مؤتمر عُمان الدولي السادس
لسلامـــة وجـودة الغـــذاء
Oman 6th International Conference
on Food Safety and Quality
12 - 14 يونيو 2023م - مسقط

# Food Contact Material's testing Regulatory Perspective

**Khalid Ghaffar (BDM – Waters Corporation USA)**

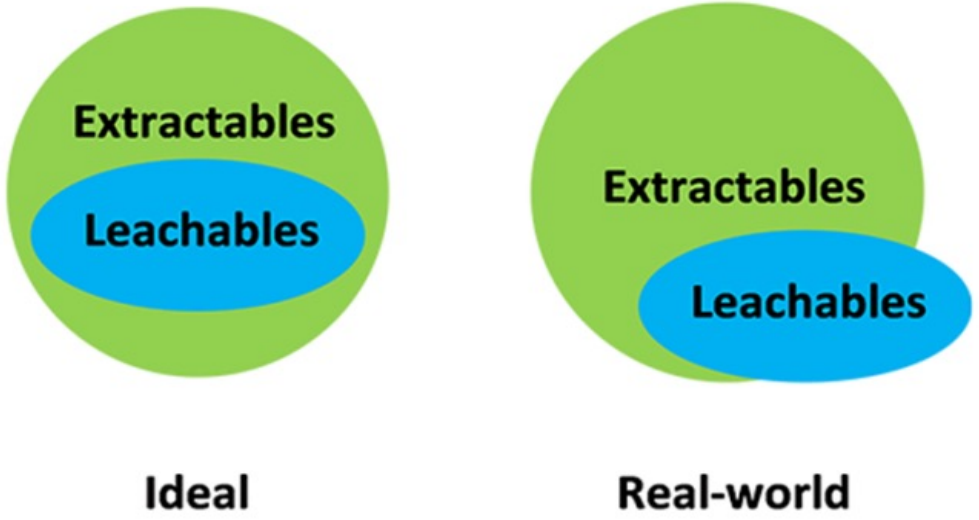
# What are extractables and leachable?

## Extractables:

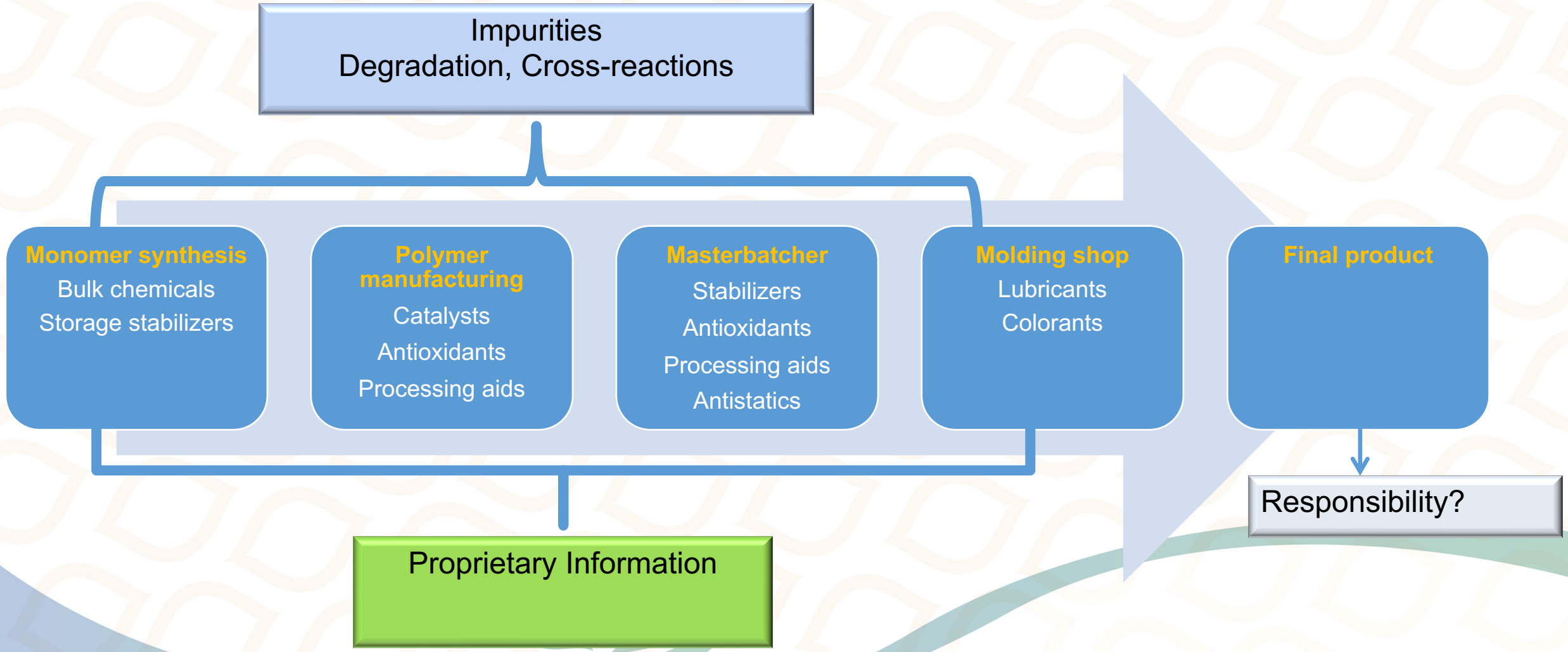
Organic and inorganic chemical species that can be released from the surfaces of components used in the manufacture and storage of products under laboratory conditions (accelerated or exaggerated temperatures, solvents or surface exposure).

## Leachable:

Organic and inorganic chemical species that can be released from the surfaces of components used in the manufacture and storage of products under conditions of normal use.

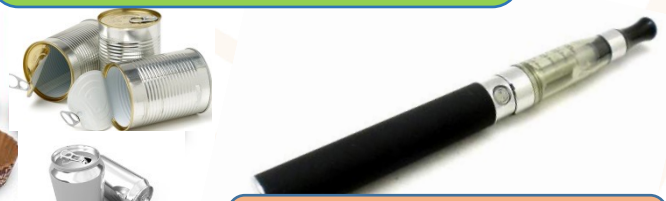


# Plastics Manufacturing Process



# Where does E&L Testing Take Place?


**Food packaging and contact materials**



**E-cigarettes**

**Implantable medical devices**

**Pharma**

**Cosmetics**

# EU Legislation

Regulation 1935/2004/EC
Regulation Framework

Regulation 2023/2006/EC:
Good Manufacturing Process

Active and intelligent: 450/2009/EC

Ceramics: 2005/31/EC (currently under review)

Plastics (including rubbers and elastomers): 10/2011/EU

Regenerated cellulose: 2007/42/EC

Unregulated materials

Adhesives
Cork
Glass
Silicones
Textiles
Waxes

Paper and board
Varnishes and coatings
Ion- exchange resins
Metals and alloys
Wood
Printing inks

# Food simulants for plastics

- Regulation 10/2011/EU Annex III

- Simplifies analyses
  - Reduces clean up
  - Reduces matrix variances and effects on mass spectrometer instruments

| Simulant Named | Content | Mimics food type |
|---|---|---|
| A | Ethanol 10 % | Aqueous |
| B | 3 % acetic acid | Acidic (tomato) |
| C | Ethanol 20 % | Diary (milk) |
| D1 | Ethanol 50 % | Fatty |
| D2 | Vegetable oil | Fatty |
| E | Tenax (poly(2,6-diphenyl-p-phenylene oxide)) | Dry (cereals) |

# Overall Migration

Migrants- compounds which partition from the packaging into the food

- Gravimetric approach
  - Material or article is weighed, exposed to appropriate testing conditions and re-weighed following the migration testing
  - Any loss in weight is considered to have migrated
  - Tested under the worst case scenario conditions

- Qualitative analysis
  - weight loss calculation only

- Quantitative analysis
  - extract analysed, typically by MS for targeted/ non- targeted analysis

- **Overall Migration Limit (OML): 10 mg.dm$^{-2}$**
  - 10 mg of substance per dm$^2$ of the food contact surface for all substances that can migrate from food contact materials to foods

# Specific Migration

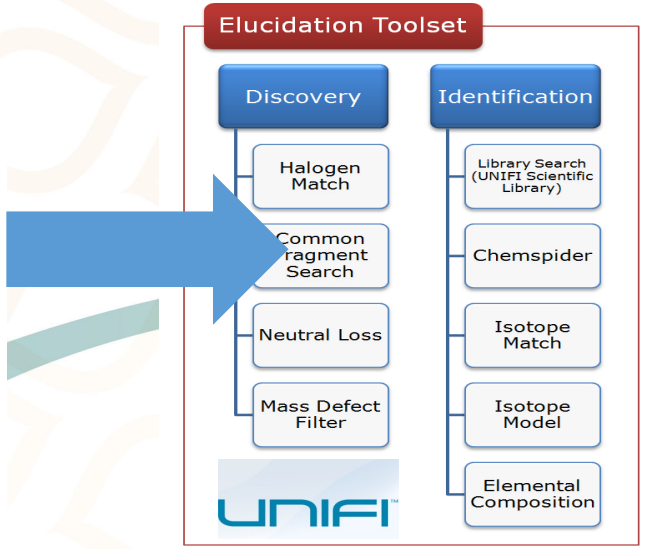
- Specific Migration Limits for plastic materials and articles as set out in Annex I of Regulation 10/2011/EU

- Specific migration is the amount of a specified component that migrates from the food contact material or article to the food during contact

- Regulations and testing ensures safety limit based on toxicological data and risk of exposure

# Non-intentionally added substances (NIAS)- impurities from starting materials, reaction and degradation products formed during manufacturing process

- NIAS specifically outlined in 10/2011/EU for plastic materials
- Compounds not specifically regulated by name (in Annex I of Regulation) must be subjected to a risk assessment by the business operator, *i.e.*: manufacturer
- These include impurities, degradation products and reaction intermediates
- Non targeted analysis workflow required for detection of possible contaminants (unknowns)



# What are the consequences of packaging failures?

- Consumers reported strange taste and odour in various cereals.
- Test attributed these symptoms on elevated levels of 2-methylnaphthalene in the packaging used.
- Kellogg Company recalled **28 million** boxes of cereal.


http://www.fda.gov/NewsEvents/PublicHealthFocus/ucm221489.htm

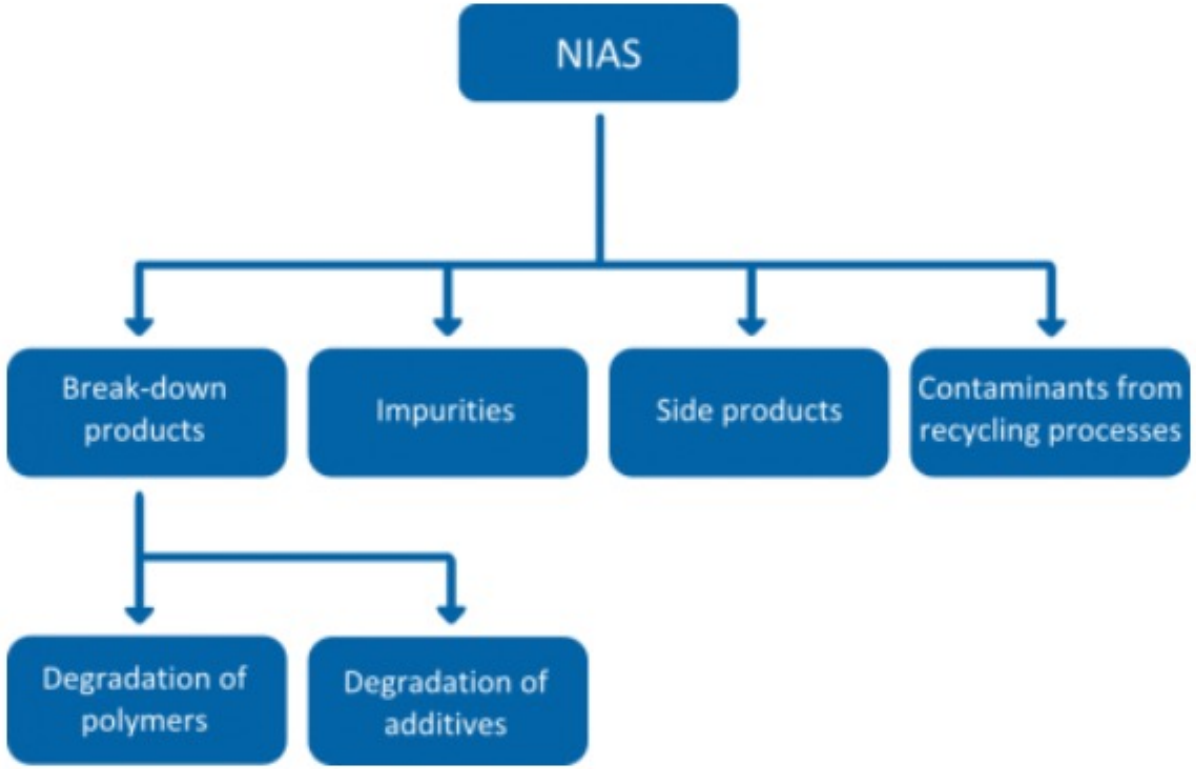
# Printing Inks

- Printing inks are complex mixtures containing pigments or dyes, binders, solvents, and additives including plasticizers.
- Printing inks are commonly used as a promotional tool and to inform the consumer of the contained product.
- Ultraviolet light (UV)-curing inks are used to print and coat food contact and pharmaceutical packaging. These formulations typically consist of monomers and pre-polymers such as acrylates, pigments, photoinitiators, and additives.
- The non-printed side of the packaging or a foil is usually in contact with the product however due to the potential for migration they are considered a potential leachable or food contact material.

# NIAS

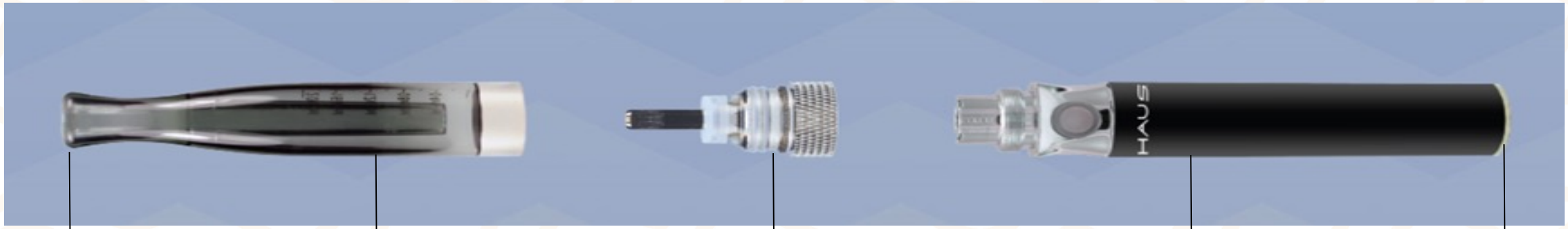
- Non-intentionally added substances (NIAS) are chemical compounds that are present in a material but have not been added for a technical reason during the production process. Their presence in food/pharma contact materials is generally not known by the consumer and often is a challenge for the producer.

- NIAS originate from break-down products of food/pharma contact materials, impurities of starting materials, unwanted side-products, and various contaminants from recycling processes.



# Extractables and Leachables of Inhalation Products

## E-cigarette Device




**Mouth Piece**

**Flavor Chamber**

**Atomizer**

**Battery**

**LED Light**


E-Liquids

**E-liquids typically contain nicotine and excipients such as propylene glycol, glycerol and a mixture of flavors**

**Characterization of extractables and leachable is important for ensuring the safety, quality and efficacy of inhalation tobacco products**

# Evolving E-cigarette Regulations - Considerations

- Challenges
  - Tobacco Product or Medical Device?
  - Lack of harmonized regional approaches to regulation
  - Lack of scientific information
- Product quality & safety standards being implemented
  - E.g. UK - Medicines and Healthcare Products Regulatory Agency (MHRA) requires complete quality information for licensing e-cigarettes including:
    - Composition of e-cigarette device, e-liquid and aerosol
    - Quality of nicotine and excipients
    - Extractables and leachable
    - Stability data during use and over product shelf-life

# Food Contact Material's testing Technology Portfolio overview

| Chemistries | Separations | Mass Spectrometry | Informatics | Standards & Reagents |
|---|---|---|---|---|
|  |   |  |  |  |

# Customer challenges to address

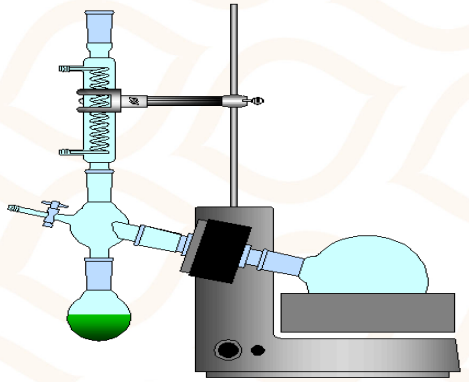
1. Regulatory requirements
2. Sample extraction and preparation
3. Sample analysis: separation, detection, identification, quantitation
4. Data mining: visualisation, processing, reporting
5. Converting data to decisions and building the knowledge base

# Sample Preparation

## TRADITIONAL

Cutting / grinding

Soxhlet extraction



Rotary evaporation

Make-up injection solution

Preparation → Extraction → Concentration → Injectable Solution

## ALTERNATIVES

Microwave Assisted Extraction

Migration cells for FCM

Automated supercritical fluid extraction (ASFE)

# Challenges in Separations

- **Sample complexity**
  - Extracts of polymeric materials often contain many components
  - Compounds on interest often at low levels
  - Method blanks often contain many components
- **Chemical diversity**
  - Compounds of interest cover very wide range of “chemical space”
- **Type of extracts**
  - Can be in aqueous solution or strong organic solvents

***“There is always a benefit from having the best possible chromatographic performance”***

# Chromatography considerations for extractable testing

## (1) Polar solvent extract

- Direct injection on LC ☺
- Solvent exchange to non-polar solvent 😐
  - Direct injection on GC

*Acquity UPLC Family*

## (2) Non-Polar solvent extract

- Solvent exchange to polar solvent 😐
  - Direct injection on LC
- Direct injection on GC ☺

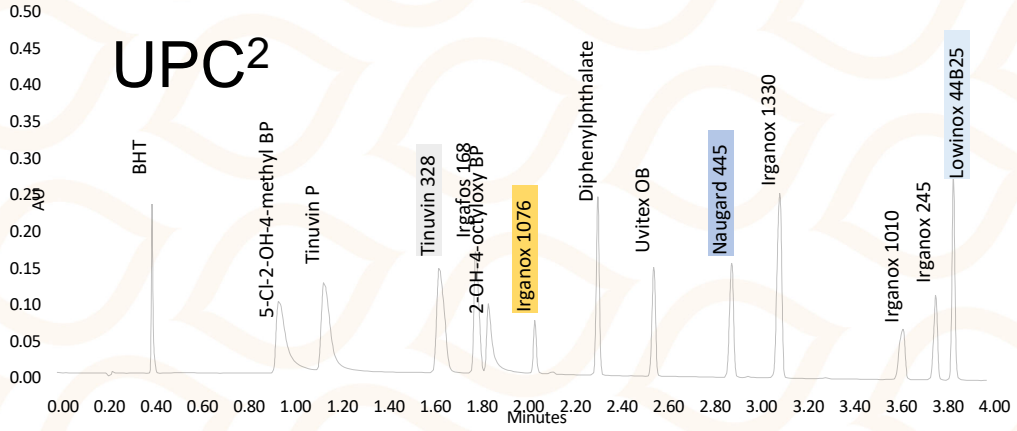
*APGC interface for GC-API-MS*

## (3) Polar *or* Non-polar solvent extract

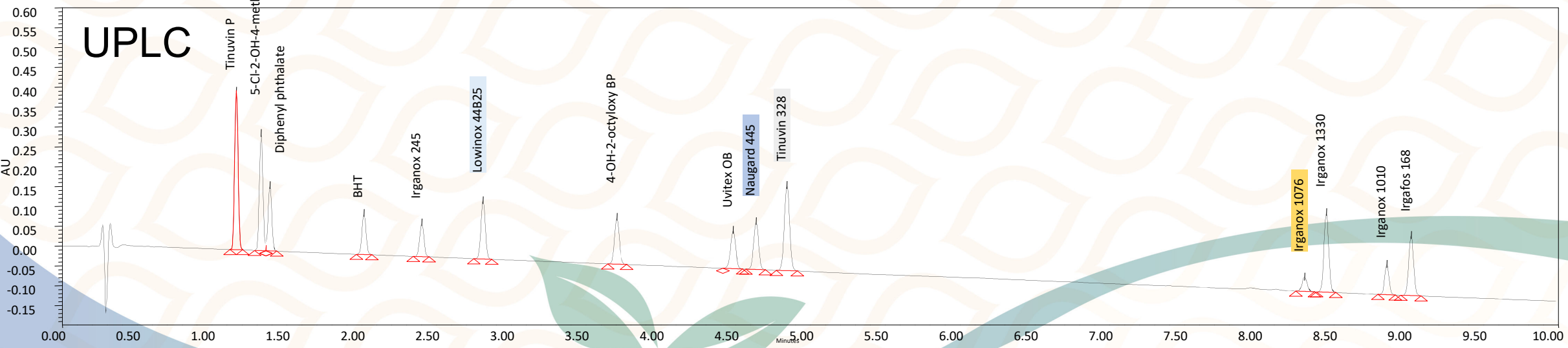
- Direct injection on CC (SFC) ☺

*Acquity UPC²*

# Chromatographic separations




4 min separation by UPC² vs. 9.5 min by UPLC



# Detection & Identification

# 4 Fundamental Questions

Are these compounds in my sample?

**Screening**

How much is in my sample?

**Quantitation**

What else is in my sample?

**Elucidation**

What is the difference between my sample and another one?

**Comparison**

***All can be important in E&L testing***

# Screening & Quantitation

**Are these compounds in my sample?**

**Screening**

**How much is in my sample?**

**Quantitation**

**Screening against a compound list, database or spectral library**

- Acquisition may be ***targeted***
  - Only look for *pre-selected* compounds
  - Quantify against standards

# Solutions for Targeted Screening & Quantitation

- **Highest performance** methods
  - Use MS/MS to provide selectivity & sensitivity in complex samples
  - Use retention time, multiple MRMs and ion ratios to confirm identity

*ACQUITY I-Class with Xevo TQ-XS*

- More **advanced** methods
  - Use mass detection
  - Eg. LC/PDA/Qda system
  - Include mass data to help detect and confirm identity

*ACQUITY H-Class with QDa*

- **Simple** routine methods
  - Eg. LC/PDA system
  - Use retention time and UV spectra to target compounds

*Alliance HPLC with PDA*

# Screening using a non-targeted acquisition

**Are these compounds in my sample?**

**Screening**

**Screening against a compound list, database or spectral library**

- Acquisition may be ***untargeted***
  - No pre-selection of compounds to look for
  - See widest range of compounds
  - Look for compounds of interest in historical datasets

  - ***Also answer another question .....***

**What else is in my sample?**

**Elucidation**

# MS Technology Positioning

***Tandem Quads*** – "Gold Standard" for targeted screening & quantitation.

**Are these compounds in my sample?**
**Screening**

**How much is in my sample?**
**Quantitation**

**What else is in my sample?**
**Elucidation**

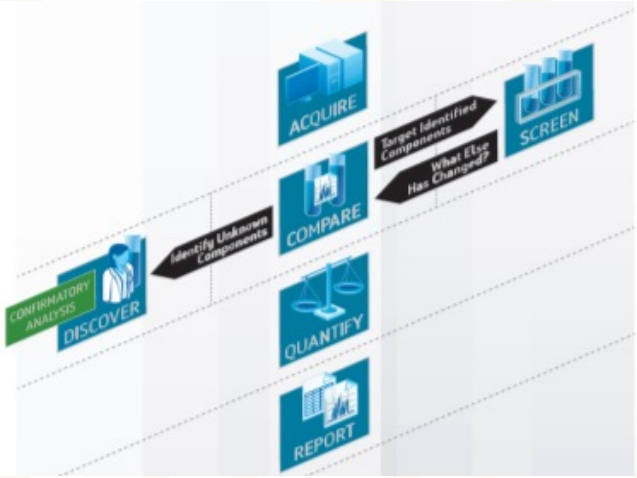
**What is the difference between my sample and another one?**
**Comparison**

***Q-Tof as HR MS***

# Scientific Information System

UNIFI

- Single environment for data …
  - Acquisition, processing, review, reporting and storage/management
- Database solution
  - -Easier to find your data, and related data
- Workflow centric solution
  - Single software for screening, quantitation, elucidation, comparison, ion mobility data processing.
- Scientific Library
  - Provides single repository for all compound information
  - Spectra, RT, fragment ions, structures, Word Docs, PDFs etc.
- Standalone Workstation or Networked solution




# Targeted and non - targeted screening in UNIFI

**UPLC, UPC² or APGC with Xevo G2-XS Qtof or VION:**
High resolution chromatographic separation
High sensitivity and accurate mass, $MS^E$ data

**Targeted screening/Quantitation**
User library

**Candidate *m/z* determination**
**Statistical analysis**

**Elemental composition**
**ChemSpider search**

**Fragment Match for confirmation of molecular fragments**

**MS/MS measurement:**
Acquire standards and compare standard results with samples

UNIFI™

# Target and Suspect Compounds

| Name | CAS No. | Synonym |
|---|---|---|
| 1,1,1-Trimethylolpropane, ethoxylated, ester with 2-ben-zoyl-benzoic acid | Not available | Polymeric benzophenone derivative |
| 1-(4-[(4-Benzoylphenyl)thio]phenyl)-2-methyl-2-[(4-methylphenyl)sulfonyl]-1-propan-1-one | 0272460-97-6 | Esacure 1001 |
| 1-Butanone, 2-(dimethylamino)-1-[4-(4-morpholi- nyl)phenyl]-2-(phenylmethyl) | 0119313-12-1 | Irgacure® 369 |
| Poly(oxy-1,2-ethanediyl), α-(2-benzoylbenzoyl)-ω-[(2-ben- zoylbenzoyl)oxy)] | 1246194-73-9 | Omnipol 2702 |
| 1,3-di({a-[1-chloro-9-oxo-9H-thioxanthen-4-yl)oxy]acetylpoly[oxy(1-methylethylene)]}oxy)-2,2-bis({a-[1-methylethylene)]}oxymethyl) propane | 1003567-83-6 | Speedcure 7010 |
| (Dimethylamino)benzoate, esters with branched polyols | Not available | Polymeric aminobenzoate derivative |
| 1-Butanone, 2-(dimethylamino)-2-[(4-methylphenyl)methyl]-1-[4-(4-morpholinyl)phenyl]- | 0119344-86-4 | Irgacure® 379 |
| Phenyl bis(2,4,6-trimethylbenzoyl) phosphine oxide | 0162881-26-7 | Irgacure® 819 |
| Pentaerythritol ethoxylate tetraacrylate | 51728-26-8 | PPTTA |
| Glycerol propoxylated, esters with acrylic acid | 52408-84-1 | GPTA |
| Trimethylolpropane triacrylate | 15625-89-5 | TMPTA |
| Ethoxylated trimethylolpropane triacrylate | 28961-43-5 | TMP(EO)TA |

# Summary of Target Ions and Calibration Ranges

| Synonym | First Most Intense Target | Adduct | Observed *m/z* of Expected Fragments | Primary Calibration Range (ng/mL) |
|---|---|---|---|---|
| Polymeric benzophenone derivative (n=6) | 832.3917 | $[M+NH_4]^+$ | 209.0594, 253.0869 | 10-10,000 |
| Esacure 1001 | 515.1339 | [M+H]+ | 331.1143 | 5-1000 |
| Irgacure 369 | 367.2381 | $[M+H]^+$ | 190.0871, 176.1442, 294.1855 | 5-1000 |
| Omnipol 2702 (n=4) | 628.2543 | $[M+NH_4]^+$ | 209.0594, 253.0869 | 5-1000 |
| Speedcure 7010 (n=8) | 905.1697 | $[M+2H]^{2+}$ | 361.0290, 320.9980, 379.0394 | 50-10,000 |
| Polymeric aminobenzoate derivative (n=6) | 840.4656 | $[M+H]^+$ | 148.0773, 192.1029 | 5-5000 |
| Irgacure 379 | 381.2532 | $[M+H]^+$ | 190.0869 | 5-1000 |
| Irgacure 819 | 441.1594 | $[M+Na]^+$ | 147.0812 | 50-5000 |
| PPT(T)A (n=5) | 590.2823 | $[M+NH_4]^+$ | 501.2334, 413.1802, 369.1526 | 5-5000 |
| GPTA (n=4) | 504.2819 | $[M+NH_4]^+$ | 241.1070, 113.0582, 183.0636 | 5-5000 |
| TMPTA | 319.1151 | $[M+Na]^+$ | [M+Na]+ | 50-1000 |
| TMP(EO)TA (n=5) | 490.2654 | $[M+NH_4]^+$ | 269.1370, 313.1633, 357.1890 | 5-5000 |

# Summary of Quantitative Results of Three Printed Sample Films

- Three different ink formulations (printed on a foil) were tested in the migration study.
- Increased migration was noted for TMPTA.
- The detected levels exceeded the 50 µg/kg SML level in formulation 1 and 3.
- At the end ink formulation 2 was taken for further evaluation.

| Migration Results | Ink Formulation 1 | | Ink Formulation 2 | | Ink Formulation 3 | |
|---|---|---|---|---|---|---|
| | µg/dm² | µg/kg | µg/dm² | µg/kg | µg/dm² | µg/kg |
| **Irgacure 379** | ND | ND | ND | ND | ND | ND |
| **Esacure 1001** | 0.1 | 0.7 | 0.4 | 2.5 | 0.2 | 1.2 |
| **TMPTA** | 60 | 360 | 2.6 | 15 | 37 | 220 |
| **TMPEOTA** | ND | ND | 1.3 | 8.1 | ND | ND |
| **PPTTA** | ND | ND | 0.7 | 4.2 | 0.7 | 4.1 |
| **GPTA** | 0.8 | 4.8 | 0.8 | 4.5 | 1.4 | 8.3 |

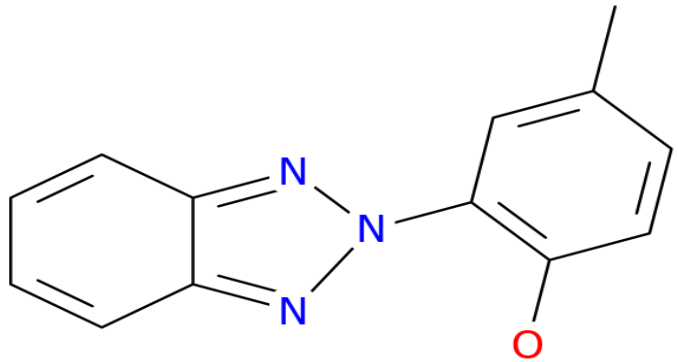
ND = not detected

# Scientific Library

Tinuvin P [CCS test]

Tools

| Property | Value |
|---|---|
| Item type | Compound |
| Item description | 2440-22-4 |
| IUPAC name | |
| Formula | C13H11N3O |
| Hill formula | C13H11N3O |
| Average molar mass | 225.2459 |
| Monoisotopic mass | 225.0902 |
| Item tag | Polymer Additive, Antioxidant, ERA |
| InChI | 1S/C13H11N3O/c1-9-6-7-13(17)12(8-9)16-14-10-4-2-3-5-11(10)15-16/h2-8,17H,1H3 |




Detection results

Add Edit Delete

| Priority | Intensity | Formula | Neutral Mass (Da) | Adduct | Charge | Fragmentation type | Expected m/z | Observed m/z | Expected RT (min) | Observed CCS (Å²) | Observed drift (ms) | Ionization |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Detection result: Instrument model: ACQUITY Sample Manager FTN, Osprey, ACQUITY Binary Solvent Manager, ACQUITY Column Manager, , Instrument serial no: , Analysis, Created by administrator on May 18, 2016 (7 items) | | | | | | | | | | | | |
| 1 | 487338 | | 225.0902 | +H | 1 | None | 226.0975 | 226.0968 | 3.600 | 148.12 | 4.28 | ESI+ |
| 2 | 9376 | C6H5 | | | 1 | CID | 77.0386 | 77.0382 | 3.600 | | 4.26 | ESI+ |
| 3 | 5087 | | | | 1 | CID | 120.0556 | 120.0552 | 3.600 | | 4.23 | ESI+ |
| 4 | 5087 | C6H6N3 | | | 1 | CID | 120.0556 | 120.0552 | 3.600 | | 4.23 | ESI+ |
| 5 | 1946 | C12H10N3 | | | 1 | CID | 196.0869 | 196.0872 | 3.600 | | 4.17 | ESI+ |
| 6 | 1508 | | | | 1 | CID | 107.0491 | 107.0490 | 3.600 | | 4.05 | ESI+ |
| 7 | 1508 | C7H7O | | | 1 | CID | 107.0491 | 107.0490 | 3.600 | | 4.05 | ESI+ |

# Review

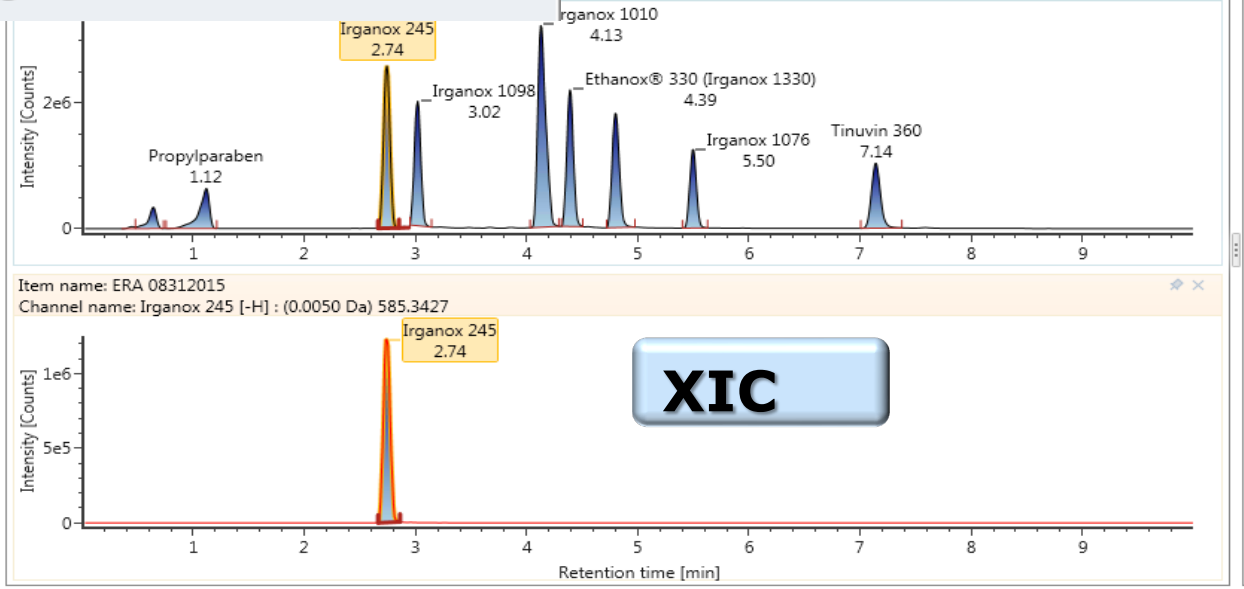
Tray: 1:A,2 | ERA 08312015 [1] | Irganox 245 | Filters

**Workflow**

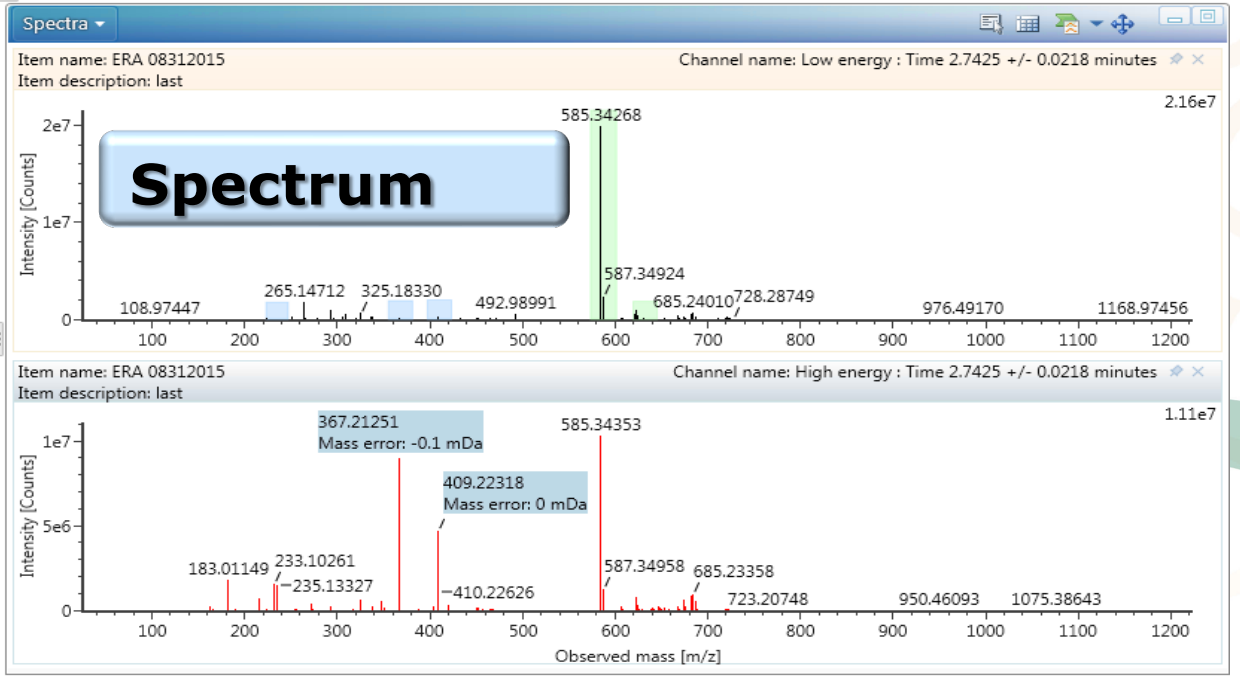
- **Summary**
  - Batch Overview
- **Accurate Mass Screening bc**
  - System suitability sample
  - Targeted Screening Overview
  - Targeted Screening Details
  - Binary compare details
  - Binary compare
  - Unknown review

**RT, Mass accuracy**

| Identification status | Neutral mass (Da) | Observed m/z | Mass e | | | | Detector counts | Response | Adducts |
|---|---|---|---|---|---|---|---|---|---|
| Identified | 474.40730 | 473.3996 | | | | | 815535 | 516128 | -H |
| Identified | 774.59510 | 773.5883 | 0.5 | 0.6 | 4.26 | 4.39 | 1261891 | 564724 | -H, +HCOO |
| Identified | 1176.78408 | 1175.7772 | 0.4 | 0.3 | 4.01 | 4.13 | 2540995 | 931926 | -H |
| Identified | 530.46990 | 529.4634 | 0.8 | 1.5 | 5.21 | 5.50 | 358988 | 244974 | -H |
| Identified | 636.48661 | 635.4784 | -0.9 | -1.4 | 2.98 | 3.01 | 1281611 | 580027 | -H |
| Identified | 586.35057 | 585.3427 | -0.6 | -1.0 | 2.72 | 2.74 | 1033970 | 612482 | -H, +HCOO |
| Identified | 152.04734 | 151.0396 | -0.4 | -2.9 | 0.72 | 0.64 | 55086 | 50003 | -H |
| Identified | 180.07864 | 179.0706 | -0.8 | -4.4 | 1.22 | 1.12 | 156010 | 139232 | -H, +HCOO |
| Identified | 357.16079 | 356.1531 | -0.5 | -1.3 | 4.09 | 4.18 | 152205 | 84380 | -H |
| Identified | 658.39952 | 657.3930 | 0.8 | 1.1 | 6.60 | 7.14 | 564639 | 351409 | -H |




**XIC**




**Spectrum**

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# Summary

Sample Extraction → Separation → Detection → Identification

*MV-10 ASFE*

*ACQUITY Arc & H-Class*

*Alliance HPLC*

*ACQUITY UPC²*

*ACQUITY QDa*

*Xevo TQ-Sμ and TQ-XS*

*APGC source For MS*

*Xevo G3*

Empower 3

MassLynx

UNIFI

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# Food Contact Material's Testing Application review

[APPLICATION NOTE]

Waters
THE SCIENCE OF WHAT'S POSSIBLE.

# Identification of Non-Intentionally Added Substances (NIAS) in Food Contact Materials Using APGC-Xevo G2-XS QTof and UNIFI Software

Nicola Dreolin and Peter Hancock
Waters Corporation, Wilmslow, UK

## APPLICATION BENEFITS

- Reliable GC-MS method for screening and structural elucidation of non-intentionally added substances (NIAS) in food packaging materials
- Atmospheric Pressure Gas Chromatography (APGC) is a soft ionization technique that produces lower levels of fragmentation than EI, enabling improved detection of challenging molecular ions and the avoidance of

## INTRODUCTION

Food comes into contact with many materials and articles during its production, processing, storage, preparation, and serving before its eventual consumption. Such materials and articles are called food contact materials (FCMs). Recently, concern about the wholesomeness and safety of food products has increased dramatically. Most of the concern usually focuses on food additives, monomers, oligomers, and non-intentionally added substances (NIAS). A non-intentionally added substance is defined in the European Union (EU) Regulation No 10/2011 as "an impurity in the substances used or a reaction intermediate formed during the production process or a decomposition or reaction product."[1,2] FCMs can, therefore, be

GC-Qtof for FCM, and compared to EI

https://connect.waters.com/files/app/file/cb774f22-eef2-499e-93fe-4a9d94e8e72d

# Chemical Analysis of Food Packaging Migrants and Other Chemical Contaminants in Infant Formula Using a TOF-Based Approach

Melvin Gay,[1] Antonietta Gledhill[2]
[1]Waters Pacific Pte Ltd, Singapore, [2]Waters Corporation, Manchester, UK

## APPLICATION BENEFITS

- Unequivocal identification of potentially harmful food packaging migrants in infant formula containers.
- Simultaneous $MS^E$ data acquisitions of both low energy precursor (MS) and high energy fragment ions ($MS^E$) in a single injection, for compound identification and confirmation.
- Structural elucidation and compound identification through the use of MarkerLynx™ MS, ChemSpider, and other software tools.

## GOAL

To identify possible food packaging migrants in infant formula containers.

## INTRODUCTION

Packaging has become an indispensible element of food manufacturing processes. Packaging not only better protects consumers from microorganisms, biological, and chemical changes in food, thus providing longer shelf life, but it also makes foods easier to transport.

Recently, food packaging issues have gained widespread importance in food safety, due to the possible migration of chemicals from food contact materials into the food. Instances, such as the leaching of bisphenol-A (BPA) and BPA diglucidyl ether (BADGE) from plastic films to aqueous food simulants [1,2] have

http://www.waters.com/webassets/cms/library/docs/720003905en.pdf

# Quantifying Primary Aromatic Amines in Polyamide Kitchenware Using the ACQUITY UPLC I-Class System and Xevo TQ-S micro

Steven Haenen and Marijn Van Hulle
Waters Corporation, Brussels, Belgium

## APPLICATION BENEFITS

- Single method for analysis of 23 PAAs
- No need for ion-pairing reagents, or the removal of acetic acid from the sample extract prior to analysis
- Sensitive detection at levels well below the EU guidelines with Xevo® TQ-S micro Triple Quadrupole Mass Spectrometry

## INTRODUCTION

Primary Aromatic Amines (PAAs) are a class of compounds of which the simplest form is aniline (Figure 1). PAAs are substances that are used, for example, in the production of certain colorants, so-called azo pigments, notably in the color range yellow – orange – red. Whereas a large number of PAAs are safe for human health, some PAAs are known human carcinogens. For kitchenware, paper napkins, baker's bags with colorful print and other printed items that come in contact with food, some PAAs may pose a health risk, if they are transferred to the food.

http://www.waters.com/webassets/cms/library/docs/720005781en.pdf

- Kitchenware by TQ-S micro and i-class
- Primary aromatic amines

# The Identification and Structural Elucidation of Potential Migrants from Paper and Board Food Packaging Using UPLC/Q-Tof MS with MS$^E$ and MassFragment

Malcolm Driffield,[1] Antony Lloyd,[1] Emma Bradley,[1] Dominic Roberts[2]
[1]The Food and Environment Research Agency, York, UK
[2]Waters Corporation, Manchester, UK

## APPLICATION BENEFITS

- MS$^E$ data acquisition allows for the simultaneous collection of both low energy precursor ion and higher energy fragment ion data from a single injection for greater confidence in compound identification, and provides comprehensive historical data review.
- ChromaLynx™ XS Software provides rapid detection, identification, and confirmation of all components in complex mixtures. It allows the user to determine chemical formulae from accurate mass information, searching a user-prepared database of compounds.
- MassFragment™ is an intelligent software tool that automates structural assignment to fragment ion spectra making data processing significantly easier, and confirmation without standards possible.

## INTRODUCTION

Recycling paper and board has clear benefits to the environment, relieving pressures on forestry resources and reducing the amount of waste disposal. Currently, there is limited control over the types of paper and board entering the recycling stream. End use of the recycled paper and board ranges from less demanding applications, such as newspapers and magazines, to cardboard boxes and cartons, and more demanding applications, such as food packaging.

In recent years, there have been issues reported in scientific literature and in the media relating to the use of recycled paper and board in food packaging. Contaminants associated with recycled paper and board have been detected in food. Mineral hydrocarbons have been found from inks used to print newspapers and magazines,[1-2] as well as phthalates, such as diisobutyl phthalate from adhesives in catalogues and brochures,[3] and photoinitiators and other components from printing on the external surface of the paper and board.[4] All of these chemical types have been shown to persist after passing through the recycling process.

This study is part of a larger project investigating suitable sources of paper and board for use in recycled food packaging.[5] Four different paper sources (plain white printer paper, newspapers and magazines, corrugated cardboard,

http://www.waters.com/webassets/cms/library/docs/720004591en.pdf

# A Simple, Fast, and Reliable LC-MS/MS Method for Determination and Quantification of Phthalates in Distilled Beverages

Dimple Shah and Jennifer Burgess
Waters Corporation, Milford, MA, USA

## APPLICATION BENEFITS

- Separation and detection of 7 phthalates in 11 minutes.
- Simple, quick "dilute and shoot" sample preparation method for routine applications where high sample throughput is required.
- Elimination of major phthalate contamination using the ACQUITY UPLC® Isolator Column.
- Selective mass spectra obtained for all seven phthalates with dominant precursor ion.
- Low limits of quantification achieved using Waters® ACQUITY UPLC H-Class System and Xevo® TQD.

## INTRODUCTION

Phthalates, esters of phthalic acid, are often used as plasticizers for polymers such as polyvinylchloride. They are widely applicable in various products including personal care goods, cosmetics, paints, printing inks, detergents, coatings, and food packaging. These phthalates have been found to leach readily into the environment and food as they are not chemically bound to plastics. As such they are known to be ubiquitously present in our environment.

Phthalates have been reported to show a variety of toxic effects related to reproduction in animal studies, which has resulted in these compounds being considered as endocrine disruptors. Screening food and beverages for phthalates contamination is required by many legislative bodies, although regulations vary from country to country in regards to acceptable daily tolerances and specific migration limits.

http://www.waters.com/webassets/cms/library/docs/720005403en.pdf

- H-class and TQD for phthalates

# Questions?

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