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

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

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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 dm² 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.

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?

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