XV Reunión Científica de la SECyTA y VII Reunión Nacional de la SEEM

Investigation of Metabolites/Transformation Products of Emerging Contaminants in the Aquatic Environment by HRMS

Félix Hernández. Institute for Pesticides and Water (IUPA), University Jaume I, Castellón, Spain

One of the communications more interesting for me due to my research topic was "INVESTIGATION OF METABOLITES/TRANSFORMATION PRODUCTS OF EMERGING CONTAMINANTS IN THE AQUATIC ENVIRONMENT BY HRMS". In recent years there is a growing interest in determining metabolites or transformation products of emerging organic contaminants in aquatic environments. The reason is because these metabolites would be able to have more toxicity than parent compounds. In addition to detect and identify metabolites and transformation products the target of this research was also to determine unknown compounds.

The used technique to achieve this aim was Liquid Chormatography-High Resolution Mass Spectrometry (LC-HRMS) due to its accurate-mass full-spectrum acquisition measurements and sensitivity provided. Specifically, Hibrid Quadrupole-Time-of-Flight Mass Spectrometry was used to detect and identify metabolites, transformation products and unknown compounds in wastewater.

Some examples of emerging contaminants were presented in the oral presentation as mephedrone (drug of abuse) to identify and detect its metabolites or transformation products as a tentative identification. Some of the detected metabolites were identify by comparation with those reported in the bibliography and other ones were identified as unknown metabolites using different predictions of its fragmentation from the parent compounds or laboratory specific conditions. For unambiguous identification of this metabolites or transformation products they would need their reference standards.

HRMS Tools for Direct Analysis of Recreative Drugs and Legal Highs

Élida Alechaga, Encarnación Moyano, Maria Teresa Galceran. Department of Analytical Chemistry, University of Barcelona

One of the most interesting presentations for me was "HRMS TOOLS FOR DIRECT ANALYSIS OF RECREATIVE DRUGS AND LEGAL HIGHS". In recent years, new psychoactive substances (Legal Highs) comprise a broad range of substances that are not controlled under international drug laws. Often they are intended to mimic the effects of existing controlled drugs. One example is JWH-O18 that is a synthetic cannabinoid. Besides, adulteration of illegal drugs with other substance is carried out commonly.

The continuous and quick development of these new drugs in recent years reveals the necessity to carry out analytical methods to identify this substance. In this presentation the researchers chose a hybrid mass analyser as Quadrupole-Orbitrap for the direct screening of these substances. MS acquisition was performed in a Q-exactive mass combining full-scan and data dependent tandem mass spectrometry acquisition. Both were used as identification criteria. Target compound identification was performed against a data base table using the MS full-scan and product ion scan. Unknown new psychoactive substances were identified using libraries and they were confirmed with reference standards.

The results show that illegal drug samples were adulterated with pharmaceuticals and possible candidates for new psychoactive drugs were identified.

María Jesús Andrés Costa