Identification algorithm for polymer mixtures based on Py-GC/MS and its application for microplastic analysis in environmental samples

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Abstract:

Microplastics pollution is an acknowledged global issue, and new strategies are required to meet the increasing demand of standardized, fast and reliable measurements. Analytical pyrolysis coupled to gas chromatography and mass spectrometry (Py-GC/MS) is a promising technique to obtain qualitative and quantitative data on microplastics mixtures through the selection of a set of characteristic pyrolysis products for each polymer. However, this data processing method is time-consuming, and no automated algorithms are currently available. In the present work, a new method for the qualitative analysis of eleven types of synthetic polymers was developed, automated and implemented in the F-Search software, with the aim of proposing a standardized procedure for data processing in Py-GC/MS analysis of plastics mixtures. The method improves on the current literature, and is based on the generation of summated mass spectra (SMS) for each polymer, obtained by extracting specific m/z and retention index coordinates corresponding to characteristic pyrolysis products. The identification of a polymer is performed by comparing its SMS with those of a built-in library. After validation, the algorithm was tested on a reference sample containing all eleven investigated polymers. The algorithm provided relative standard deviations around 10%, and the results were used to estimate the lowest amount of polymer detectable in a sample, which was found lower than μg for most polymers. The performance of the algorithm was also evaluated on a real sample from ocean water trawling, providing positive results for four different polymers. The performances of the algorithm are discussed, and possible future developments are outlined.

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Frontier Labs Products used:

F-Search, IQ-mill-2070, EGA/Py-3030D, AS-1020E, UA-5