

WORKFLOW FOR THE IDENTIFICATION OF BIOTRANSFORMATION PRODUCTS OF AMINE-CONTAINING PSYCHOTROPIC DRUGS IN THE AQUATIC ENVIRONMENT

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Pharmaceuticals are continuously discarded into the aquatic system through wastewater treatment plants (WWTPs). The microbial degradation of these organic micropollutants and formation of transformation products (TPs) under aerobic conditions is the fundamental process for their elimination. It is of paramount importance to understand the microbial metabolic pathways so as to obtain knowledge of how fast micropollutants degraded and to assess the exposure to their potential TPs as they can be more polar and consequently environmentally persistent [1].

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 selective psychotropic drugs, containing amine moieties. Biodegradation and transformation products were identified using liquid chromatography quadrupole-time-of-flight mass spectrometry (LC-QToF-MS). Data were acquired through broad-band collision induced dissociation (bbCID) mode, providing MS and MS/MS spectra simultaneously under positive and negative electrospray ionization (two separate runs). A workflow for target, suspect and non-target screening was developed. Data treatment was performed by using metabolite tools accompanying Bruker's maxis impact ESI-QToF-MS and the structure elucidation of the candidate transformation products was based on accurate mass and isotopic pattern measurements by HRMS and tentative interpretation of MS/MS spectra. Finally a biodegradation pathway was proposed based on the TP structures identified. Despite the structure similarities, different degradation constants were calculated for each compound.

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References

1. B. O. Clarke and S.R. Smith, *Environ. Int.* **37**, (2011) p. 226-247.