

Gas chromatography

# Lead discovery

Delivering broader and deeper insights

Orbitrap Exploris GC 240 mass spectrometer



# Lead discovery with breakthrough performance

Take research capability to a new, unprecedented level of performance with the Thermo Scientific™ Orbitrap Exploris™ GC 240 mass spectrometer and accelerate your scientific discovery. With the unique ability to deliver the very highest-quality, information-rich data, your most complex analytical challenges are simplified.



Performance | Discovery | Versatility

The Thermo Scientific Orbitrap Exploris GC 240 mass spectrometer with the Thermo Scientific™ TriPlus™ RSH SMART autosampler.

- **Ultimate performance and accuracy**

Get the right answer first time and the flexibility to adapt to evolving research demands. The Orbitrap Exploris GC 240 mass spectrometer brings breakthrough 240,000 mass resolving power, MS/MS capability, and leading sensitivity to researchers across all applications. Lead discovery and be confident that you have the very highest data quality and comprehensive quantitative information to advance your research.

- **Power discovery with ease**

Focus on results, not instrument setup. Intuitive instrument control and method templates ensure that exceptional data are accessible to all members of your scientific team. Integrated informatics solutions for quantitation and compound discovery facilitate detailed characterization of your most challenging samples to turn data into scientific understanding. The compact Orbitrap Exploris GC 240 mass spectrometer provides definitive gains in resolution, consistent mass accuracy, and robustness to enhance laboratory capability.

- **Versatility for diverse analytical challenges**

Address diverse analytical challenges today and into the future with ultimate GC-MS performance and flexibility. Expand analytical possibilities with the Thermo Scientific™ ExtractaBrite™ electron ionization/chemical ionization (EI/CI), direct analysis probes, MS/MS capability, and GC modularity. Switching between techniques, ion sources, probes, and columns is fast and easy.

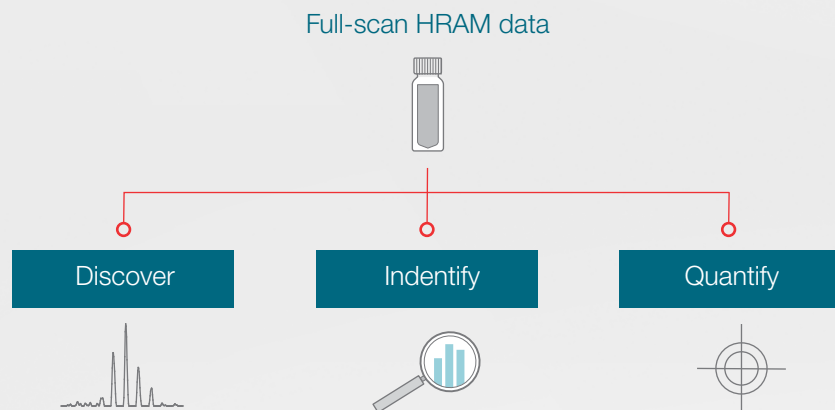


# Accelerate exploration with outstanding data quality

Gain a broader and deeper understanding of every sample you analyze with the unprecedented performance that the Orbitrap Exploris GC 240 mass spectrometer delivers. Discover features in your data that would go unnoticed using other technology and gain the power to make confident identifications with uncompromising sensitivity and mass resolving power.

## Work smarter to discover more

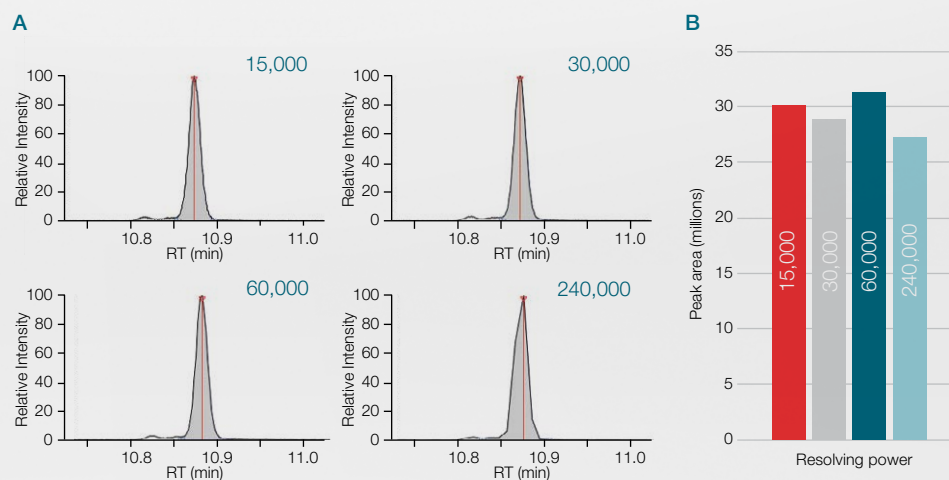
Undetected compounds can have significant implications for your research. The Orbitrap Exploris GC 240 mass spectrometer provides the mass resolving power to cut through the most difficult sample matrices, ensuring you know which compounds are present and at what concentrations. Easily interrogate and re-interrogate full-scan high resolution accurate mass (HRAM) data to answer questions not possible using targeted acquisition. Decide post-acquisition which compounds to analyze and never again be limited to only the ions measured at the time of data acquisition.



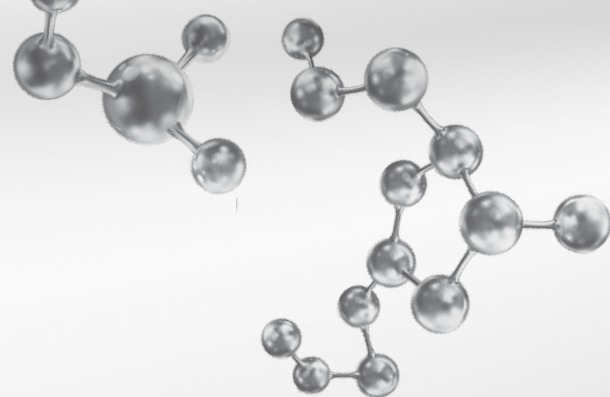
**Research flexibility.** A single full-scan accurate mass data file answers multiple questions with confidence. Discover emerging compounds, make fast and confident identifications, and determine reliable quantitative information.

## Uncompromising sensitivity delivers deeper insights

Full-scan HRAM data with part-per-trillion-level sensitivity, sub-1 ppm mass accuracy, and 240,000 mass resolution (at  $m/z$  200) delivers high-capacity component detection in complex samples. Critical to every application, there is never a need to compromise between resolution and sensitivity.



Access the highest resolving power (RP) and sensitivity without compromising data quality. [A] Effect of resolving power on sensitivity (as absolute peak area response) for pyriproxyfen, in a QuEChERS soil extract at a concentration of 100 ng/mL, showing the extracted ion chromatograms of the  $m/z$  fragment ions, and [B] the corresponding peak area responses obtained at 15,000, 30,000, 60,000, and 240,000 RP.

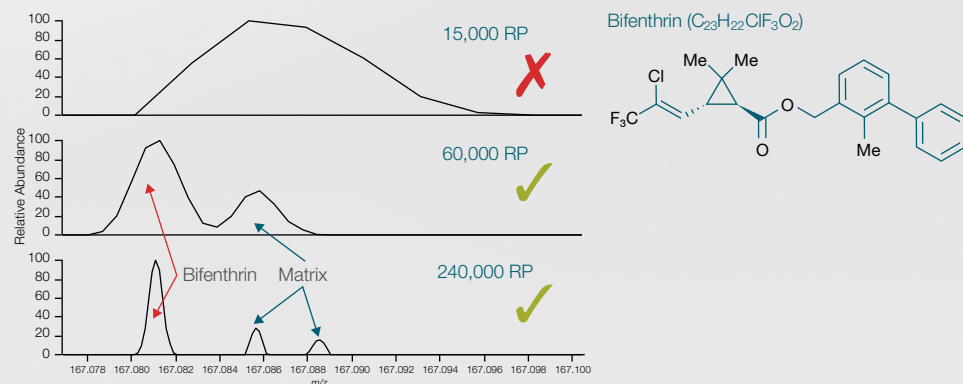


For metabolomics experiments, the capability to achieve such high selectivity and maintain sensitivity is revolutionary for our research; having easy access to this data certainty and such wide coverage opens up new research avenues for us.”

Dr John Bowden, University of Florida

## Outstanding mass resolving power provides data certainty

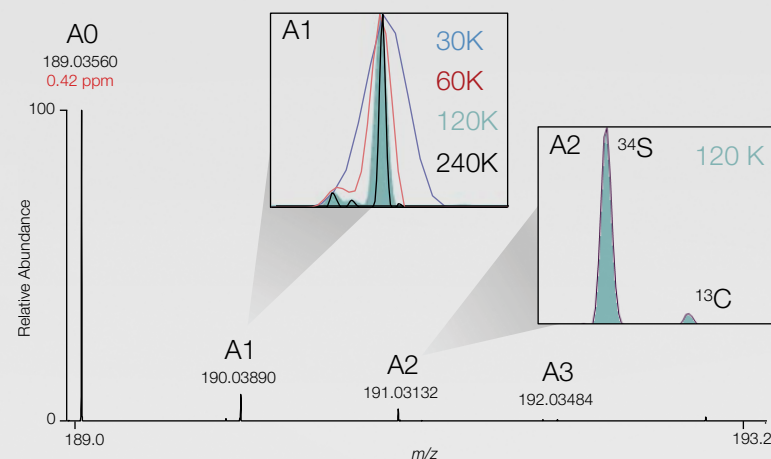
High-resolving power enables you to differentiate between chemical background ions and target ions of interest. Baseline resolution and confident identification of compounds in high matrix samples requires high mass resolving power. Excellent mass accuracy and resolution greater than 120,000



| RP (set by instrument) | Mass (m/z) | Proposed elemental composition(s) | Theoretical mass (m/z) | Mass accuracy (ppm) |
|------------------------|------------|-----------------------------------|------------------------|---------------------|
| 15,000                 | 167.08629  | $C_8H_{15}^{37}ClF$               | 167.08113              | 30.8                |
|                        |            | $C_{13}H_{11}$                    | 167.08629              | 4.5                 |
| 60,000                 | 167.08111  | $C_8H_{15}^{37}ClF$               | 167.08113              | -0.14               |
| 60,000                 | 167.08629  | $C_{13}H_{11}$                    | 167.08553              | 1                   |
| 240,000                | 167.08111  | $C_8H_{15}^{37}ClF$               | 167.08113              | -0.15               |
| 240,000                | 167.08629  | $C_{13}H_{11}$                    | 167.08553              | 0.81                |
| 240,000                | 167.08851  | -                                 | -                      | -                   |

Mass spectra of bifenthrin 10 ng/mL in soil acquired at 15,000, 60,000, and 240,000 RP. Matrix interference at 15,000 RP prevented separation of the pesticide from the matrix, resulting in a higher than expected mass difference. The bifenthrin fragment ion m/z 167 was partially resolved at 60,000 RP and fully resolved at 240,000 RP.

provide access to isotopic pattern determination and reduces the number of potential elemental compositions, providing more assurance in compound assignments.



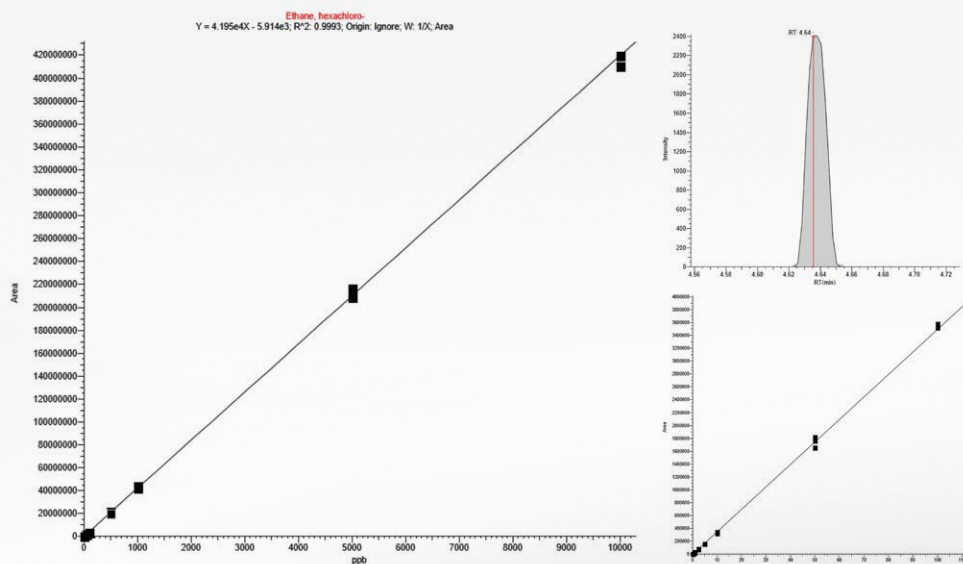
Analysis of tricyclazole demonstrating excellent mass accuracy, and at resolutions greater than 120,000, access to isotopic pattern determination as shown for the A1 and A2 isotopic clusters. Combining these capabilities reduces the number of potential elemental compositions and provides assurance in assignments.

# Experience accurate quantitation irrespective of sample complexity

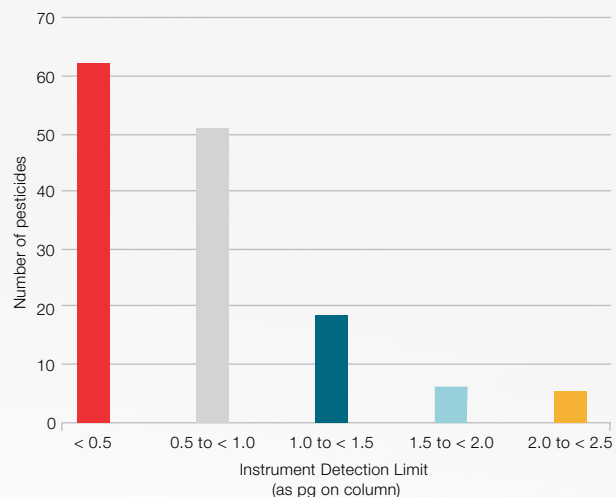
Once a component is identified, the next question is usually “how much is there?” Use the Orbitrap Exploris GC 240 mass spectrometer to accurately determine analyte concentration with quantitative accuracy across six orders, even in the most complex matrices. The instrument has the quantitative power of a GC triple quadrupole mass spectrometer combined with the precision and full-scan HRAM capability that only Thermo Scientific™ Orbitrap™ technology offers. When your discovery workflows move to accurate quantitation, with the Orbitrap Exploris GC 240 mass spectrometer you already have the capability.

## Quantitating power beyond other GC-MS systems

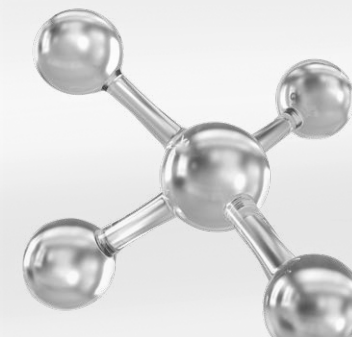
With full-scan data acquisition, the Orbitrap Exploris GC 240 mass spectrometer enables flexible data processing for screening and quantitative workflows. In addition, the instrument provides leading sensitivity, quantitative accuracy, and linearity across a wide dynamic range, even in the most complex sample matrices.



This analysis of hexachloroethane using full-scan data acquisition at a resolution setting of 60,000 provided calibration data that was linear over six orders (from 0.1 to 10,000 pg on column) with three repeat injections of each calibration level. An expansion of 0.1 to 100 pg on column is shown, highlighting the lower calibration points. Extracted ion chromatogram for  $m/z$  165.87191 corresponding to 0.1 pg on column shown. The combination of mass accuracy and resolution allows the use of narrow mass extraction windows to increase specificity.



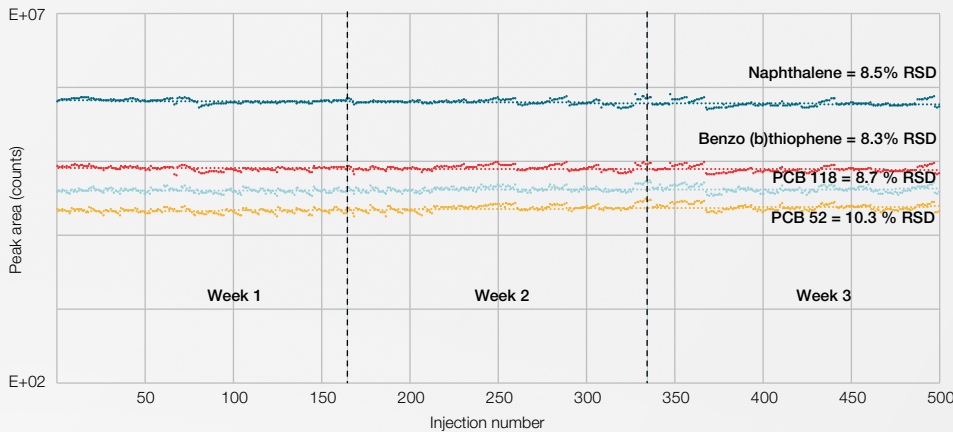
Instrument detection limit (IDL) as pg on column determined for 142 pesticides in whole flour using the Orbitrap Exploris GC 240 mass spectrometer.



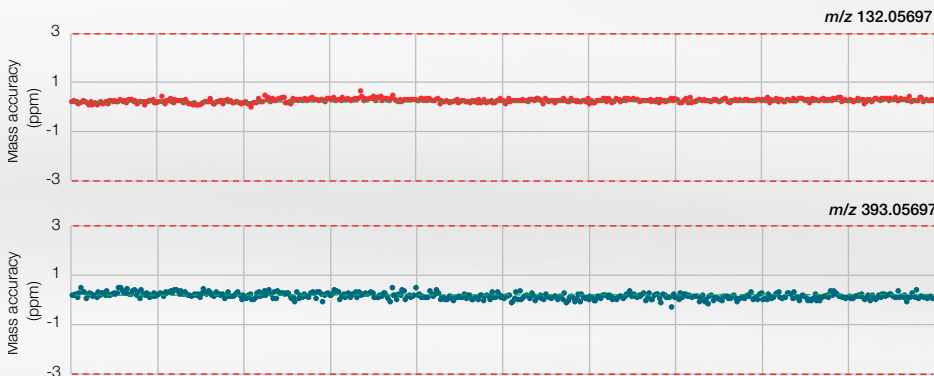
# Obtain consistent accuracy for all applications

## Robustness for all applications

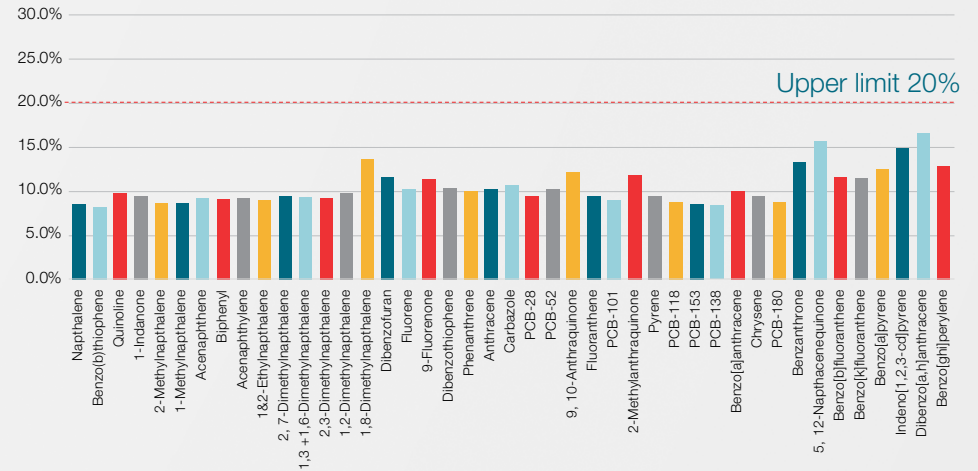
Maintaining sensitivity and performance is critical to every analysis, from routine quantitation to complex metabolomics experiments. Obtain the same response injection after injection to ensure stability across samples.



Repeatability across 500 injections of PAHs and PCBs in soil QuEChERS extracts post spiked at 10 pg/ $\mu$ L.



Mass accuracy stability of low mass early eluting (upper) 1-indanone,  $n=500$  injections at 10 pg/ $\mu$ L spiked soil QuEChERS extract ( $m/z$  132.05697). (Lower) PCB 180 ( $m/z$  393.80195).



\*Inlet septa were replaced every 100 injections. Apart from this no other inlet maintenance was undertaken.

Absolute peak area %RSDs (without internal standard adjustment) for PAHs and PCBs calculated from  $n=500$  injections of a QuEChERS soil sample post spiked at 10 pg/ $\mu$ L (ppb).

## Popular scan modes

**Full Scan:** Obtain comprehensive data coverage by capturing all ions in a user-defined mass range with high mass accuracy. Extract desired  $m/z$  values immediately after data acquisition or later using retrospective data analysis.

**Targeted Selection Ion Monitoring (t-SIM):** Achieve higher sensitivity by setting a narrow mass range (quadrupole settings as narrow as 0.4 Da).

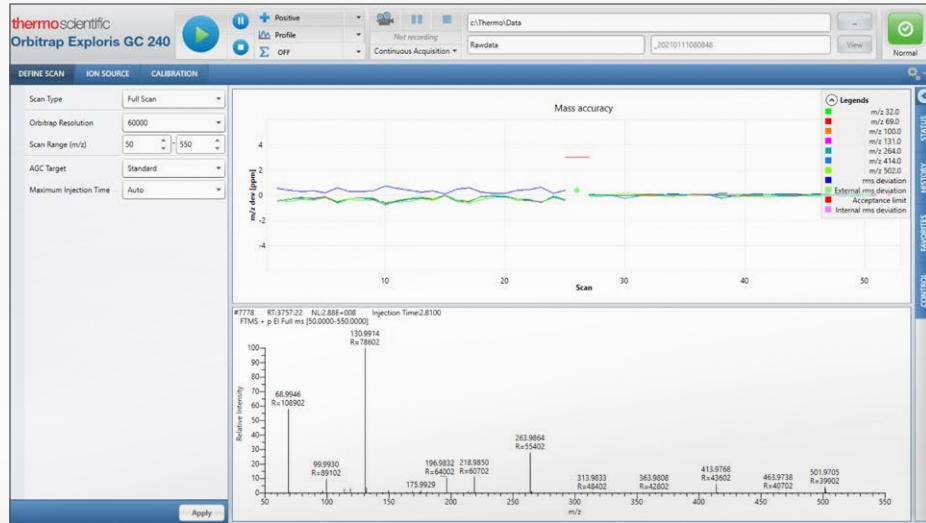
**Targeted-MS/MS:** Gain additional information in complex matrices. A high-resolution product-ion spectrum is only generated for precursor ions detected in a narrow mass range per a mandatory inclusion list.

# Accelerate discovery with ease

An unrivalled combination of high-sensitivity full-scan HRAM data, and intelligent identification using Compound Discoverer software unlocks answers to questions about the full nature of every sample you analyze. Add next-generation software containing built-in method templates and ready-to-use intelligent parameters, and you can analyze complex samples without extensive expertise or effort.

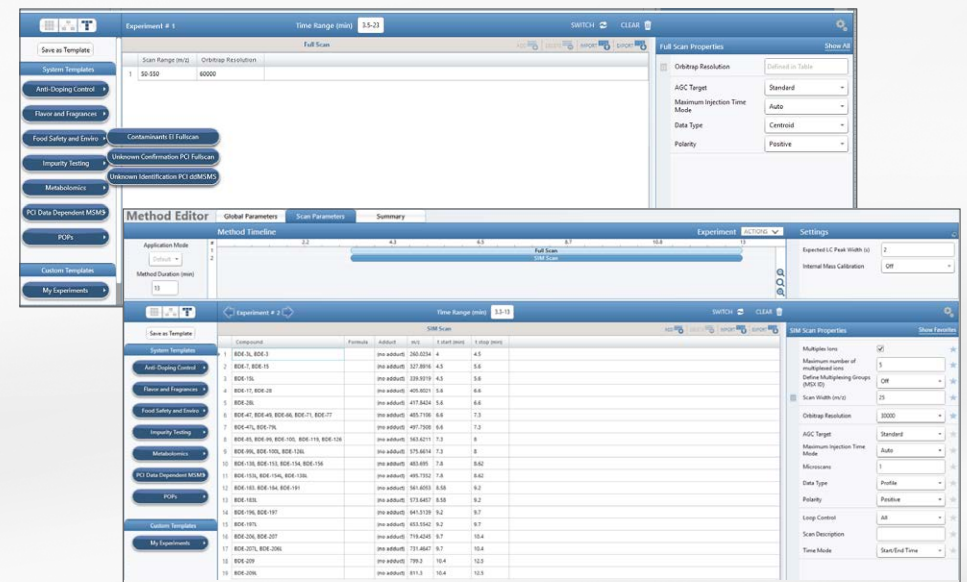
## Focus on your science, not instrument operation

The instrument control software maximizes ease of use, flexibility, and data quality so you can concentrate on your science instead of method setup. The intuitive Method Editor features a drag-and-drop, user-friendly interface with optimized method templates for a wide range of applications, simplifying everyday usability. Consistency among software streamlines training, provides familiarity of operation, and makes transitioning methods from research to everyday analyses easy.



## Benefits

- Walk-up tune and calibration, with single-method control of tune and data-acquisition parameters simplifies error-free operation
- Ready-to-use application-specific templates reduce method development time
- Auto-settings provide high-quality data for most experiments, permitting users to get started quickly
- Drag-and-drop method editing with tooltips offers flexibility in an easy-to-visualize format



Method templates provide “go to” parameters for easy data collection or can be used as a starting point for method development.



# See everything and discover more in profiling and metabolomics experiments

## Rapidly unlock insights with Compound Discoverer software

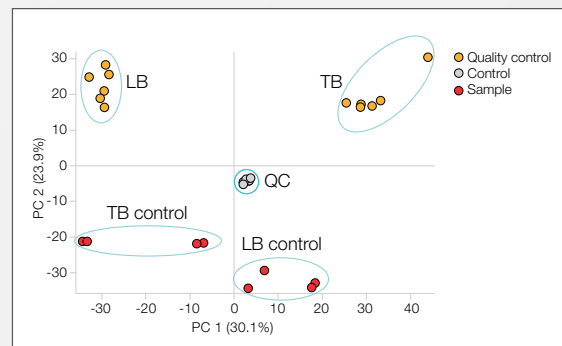
Detailed sample understanding requires the complete qualitative and quantitative data provided by the Orbitrap Exploris GC 240 mass spectrometer to maximize the number of well-defined components obtained. Whether its from small or large datasets, Thermo Scientific™ Compound Discoverer™ software transforms information-rich data into known compounds. The software includes a full suite of integrated workflows and advanced software tools that automatically detect components, generate clean spectra, and identify compounds. Excellent sensitivity and mass resolution across a wide dynamic range enable the software to work at its optimum to quickly deliver results.

## Find real differences

Use the statistical comparison tools in Compound Discoverer software to quickly and confidently isolate the features of interest in your samples. Find real differences between sample sets, see trends in components across a study, or identify components between multiple sample groups—all in interactively linked displays. Perform metabolomic experiments, and map detected compounds.

## Discover what's important

Refined mass spectra can be screened against spectral libraries to generate candidate compound lists and confirm identities using search index, high resolution filtering, and retention indexing.

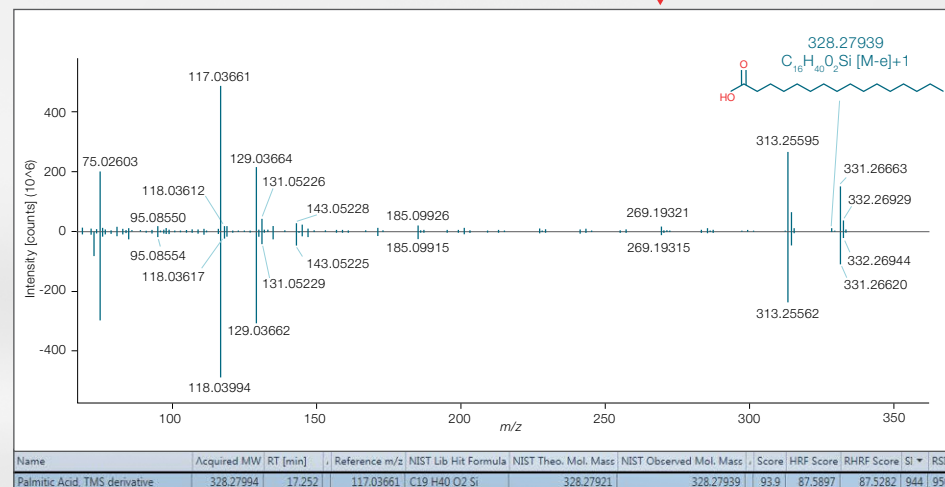


Metabolomics experiment showing differences between sample groups, control, and QC data. Compound Discoverer software provides advanced statistical comparison capabilities, such as PCA plots, to quickly make supported scientific discoveries.



Comparison between sample groups. Peaks of interest can be quickly isolated using a volcano plot.

Palmitic acid TMS acquired spectrum matched to a metabolomics library spectrum, with a search index score of 944.

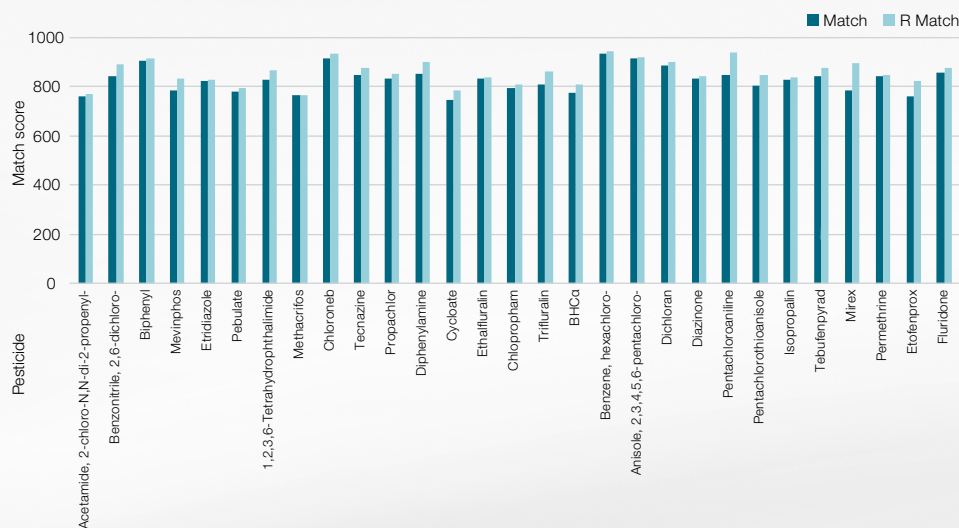


# Gain ultimate certainty for compound identification

Add comprehensive spectral library matching to breakthrough performance and access the highest-confidence identification and quantitative workflows available today. Full-scan HRAM data with spectral matching, isotope patterns, retention indices, and elemental compositions allow multi-point compound identification. Gain certainty in proposed elemental compositions for both confirmation and unknown identification.

## Identify components using libraries

The Orbitrap Exploris GC 240 mass spectrometer uses extensive, readily available nominal mass electron ionization (EI) libraries such as the NIST and Wiley libraries to generate candidate compound lists. In addition to classic search index (SI) scoring, HRAM data enables use of a second parameter to score hits: high resolution filtering (HRF). For every ion in the spectrum, HRF uses accurate mass information to discriminate against unlikely candidates based on elemental composition.



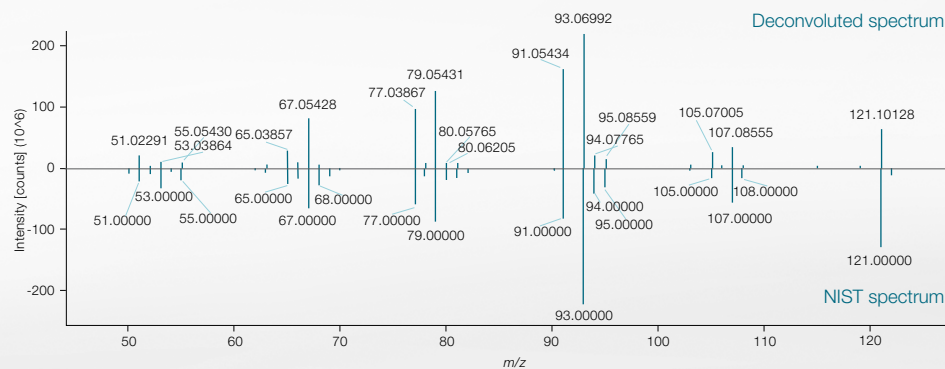
Library search scores for a selection of pesticides from an Orbitrap Exploris GC 240 mass spectrometer analysis of a mixed pesticide standard in a whole flour matrix (a score of 1,000 equals a perfect match). Forward search scores (Match) and reverse search scores (R Match) when searched again the NIST library are given for each pesticide.

## Orbitrap GC-MS HRAM contaminants library

The Thermo Scientific™ Orbitrap™ GC-MS HRAM contaminants library provides tools that support rapid and customizable method setup for contaminant screening. The library includes a Thermo Scientific™ TraceFinder™ compound database and HRAM library of more than 800 food and environmental contaminants.

## Orbitrap GC-MS HRAM metabolomics library

The Thermo Scientific™ Orbitrap™ GC-MS HRAM metabolomics library contains more than 900 retention-indexed unique entries from more than 900 metabolites for broad coverage of primary and secondary metabolites (including terpenes) in plants, animals, and microbes.

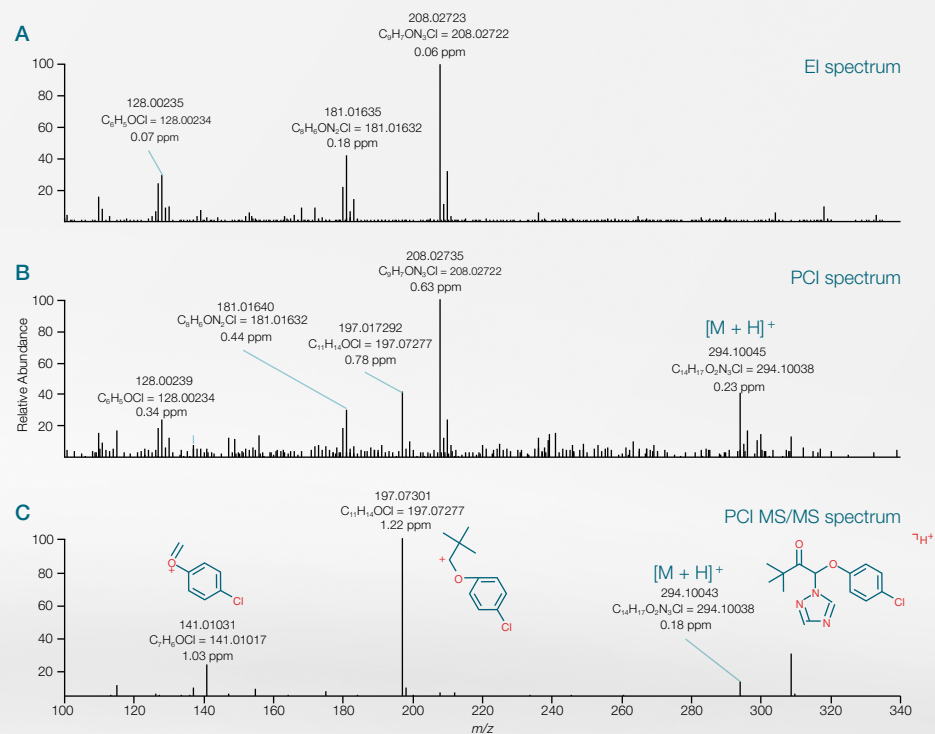


| Matched Compound | Formula                         | Score | HRF Score | SI  | RSI | RI Delta | Elements Found[%] | Theo Mol Mass | Observed Mol. Mass | RI Column type   | RI Diff[%] |
|------------------|---------------------------------|-------|-----------|-----|-----|----------|-------------------|---------------|--------------------|------------------|------------|
| Camphene         | C <sub>10</sub> H <sub>16</sub> | 95.0  | 97.7356   | /94 | 801 | 4        | 100.0             | 136.12465     | 136.12457          | StandardNonPolar | 0.4        |

The deconvoluted spectrum of camphene mirrored with NIST library spectrum, shown in the Compound Discoverer results browser. Search index and HRF score used to confirm identification.

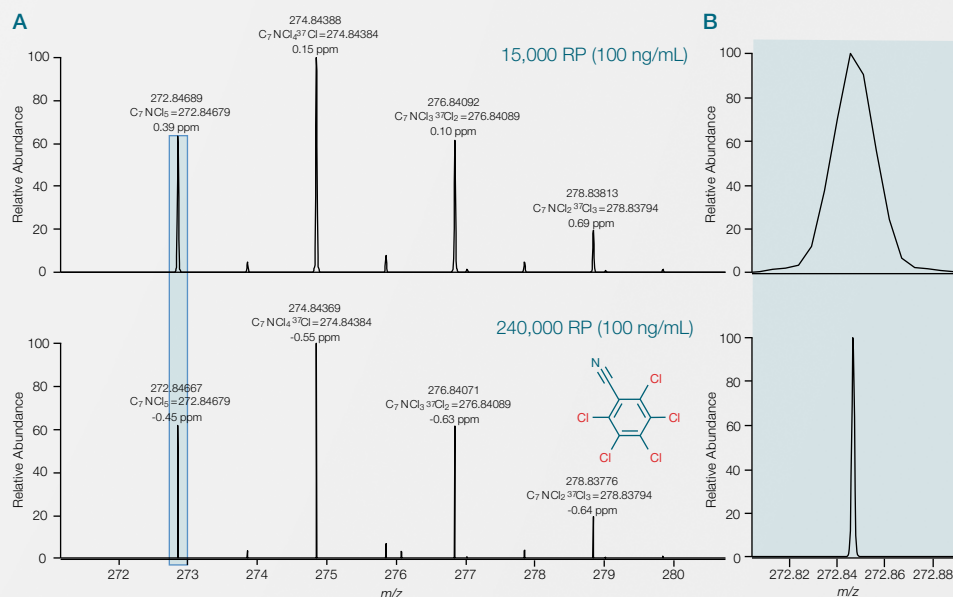
## Obtain molecular ions and perform MS/MS for identification certainty

Molecular ion confirmation often requires chemical ionization (CI) or variable energy electron ionization (VeV) spectrum. Using the Orbitrap GC Exploris 240 mass spectrometer, you can directly measure molecular ions in full-scan data or after fragmentation using optional higher energy collisional dissociation (HCD) to investigate compound structures.

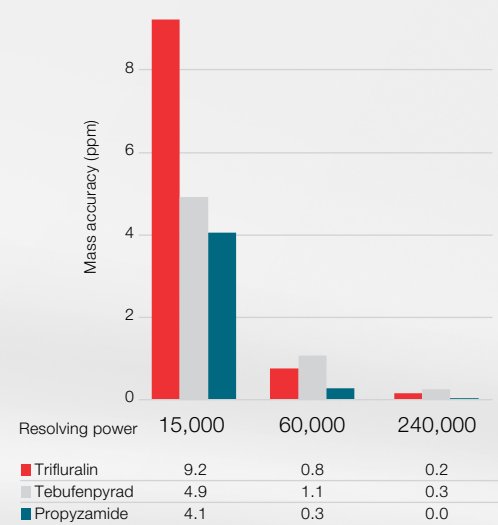


Comparison of the [A] EI, [B] PCI, and [C] PCI MS/MS spectra obtained from an analysis of triadimefon in a QuEChERS soil extract, illustrating that PCI and PCI MS/MS data can be used to provide additional compound confirmation. [A] The molecular ion for triadimefon corresponding to  $C_{14}H_{16}ClN_3O_2$  (exact mass  $m/z = 293.993105$ ) was not present in the EI spectrum. [B] In the PCI spectrum, the triadimefon pseudo molecular  $[M+H]^+$  ion was observed with sub-1-ppm mass accuracy. [C] The PCI MS/MS spectrum following  $m/z 294.10038$  fragmentation in the HCD collision cell.

## Spectral fidelity combined with mass accuracy



Spectral fidelity for pentachlorobenzonitrile ( $C_7Cl_5N$ ) at 15,000 RP and 240,000 RP in a QuEChERS soil extract. [A] EI mass spectra of the molecular ion cluster at each level. [B] Zoomed-in EI mass spectra of the molecular ion ( $m/z 272.84679$ ) in the ion cluster at 15,000 RP and 240,000 RP.



Effect of resolving power on the mass accuracy of three example compounds. 60,000 RP is required to completely separate compounds from interfering matrix ions to deliver low number of possible formulae.

# Power targeted workflows with Thermo Scientific software solutions

Research requires powerfully flexible and intelligent identification and quantitation workflows that are accessible to users with different MS expertise levels. Both Thermo Scientific™ Chromeleon™ chromatography data system (CDS) software and TraceFinder software are workflow solutions that increase productivity from method setup to acquiring and processing data, and reporting.

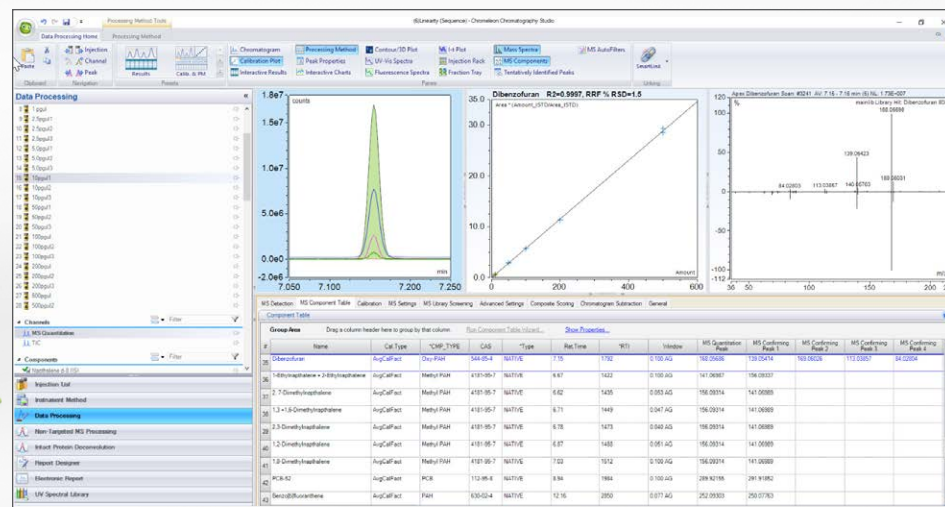
Providing reportable results in a timely manner requires access to a truly connected data processing ecosystem. Regardless of application, Thermo Scientific small-molecule data analysis solutions streamline unknown identification, screening, and quantitation using a powerful suite of software tools.



## Chromeleon CDS software

Enterprise-ready, regulatory-compliant quantitation

- Streamline chromatography and MS software training using the first CDS with quantitative MS analysis control
- Prepare for audits confidently with support for GLP, GMP, and 21 CFR Part 11 regulations
- Connect multiple sites and locations to a central data center with network failure protection
- Easily connect to third-party software applications and multi-vendor LC and GC chromatography instruments



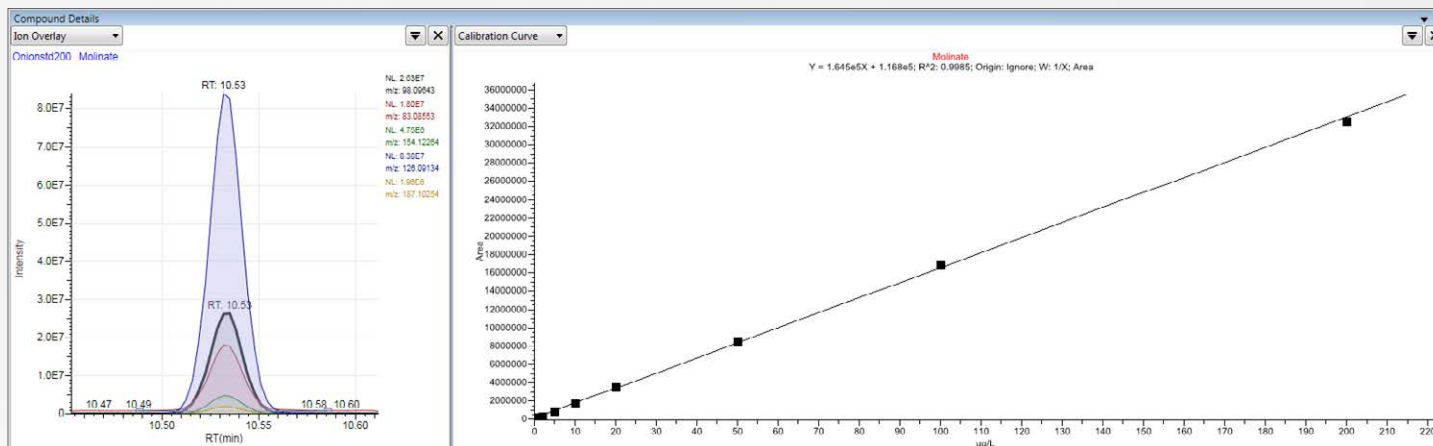
Chromeleon CDS data review browser for quantitation and confirmation of environmental contaminants.



## TraceFinder software

High-throughput screening and quantitation

- Save time training staff using a single platform for both screening and quantitation
- View only desired data parameters with a customizable user interface
- Efficiently analyze and report data with customizable flagging and report templates



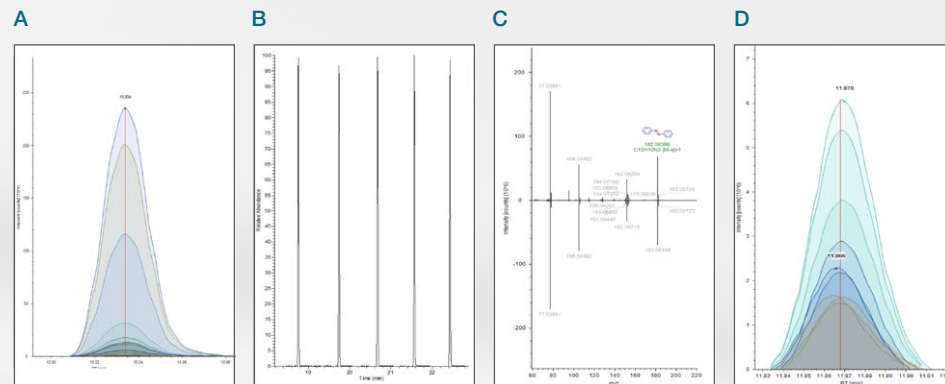
TraceFinder software browser showing extracted ion overlay of the quantitation ion plus four confirming ions for molinate ( $\pm 5$  ppm extraction window) and matrixed matched calibration series [right].



## Compound Discoverer software

Small-molecule unknown identification

- Streamline and customize HRAM data analysis to simplify and gain insights fast. Node based workflows include GC EI and CI deconvolution with statistical analysis tools.
- Confidently identify unknowns using nominal mass and high resolution mass spectral libraries
- Specify desired data flows using drag-and-drop workflow nodes
- Review only data you choose with customizable data visualization



Compound Discoverer software EI and CI node functionality. [A] Peak deconvolution. [B] Retention indexing. [C] Library search. [D] Cross sample peak grouping.

# Fourth-generation quadrupole-Orbitrap mass spectrometer

The Orbitrap Exploris GC 240 mass spectrometer combines proven technology refined over more than 20 years with advanced performance and speed capabilities, day-to-day reliability, and a compact footprint. Now both novice and expert high-resolution MS users can efficiently obtain highly reliable and accurate results.

## Thermo Scientific ExtractaBrite EI/CI ion source

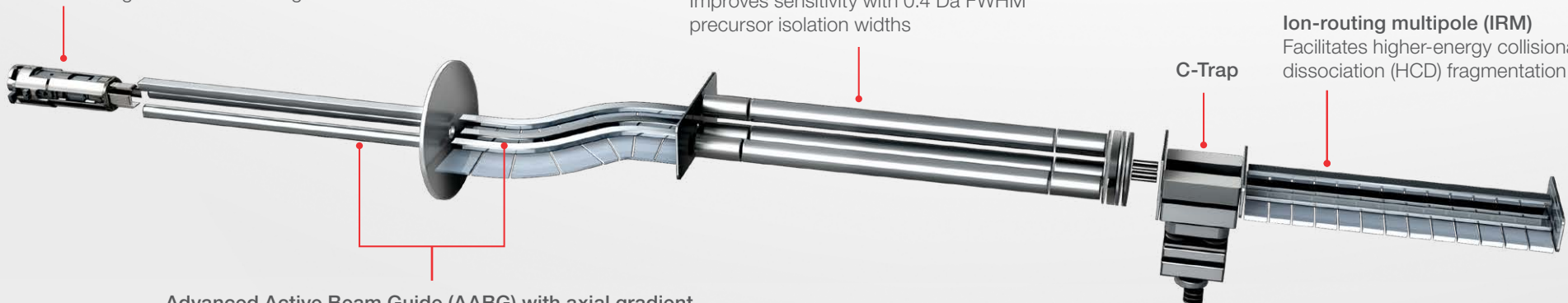
Robust electron impact (EI) and chemical ionization (CI) performance. Fully removable for maintenance or column changes without breaking vacuum

## Advanced Quadrupole Technology (AQT)

Improves sensitivity with 0.4 Da FWHM precursor isolation widths

## Ion-routing multipole (IRM)

Facilitates higher-energy collisional dissociation (HCD) fragmentation



## Advanced Active Beam Guide (AABG) with axial gradient

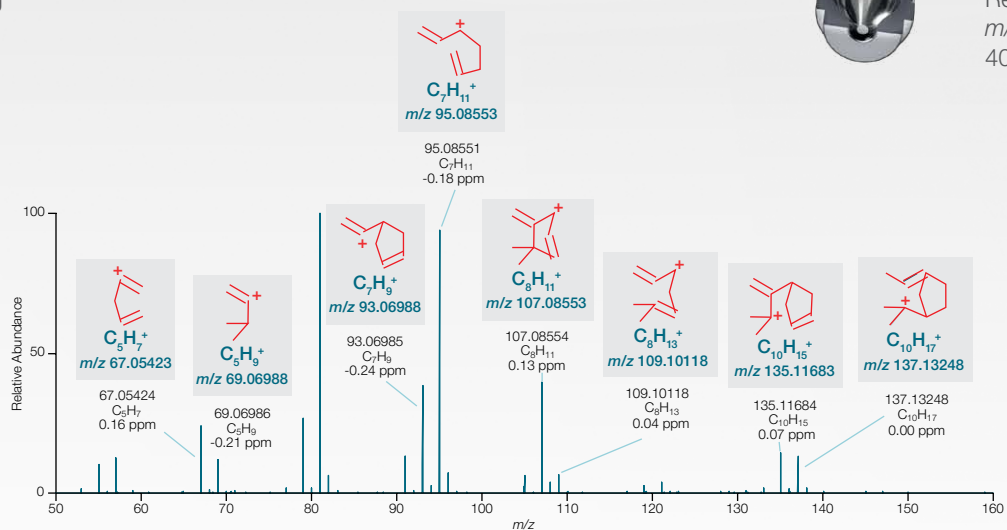
Reduces noise and increases robustness by preventing neutrals from entering the quadrupole mass filter, and by eliminating effects of local charging

## High-field Orbitrap mass analyzer

Resolution up to 240,000 (FWHM) at  $m/z$  200 and acquisition rates up to 40 Hz (at 7500 resolving power)

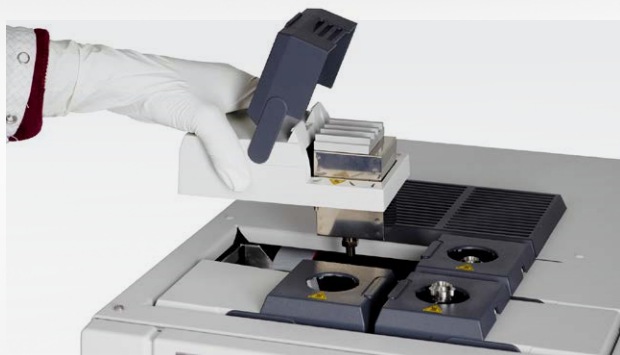


Quickly change column, source or switch to CI with the vacuum probe interlock.



PCI MS/MS analysis of an unknown chemical with  $m/z$  137 following  $m/z$  137.13252 fragmentation in the HCD collision cell showing product ions annotated with measured mass, elemental composition, theoretical mass, mass accuracy (ppm), and proposed structure.

# Step into modern gas chromatography



Access unprecedented flexibility. Switch instant-connect injectors and detectors in minutes without tools.

## Modularity increases uptime

The unique modular design of the Thermo Scientific™ TRACE™ 1600 Series GC empowers users with new time-saving capabilities and unmatched flexibility. Swapping modules is easy by removing and replacing just three screws, accessible from the top of the GC system. The entire process takes less than five minutes without requiring specialized service assistance. This modularity provides maximum uptime with offline cleaning and servicing of the GC inlet when a spare module is purchased.

Also, rapid response to different application needs or sudden workload requirements is possible with a limited investment in modules.

Take advantage of a comprehensive range of the Thermo Scientific™ iConnect™ injectors and detectors interchangeable modules, available at your fingertips at any time for any need:

- iConnect split/splitless (SSL) injector
- iConnect Programmable Temperature Vaporizer (PTV) injector
- iConnect Cold On-Column (COC) injector
- iConnect Flame Ionization Detector (FID)
- iConnect micro-volume Thermal Conductivity Detector (TCD)
- iConnect Electron Capture Detector (ECD)
- iConnect Nitrogen Phosphorous Detector (NPD)
- iConnect Flame Photometric Detector (FPD)
- iConnect Pulsed Discharge Detector (PDD)

# Add productivity with automated sample handling

The TriPlus RSH SMART autosampler offers advanced robotic sample handling to extend automation beyond liquid injection, headspace, and solid-phase microextraction (SPME). Your results will benefit from improved precision and reproducibility, while your laboratory will increase productivity with sample handling flexibility. Several tools are available to reliably automate the most common sample preparation procedures, such as dilution, internal standard addition, and complex derivatization methods, including online microSPE cleanup of QuEChERS extracts.

Automation is enhanced by the innovative SMART technology that tracks consumables' ID and usage parameters through a chip embedded in SMART syringes and SPME/SPME Arrow fibers, triggering consumable health notifications to maintain system uptime and high-quality, reliable data.

## Key benefits

- Improved data repeatability
- Increased automation and laboratory efficiency
- Reduced cost per sample

The TriPlus RSH SMART autosampler delivers exceptional precision, flexibility, and productivity with robotic sample handling.



**Almanac web-based monitoring and management**

Stay connected to your science. See how the Thermo Scientific™ Almanac™ application can help you get the most out of your instruments.

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**Technical and online support: peak performance for your instruments**

Helping you keep your instruments running at peak performance is our goal. Whether you're looking for an instrument manual or spare parts, want to submit a repair request, or check on the status of your warranty or service contract, we have every support option you're looking for.

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**Protecting your investments: unparalleled laboratory services**

Unity™ Lab Services provides a single source for integrated lab service, support, and supply management. Our customized service offerings and world-class service experts have the flexibility and experience to address your laboratory's needs. We provide a complete portfolio of services and support solutions designed to help you improve productivity, reduce total cost of ownership, and ensure performance throughout your laboratory.

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**Thermo Scientific TraceFinder software**

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**Thermo Scientific Compound Discoverer software**

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