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Persistent organic pollutants (POPs) in food

Application summary compendium

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Persistent organic pollutants (POPs) in food

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Introduction

Persistent organic pollutants (POPs) are man-made chemicals which are persistent and stable contaminants in the environment, globally present and have known toxicological effects on animals and man. They are defined by the United Nations under the Stockholm Convention. Under the convention there is international agreement to eliminate POPs whether produced intentionally or produced unintentionally as by-products (e.g., from incineration). Certain organochlorine pesticides including DDT as well as PCBs, dioxins and dibenzofurans, PBBs and PBDEs are recognized as POPs. Other chemicals including fluorinated substances, chlorinated naphthalenes, pentachlorophenol and chlorinated paraffins have reached various stages of being officially designated as POPs. Some POPs were in the past deliberately used as agrochemicals, while others have and continue to be dispersed in the environment though industrial accidents and poor waste-disposal strategies. Aerial dispersal via gases and particulates, atmospheric transfer and rainfall, combined with direct leaching from waste materials into soil and water have led to ubiquitous environmental contamination. Methods of analysis for POPs are generally based on appropriate extraction, cleanup and GC-MS determination and occasionally LC-MS analysis.

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Determination of persistent organic pollutants in fish tissues by accelerated solvent extraction and GC-MS/MS

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Overview

The capacity of the halogenated hydrocarbons to bioaccumulate in fatty tissues and biomagnify up the food chain, in combination with their resistance to degradation and their toxicity, make this class of chemicals a serious threat to environmental and human health. 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. Accelerated solvent extraction was developed to meet the new requirements of increased throughput and reduced solvent usage in sample preparation.

Method

The extractions were carried out using a Thermo Scientific™ Dionex™ ASE™ 350 Accelerated Solvent Extractor. The samples were analyzed using a Thermo Scientific™ TRACE™ 1310 Gas Chromatograph equipped with a Thermo Scientific™ Instant Connect Split/Splitless Injector and a Thermo Scientific™ TSQ™ 8000 Evo Triple Quadrupole GC-MS/MS system.

Conclusion

An analytical method was developed and applied to evaluate POP residues in tuna samples from different Food and Agriculture Organization (FAO) catch areas. The method proved to be simple and rapid, requiring small sample sizes and minimizing solvent consumption, due to the use of accelerated solvent extraction with an inline clean-up step. Detection via MS/MS provides both quantitative information and confirmation of POP residues in tuna. Corroborating the one-step accelerated solvent extraction method as a valid faster alternative to classic extraction methods because the analytical quality is comparable.

Read the full application note.

Dionex ASE 350 Accelerated Solvent Extractor

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

Determination of pesticides and persistent organic pollutants in honey by accelerated solvent extraction and GC-MS/MS

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Overview

Honey is a natural product that is widely used for both nutritional and medicinal purposes. It is generally considered a healthy substance that is free of impurities. However, many pollutants in the environment can contaminate honey, other bee products, and the bees themselves. Studies have documented the occurrence of organochlorines (OCs), polychlorobiphenyls (PCBs), organophosphates (OPs), and polybromodiphenylethers (PBDEs) in honey. The complexity of honey requires selective sample preparation because carbohydrates and other matrix substances may be co-extracted with the analytes. 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.

Method

The extractions were carried out using a Thermo Scientific™ Dionex™ ASE™ 350 Accelerated Solvent Extractor. The samples were analyzed using a Thermo Scientific™ TRACE™ 1310 Gas Chromatograph equipped with a PTV injector and a Thermo Scientific™ TSQ™ 8000 Evo Triple Quadrupole GC-MS/MS system.

Conclusion

An analytical method was developed and successfully applied to evaluate pesticides and POP residues in organic honey samples produced in three different Italian regions, which are characterized by different contamination sources. The method proved to be simple and rapid, requiring small sample sizes and minimizing solvent consumption, due to the ASE with an inline clean-up step. MS/MS detection provided both quantitative information and the confirmation of POP residues in honey, corroborating the one-step ASE method as a valid alternative to classical extraction methods.

Read the full application note.

Dionex ASE 350 Accelerated Solvent Extractor

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Using GC-MS/MS as a confirmatory method for dioxin-like PCBs in food and feed

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Overview

Polychlorinated biphenyls (PCBs) are a group of highly toxic organochlorine compounds that have a possible 209 congeners, depending on the number and position of the chlorine atoms. 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. DL-PCBs have been classified as persistent organic pollutants (POPs) and have been regulated under the Stockholm Convention for POPs since 2001.

Method

Sample introduction was performed with a Thermo Scientific™ TriPlus RSH™ autosampler. Compound separation was achieved using a Thermo Scientific™ TSQ™ 8000 Evo triple quadrupole GC-MS/MS instrument coupled with a Thermo Scientific™ TRACE™ 1310 GC system. Thermo Scientific™ TargetQuan 3.1 software, designed specifically to comprehensively process MS, MS/MS, or HRMS data for routine quantification of persistent organic pollutants in a regulated environment, was used.

Part Number	Description
26096-1540	Thermo Scientific™ TraceGOLD™ TG-5SilMS column, 60 m × 0.25 mm × 0.25 µm

Conclusion

The results of this evaluation demonstrate that the TSQ 8000 Evo GC-MS/MS system is an extremely effective tool for routine analysis of DL-PCBs, meeting all the European Commission requirements for DL-PCB confirmation in food and feed samples.

Read the full poster note.

TSQ 8000 Evo Triple Quadrupole GC-MS/MS system

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

A novel high-resolution accurate-mass, Orbitrap-based GC-MS platform for routine analysis of short-chained chlorinated paraffins

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Overview

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. SCCPs are intentionally manufactured and used as lubricants and coolants in the metal processing industry or as plasticizers and flame retardants in plastic products. In this study, the performance of a novel benchtop, high-resolution, accurate-mass Orbitrap-based GC-MS was tested for the analysis of SCCPs.

Method

Injection of liquid samples was performed automatically using a Thermo Scientific™ TriPlus™ RSH™ autosampler. A Thermo Scientific™ Exactive™ GC Orbitrap™ mass spectrometer was coupled to a Thermo Scientific™ TRACE™ 1310 gas chromatograph for gas-phase separation of target compounds using the consumables shown in the table below. Data was processed with Thermo Scientific™ TraceFinder™ software.

Part Number	Description
453A0344-UI	Thermo Scientific™ LinerGOLD™ GC liner, single taper
26096-1300	Thermo Scientific™ TraceGOLD™ TG5-SilMS column, 15 m × 0.25 mm × 0.25 µm

Conclusion

These preliminary results demonstrate that the Exactive GC 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, combined with its uncomplicated instrumental setup.

Read the full technical note.

Exactive GC Orbitrap GC-MS system

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

High-throughput analysis of polychlorinated dioxins/furans (PCDD/Fs) with dedicated DualData XL DFS Magnetic Sector GC-HRMS

Heinz Mehlmann, Dirk Krumwiede, Thermo Scientific, Bremen, Germany

Overview

By using the DualData XL Acquisition configuration of the Thermo Scientific™ DFS™ Magnetic Sector GC/HRMS, the sample throughput for dioxin/furan analyses can be increased. The analytical system can be set-up to perform different analyses, such as PCDD/F, PCBs, and PBDEs, and change automatically between columns within a measurement sequence. The analytical performance with DualData XL Acquisition and conventional GC-MS configuration was compared using the same set of polychlorinated dioxins and furans, PCBs, and PBDE samples as model compounds.

Method

The Thermo Scientific™ TriPlus™ RSH™ autosampler with extended x-rail served both GCs from one common sample tray. The configuration consisted of two Thermo Scientific™ TRACE™ 1310 GCs equipped with the DualData XL Module, using two columns coupled to the Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS.

Part Number	Description
26AF154P	Thermo Scientific™ TR-Dioxin™ column 60 m × 0.25 mm × 0.25 µm

Conclusion

The DualData XL Module for the DFS Magnetic Sector GC-HRMS allows a higher sample throughput with no loss in performance such as peak shape or sensitivity. The GC separation integrity, ruggedness, and long-term stability of the column switching system were proven in an unattended sample.

- Increase of productivity up to double sample throughput.
- Excellent peak shape using MCD wafer technology.
- No loss in sensitivity compared to a standard dual GC system.
- Applicable to different POPs such as dioxins, PCBs, and PBDEs.

Read the full technical note.

DFS Magnetic Sector GC-HRMS system

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

A new GC–ICP–MS method for compound specific determination of brominated flame retardants

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Overview

Polybrominated diphenyl ethers (PDBEs) are brominated flame retardants (BFRs), which are commonly found in electrical and electronic equipment and household textiles. Due to their ubiquitous use and poor recycling practices for electronic waste, these substances are now found in consumer goods that do not require flame retardancy, such as kitchen utensils, children's toys, and food contact materials. A method based on ICP-MS detection was developed with a goal to accurately and rapidly quantify BFRs in plastic materials and subsequently in consumer products.

Method

A Thermo Scientific™ TRACE™ 1310 gas chromatograph (GC) was interfaced with a Thermo Scientific™ iCAP™ Q ICP-MS. Sample introduction was via a Thermo Scientific™ TriPlus™ RSH autosampler.

Conclusion

By virtually eliminating the decomposition of higher brominated compounds into the lower brominated ones, quantification of the complete range of congeners was possible. Thanks to the programmed flow, chromatographic run times are reduced, and by employing just one GC column, the number of analyses per sample is halved.

Read the full poster note.

iCAP RQ ICP-MS

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

Sensitive and accurate quantitation of perfluorinated compounds in human breast milk using selected reaction monitoring assays by LC/MS/MS

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Overview

The potential toxicity of perfluorinated compounds (PFCs) 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 in 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.

Method

Six PFCs in neat solution and in human breast milk matrix were analyzed. Human breast milk was diluted in acetonitrile followed by weak anion SPE, chromatography separation was performed using a Thermo Scientific™ Hypersil GOLD™ PFP HPLC column. LC-MS/MS was performed on a Thermo Scientific™ TSQ Vantage™ triple quadrupole mass spectrometer using selected reaction monitoring (SRM) and H-SRM.

Part Number	Description
25402-103030	Thermo Scientific™ Hypersil GOLD™ PFP column, 100 mm x 3 mm 1.9 µm column

Conclusion

PFCs were accurately and reproducibly detected at ppt levels in neat solution and in human milk. This approach does not require trapping or column switching techniques to ensure exceptional sensitivity in high chemical backgrounds.

Read the full application note.

Discover the NEW Thermo Scientific™ TSQ Quantis™ triple quadrupole mass spectrometer

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Highly selective detection and identification of nitrofuran metabolites in honey using LC-MS/MS

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[3]Eidomet, Buenos Aires, Argentina

Overview

Nitrofuran metabolites were accurately quantitated at levels as low as 0.3 ppb in a matrix consisting of honey using LC-MS/MS. Honey, as well as other food products, provides a complex matrix that increases the difficulty of sample preparation. Efficient chromatography is critical to provide good separation of the various metabolites from each other and any contaminants that might be present. The most important requirement is a very high level of sensitivity and linearity in the mass spectrometer to achieve the required high levels of accuracy in quantifying the metabolites.

Method

An LC-MS/MS assay to detect and identify nitrofuran metabolites developed. Sample analysis was performed on a Thermo Scientific™ mass spectrometer using positive electrospray ionization (ESI) in SRM mode.

Conclusion

The extraction method appears to be extremely robust and reliable with good recovery efficiency (better than 80%), allowing unambiguous routine identification and quantification of all nitrofuran metabolites in honey. The LC-MS/MS-based method described here provides high speed, excellent sensitivity, and specificity of detection.

Read the full application note.

Thermo Scientific TSQ Quantis triple quadrupole mass spectrometer

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

A strategy for an unknown screening approach on food and environmental samples using HRAM mass spectrometry

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Overview

The analysis of food and environmental samples for contaminants by LC-MS has become a quick and cost-effective routine application when run in a targeted fashion, but this method disregards events or circumstances not taken into account beforehand. Run in a non-targeted fashion, this method is known to be laborious and time-consuming, making it everything but a routine application. New-generation software now links quantitative and (unknown) screening approaches into one smoothly integrated workflow, tying together component detection capabilities of unknown screening workflows with the identification capabilities of targeted screening and quantification software.

Method

Four samples of surface water from different sources were taken and analyzed without any further treatment. In addition, one neat standard as a control sample and one tap-water sample as a reference sample were run in the same sequence. Chromatographic separation was performed using the HPLC columns shown in the table.

Part Number	Description
Trapping column	Thermo Scientific™ Hypersil GOLD™ C18 column, 20 mm × 2.1 mm × 12 µm trapping column
17626-032130	Thermo Scientific™ Accucore™ RP-MS 18 column, 30 mm × 2.1 mm × 3 µm column

Conclusion

The resolving power of the Thermo Scientific™ Exactive™ Plus Orbitrap™ MS system provides separation of the analyte peaks from the background and matrix signals, thus yielding the selectivity and reliability of the obtained results.

Read the full poster note.

Thermo Scientific™ Q Exactive™ Plus Hybrid Quadrupole-Orbitrap™ mass spectrometer

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