



Persistent organic pollutant analysis

Comprehensive workflows for regulatory compliance

Persistent organic pollutant analysis

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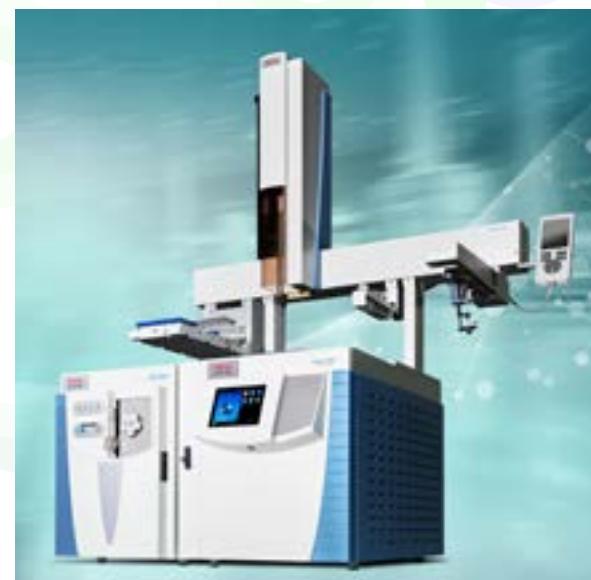
GC-MS solutions

Thermo Scientific™ TSQ™ 9000 GC-MS/MS, Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system

Thermo Scientific™ Q Exactive™ GC Orbitrap™ LC-MS/MS

Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS

Data analysis tools and software



POPs analysis: a global concern

Persistent organic pollutants (POPs) are toxic chemicals, produced either intentionally or as byproducts of industrial activity, that don't break down easily.

Due to the persistent nature of POPs, many of these compounds bioaccumulate in the fatty tissue of animals and migrate naturally up the food chain. It is through this biomagnification mechanism that these contaminants negatively influence human health and development. Particular concerns exist over the accumulation of POPs compounds in human breast milk.

In addition to adverse health and environmental risks, POPs exposure events can negatively impact the world's economy as well. Food contamination incidents can quickly become global news, damage brands, and affect trade at the international level.

Global concern over the presence and impact of POPs contamination has produced a need for strategies to restrict, reduce, and eliminate such chemicals in the environment.

In an effort to manage these contaminants, the Stockholm Convention on POPs (an international treaty from the United Nations Environment Programme to restrict or eradicate POPs) was ratified by more than 160 nations. As a result, all parties must try to eliminate or reduce the release of POPs into the environment. Two key members – the United States (US) and European Union (EU) – have put strict testing requirements into place through the US Federal Department of Agriculture (FDA), US Environmental Protection Agency (EPA), and EU Commission.

International focus on POPs, for both health and economic reasons, has led to the continuous monitoring of POPs in food, food additives, and the environment in an effort to measure and control exposure. While fatty foods such as fish, milk, and cheese are most frequently analyzed due to their high potential for contamination, the entire food industry should be aware of the potential for POPs contamination and adopt strategies to actively manage this concern.



POPs analysis: a global concern

Emerging Contaminants

New BFRs, dicofol, short-chained chlorinated paraffins, chlorinated naphthalenes, hexachlorobutadiene, pentachlorophenol and other emerging unknowns

Eliminate, Restrict, and Reduce

Dioxins and furans (PCDD/Fs), PCBs, BFRs, PFOS, PFOA, BDE-209, organochlorine pesticides (OCPs), metabolites / breakdown products / production intermediates / production byproducts and many more

Routine LC and LC-MS Analysis

Thermo Scientific™ TSQ Quantis™ LC-MS/MS
Thermo Scientific™ TSQ Altis™ LC-MS/MS
Thermo Scientific™ TSQ Fortis™ LC-MS/MS
Thermo Scientific™ Orbitrap Exploris™ 120 LC-MS
Thermo Scientific™ Vanquish™ Core UHPLC
Thermo Scientific™ Vanquish™ Flex UHPLC
Thermo Scientific™ Vanquish™ Duo for Tandem LC-MS

Routine GC and GC-MS Analysis

TSQ 9000 GC-MS/MS
DFS Magnetic Sector GC-HRMS

Research Analyze Analysis

Exactive GC Orbitrap GC-MS system
Q Exactive GC Orbitrap LC-MS/MS

Comprehensive capabilities for POPs workflows

Sample Login

Sample Preparation

Sample Analysis

Data Analysis



Easily track samples through the facility down to specific cabinet or freezer locations.

Simplify, accelerate, and automate sample preparation to increase productivity and reduce cost per sample.



Rapidly separate and analyze complex samples with industry-leading chromatography and mass spectrometry solutions.

Maximize the functionality and efficiency of sample analysis and data interpretation with comprehensive software.



Optimum system performance

GC columns and consumables

Analysis for POPs content is performed on a variety of sample types including food, water, and soil. Our broad range of high-quality chromatography columns and consumables is designed to ensure that analytical systems operate at peak performance providing optimal sample assessment regardless of matrix type.

Thermo Scientific™ TraceGOLD™ GC columns provide excellent quality and performance by offering:

- Ultra-low bleed
- Excellent reproducibility, column-to-column and run-to-run
- Superior inertness



Our comprehensive range of high-quality GC consumables has been thoroughly tested on Thermo Scientific GC and GC-MS systems to ensure confidence in your measured results.

- Thermo Scientific™ LinerGOLD™ GC liners – Deliver increased accuracy and precision in analysis
- Septa in blister packs – Enhance GC septa cleanliness
- Precision-manufactured GC syringes – For accurate sample introduction
- Ferrules – Available in a variety of materials and dimensions to match your system

Supporting all techniques

LC columns and consumables

Thermo Scientific LC and LC-MS columns and consumables are designed to meet the challenging requirements of POPs analysis:

- Thermo Scientific™ Accucore™ columns – Ultimate Core Performance, speed and selectivity combined
- Thermo Scientific™ Acclaim™ columns – Optimal selectivity through innovative chemistry
- Thermo Scientific™ Hypersil GOLD™ columns – Outstanding peak shape for your separations



Thermo Scientific™ AVCS (Advanced Vial Closure System) and SureStop™ vials provide the next generation of sample handling. The AVCS design allows for consistent sealing, eliminating user-to-user variance. The SureStop vial provides optimal cap positioning and eliminates cap tilt and septa displacement due to over-tightening.

Accelerated solvent extraction

Walk-away automation for improved productivity

Thermo Scientific™ Dionex™ Accelerated Solvent Extraction (ASE) Systems

The Dionex ASE 350 and ASE 150 systems are used for the extraction of organic pollutants from solid and semisolid samples. Elevated temperature and pressure are used with organic and aqueous solvents to increase the efficiency of the extraction process. Flow-through technology allows in-line filtration, and in-cell cleanup eliminates the need for offline cleanup procedures such as gel permeation chromatography. Use of the novel water absorbing polymer Dionex ASE Prep MAP expands the capabilities of the accelerated solvent extraction technique and allows for the extraction of analytes from samples containing up to 85% water.

Dionex ASE instruments meet the requirements of the US EPA Method 3545A for extraction of persistent organic pollutants from environmental matrices including soils, sediments, sludges, tissues, air sampling cartridges, and fly ash. These systems are also suitable for extraction of pollutants from high-fat content and dry foods such as avocados and tea. Dionex ASE systems are equivalent to or better than Soxhlet, automated Soxhlet, sonication, and shaking techniques.

Comparative accelerated solvent extraction technique / Soxhlet extraction of sediment contaminated with low concentrations of dioxins. See chart details in our [Application Note 323, Extraction of PCDD/Fs from Environmental Samples Using Accelerated Solvent Extraction Technique.](#)

Average Values (ng/kg) from HS-2 –Comparison of Soxhlet vs. Accelerated Solvent Extraction Technique						
Group Totals	Soxhlet Extraction (n=4)			Accelerated Solvent Extraction Technique (n=2)		
	Value	% RSD	Isomers	Value	% RSD	Isomers
Total T ₄ CDD	3.9	14	2	2.5	34	5
Total P ₅ CDD	17	7.8	6	10	10	9
Total H ₆ CDD	510	5.6	8	570	1.3	7
Total H ₇ CDD	4700	8.3	2	5100	11	2
Total O ₈ CDD	6500	4.2	1	7100	0	1
Total T ₄ CDF	39	11	13	24	3	14
Total P ₅ CDF	33	13	8	28	0	11
Total H ₆ CDF	89	3.2	6	87	12	10
Total H ₇ CDF	293	3.3	4	310	0	4
Total O ₈ CDF	300	3.8	1	280	2.6	1
Congeners	Value	% RSD	Isomers	Value	% RSD	Isomers
2,3,7,8-Total T ₄ CDD	n.d. (1)		62	n.d. (1)		71
1,2,3,7,8-Total P ₅ CDD	1.6	4.6	69	n.d. (1)		75
1,2,3,4,7,8-Total H ₆ CDD	4.5	4.8	74	5.2	11	73
1,2,3,6,7,8-Total H ₆ CDD	19	4.3	75	21	0	50
1,2,3,7,8,9-Total H ₆ CDD	24	4.3	74	28	2.6	61
1,2,3,4,6,7,8-Total H ₇ CDD	1200	8.1	80	1300	0	93
2,3,7,8-Total T ₄ CDF	8.5	11	62	6.6	5.4	65
1,2,3,7,8-Total P ₅ CDF	1.9	17	68	2	0	72
2,3,4,7,8-Total P ₅ CDF	3.7	7.9	71	3.7	3.8	59
1,2,3,4,7,8-Total H ₆ CDF	17	7.3	79	17	4.3	70
1,2,3,6,7,8-Total H ₆ CDF	3.7	5.6	80	4	5.4	49
2,3,4,6,7,8-Total H ₆ CDF	3.7	18	81	4.4	3.2	61
1,2,3,7,8,9-Total H ₆ CDF	n.d. (1)		83	n.d. (1)	0	75
1,2,3,4,6,7,8-Total H ₇ CDF	91	1.6	83	96	3.7	82
1,2,3,4,7,8,9-Total H ₇ CDF	5.2	6.7	84	5.3	6.7	83

Solid-phase extraction and evaporation

Broad support for sample preparation techniques

Thermo Scientific™ Dionex™ AutoTrace™ 280 Automated Solid-Phase Extraction (SPE) System

The Dionex AutoTrace 280 SPE instrument is a powerful, high-throughput workstation that provides walk-away automation, suitable for US EPA 500, 600, and 1600 Methods. A comprehensive range of [SPE accessories](#) provides clean, consistent extractions. SPE phases include C18, activated carbon, and polymeric resins in multiple chemistries, as well as SAX, SCX, WCX, WAX, and a hydrophobic reversed phase that will accommodate drinking, ground, surface, and wastewater samples.



Dionex AutoTrace 280 System



Thermo Scientific™ Dionex SolEx™ SPE Cartridges



Thermo Scientific™ HyperSep™ SPE Cartridges and Plates



Dionex ASE 350 System



Rocket Synergy 2 Evaporator

The Thermo Scientific™ Rocket Synergy™ 2 Evaporator

Concentration and evaporation is an important step in achieving accurate analytical results with sample extracts. The Rocket Evaporator automates this process and can be used either to dry samples completely or to concentrate them directly into autosampler vials. This system can process large volumes of solvent extract (up to 450 mL) and also allows direct transfer of 60 mL extract from the accelerated solvent extraction system to eliminate manual sample transfer steps.

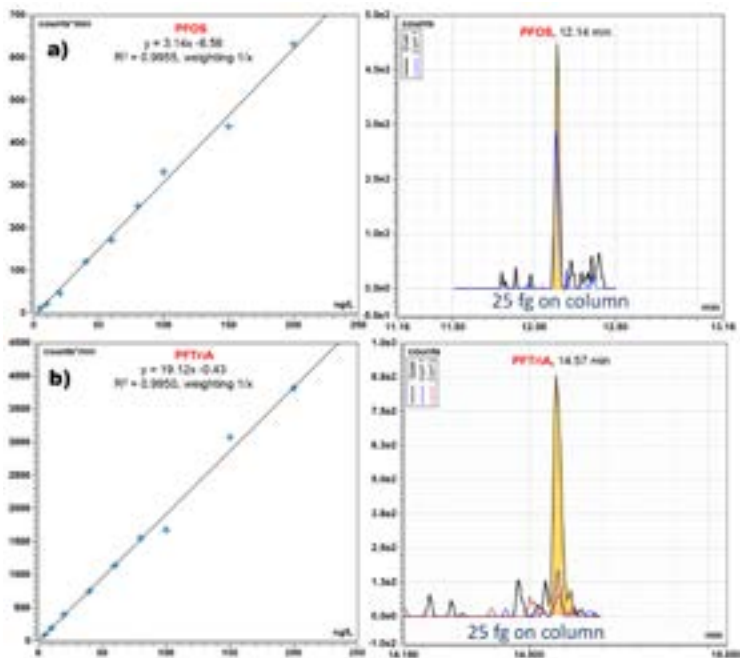
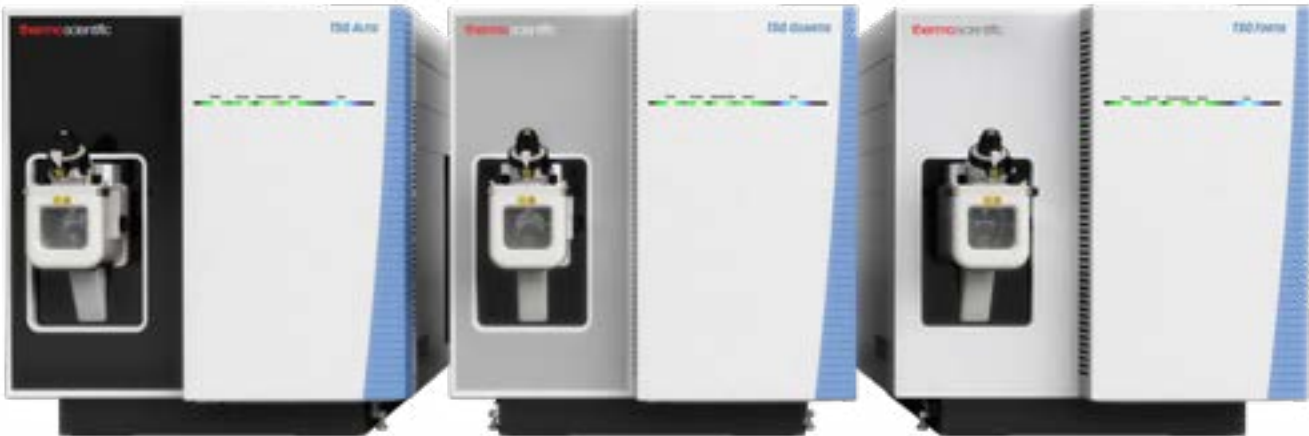
Extreme quantitative performance

LC-MS Triple Quadrupoles

Continual changes in POPs research and regulatory requirements drive the need for ever-lower limits of detection and quantitation. The Thermo Scientific™ TSQ Quantis™, TSQ Altis™, and TSQ Fortis™ mass spectrometers use active ion management to exceed even the most stringent analytical requirements with superb sensitivity, speed, and dynamic range. It does so with an ease of operation—from method development through routine maintenance—that allows users to spend more time thinking about their research and less time worrying about instrument setup and operation.

The emerging contaminants PFOS and PFOA are extremely persistent in the environment and resistant to typical environmental degradation processes. Use of LC-MS/MS has enabled more sensitive determinations of individual PFOS and PFOA¹. The unique features of the Thermo Scientific LC-MS/MS platforms allow sensitive detection and quantitation in matrix to address these more stubbornly resilient POPs compounds.

¹EFSA 2008; Jahnke and others 2007b; Washington and others 2008.



Representative calibration curves for a) PFOS and b) PFTriA, and chromatograms of an injection of 1 ng/L, which is five times lower than the reporting limit of quantitation

HRAM screening and quantitation

LC-MS Orbitrap technology

Ensuring the safety of the world's environment and food supply is critically important, no matter what you're looking for in the samples.

Targeted screening and quantitation

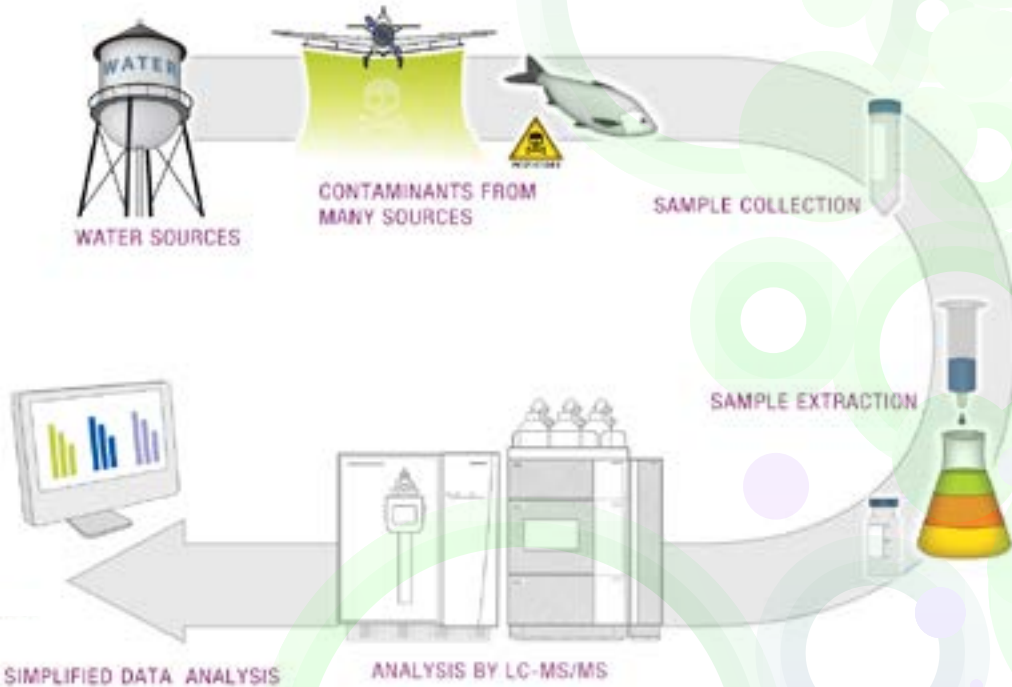
Thermo Scientific™ Orbitrap™ technology can screen samples for targeted contaminants such as pesticides, herbicides, and other pollutants, followed by quantitation of the contaminants.

Unknown screening

Screening samples for unknown contaminants is one of the most challenging workflows in the laboratory. It requires a different experimental and data analysis approach which can also be addressed with Orbitrap technology.

High-resolution, accurate-mass (HR/AM) mass spectrometry is ideally suited for this difficult analysis. Using the high-resolution capabilities and fast scanning speed of Orbitrap-based platforms, screening for hundreds of contaminants can be performed in less time than ever before. Results can be delivered quickly so the safety of our environment can be ensured.

- Targeted mass lists are used to trigger MS/MS analysis of compounds of interest
- The system rapidly and automatically performs MS/MS on the components detected in the MS spectrum with HR/AM at a speed amenable to UHPLC
- Full-scan MS and MS/MS allow quantitation and confirmation of identity in the same run
- After data is acquired and components are identified, the data can always be re-evaluated for new compounds of interest

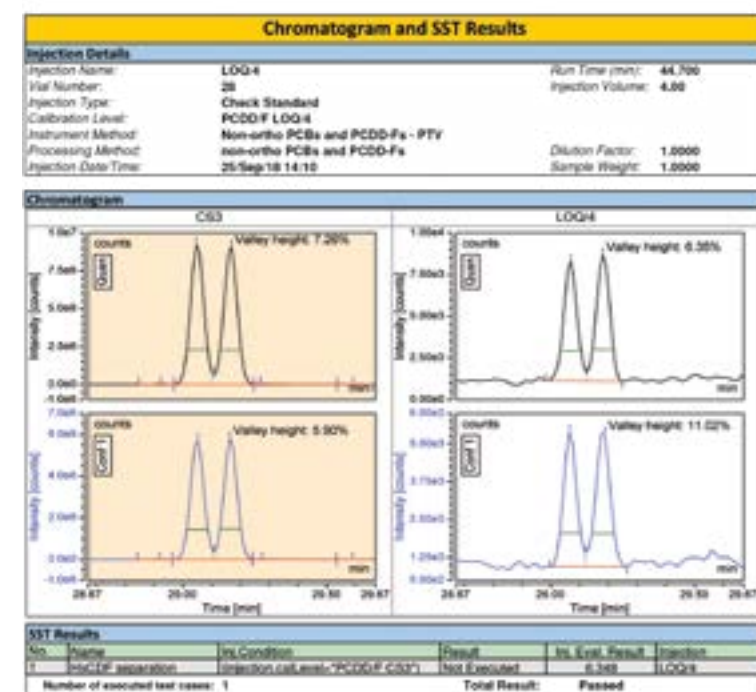


Screening and confirmation

TSQ 9000 AEI GC-MS/MS Triple Quadrupole

Highlights for dioxin analysis include:

- Compliance with all EU requirements for Dioxin/PCBs in food and feed
- Operational simplicity and out-of-box implementation
- Comprehensive suite of Thermo Scientific™ Chromeleon™ CDS productivity tools with pre-loaded calculation and reporting templates as required by regulations
- Method robustness validated over a large variety of samples
- Unmatched uptime via the new ultra-robustness source designed for high matrix tolerance



Key information includes average response factor, response factor deviation and Ion ratio.

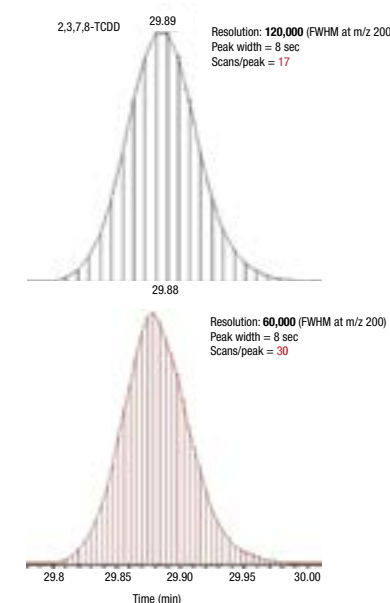
System suitability results built into the method allow for intelligent run control, ensuring samples are only analyzed if the system passes specification, saving repeat analysis time, acquisition and processing of non-compliant data.

The ultimate POPs research tool

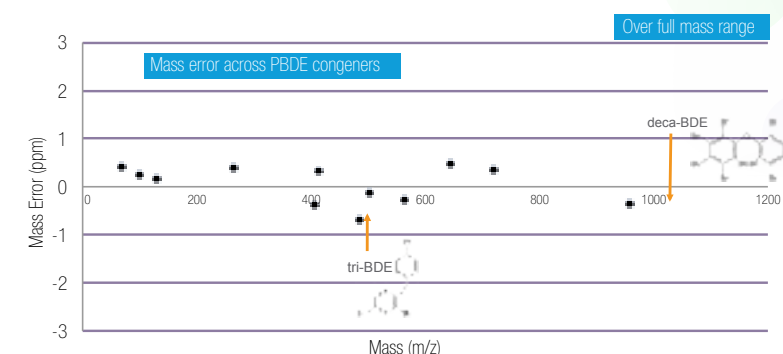
Q Exactive GC Orbitrap GC-MS

The Q Exactive GC system makes it a reality to collect comprehensive qualitative and quantitative sample information with high levels of selectivity, sensitivity, and confidence; especially in highly complex samples.

It is an easy-to-use, dedicated benchtop GC-MS system that provides the highest confidence for emerging POPs research with unmatched performance in compound discovery, identification, and quantitation for a comprehensive understanding of your samples.



Accurate peak profiling with high resolving power in full scan.



Excellent mass accuracy across the mass range for confident elemental composition assignment.

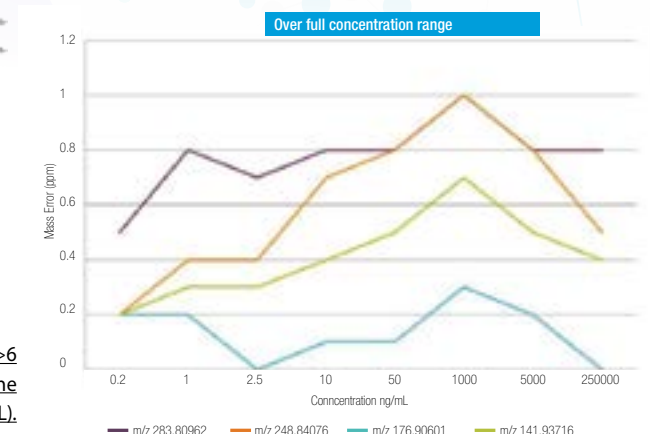
Mass accuracy over >6 orders (Hexachlorobenzene 0.2 – 250,000 ng/mL).



Q Exactive GC Orbitrap GC-MS/MS

"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



The gold standard

Global compliance in dioxin and POPs

The DFS Magnetic Sector GC-HRMS is the gold standard for performing Dioxin and Persistent Organic Pollutants (POPs) analysis. It empowers you to achieve full compliance with any official Dioxins, PCB, or PBDE method around the world.

For over a decade, the global scientific community has chosen Thermo Scientific DFS Magnetic Sector GC-HRMS for its superior performance in routine quantitative analysis of Dioxins and POPs. Today, the DFS Magnetic Sector GC-HRMS continues to set the gold standard in providing robust performance and high-confidence results in full compliance with any official method or regulations (for example US EPA1613).



Thermo Scientific DFS Magnetic Sector GC-HRMS

The Gold Standard

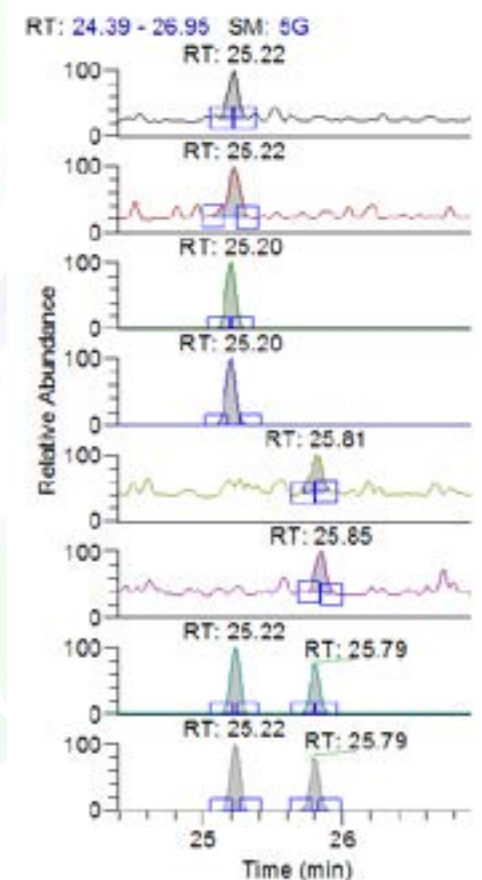
DFS magnetic sector GC-HRMS for ultimate sensitivity and robustness

Reporting with ultimate confidence

Reporting of non-compliant food and feed samples can result in expensive product recalls and bans, which can quickly become headline news. So you need to be sure of your analysis and the data. The DFS Magnetic Sector GC-HRMS provides defensible confirmatory quantitation down to the very low femtogram level. No other technology provides higher precision and sensitivity.

DFS Magnetic Sector GC-HRMS:

- Ultimate sensitivity in routine quantitation
- Highest available dioxin sensitivity at maximum robustness due to the large-volume ion source
- Best dioxin installation spec available: 20 fg 2378-TCDD gives a S/N $\geq$ 200:1 (4s)
- Worldwide compliance with official methods (e.g. US EPA 1613, 1668, & 1614; JIS K 311 & 312; etc.)
- Unique dual GC configuration for flexibility
- High transmission for high masses (i.e. high sensitivity for BDE-209)
- Flexibility for reference gases, e.g. PBDE uses perfluorokerosene (PFK) or perfluorotributylamine (FC-43), etc.
- LOD/LOQ calculation using S/N
- Results proven by routine use in top-notch environmental labs



Serum sample on 60 m column: ca. 3 fg TCDF
ca. 2 fg TCDD.

Powering dioxins and POPs analysis with software solution

DFS software package

Quantify POPs routinely and easily in this highly regulated environment using [Thermo Scientific™ DFS™ Software Package](#)

Your routine quantifications of POPs are important and you can't afford that they are not compliant with regulations and your business requirements. Laboratories need that their Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS is supported by a software solution enabling compliance and reliability of results, backed by automation.

The DFS Software Package includes automated features supporting full compliant routine quantifications of POPs, with the automation required to meet your lab needs. Designed with ease-of-use in mind, the DFS Software Package ensures full data confidence while delivering maximum flexibility, even in regulated labs.

Thermo Scientific™ DFS SmartTune™ Operating Software

Robust analysis in complex matrices

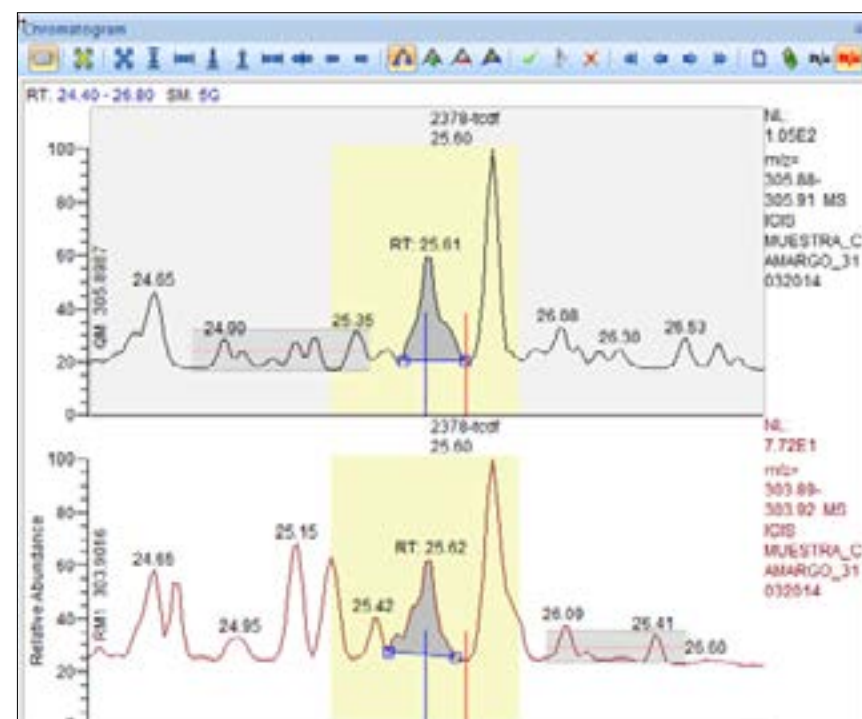
New concerns in food and environmental safety emerge every day. Challenging samples require robust hardware and software analytical solutions. With the Smart MID Feature of the DFS Software Package you can avoid that complex matrix affect the system calibration, preventing the risk of redoing the analysis and being more confident.

Thermo Scientific™ DFS TargetQuan™ Data Evaluation Software

Full transparency of software processes Dioxins and POPs represent a global concern for the environmental and human health.

Official regulatory bodies, aiming at standardizing the monitoring of dioxins and POPs in food, feed and environmental samples, requires full transparency of analytical methods and results.

The DFS Software Package enables analysts to report LOQ and LOD calculations, ensuring compliance and confidence of results.



Chromatographic view with displayed noise range.

Direct knowledge for POPs quantitation

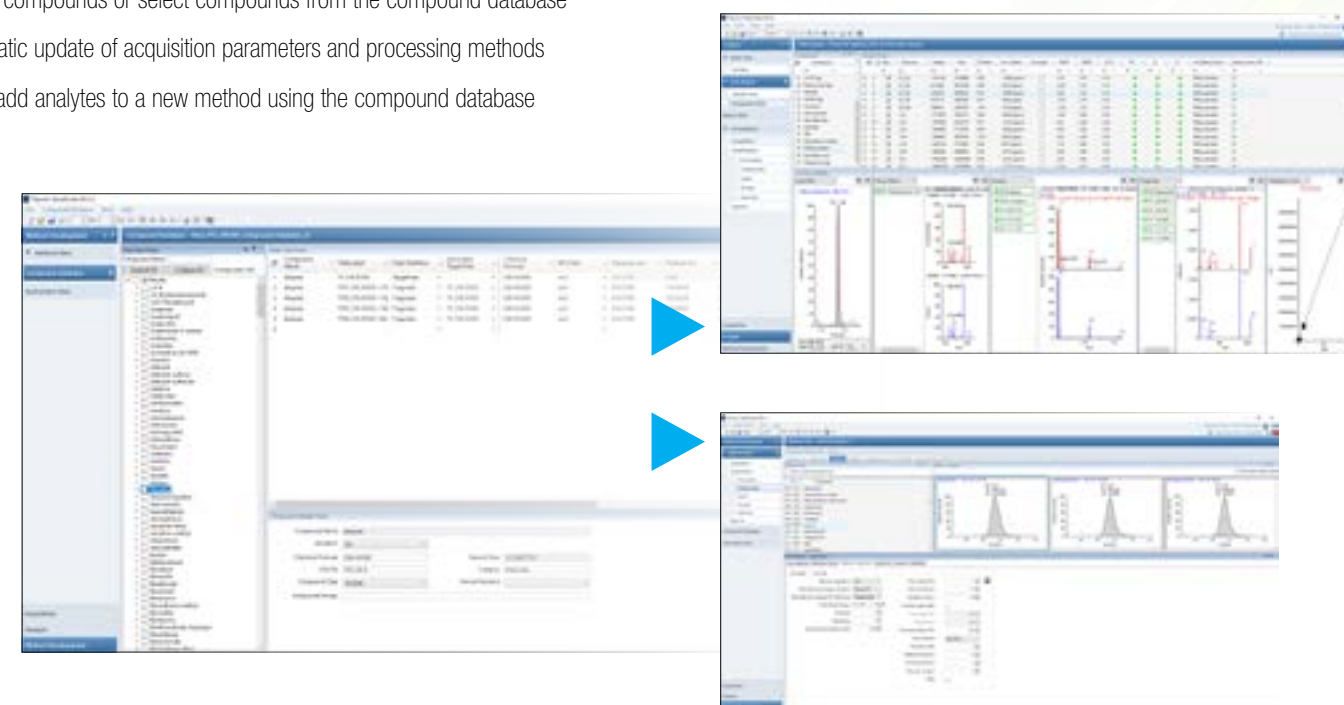
TraceFinder software

Perform targeted screening, routine quantitation, and quantitative and qualitative review of GC, GC-MS, GC-MS/MS, LC, LC-MS, and LC-MS/MS data with [Thermo Scientific™ TraceFinder™ Software](#)

This easy-to-use software provides quantitative workflows and reports for routine POPs analysis. It's compatible with Thermo Scientific GC-MS and LC-MS systems, and most GC and LC detectors.

Flexible method development

- Choice of method development approaches optimizes your workflows
- Import compounds or select compounds from the compound database
- Automatic update of acquisition parameters and processing methods
- Easily add analytes to a new method using the compound database



From targeted screening to unknown screening simplified within one method

- Easy-to-use built in software tools to quickly add unknown screening workflows to targeted
- Build personalized screen libraries ([mzVault](#)) or use established industry standard curated libraries from [mzCloud](#)

Thermo Scientific digital communities

Online POPs analysis resources

Stay involved and informed. Thermo Scientific Environmental and Food analysis communities provide in-depth information to keep you informed on hot topics and updates to environmental regulations. Explore a wealth of knowledge to guide you through research and routine POPs analysis.

Interact with experts and environmental analysis community leaders and share experiences and guidance. Learn about comprehensive solutions and streamlined workflows to increase laboratory throughput and improve productivity.

- Knowledge library
- Informative articles
- Featured webinars
- Applications
- Customer testimonials
- Expert guidance

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Environmental Community



www.thermofisher.com/environmental

Food and Beverage Community



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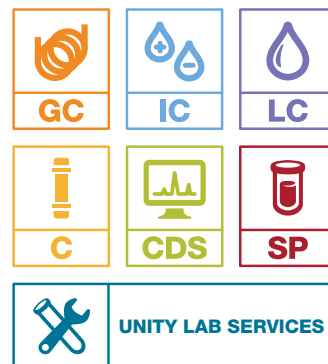
Analyte Guru Blog



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The collective power of chromatography

Whether you are working to achieve the next breakthrough in research or looking to have full confidence and precision in your routine results, Thermo Fisher Scientific chromatography products can offer you a complete workflow solution. Drive innovation, improve your productivity and achieve operational excellence to deliver a maximum return on your investment. With the largest portfolio of chromatography solutions, we remain a steadfast and committed partner in your endeavor to improve the world around us.



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Find out more at thermofisher.com/chromatography and thermofisher.com/icms