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Persistent organic pollutants in food

Solutions for POPs in food testing

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Complete POPs in food solutions

Environmental pollutants in foods and beverages—such as persistent organic pollutants, also known as POPs—are of great interest when it comes to food safety. Dioxins, polychlorinated biphenyls (PCBs), organochlorine pesticides (OCPs), and polybrominated diphenyl ethers (PBDEs) are among the most common. Other chemicals including fluorinated substances, chlorinated naphthalenes, pentachlorophenol, and chlorinated paraffins are in various stages of becoming officially designated as POPs.

Dioxins in food, such as polychlorinated dibenzo-*p*-dioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), and polychlorinated biphenyls (PCBs), constitute a group of highly toxic organic compounds formed unintentionally, mainly in waste combustion processes or as by-products of industrial manufacturing of certain chemicals, such as chlorinated pesticides.

Resistant to environmental degradation, POPs bioaccumulate up the food chain and often occur as residues in fatty foods including meat, fish, eggs, or other dairy products. They can have significant effects on humans and animals as they migrate through the food chain. The EU has demanding regulatory limits for OCPs, PCBs, and PCDDs/PCDFs in animal feed and animal and fish products for human consumption.

More information on POPs, from improvements in instrumentation and methods, drive the need for ever-lower limits of detection and quantitation, for both known and unknown compounds. Using state-of-the-art high-resolution mass spectrometry (HRMS), we provide solutions for some of the most challenging food safety and environmental pollutant determinations.

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Accelerated solvent extraction

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The Thermo Scientific™ Dionex™ ASE™ 350 Accelerated Solvent Extraction system is used for the extraction of organic pollutants from solid and semisolid samples. This system is suitable for extraction of pollutants from high-fat content and dry foods such as avocados and tea. The Dionex ASE system is equivalent to or better than Soxhlet, automated Soxhlet, sonication, and shaking techniques.

Use of the novel water-absorbing polymer Thermo Scientific™ Dionex™ ASE Prep MAP dispersant and sorbent expands the capabilities of the accelerated solvent extraction technique and allows for the extraction of analytes from samples containing up to 85% water.

Thermo Scientific Dionex ASE 350 Accelerated Solvent Extractor system

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POPs in fish tissue

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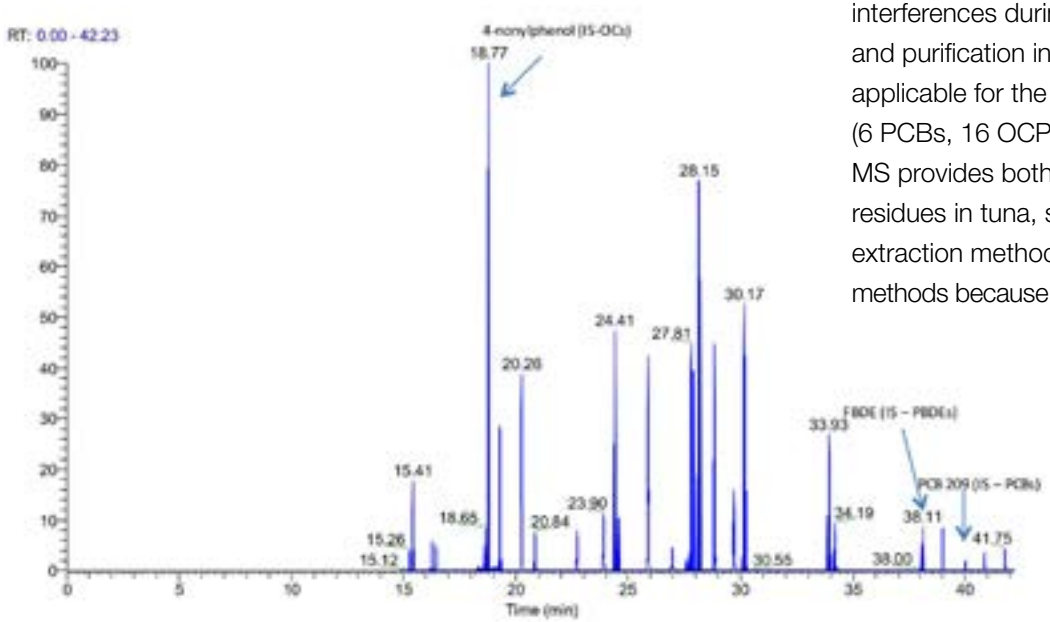
Techniques such as Soxhlet and sonication are used for the extraction of halogenated hydrocarbons from food and environmental samples prior to their analytical determination. These techniques are, however, very labor intensive and suffer from high solvent consumption. The accelerated solvent extraction technique meets the new requirements of increased throughput and reduced solvent usage in sample preparation as extractions can be completed quickly using minimal solvent. Recent advances using accelerated solvent extraction systems, as described in several publications,[1-19] include procedures for selective removal of interferences during sample extraction, thus combining extraction and purification into a single step. The method reported here is applicable for the determination of 29 halogenated hydrocarbons (6 PCBs, 16 OCPs, and 7 PBDEs) in fish tissues. Detection via MS/MS provides both quantitative information and confirmation of POP residues in tuna, substantiating that the one-step accelerated solvent extraction method is a valid faster alternative to classic extraction methods because the analytical quality is comparable.



Total ion current (GC-MS/MS) chromatogram of tuna spiked sample.

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Dioxins in oysters

Accelerated solvent extraction is a high-temperature, high-pressure extraction technique that is widely used for sample extractions in the environmental, chemical, and food analysis industries. Extractions at higher temperatures and pressures allow faster extraction of analytes relative to conventional solid-liquid-based extraction techniques such as Soxhlet. Spiked oyster samples were either treated with Dionex ASE Prep MAP and Dionex ASE Prep DE (1:1) or by using sodium sulfate as the drying agent prior to in-cell extraction in the Dionex ASE 350 system. The data shows that Dionex ASE Prep DE is an effective drying agent for wet oyster samples with excellent recoveries for the six OCPs.

In-cell moisture removal of oyster sample using Dionex ASE Prep MAP and Dionex ASE Prep DE

	% Recovery oyster dried with Dionex ASE Prep MAP and Dionex ASE Prep DE*	% Recovery oyster dried with sodium sulfate**
Compound	(n = 3)	(n = 3)
Lindane	91	81
Heptachlor	93	64
Aldrin	94	66
Dieldrin	105	75
Endrin	106	70
DDT	114	69
Total	101	71

* Data is courtesy of Department of Toxicology, Texas Tech University, Lubbock, TX, USA
** In-cell drying with sodium sulfate is not recommended using the ASE instrument

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DFS GC-HRMS

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Achieve outstanding sensitivity for analysis of dioxins and persistent organic pollutants in food with the Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS system. The DFS GC-HRMS system with double-focusing delivers ultimate mass spectrometry performance for target compound analysis. It also offers worldwide full compliance with any official dioxin, PCB, or PBDE method (for example, EPA 1613, 1668, or 1614). Exploit the benefits of the highest available dioxin sensitivity and robustness, delivered by our large-volume ion source. A product of 50 years of experience in developing magnetic sector MS, the DFS GC-HRMS system has all the features you need for your food applications.

DFS™ Magnetic Sector GC-HRMS system

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Analysis of polychlorinated dioxins/furans

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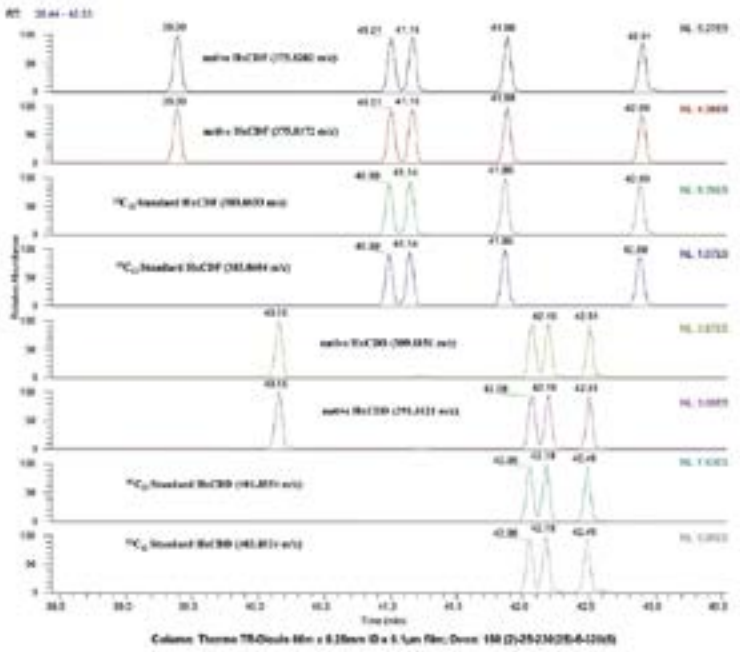
Magnetic sector high-resolution GC-MS is the gold standard for high sensitivity analysis of dioxins and other POPs. For decades it has proven its proficiency in this field of analysis and thus has become the established analysis technique available in leading dioxin laboratories throughout the world. The analytical performance with the DualData XL Acquisition configuration and conventional GC-MS configuration was compared using the same set of polychlorinated dioxins and furans, PCBs, and PBDE samples as model compounds.



Example of peak integrity of dioxin trace analysis (Hexa CDD/F) using the DualData XL Acquisition configuration.

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GC and GC-MS

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Meet your stringent requirements for performance, reliability, and value with Thermo Scientific™ gas chromatography-mass spectrometer (GC-MS) systems. Combine powerful GC-MS instruments with productivity-enhancing software to create complete solutions for the most challenging POPs testing. Achieve analysis of dioxins in food and feed and meet demanding performance criteria.

GC instruments from Thermo Fisher Scientific provide outstanding performance for routine analyses, advanced capabilities, and the flexibility to increase sample throughput. Instant-connect injectors and detectors enable you to change modules in minutes to reconfigure the instrument for new workflows, develop new methods, and eliminate maintenance downtime. Current developments in GC-MS triple quadrupole technology deliver high sensitivity and selectivity in the small molecule mass range and allow the detection of compounds at low concentrations, even in complex matrix samples. A simple and standard approach using electron impact ionization (EI) enables a very straightforward method for low-level analysis.

Thermo Scientific™ TSQ™ 8000 Evo Triple Quadrupole GC-MS/MS system

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Dioxin-like PCBs in food and feed

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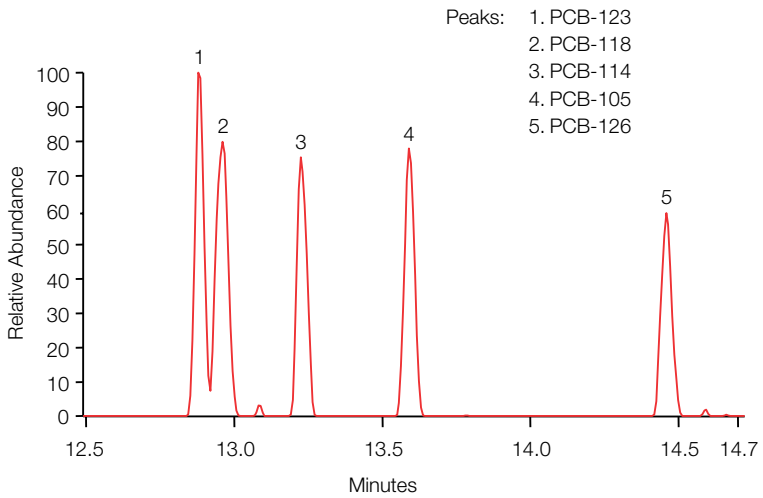
Polychlorinated biphenyls (PCBs) are a group of highly toxic organochlorine compounds with 209 possible congeners, depending on the number and position of the chlorine atoms. These congeners can be divided into two groups based on their structural and toxicological characteristics. The first group comprises 12 congeners that have a structure and toxicity similar to dioxins. These are termed “dioxin-like PCBs” (DL-PCBs) and are the focus of this study. The other group, forming the majority, do not exhibit the same degree of toxicity and these are called “non-dioxin-like PCBs” (NDL-PCBs). The potential for human exposure to these compounds makes accurate detection and quantification of DL-PCBs in the environment, particularly in food and animal feed, very important. The instrumental method used was based on that described in previous work analyzing PCDD/Fs using GC-MS/MS. The results obtained demonstrate that GC-MS/MS is a highly sensitive and selective analytical system that can be confidently used for DL-PCB detection and confirmation in food and feed samples.



Example of chromatographic separation of the pentachlorobiphenyl congeners in the CS-1 standard (1 pg/µL).

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POPs in honey

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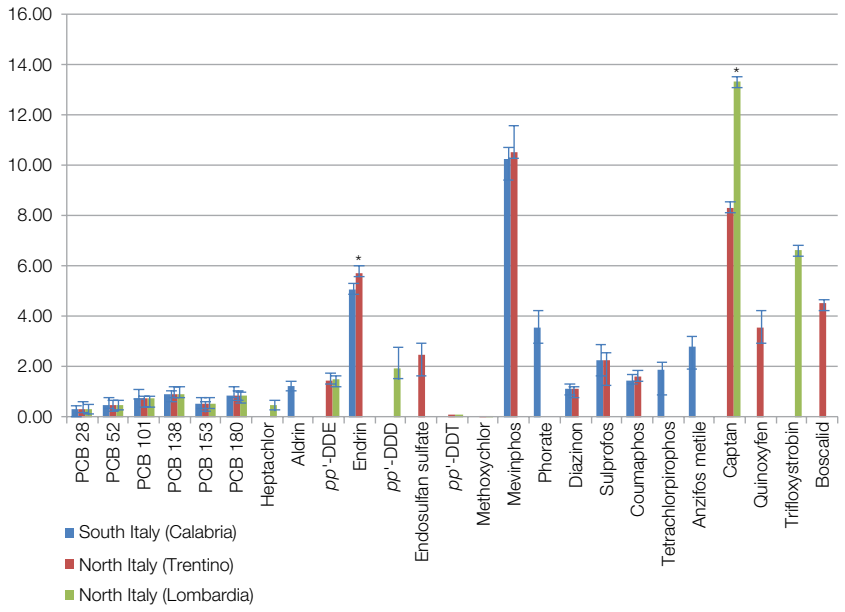
Honey is a natural product that is widely used for both nutritional and medicinal purposes. It is generally considered a natural and healthy product of animal origin and free of impurities. Consumer preference for natural products and the demand for quality ingredients and clean-label products, including organic honey, is increasing. Many pollutants in the environment can contaminate the bees themselves in addition to their pollen, honey, and other bee products. Environmental pollutants include pesticides, heavy metals, bacteria, and radioactive materials. Among the environmental contaminants, studies have documented the occurrence of organochlorines (OCs), polychlorobiphenyls (PCBs), organophosphates (OPs), and polybromodiphenylethers (PBDEs) in honey. The European Commission has set the maximum residue level values (MRLs) for feed as well as for food of animal origin for these chemicals. The method reported here is applicable for the determination of four different classes of compounds (6 PCBs, 7 PBDEs, 16 OCs, and 19 OPs) in honey. Eleven additional compounds, belonging to different classes and commonly used as agrochemicals, have also been investigated.



Distribution of detected contaminants (ng/g) in organic honey samples according to their sampling area.

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PCDD/Fs in food and feed samples

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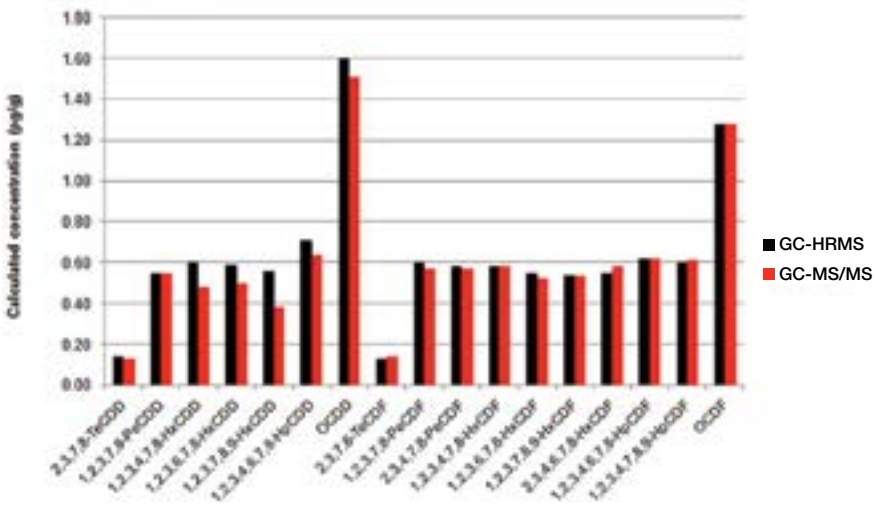
Legislation in the European Union previously required the confirmation and quantification of PCDD/Fs in contaminated samples by gas chromatography/high-resolution mass spectrometry (GC-HRMS) instruments, considered the “gold standard” approach. However, technological advances in gas chromatography/triple-quadrupole mass spectrometry (GC-MS/MS) technology allowed high sensitivity and selectivity to be achieved. These improvements have led to GC-MS/MS being considered a reliable tool that can be used to control the maximum levels for PCDD/Fs in food and feed as a full confirmatory method. The dioxin content of each sample, expressed as WHO-PCDD/F-TEQ pg/g, was determined for each sample analyzed, and the results were compared with the existing data obtained for the same samples from the GC-HRMS. The calculated concentrations of each individual PCDD/F congener (as TEQ pg/g) were compared with the values obtained from the GC-HRMS. The data shows excellent agreement.



Individual contribution of each PCDD/F congener to the feed sample dioxin content (as TEQ pg/g) and comparison of Thermo Scientific™ TSQ™ 8000 Evo GC-MS/MS system results with the GC-HRMS values.

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GC-HRAM

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Bring the power of the first-ever combination of high-resolution gas chromatography (GC) and high-resolution, accurate-mass (HRAM) Orbitrap™ mass spectrometry to your laboratory. The Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system provides comprehensive characterization of samples in a single analysis for the highest confidence in compound discovery, identification, and quantitation. This system offers the quantitative power of a GC triple quadrupole MS combined with the high-precision, full-scan HRAM capabilities only available in combination with Thermo Scientific™ Orbitrap™ technology.

The Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system is the first-ever combination of high-resolution gas chromatography and high-resolution, accurate-mass (HRAM) Orbitrap mass spectrometer. 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.

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

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Short-chained chlorinated paraffins

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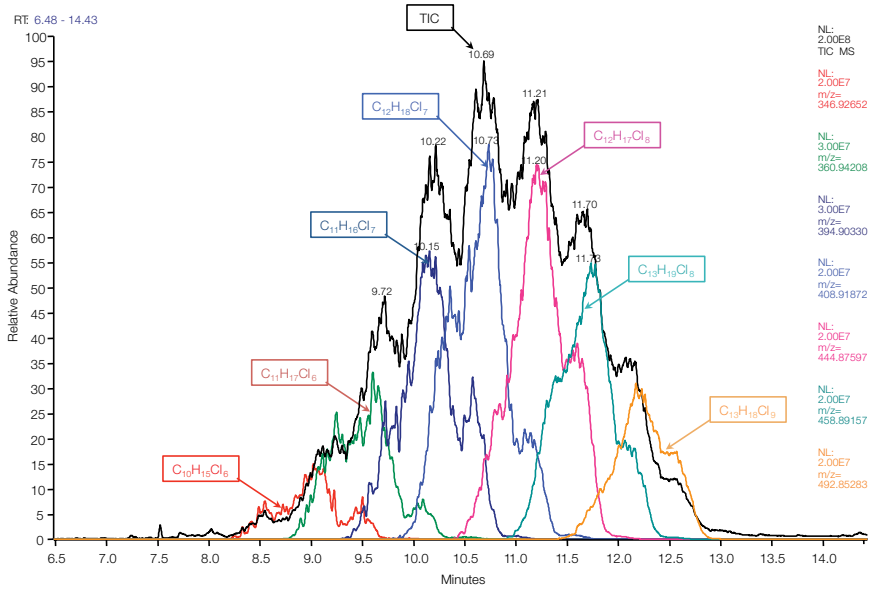
Short-chained chlorinated paraffins (SCCPs) are emerging contaminants that, once released, remain in the environment for long periods with the potential to bio-accumulate in living organisms. Detection and quantification of SCCPs pose analytical challenges due to the fact that these compounds are present in the environment at low levels, as very complex isomeric mixtures, and are difficult to separate chromatographically. Complete separation of SCCPs is also challenging because of the very high numbers of isomers and homologues with similar physiochemical properties. In this study, the performance of a novel benchtop high-resolution, accurate-mass Orbitrap™-based GC-MS was tested for the analysis of SCCPs. The Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system is a potential solution to the difficult challenges related to the detection and quantification of SCCPs due to its excellent sensitivity, linearity, and selectivity and in combination with its uncomplicated instrumental setup.



High-resolution, accurate-mass selectivity demonstrated for the C_{10}-C_{13} 63% technical mix acquired in NCI at 60k resolution. Examples of extracted ion chromatograms for individual homologues with various chlorination degrees are shown.

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Identification of novel brominated flame retardants

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Due to legislative restrictions on the manufacture and use of some brominated flame retardants (BFRs), several new chemicals (NBFRs) have been developed. To explore their presence in different food and environmental compartments, and ultimately understand their environmental fate, analytical methods for targeted analysis are required. Classically, these compounds are determined by GC-based instrumental methods. In recent years, LC-based methods coupled to low-resolution mass spectrometers have also been developed. Advances in high-resolution mass spectrometry facilitate accurate measurements and identification of unknowns, including degradation and transformation products. Several legacy BFRs and NBFRs were identified in dust samples. This indicates the relevance of dust-containing chemicals as an entry pathway to human and environmental exposure. Mass defect plots are a useful technique to simplify any chosen mass spectrum greatly. Thermo Scientific™ Compound Discoverer™ software is a powerful tool for unknown screening and structural identification of compounds in food and environmental sciences.

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Selected (N)BFRs in dust sample.

Suspect compound	Formula	Quasi-molecular ion and *m/z*		Δ *m/z* (ppm)	Time (min)
EH-TBB	$C_{15}H_{18}Br_4O_2$	$[M-Br+O]^-$	484.87706	0.08	10.24
BEH-TBP	$C_{24}H_{34}Br_4O_4$	$[M-C8H17+H-Br]^-$	512.87402	0.98	11.16
DBDPE	$C_{14}H_4Br_{10}$	$[M-Br+O]^-$	906.28362	0.82	12.06
TBBP-A	$C_{15}H_{12}Br_4O_2$	$[M-H]^-$	542.74571	0.09	8.30
HBCD	$C_{12}H_{18}Br_6$	$[M-H]^-$	640.63746	0.23	9.02

Compounds: (2-ethylhexyltetrabromobenzoate (EH-TBB), bis(2-ethylhexyl) tetrabromophtalate (BEH-TBP), decabromodiphenyl ethane (DBDPE), tetrabrombisphenol A (TBBP-A), hexabromcyclododecane (HBCD)

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LC-MS

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MS detection has become more affordable, accessible, and even mandatory in many fields of research. Simply detecting a peak is no longer sufficient; today it is necessary to know the identity of the compound causing the response, often in accordance with internationally accepted criteria. When our pioneering Thermo Scientific™ Vanquish™ UHPLC platform is combined with our best-in-class mass spectrometers, you achieve an extra level of confidence.

The Thermo Scientific™ TSQ Altis™ and TSQ Quantis™ triple quadrupole mass spectrometers are the perfect match for a wide range of quantitation workflows that utilize selected reaction monitoring (SRM) analyses.

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Vanquish UHPLC and TSQ Altis triple quadrupole mass spectrometer

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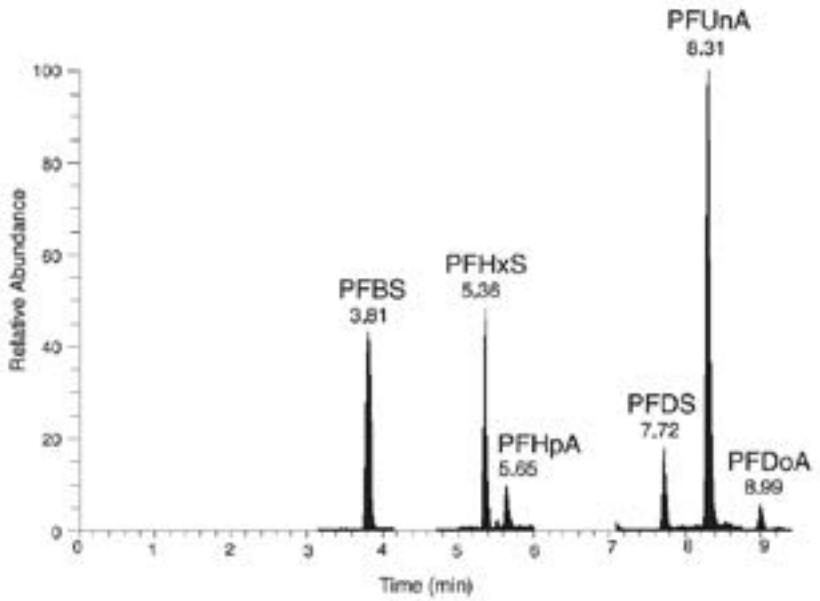
Perfluorinated compounds in human breast milk

Perfluorinated compounds (PFCs) are ubiquitous and persistent pollutants that bioaccumulate in animals and humans. The potential toxicity of these chemicals has fueled efforts to develop robust analytical techniques for measuring low levels of PFCs in human matrices. Quantitative selected reaction monitoring (SRM) assays were developed for six PFCs. PFCs were accurately and reproducibly detected at ppt concentration in neat solution and human milk matrix. Exceptionally sensitive and accurate, this integrated LC-MS platform is ideally suited for robust ultra-trace analysis of PFCs in a wide range of matrices.



The separation and detection of the PFCs in human milk matricies.

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LC-HRAM

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Identify and confirm more compounds rapidly and with confidence. The Thermo Scientific™ Vanquish™ UHPLC platform is a great match for our unique Orbitrap™ technologies including the Thermo Scientific™ Exactive™ line of benchtop mass spectrometers.

Take full advantage of all the benefits of high-resolution, accurate-mass detection by LC-MS to identify, characterize, and quantify unknown and known compounds within complex matrices.

Vanquish UHPLC and Q Exactive Focus LC-MS system

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Peer reviewed journal articles

Peer reviewed journal articles:
GC-MS methods

Title	Authors	Publication
Meeting the European Commission performance criteria for the use of triple quadrupole GC-MS/MS as a confirmatory method for PCDD/Fs and dl-PCBs in food and feed samples	Manuela Ábalos, Cristian I. Cojocariu, Paul Silcock, Dominic Roberts, Diana M. Pemberthy, Jordi Sauló, Esteban Abad	Analytical and Bioanalytical Chemistry May 2016, Volume 408, Issue 13, Pages 3511–3525
Dibenzo-*p*-dioxins and dibenzofurans in human breast milk collected in the area of Taranto (Southern Italy): first case study	Giuliana Bianco, Rosalia Zianni, Giuseppe Anzillotta, Achille Palma, Vincenzo Vitacco, Laura Scrano, Tommaso R. I. Cataldi	Analytical and Bioanalytical Chemistry March 2013, Volume 405, Issue 7, Pages 2405–2410
Survey of persistent organochlorine contaminants (PCDD, PCDF, and PCB) in fish collected from the polish baltic fishing areas	Jadwiga Piskorska-Pliszczynska, Sebastian Maszewski, Malgorzata Warenik-Bany, Szczepan Mikolajczyk, and Lukasz Goraj	The Scientific World Journal Volume 2012 (2012), Article ID 973292, 7 Pages
PCDD and PCDF levels in paper with food contact	H. Beck, A. Droß, W. Mathar	Chemosphere Volume 25, Issues 7–10, October–November 1992, Pages 1533–1538

Find out more at **www.thermofisher.com/food-safety**

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