



Redefining Routine GC-MS

Thermo Scientific Exactive GC
Orbitrap GC-MS System



The Frontier of Routine GC-MS

The power of the multi-award-winning Orbitrap™ GC-MS technology has so far allowed research scientists to break new ground and gain a broader and deeper understanding of their samples through the use of high-resolution, accurate-mass (HRAM) analysis. The introduction of the Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system brings that power into the routine environment for the first time. This system allows scientists working in fields such as food safety, environmental, industrial, forensics and anti-doping to revolutionize their workflows by taking their analytical capability to the next level.

The Exactive GC system is an easy-to-use, dedicated GC-MS that provides an unprecedented level of highly sensitive, routine-grade performance for both targeted and non-targeted analysis, along with high confidence quantitation for the ultimate sample analysis workflow. This is achieved through the superior resolving power, mass accuracy, linear dynamic range and sensitivity that only Orbitrap technology can deliver, combined with the intelligent data processing workflows provided by Thermo Scientific™ TraceFinder™ Software.



“This is clearly a major step forward.”

Dr. Hans Mol
RIKILT, Netherlands
Natural Toxins and Pesticides



“GC Orbitrap technology will bring a new level of performance to high resolution GC-MS.”

Prof. Jana Hajšlová
University of Chemical Technology
Prague, Czech Republic
Food Safety and Food Authenticity



“The chance to look for unknown substances, that today remain to be discovered, is a real advance in MS.”

Dr. Esteban Abad Holgado
Spanish Council for Scientific Research,
Barcelona, Spain
Environmental Analysis



“I believe that, in screening applications, one panoramic high-resolution accurate-mass spectrum is worth thousands of transitions.”

Dr. Alexander Makarov
Director of Research
Life Science Mass Spectrometry
Thermo Fisher Scientific

Ultimate Performance for Targeted Screening and Quantitation

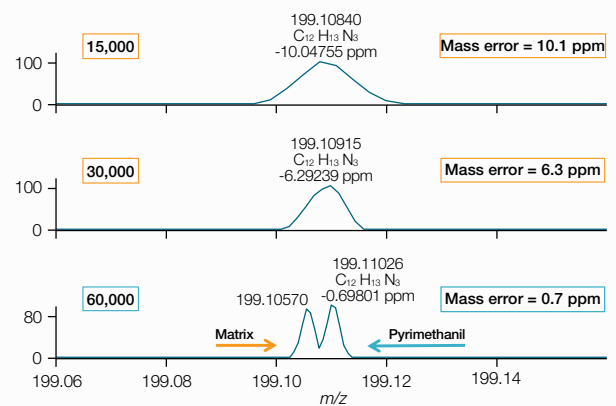
High selectivity full-scan analysis brings new possibilities to the routine environment: ease of analytical set-up, almost unlimited scope, efficient automatic data processing and retrospective data analysis. The Exactive GC system has the quantitative power of a GC triple quadrupole MS combined with the full-scan high-resolution, accurate-mass (HRAM) capability that only Orbitrap GC-MS technology can offer. This combination will change your workflows, forever.

Confident low-level detection and identification for high efficiency screening workflows

The Exactive GC system offers routine full-scan operation, possible at 15k, 30k, or 60k resolution (at m/z 200) with sub-1 ppm mass accuracy and full-scan sensitivity down to part-per-trillion concentrations. This capability drives truly powerful broad-scope screening methods for food safety, environmental, anti-doping and many other applications where confident ultra trace-level detection is required in difficult matrices.

For pesticides, I could safely see very low levels.

– Jana Hajšlová



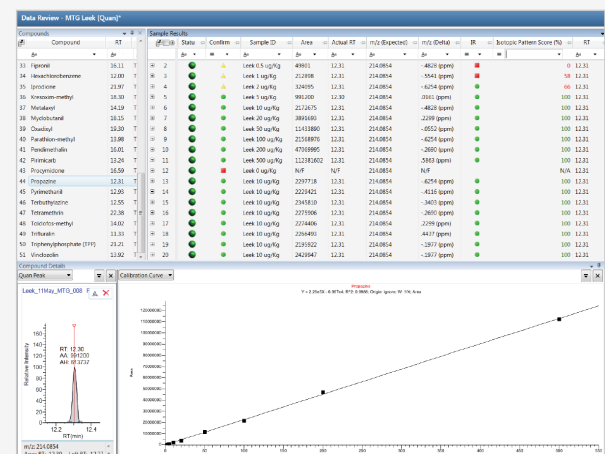
Impact of resolving power on the mass accuracy of Pyrimethanil at 10 $\mu\text{g}/\text{Kg}$ in leek acquired at different resolutions of 15K, 30K, and 60K. A resolution of 60K is required to resolve the Pyrimethanil ion from the matrix interference to achieve a mass accuracy compatible with the regulatory guidelines of <5ppm.

Quantitation capability far beyond that of other HRAM GC-MS systems

Even when using non-targeted full-scan acquisition, the Exactive GC system provides the quantitative capability of a GC triple quadrupole instrument operating in selected reaction monitoring (SRM) mode. Sensitivity (<ppb), quantitative accuracy, precision, and linearity (>6 orders) are excellent, even in complex matrices. This is an unprecedented level of performance in GC-MS, only possible with Orbitrap GC-MS technology.

This technology provides an easier, more efficient, and more comprehensive way of doing GC-based pesticide residue analysis.

– Hans Mol

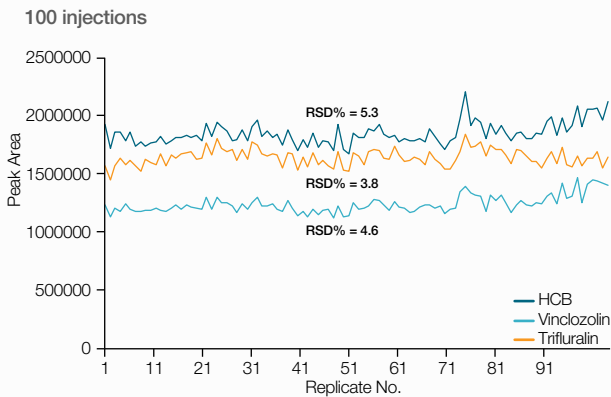


TraceFinder software uses the Exactive GC system data and combines compound detection, identification and quantitation to enable routine trace pesticide analysis to regulatory requirements. It also allows customizable, automated flagging for detected compounds along with flexible reporting tools.

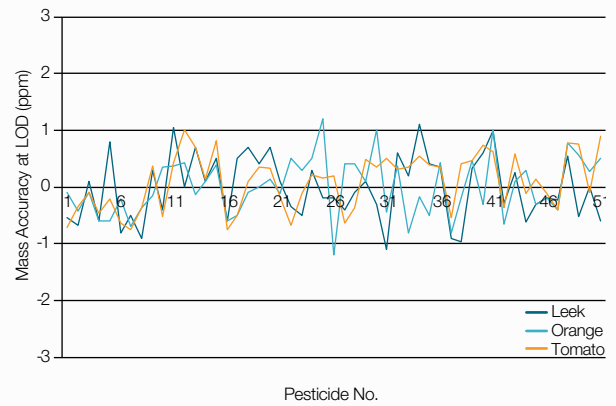
detect

identify

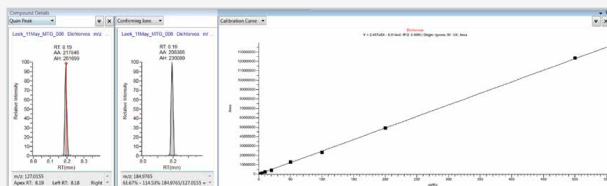
quantify



100 repeat injections of a tomato extract spiked at 10 µg/Kg shows sensitivity is maintained over the 66 hours of continual operation.



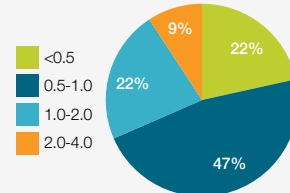
Mass accuracy at the limit of identification (0.5-5 µg/Kg) for 151 pesticides in leek, orange and tomato matrices. The consistent low mass errors provides high confidence in positive identifications.



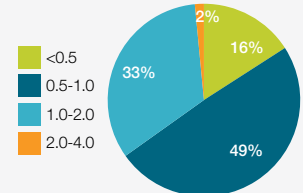
TraceFinder software view of leek matrix matched calibration curve of dichlorvos (0.5-500 µg/Kg) including extracted quantifier and qualifier ions at 1 µg/Kg. Acquired using 60K resolution at m/z 200.

GC Orbitrap vs. GC-MS/MS

GC Orbitrap



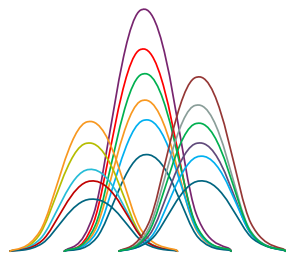
GC-MS/MS



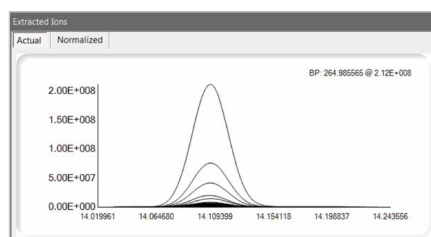
Instrument detection limit (IDL) of 150 pesticides in mixed vegetable matrix using a GC Orbitrap system (full-scan 60k at m/z 200) and GC-MS/MS system (SRM) with a fast GC separation.*

*Data collected on the Q Exactive GC system. The Exactive GC system provides the same level of performance when operated under the same conditions. Please refer to Exactive GC Specification Sheet (PS10506) and Exactive GC Technical Note (TN10511).

detect and refine

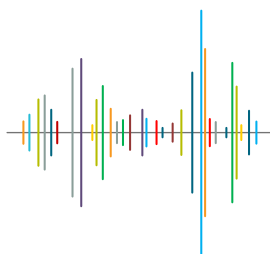


Part-per-trillion level sensitivity of the Exactive GC system in full-scan, with a wide dynamic range and HRAM drives high capacity component detection, even in your most complex samples. Specially designed algorithms perform spectral deconvolution, and generate high-fidelity spectra for each component detected.

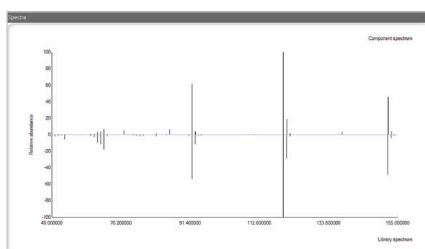


Accurate mass deconvolution extracts hundreds of components and provides a comprehensive profile of a brandy sample. Peak cluster shown has been extracted and can be library searched to identify the compound.

generate candidates

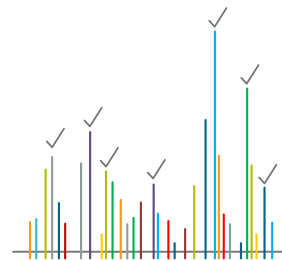


Refined mass spectra are then screened against spectral libraries to generate candidate compound lists based upon thresholded library match scores.



Component spectrum from peak at 7.8 minutes is library searchable and matched to multiple candidates in NIST 2014 spectral library.

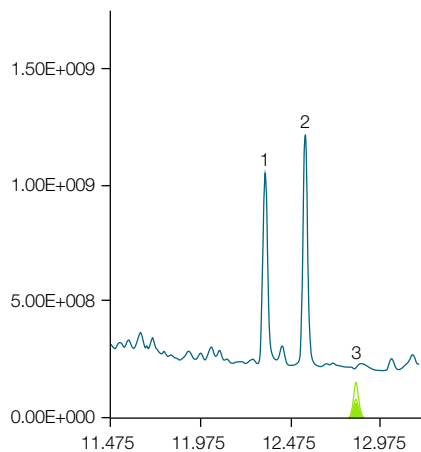
filter and identify



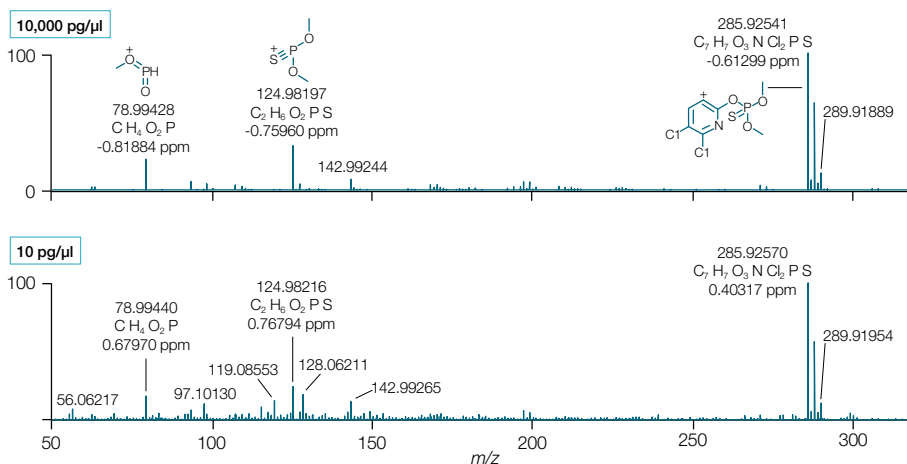
High-resolution filtering (HRF) algorithm uses accurate-mass information to discriminate against unlikely candidates based on elemental composition for every ion in the mass spectrum. This provides a high confidence identification of components detected.

Score	Matched Compound	Formula	CAS	SI	HRF Score
95.8	Benzoic acid, 2-(1-methylpropyl)oxy-, methyl ester	C12H14O3		854	99.2793
95.8	Benzoic acid, 2-(isopropyl)oxy-, methyl ester	C11H14O3		852	99.2793
95.8	Benzoic acid, 2-(2-methylpropyl)oxy-, methyl ester	C12H16O3		806	99.2793
95.4	Benzoic acid, 2-(2-methylbutyl)oxy-, methyl ester	C13H18O3		785	99.2793
95.1	Aspirin methyl ester	C13H14O4	580-42-9	807	94.8006
95.1	Benzoic acid, 2-iodoxy-, methyl ester	C12H13O3	5446-96-8	770	99.2793
95	Benzoic acid, 2-(3-methylbutyl)oxy-, methyl ester	C13H18O3		764	99.2793
94.8	Benzoic acid, 2-(pentyl)oxy-, methyl ester	C13H18O3	21018-10-0	751	99.2793

The list of proposed candidates are filtered based on a combination of search index and HRF to quickly propose an identity with a high degree of confidence. In this example, the list of 35 candidates are sorted based on search index and HRF to tentatively identify the compound as benzoic acid, methyl ester.



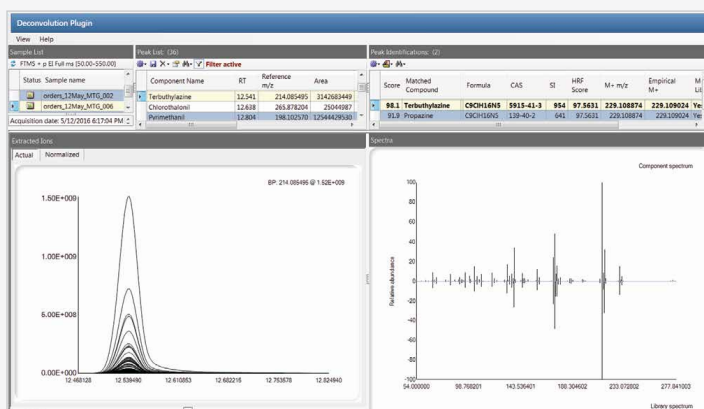
Accurate mass deconvolution extracts both high and trace level components to provide clean mass spectra and a comprehensive profile of a sample. Shown here are major peaks (1–2) in the TIC and a minor component in green (3).



Full-scan spectra of chlorpyrifos-methyl at 10,000 and 10 pg/μl with fragment assignment using Thermo Scientific™ Mass Frontier™ software. Spectral fidelity and sub 1 ppm mass accuracy is maintained across the spectrum at both low and high concentrations.

Intelligent Non-Targeted Screening

Automatic compound identification in a non-targeted way was once science fiction. Today, with the Exactive GC system and TraceFinder software, it's a reality. The sensitivity, selectivity and dynamic range of the Exactive GC system provides an unprecedented level of component coverage in GC-MS, and TraceFinder software intelligently mines data sets using automated software workflows that ultimately identify components within the sample. Data interpretation is available in minutes, instead of weeks, and an entirely new host of new possibilities is unleashed within your laboratory.



Adjustable scope of analysis

TraceFinder software allows the use of multiple library sources for automatic compound identification and these can be both nominal mass or exact mass. These can be existing spectral libraries that have been developed in-house, commercially available libraries such as NIST or Wiley or official Orbitrap GC-MS libraries. The scope of your non-targeted analysis can be easily adjusted; to narrow the scope: a more restricted library or sub-library can be configured; to broaden the scope: larger libraries or combinations of libraries can be used.

Bringing GC and Orbitrap Technology Together

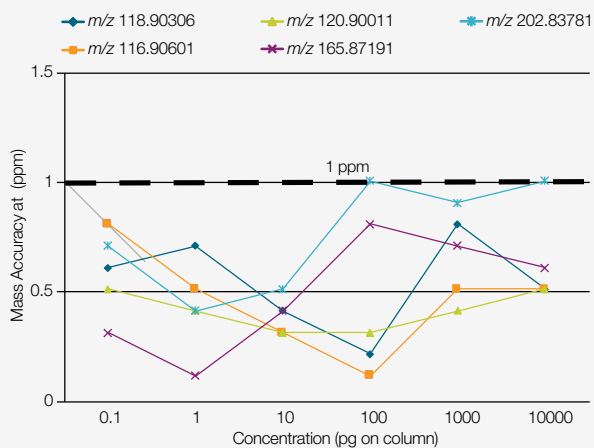
C-TRAP

Curved linear trap for precise ion injection—delivers excellent in-spectrum dynamic range and ensures outstanding HRAM performance across a wide range of concentrations through automatic gain control (AGC).

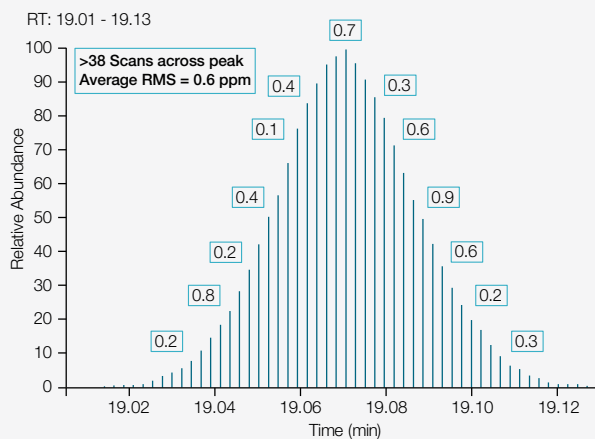


ORBITRAP MASS ANALYZER

High resolving power up to 60,000 FWHM at m/z 200, sub-ppm mass accuracy with a high acquisition rate, driving unrivaled spectral quality.



Mass accuracy of hexachloroethane ions <1 ppm over six orders of magnitude (0.1 to 10,000 pg. on column). High quality mass measurements are maintained for both trace and high concentration components.



Extracted ion chromatogram of chlorobenzilate (m/z 251.0025 \pm 5 ppm mass window) in leek spiked at 10 μ g/Kg showing >38 scans/peak (peak width 6 sec). Data acquired in full-scan at 60K FWHM resolving power. Excellent accurate mass (ppm) achieved for each individual scan (every third scan labeled). Average (RMS) mass difference of 0.6 ppm across the peak.

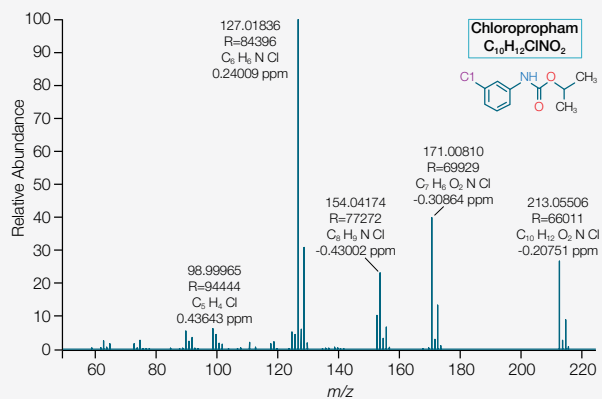
BENT FLATAPOLE

For lowest possible noise and maximum robustness.



Thermo Scientific™ ExtractaBrite™ ION SOURCE

Robust, rugged electron impact (EI) and chemical ionization (CI) performance – proven in routine applications in the Thermo Scientific™ ISQ™ and TSQ™ 8000 series GC-MS systems. Fully removable without breaking vacuum for maintenance or switching to chemical ionization (CI). Also exchangeable for a unique source plug, making GC columns easily exchanged, without venting the MS system.



60K (FWHM at m/z 200) acquisition spectrum of chloroproprham.



The operation and software handling is very simple.

– Jana Hajšlová

Transcend the traditional

Step into modern gas chromatography. Tailor the Thermo Scientific™ TRACE™ 1310 Gas Chromatograph to your needs with its proprietary user-exchangeable Instant Connect Injector and Detector modules. Swapping modules is easy to do by removing and replacing three screws, accessible from the top of the GC. The entire process takes less than five minutes without requiring specialized service assistance. This modularity enables budget-conscious laboratories to purchase a base-configured GC today, then easily expand their capabilities to accommodate new applications and throughput demands tomorrow.

Instant Connect Injectors

Instant Connect SSL

The Thermo Scientific™ Instant Connect SSL (Split/Splitless) Injector features an optimized thermal profile developed to avoid sample discrimination in split and splitless mode, allowing the broadest range of analytes to be accurately injected. Its cool injector head guarantees minimum thermal stress to the septum, therefore reducing bleed and extending septa lifetime. Also available with concurrent back-flushing.

Instant Connect-PTV

The Thermo Scientific™ Instant Connect PTV (Programmed Temperature Vaporizing) Injector combines the “discrimination-free” performance of a cold injector with the robustness of a vaporizing injector. Merging fast heating and cooling performance with the inertness of the injector chamber and large sample capacity, this injector is the ideal choice for trace analysis in dirty matrices and for thermally labile compounds. Also available with concurrent back-flushing.

Instant Connect Helium Saver Module

A unique solution to a difficult problem, this proprietary split/splitless injector module greatly reduces helium consumption, by using helium only to supply carrier gas flow to the capillary column, while using nitrogen for all other injection processes, including the septum purge, split, and sample vaporization.

Instant Connect Detectors

Instant Connect-FID

The Thermo Scientific™ Instant Connect-FID (Flame Ionization Detector) offers the highest sensitivity and a wide dynamic range with rapid acquisition speed, making it ideal for extremely fast GC applications.

Instant Connect-TCD

The newly-designed micro-volume Thermo Scientific™ Instant Connect-TCD (Thermal Conductivity Detector) is used in a wide variety of capillary and packed column applications. Due to its exceptional thermal stability and fast response, this non-destructive detector provides exceptional sensitivity over the widest range of applications.

Instant Connect-ECD

The new Thermo Scientific™ Instant Connect-ECD (Electron Capture Detector) is optimized for trace analysis in challenging samples. Its miniaturized cell, equipped with a purged, removable anode, has been designed to guarantee the utmost sensitivity while maximizing robustness towards the matrix effect.

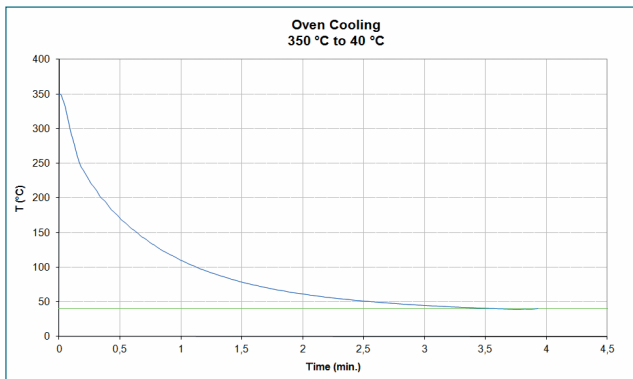
Instant Connect-NPD

Built upon the proven sensitivity of the Thermo Scientific™ Nitrogen Phosphorous Detectors (NPD), the new Instant Connect-NPD brings exceptional flexibility to the determination of specific components with the adoption of multiple dedicated ion sources.

Instant Connect-FPD

The Thermo Scientific™ Instant Connect-FPD (Flame Photometric Detector) provides excellent sensitivity and response stability for the most demanding sulphur applications, as well as phosphorous or tin determinations. Its extended operating temperature range and dual wavelength capability further expand its applicability.

Warm-up Times. From OFF Conditions to Readiness (minutes)		
Oven at 50 °C	TRACE 1300 Series GC system	Standard GC system
Injector and Detectors at 250 °C	3.5	10.2



The TRACE 1300 Series GC system quickly reaches near ambient temperatures.

Fast oven temperature cycling and excellent retention time performance mean that high-precision, high-productivity data sets can be realized. This type of data is especially important to facilitate statistics in larger batches, e.g., in “-omics”-type studies with many biological or technical replicates.



Exceptional Retention Time Stability

Outstanding retention time stability is achieved, even in the most complex GC and GC-MS applications, through the use of innovative and unique IEC (integrated electronic control) modules. This stability guarantees industry-leading 0.001 psi control through the entire working range. These miniaturized gas controls, integrated within every injector or detector module for compact, self-sufficient, fully-featured devices, deliver strictly controlled pressure or flow to columns and detectors. Setting constant or ramped pressures and flows is easy through the software or the local user interface, while the electronic control maintains the stability during every run for exceptional retention time, accuracy, and precision. To further enhance analytical performance, the IEC module also supports the automated leak check of the injector and column installed and column evaluation procedures.

Hydrocarbon	Mean RT Min.	Std. Dev. Min.	Hydrocarbon	Mean RT Min.	Std. Dev. Min.
C12	4.6200	0.0003	C28	12.4725	0.0005
C14	6.0192	0.0004	C30	13.1348	0.0006
C16	7.2268	0.0005	C32	13.7557	0.0006
C18	8.3051	0.0005	C34	14.3395	0.0007
C20	9.2825	0.0006	C36	14.8908	0.0005
C22	10.1767	0.0006	C38	15.4118	0.0007
C24	10.9997	0.0004	C40	15.9063	0.0006
C26	11.7629	0.0005			

Retention time stability on 10 consecutive runs of hydrocarbon mix. Retention time standard deviation is always $\leq 1/1000$ minute.

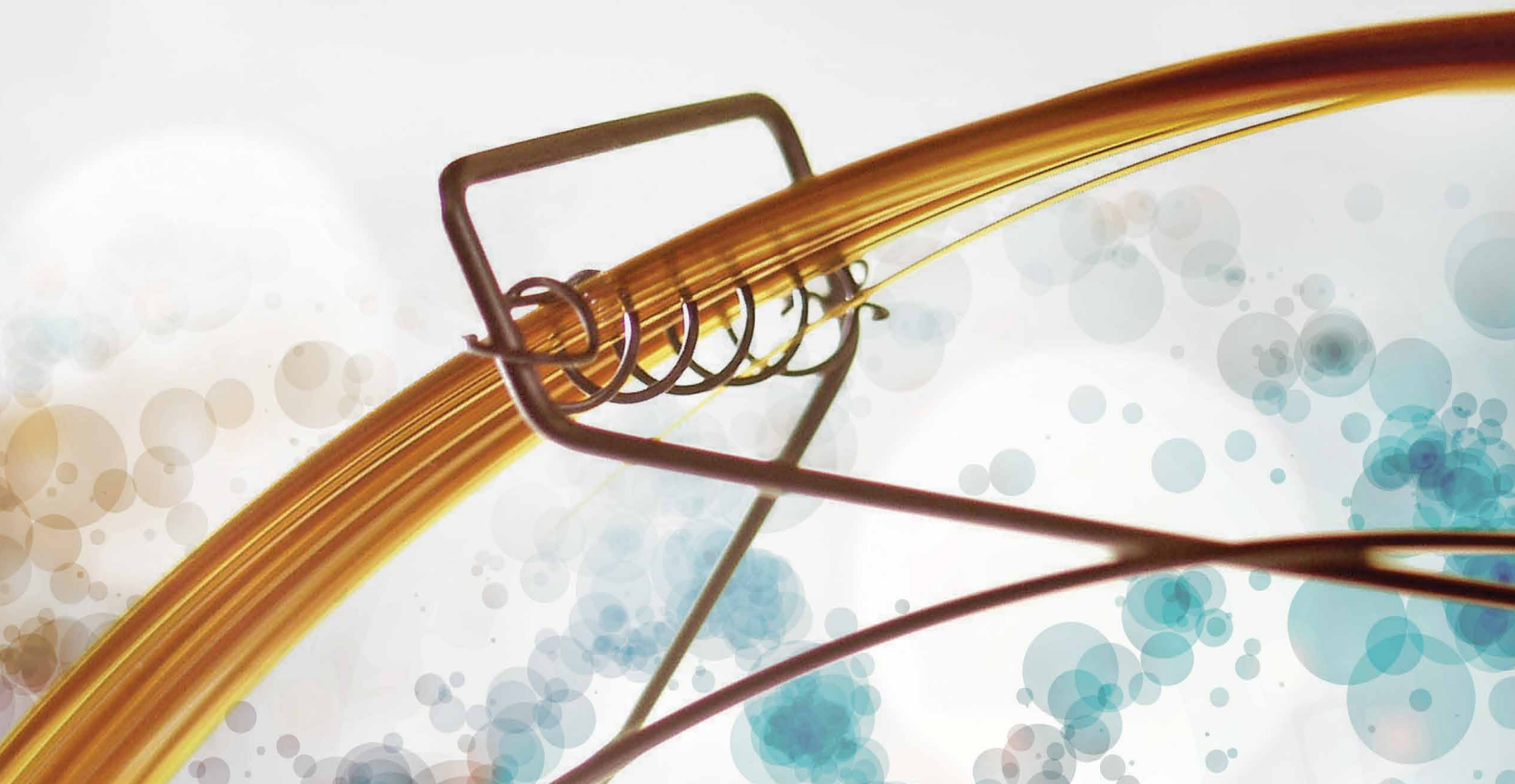
A step ahead in automated sampling

A perfect match for the Exactive GC system, the Thermo Scientific™ TriPlus™ RSH autosampler utilizes robotic sample handling to expand automated capabilities beyond liquid, headspace, and solid-phase microextraction (SPME) injections to advanced sample handling cycles. Your results benefit from improved precision and reproducibility, while your laboratory gains unique advantages from the system’s unattended operations and sample handling flexibility.

- Automate basic sample and standards preparation procedures such as dilution, internal standard addition, and derivatization.
- High precision injection from low volumes to maximize your analysis opportunities with your most precious samples.
- Automated toll exchange to switch between different syringes and techniques “on-the-fly”.

1 μ L splitless injection		40 ppm C20 in toluene
Volume in vial (μ L)	Peak area	
50	81244277	
40	80268993	
30	82088809	
20	82095395	
10	84436788	
5	84312030	
RSD%	2.0	

The TriPlus RSH autosampler provides excellent repeatability with microsamples, down to 5 μ L in a vial. This feature is particularly interesting for trace analysis, radioactive samples, or samples requiring expensive internal standards.



Thermo Scientific Chromatography Columns and Consumables

Get the most out of the Exactive GC system by pairing it with advanced, high-performance Thermo Scientific products. Our wide range of consumables and accessories offer customers applications-focused solutions in the environmental, food safety, toxicology, clinical, petrochemical, pharmaceutical, and general analytical industries.

- Thermo Scientific™ TraceGOLD™ columns – low bleed, high reproducibility
- Consumables tested and certified on the Thermo Scientific™ TRACE™ 1300 Series GC systems
- Vials guaranteed for Thermo Scientific autosampler systems
- Thermo Scientific™ GFM Pro Gas Flowmeter and Thermo Scientific™ GLD Pro Gas Leak Detector for system installation and maintenance
- Derivatization reagents and derivatization-grade solvents

Learn more: thermofisher.com/chromexpert

Find out more at thermofisher.com/ExactiveGC

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BR10505-EN 0716S