Thermo Scientific
Pesticide Explorer Collection

Start-to-finish

workflows for pesticide analysis

Thermo
SCIENTIFIC

Comprehensive Pesticide Analysis Solutions

Pesticide Explorer Collection

Selection table	Triple Quadrupole Solutions		Orbitrap Solutions	
	1–Standard Quan	2–Premium Quan	3–HRAM Quan	4–HRAM Quan/Qual
Lab Profile				
Routine - Standard Quantitation	●			
Routine - High Sensitivity Quantitation		●		
Routine - Targeted HRAM Quantitation			●	
Routine Plus - Targeted and Non-targeted Screening and Quantitation				●
Workflow and Components	**Targeted**	**Targeted**	**Targeted**	**Targeted + Non-targeted**
Thermo Scientific™ QuEChERS kit	●	●	●	●
Pre-set Methods (LC-MS)	●	●	●	●
Thermo Scientific™ Accucore™ aQ C18 LC columns (100 x 2.1 mm, 2.6µm)	●	●	●	●
Thermo Scientific™ UltiMate™ 3000 LC system (HPG-3400RS)	●	●	●	●
MS System				
Thermo Scientific™ TSQ Endura MS	●			
Thermo Scientific™ TSQ Quantiva MS		●		
Thermo Scientific™ Q Exactive™ Focus MS			●	●
Software				
Thermo Scientific™ TraceFinder™ software	●	●	●	●
Thermo Scientific™ Compound Discoverer™ software				●
Thermo Scientific™ SIEVE™ software				●
Thermo Scientific™ HRAM MS/MS Spectral Library			●	●
Quick-Start Manual	●	●	●	●
3-day training	●	●	●	●

The Thermo Scientific™ Pesticides Explorer Collection is a comprehensive set of liquid chromatography-mass spectrometry (LC-MS) solutions designed for laboratories performing routine quantitation, targeted and non-targeted screening of pesticide residues in food matrices. Each configuration includes all the workflow components needed—consumables, hardware, software and built-in instrument and data processing methods—pre-configured and tested, from your single trusted supplier, Thermo Fisher Scientific.

Choice of configurations simplify complex pesticide methods

To ensure your immediate success, the Pesticide Explorer Collection is available in four pre-configured, pre-tested solutions.

For laboratories performing routine targeted quantitation, the Pesticide Explorer Collection offers two triple quadrupole mass spectrometer workflow-based configurations for Standard and Premier Quantitation. The Standard Quantitation configuration includes the TSQ Endura triple quadruople mass spectrometer and ensures compliance against regulated levels of detection. For quantitative applications demanding the highest possible sensitivity, the Premier Quantitation configuration features the TSQ Quantiva triple quadruople mass spectrometer to meet or exceed regulatory limits.

For laboratories offering specialized analytical services, there is a choice of two Thermo Scientific™ HRAM Orbitrap configurations for quantitation and screening employing the Thermo Scientific™ Q Exactive™ Focus mass spectrometer. HRAM capability significantly enhances quantitative accuracy even when analyzing complex sample matrices with limited prior clean up as well as the ability to quantify and confirm in one single analysis.

Configurations available in the Pesticide Explorer Collection

- Pesticide Explorer Collection – Standard Quantitation
- Pesticide Explorer Collection – Premier Quantitation
- Pesticide Explorer Collection – Orbitrap HRAM Quantitation
- Pesticide Explorer Collection – Orbitrap HRAM Screening and Quantitation

Robust, Routine Workflows for Triple Quadrupo

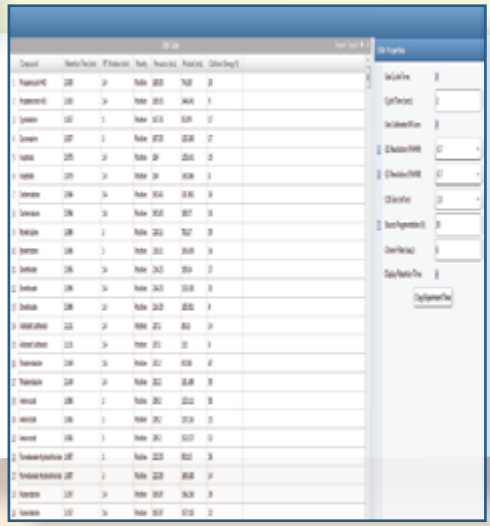
The Standard and Premier Quantitation configurations provide everything needed to perform robust, routine workflows for SRM-based quantitation of pesticides, from the QuEChERS sample extraction kit to proven multi-class pesticide residue analysis methods. Pre-configured methods for each solution are easy to access on the USB drive included with the Pesticide Explorer Collection installation guide.

Select compounds from the compound database to automatically create the instrument and processing method.

Users can quickly and easily set up a new method using the TraceFinder software compound database, or by uploading and modifying pre-configured methods.

UltiMate 3000 LC System with TSQ Endura MS or TSQ Quantiva MS

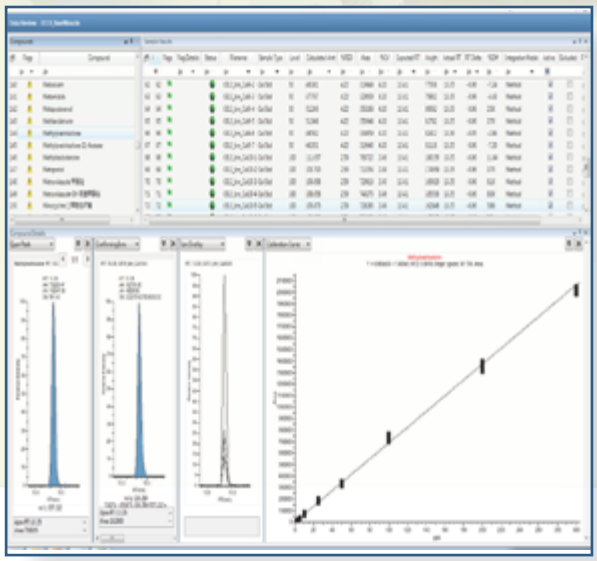
SELECT



Flexibility in the instrument method allows you to create or edit pre-configured methods with SRM transitions and retention times with ease.

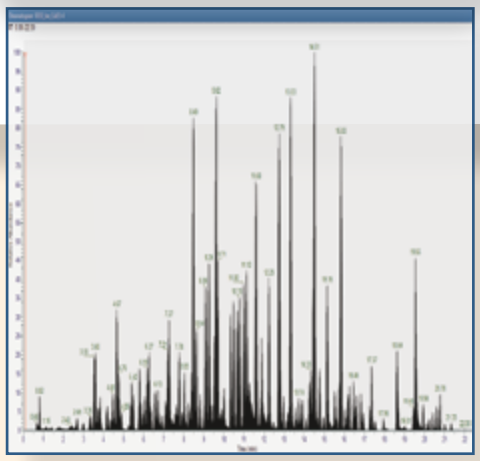
Select a pre-configured TSQ-tested method with column and conditions. Load and go!

le-Based Quantitation



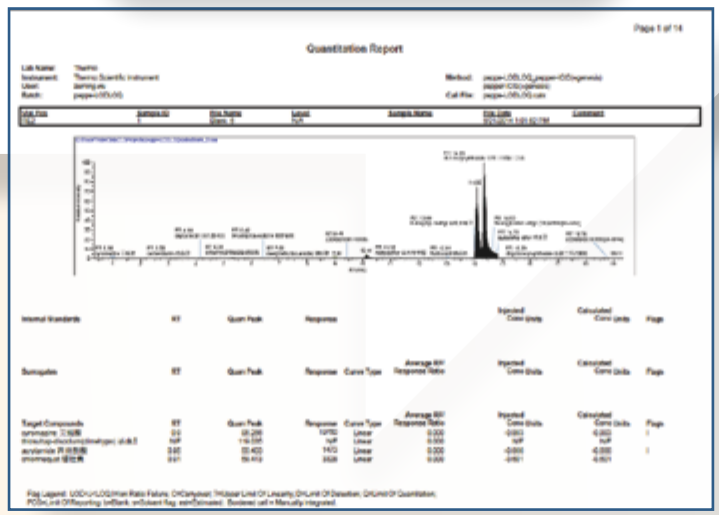
The color flagging features in TraceFinder software enable the analyst to quickly review and confirm results.

LOAD METHOD AND ACQUIRE DATA



Data is acquired under optimal conditions for large multi-component pesticide residue analysis.

REVIEW AND REPORT

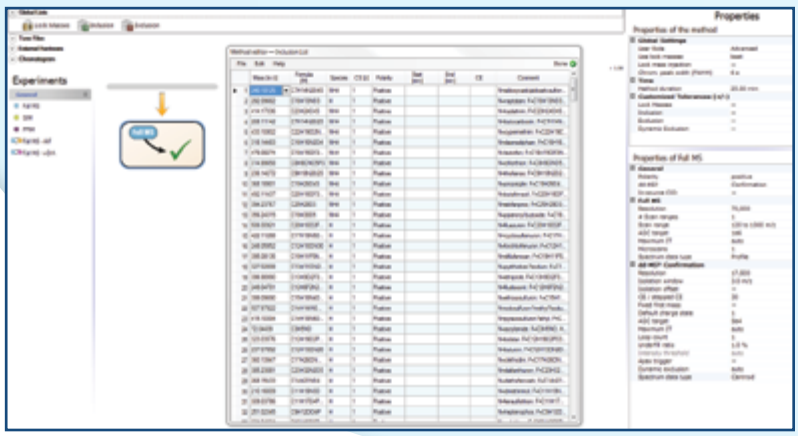


After data review, generate high-quality standard and custom reports to rapidly turn your samples into results.

Routine Workflows for Orbitrap HRAM Targeted

The Orbitrap HRAM Quantitation configuration provides high resolution accurate mass analysis, a unique capability that enables quantitation without compromise in sensitivity, accuracy, precision, or linear dynamic range. High resolving power is particularly useful for the analysis of contaminants in complex matrices and can overcome the masking effects of isobaric inferences, allowing detection of analytes at very low concentrations.

Reduce method development time by using the HRAM spectral fragmentation library and compound database to identify compounds with speed and confidence.

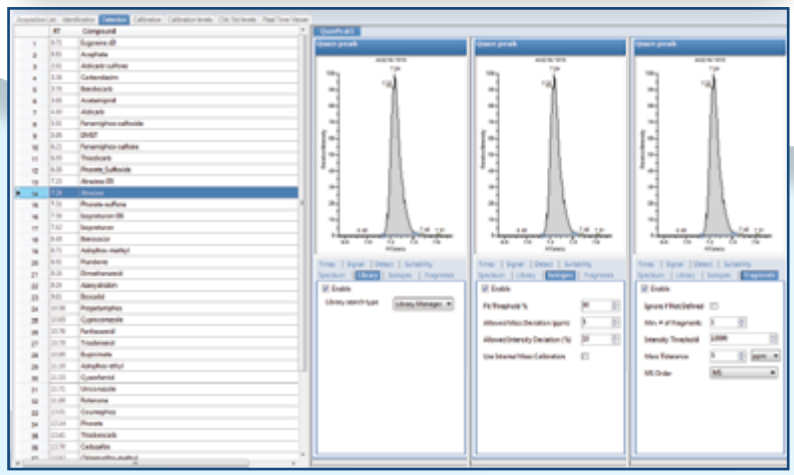


Pre-configured instrument methods for targeted quantitation enable the user to quickly start acquiring data.

SELECT

Q Exactive Focus MS and UltiMate 3000 LC System

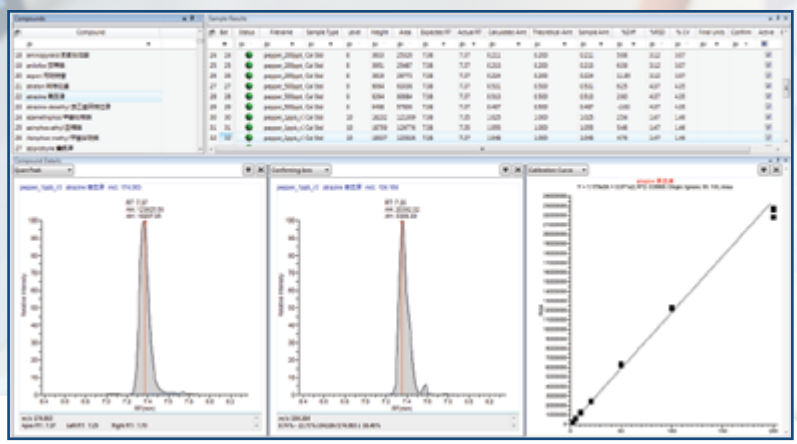
LOAD METHOD AND ACQUIRE DATA



Master Method templates available with the Pesticide Explorer Collection instantly allows users to acquire and process data for quantitation.

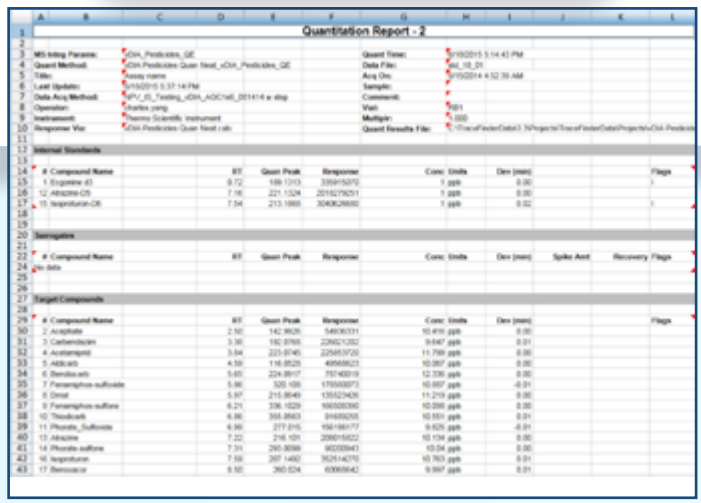
Quantitation

Review results rapidly by flagging method criteria and/or regulatory levels. Choose from a large number of pre-defined and customizable report templates meeting a variety of regulatory requirements. View the result of changes to the data processing method immediately without manual intervention.



In data review, the analyst is able to quickly glance through all compounds and samples in a single view.

REVIEW AND REPORT

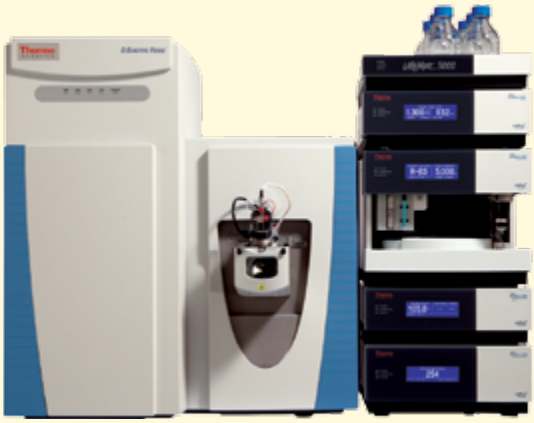


Customizable reports can easily be exported in MS Excel format for possible LIMS integration.

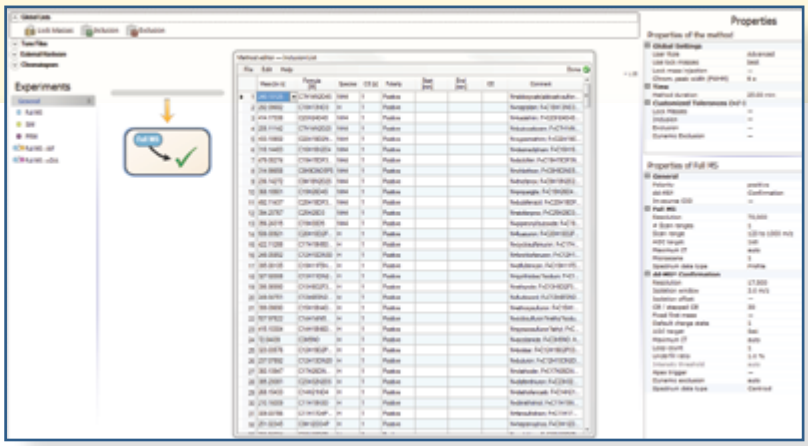
New Analytical Capability Workflows For

The Q Exactive Focus mass spectrometer produces data that can be used for highly sensitive and selective quantitation as well for in-depth screening. Built-in databases designed for food safety and environmental analyses make quantitation, and targeted as well as non-targeted screening from a single data set seamless, with the option to reanalyze data retrospectively at a future date without the need for sample reinjection. Even without using reference standards, TraceFinder software allows the user to perform relative quantitation between multiple samples in their workflow.

Targeted Screening



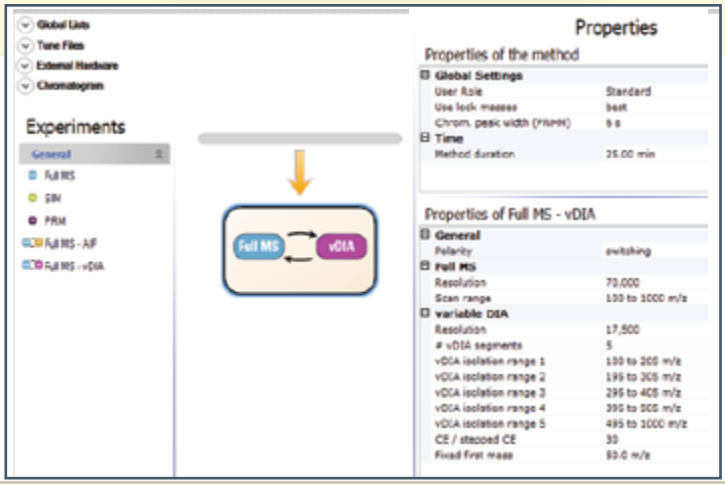
Q Exactive Focus MS and UltiMate 3000 LC System



With full-scan, targeted data-dependant MS/MS, the analyst enjoys greater flexibility to detect large sets of compounds in a single run.

METHOD SELECTION

Non-targeted Screening

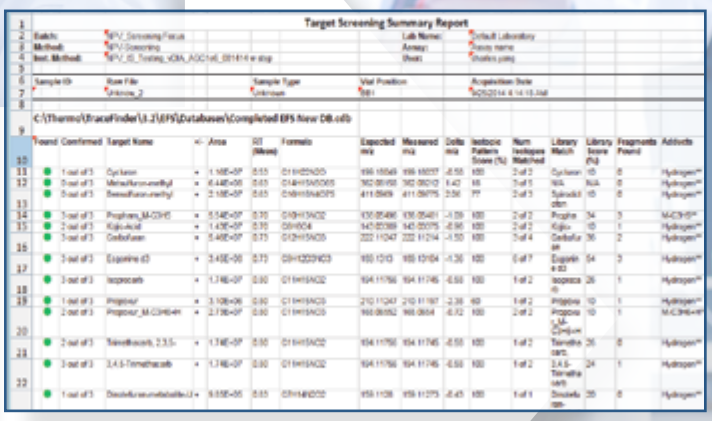


With variable data independent acquisition (vDIA), full-scan MS and MS/MS HRAM analysis, no sample-specific method optimization is necessary, and the risk of missing important non-targeted compounds is greatly reduced.

Orbitrap HRAM Screening and Quantitation

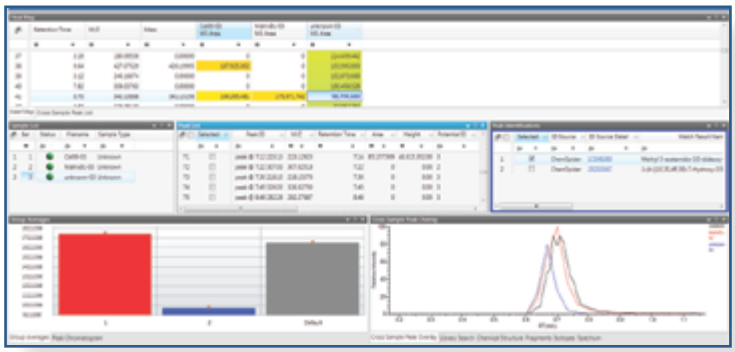
Built-in databases in TraceFinder software allow the user to perform quantitation.

View positive hits during data review; confirmation is easily done using fragmentation, spectra, retention time, and isotope pattern information.



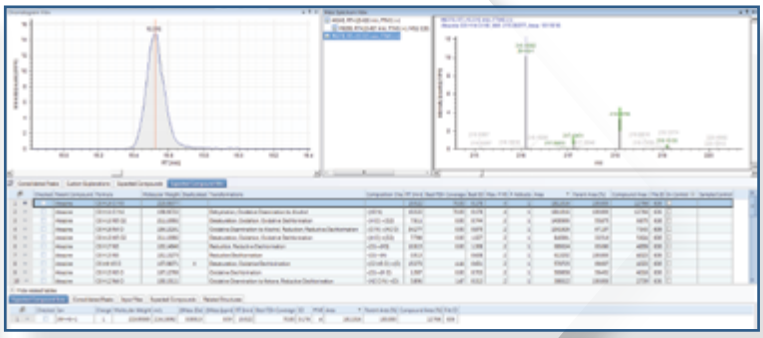
Detailed reports are generated and exported for printing and also customizable for individual customers.

CONFIRM RESULTS



When integrated into the TraceFinder workflow, SIEVE software extracts compound spectra from complex data and performs differential and statistical analysis to determine the compounds that vary significantly within the sample set.

REVIEW AND REPORT



Compound Discoverer software can be used to identify the degradents and metabolites of known target compounds.

Power of HRAM MS/MS Spectral Libraries and Compound Databases

The Thermo Scientific Pesticide Explorer Collection includes the High-Resolution Accurate-Mass MS/MS Spectral Libraries and TraceFinder compound databases. These were designed specifically for targeted screening, quantitation and analysis of non-targeted contaminants in food, environmental, clinical research and forensic toxicology sample matrices. Fully integrated and searchable using TraceFinder software with over 2,600 compounds and more than 15,000 spectra, the HRAM MS/MS Spectral Libraries can be used to screen and identify a variety of known and unknown compounds with speed and confidence. To reduce method development time and increase confidence in compounds detected, the HRAM MS/MS compound database includes retention times that were determined using the same internal standards.

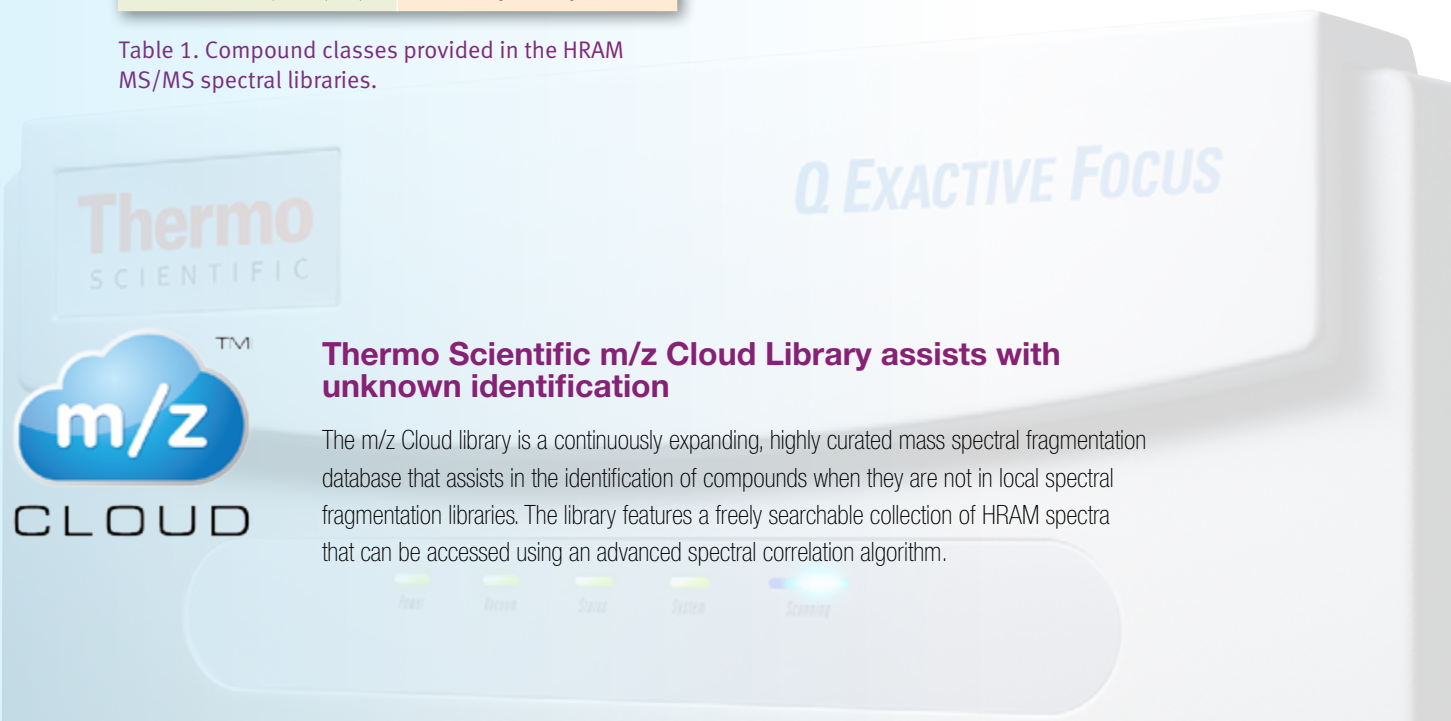
Laboratories using The Pesticide Explorer Collection comprising of either the Orbitrap HRAM Quantitation or Orbitrap HRAM Screening and Quantitation configuration will enjoy the time-savings provided by an "off-the-shelf" database of MS/MS spectra – no need to build your own libraries! To meet specific laboratory requirements, the libraries can be expanded and customized by adding new compounds and spectra.

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.

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.



Thermo Scientific m/z Cloud Library assists with unknown identification

The m/z Cloud library is a continuously expanding, highly curated mass spectral fragmentation database that assists in the identification of compounds when they are not in local spectral fragmentation libraries. The library features a freely searchable collection of HRAM spectra that can be accessed using an advanced spectral correlation algorithm.

Comprehensive, High Productivity Reporting

The heat map reporting templates allow for the quick evaluation of the presence of components and their relative abundance across the sample set.

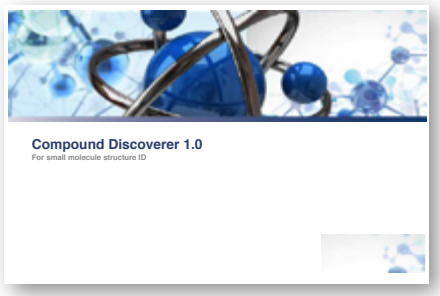
As the identification of pesticide residues becomes increasingly important, so does that ability to review and report results quickly and accurately. In particular, high productivity multi-residue analyses require accurate and robust reporting across multiple regulatory agencies. The TraceFinder software reporting system allows creation and automated generation of quantitative and qualitative reports covering a broad array of pesticide residue analysis methods. The reports can be tailored to meet specific reporting needs.

Powerful Software Empowers Your Pesticide Analyses

TraceFinder software provides an extensive suite of targeted quantitation and screening LC-MS workflows, experiments and reports for environmental and food safety applications as well as protects the integrity of the analytical data.

Further updates on the TraceFinder compound database are offered to registered users at **https://thermo.flexnetoperations.com**

SIEVE software enables label-free, semi-quantitative differential analysis of complex LC-MS data sets. Whether your analytes are large or small molecules or whether you are comparing two or hundreds of samples, SIEVE software confidently and reproducibly identifies components with statistically significant inter-sample differences in abundance.



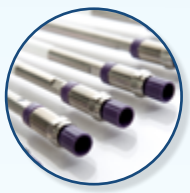
Designed to save time, Compound Discoverer software includes an extensive set of tools to ensure confident compound identification and structural elucidation in pharmaceutical metabolism, impurity analysis, forensic toxicology, and food and environmental applications.

Single Provider Solution Ensures Your Success

The Pesticide Explorer Collection provides start-to-finish workflows tailored to help food monitoring and testing laboratories reduce startup time and cost. The collection provides compelling productivity and efficiency enhancements for both startup laboratories and laboratories adding new analytical capabilities to address evolving customer and industry demands. Regardless of staff or laboratory expertise, the Pesticide Explorer Collection is designed to make it easier for both new and experienced users to obtain reliable, unambiguous, high-quality LC-MS/MS results. At Thermo Fisher Scientific, we'll match you to the right products - through experienced commercial support combined with the most comprehensive line of instruments, equipment, consumables, chemicals, reagents and software available.

QuEChERs products are a convenient and effective approach for determining pesticide residues in fruit, vegetables and other foods. The extraction and clean-up products are easy to use and enable researchers to determine greater numbers of pesticides than with standard SPE.

Perform the full range of HPLC or nano HPLC applications on one system platform using UltiMate 3000 RSLC systems. For added mobile phase flexibility, the included Thermo Scientific™ Dionex™ Ultimate™ HPG-3400RS Rapid Separation Binary Pump is included, provides true ballistic gradients with excellent retention time precision.



Simplify and improve your analytical results with Thermo Scientific™ HPLC columns. Available in particle sizes and column designs to meet all separation needs, they improve resolution, enhance sensitivity, and deliver faster analysis and consistent performance.

Meet today's challenges with us to safeguard the global food supply. Triple quadrupole MS delivers SRM sensitivity and speed to detect targeted compounds more quickly and HRAM solutions using Thermo Scientific™ Orbitrap™ MS enables screening with accurate quantitation of hundreds of contaminants.

Screening, identification, and quantification of food and environmental contaminants are faster and more confident with High-Resolution Accurate-Mass MS/MS Spectral Libraries. The libraries provide high-resolution, accurate-mass (HRAM) MS/MS spectra for identification, confirmation, and quantification of thousands of compounds.

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Africa +43 1 333 50 34 0
Australia +61 3 9757 4300
Austria +43 810 282 206
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China 800 810 5118 (free call domestic) 400 650 5118
Denmark +45 70 23 62 60
Europe-Other +43 1 333 50 34 0
Finland +358 10 3292 200
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9494
Italy +39 02 950 591
Japan +81 45 453 9100
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