Non targeted analysis in polypropylene for food packaging by LC-MS

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Abstract

Films and containers for food packaging are made largely in base of polypropylene (PP). PP is a material used to package different types of food and its use has increased due to its utilization as substitute of polycarbonate in baby bottles.

In this work PP powders and pellets kindly supplied by the industry were analyzed by liquid chromatography-mass spectrometry (LC-MS) in order to identify unknown compounds, present in these samples that are intended to be used in the manufacture of PP for food packaging. Both were extracted with acetonitrile at 70 °C for 24 hours previous its analysis. Two LC-MS systems were used; a triple quadrupole (QqQ) and quadrupole-time of flight (QTOF) mass spectrometer. Two different internal standards were used for the APCI (Atmospheric pressure chemical ionization) and ESI (Electrospray ionization) analysis both in positive and negative mode

Using these analytical techniques, the presence of unknown non-volatile compounds in the extracts was determined; when the APCI+ source and the QTOF spectrometer are used more peaks are detected. The main challenge is the identification of these non-intentionally added substances (NIAS) to determine if they are impurities or if they are formed by reaction or degradation process during the material production.

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Image

Source	ESI		APCI	
polarity	Negative	Positive	Negative	Positive
Mass range: m/z	50-1400	50-1400	50-1400	50-1400
Nebulizer: bar	3	3	2.5	2.5
Dry Gas: l/min	9.3	9.0	4	4
Dry Heater: ºC	200	200	250	250
Capillary: V	3500	4500	4500	4000
APCI heater			400	400
Crown			8000	4000
Mobile phase	ACN: Water	ACN 0.1% HCOOH: Water 0.1% HCOOH	ACN: Water	ACN 0.1% HCOOH: Water 0.1% HCOOH

Figure 1. Spectrometric conditions used in the analysis of PP extracts by QTOF.

Recent Publications

1. M. Onghena, E. Van Hoeck, N. Negreira, L. Quirynen, J. Van Loco, A. Covaci (2016) Evaluation of the migration of chemicals from baby bottles under standardised and duration testing conditions, Food Addit. Contam. Part a-Chem. Anal. Control Expo. Risk Assess. 33 (5):893–904
2. Paula Vera, Elena Canellas, Cristina Nerín (2018) Identification of non-volatile migrant compounds and NIAS in polypropylene films used as food packaging characterized by UPLC-MS/QTOF. Talanta 188:750-762.
3. H.T. Chi, Y. Liu, X. Gao, W.L. Liu, G.H. Hu, Y.J. Luo (2015) Study on migration model of antioxidants in food contact polypropylene plastics, Chin. J. Anal. Chem. 43 (3):399–403.
4. J. Alin, M. Hakkarainen (2010) Type of polypropylene material significantly influences the migration of antioxidants from polymer packaging to food simulants during microwave heating, J. Appl. Polym. Sci. 118 (2):1084–1093.
5. M. J. Martínez-Bueno, S. Cimmino, C. Silvestre, J. L. Tadeo, A. I. Garcia-Valcárcel, A. R. Fernández-Alba and M. D. Hernando (2016) Characterization of non-intentionally added substances (NIAS) and zinc oxide nanoparticle release from evaluation of new antimicrobial food contact materials by both LC-QTOF-MS, GC-QTOF-MS and ICP-MS. Anal. Methods. 8: 7209-7216.



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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