Thermo Scientific HRAM MS/MS
Spectral Libraries and
Compound Databases

Comprehensive compound identification

with maximum speed and confidence

Thermo SCIENTIFIC

Harness the power of HRAM MS/MS

Spectral Libraries and Compound Databases

Harness the power of Thermo Scientific™ high-resolution accurate-mass (HRAM) MS/MS spectral fragmentation libraries and compound databases to identify compounds with speed and confidence. The libraries and compound databases are specifically designed for targeted screening and quantitation as well as unknown analyses of very simple to very complex food, environmental, clinical research and forensic toxicology samples.

The compound databases include predefined retention times, making method development fast and flexible. The libraries include multiple spectra and fragments for every compound entry, providing high confidence compound identifications. Two spectral libraries are available for use with Thermo Scientific™ TraceFinder™ software:

- Thermo Scientific HRAM MS/MS spectral fragmentation library for food safety and environmental compounds
- Thermo Scientific HRAM MS/MS spectral fragmentation library for forensic toxicology compounds*

* Also available for use with Thermo Scientific™ ToxFinder™ software.

Identify a Broad Range of Compounds

With spectra for over 2,600 compounds, the HRAM MS/MS spectral libraries can be used to rapidly screen and identify a variety of known and unknown compounds (Table 1).

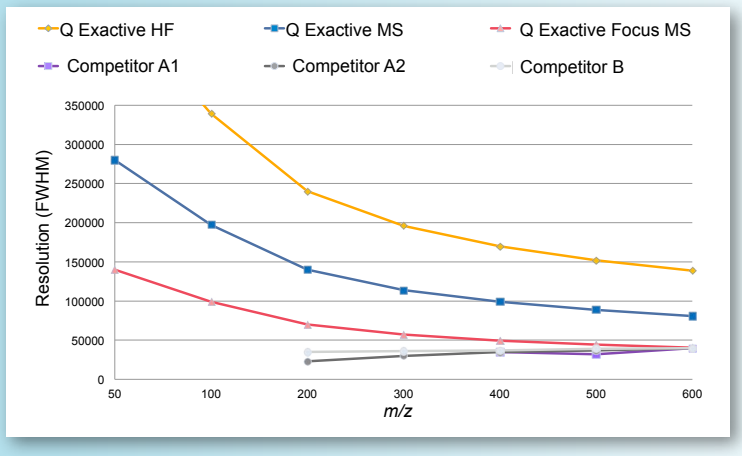
The HRAM MS/MS spectral libraries will continue to grow as Thermo Fisher Scientific adds more compounds and spectra.

Access the most up-to-date spectral library information at www.thermoscientific.com/HRAMlibrary.

COMPOUND CLASS	
Food Safety and Environmental	**Forensic Toxicology**
Emerging Environmental Contaminants	Drugs of Abuse
Pesticides	Natural and Industrial Toxins
Veterinary Drugs	Prescription Drugs
Mycotoxins	Performance Enhancing Drugs
Perfluorinated Compounds (PFCs)	Other Drug Monitoring Research

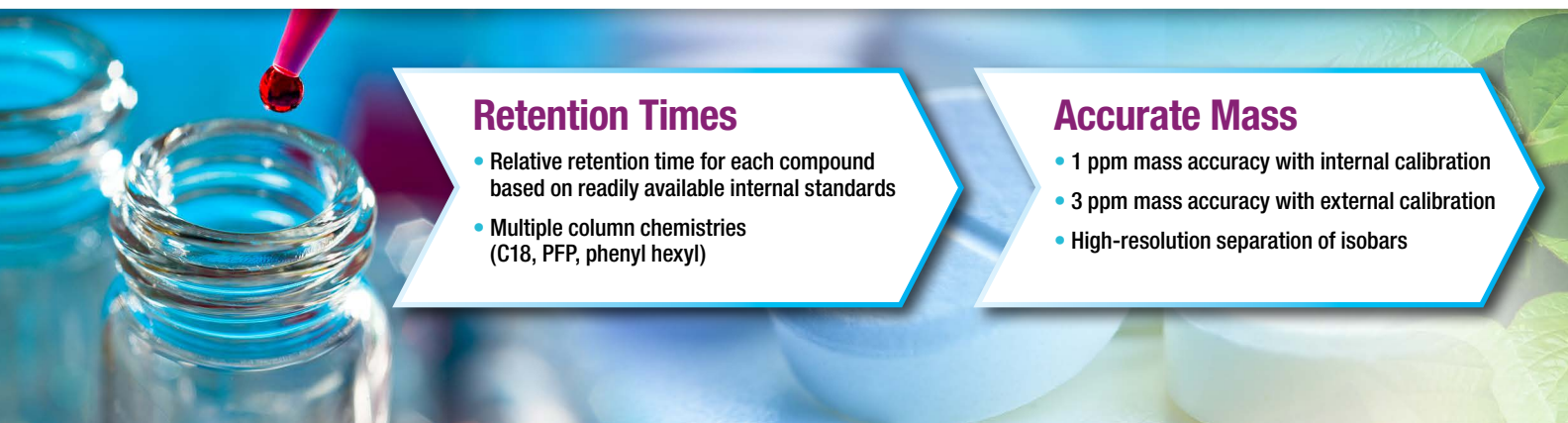
Table 1. Compound classes provided in the HRAM MS/MS spectral libraries.

Identify Compounds with Confidence



HRAM MS/MS library spectra are collected at a remarkable 140,000 (FWHM) at *m/z* 200 resolution using the Thermo Scientific™ Q Exactive™ hybrid quadrupole-Orbitrap™ mass spectrometer. High-resolution spectra minimize false positives, false negatives, and matrix interferences, enhancing your confidence in identification of known and unknown compounds.

Figure 1. The Orbitrap mass analyzer technology provides superior resolution for all MS/MS fragments throughout the mass range over other high-resolution instruments.



Retention Times

- Relative retention time for each compound based on readily available internal standards
- Multiple column chemistries (C18, PFP, phenyl hexyl)

Accurate Mass

- 1 ppm mass accuracy with internal calibration
- 3 ppm mass accuracy with external calibration
- High-resolution separation of isobars

Find More Matches

The HRAM MS/MS spectral libraries and compound databases are comprehensive. Five to six HRAM MS/MS spectra per compound, collected at different collision energies, ensure a hit regardless of the mass spectrometer method used in your laboratory. You can use mzCloud™, a growing online repository of thousands of compounds, to update your library. The most up-to-date spectral library information may be accessed at www.thermoscientific.com/HRAMlibrary.

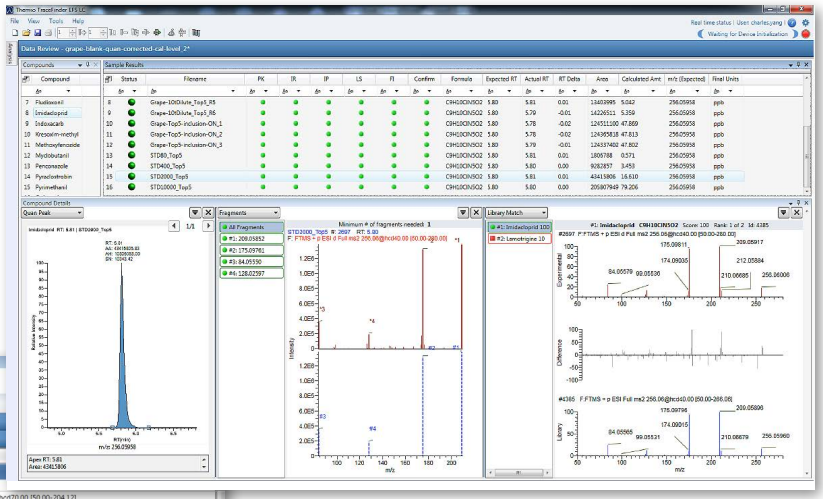


Figure 2. Imidacloprid is quantified and confirmed by HRAM MS/MS spectral library fragment matching.

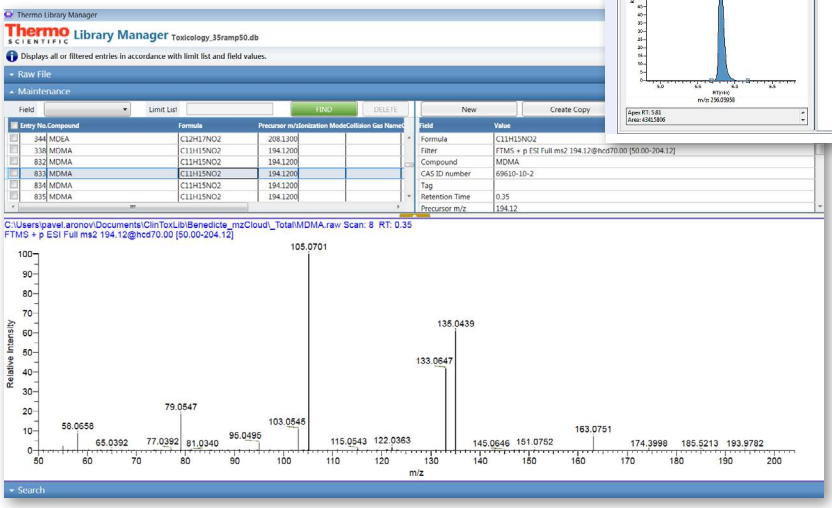


Figure 3. Multiple spectra are provided for the compound MDMA.

Compound Groupings	Unique Entries	Total Spectra
Environmental and Food Safety	1,634	8,906
Clinical Research and Forensic Toxicology	926	4,630

Table 2. Unique entries and total spectra in the HRAM MS/MS spectral libraries.

Reduce Method Development, Save Time

The HRAM MS/MS compound database includes retention times (RT's) and relative retention times (RRT's) determined using the same internal standards. This reduces method development time and increases confidence in compounds detected when performing screening and quantitation.

The libraries are fully integrated with and searchable using TraceFinder and ToxFinder software platforms. Laboratories not required to build their own libraries will enjoy the time savings provided by an "off-the-shelf" database of many spectra. To meet specific laboratory requirements, the libraries may be customized by adding new compounds and spectra.

Isotopic Pattern

- High-resolution results in baseline separation of ^{13}C, ^{15}N, ^{18}O and ^{34}S isotopes

MS/MS

- Multiple spectra at different collision energies for each compound
- HRAM fragmentation acquired at better than 5 ppm mass accuracy

Maximize your productivity

Stay informed!
Scan this QR code to view updates to the HRAM Library.

HRAM MS/MS Spectral Libraries and Compound Databases

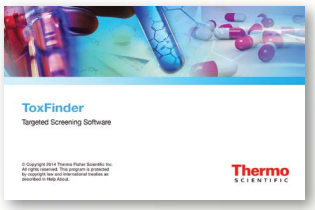
Access the most up-to-date spectral library information at www.thermoscientific.com/HRAMlibrary or scan the QR code to the left to instantly view updates made to the HRAM MS/MS Spectral Library.

Q Exactive Hybrid Quadrupole-Orbitrap Mass Spectrometer

The Q Exactive mass spectrometer combines quadruple precursor ion selection with high-resolution, accurate-mass (HRAM) Orbitrap detection to deliver exceptional performance and versatility. It is useful for untargeted or targeted screening and a broad range of qualitative and quantitative applications in environmental and food safety testing, clinical research and forensic toxicology, drug discovery, and proteomics.

TraceFinder Software

TraceFinder software is an easy-to-use, workflow-driven software for laboratories performing quantitation and targeted screening using GC-MS and LC-MS. TraceFinder software increases productivity with powerful method development, simplified data acquisition, comprehensive data review, and extensive reporting features including custom report options.



ToxFinder Software

ToxFinder software is a streamlined, intuitive software that supports experiment-specific workflows for screening and routine semi-quantitation. ToxFinder software expedites method development with easy to set up databases, experiment-based method templates, and advanced algorithms for finding, confirming and quantitating compounds of interest.

m/z™ CLOUD

mzCloud Library

The mzCloud library is an advanced mass spectral database that assists analysts in identifying compounds even when they are not present in the library. The database features a freely searchable collection of high-resolution, accurate-mass spectra using a third generation spectra correlation algorithm. mzCloud is the result of a consortium of dedicated research and scientific groups aiming to establish a comprehensive library of high-quality spectral trees. Their objective is to improve the structural elucidation of unknowns in fields such as metabolomics, forensic toxicology and environmental sciences.

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