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High-resolution mass spectrometry with data independent acquisition for the comprehensive non-targeted analysis of migrating chemicals coming from multilayer plastic packaging materials used for fruit purée and juice

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Abstract

EU legislation requires that chemicals migrating from food packaging into food do not endanger human health. A proper safety assessment must go further than simply testing for known ingredients used to make the packaging materials. The identification of all potential migrants, including non-intentionally added substances (NIAS), is required to assess the safety of these materials. In this study, the benefits of using LC-ESI-Q-TOF-MS equipment combined with the data-independent acquisition method SWATH (Sequential Windowed Acquisition of All THeoretical MS) have been evaluated for the identification of unexpected migrants from multilayer plastic packaging materials. Identification of non-target peaks followed by filtering strategies facilitated the comprehensive identification procedure of unexpected migrants present in the food simulants. MS and MS/MS data from the most abundant ions in the samples were processed using formula finding and searched against open chemical and spectral databases, such as ChemSpider and METLIN, combined with bibliographic search. This approach has allowed the identification of 26 potential migrants, of which 23 were NIAS. Cyclic oligomers, possibly coming from polyurethane adhesives, were the main migrants in the studied materials. Evaluation of the toxicity of the tentatively identified migrants was carried out, showing that most of them classified in the higher toxicity class according to Cramer rules. Most of the compounds detected in this study were previously reported in other studies of NIAS migration from plastic packaging materials, except for five of the tentatively identified oligomers that were found for the first time in this study. This study shows the high potential of non-targeted approaches using high resolution accurate mass spectrometry (HRAMS) with SWATH acquisition for the characterization of food packaging materials aimed at food safety evaluation.

1. Introduction