Novel workflow for identification and determination of antibiotics and their transformation products in wastewater by liquid chromatography coupled to high resolution-mass spectrometry

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Extended abstract

Contaminants of emerging contaminants (EC) have been detected and reported in various environmental compartments [1-3]. However, knowledge on the occurrence of antibiotics (A) and their transformation products (TPs) is still scarce [2]. A list of 676 antibiotics and major TPs reported in literature was compiled. The collection of compound information was done in a systematic and reproducible way and included chemical identifier information (SMILES, InChIKey, InChI and CAS), connection with chemical databases (ChEBI, HMDB, KEGG, LIPID MAPS, PubChem and ChemSpider) and category based on chemical structure (i.e. Aminoglycosides, b-lactams/Cephalosporins, b-lactams/Penicillins, Sulfonamides). The compound list is available in NORMAN network website (http://www.norman-network.com/?q=node/236) and is part of NORMAN-SusDat database (http://www.norman-network.net/datatable/). Moreover, literature review conducted in context of this study, revealed that only a small fraction of these compounds (less than 10%) has been investigated so far. A second list with in-silico predicted TPs was also compiled. The current problem of in-silico prediction tools is that they produce a very large number of TPs, even when likelihood thresholds are implemented [4]. In our case, the number of predicted structures (~20,000) was high enough and therefore could only be managed by a systematic and automatic procedure. Therefore, a novel wide-scope suspect screening scheme was developed to evaluate the occurrence of A and TPs. The presented workflow will address that developments in high resolution mass spectrometry and retention time prediction. Workflow will highlight new cheminformatic tools that make quick, effortless and effective search of hundreds of substances known or suspected to be present in the environment.

Keywords: Antibiotics; Transformation products; Suspect Screening; Cheminformatic tools

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