Thermo Scientific
Protecting the Environment

Persistent organic pollutant analysis

Comprehensive workflows for regulatory compliance

Thermo SCIENTIFIC

Persistent Organic Pollutant Analysis

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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

Emerging Contaminants

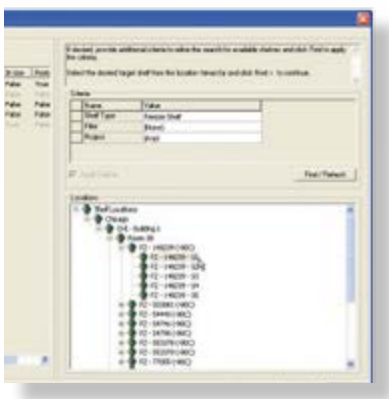
New BFRs, dicofol, short-chained chlorinated paraffins, chlorinated naphthalenes, hexachlorobutadiene, pentachlorophenol and other emerging unknowns

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

Comprehensive capabilities

Sample Login > **Sample Preparation** >



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.

Global Concern

Routine LC and LC-MS Analysis

Thermo Scientific™ TSQ Endura™ LC-MS
Thermo Scientific™ TSQ Quantiva™ LC-MS
Thermo Scientific™ Q Exactive™ Focus Hybrid Orbitrap™ LC-MS

Routine GC and GC-MS Analysis

Thermo Scientific™ TSQ™ 8000 EVO GC-MS/MS
Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS

Research Analyze Analysis

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

for POPs workflows

Sample Analysis > **Data Analysis**

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 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 PCCD/Fs from Environmental Samples Using Accelerated Solvent Extraction Technique.*

Dionex ASE 350 System

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_4CDD	3.9	14	2	2.5	34	5
Total P_5CDD	17	7.8	6	10	10	9
Total H_6CDD	510	5.6	8	570	1.3	7
Total H_7CDD	4700	8.3	2	5100	11	2
Total O_8CDD	6500	4.2	1	7100	0	1
Total T_4CDF	39	11	13	24	3	14
Total P_5CDF	33	13	8	28	0	11
Total H_6CDF	89	3.2	6	87	12	10
Total H_7CDF	293	3.3	4	310	0	4
Total O_8CDF	300	3.8	1	280	2.6	1
Congeners	**Value**	**% RSD**	**Isomers**	**Value**	**% RSD**	**Isomers**
2,3,7,8-Total T_4CDD	n.d. (1)		62	n.d. (1)		71
1,2,3,7,8-Total P_5CDD	1.6	4.6	69	n.d. (1)		75
1,2,3,4,7,8-Total H_6CDD	4.5	4.8	74	5.2	11	73
1,2,3,6,7,8-Total H_6CDD	19	4.3	75	21	0	50
1,2,3,7,8,9-Total H_6CDD	24	4.3	74	28	2.6	61
1,2,3,4,6,7,8-Total H_7CDD	1200	8.1	80	1300	0	93
2,3,7,8-Total T_4CDF	8.5	11	62	6.6	5.4	65
1,2,3,7,8-Total P_5CDF	1.9	17	68	2	0	72
2,3,4,7,8-Total P_5CDF	3.7	7.9	71	3.7	3.8	59
1,2,3,4,7,8-Total H_6CDF	17	7.3	79	17	4.3	70
1,2,3,6,7,8-Total H_6CDF	3.7	5.6	80	4	5.4	49
2,3,4,6,7,8-Total H_6CDF	3.7	18	81	4.4	3.2	61
1,2,3,7,8,9-Total H_6CDF	n.d. (1)		83	n.d. (1)	0	75
1,2,3,4,6,7,8-Total H_7CDF	91	1.6	83	96	3.7	82
1,2,3,4,7,8,9-Total H_7CDF	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

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 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

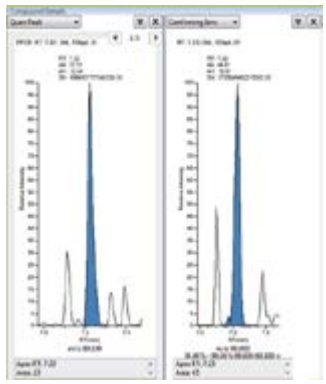
LC-MS Triple Quadrupoles

Continual changes in POPs research and regulatory requirements drive the need for ever-lower limits of detection and quantitation. The Thermo Scientific™ TSQ 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.

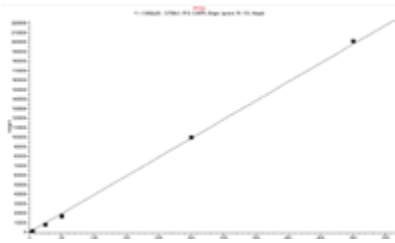
The emerging contaminants PFOS and PFOA are extremely persistent in the environment and resistant to typical environmental degradation processes. Use of LC-MS/MS has enabled more sensitive determinations of individual PFOS and PFOA[1]. The unique features of the Thermo Scientific LC-MS/MS platforms allow sensitive detection and quantitation in matrix to address these more stubbornly resilient POPs compounds.

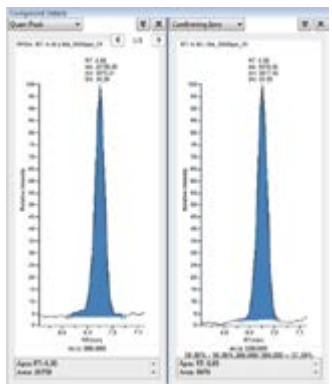
[1]EFSA 2008; Jahnke and others 2007b; Washington and others 2008.

Compound	Retention Time (min)	Polarity	Precursor/Product ion pair	CE
PFOA	8.7	Neg.	413 / 169	20
PFOA	8.7	Neg.	413 / 369	15
PFOS	8.9	Neg.	499 / 80.1	45
PFOS	8.9	Neg.	499 / 99	40

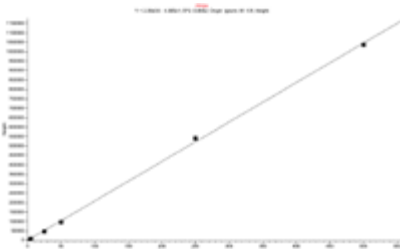


PFOA @ 5 mg/L





PFOS @ 5 mg/L



Separation and detection of PFOS and PFOA compounds using MS/MS including calibration curves from 0-5000 ppt.

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

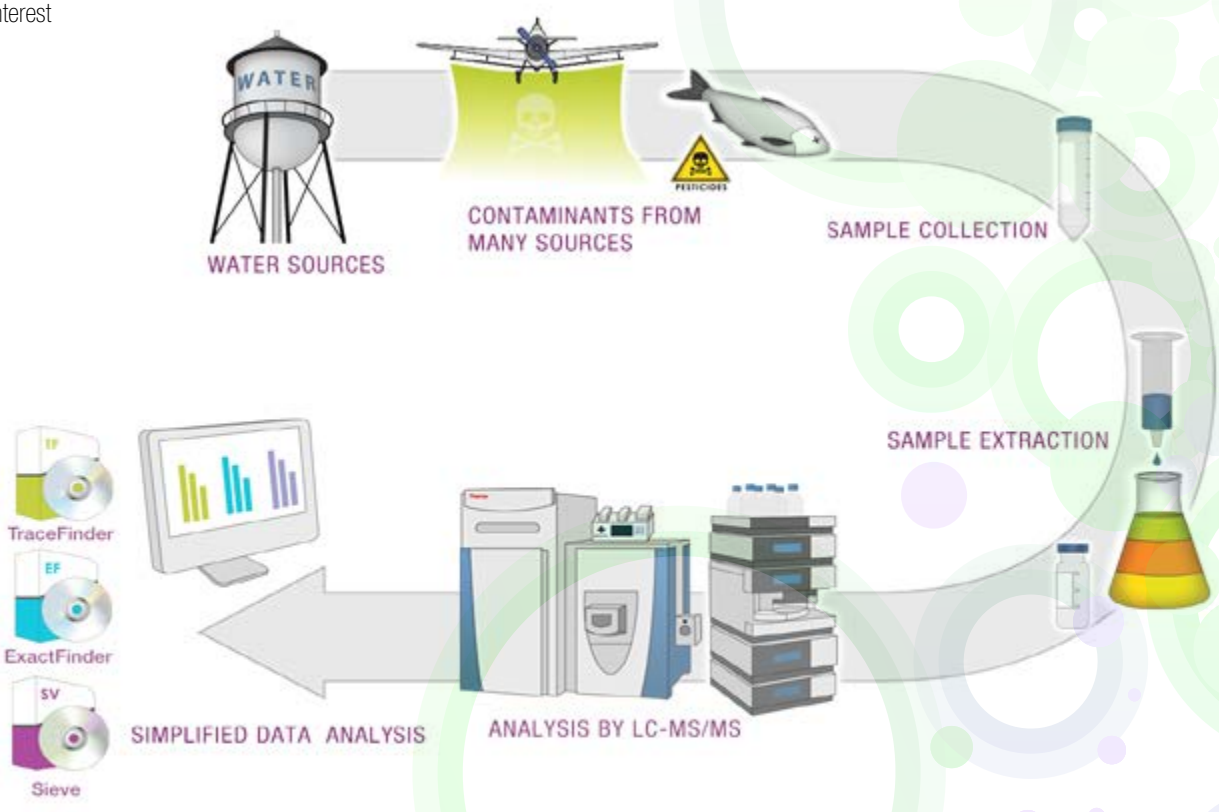
Thermo Scientific™ Orbitrap™ technology can screen samples for targeted contaminants such as pesticides, herbicides, and other pollutants, followed by quantitation of the contaminants.

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



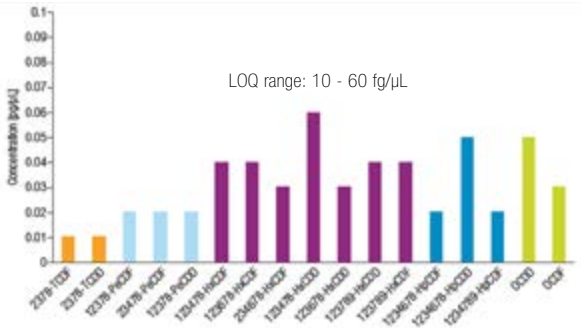
Screening and Confirmation

TSQ 8000 Evo GC-MS/MS Triple Quadrupole

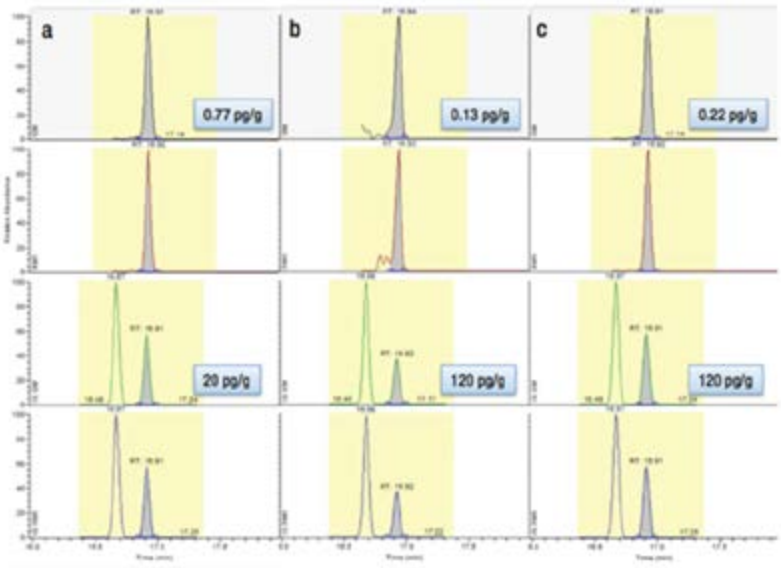
The Thermo Scientific™ TSQ™ 8000 Evo GC-MS/MS system has been designed with the productive POPs lab in mind.

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



Example LOQ calculated from CSL x5 and CSL x10 dilution (n = 10 injections) and taking into account the ion ratio, response factors and precision limits.



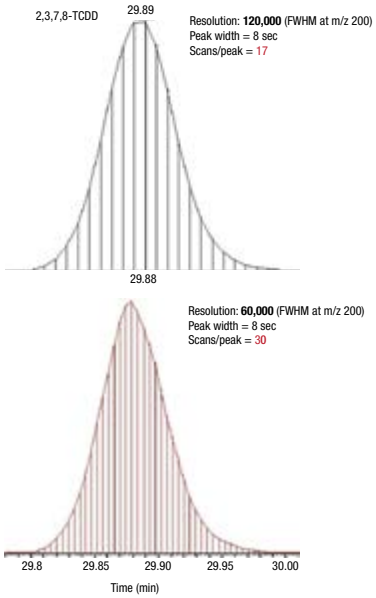
Example of chromatographic separation of 2378-TCDD and its internal standard 13C-2378-TCDD present in fish (a), feed (b), and milk powder (c) samples.

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.

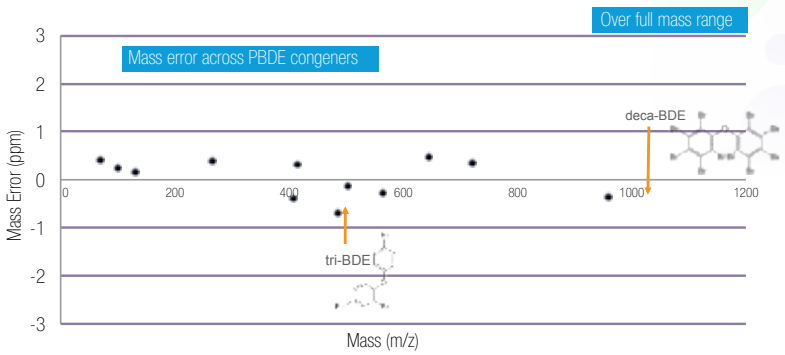


Accurate peak profiling with high resolving power in full scan.

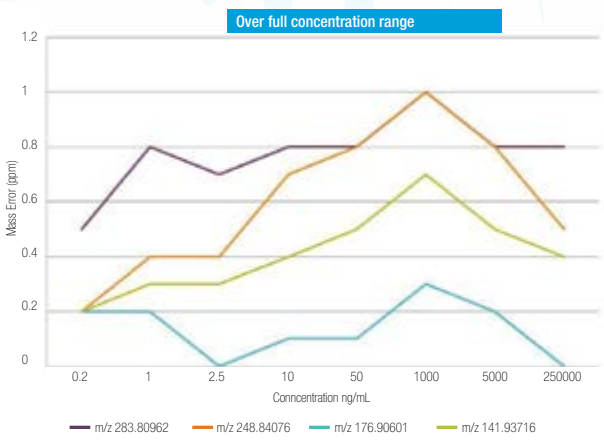
Q Exactive GC Orbitrap
GC-MS/MS

"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



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



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

The Gold Standard
in Dioxin and POPs Analysis

The Thermo Scientific™ DFS™ GC Magnetic Sector High Resolution Mass Spectrometer (HRMS) provides the ultimate sensitivity and maximum robustness for your analysis.

The DFS Magnetic Sector GC-HRMS is the highest performing mass spectrometer ever built for target compound analysis. Specifically designed for dioxin and POPs analysis, it provides full compliance worldwide with any official method for detecting dioxins, PCBs, or PBDEs such as those from the US EPA or EU Commission.

Dual GC DFS Magnetic Sector GC-HRMS

The Gold Standard

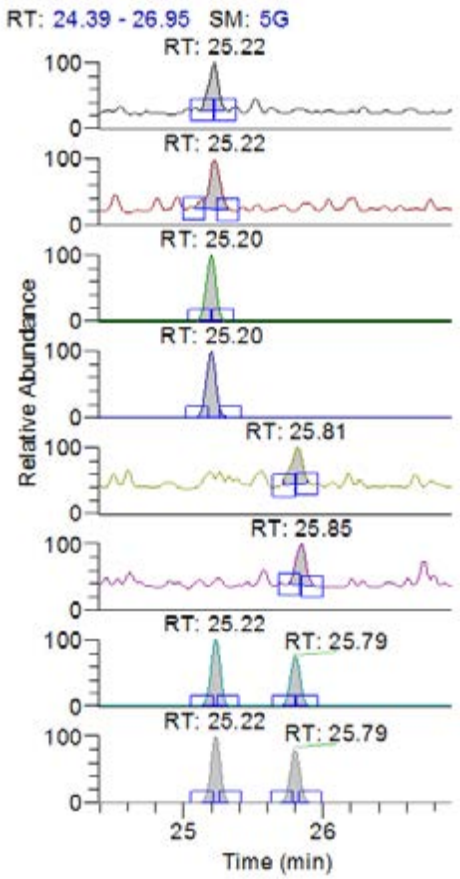
DFS Magnetic Sector GC-HRMS for Ultimate Sensitivity and Robustness

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 defendable 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 ≥ 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.

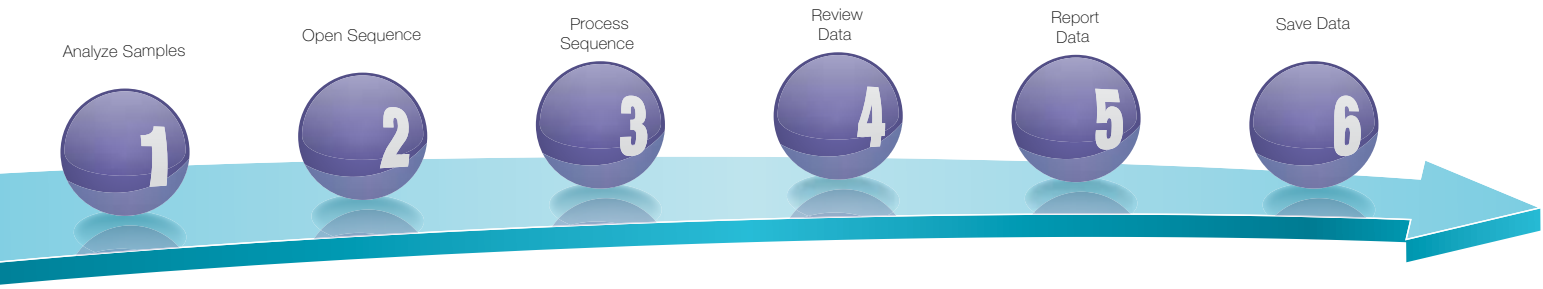
POPs Data Analysis

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 known from US EPA 1613 or 1668 where precise quantitation is performed through isotope dilution. Data processing is independent of instrumentation and is used for MS, MS/MS, and HRMS data; you can use just one software for both screening and quantitation.

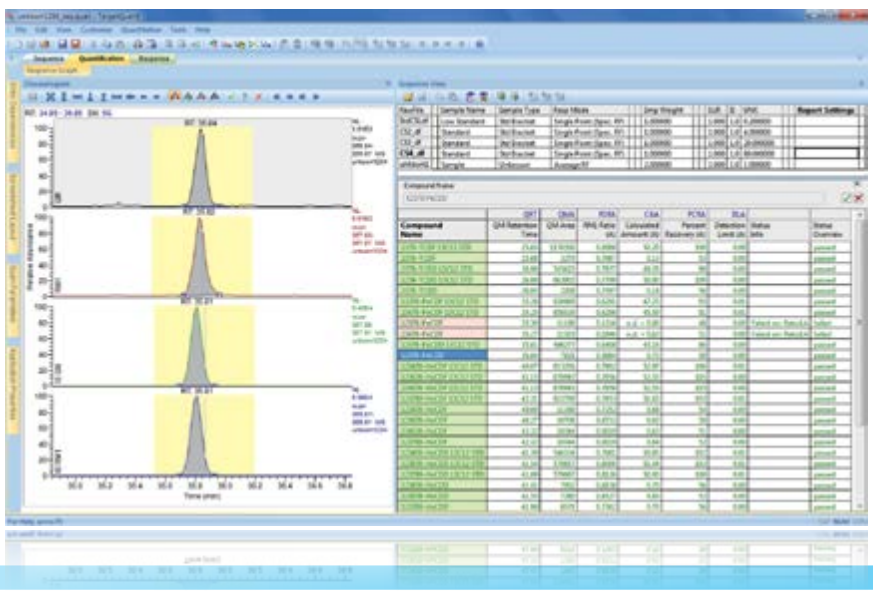


Calculating toxic equivalence quotients (TEQs)

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.

EPA 1613 B compliance

Templates are included for all major legislative methods. TargetQuan allows quantitation based on the average response of selected compounds and performs retention time corrections. This helps ensure compliance with US EPA 1613 protocols.



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.

Direct Knowledge for POPs Quantitation

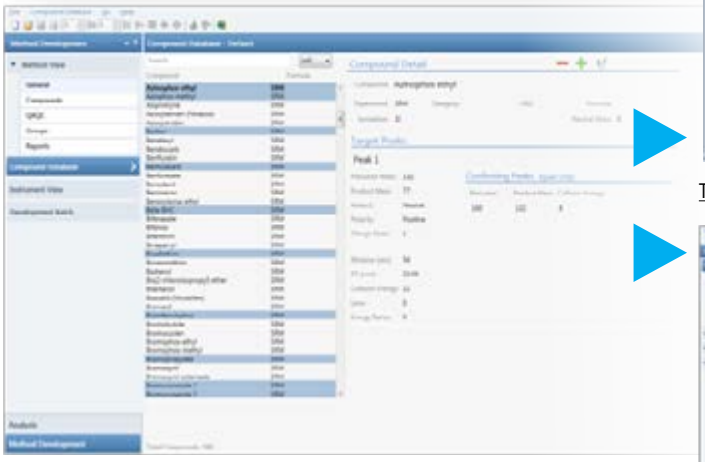
TraceFinder Software

Perform targeted screening, routine quantitation, and qualitative review of GC, GC-MS, LC, and LC-MS data with Thermo Scientific™ TraceFinder™ software.

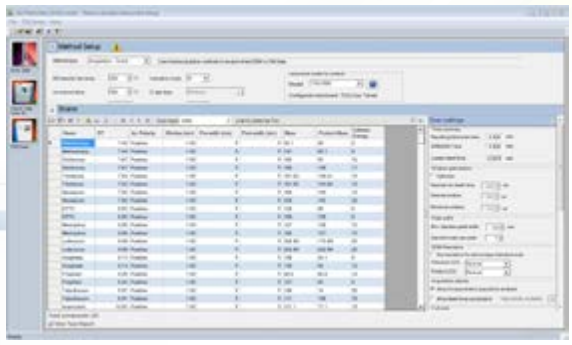
This easy-to-use software provides quantitative workflows and reports for routine POPs analysis. It's compatible with Thermo Scientific GC-MS and LC-MS systems, and most GC and LC detectors.

Flexible method development

- Choice of method development approaches optimizes 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

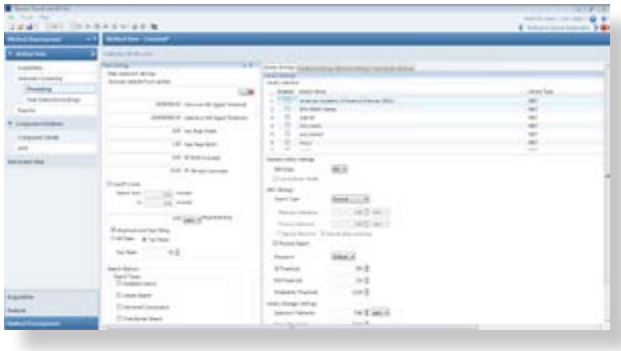


TraceFinder compound data store



Thermo Scientific™ Xcalibur™ software method editor

TraceFinder data processing



Enhanced targeted screening and quantitation; simplified screening for unknowns

- Easy-to-use tools substantially simplify workflows with support for SRM, HR/AM, MS/MS and MS2/MS3 experiments
- Build personalized screening libraries or use established industry standard libraries including NIST and Wiley

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**

POPs Symposium

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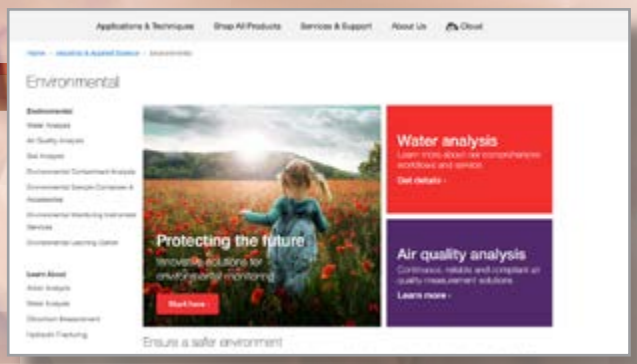
Environmental Community



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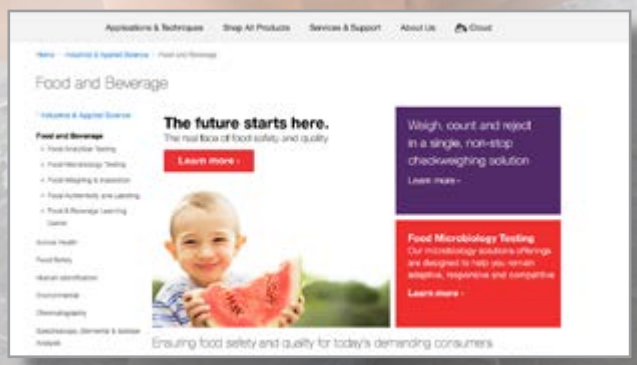
Food and Beverage Community



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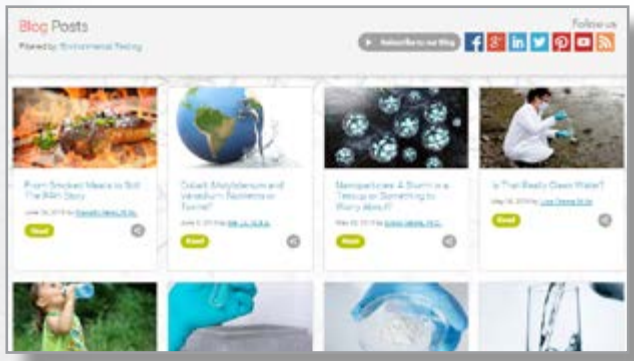
Analyte Guru Blog



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