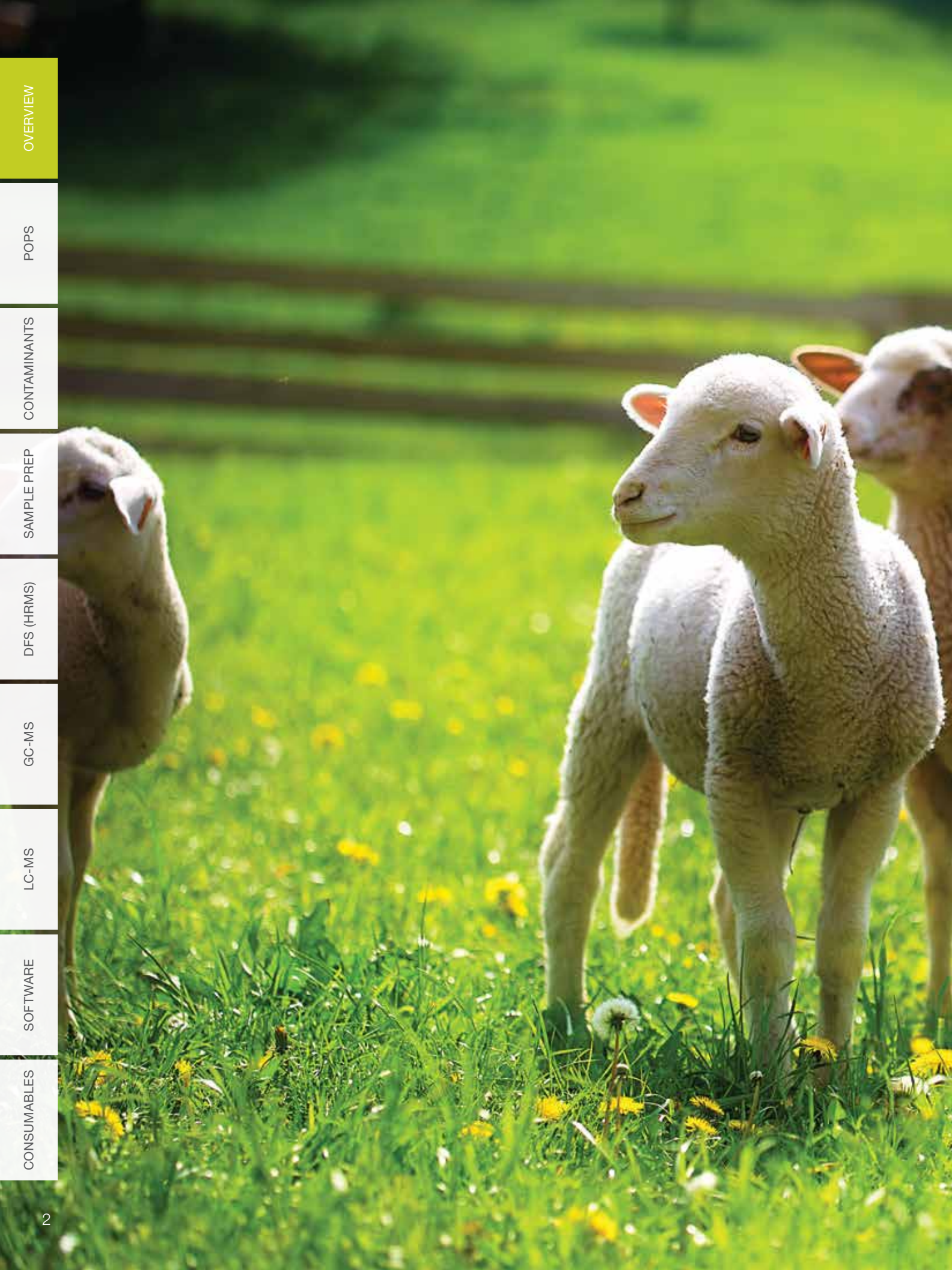


Persistent organic pollutants (POPs) in food

Identification and quantitation workflows



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POPs analysis protecting our food chain

Persistent organic pollutants (POPs) are toxic chemicals, produced either intentionally or as byproducts of industrial and agricultural activity.

Due to the persistent nature of POPs, many of these compounds migrate naturally from the environment into plant food sources and up the food chain where they bioaccumulate in the fatty tissue of animals. It is through this biomagnification mechanism that these contaminants negatively influence human health and development. Particular concerns exist over the accumulation of POPs 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 brand reputation and affect trade at an international level.

Global concern over the presence and impact of POPs contamination has produced a need for strategies that restrict, reduce, and eliminate such chemicals in the environment ultimately preventing them from entering the food chain.

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, requiring all parties to assist in efforts to eliminate or reduce the release of POPs into the environment.

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

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Emerging contaminants

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

Eliminate, restrict, and reduce

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

Comprehensive capabilities for POPs workflows



Sample Login

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

Sample Preparation

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



LC and LC-MS analysis

Thermo Scientific™
TSQ Endura™ Mass Spectrometer

Thermo Scientific™
TSQ Quantiva™ Mass Spectrometer

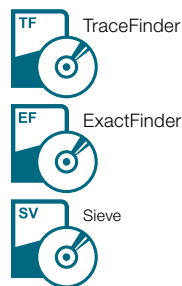
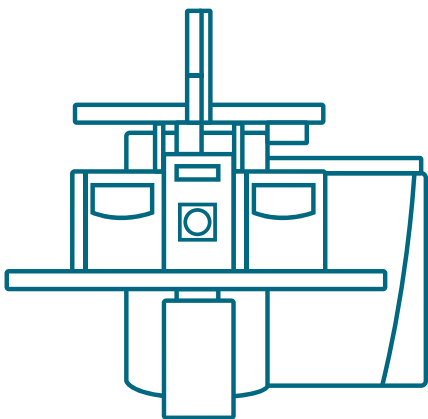
Thermo Scientific™
LC Orbitrap™ series

GC and GC-MS analysis

Thermo Scientific™
TSQ™ 8000 EVO GC-MS/MS

Thermo Scientific™
DFS™ Magnetic Sector GC-HRMS

Thermo Scientific™
GC Orbitrap™ series



Sample Analysis

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

Data Analysis

Maximize the functionality and efficiency of sample analysis and data interpretation with POPs workflow supporting software.

Persistent organic pollutants are toxic compounds that have adverse effects on health.

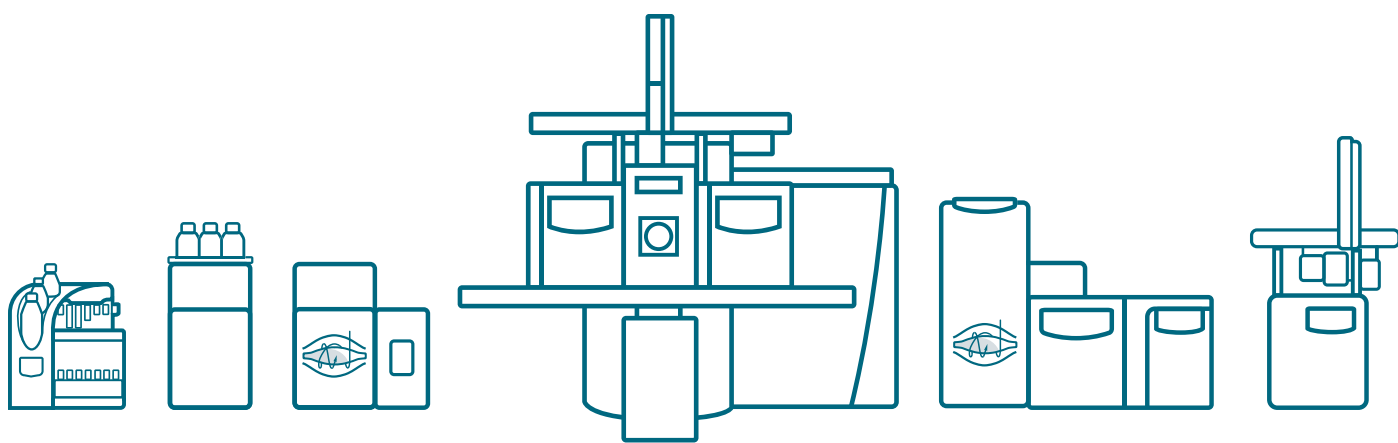
POPs compounds can be derived unintentionally or intentionally. When produced **unintentionally** they are usually created as a result of an industrial process and combustion. The most widely known compounds derived in this manner are dioxins.

Intentionally produced POPs include compounds used and/or produced for use in industries such as agriculture, manufacturing and industrial processing. The most commonly known of these are Polychlorinated biphenyls (PCBs) and organochlorine pesticides such as DDT.



The banned list

Compound	Description	Intentionally Produced	Unintentionally produced
Aldrin	An agricultural insecticide it was used to eradicate termites and other pests in cotton and corn crops.	✓	
Chlordane	With a half-life of approximately one year, this chemical was used as an insecticide on crops that include potatoes, sugar cane and sugar beet, fruits, nuts and vegetables. It was also used in domestic homes to treat lawns and pests.	✓	
Dieldrin	The oxidized form of aldrin, it has a half-life of up to five years and is highly toxic to aquatic animals. It was used to control termites, cotton pests and insect – borne diseases.	✓	
DDT (Dichlorodiphenyltrichloroethane)	Used to protect against malaria and lice borne typhus, during the second world war, it was later used as an agricultural insecticide, mainly on cotton crops. Its residues can remain in soil for up to 10-15 years after application.	✓	
Dioxins	By-products of high temperature industrial processes for example the production of pesticides and through incomplete combustion such as the burning of hazardous waste and domestic waste.		✓
Endrin	Used to control rodents and also as an insecticide, sprayed on crops such as corn and cotton.	✓	
Furans	Produced as by-products of high temperature industrial processes such as the incineration of medical and household waste. Also produced during the production of PCBs and some pesticides.		✓
Heptachlor	Used to eradicate crop and cotton pests and malaria carrying mosquitos.	✓	
HCB (Hexachlorobenzene)	Selective fungicide used for seed treatments.	✓	
Mirex	With a half-life of up to 10 years, this was used as a flame retardant in electrical goods, plastics and rubber as well as an insecticide.	✓	
PCBs (Polychlorinated biphenyls)	They were used in the electrical transformers, capacitors and other various electrical items as they are good insulators and are non-flammable. Also used in paint additives and in plastics and also in carbonless copy paper and heat exchange fluids.	✓	
Toxaphene	Applied to control pests in crops such as cereals, grains, cotton, fruits nuts and vegetables with a half-life of up to 12 years. It was also used to control unwanted fish stocks.	✓	



Accelerated solvent extraction

Walk-away automation for improved productivity

Thermo Scientific™ Dionex™ ASE™ 150/350 Accelerated Solvent Extractor

The Dionex ASE 150/350 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.

These systems are suitable for extraction of pollutants from high-fat content and dry foods such as fish and tea. Dionex ASE systems are equivalent to or perform better than Soxhlet, automated Soxhlet, sonication, and shaking techniques.



Dionex ASE 350 System.



Rocket Evaporator System.

The Thermo Scientific™ Rocket™ Evaporator System

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 reduce 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.



The Gold Standard in Dioxin and POPs analysis

The Thermo Scientific™ DFS™ Magnet Sector GC-HRMS (HRMS) System provides the ultimate sensitivity combined with maximum robustness for your routine analysis.

The DFS Magnetic Sector GC-HRMS System is the highest performing mass spectrometer ever built for target compound routine analysis of Dioxins and POPs in all kinds of sample matrices. Specifically designed for dioxin and POPs analysis, it provides full compliance worldwide with any regulatory method for detecting dioxins, PCBs, or PBDEs in food matrices.



Dual GC DFS Magnetic Sector GC-HRMS System.

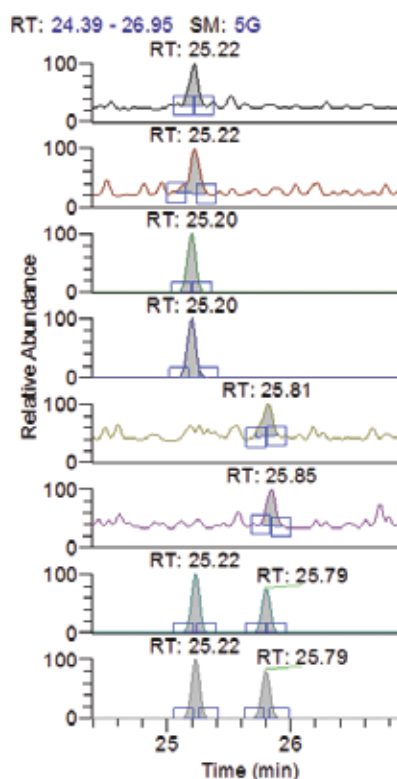
DFS magnetic sector GC-HRMS for ultimate sensitivity and robustness

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. Laboratories need to ensure the validity of your analysis and the data to prevent these occurrences. The DFS Magnetic Sector GC-HRMS provides dependable confirmatory quantitation down to the very low femtogram level. No other technology provides higher precision and sensitivity.

DFS Magnetic Sector GC-HRMS System:

- Ultimate sensitivity in routine quantitation.
- Highest available dioxin sensitivity with 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, and 1614; JIS K 311 and 312; etc.).
- Unique dual GC configuration for flexibility.
- Unique DFS DualData XL option for ultimate productivity – up to doubled sample throughput
- 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.



Serum sample evaluated using a 60 m column: ca. 3 fg TCDF ca. 2 fg TCDD.

The ultimate POPs research tool

Exactive GC Orbitrap GC-MS System

The Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS 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 high resolution/accurate mass (HRAM) capabilities for the highest confidence in emerging POPs research with unmatched performance in compound discovery, identification, and quantitation for a comprehensive understanding of your samples.

“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*



Exactive
GC Orbitrap
GC-MS System.



TSQ 8000 Evo
Triple Quadrupole System.

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Screening and confirmation

TSQ 8000 Evo GC-MS/MS Triple Quadrupole System

The Thermo Scientific™ TSQ™ 8000 Evo GC-MS/MS System has been designed with the productive POPs lab in mind.

Highlights for dioxin analysis include:

- Advanced, built-in robotics in the Thermo Scientific™ TriPlus™ RSH autosampler to deliver exceptional precision, sample handling flexibility, and reliable weekend-long unattended operation.
- Complete modularity in the Thermo Scientific™ TRACE™ 1300 Series gas chromatograph so changing Instant Connect injector or detector types takes only minutes.
- The rugged Thermo Scientific™ Extractabrite™ ion source can be easily replaced without taking time to vent the system.
- EvoCell collision cell technology provides high-performance SRM at high velocity, without compromising sensitivity.
- Uniquely tailored software for workflow-oriented POPs quantitation.
- Full compliance with the latest regulations for analyzing dioxins in food and feed, meeting stringent European Union performance criteria.



Extreme quantitative performance

LC-MS triple quadrupole technology

Continual changes in POPs research and regulatory requirements drive the need for ever-lower limits of detection and quantitation. The Thermo Scientific™ TSQ Quantiva™ Triple Quadrupole Mass Spectrometer uses 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 Perfluorooctanesulfonic acid (PFOS) and Perfluorooctanoic acid (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 PFOA. 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.



HRAM screening and quantitation

LC-MS Orbitrap and triple quadrupole technology

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

Targeted screening and quantitation

Thermo Scientific™ Orbitrap™ mass analyzer 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 food supply chain 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 fragmentation of the components detected in the full scan spectrum acquired with HRAM and at a speed compatible with 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 emerging compounds of interest.



Exactive™ Hybrid Quadrupole – Orbitrap™ Mass Spectrometer and Vanquish UHPLC System.



TSQ Triple Quadrupole MS Mass Spectrometer.

POPs data analysis

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TargetQuan software

Quantify POPs routinely and easily in this highly regulated environment using Thermo Scientific™ TargetQuan 3 software.

POPs quantitation has very specific requirements demanded from an extensive regulatory framework and the need to understand a sample's overall toxicity. The persistent, chronic toxicity of these compounds means extremely low-level determinations are needed using highly accurate and precise isotope dilution techniques. Quantitative calculations can quickly become demanding and complex which impedes laboratory efficiency and slows time-to-result.

TargetQuan 3 software is designed for POPs analysis reflecting special calculation schemes where precise quantitation is performed through isotope dilution. Data processing is independent of instrumentation and is used for MS, MS/MS, and HRMS data; enabling use of just one software for both screening and quantitation.

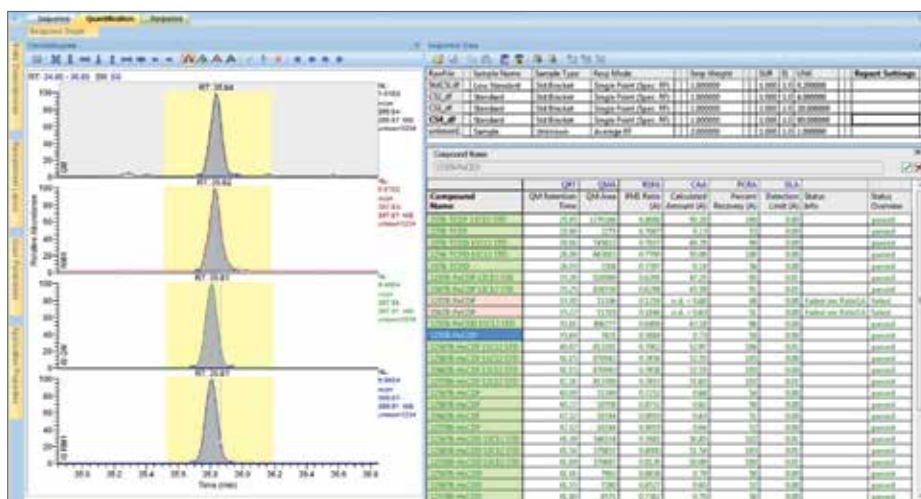
Calculating toxic equivalence quotients (TEQs)

TargetQuan automates the complex calculations required for dioxin analysis. Its isotope dilution methodology uses robust internal standardization and response factors to calculate the concentration of contaminants. Toxic equivalence factors are applied for analytes and the sample's final TEQ is calculated:

- No spreadsheets
- No transposition errors
- Complete audit traceability

Comprehensive, automated QA/QC checking

A simple user interface and intuitive workflow hide complex, powerful QA/QC processes in TargetQuan. Comprehensive automatic checking of all QA/QC factors is performed rapidly and automatically, minimizing the need for user intervention and freeing the chemist for other tasks.



TargetQuan 3 software.

Direct knowledge for POPs quantitation

TraceFinder software

Perform targeted screening, routine quantitation, and qualitative review of GC, GC-MS, LC, and LC-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 to optimize your workflows.
- Import compounds or select compounds from the data store.
- Automatic update of acquisition parameters and processing methods.
- Easily add analytes to a new method using the compound data store.

Enhanced targeted screening and quantitation; simplified screening for unknowns

- Easy-to-use tools substantially simplify workflows with support for SRM, HRAM and MS/MS experiments.
- Build personalized screening libraries or use established industry standard libraries such as NIST and Wiley.



Optimum system performance

GC columns and consumables

Analysis for POPs content is performed on a variety of sample types including foods and beverages. Our broad range of high-quality chromatography columns and consumables are 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 Thermo Scientific™ 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.



Thermo Scientific digital communities

Online POPs analysis resources

Stay involved and informed. Join the Thermo Scientific Food analysis community providing in-depth information to keep you informed on hot topics and updates to food regulations. Explore a wealth of knowledge to guide you through research and routine POPs analysis.

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

POPs online



thermofisher.com/POPsinFood

Online applications library



thermofisher.com/appslab

POPs center of excellence



thermofisher.com/pops-center-of-excellence

Find out more at thermofisher.com/food-safety

 facebook.com/ChromatographySolutions

 twitter.com/ChromSolutions

 analyteguru.com

Stay Ahead! Scan the QR code or follow the URL to discover the latest in POPs instrumentation.

