DEGRADATION AND BY-PRODUCTS IDENTIFICATION OF BENZOTHIAZOLES AND BENZOTRIAZOLES DURING CHLORINATION BY LC-HR-MS/MS

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Nowadays, chlorination is the most prevalent disinfection method applied for water treatment in Europe. Chlorine can be supplied as sodium hypochlorite (NaOCl) which reacts in water to produce the disinfectants hypochlorous acid (HOCl) and hypochlorite ion (OCl^-), otherwise known as free chlorine [1]. Although the primary purpose of chlorination is the elimination of micropollutants via oxidation, several investigations have shown that chlorine reacts with micropollutants leading in the production of undesired by-products. 1,3-benzothiazoles (BTHs) and 1,2,3-benzotriazoles (BTRs) are classified as high production volume emerging environmental pollutants due to their broad industrial and domestic application [2], and even though recently several analytical methods have been applied for their determination [2,3], there is still a lack of research for their by-products' identification.

Initially, the degradation of three BTHs (BTH, 2-OH-BTH and 2-amino-BTH) and four BTRs (1-H-BTRi, TTRi, XTRi and 1-OH-BTRi) during chlorination was investigated by UHPLC-MS/MS (QqQ). Although chlorination appeared to be an insufficient degradation process for BTH and 1-H-BTRi, all their examined substituted derivatives seem to be significantly degraded when the molar ratio of sodium hypochlorite and the target analytes was between 5000:1 – 1000:1. Then, LC high resolution MS/MS (q-TOFMS) was used to investigate the formation of by-products in the chlorinated samples. Two suspect by-products of 2-amino-BTH and one of XTRi were tentatively identified based on their probable structure, mass accuracy, retention time and fragmentation and isotopic pattern. An interesting observation was the formation of 1-H-BTRi as a degradation product of 1-OH-BTRi during chlorination. Moreover, post-acquisition non-target treatment of the MS data revealed several unknown by-products of the tested analytes and their structure elucidation is still in progress.

Acknowledgments

This research has been co-financed by the European Union and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) – ARISTEIA 624 (TREMEPOL project).

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