

Identification and quantification workflows

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Food contact materials

A Food Contact Material (FCM) is any material approved for food use that comes in contact with food or drink products during manufacturing, packaging, preparation, and storage. They can be made from a variety of materials including plastics, rubber, paper, and metal. The safety of a FCM must be evaluated, as chemicals can migrate from the materials into the food. Food packaging must be manufactured in compliance with regulations, including good manufacturing practices, so that any potential transfer of chemical substances from the packaging to foods does not raise food safety concerns, change the composition of the food or have adverse effects on the taste or odor of the product.

Identify all suspects in food packaging

- migration limits that may impact consumer health.
- (NIAS).

Factors Affecting Migration





Heat Higher temperatures increase migration.

Time Long storage time increases migration potential.



Regulations US FDA 21 CFR 174 to 21CFR 190. EU Regulation 10/2011.

and Quantification

These challenges require an arsenal of analytical techniques and workflows to meet the ever demanding challenges of compliance with global regulations.



Confident Identification The analysis of packaging impurities involves a diverse range of chemicals; from volatiles to high molecular weight non-volatile molecules and even metals.



• A FCM must not transfer chemicals to, or cause changes to, foods above regulated

• Testing is driven by regulation and demands migration studies that assess all known intentionally added substances (IAS) and 'unknown' non-intentionally added substances



Food type Fatty/acidic foods & liquids have influence on migration.



Packaging size Ratio of packaging surface to foodstuff volume.



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Extract smarter

Traditional Soxhlet or reflux techniques are labor intensive (>24 hours) and consume large quantities of solvent (>150 mL/sample).

Accelerated solvent extraction delivered by the Thermo Scientific[™] Dionex[™] ASE[™] 350 System is an automated alternative with several advantages, including efficient extraction, reduced extraction time (<0.5 h/sample) and reduced solvent use (<30 mL/sample).

Conditions can be carefully controlled to ensure that the material is not deformed or damaged during the extraction process.

The ASE technique delivers comparable and more efficient extractions than the traditional Soxhlet methods; while saving time and solvent and delivering confidence through control by compliant Thermo Scientific[™] Chromeleon Chromatography Data System Software.



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Quality columns you can rely on for accurate results

Hypersil GOLD HPLC columns



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Volatiles

Low molecular weight, nonpolar organic compounds are typically volatile and have the highest probability to migrate from or through polymeric packaging. Testing of the food contact material or packaging material is typically conducted by headspace sampling followed by gas chromatography and mass spectrometry.

No more volatile unknowns

In many food packaging testing laboratories, sample preparation often accounts for more than twice the time spent on actual chromatography. Improved sample handling can reduce turnaround times and significantly lower the cost per analysis. Automate and accelerate organic volatiles determinations, to increase sample turnaround and lower the cost per analysis, with the powerful Thermo Scientific[™] TriPlus[™] 300 Headspace Autosampler.







Modular GC allows your choice of injectors, together with helium saver options and the widest range of advanced column technologies, including Thermo Scientific™ **TraceGOLD**[™] GC column phases for volatiles.



Sensitive mass spectrometers delivers both quantitation and gualification of volatiles. Thermo Scientific[™] ISQ[™] Series Quadrupole GC-MS features a new source design ideal for continuous high-throughput operation.



processing.







Click to learn more about **GC-MS** Systems

Volatiles are released from materials using headspace sampling. Certain methods suggest the use of valve-and-loop headspace sampling systems. Ultraclean Thermo Scientific[™] Chromacol[™] headspace vials ensure low background and leak free seals.

Simple to operate and fully compliant Thermo Scientific™ Chromeleon[™] Chromatography Data System (CDS) Software provides mass spectrometry data acquisition and

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Semivolatiles

Semi-volatile compounds are among the most frequently detected migration impurities. Testing is performed through liquid injection of an extract of the material or product. Often extracts are derivatized to increase analyte volatility. Testing demands absolute confidence in unknown identification and quantification.

Confident identification

spectra; achieve exceptional mass accuracy for

Orbitrap comes to GC-MS The Thermo Scientific™ Exactive[™] GC Orbitrap[™]

GC-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.



Exceptional <1ppm mass accuracy is achieved on every scan, on every mass, and at every concentration.







Click to learn more about GC Orbitrap Systems

Ultra clean Thermo Scientific™ MS Certified vials ensure the lowest backgrounds to reduce false positives.



Simplify preparation with accurate, automated sample handling. Prepare standards, spike samples and automate derivatization with the Thermo Scientific[™] TriPlus[™] RSH **Autosampler**. With built-in robotics that deliver exceptional precision, flexibility, and reliable operation.



Absolute confidence in your analyte identification demands: HRAM GC-MS with <1ppm mass accuracy, femtogram sensitivity and 6 orders linear dynamic range.

Perform targeted screening, routine quantitation, and qualitative review of data with Thermo Scientific™ TraceFinder[™] Software. Use advanced high resolution filtering (HRF) algorithms to provide a new dynamic in confident identification of unknowns.



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Non-volatiles

Non-volatile impurities are among the most difficult to identify. The sheer diversity of polymer additives and monomers represent an ongoing analytical challenge. Confident identification using a range of targeted libraries or advanced high resolution accurate mass (HRAM) cloud based spectral libraries simplify the workflow.

Proven performance for migrates a Thermo Scientific[™] Exactive[™] Spectrometer and Thermo Scientific™ Vanquish[™] UHPLC platform.





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Robust chromatographic separations are delivered by Thermo Scientific™ **Vanguish[™] UHPLC** platform with orthogonal detection techniques such as Charged Aerosol Detection providing universal coverage for unknowns, complementing MS detection and identification. Because CAD does not provide structural information.





Thermo Scientific[™] Compound Discoverer[™] Software ensures confident compound identification and structural elucidation with advanced algorithms that quickly process and identify compounds based on multiple search approaches; including HRAM libraries, cloud based libraries like mzCloud, and compound databases. Searches are conducted in parallel and a single unified report is delivered.









Click to learn more about LC Orbitrap Systems

Quick exchange ionization modes including APCI & ESI are complemented by fast polarity MS switching. Record both +/- scans within a single acquisition for complete ionization coverage. MSⁿ capabilities and exceptional mass accuracy, make the **Thermo Scientific[™] Exactive[™] Series** of mass spectrometers the





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Elemental impurities

Elemental impurities are common in printed materials, pigments, foil based packaging and delivery systems.

Robust, compliant analysis at the lowest levels is provided by ICP-MS or ICP-OES.

Automate more

Your time is precious. Spend less time at the instrument by using automated, unattended system set-up routines like the advanced singleclick 'Get Ready' function in **Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™** (ISDS) Software.





Simplicity, productivity, robustness

Gain complete confidence with accurate results. Enjoy minimal maintenance thanks to our intelligently

engineered design. The Thermo Scientific™

Automation of the lab workflow has taken a step forward with integration of intelligent auto-dilution, eliminating manual intervention, increasing productivity.



The Thermo Scientific[™] iCAP[™] RQ ICP-MS delivers simplicity, productivity and robustness, combined with the flexibility for unattended 24/7 operation in routine, compliant environments.



Designed to comply with the most rigorous data audit and security measures, Qtegra ISDS Software is FDA 21 CFR Part 11 ready and comes with full IQ/OQ procedures for simple implementation in GMP/GLP regulated environments.







Click to learn more about Trace Elemental Analysis

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Go from sample to results the fast and easy way

Whether you are performing routine product analysis, looking for potential migrates or carrying out food contact material or NIAS studies, the Thermo Scientific informatics and chromatography software solutions help you manage your entire laboratory process. Simplify your MS and MS/MS analyses with our mass spectrometry software platforms that feature intuitive and user-friendly interfaces that easily acquire, analyze, manage and report data generated by LC-MS, GC-MS and ICP-MS systems. Combine our software platforms with our extensive and searchable spectral libraries for easier quantification and Identification of your analytes.

Thermo Scientific[™] SampleManager[™]

Provides comprehensive data and operations management and lab execution in a single solution. When integrated with Thermo Scientific[™] Chromeleon[™] CDS software you can benefit from a complete software platform that simplifies analysis and unlocks the value of your data.

Chromeleon[™] 7.2 Chromatography Data System (CDS) Software

Streamline your entire chromatography workflow, giving you better results faster. Its advanced processing tools ensure quick, consistent results. Chromeleon is also the first CDS to unify workflows for chromatography and routine quantitative MS analysis. Chromeleon eWorkflows contain everything you need to perform a run including the sequence, instrument and processing methods and final reports simplifying the management and execution of routine analysis.

Thermo Scientific[™] TraceFinder[™] Software

Offer increased flexibility and an array of capabilities in performing targeted screening and routine guantitation with either high resolution accurate mass (HRAM) and/or triple stage quadrupole (TSQ) mass spectrometers with Thermo Scientific[™] TraceFinder[™] Software. Not only does TraceFinder provide method development tools for all molecule types, it also generates new methods from existing data.

Click to learn more about Software Solutions

Ensure confident compound identification and structural elucidation with advanced algorithms that guickly process and identify changes between different sample groups and identify compounds based on multiple search approaches; including HRAM libraries, cloud based libraries like mzCloud[™], and compound databases. Searches are conducted in parallel and a single unified report is delivered.

Thermo Scientific[™] AppsLab Library of Analytical **Applications**

An online repository for methods created and tested by Thermo Fisher Scientific application chemists. These applications can be downloaded through one-click eWorkflows directly into Chromeleon CDS and are ready to run.

Qtegra[™] Intelligent Scientific Data Solution[™] Software

Minimize training, automate workflows, simplify your experience, and improve efficiency with the innovative Thermo Scientific™ Qtegra[™] Intelligent Scientific Data Solution[™] (ISDS) platform software. This shared software approach provides control and data processing for a range of elemental and isotopic analysis technologies including ICP-OES and ICP-MS. Designed for workflow, scalability, compliance and data management, Qtegra ISDS Software provides essential tools for consistent, accurate analysis. ChromControl[™] and npQuant[™] plug-ins to make applications for speciation and nanoparticles even easier.



Thermo Scientific[™] Compound Discoverer[™]



Thermo Scientific[™] AppsLab Library of Analytical Applications - One-click workflows for use with Chromeleon CDS.



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



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