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Analysis of different high production volume chemicals and their chlorination by-products in waters by ultrasound-assisted emulsification–microextraction

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Ultrasound-assisted emulsification–microextraction (USAEME) demonstrated its applicability for the analysis in waters of 2-phenylphenol (PP), 4-*tert*-butylphenol (TBP), benzothiazole (BTZ) and piperonyl butoxide (PBO), belonging to different chemical families, and all of them characterised by its high production volume. In the developed USAEME procedure, compounds were extracted in chloroform from 10 mL of water sample during only 5 min. The addition of derivatising reagents has been studied as part of the optimisation process. The optimised procedure provided an efficient and exhaustive extraction with the advantage that the extract was ready for GC analysis. The method was validated using real environmental water samples, obtaining recoveries between 68 and 111%, RSD values ≤10%, and limits of quantification at the sub-ng per millilitre level (0.004–0.072 μg L^{-1}). The application of the method to the determination of the targets in different environmental waters showed their presence in most samples.

In addition, the method allowed the study of the behaviour of the compounds in the presence of chlorine as disinfection agent, reporting for the first time that BTZ and PBO remained stable even at 4 mg L^{-1} of chlorine concentration, whereas the phenolic compounds (TBP and PP) required low chlorination levels to be transformed into mono- and di-chlorinated derivatives.

Keywords: USAEME; ultrasound-assisted emulsification–microextraction; water analysis; microextraction; chlorination by-products

1. Introduction

The increasing concern about residues from industrially important compounds demands the evaluation of their occurrence and fate in the environment. The worldwide annual production of many chemicals with application, among others, in the pesticide industry is estimated at several million tons. High production volume chemicals encompass different chemicals that easily enter the aquatic environment and can be found as emerging pollutants in waters. It is quite difficult to establish general criteria to select which of these chemicals should be or not be considered for analysis [1]. More interesting is developing suitable tools for analysing diverse chemicals becoming potential pollutants. The present work focuses on four compounds belonging to very different chemical families: 2-phenylphenol, 4-*tert*-butylphenol, benzothiazole and piperonyl butoxide. Phenylphenol (PP) has application as a disinfectant, bactericide and virucide. In

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