thermo scientific

A new chapter in GC-MS

Thermo Scientific Q Exactive GC Orbitrap GC-MS system

ThermoFisher SCIENTIFIC

Unprecedented Depth in GC-MS Analysis

The Thermo Scientific™ Q Exactive™ GC Orbitrap GC-MS/MS system has finally arrived. For years, scientists have demanded this highly anticipated, high-resolution, accurate-mass (HRAM) system in fields ranging from metabolomics to food safety, industrial, clinical, and pharmaceutical analysis. These scientists understand the power that only Thermo Scientific™ Orbitrap™ technology can bring to the detailed characterization of their most challenging samples.

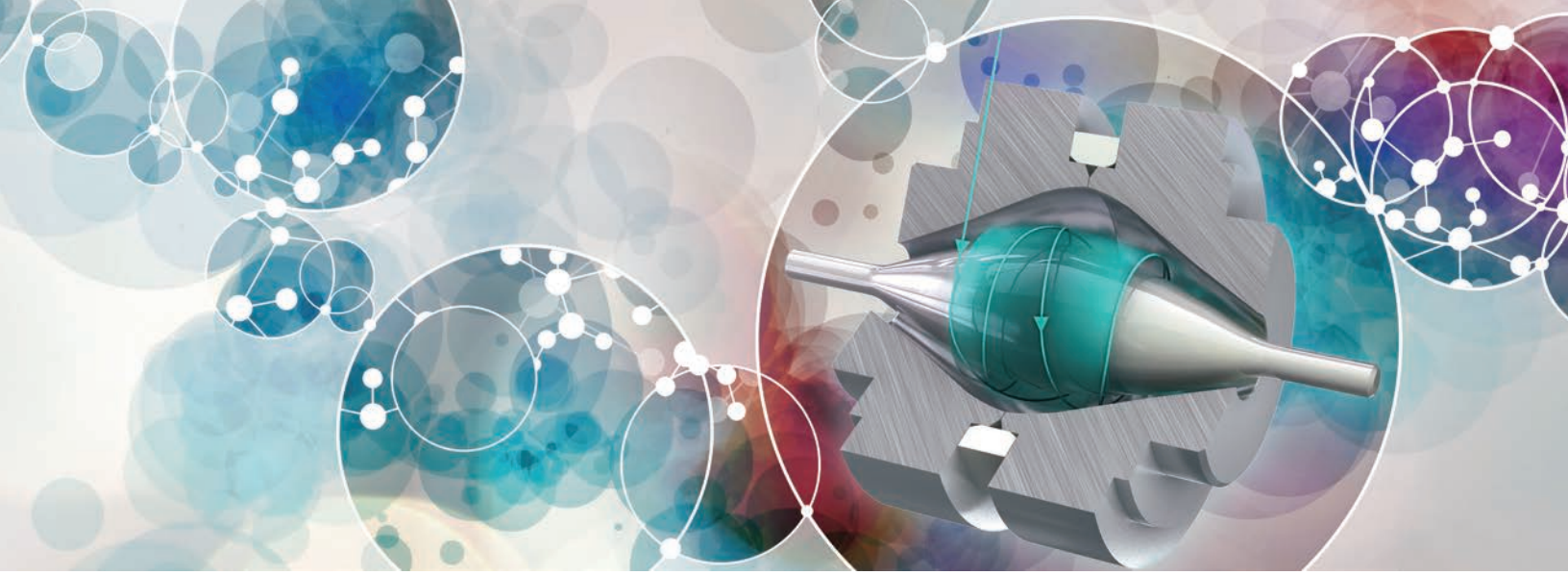
Until now, GC-MS technology has been limited in its ability to collect comprehensive qualitative and quantitative sample information with high levels of selectivity, sensitivity and confidence; especially in highly complex samples.

Today, the Q Exactive GC system makes this comprehensive analysis a reality. It is an easy-to-use, dedicated benchtop GC-MS system that provides the highest confidence in compound discovery, identification, and quantitation for a comprehensive understanding of your samples. This unmatched performance is achieved through the superior resolving power, mass accuracy, and sensitivity that only Orbitrap technology can deliver.

The capabilities of the Q Exactive GC system create a paradigm shift for analysis of GC-amenable compounds and signal the start of an exciting new chapter in GC-MS…

"GC Orbitrap technology significantly expands the firepower of GC-MS, which will spark an acceleration in discovery for small molecule analysis across multiple applications."

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



“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 introduction of the Q Exactive GC system is a game changer in this space.”

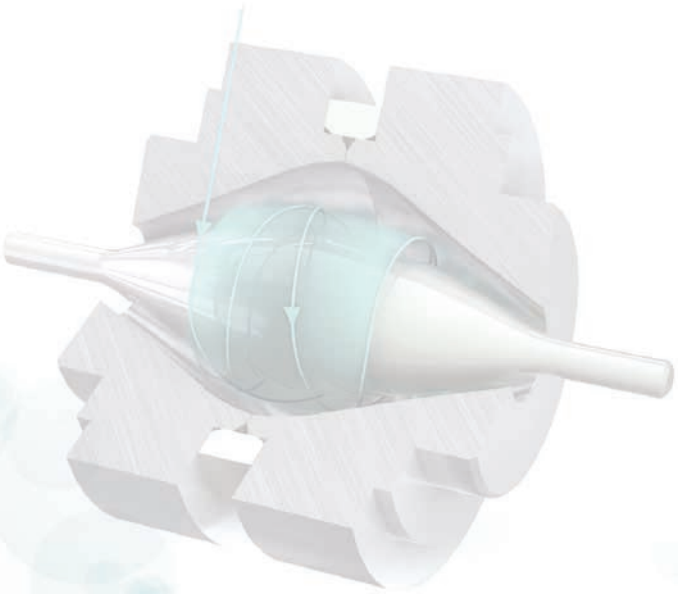
Prof. Joshua Coon
Department of Chemistry
University of Wisconsin, USA
Proteomics and Metabolomics

“This is the technology platform I have been waiting for since I started in metabolomics.”

Dr. Karl Burgess
Glasgow Polyomics
University of Glasgow, UK
Metabolomics

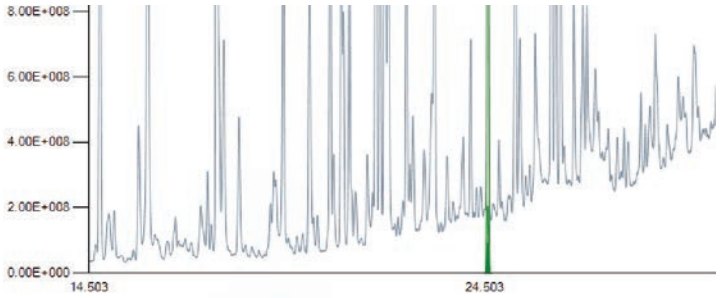
The ultimate profiling tool

Superior compound discovery and identification: the Q Exactive Orbitrap GC-MS/MS system provides you with the power to discover features within a sample that went unnoticed with previous GC-MS technology. This unrivalled combination of high-resolution gas chromatography separations and highly sensitive HRAM acquisitions and intelligent identification software will help unlock answers to questions about the very nature of each sample you inject.



High capacity component detection

Part-per-trillion level sensitivity of the Q Exactive GC system in full-scan with a wide dynamic range and HRAM drives high capacity component detection, even in your most complex samples.

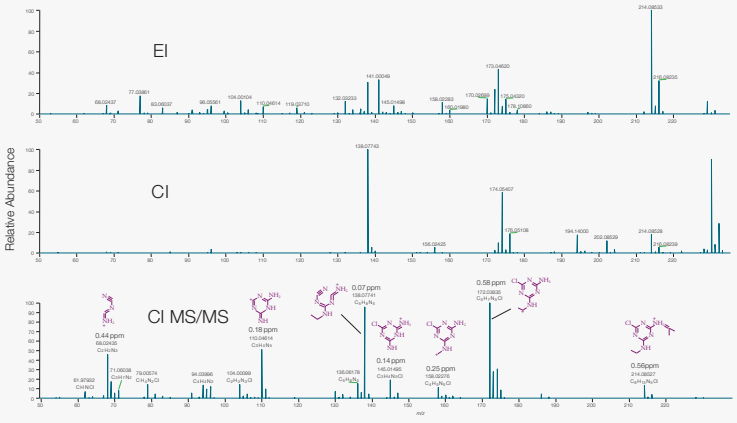


Full-scan acquisition (60,000 resolution at *m/z* 200) of a food packaging sample from an extractables and leachables study. A single, unidentified component is visible within the complex matrix background.

High confidence confirmation

For further information and/or confirmations of compounds, positive chemical ionization (PCI) can be used to yield molecular ions. These ions can be measured directly in the Orbitrap or after fragmentation in the HCD for further HRAM investigation into the compound structure.

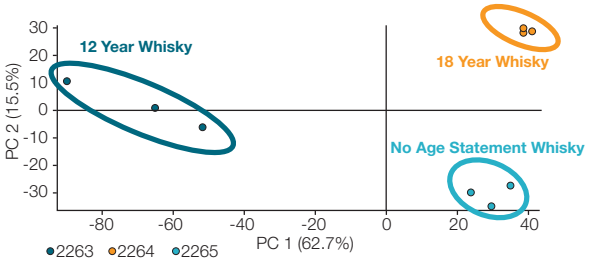
This technology will greatly facilitate the identification of unknown compounds.
– Joshua Coon



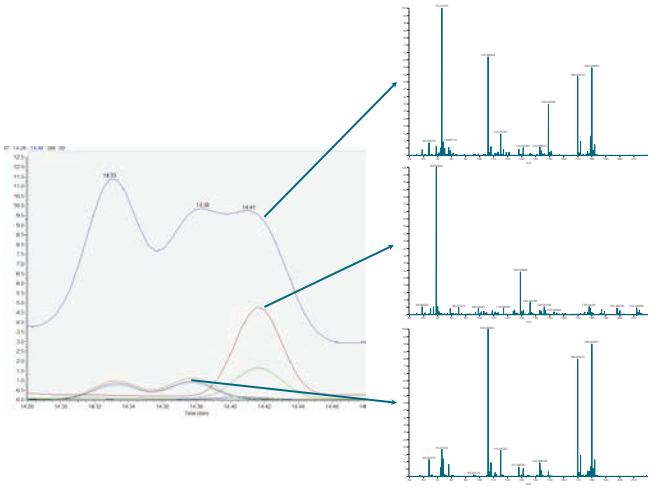
EI, PCI, and PCI – MS/MS spectra (60,000 resolution at *m/z* 200) of terbuthylazine with fragment structure assignment using Thermo Scientific™ Mass Frontier™ spectral interpretation software.

Highly resolved components for chemometric analysis and compound identification

In addition to the highest quality raw data, the Q Exactive GC system uses newly developed specialist deconvolution software tools to automatically detect components within your sample and generate clean spectra for further data processing steps.



Principle component analysis (PCA) generated using Thermo Scientific™ Compound Discoverer™ 2.0 software from a study profiling single malt whiskies of different age declaration using the Q Exactive GC system.



Co-eluting compounds are deconvoluted to obtain clean mass spectra

The Q Exactive GC brings highly resolved data that allows for advanced deconvolution providing high quality inputs for downstream contextualization software. And the ability to predict elemental formulae of each EI fragment is hugely powerful for metabolite identification.

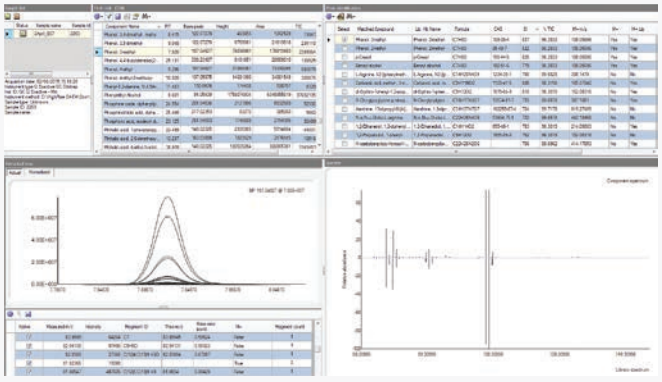
– Karl Burgess

Powerful software for intelligent identification

The Q Exactive GC system uses vast, readily available nominal mass electron ionization (EI) libraries (such as NIST and Wiley) to generate candidate compounds. Hits can be verified automatically using Kovats retention indices and intelligent exact mass interpretation of the fragmented mass spectrum acquired. Customized HRAM libraries can also be used.

Analyzing whiskey and pesticide samples, to my surprise, many compounds where automatically identified.

– Jana Hajšlová



High quality deconvolution of spectra from a Scotch whiskey sample during an authenticity study. Automatic identification of unknown peaks was performed using intelligent identification software.

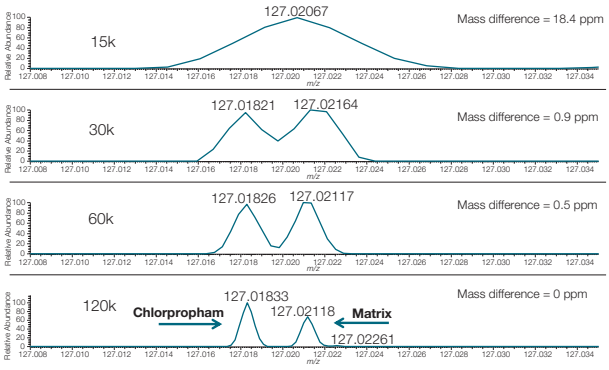
The ultimate screening tool

Analyzing compounds present at low concentrations, quantitatively, with high selectivity using full-scan acquisition has been out of reach for GC-MS users for too long. Many leading laboratories in various fields require simultaneous targeted and untargeted sample screening, but that need went unmet until now. Today, the Q Exactive GC system has the quantitative power of a GC triple quadrupole MS combined with the high precision, full-scan high resolution/ accurate mass capability that only Orbitrap technology can offer. This combination will change your workflows, forever.

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

The Q Exactive GC system offers routine operation, possible at 60k–120k 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 screening methods for food safety, environmental, anti-doping, and many other applications where ultra trace-level detection is required in difficult matrices.

For pesticides, I could safely see very low levels.
– Jana Hajšlová

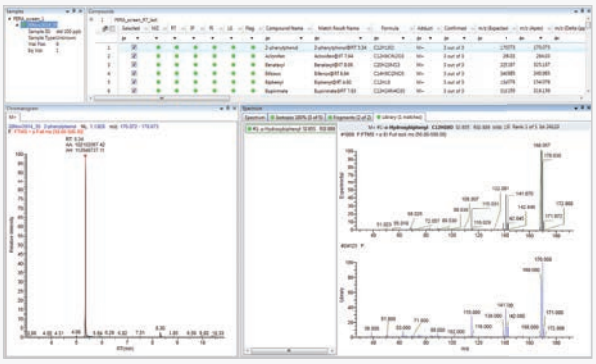


Acquisition at 15k yield false negative results based upon identification criteria. Chlorphropham example XIC shows resolution values of 60k and 120k, providing interference-free, confident detection with excellent mass accuracy.

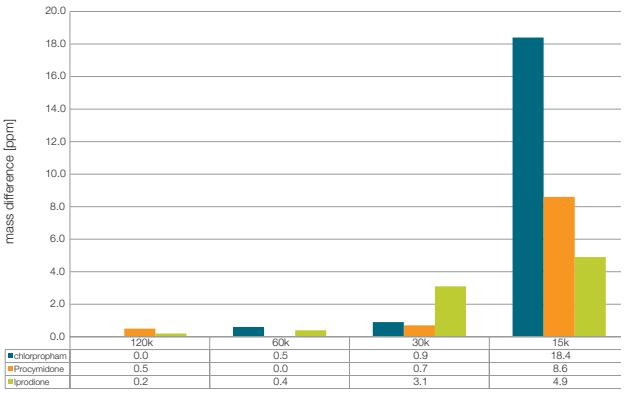
Quantitation capability beyond that of other benchtop HRAM GC-MS systems

Using full-scan acquisition, the Q Exactive GC system provides the quantitative capability of a GC triple quadrupole instrument operating in selected reaction monitoring (SRM) mode. Sensitivity, quantitative accuracy, precision, and linearity are excellent, even in complex matrices.

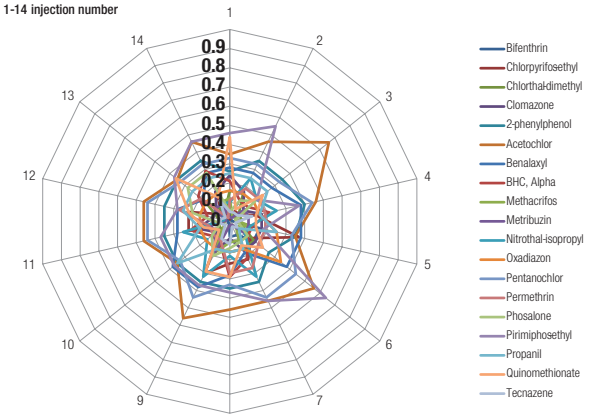
The wide dynamic range of the system, along with its high sensitivity, will bolster all quantitative experiments dramatically.
– Joshua Coon



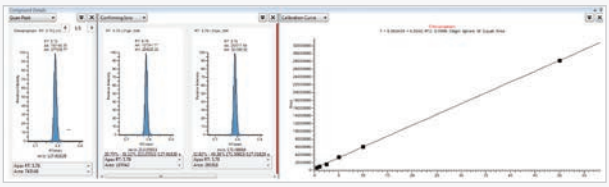
Thermo Scientific™ TraceFinder™ software uses Q Exactive GC system data and combines compound detection, identification, and quantitation to enable high efficiency screening. It also allows customizable, automated flagging for detected peaks along with highly flexible reporting tools.



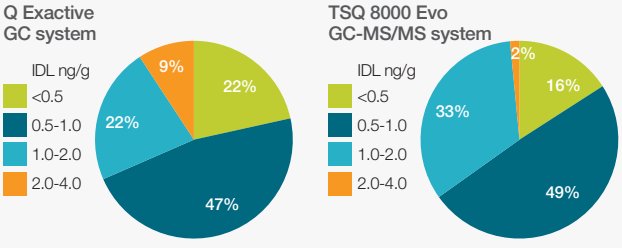
Effect of resolution (specified @ *m/z* 200) on mass accuracy for pesticides in leek samples at 10 ng/g.



Mass accuracy across n=14 repeat injections of a baby food sample spiked with several pesticides at 5 ng/g.



Wheat matrix calibration curve of chlorpropham (0.5 ppb–50 ppb) including extracted quantifier and qualifier ions at 0.5 ppb. Acquired using 60k resolution at *m/z* 200.



Instrument detection limit (IDL) of 150 pesticides in mixed vegetable matrix using the Q Exactive GC system (full-scan 60k at *m/z* 200) and Thermo Scientific™ TSQ™ 8000 Evo GC-MS/MS system (SRM) with a fast GC separation.

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

Bringing GC and Orbitrap technology together

ADVANCED QUADRUPOLE TECHNOLOGY (AQT)

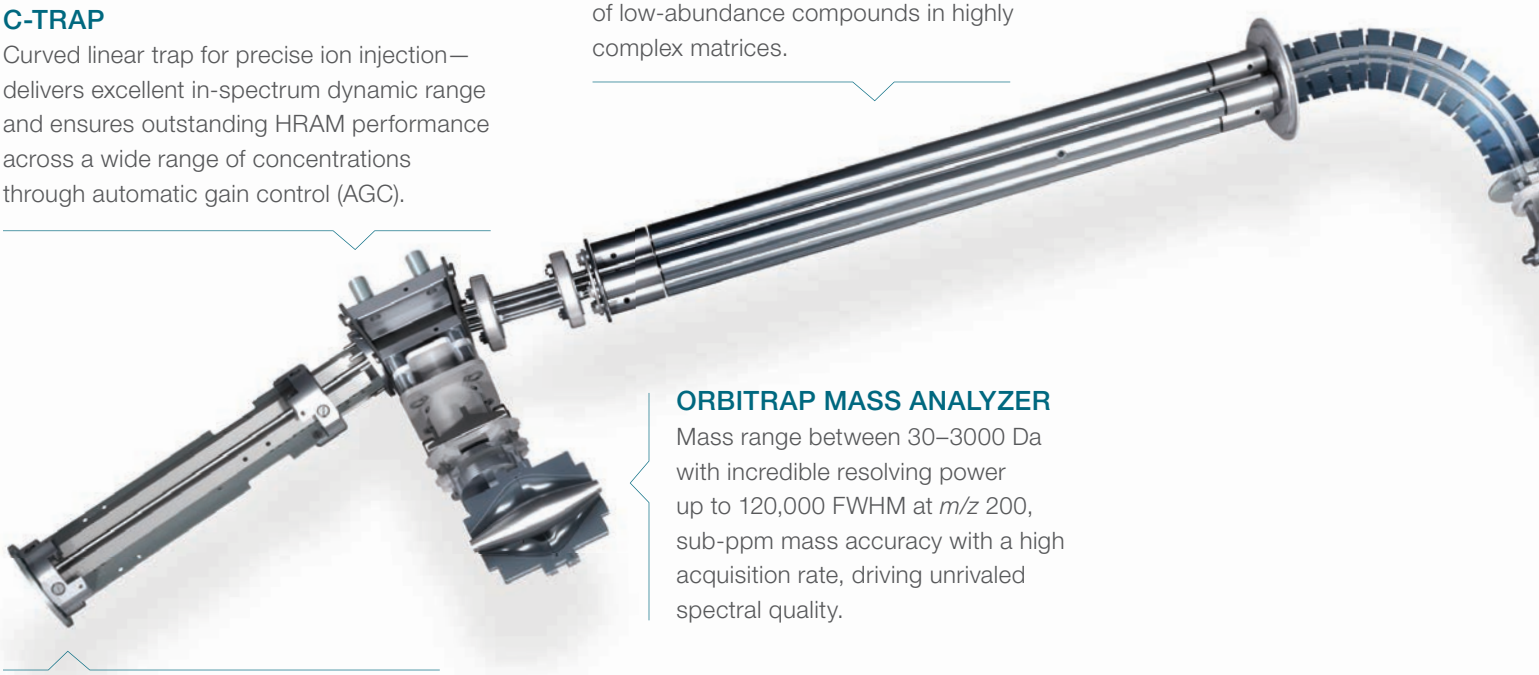
High transmission of selected masses for low-level detection and quantitation of low-abundance compounds in highly complex matrices.

BENT FLATAPOLE

For lowest possible noise and maximum robustness.

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).

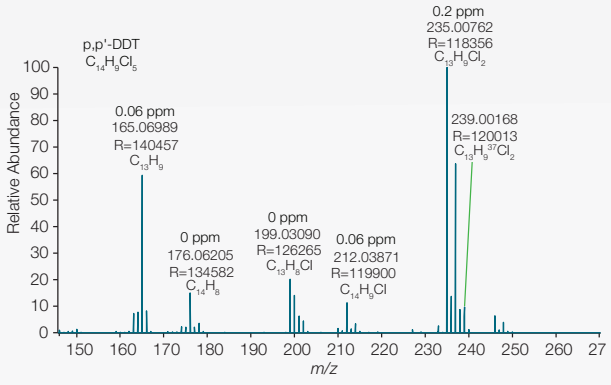


ORBITRAP MASS ANALYZER

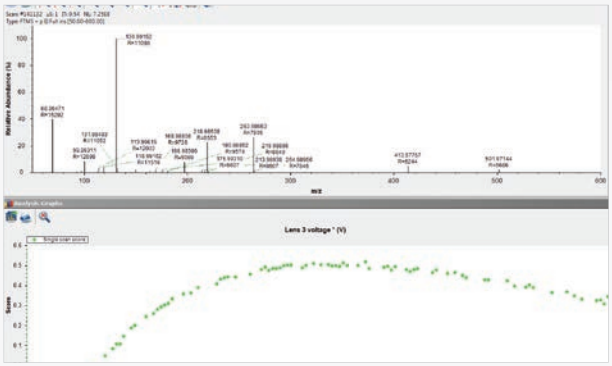
Mass range between 30–3000 Da with incredible resolving power up to 120,000 FWHM at *m/z* 200, sub-ppm mass accuracy with a high acquisition rate, driving unrivaled spectral quality.

HCD COLLISION CELL

Higher-energy collisional dissociation for MS/MS characterization of ions—used in combination with chemical ionization to help elucidate chemical structures.



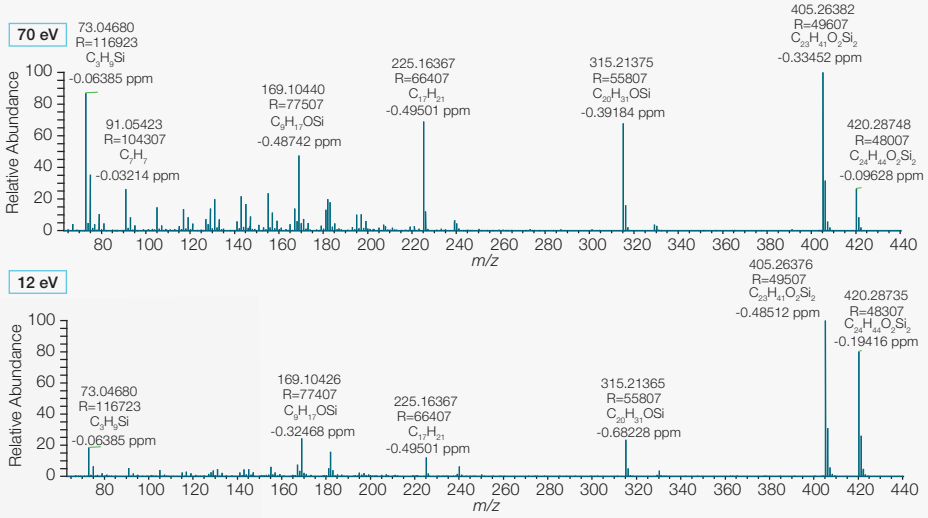
Full-scan spectrum of p,p'-DDT acquired at 120,000 resolution (@ *m/z* 200).



Fastest route to powerful data

With the Q Exactive GC system it is easy to obtain powerful results. The instrument control page provides clear instrument status information, leak check is automated, and mass spectrometer tuning and calibration takes less than a minute.

The operation and software handling is very simple.
– Jana Hajšlová



Epitestosterone shown with standard EI and VeV EI. Using VeV, the molecular ion signal and high mass fragment abundance are greatly increased, improving sensitivity for quantitative analysis and further MS/MS fragmentation experiments.

Variable electron voltage (VeV) technology enables lower electron voltage (eV) settings for Electron Ionization (EI). It is a softer EI technique, which promotes higher mass signals and increases sensitivity for compounds prone to extensive fragmentation.

Key benefits:

- Increased sensitivity—Compounded by the unrivalled full-scan sensitivity of Orbitrap
- Increased confidence in identification—VeV promotes molecular ion and diagnostic high mass signals
- Fully automated for optimum performance—Following the simplicity of Orbitrap GC-MS operation, VeV set-up is easy, with fast, fully automated tuning

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 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.

Direct probes are used without requiring a break in the vacuum, and they enable the performance of MS and MS/MS experiments on solids and liquids/solutions in real-time while effortlessly switching between electron ionization (EI) and chemical ionization (CI).

Direct Insertion Probe (DIP)—Slower volatilization with heated capillary tube for solid samples. The DIP can be utilized for rapid analysis of solids or trace components in solid matrices such as organic synthesis products, forensic samples, tissue, etc.

Direct Exposure Probe (DEP)—Rapid heating filament for liquids or solutions. The DEP is ideal for rapid molecular weight confirmation of solids dissolved or suspended in a suitable solvent.

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 backflushing.

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 backflushing.

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.

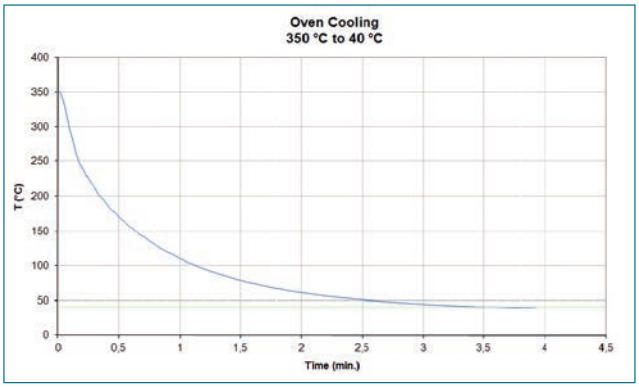
Instant Connect-NPD

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 appliations, as well as phosporous 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 Injector and Detectors at 250 °C	TRACE 1300 Series GC system	Standard GC system
	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.

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".

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 ≤1/1000 minute.

1 µL splitless injection	40 ppm C20 in toluene
Volume in vial (µL)	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 µL in a vial. This feature is particularly interesting for trace analysis, radioactive samples, or samples requiring expensive internal standards.

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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/QExactiveGC**

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