SCREENING OF METABOLITES AND TRANSFORMATION PRODUCTS OF PHARMACEUTICALS AND ILLICIT DRUGS BY UHPLC-QTOF MS IN EFFLUENT WASTEWATER SAMPLES FROM ATHENS

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The presence of pharmaceuticals and illicit drugs (PIDs) in the environment is a matter of major concern because of their wide consumption and their potential negative effects on the water quality and living organisms. After consumption, PIDs can be excreted in unchanged form as the parent compound and/or as free or conjugated metabolites. Some of these compounds seem not to be completely removed during wastewater treatments, and might finally arrive to surface and ground waters. This has forced sewage water treatment plants to perform alternative treatment technologies to guarantee water quality. In order to evaluate the hazard in the water cycle, not only removal of the parent compounds and metabolites in the treatment processes must be taken into account, but also the possible formation of transformation/degradation products (TPs). Therefore, detection and identification of TPs in effluent wastewater is of great importance to know the overall contribution of chemicals in the aquatic environment.

In this study, hybrid quadrupole time-of-flight mass spectrometry (QTOF MS) in MS^E mode, together with the aid of a specialised processing-data application manager, has allowed the screening of more than 200 PIDs TPs/metabolites in Athens effluent. The satisfactory sensitivity in full-acquisition mode, high-resolution, accurate-mass measurements and MS/MS capabilities of QTOF MS make this technique a powerful analytical tool for the identification of organic contaminants including their TPs. Moreover, it is remarkable that large screenings can be made even without reference standards, as the valuable information provided by HRMS allows the tentative identification of the compound detected. In this work, TPs/metabolites previously identified in degradation experiments performed at our laboratory for pharmaceuticals as omeprazole, venlafaxine, gemfibrozil, ibuprofen, irbesartan and ofloxacin, were investigated. In a similar way, TPs of cannabis and cocaine were also searched for (Bijlsma, 2013; Boix, 2014a,b). Additionally, a second database was compiled, including theoretical exact masses of metabolites reported in the literature and also those for which reference standards were commercially available. Preliminary results show the frequent detection of metabolites/TPs of pharmaceuticals like omeprazol, irbesartan, venlafaxine, clindamycin, clarithromycin, clopidogrel or dipyrone, among others.

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