Abstract
Biodegradation is considered to be the key process for the elimination of the majority of pharmaceuticals in the environment. During wastewater treatment or once they are disposed in the aquatic environment, pharmaceuticals may transformed to new, structurally-related compounds which are called transformation products (TPs). Since most of these compounds are unknown, their identification is essential not only to provide a comprehensive risk assessment on micropollutants in the environment, but also to design improved removal technologies for (pseudo)persistent trace contaminants.

In this study, batch reactors seeded with activated sludge from the WWTP of Athens were set up to assess biotic, abiotic and sorption losses of a SSRI drug, citalopram. TPs were identified by reversed-phase liquid chromatography quadrupole-time-of-flight mass spectrometry (RP-LC-QToF-MS). Hydrophilic interaction liquid chromatography (HILIC) was also used as a complementary, orthogonal, technique for the identified TPs, instead of NMR. A workflow for suspect and non-target screening was developed. A suspect list of possible TPs was compiled by literature and in silico prediction tools (EAWAG-BBD Pathway Prediction System and Bruker’s Metabolite Predict). Structure elucidation of TPs was based on accurate mass and isotopic pattern measurements and interpretation of MS/MS spectra by the observed fragmentation pattern and library-spectrum match.

In total, thirty TPs were identified. Four out of them were fully identified and confirmed by reference standards (desmethylcitalopram, citalopram amide, citalopram carboxylic acid and 3-oxo-citalopram). A probable structure based on diagnostic evidence and tentative candidates were proposed for the additional five and four TPs, respectively. Finally, a transformation pathway based on the identified compounds was presented.

EXPERIMENTAL

KINETIC EXPERIMENT
Degradation of citalopram

RESULTS & DISCUSSION

TRANSFORMATION PATHWAY OF CITALOPRAM

EXAMPLE IDENTIFICATION OF CTR 343

CONCLUSIONS

* Suspect and non-target screening was performed for the identification and structure elucidation of TPs.
* HILIC was used complimentary to RP (identical MS/MS spectra of TPs in RP and HILIC).
* 13 TPs were identified in total.

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