thermo scientific



New opportunities for analytical testing



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

Evolved to exceed the demands of everyday testing, the Thermo Scientific™ Orbitrap Exploris™ GC mass spectrometer simplifies operations and delivers consistently accurate results. Transform analytical workflows to keep pace with changing demands, maximize system uptime, and expand laboratory capability.

Simplify | Confidence | Everyday

Power productivity

Simplify analytical workflows with the compact Orbitrap Exploris GC mass spectrometer that brings the versatility of full-scan high-resolution accurate mass data to screening and quantitation. With proven robustness and reliability across all applications, the system delivers accurate results sample after sample.

Ensure certainty in results

Reduce time evaluating data and increase confidence with exceptional levels of selectivity, sensitivity, and linear dynamic range that come together to deliver accurate results, in all sample matrices. Full-scan high-resolution MS data allows multipoint compound identification with spectral matching, isotope patterns, retention indices, and elemental compositions to reduce time to result.

Maximize uptime

Deliver results on time and with ease. With an intuitive instrument control and method templates, the system is fully accessible to all members of your analytical team and provides complete confidence that the system is always operating at maximum performance.



Environmental



Food safety



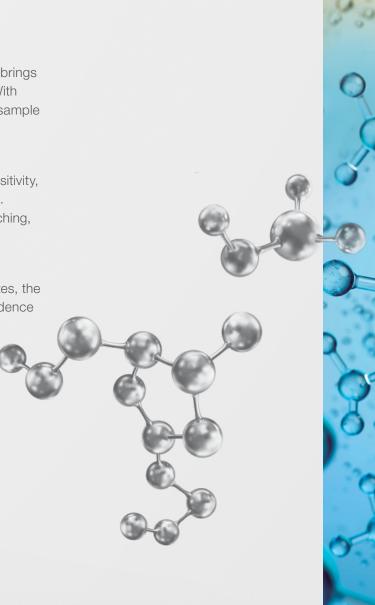
Anti-doping



Clinical and toxicology



Industrial

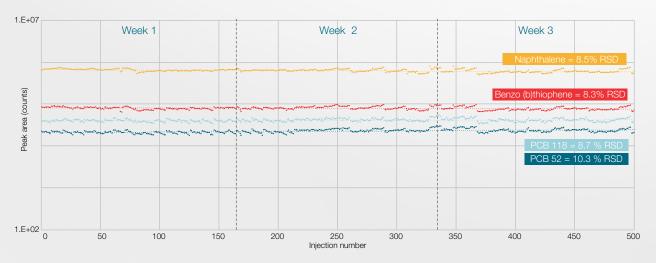


Expand analytical capability with simplicity

The Orbitrap Exploris GC mass spectrometer provides high-confidence detection and precise quantitation in complex matrices, with minimal method development for maximum productivity. As one of the next-generation Thermo Scientific™ mass spectrometers, the Orbitrap Exploris GC mass spectrometer brings together exceptional levels of mass resolution, sensitivity, speed, and linear dynamic range without detector saturation to deliver accurate results even for your most challenging samples.

Transform profitability

The efficiency of operations from sample receipt to report drives profitability in analytical testing laboratories. Every step in the process is critical and every instrument needs to provide a return on investment. The Thermo Scientific Orbitrap Exploris GC mass spectrometer delivers new opportunities for analytical services to simplify operations and improve efficiency. With outstanding real-world performance and analytical flexibility, the system can reduce costs and increase the quality of quantitative results.



Repeatability for high-throughput analysis of 500 replicate injections of a QuEChERS soil extract post spiked with PAHs and PCBs at $10 \text{ pg/}\mu\text{L}$ (ppb) without internal standard correction.

Benefits that boost productivity

Increase scope

Gain the flexibility to quickly add new compounds without compound optimization and decide post acquisition which analytes to measure.

Fast system setup

Walk up, tune, and calibrate in under five minutes with full confidence that the system is operating at maximum performance for all users.

Efficient review and reporting

Use multiple points of identification to quickly confirm or reject detections, increasing peace of mind. Spectral matching, isotope patterns, retention indices, and elemental compositions provide high confidence in results.

Accurate quantitation

Six orders of linear dynamic range covers the concentrations encountered in even the most complex sample matrices.

Method consolidation

Combine acquisition methods onto a single system, reducing the need for multiple systems and streamlining data processing.

Retrospective analysis

Interrogate previously acquired high-resolution accurate-mass (HRAM) data in multiple ways to answer additional analytical questions without additional sample injections.



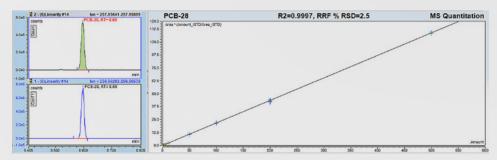
Compared to existing triple-quadrupole methods, the selectivity of GC Orbitrap is much higher, the sensitivity is at least comparable, and the repeatability and reproducibility are better."

Dr. Jim Garvey, Department of Agriculture, Food and the Marine, Ireland

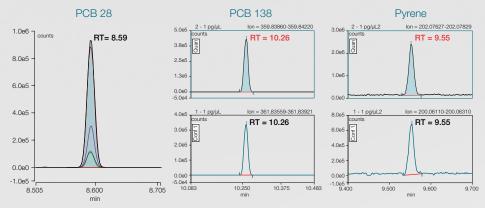


Sensitive, high-capacity component detection

HRAM data with part-per-trillion-level sensitivity in full scan and a wide dynamic range drives high-capacity component detection in complex samples. This capability opens up new opportunities and enables your laboratory to answer many questions about samples from a single injection. Even when using non-targeted full-scan acquisition, the Orbitrap Exploris GC system provides the quantitative capability of a GC triple quadrupole instrument operating in selected reaction monitoring (SRM) mode. Orbitrap Exploris GC mass spectrometers deliver the new level of performance that you demand for everyday quantitative applications.

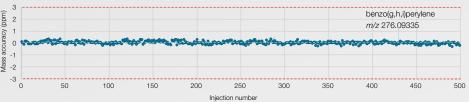


Thermo Scientific™ Chromeleon™ chromatography data system (CDS) software view of soil matrix-matched calibration curve of PCB 28 (0.1–500 µg/kg), including extracted quantifier and qualifier ions at 0.1 µg/kg. Data were acquired using 60,000 mass resolving power at m/z 200.



Gain data certainty with sensitive multi-ion confirmation to streamline data reviewing and reduce turnaround time (1 pg/µL injection of QuEChERS soil extracts).

500 repeat injections of 10 pg/µL spiked soil QuEChERS extract



Mass accuracy stability across 500 repeat injections of a 10 pg/ μ L spiked soil QuEChERS extract. Mid-mass, late-eluting (PAH) benzo(g,h,i)perylene (RT = 15.5 min, m/z 276.09335.)

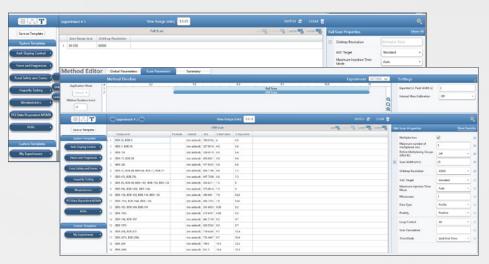
Focus on results, not instrument operation

When next-generation mass spectrometer design is combined with next-generation software containing built-in method templates and ready-to-use intelligent parameters, you can analyze complex samples without extensive expertise or effort. The instrument control software maximizes ease of use, flexibility, and data quality so your lab can concentrate on results instead of setting up methods. Consistency among software streamlines training, provides familiarity of operation, and makes transitioning methods easy.

Powerfully intuitive instrument control

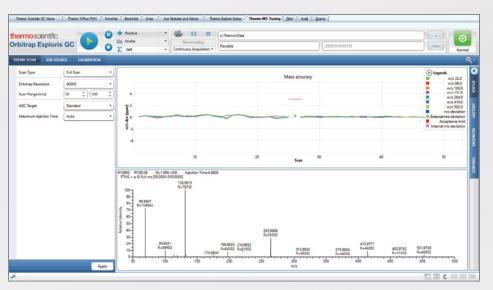
The intuitive Method Editor features a drag-and-drop user-friendly interface with optimized method templates for a wide range of applications, simplifying everyday usability.

- 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 any user to get started quickly
- Drag-and-drop method editing with tooltips offers flexibility in an easy-to-visualize format



Software tailored to analytical testing

Acquiring data and reporting results in a timely manner is a necessity for fast turnaround applications. Both Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) and Thermo Scientific™ TraceFinder™ software offer a powerful solution with pre-configured, customizable methods and reports with advanced features including advanced calculations, charting, and results flagging.



Intuitive user interface for system set up and operation. Tune and calibrate the system in under five minutes.

Experience next-generation reliability and uptime

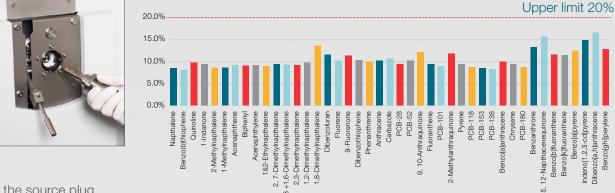
The Orbitrap Exploris GC mass spectrometer joins the family of next-generation Thermo Scientific mass spectrometers, which are built on a common architecture with the guiding principle of robust real-world performance. Frequent unplanned or planned downtime can impede your laboratory's ability to achieve its goals. By minimizing downtime, the Orbitrap Exploris GC mass spectrometer ensures your lab achieves high throughput all day, every day.

Continuous performance

- Reduce planned downtime when using the vacuum probe interlock (VPI), and the Thermo Scientific™ ExtractaBrite[™] electron impact (EI)/chemical ionization (CI), which is fully removable under vacuum, even when hot, for routine cleaning or swapping with a spare source
- When you need to confirm the molecular ion of an unknown, you can switch between El and Cl modes in minutes using the VPI

30.0%

25.0%



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

• Quickly change a column without breaking vacuum using the source plug

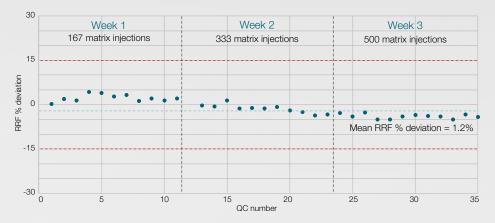


Chart showing the RRF % deviation values for PCB 153 calculated for a low-level QC standard (40 pg/uL) injected after every 20 sample injections across three weeks of continuous analysis. Absolute peak area %RSDs (without internal standard adjustment) for all PAHs and PCBs from n=500 injections of a QuEChERS soil sample.

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 setting 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.

Be certain with multipoint compound identification

Add comprehensive HRAM spectral library matching to breakthrough performance to access the highest-confidence screening and quantitative workflows available today to speed up time to result. Full-scan HRAM data with spectral matching, isotope patterns, retention indices, and elemental compositions allow multi point compound identification, eliminating false results and accelerating report generation. Accurate masses provide certainty in proposed elemental compositions for both confirmation and unknown identification workflows.

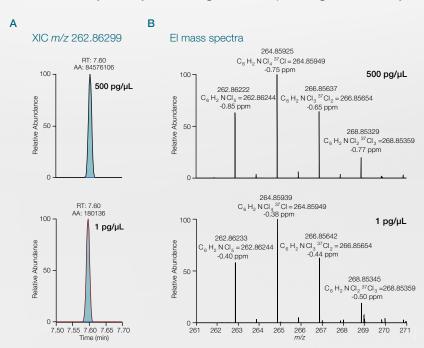
Intelligent screening to increase scope

When used with Chromeleon CDS and TraceFinder software, the Orbitrap Exploris GC mass spectrometer offers a powerful, yet easy to use, screening solution with the durability demanded by laboratories focused on highthroughput analyses. Both software take advantage of multiple library sources

Match
R Match 1000 400 200 Trifluralin BHCa

Library search scores for pesticides from an Orbitrap Exploris GC 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.

(nominal mass and exact mass) to automate compound identification, including commercially-available libraries and Thermo Scientific™ Orbitrap™ HRAM GC-MS libraries. Sensitivity and dynamic range offer deeper insights into every sample.

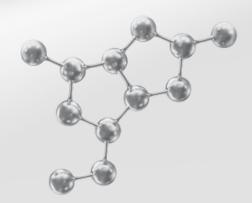


Spectral fidelity for pentachloroaniline at two levels (1 and 500 pg/µL) in whole flour matrix using the Orbitrap Exploris GC mass spectrometer. [A] extracted ion chromatograms (XIC) for pentachloroaniline at each level annotated with peak retention time (RT) and peak area (AA); and [B] a zoomed-in view of El mass spectra of the molecular ion cluster at each concentration level, annotated with the measured mass, elemental composition, theoretical mass, and mass accuracy (ppm).



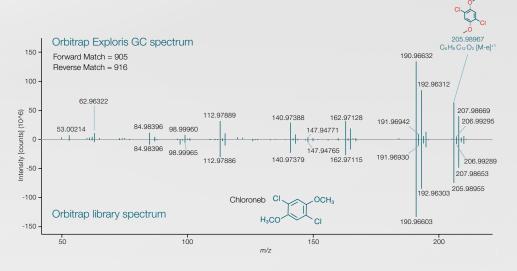
With GC Orbitrap we could easily reach our target limits of quantification and the selective full scan data enables us to work more efficiently, especially through data processing."

David Haas, Eurofins, Germany



Orbitrap GC-MS contaminants library

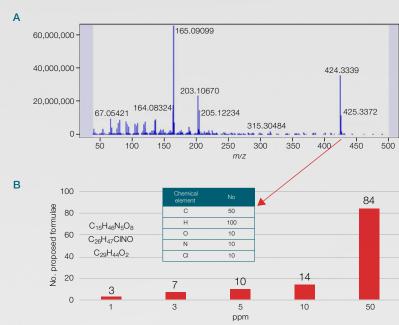
The Thermo Scientific™ Orbitrap™ GC-MS contaminants library provides tools that support rapid and customizable method setup for contaminant screening. The library includes a TraceFinder software compound database and HRAM library of more than 800 food and environmental contaminants. The user guide explains how to customize the library by adding new compounds acquired using an Orbitrap GC mass spectrometer system.



Example spectrum library match for chloroneb. Full scan data allows for multiple identification points, including accurate mass ions, spectral matching, isotope pattern comparison, and ion ratio confirmation.

Identify the unknown

When it comes to unknown compounds that do not have a satisfactory library match, high mass accuracy and isotope patterns enable the right elemental composition to be proposed so you can get the right answer fast.



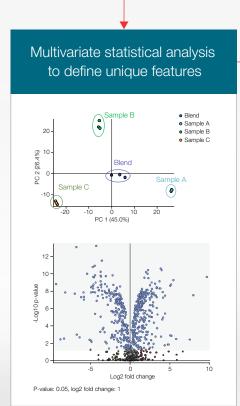
Whole flour extract containing an unknown peak at retention time 10.05 min; [A] El mass spectra for the unknown peak; [B] number of proposed formulae (annotated on top of the bars) with different mass tolerances applied; and inset table detailing the selected chemical elements used, and proposed formulae for a mass tolerance of 1 ppm.

Broaden your scope, boost opportunity

Target compound lists are likely to increase and limits of detection and quantitation fall. Imagine if you could expand your scope of analysis, consolidate multiple methods onto a single system, or open up new business opportunities with sample profiling. All without the need for reanalysis or time-consuming method development. The Orbitrap Exploris GC mass spectrometer makes this a reality. Full-scan HRAM data combined with Thermo Scientific™ Compound Discoverer™ software enables analysts to gain a comprehensive understanding of their samples through intelligent informatics workflows. In addition, you can re-interrogate data to answer analytical questions arising later.

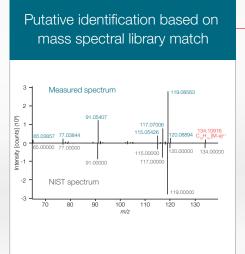
Full scan EI and CI data deconvoluted

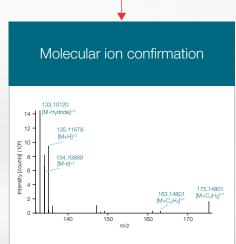
Workflow to assess the volatile profile of oregano samples. Full-scan data were acquired in EI and PCI modes: multivariate statistical analysis was performed to identify unique features contributing to the group differences in the EI data; putative peak identification was made using a mass spectral library match (NIST20 and Thermo Scientific™ Orbitrap™ GC-MS HRAM Metabolomics Library); compound identification was confirmed using soft ionization PCI data and the presence of pseudo-molecular and/or adduct ions.



Take sample profiling further with Compound Discoverer software

Easily interrogate and re-interrogate full-scan HRAM data to answer questions not possible using targeted acquisition data. Samples can be screened for a target list of compounds or interrogated for unknowns. Decide post-acquisition which compounds to analyze and never again be limited to only the ions measured at the time of data acquisition.







Fully understand what's in your samples

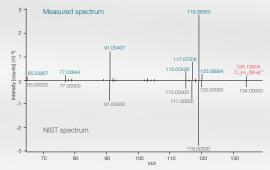
Advanced compound discovery and identification workflows enable you to gain a comprehensive understanding of your samples. With a full suite of advanced software tools, Compound Discoverer software transforms your full-scan HRAM data into known compounds. Because identifying differences among samples or sets of samples can be particularly challenging, Compound Discoverer software also provides intelligent informatics workflows, including differential analyses, to quickly uncover statistically significant differences.

	RT [min]	Chemical Formula	Reference m/z		EI			PCI		Total	Log2 Fold Change				
Name				Measured m/z	Theoretical m/z	Mass error (±5	[M+H] ⁺	[M+C ₂ H ₅] ⁺	[M+C ₃ H ₅]*	Score	Sample A / Sample C	Sample B / Sample C	Sample B / Sample A		
α-Thujene	8.64	C10H16	91.05417	136.12463	136.12465	-0.1	137.13254	165.16379	177.1638	93.4	4.0	3.3	-0.7		
α-Pinene	8.79	C10H16	91.05423	136.12469	136.12465	0.3	137.13252	165.16377	177.16377	93.4	3.4	3.0	-0.4		
p-Cymene	10.21	C10H14	119.0856	134.10892	134.10900	-0.6	135.11688	163.14818	175.14815	96.2	3.7	2.8	-0.9		
y-Terpinene	10.84	C10H16	91.05424	136.12457	136.12465	-0.6	137.13234	165.13659	177.16353	95.2	2.3	2.6	0.3		
β-Ocimene	11.40	C10H16	93.06971	136.12466	136.12465	0.1	137.13266	165.16393	177.16391	90.2	-4.4	-0.6	3.9		
Camphor	12.09	C10H16O	95.08548	152.11957	152.11957	0.0	153.12727	181.15852	193.15848	96.6	0.6	1.1	0.5		
Thymoquinone	13.54	C10H12O2	149.0596	164.08311	164.08318	-0.4	165.09077	193.12198	205.12195	94.4	0.1	0.4	0.3		
Methyl thymyl ether	13.61	C11H16O	149.0962	164.11960	164.11957	0.2	165.12726	193.15863	205.15863	97.4	1.5	2.0	0.4		
Thymol	14.23	C10H14O	135.0804	150.10382	150.10392	-0.6	151.11169	179.1431	191.1431	96.1	2.8	-0.3	-3.1		
Carvacrol	14.42	C10H14O	135.0805	150.10384	150.10392	-0.5	151.11163	179.14302	191.14294	95.7	0.3	0.2	0.0		
Eugenol	15.36	C10H12O2	164.0831	164.08321	164.08318	0.2	165.091	193.12228	205.12231	96.9	-1.5	0.2	1.7		
Methyleugenol	16.02	C11H14O2	178.0989	178.09885	178.09883	0.1	179.1066	207.13788	219.13788	96.2	-2.6	0.2	2.9		
y-Elemene	17.00	C15H24	189.1639	204.18726	204.18725	0.0	205.19524	233.22658	245.22647	92.1	0.5	0.2	-0.3		
β-Caryophyllene	17.15	C15H24	91.05417	204.18721	204.18725	-0.2	205.19489	233.22615	245.22627	95.3	0.5	-0.1	-0.6		
Humulene	17.76	C15H24	93.06991	204.18729	204.18725	0.2	205.19513	233.22646	245.22649	94.5	1.8	-0.1	-1.9		
Isoledene	18.06	C15H24	105.0699	204.18713	204.18725	-0.6	205.19519	233.22652	245.22665	96.2	1.2	0.9	-0.3		
Germacrene D	18.22	C15H24	147.1167	204.18727	204.18725	0.1	205.19514	233.22649	245.22647	95.5	-0.9	0.9	1.7		
Alloaromadendrene	18.58	C15H24	91.05424	204.18716	204.18725	-0.4	205.19485	233.22614	245.22618	95.8	-0.6	0.7	1.3		
y-Muurolene	18.78	C15H24	161.1327	204.18719	204.18725	-0.3	205.19499	233.22635	245.22636	93.6	-0.3	0.2	0.5		
Isospathulenol	19.94	C15H24O	91.05419	220.18230	220.18217	0.6	221.19	249.22171	261.22125	94.5	-1.3	0.0	1.3		
Caryophyllene oxide	20.10	C15H24O	91.05419	220.18199	220.18217	-0.8	221.18999	249.2213	261.22129	94.7	-0.2	-0.3	-0.1		

Predominant fold change values for the predominate volatile constituents of *Oreganum vulgare* samples with different geographical provenances. In particular, sample A showed a significantly higher level of cymyl-type compounds such as p-cymene (four-fold change), y-terpinene (two-fold change), and thymol (three-fold change).

Α				В
	3.0 -	10.21		
	2.5 -		Sample A	
ints] (10 ⁹)	2.0 -			С
Intensity [counts] (10 ⁹)	1.5 –		Sample B	
	1.0 –			
	0.5 _		Sample C	
	10.16	10.19 10.22	10.25	
		RT [min]		

Library	Library search results Deconvolved Compounds																						
8	Matched	ompound 4	- Chec	ked Formula	CAS Num	Score	HRF Score	RHRF Score	SI	RSI	RI Delta	Elements Fo	Theo Mol Mass	Observed Mol. Mass	M+ In Lib	M+ found	Selected	RI Column type	Library RI	RI Diff[%]	Library	Library Ic	Library Hit key
72	p-Cymen		J.E	C10H14	99-87-6	95.2	98.0736	98.0972	796	796	2	100.0	134.10900	134.10916	Yes	Yes	True	StandardNonPolar	1014	0.2	mainlib	109426	mainlib109426
70	p-Cymen		E	C10H14	99-87-6	95.6	98.0736	99.4404	818	819	2	100.0	134.10900	134.10916	Yes	Yes	False	StandardNonPolar	1014	0.2	replib	21491	replib21491
70	p-Cymen		E	C10H14	99-87-6	97.5	98.0736	99.4587	913	916	0	100.0	134.10900	134.10916	Yes	Yes	False	None	0	0	orbitrap,	302	orbitrap_metabolomics_v1302



Compound Discoverer software peak deconvolution results for a compound eluting at RT = 10.21 min putatively identified as p-cymene (*m/z* 119.08563). [A] XIC for p-cymene in three sample groups; [B] result table with deconvoluted compound, retention index, and library search results for the NIST20 and Orbitrap GC-MS HRAM Metabolomics Library; and [C] measured El spectrum of p-cymene versus NIST20 library spectrum.

Power GC-MS with Thermo Scientific software solutions

Providing fast and accurate results requires screening, quantitation, and discovery workflows that are accessible and efficient for users with different levels of MS expertise. Both Chromeleon CDS and TraceFinder software are workflow solutions that increase laboratory productivity from method setup to acquiring and processing data, and reporting results. Compound Discoverer software makes sample profiling and unknown analysis fast and easy with intelligent and flexible functionality to really get the most from your data.

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.

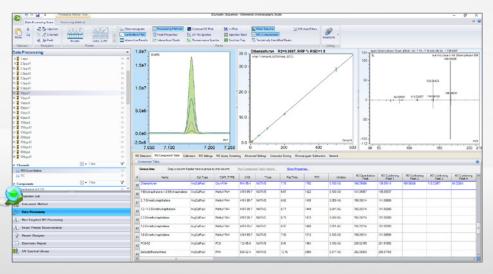




Chromeleon CDS

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

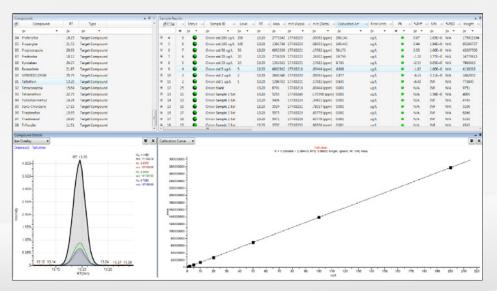




TraceFinder software

High-throughput screening and quantitation

- TraceFinder software provides a single platform for both screening and quantitation, including peak deconvolution and spectral library matching
- View only desired data parameters with a customizable user interface
- Efficiently analyze and report data with customizable flagging and report templates



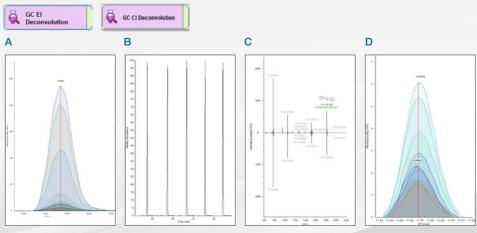
TraceFinder software data review of tefluthrin in onion with extracted ion overlay of the quantifier ion and three confirming ions (± 5 ppm window) and matrix matched calibration series.



Compound Discoverer software

Small-molecule unknown identification

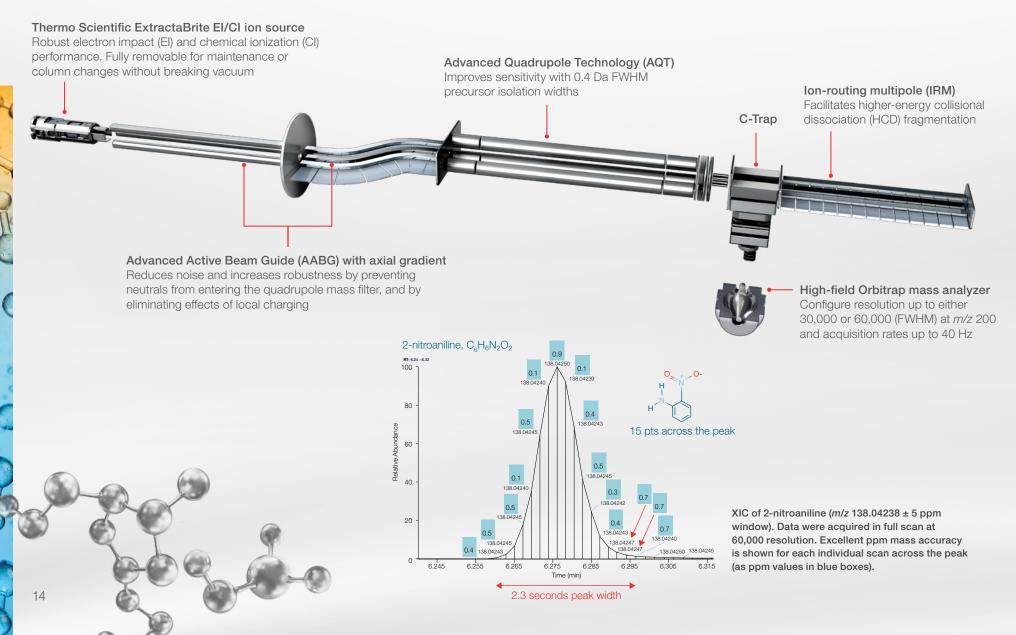
- Streamline and customize HRAM data analysis to simplify and gain insights fast.
 Node based workflows include GC EI and CI deconvolution with statistical analysis tools.
- Confidently profile your samples, compare sample groups, and identify unknowns faster using nominal mass and high- resolution mass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



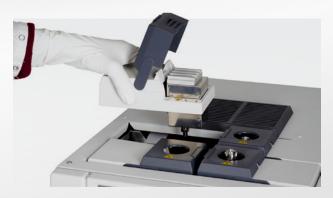
Compound Discoverer software EI and CI node functionality. [A] Peak deconvolution. [B] Retention indexing. [C] Library search. [D] Cross sample peak grouping.

Fourth-generation quadrupole-Orbitrap mass spectrometer

The Orbitrap Exploris GC 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.



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™ 1300 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 spare modules. Take advantage of a comprehensive range of the Thermo Scientific™ Instant Connect injectors and detectors interchangeable modules, right available at fingertip at any time for any need:

- Instant Connect Helium Saver split/splitless (SSL) injector
- Instant Connect Cold On-Column (COC) injector
- Instant Connect Flame Ionization Detector (FID)
- Instant Connect micro-volume Thermal Conductivity Detector (TCD)
- Instant Connect Electron Capture Detector (ECD)
- Instant Connect Nitrogen Phosphorous Detector (NPD)
- Instant Connect Flame Photometric Detector (FPD)
- Instant Connect Pulsed Discharge Detector (PDD)

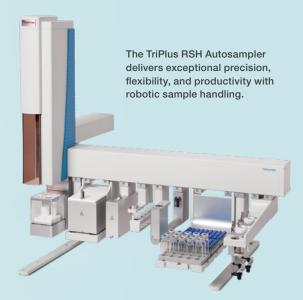
Add productivity with automated sample handling

The Thermo Scientific TriPlus RSH 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.

Ready-to-use prep cycles are available or it is possible to easily create custom workflows using the Thermo Scientific™ Sampling Workflow Editor software, with intuitive drag-and-drop visual programming.

Key benefits

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



thermo scientific



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.

thermofisher.com/almanac



Technical and online support: peak performance for your instruments

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