Identification of unknown compounds in PE and PP for food contact materials

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Abstract

Packaging materials are complex mixtures and can contain unknown compounds due to unexpected reactions or degradation of substances present in the materials used for their manufacture.

Polyethylene (PE) and polypropylene (PP) are polymers widely used for packaging applications, which may undergo changes during their manufacture. One of the challenges in the food packaging field is the identification of unknown compounds present in the final material and that could be originated during its processing.

In the present work a non-targeted analysis for the identification of unknown compounds was applied. Different PE and PP were analyzed. Samples consisted of raw materials as well as the additives used in its manufacture.

Each sample was analyzed by gas chromatography coupled to mass spectrometry (GC-MS) after solvent extraction to detect semi-volatile compounds and GC-MS coupled to Purge and Trap (GC-MS-P&T) in case of volatile compounds.

To be analyzed by GC-MS, samples were previously extracted with hexane at 70°C for 4 hours and with a mixture of Hexane: Ethanol (3:1 v/v) at 20°C for 8 hours.

Likewise, each sample was directly subjected to a slight heating (Purge) during which the volatiles present were dynamically dragged through a stream of Helium being retained in a trap. Subsequently the trap was subjected to rapid heating and the retained compounds were eluted to the chromatograph where they were analyzed.

The presence of alkanes as more abundant components was confirmed by both techniques, as well as the presence of 2,4-di-tertbutylphenol as can be seen in Figure 1. This compound is a product of degradation of the antioxidants used in the processing of this material.

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Image

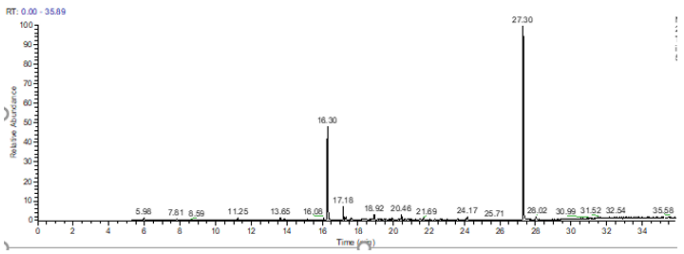


Figure 1. Chromatogram of one of the additives of polyethylene extracted with hexane at 70ºC for 4h. The majority peak (60%) is identified as 2,4-di-tert-butylphenol CAS 96-76-4 (tr: 27.30 min) and the next in abundance (25%) as an alkane (tr: 16.3 min.).

Recent Publications

1. C. Nerín, P. Alfaro, M. Aznar, C. Domeño (2013) The challenge of identifying non-intentionally added substances from food packaging materials: A review. Analytical Chimica Acta 775: 14-24.
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3. D Brocca, EArvin, H Mosbæk (2002) Identification of organic compounds migrating from polyethylene pipelines into drinking water. Water Research 36 (15): 3675-3680.
4. M.Hoppe, P. de Voogt, R.Franz (2016) Identification and quantification of oligomers as potential migrants in plastics food contact materials with a focus in polycondensates – A review. Trends in Food Science & technology 50: 118-130.
5. C. Carrero-Carralero, J.Escobar- Arnanz, M. Ros, S. Jiménez- Falcao, M. L. Sanz L. Ramos. An untargeted evaluation of the volatile and semi-volatile compounds migrating into food simulants from polypropylene food containers by comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry. Talanta 195: 800-806.



Biography

Patricia Vázquez Loureiro is a PhD Student in the Department of Analytical Chemistry, Nutrition and Food Science in the University of Santiago de Compostela. Her works are focus on packaging materials and food safety and she has experience in the analysis of compounds of interest in food products as well as in method developments or different extraction sample procedures. She has worked with both liquid and gas chromatography coupled to mass spectrometry (LC-MS/MS and GC-MS) and liquid chromatography with fluorescence detector to identify and quantify compounds of interest.

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