

Abstract

In the present work, the development and validation of a simple, low-cost and sensitive method for the direct determination of nine analytes in beverages belonging to four types of compounds, is reported. The analytes were chosen based on a preliminary migration study conducted on crown cap polymer liners and on the probability of their occurrence in real samples as a consequence of migration. The analytes were preconcentrated using solid-phase microextraction (SPME) and analyzed by gas chromatography – tandem mass spectrometry (GC-MS/MS).

The following SPME parameters were optimized: fiber stationary phase selection, NaCl addition effect, extraction time and temperature effects, and the matrix effect. With respect to the latter, a simple GC-FID method was implemented for the monitoring of organic solvent residues in samples and analytical solutions. By using GC column with novel stationary phase (ultra inert modification of a HP-5) it is possible to analyze more polar compounds directly without a derivatization step, which is considered as one of the important advantages of the developed method. The affordable compound phenyl dichlorophosphate was proven to be not only comparable, but even a better alternative to isotopically labeled analogues as internal standards. The LODs of the SPME-GC-MS/MS method were in the range of 0.005 – 0.2 µg/L, the relative standard deviations 0.8 – 5.4 %, and the mean accuracies (recoveries) of determination 98 – 109 %.

A migration study at 50 °C in a timespan of 6 months was conducted in bottles filled with various model solutions for migration testing and closed with crown caps. A migration study was also performed in a plastic fermenter where butylated hydroxytoluene was proven to migrate from the contact surface of the fermenter. Commercially available and homemade alcoholic beverages and vinegars were analyzed. Traces and larger concentrations of all the analytes with the exception of *tert*-butyl hydroquinone and tris(2-butoxyethyl)phosphate were detected.

Keywords: food contact material, contact embalage, migration of compounds, SPME, GC-MS/MS, parabens, phenolic antioxidants, plasticizers