

Analysis of 44 drugs of abuse and metabolites in wastewater and river water using a hybrid quadrupole time-of-flight tandem mass spectrometry

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The presence of drugs of abuse in the aquatic environment has been recognized as an important issue for the ecosystem due their possible negative effect on it (Richardson, 2011). Incomplete removal of these substances during wastewater treatment could be one of the causes of their release in the environment (Zuccato and Castiglioni, 2009). Pollution by illicit drug residues at very low concentrations is generalized in populated areas, with potential risks for human health and the environment (Zuccato, 2008; Castiglioni et al 2007). The aim of this study was to screen and quantify 44 drugs of abuse and metabolites of wastewater samples using a hybrid quadrupole time-of-flight tandem mass spectrometry and furthermore carry out a post-target screening to identify additional compounds present in the water samples.

Wastewater samples were collected from the influent and effluent of three wastewater treatment plants (WWTPs) in Valencia and river water samples from Turia River Basin. Illicit drugs were extracted by solid-phase extraction (SPE). The chromatography was performed with an Agilent 1260 Infinity ultra high performance liquid chromatography (UHPLC). The UHPLC system was coupled to a hybrid quadrupole time-of-flight ABSciex Triple TOFTM 5600. All analytes were analyzed in positive mode. Acquiring full scan MS data was employed for quantification of drugs of abuse, and automatic data dependent information product ion spectra (IDA-MS/MS) was checked for identifying emerging illicit drugs and other compounds in water samples. The use of a database containing 1212 compounds achieved high confidence results for a wide number of contaminants.

In the present study, the presence of compounds that belong to amphetamines group (amphetamine, methamphetamine, ephedrine, MDMA, MDA and MDEA), tryptamines (bufotenine), pirrolidinophenone group (α -PVP and 4'-MePHP), arylcyclohexylamines (ketamine), cocaine derivatives (cocaine, benzoylecgonine, cocaethylene and ecgonine methyl ester) and morphine derivatives (codeine, EDDP, morphine and methadone) and cannabinoids (THC) were detected in the influent, effluent or river water samples. These compounds were quantified, reaching cocaine derivatives the highest values. Regarding post-target screening approach, more than 120 contaminants, mostly pharmaceuticals, but also mycotoxins and polyphenols were unambiguously identified. This new approach to data evaluation by non-target screening analyses opens the possibility of various other applications, for example in open and groundwater or for monitoring natural attenuation.

Acknowledgements

This work has been supported by the Spanish Ministry of Economy and Competitiveness through the project CGL2011-29703-C02-02. MJ Andrés Costa also acknowledges to this Ministry the FPI grant to perform her PhD.

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