

QUALITATIVE SCREENING FOR EMERGING CONTAMINANTS AND THEIR METABOLITES/TRANSFORMATION PRODUCTS IN SEWAGE SLUDGE OF ATHENS BY UHPLC-QTOF MS

BOROVA V.1, BLETSOU A.1, PSOMA A.1 and THOMAIDIS N.S.1

¹ Department of Chemistry, University of Athens, Panepistimiopolis Zografou 157 84 Athens, Greece E-mail: ntho@chem.uoa.gr

Municipal wastewater contains a wide variety of contaminants, called emerging pollutants (EPs). Among them the active ingredients of pharmaceuticals, illicit drugs and new psychoactive substances, are important classes. After the intake, these active compounds undergo metabolic processes in organisms. Both parent compounds and their metabolites are excreted into raw sewage and then are degraded up to a point through the processes applied in waste water treatment plants (WWTPs), mainly through mineralization, absorption and biodegradation. The sewage sludge represents the insoluble residue produced during wastewater treatment. Although it is treated, still many EPs and their metabolites/transformation products (TPs) are adsorbed and not efficiently removed. This can result in the introduction of these contaminants into the food chain because of their accumulation into plants, when the sludge is used as a fertilizer on agricultural or disposed to land filed, causing potential negative effects.

In this study, a wide-scope screening method was developed for the detection of pharmaceuticals, illicit, new psychoactive drugs and their metabolites/TPs. The analytical procedure includes a simple ultrasound-assisted extraction [1], followed by liquid chromatography coupled to a hybrid quadrupole time of flight mass spectrometer with an ESI source operated in positive and negative mode, allowing the detection of a broad range of compounds in complex environmental samples, as sewage sludge. A broadband collision induced dissociation (bbCID) acquisition mode was performed recording spectra over the range m/z 40-1000 with a scan rate of 2 Hz and providing MS (low energy: 4 eV) and MS/MS (high energy: 25 eV), spectra at the same time. The detection of the substances was accomplished by retention time matching (± 0.2 min), mass accuracy (≤ ± 5 ppm), and the isotopic fit (≤ 200 mSigma) using a in-house database. The procedure was used to screen a wide variety of emerging contaminats in sewage sludge, during 7 consecutive days in March 2014 and in March 2015, , from Athens. More than 100 compounds were identified both years including the drugs MDA, EDDP and methadone, the antidepressants venlafaxine, citalopram, mirtazapine, trazodone, maprotiline, the antiepileptic carbamazepine, lamotrigine, the antibiotics clarithromycin, azithromycin, ciprofloxacin, the analgesics tramadol, paracetamol and some rarely reported ones, like the metabolites and TPs of venlafaxine, diltiazem, and clarithromycin.

Keywords: emerging contaminants, metabolites, transformation products, QTOFMS, illicit drugs, NPS

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