Untargeted Chemical Screening of Food Packaging Composition & Migration: Our Current Approach



H. Simian, Y.-A. Hammel, J. Varela and S. Koster Packaging Food Safety group, Nestlé Research Center, Switzerland

Context & Needs

Packaging materials can contain a wide range of known and unknown substances



Food packers are responsible for the Safety & Compliance of their Packaging materials

Complexity of the supply chain

- Many actors implicated from chemical industry to converters
- Lack of chemical knowledge, especially at converter level
- Information difficult to convey to end user (food packer)

Diversity of regulations:

- Lack of supra-national regulations for authorized substances (IAS)
- No harmonization between national regulations
- NIAS are not regulated but... their safety must be assessed based on internationally recognized scientific principles

Packaging Composition & Migration must be checked for Safety, Compliance and Quality

Packaging Food or Food Simulant



Analytical Procedures





- Column: 5 % phenyl 95 % methyl polysiloxane, 30 m x 0.25 mm ID, df 0.25 µm
- Acquisition mode: EI + CI, Full Scan, m/z 35-1000 Da
- Semi-quantification by FID using **BHA** as unique internal standard





- Column: Waters Acquity BEH C8, 2.1 x 100 mm, 1.7 µm • Mobile phase: A: Water +0.1% Formic acid + 0.5 mM ammonium formate / B: Methanol +0.1% Formic acid + 0.5 mM ammonium formate
- Acquisition mode: ESI+, Full Scan, m/z 80-1200 Da & Data Independent Acquisition (DIA) • Resolution: 70`000

Data Treatment & Interpretation process

TIC Deconvolution



Retention index calculation and ~ 300 peaks by deconvolution



~ 900 peaks by deconvolution

Tier 1 Search in targeted/injected substances database

Average of 35.253 to 35.290 min.: D14091012.D\data.ms (-)	
149	
	Average of 35.253 to 35.290 min.: D14091012.D\data.ms (-) 149



Example **1**: Di(2-ethylhexyl) phthalate



Tier 2

Database-assisted identification using an in-house packagingrelated database (~4000 IAS + NIAS with exact MW and ~1000 retention indices)

Example **2**: **Glyceryl 2-monostearate**



- Match with spectrum from Wiley/NIST reference library
- Match of nominal MW with few substances in the database
- Retention index to support



Tier 3 Investigation of unknowns





Next steps & Challenges

- GC-HRMS (EI/CI) to implement
- Automatic deconvolution and searches for routine/high sample throughput
- Lack of standards for confirmation of NIAS identity and quantification
- Test of LC semi-quantification by Charged Aerosol Detector (CAD) or other approaches

Conclusions

- Complementarity of GC and LC
- Complete workflow from an unique LC-HRMS acquisition (Full scan + CID)
- Need of tools to improve treatment and reduce manual data handling
- Better knowledge /partnership with packaging suppliers needed