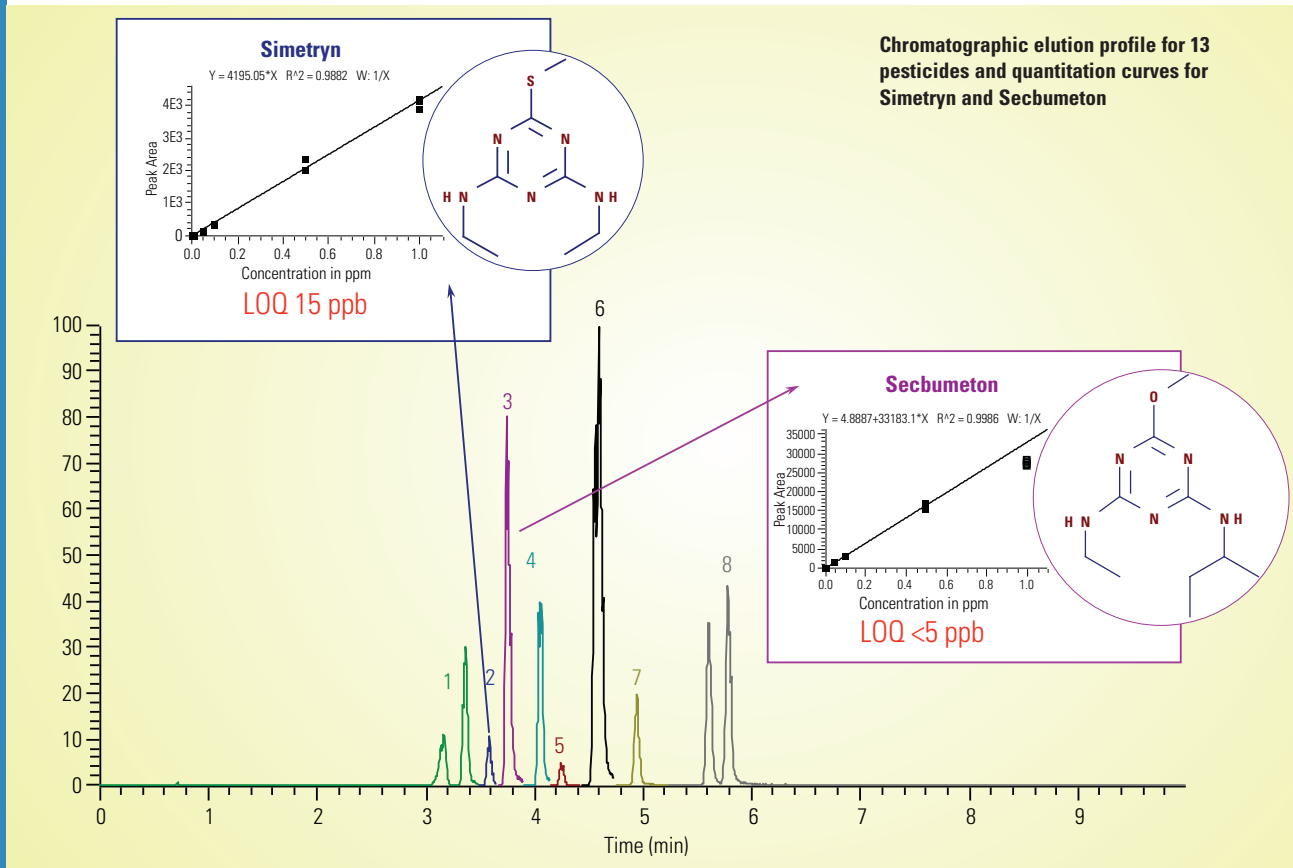
The Solution for Pesticide Screening

Rapid and reliable compound detection, structural confirmation and quantitation

Multi component detection is the standard in pesticide analyses. The ability to detect for numerous targets is essential for any screening technology. The LCQ Fleet system with fast scan speed and polarity switching allows multiple components to be screened, and quantified, simultaneously – requiring no previous knowledge of retention times or product ion masses.

However, if retention time information is available, many more targets can be screened and quantified as shown below. In this example, 13 pesticides are quantified in 8 segments in a 3 minute elution window. High quality MS/MS spectral information and fast polarity switching time make multi-component pesticide detection routinely possible on the LCQ Fleet system.

- Fast (100 ms) positive/negative switching allows the analysis of more compounds with less sample in less time
- High sensitivity and specificity for more accurate results at a lower detection level compared to traditional methods
- Standard normalized collisional energy generates reproducible spectra for library searching
- Proven reliability and ease of use for LC-MS^n



Chromatographic elution profile for 13 pesticides and quantitation curves for Simetryn and Secbumeton

The Next Dimension in LC Detection

Photodiode Array

- Retention time

Photodiode arrays are a long standing method of detection for HPLC. The Thermo Scientific Accela PDA detector delivers accurate retention time information and also gives an indication of functional groups in the molecule.

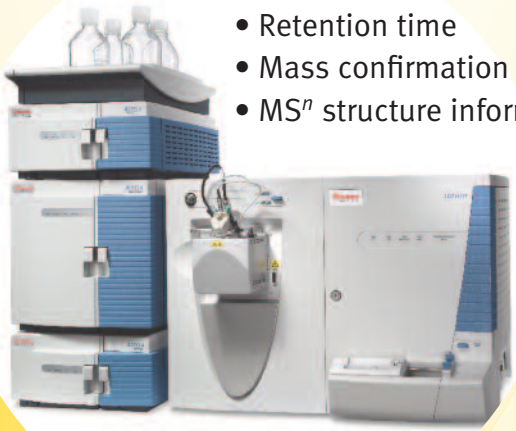
Thermo Scientific MSQ Plus

- Retention time
- Mass confirmation

Further information is made available when a mass spectrometer is used for detection (LC-MS). The MSQ™ Plus mass spectrometric detector provides accurate retention time as well as mass-to-charge ratio (*m/z*) confirming the molecular weight of the target.

Thermo Scientific LCQ Fleet

- Retention time
- Mass confirmation
- MS^n structure information



Structural information about the analyte is provided when tandem mass spectrometry is used for detection (LC-MS/MS). The LCQ™ Fleet system delivers rapid tandem mass spectral data for reliable structure elucidation.

	Accela PDA	MSQ Plus	LCQ Fleet
Retention Time	☑	☑	☑
Mass Confirmation		☑	☑
Structural Information			☑

Laboratory Solutions Backed by Worldwide Service and Support

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