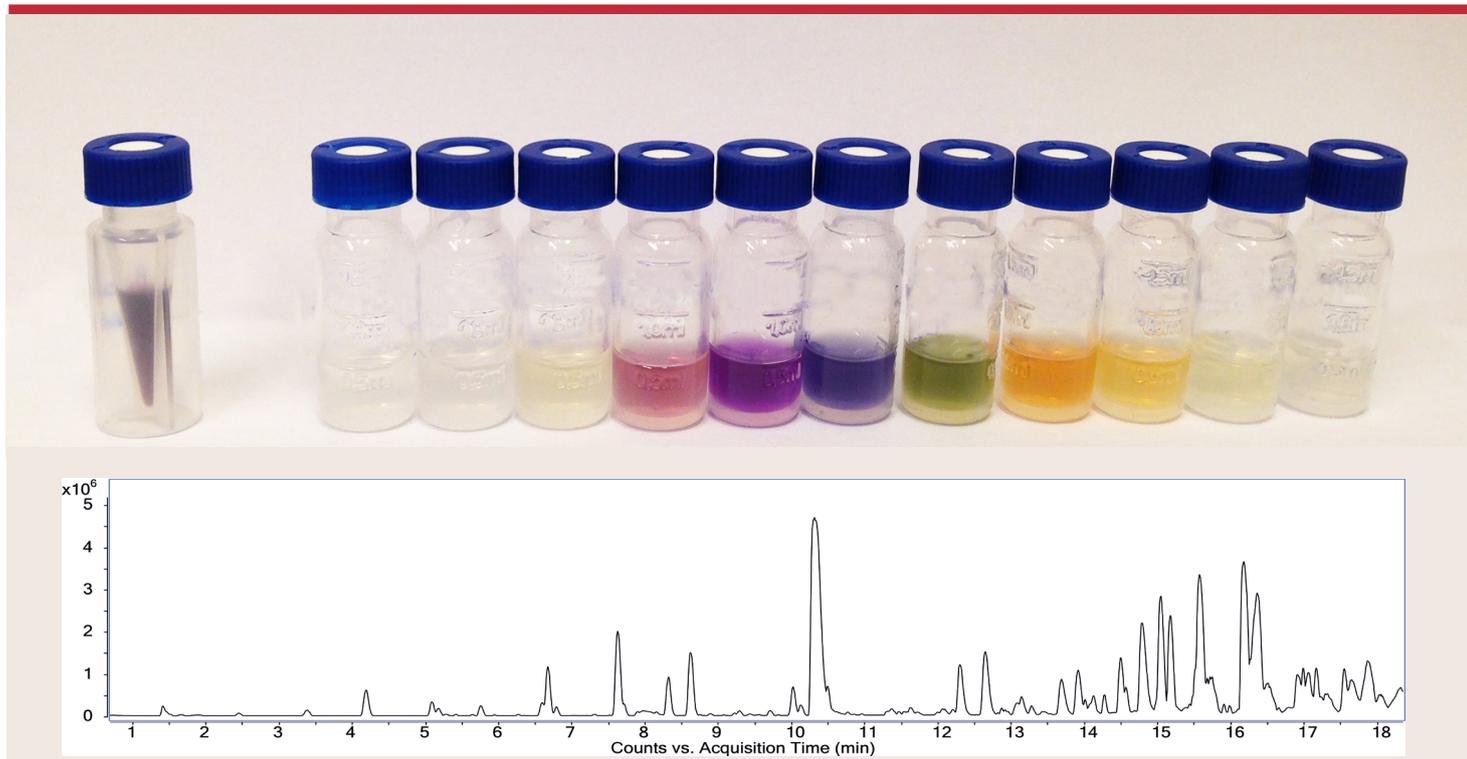


Linda Bengtström
Summary of PhD thesis

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Chemical identification of contaminants in paper and board food contact materials



Summary

Paper and board are used for a variety of food contact materials, such as baking paper, microwave popcorn bags and packaging for cereals as well as fast foods. Despite this extensive use, there are currently large data gaps about the chemical composition of different paper and board food contact materials and the toxicological effects of these compounds.

The aim of this study was to develop a rationalised interdisciplinary strategy for the screening and identification of compounds with potential adverse health effects in paper and board materials. The first step in the proposed strategy was to develop a comprehensive extraction process that is compatible with both chemical and toxicological analyses. For this purpose, a purge-and-trap method was developed for the collection of small volatile organic compounds; in addition semi- and non-volatile compounds were extracted by a boiling ethanol reflux system.

After an initial *in vitro* screening of 20 different paper and board samples for endocrine disruptive effects, mutagenicity and effects on metabolism of foreign compounds, five samples with adverse effects were selected for fractionation. The fractions were tested in cell assays in a second screening. The fractionation was used to reduce the number of compounds to be identified as well as the matrix effect.

Next, the fractions were analysed by gas chromatography and liquid chromatography coupled to high resolution mass spectrometry. These two techniques were designed to be as complimentary as possible and by them in combination increased the possibility to identify compounds with potential adverse health effects. Several steps in the tentative identification by gas chromatography can be automated, due to the standardisation of this technique that enables searches in vast mass spectral libraries. Such libraries are missing for liquid chromatography, and a large part of the tentative identification must be performed manually. To facilitate the tentative identification by liquid chromatography, an accurate mass database containing approximately 2100 entries of compounds with reported use in paper and board was built. The results from this study indicate that both isotope ratio and hits in the accurate mass database greatly increases the possibility of a correct tentative identification.

After lists of tentatively identified compound had been produced for a certain toxicological assay, compound were selected for further testing based on previously reported effects, structural similarities to known ligands, and availability of analytical standards for identified compounds. Any positive annotation through databases should be regarded as tentative, and therefore analytical standards were used to confirm the identification.

After confirmation, equivalence factors for the initially observed toxicological effect and from all the confirmed compounds tested in the same toxicological assay were calculated. The initially observed effects on the metabolism of xenobiotics could to a minor extent, though not fully, be attributed to dyes used in printing inks. In addition, it was concluded that the endocrine disruptive effects could largely be explained by monomers and plasticisers present in a recycled fibre sample and by sizing agents in virgin fibres.