Chemicals in Paper and Board Food Contact Material: Towards More Knowledge, Analytical and Prioritization Analysis

Pieke, Eelco Nicolaas; Granby, Kit; Boriani, Elena

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

DTU Food
National Food Institute

Chemicals in Paper and Board Food Contact Material: Towards More Knowledge, Analytical and Prioritization Analysis

Eelco Nicolaas Pieke[1], Kit Granby[1], Elena Boriani[1,2]

Technical University of Denmark (DTU): [1)] National Food Institute, [2)] Global Decision Support Initiative

The level of information regarding chemicals present in non-plastic Food Contact Materials (np-FCM) is insufficient [1]. The process of discovering, identifying and risk assessing new compounds is challenging and time-consuming. This works aims to provide a framework for rapid identification and quantification of emerging substances in paper and board FCM, while also exploring preliminary risk assessments (RA) useful for prioritization.

Migration Testing

Non-specific migration occurring from paper / board FCM (e.g., pizza box, fries box) in contact with liquids is evaluated by fully immersing 1 dm^2 of cut-out paper samples of in 50% ethanol / water (Food Simulant D1) for 24 hours at 40°C

Identification of Unknowns

High resolution LC-MS (QTOF) with accurate mass fragmentation is combined with data mining algorithms to obtain a tentative identification. The method is designed to act as naïve untargeted exploration. The goal is to obtain as much information as possible while having minimum restrictions.

Concentration Estimates

Semi-quantification (SQ) in LC-MS is error-prone due to large response variations. We developed a non-specific SQ method for estimating the concentration of unknown compounds within a 3-fold range. The method was designed to be wide rather than deep: we believe concentration estimates spanning 3-fold error are better than no data.

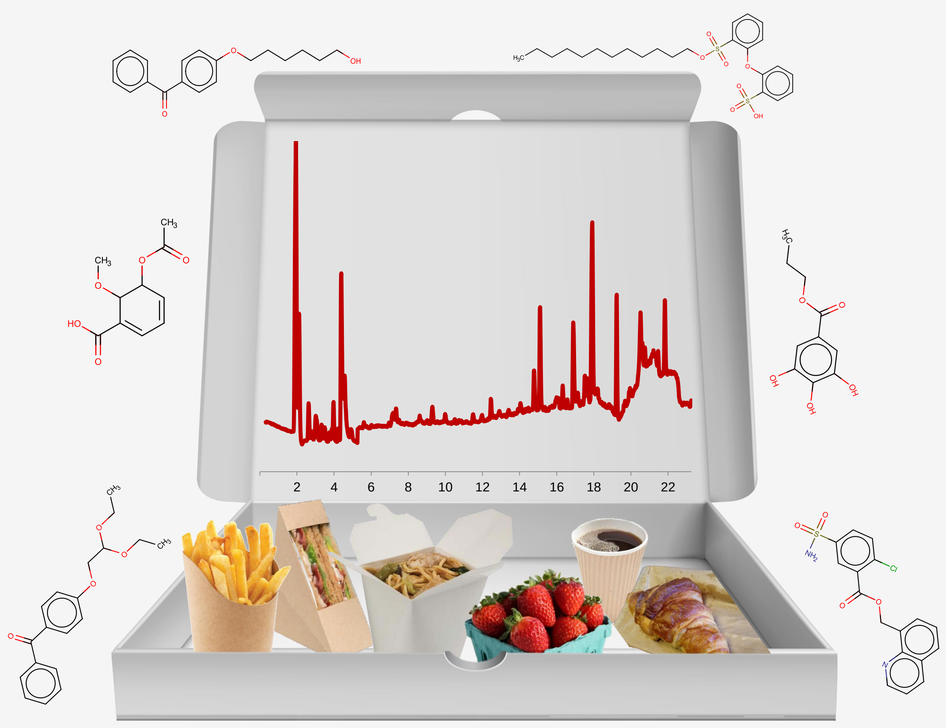

Figure 1. For a non-harmonized FCM, paper and board are used with a surprising variety of food. Yet, knowing whether it is safe to use paper and board for a specific application depends both on what is present and what can actually migrate.

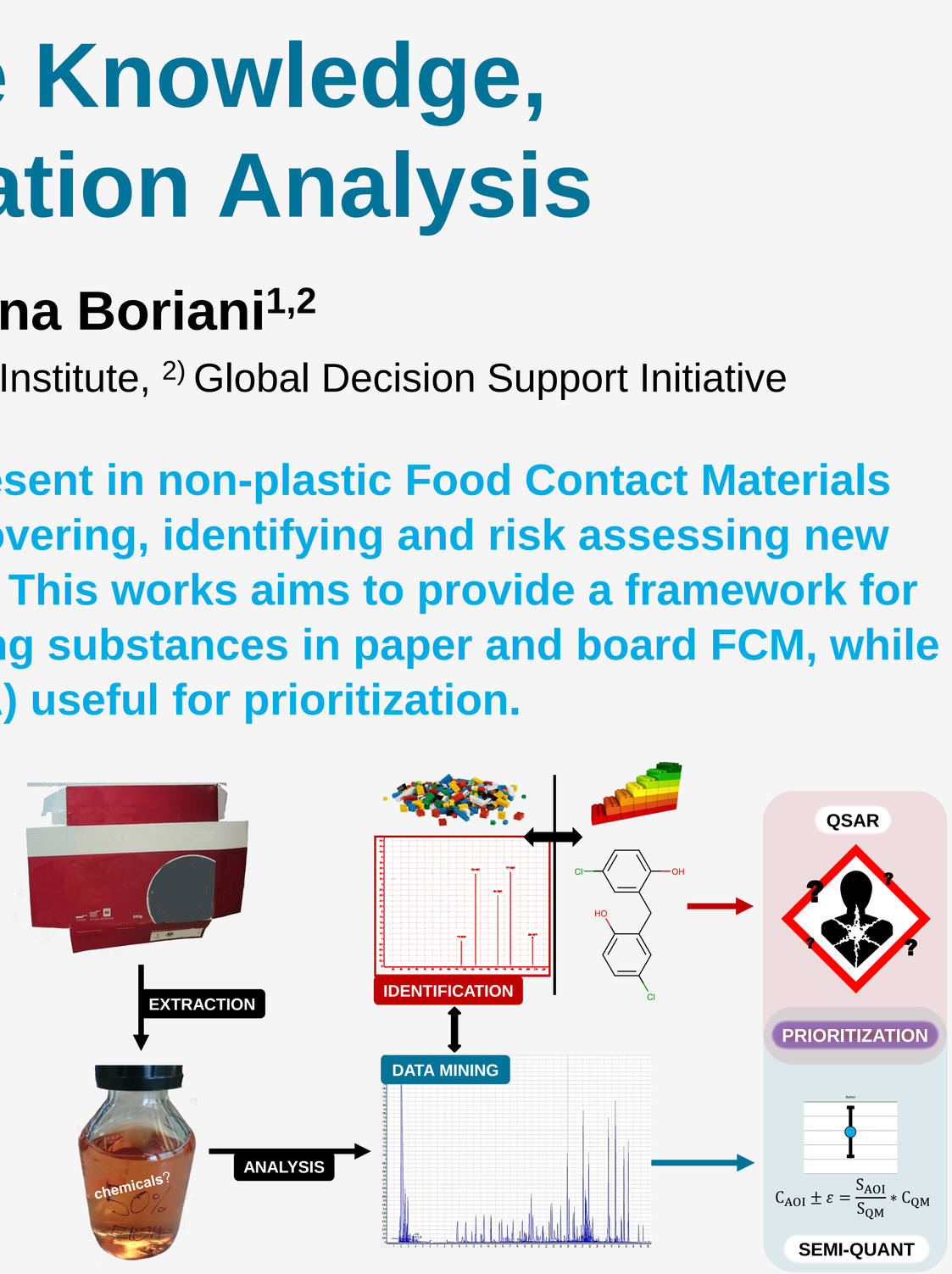

Figure 2. Flowchart depicting the route from sample to preliminary prioritization. First, samples are extracted, filtered, and then analysed by LC-MS. Then, the chromatogram and mass spectra are data-mined for concentration data and tentative structural information. Finally, predictive models are used to estimate the concentration level ("exposure") and the toxic properties ("hazards") of each substance of interest.

We think that by finding new compounds and ranking according to potential risk, we can support making better decisions. Exploring the risks via preliminary estimates is a first step towards prioritization and risk management.

Toxicological Predictions

Quantitative structure-activity relationship (QSAR) models are used to predict toxicological effects of tentatively identified substances. We use QSAR models as a tool to classify substances of high concern against those of low concern (also see **S1-07-A** poster)

Combining the Data

Current collaborations with *ANSES* (Paris, France) is focusing on distilling the available data for prioritization. A key parameter is communication: how can data with a number of uncertainties (e.g., QSAR, SQ) be communicated properly to industry, decision makers, and the public?

1. ENVI Committee (July 18, 2016). "Report on the implementation of the Food Contact Materials Regulation ((EC) No 1935/2004)." *European Parliament*