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Enantiomeric profiling and drug consumption estimation

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Abstract

Background: Recent trends in new psychoactive substances (NPS) abuse have raised a serious public health issue that affects all communities. NPS comprise a wide range of substances, such as synthetic cathinones, synthetic cannabinoids, opioids, and benzodiazepines [1, 2]. These substances end up in the environment as excretion products or by direct disposal [3]. Wastewater-based epidemiology (WBE) combined with the evaluation of enantiomeric fractions (EF) is used for complementing the drug monitoring methods traditionally used to estimate drug consumption. However, the adsorption of these substances to suspended particulate matters (SPM) has been neglected, leading to a potential underestimation of the consumption patterns [3, 4]. **Objective:** This study was aimed to better understand and to get knowledge on: (i) the enantiomeric profiling and consumption estimation of amphetamine-type substances (amphetamine (AMP), methamphetamine, 3,4-methylenedioxymethamphetamine) and synthetic cathinones (buphedrone, butylone, 3,4-dimethylmethcathinone and 3-methylmethcathinone); (ii) the behaviour and distribution of NPS in SPM. **Methods:** In this study, 24-h composite raw wastewaters were collected from a wastewater treatment plant (WWTP) located in the north of Portugal. After the extraction, the SPM and influent extracts were analyzed using an indirect analytical method. Briefly, samples were subjected to chiral derivatization using (*R*)-(−)-α-methoxy-α-(trifluoromethyl) phenylacetyl chloride, leading to the formation of diastereomers that were further analyzed by gas chromatography coupled to mass spectrometry (GC–MS), as described elsewhere [3]. **Results:** Both enantiomers of AMP, MDMA and 3,4-DMMC and (*S*)-MAMP and the first eluted enantiomer of BPD and 3-MMC were detected. The selected NPS were found at concentrations between LOQ and 0.4 ng mg^{-1} and <LOQ and 315,82 ng L^{-1} in SPM and influents, respectively. Regarding the consumption estimation, AMP showed the highest values (<166,05 mg d^{-1} 1000 inh^{-1}). **Conclusions:** The method allowed the characterization of the adsorption as well as the assessment of consumption patterns, occurrence, and the EF of the target chiral NPS.

Keywords: synthetic cathinones; suspended particulate matter; amphetamine type substances; wastewater treatment plants; chirality

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