

# Non-target analysis of intentionally and non-intentionally added substances from virgin and recycled paper/paperboard for food contact materials

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## Abstract

Paper and paperboard food contact materials (P/B FCMs) are one of the main important sources of food contamination. During the manufacturing, storage, and use of food packaging, their direct or indirect contact with food can induce the migration of intentionally and non-intentionally added chemicals. Their occurrences are crucial to account for dietary exposure and to protect consumer's health. However, limited information on food packaging chemicals' identity and potential effects on human health is lacking. The present study was aimed to identify chemicals migrating from the P/B FCMs by non-target analysis with ultra-performance liquid chromatography coupled with quadrupole-time of flight mass spectrometer (LC-QTOF-MS) and gas chromatography mass spectrometer (GC-MS).

A modified analytical procedure for an automated data processing of LC-QTOF-MS and GC-MS has been developed and evaluated with MS-DIAL, MassHunter and python software.

A total of 296 migrated chemicals were putatively identified as residues in virgin and recycled paper and paperboard intended for use as food packaging materials. They represented natural compounds, fatty acid ethyl esters, additives in FCMs, common phthalates, organophosphorus flame retardants substances and per/poly fluoroalkyl substances, alkanes, siloxanes, ketones, and chemicals used as stabilizer in packaging.

A non-targeted approach for identification of migrated chemicals with LC-QTOF-MS and GC-MS was established and evaluated. The information on the identity of chemicals migrating from food packaging materials is important to guide recommendations on the safety of chemicals used in P/B FCMs and provide a science-based data to illustrate risk management strategies.

Key words: Paper contact materials, Non-targeted analysis, UPLC/HRMS, GC-MS, In-house database