

UHPLC-HRMS based targeted and untargeted screening of plasticizers in the marine environment

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The cumulative amount of plastics entering our aquatic environment is predicted to increase by an order of magnitude by 2025, resulting in the extensive entree of plasticizers. Plasticizers, i.e. phthalate acid esters and alkylphenols, are easily released into the aquatic environment as a result of their weak physical bonding to plastic polymers. As it has been shown that continuous exposure to plasticizers results in a plethora of adverse ecological effects, monitoring phthalate acid esters and alkylphenols in the marine environment is of great importance to provide insight in the widespread occurrence of these compounds in our aquatic ecosystems.

Therefore, this study engaged on the analysis of the abovementioned compound groups in seawater samples obtained from different locations in the Belgian Part of the North Sea during different seasons (2016-2017). The seawater samples were analyzed using an in-house developed and validated ultra-high-performance liquid chromatographic high-resolution mass spectrometric (UHPLC-HRMS) method. This novel analytical method was specifically designed to minimize false-positive detections resulting from laboratory contamination of plasticizers. Performing the targeted analysis of 27 plasticizers revealed the prevalence of 16 unique plasticizers in the seawater samples. Alkylphenols and phthalates were respectively detected at concentrations ranging from 24 to 8000 ng L⁻¹ and 20 to 2580 ng L⁻¹. Moreover, multivariate statistics displayed the highest concentrations of ethylphenol and dibutyl phthalate in the harbor of Ostend. Next to the native plasticizers, also primary plasticizer metabolites (mono-phthalates) were ubiquitously detected with concentrations ranging between 25 and 2550 ng L⁻¹. Subsequent to the targeted screening, untargeted analysis of the same seawater samples revealed 3688 different unknown compounds. Further data analysis for identification purposes occurred through online environmental database search, including MarineLit, Marine Drugs, EPA, drugsbank, ACTor and EAWAG biodegradation. In conclusion, the ubiquitous prevalence of plasticizers in our marine waters suggests that plasticizers will have reached different trophic levels throughout our aquatic ecosystem and may thus contribute to adverse ecological effects threatening the quality of our marine environment.

Acknowledgments

The authors acknowledge the Belgian Science Policy (BELSPO) for funding the NewSTHEPS project (BR/143/A2/NEWSTHEPS; www.newstheps.be) in which this work fits.