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## Food contact materials

## Applications summary compendium



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## Food contact materials testing

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#### The Analytical Scientist article Food contact materials

### Living in a material world

John Gilbert, Director at FoodLife International, York, UK

Today, a food contact material is, by definition, one that is approved for food applications – the EU, for example, has a positive list of starting materials and plastics additives restricted to substances that are deemed safe for food packaging. Polyolefins (HDPE, LDPE and PP), PET and polystyrene are probably the most important plastics in common use in bottle, sheet and film formats. Films can be particularly complex in construction, involving multiple laminate layers to achieve the desired properties, sometimes with adhesive between layers, and printing on the outer surface. Coated paperboard is also widely used; for example, in drinks cartons.

Although polymers are generally inert, high-molecular weight, cross-linked substances that don't migrate – the residual monomers used to prepare them can, and since it's not possible to get a complete conversion to the polymer, oligomers may remain. Moreover, as indicated above, plastics need numerous additives to make them suitable for packaging – antioxidants, heat stabilizers, UV absorbers, plasticizers and colorants, and so on – there are literally hundreds of potential substances, which represents a significant analytical challenge.

It's fair to say that food-packaging analysis is very niche compared with, for example, pesticide residues, but there is a lot of awareness within the packaging industry – and the food industry certainly realizes it must comply with regulations.

#### **Analytical drivers**

Over the years, a great deal of food packaging regulation has actually been driven by developments in analytical techniques. Going back to the 1970s, MS and GC-MS were around, but the techniques were relatively specialized. People were using headspace GC with FID, and LC-MS was yet to be developed. As instrumental techniques have become more sensitive – and as costs have come down – methods have been developed and regulations established using the techniques available. Indeed, today's regulations were beyond the realms of possibility back in the 1970s because the technology simply wasn't available. Substances of below 1000 daltons in molecular weight are of particular interest, but can vary from simple volatile chemicals like vinyl chloride, acrylonitrile, vinylidene chloride through to complex mixtures of substances of much higher molecular weights like mineral oils. Migrants range in polarity from highly polar to non-polar organic molecules through to classical metals, as well as metal nanoparticles. Therefore, the full range of analytical tools must be employed in migration testing, including headspace GC-MS for volatiles, LC-MS/MS, LC-highresolution accurate mass (HRAM) MS (Orbitrap) through to AAS and ICP-MS. Even DART-Orbitrap MS has been investigated for direct analysis of both plastics materials as well as extracts from plastics without any cleanup.

#### **NIAS work**

In 2011, Commission Regulation (EU) No. 10/2011 brought together numerous previous regulations and introduced the concept of non-intentionally added substances (NIAS). The new regulations place responsibility on food producers to demonstrate due diligence for untargeted substances – a challenging feat. With NIAS, the substance could be a decomposition product from additives used in the plastic packaging or an adventitious contaminant – there is a huge range of possibilities. And that has led to a real interest in non-targeted analysis using LC-HRAM (Orbitrap-based) systems, where the ability to gain fullscan data at accurate mass is extremely useful.

Right now, NIAS regulations are very general; they simply state that not only are you responsible for showing compliance to the positive list of substances, you also have to prove you have considered other potential contaminants, which by NIAS definition are unknown. It's very typical in the regulatory world to begin with an indication of intention and then firm up on the detail of compliance later on.



#### The *Analytical Scientist* article (continued) Food contact materials

### Living in a material world

John Gilbert, Director at FoodLife International, York, UK

In time, someone might suggest an approach for providing assurance, and someone else will suggest it is validated. If CEN adopts it, it will become a definitive CEN standard for NIAS measurement. But, of course, these things take time.

Right now, I would say that the industry is largely selfpolicing – especially given that food control or public analysts have limited resources. But that doesn't mean it isn't proactive. The big worry for the food industry is a sudden scare and the resultant damage in reputation – and there have been several related to packaging. Photoinitiators represent a recent scare – especially as they decompose into free radicals when exposed to sunlight. Bisphenol A is also on the list, as it can migrate into food from the epoxy resin coating on the can or from polycarbonate food containers in certain circumstances.

I believe that in due course, contract labs will offer comprehensive analysis using HRAM mass spectrometry for migrating substances from food packaging, just as they do for other residues and contaminants.

#### The future of food contact materials

Packaging never stands still; innovation is continual. Take nanotechnology – the industry is looking for ways to improve the performance of packaging with nanoclays and other materials, such as nano-silver.

There's also a great deal going on in active packaging, where examples include 'moisture absorbers' used in meat trays, 'scavengers' found in small sachets used to absorb residual ethylene or oxygen, or 'releasing systems' that slowly release antimicrobial agents to extend shelf-life. There is also interest in whether it's possible to incorporate antimicrobial substances into the packaging itself. Clearly, the food cannot be contaminated in the process. Indeed, all of these innovations represent new analytical challenges. And with nanomaterials, unlike other contaminants, it is not simply a case of measuring compound concentrations – particle size and particle size distribution are also important. There's a good paper that uses Thermo Scientific ICP-MS to look at the migration of silver nanoparticles incorporated into plastic chopping boards into chicken meat (1).

The regulators have to balance food safety (from a contaminant point of view) on one hand, but on the other, limit controls that get in the way of packaging innovations that are advantageous to the producer, retailer, and consumer. Indeed, it is all too easy to think negatively about packaging when you consider substance migration and contaminants. But the reality is that packaging has made a huge difference to the food chain in terms of extending shelf life and availability; we no longer have to rely on locally available food products, and I would say the advantages far outweigh the disadvantages – it's just a question of striking the right balance and using the right analytical tools and techniques to ensure safety.

In my opinion, the push for sensitivity has largely ended (which was getting a little ridiculous in terms of identifying miniscule amounts of anything and everything). I believe specificity is also adequate – as long as the analysis is performed properly. What the food and packaging industries want is the ability to cover more analytes, at lower cost – and with greater speed. And as attention turns increasingly to non-intentionally added substances, we'll see a concomitant growth in untargeted analyses.

To watch John Gilbert's comprehensive webinar on: "Analytical challenges in measuring migration from food contact materials" – **register here.** 

#### Read the full article.



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### Comparison of Soxhlet and accelerated solvent extraction for leachable and extractable analysis of packing material

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#### **Overview**

This application note compares Soxhlet and accelerated solvent extraction techniques in packing material extractable studies. The accelerated solvent extraction technique is an automated technique with several advantages, including efficient extraction, reduced extraction time (<0.5 h/sample), reduced solvent use (<30 mL/sample), and flexibility in solvent selection. Using the method and sequence editor in the Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> ASE<sup>™</sup> 350 Accelerated Solvent Extractor system, three solvents and their mixture can be used as an extraction solvent in different methods in a single sequence run. The accelerated solvent extraction technique is an efficient technique to extract compounds from polymeric materials reliably.

#### Method

Polymer packaging was extracted using the Dionex ASE 350 Accelerated Solvent Extractor system and Soxhlet, respectively. The extracts were analyzed using a Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> UltiMate<sup>™</sup> 3000 HPLC system coupled with a Thermo Scientific<sup>™</sup> Q Exactive<sup>™</sup> Hybrid Quadrupole-Orbitrap<sup>™</sup> mass spectrometer.

#### Part Number Description

17126-102130

Thermo Scientific<sup>™</sup> Accucore<sup>™</sup> C18 column, 2.1 × 100 mm × 2.6 μm

#### Conclusion

The accelerated solvent extraction technique delivers comparable or more efficient extractions than the traditional Soxhlet extraction method using less time and less solvent. Extractions using two solvents of varying polarity are necessary in controlled extraction studies because different solvents can provide additional information on extractables.

#### Read the full application note.



Dionex ASE 350 accelerated solvent extractor



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## Static headspace analysis of residual solvents in flexible packaging and quantitation with multiple headspace extraction following EN 13628-1: 2002

Silvia Gemme and Massimo Santoro, Thermo Fisher Scientific, Milan, Italy

#### **Overview**

Flexible packaging is essential in ensuring the safety, guality, and shelf-life of packaged consumer products. Such packaging, commonly referred to as cling film or plastic wrap, is often comprised of layers bonded together with adhesives (multilayer) and imprinted with product information. During the process of manufacturing, shipping or storage, the packaging itself might leach solvents from the adhesives and printing inks or finishes into the very product it was meant to protect. When these are food products, those solvents can pose significant health risks and negatively impact the taste, aroma, or appearance of the product.

#### Method

Headspace analysis was conducted using a Thermo Scientific<sup>™</sup> TriPlus<sup>™</sup> 300 Headspace autosampler. Equipped with the standard 1 mL loop and connected to a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> 1310 Gas Chromatograph (GC). The system was further configured with an instant connect Split/Splitless (SSL) injector and a Thermo Scientific<sup>™</sup> Instant Connect Flame Ionization Detector (FID) module. The Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> Chromeleon<sup>™</sup> 7.2 Chromatography Data System was used to control the system, acquire data and generate all reports.

Part Number	Description
26085-3330	Thermo Scientific <sup>™</sup> TraceGOLD <sup>™</sup> TG-624 (60 m × 0.25 mm × 1.4 um) column
453A1335	Thermo Scientific <sup>™</sup> HS/SPME straight liner
60180-506	20 mL headspace vials
60180-520	Magnetic caps and PTFE/silicone septa

Conclusion

The data obtained in this application demonstrate that the technique of headspace gas chromatography using MHE in an automated fashion easily meets the requirements of the EN 13628-1: 2002 standard and provides excellent quantitation results without any sample preparation.

#### Read the full application note.



#### **TriPlus 300 Headspace autosampler**

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## Unattended automated standard addition and headspace analysis for the quantitative determination of VOCs in food packaging

Stefano Pelagatti,<sup>1</sup> Silvia Gemme,<sup>1</sup> Andrea Caruso,<sup>1</sup> Fausto Pigozzo,<sup>1</sup> Massimo Santoro,<sup>1</sup> and Eric Phillips<sup>2</sup> <sup>1</sup>Thermo Fisher Scientific, Milan, Italy; <sup>2</sup>Thermo Fisher Scientific, Austin, Texas, USA

#### **Overview**

Headspace analysis by means of a dedicated autosampler is a standard technique for the determination of volatile organic compounds (VOCs) possibly present in food packaging materials. The main challenge with this kind of analysis is the quantification of volatile compounds that are present because these samples are typically layered solids that generate adsorption and migration effects. Until now, preparation of samples for standard addition calibration has been performed off-line but by performing sample preparation by means of the same robotic sampler used for headspace analysis enables the quantification sequence to be run automatically in an unattended way.

#### Method

A Thermo Scientific<sup>™</sup> TriPlus<sup>™</sup> RSH autosampler was coupled to the Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> 1310 GC, coupled with the Thermo Scientific<sup>™</sup> ISQ<sup>™</sup> Series Single Quadrupole GC-MS, for analysis of the samples. The GC was configured with an instant connect split/splitless (SSL) module, operated in split mode.

Part Number	Description
26059-3330	Thermo Scientific <sup>™</sup> TraceGOLD <sup>™</sup> TG-624
20039-3330	(60 m × 1.4 μm × 0.25mm) column

#### Conclusion

A completely automated method for analyzing and quantifying VOCs in food packaging materials is presented. The combination of sample preparation steps and an analytical step in the same sequence allows high accuracy in quantification, high sample throughput, and minimizes error-prone manual manipulations.

#### Read the full application note.



ISQ Series Single Quadrupole GC-MS systems



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#### Application summary AN10479 Food contact materials

# SPME-GC-MS/MS for identification and quantification of migration contaminants in paperboard food packaging

Katerina Bousova,<sup>1</sup> Michal Godula,<sup>2</sup> and Michele Suman<sup>3</sup> <sup>1</sup>Thermo Fisher Scientific, Special Solutions Center Europe, Dreieich, Germany <sup>2</sup>Thermo Fisher Scientific, Prague, Czech Republic <sup>3</sup>Barilla Food Research Labs, Parma, Italy

#### **Overview**

Packaging of foods is a key activity of the food industry. It helps protect the food from damage while keeping it fresh and free from microbial degradation. However, the materials used in food packaging can also cause degradation of the packaged food. Inappropriately packaged food may develop an unpleasant odor or off-flavor. It is important for food producers to ensure that packaging does not contribute to off-flavors or other toxic compounds that might be harmful to consumers. During the study, a simulated food product is placed in contact with the packaging material for a precisely defined period of time, under specially defined conditions, and subsequently analyzed.

#### Method

These experiments use a Thermo Scientific<sup>™</sup> TSQ<sup>™</sup> 8000 GC-MS/MS system, including a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> 1310 gas chromatograph equipped with a Thermo Scientific<sup>™</sup> TriPlus<sup>™</sup> RSH autosampler and SPME module (SPME NL: 50.5 mm). Data acquisition for quantification and confirmation is performed in the timedselected reaction monitoring (timed-SRM) mode using Thermo Scientific<sup>™</sup> TraceFinder<sup>™</sup> 3.2 software.

10177894 Thermo Scientific <sup>™</sup> TraceGOLD <sup>™</sup> TG-5Sil		Part Number
30 m × 0.25 mm × 0.25 μm column	IMS,	10177894

#### Conclusion

The reported in-house validated method enables determination and quantification of 12 possible migrants from paperboard packaging. This fully automated SPME method can increase laboratory throughput. The results obtained from in-house validation, according to the IUPAC/AOAC harmonized protocol, confirmed that this method is suitable for monitoring the content of unwanted contaminants in paperboard intended for contact with food.

#### Read the full application note.



TSQ 8000 Evo Triple Quadrupole GC-MS/MS



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



#### Application summary AN20735 Food contact materials

## Determination of phthalate esters in soft drinks by GC-MS

Anila I. Khan, Thermo Fisher Scientific, Runcorn, UK



#### **Overview**

Phthalate esters are the main plasticizers used as softening agents in the production of PVC. There have been reports from the U. S. Food and Drug Administration that certain foods and beverages, particularly fruit juices, contain high levels of phthalates. In this application note, an analytical procedure for the quantitative analysis of 15 phthalate esters is reported. The extraction of the phthalate esters is based on liquid-liquid extraction.

#### Method

The analysis was carried out using a Thermo Scientific<sup>™</sup> TraceGOLD<sup>™</sup> TG-5MS GC column in a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> GC Ultra gas chromatograph and Thermo Scientific<sup>™</sup> ISQ<sup>™</sup> GC single quadrupole mass spectrometer, using Thermo Scientific<sup>™</sup> Xcalibur<sup>™</sup> data processing software.

Part Number	Description
26098-1420	TraceGOLD TG-5MS, 30 m × 0.25 mm × 0.25 μm column
31303211	Thermo Scientific BTO, 17 mm
45350033	Thermo Scientific <sup>™</sup> Splitless Straight Liner, 5 × 8 × 105 mm
36500525	10 μL fixed needle syringe for a Thermo Scientific™ TriPlus™ autosampler

#### Conclusion

A method for the quantification of phthalate esters in soft drinks has been developed. The ultra-low bleed characteristics of the column enable the detection of low levels of phthalate esters using the ISQ mass spectrometer in SIM mode.

#### Read the full application note.



ISQ Series Single Quadrupole GC-MS systems



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## Determination of phthalates in liquor beverages by single quadrupole GC-MS

Jianxia Lv,<sup>1</sup> Lina Liang,<sup>1</sup> and Hans-Joachim Huebschmann<sup>2</sup> Thermo Fisher Scientific, <sup>1</sup>Beijing, China, <sup>2</sup>Singapore

#### **Overview**

Phthalates (Phthalate Acid Esters, PAEs) have widespread use in the polymer industry as plasticizers and softeners to increase the plasticity of polymer materials and their toughness and strength. Phthalate plasticizers also migrate from plastic containers or closures into soft drinks and alcoholic beverages. This study follows the China regulation GB/T 21911-2008 for the determining of phthalates in food.

#### Method

All measurements were performed using the Thermo Scientific<sup>™</sup> ISQ Series single quadrupole GC-MS system with a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> 1310 GC equipped with the instant connect SSL injector module (split/ splitless injector) and a Thermo Scientific<sup>™</sup> AS 1310 liquid autosampler.

#### Part Number Description

26094-1420

Thermo Scientific<sup>™</sup> TraceGOLD TG-35MS 30 m × 0.25 mm × 0.25 µm column

#### Conclusion

In this study for the determination of phthalate plasticizer residues in liquor, the ISQ Series GC-MS met the special testing requirements set by the China method GB/T 21911-2008 for determining phthalates in food.

#### Read the full application note.



ISQ Series Single Quadrupole GC-MS systems



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



#### Application summary AN20639 Food contact materials

## Analysis of benzophenone and 4-hydroxybenzophenone in breakfast cereal

Anila I. Khan, Thermo Fisher Scientific, Runcorn, UK



#### Overview

The Food Standard Agency (FSA) published a method for analyzing benzophenone and 4-hydroxybenzophenone from food. Benzophenone is a chemical migrant, associated with inks and coating in food packaging that can migrate to the surface of the food. Directive 2002/72/ EC has a specific migration limit (SML) for benzophenone at 0.6 mg/kg.

Part Number	Description
60105-337	Thermo Scientific <sup>™</sup> HyperSep <sup>™</sup> Dispersive SPE multipacks
60105-225	Thermo Scientific HyperSep Dispersive SPE clean-up product
26089-1420	Thermo Scientific <sup>™</sup> TraceGOLD <sup>™</sup> TG-17MS, 30 m × 0.25 mm × 0.25 µm column
31303211	BTO, 17 mm septa
453T2999	Splitless FocusLiner <sup>™</sup> for 50 mm needle, 5 × 8 × 105 mm
29053488	100% graphite ferrules 0.1–0.25 mm ID
29033496	Graphite/Vespel <sup>®</sup> ferrules for transfer line 0.1–0.25 mm ID
365D0291	10 µL fixed needle syringe
60180-599	9 mm Wide Opening Screw Thread Vial Convenience Kit

#### Method

A modified sample preparation approach, described in the European EN15662 QuEChERS procedure, was used for extracting benzophenones from breakfast cereal. A Thermo Scientific<sup>™</sup> TriPlus RSH<sup>™</sup> autosampler coupled to a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> Gas Chromatograph was used to separate the extracts with detection by the Thermo Scientific<sup>™</sup> ISQ<sup>™</sup> mass spectrometer in SIM mode.

#### Conclusion

The QuEChERS sample preparation method provided a fast and simple approach for extracting and analyzing benzophenone and 4-hydroxybenzophenone in breakfast cereal, achieving high recoveries and good reproducibility.

#### Read the full application note.



ISQ Series Single Quadrupole GC-MS systems



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## Characterizing unknowns in food packaging using GC Orbitrap mass spectrometry

Dominic Roberts,<sup>1</sup> Jesus Varela,<sup>2</sup> Yves-Alexis Hammel,<sup>2</sup> and Paul Silcock<sup>1</sup> <sup>1</sup>Thermo Fisher Scientific, Runcorn, UK <sup>2</sup>Nestle, Lausanne, Switzerland

#### **Overview**

Packaging is an essential element of a safe food supply chain with its main purpose to preserve the food it covers and to maintain its quality over the course of the products shelf life. It is also well known that the chemical components used in the packaging can migrate into the food and present an even greater threat. Food and beverages can interact strongly with any surface that they come into contact with and can potentially impact the quality of the product. This study focused on the utilization of a GC Orbitrap system for fast and confident identification of unknown compounds in food packaging.

#### Method

A Thermo Scientific<sup>™</sup> Q Exactive<sup>™</sup> GC Orbitrap<sup>™</sup> GC MS/MS hybrid quadrupole-Orbitrap mass spectrometer was used. Sample introduction was performed using a Thermo Scientific<sup>™</sup> TriPlus<sup>™</sup> RSH autosampler, and chromatographic separation was obtained with a Thermo Scientific<sup>™</sup> TRACE<sup>™</sup> 1310 GC system. Data was acquired using the Thermo Scientific<sup>™</sup> TraceFinder<sup>™</sup> software, with Thermo Scientific<sup>™</sup> MassFrontier<sup>™</sup> spectral interpretation software used for structural elucidation.

Part Number	Description
26096-1421	Thermo Scientific <sup>™</sup> TraceGOLD <sup>™</sup> TG-5SilMS 30 m × 0.25 mm × 0.25 µm with a 10 m guard column
453A0344-UI	Single gooseneck liner

#### Conclusion

The results of this study demonstrate that the Q Exactive GC Orbitrap GCMS/MS hybrid quadrupole-Orbitrap mass spectrometer, in combination with easy-to-use software tools, is a powerful tool for the profiling of complex samples and the identification of unknown chemicals.

Penne

#### Read the full application note.



Q Exactive GC Orbitrap GC-MS system



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



#### Application summary AB161 Food contact materials

## Determination of bisphenols using HPLC-ECD

Paul Gamache and Ian Acworth, Thermo Fisher Scientific, Chelmsford, MA, USA



#### **Overview**

Bisphenols A and B are monomers used in the production of epoxy resins and plastics and are widespread in food and drink packages, as coatings of metal cans and water pipes, as microwave susceptors (used to crispen food) and in some dental resins. Bisphenol A and liquid obtained from vegetables from plastic coated cans have been shown to be estrogenic in MCF-7 and human breast cancer cells.

#### Method

The global method presented here uses the Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> UltiMate<sup>™</sup> 3000 HPLC system with Coulometric array detection to measures both bisphenols and the isoflavonic phytoestrogens. A Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> CoulArray<sup>™</sup> Coulometric Array Detector was used.

#### Part Number Description

25003-153030

Thermo Scientific<sup>™</sup> Hypersil GOLD<sup>™</sup> C18, 3 µm, 3 × 150 mm column

#### Conclusion

The coulometric electrode not only offers unrivaled sensitivity and selectivity but it also offers unparalleled stability and is maintenance free for outstanding routine operation. Using gradient HPLC with the CoulArray detector the presumptive xenoestrogens, bisphenols, can be assayed on the same system as the phytoestrogens and the synthetic estrogen, DES. By using reversed phase gradient HPLC with near-normal phase conditions, the wide range of polarities can be eluted in a single run.

#### Read the full application brief.



UltiMate 3000 CoulArray Coulometric Array Detector



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## Determination of phthalates in drinking water by UHPLC with UV detection

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#### **Overview**

Phthalates are a class of chemical compounds widely used as plasticizers for polyvinyl chloride resins, adhesives, and cellulose film coating. Phthalates are potentially hazardous to human health—especially to children's health—due to their classification as endocrine disruptors. The aim of this paper is to develop an efficient, high-performance liquid chromatography (HPLC) method for the simultaneous determination of 19 phthalate compounds in drinking water.

#### Method

The analysis was carried out using a Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> UltiMate<sup>™</sup> 3000 Rapid Separation LC (RSLC) system with DAD-3000RS Diode Array Detector with data processing carried out using Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> Chromeleon<sup>™</sup> Chromatography Data System software.

#### Part Number Description

075724

Acclaim C30 column 3  $\mu m,$  3.0  $\times$  150 mm

#### Conclusion

The work shown here describes an efficient HPLC method using UV detection for the determination of phthalates in drinking water samples. All 19 phthalates listed in key environmental regulatory documents—EU Directive 2005/84/EC; U.S. EPA Methods 606 and 8061A; the Chinese HJ/T 72-2001; and the Standardization Administration of China (SAC) GB/T 20388-2006 and GB/T 21911-2008—are well separated.

#### Read the full application note.



#### UltiMate 3000 Basic Automated system



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Analysis of plasticizer contaminants in beverages and milk using an automated system based on turbulent-flow chromatography coupled to LC-MS/MS

Ebru Ates, Klaus Mittendorf,

Thermo Fisher Scientific Food Safety Response Center, Dreieich, Germany

#### Overview

Phthalates are endocrine active chemicals used in a variety of consumer products. In some markets, restricted levels of certain phthalates are permitted for use in food contact materials, but they are not permitted as direct food additives. Contamination arises from numerous sources such as the environment and food packaging. Crosscontamination with phthalates can easily arise during trace analysis in the laboratory and there are significant advantages in minimizing sample handling through online automated analysis.

#### Method

Samples of orange juice, bitter lemon and milk were spiked. Online sample prep with LC analysis performed by Thermo Scientific<sup>™</sup> Transcend<sup>™</sup> TLX system powered by Thermo Scientific<sup>™</sup> TurboFlow<sup>™</sup> technology. MS analysis is carried out using a Thermo Scientific<sup>™</sup> TSQ Quantum<sup>™</sup> Access MAX triple quadrupole mass spectrometer controlled by Thermo Scientific<sup>™</sup> Aria<sup>™</sup> MX software. Data acquisition and processing are performed using Thermo Scientific<sup>™</sup> Xcalibur<sup>™</sup> 2.1 software.

Part Number	Description
25003152130	Thermo Scientific™ Hypersil GOLD™, 150 × 2.1 mm 3 µm column
CH953280	C18 XL 0.5 × 50 mm
3205111	LC vials
3151266	LC vial caps

#### Conclusion

A method for the determination of plasticizers in beverages and milk has been developed to enable fast and costeffective automated determination of selected plasticizers. Online TurboFlow sample preparation coupled to the analytical HPLC separation equipped with a triple quadrupole detector enables very selective and effective determination of plasticizers.

#### Read the full method guide.



<u>TSQ Quantum</u><sup>™</sup> <u>Access MAX triple quadrupole mass</u> <u>spectrometer</u>



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## Phthalate screening in food packaging by ambient ionization high resolution MS/MS mass spectrometry

Catharina Crone,<sup>1</sup> Markus Kellmann,<sup>1</sup> Frans Schoutsen,<sup>2</sup> Elizabeth Crawford<sup>3</sup> <sup>1</sup>Thermo Fisher Scientific, Bremen, Germany; <sup>2</sup>Thermo Fisher Scientific, Breda, The Netherlands; <sup>3</sup>IonSense, Inc., Saugus, MA, USA

#### **Overview**

Phthalates (Phthalate Acid Esters, PAEs) are widely used in industry as plasticizers in everyday products like toys, flooring, personal care products, and food packages. These compounds can be present up to a high ratio in some materials. As substances classified as semi-volatile organic compounds (SVOC), they are evaporating into the environment over a long time. This Poster demonstrates the analysis of phthalic acid diesters on a high-resolution accurate mass Orbitrap<sup>™</sup> analyzer based system coupled to a "Direct Analysis in Real Time" (DART<sup>™</sup>) ionization source.

#### Method

All data was acquired using a Thermo Scientific<sup>™</sup> Q Exactive<sup>™</sup> mass spectrometer, coupled to a direct analysis in real time DART<sup>™</sup> SVPA ion source (IonSense Inc., Saugus, MA, USA). The DART source was operated at 200 °C using helium as carrier gas. In total, 13 lid gaskets, 9 milk packages, 5 bags and fruit containers were tested.

#### Conclusion

DART combined with Orbitrap<sup>™</sup> based HRAM MS/MS was shown to be a very fast and convenient way for screening for additives in food packaging and other goods. Due to ambient phthalate content, the background has to be carefully monitored before starting the analysis of each sample to avoid contamination. For future work, defined solid standards have to be prepared to go on with the quantitative approach.

#### Read the full poster note.



Q Exactive Hybrid Quadrupole-Orbitrap mass spectrometer



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## Analysis of known and unknown food contact materials by means of HPLC-High-Resolution-Accurate mass spectrometry

Laszlo Hollosi and Michal Godula, Food Safety Response Center Thermo Fisher Scientific, Dreieich, Germany

#### **Overview**

Packaging materials (PM) and non-intentionally added substances (NIAS) are currently one of the hottest research topics in food safety relevant applications. Current research especially focuses on identification of non-expected or up-to-now unknown compounds. This poster aims to present such approaches supported by High-Resolution MS (HRMS) based LC-MS methods for identification of known authorized or unauthorized substances.

#### Method

All data was acquired using a Thermo Scientific<sup>™</sup> Exactive<sup>™</sup> GC Orbitrap<sup>™</sup> high-resolution benchtop mass spectrometer coupled to Transcend TLX-1 system. Identification of known and unknown compounds was carried out using TraceFinder 3.1 quantitative and screening methods.

#### Part Number Description

25203-102130

Thermo Scientific<sup>™</sup> Hypersil GOLD<sup>™</sup> C8 HPLC, 100 × 2.1 mm, 3 µm

#### Conclusion

All test compounds could be identified correctly. HRMS is essential for high confidential identification of both known and unknown compounds. Adequate software support with correct databases is necessary to apply in order to get correct results.

#### Read the full poster note.



Q Exactive Focus Hybrid Quadrupole-Orbitrap mass spectrometer



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## Characterization of nanoparticles using ICP-MS: advantages and challenges for nanoparticles in food

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#### **Overview**

Nanoparticle characterization in food faces many challenges due to the presence of complex matrix and the lack of fully developed and validated sample preparation protocols. An approach based on enzymatic extraction, Field Flow Fractionation (FFF) and final nanoparticle characterization with sp-ICP-MS was investigated for a chicken meat paste.

#### Method

A Wyatt Technology<sup>™</sup> Eclipse<sup>®</sup> equipped with a short channel was coupled to the Thermo Scientific<sup>™</sup> iCAP<sup>™</sup> Qc<sup>™</sup> ICP-MS. The mobile phase was delivered to the Eclipse chassis using a Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> ICS-5000<sup>™</sup> and injections were performed using the sample loop of the Thermo Scientific<sup>™</sup> Dionex<sup>™</sup> AS-AP ICS-5000 autosampler. A iCAP Qc was used for all experiments. Thermo Scientific Qtegra<sup>™</sup> software was used throughout for iCAP Q control and all data acquisition. Thermo Scientific Chromeleon<sup>™</sup> software was used to drive the Wyatt Eclipse and ICS-5000 in a single method.

#### Conclusion

Both FFF-ICP-MS and sp-ICP-MS bring analytical advantages to the characterization of NPs and act as complementary techniques. The integrated FFF-ICP-MS package is fully automated with bidirectional control and emergency shut-off features. The completely metal free FFF/IC system operates with a single pump and offers a switch option that allows the user to change from FFF to IC quickly. The high base sensitivity and low backgrounds of the iCAP Q offer a particular advantage in sp-ICP-MS.

#### Read the full poster note.



**ICAP RQ ICP-MS** 



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Application summary method guide 40184 Food contact materials

## Atomic absorption full method tin in canned fruit juice



#### Overview

Inorganic tin and its compounds are poorly absorbed in the intestinal tract and lasting harmful effects have not been documented. However, even small amounts of the metal can adversely affect the flavor and storage properties of food products. The metal is introduced as a contaminant during processing of food products and can accumulate during storage due to leaching from the containers. The traditional flame atomic absorption spectrometric determination of tin is relatively insensitive, and accurate quantification at low concentrations is difficult. Tin can be successfully determined by Graphite Furnace Atomic Absorption Spectrometry using an accurate background correction system provided care is taken to minimise losses during the program cycle.

#### Method

Standard solutions containing 25, 50, and 100  $\mu$ g/L of tin in 10% v/v hydrochloric acid and an acid blank were prepared. Two samples of canned orange and pineapple juice were spiked at 125 and 250  $\mu$ g/L, and analyzed for method validation.

#### Conclusion

A simple method for the routine determination of tin in canned fruit juices is presented. Use of matrix modification with ammonium nitrate allows calibration against simple aqueous standards, and the minimal residual background signal is easily corrected by the Quadline background correction system.

#### Read the full method guide.



iCE<sup>™</sup> 3500 AAS Atomic Absorption spectrometer



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