IDENTIFICATION OF BIOTRANSFORMATION PRODUCTS OF CITALOPRAM FORMED IN ACTIVATED SLUDGE

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Abstract

Citalopram (CTR) is a highly consumed antidepressant which is removed incompletely by conventional wastewater treatment. Although it is highly detected in effluent wastewaters, little is known about its behavior and transformation processes that undergo during wastewater treatment. The present study aims to expand the knowledge on fate and transformation of CTR during the biological breakdown process. For this purpose, biotransformation batch reactors were set up to assess biotic, abiotic and sorption losses of this compound. One of the main objectives of the study was the identification of the formed transformation products (TPs) by applying suspect and non-target strategies based on liquid chromatography quadrupole-time-of-flight mass spectrometry (LC-QTOF-MS). In this regard, the complementary use of reversed phase chromatography (RP) and hydrophilic interaction liquid chromatography (HILIC) in the identification of polar TPs, the deep evaluation of the obtained MS/MS spectra, as well as the use of in-house developed quantitative structure-retention relationship (QSRR) retention time prediction models provided valuable support to identification. Fourteen TPs were detected. Thirteen of them were tentatively identified. Four compounds were confirmed (N-desmethylCTR, CTR amide, CTR carboxylic acid and 3-oxo-CTR) through the purchase of the corresponding reference standard. Probable structures based on diagnostic evidence were proposed for the additional nine TPs. A transformation pathway for the biotransformation of CTR was proposed. The presence of the identified TPs was assessed in real wastewater samples through retrospective analysis resulting in the detection of five compounds. Finally, the potential ecotoxicological risk posed by CTR and its TPs to different trophic levels of aquatic organisms, exposed to the studied effluents, was evaluated by means of risk quotients.

Keywords: Citalopram; biodegradation; transformation products; retrospective analysis, LC-QTOF-MS; HILIC.