

# How far have plasticizers and additives penetrated our aquatic environment?

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## Abstract

Phthalates and phenols are a large group of ubiquitous, high-volume industrial chemicals that are added to plastics and many other daily products, such as building materials, toys, paints, adhesives and medical equipment. Due to the weak physical bonds between a polymer and the plasticizers or additives, they can easily be released directly or indirectly (i.e. through metabolism, manufacturing processes) in the aquatic environment. Continuous exposure to these substances can exert toxic, mutagenic, and carcinogenic effects on organisms by interfering with their endocrine system. Therefore, monitoring phthalate esters and phenolic compounds in the marine environment, whether or not in the metabolised form, will provide insight into the degree of occurrence that these compounds have already reached in our aquatic system.

The aim of this study was to develop a multi-residue method for the simultaneous determination of 20 phthalate esters and 10 phenolic compounds in the marine environment. The analytes were separated with an ultra high performance liquid chromatograph (UHPLC) using a 1.9  $\mu\text{m}$  Hypersil Gold column (100 mm x 2.1 mm), and quantified in full-scan by a Q-Exactive Benchtop™ high resolution mass spectrometer (HRMS). Chromatographic variables, such as mobile phase, mobile phase modifier, flow and column oven temperature, were optimised to enhance phenol sensitivity. Additionally, a trap column (1.9  $\mu\text{m}$ , 50 mm x 2.1 mm) was used for eliminating phthalate contamination originating from the analytical instrument. Furthermore, the mass spectrometric variables (such as position source, sheath gas, auxiliary gas, sweep gas, discharge current, capillary temperature, S-lens RF, and vaporizer temperature) were optimised. Next, a suitable extraction was designed for capturing a broad polarity range (Log  $K_{ow}$  ranging between 1 and 12), including the diphtalates, monophthalates and phenols.

Future perspectives comprise the validation of the developed UHPLC-HRMS method according to CD 2002/567/EC and the analysis of phthalates and phenols in the Belgian Part of the North Sea. A major advantage of our newly developed method lies in its ability to identify suspected and unknown compounds, besides the list of aforementioned target compounds. Finally, this work will be an important step towards environmental forensic profiling, future European legislation and a contribution to the Marine Water Framework Directive.

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