L112*
DETERMINATION OF MIGRATING COMPOUNDS FROM PLASTIC BABY BOTTLES BY GC–QQQ–MS AND LC–QQQ–MS

Onghena Matthias[1*], Negreira Noelia[2], Van Hoeck Els[3], Quirynen Laurent[4], Van Loco Joris[5], Covaci Adrian[6]

[1, 2, 4, 6] Toxicological Centre, Faculty of Pharmaceutical Sciences, University of Antwerp, Wilrijk-Antwerp, Belgium
[3, 5] Department of Food, Medicines and Consumer Safety, Scientific Institute of Public Health (WIV-ISP), Brussels, Belgium
**Corresponding author – E-mail: matthias.onghena@uantwerpen.be, Phone: +32471814659*

After the European Union prohibited the production of Bisphenol-A-containing polycarbonate baby bottles (EU 10/2011), alternative materials, such as e.g. polypropylene, polyethersulphone, etc. have appeared on the Belgian market. The first aim of this study was the identification of major organic compounds migrating from these new baby bottles. After sterilisation by boiling during 10 min, 3 consecutive migrations with simulant D1 (water:EtOH (50:50) were performed at 70°C during 2h (EU 10/2011). Afterwards, the migration solutions were analysed using a liquid-liquid extraction with EtOAc:*n*-hexane (1:1). Various compounds, such as alkanes, phthalates, antioxidants, etc. were identified by GC–MS using commercial mass spectral libraries. Unidentified peaks were further investigated by GC–(EI)–TOFMS and GC–(APCI)–QTOFMS for structural identification. Additionally, extracts were analysed by LC-QTOF–MS to determine the less volatile migrants, such as Bisphenol-S. Based on these results, the most toxic migrating compounds were monitored and quantified using validated GC– and LC–QqQ–MS methods. An evaluation of the effect of several "real-life use conditions" such as microwave, sterilisation and dishwasher on the profile of the different migrants was determined and compared with the standard EU "repetitive use conditions" (3 migrations, 2h at 70°C). Analysis of the 3rd migration step of the standard conditions (which has to comply with the EU legislative migration limits) showed that for some baby bottles several not authorised compounds were observed exceeding the established "no-detection limit" of 10 µg/kg. Substances such as 2,4-di-*tert*-butylphenol (up to 118 µg/kg), 2-butoxyethyl acetate (up to 945 µg/kg) and 4-propylbenzaldehyde (up to 27 µg/kg) were detected in several bottles as well as some phthalates. The silicone bottle even exhibited concentrations of TXIB around 350 µg/kg, whereas this compound is only authorised for use in single-use gloves. For all detected compounds authorised by the EU 10/2011 with a specific migration limit (SML) such as benzophenone (600 µg/kg, found up to 97 µg/kg), concentrations were below the SMLs. Analysis of the extracts from the microwave experiments showed similar trends, but lower concentrations than those observed in the repetitive use experiments. Furthermore, a downwards tendency of these concentrations towards the subsequent microwave cycli was perceived. 4-propylbenzaldehyde was detected in one specific polypropylene bottle at max. 9 µg/kg after the first microwave treatment, whereas its concentration was 3 times higher in the 3rd step of the repetitive experiment. Other parameters, such as the influence of the sterilisation or the dishwasher on the concentrations of these migrants are still ongoing, yet these first results suggest that the conventional migration experiment prescribed by the EU overestimates the actual concentrations of compounds migrating from plastic baby bottles.

Keywords: *baby bottles, plastics migration, BPA alternatives, GC–QQQ–MS, LC–QQQ–MS*

L113
LIQUID CHROMATOGRAPHY TANDEM MASS SPECTROMETRY (LC–MS/MS) DETECTION OF GLYCIDYL ESTERS AND MCPD ESTERS IN INFANT FORMULA

Jessica Leigh[1*], Shaun MacMahon[2], Lowri DeJager[3], Timothy Begley[4]

[1, 2, 3, 4] US FDA-CFSAN, College Park, MD, United States of America
**Corresponding author – E-mail: jessica.leigh@fda.hhs.gov, Phone: 2404023046*

Fatty acid esters of 3-chloro-1,2-propanediol (3-MCPD), 2-chloro-1,3-propane diol (2-MCPD), and glycidol are process-induced chemical contaminants found in refined edible vegetable oils. Formed during the deodorization of oils during refining, these compounds are considered potentially carcinogenic and/or genotoxic, making their presence in edible oils and processed foods containing these oils a potential health risk. Recently, there has been increasing attention to the use of these refined oils in commercial infant formulas. Since formula is typically an infant's sole source of nutrition, and due to infant's low body weights, the presence of MCPD and glycidyl esters poses a potential health risk. At present, published validated methods for extracting and quantifying these contaminants in processed foods are limited to mayonnaise and salad dressings. The current work focuses on developing methodology for extracting and quantifying these chemica l contaminants from commercial infant formulas in order to determine levels of exposure. A method for extracting MCPD and glycidyl esters from infant formula will be described in this presentation. The extraction efficiencies of MCPD monoesters, MCPD diesters and glycidyl esters in a homemade infant formula with known MCPD/glycidyl ester concentrations will also be discussed. Results indicate that extraction efficiencies of greater than 90% can be achieved for all monoester, diester, and glycidyl ester species using the developed extraction procedure. Quantitation of MCPD and glycidyl esters was performed using a liquid chromatography tandem mass spectrometry (LC–MS/MS) method that was previously developed for the quantitation of these species in edible oils. Validation results indicate the extraction and quantitation methods developed for infant formula are sensitive and robust. Using the validated methodology, a survey of a number of commercially available infant formulas (in both the United States and abroad) was conducted in order to assess infant exposure to MCPD and glycidyl esters.

Keywords: *processing contaminants, MCPD esters, glycidyl esters, LC-MS/MS, infant formula*