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

Resumen razonado (en inglés) de la comunicación que le hayan parecido más interesantes de la XV SECyTA (200-250 palabras aproximadamente).

The Plenary Lecture given by Dr. Facundo M. Fernandez from Georgia Institute of Technology, Atlanta, entitled "Ambient ionization with plasmas and charged droplets" dealt with the newest approaches and developments in the ambient ionization mass spectrometry field. Especial attention was given to the ones that are already commercially available. Ambient ionization techniques are based on the direct open air surface analysis under ambient conditions, from which the most extended are Desorption Electrospray Ionization (DESI), Direct Analysis in Real Time (DART) and Laser-Ablation Electrospray Ionization (LAESI). These methods allow the analysis of whole samples with simple or any previous sample treatment and also without any separation technique prior to mass spectrometry detection. They are a powerful tool in metabolomics and imaging applications when coupled to high resolution mass spectrometers.

Several applications were shown, including multimodal biological tissue imaging, rapid metabolome fingerprinting and preliminary analysis of solid samples. An example application was the preliminary analysis of suspected fake drugs (a prominent problem in developing countries); different ambient ionization sources were applied directly to the solid drug samples in order to rapidly detect whether they were fraudulent or not. Moreover, three-dimensional robotic surface sampling can be performed to solid, relatively large samples in order to obtain an insightful knowledge of their surface composition.

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The Plenary Lecture given by Dr. Félix Hernández from University Jaume I, Spain, entitled "Investigation of metabolites/transformation products of emerging contaminants in the aquatic environment by HRMS" dealt with the potential of liquid chromatography coupled to high resolution mass spectrometry (LC-HRMS) for the analysis of metabolites and/or transformation products that are not usually taken into account in environmental analysis. These metabolites/TPs may be present in waters at higher concentrations than the parent contaminant compound and their toxicity and effects are not usually known or fully understood. For this reason, it is important to know which metabolites/TPs may be present in a given sample, for which different strategies were presented.

Several examples of emerging contaminants investigations by QTOF MS were given, including detection and identification of analytes already reported in bibliography, investigation of unknown analytes related to parent compounds, computational prediction of TPs and laboratory experimentation on selected aquatic contaminants under different conditions in order to discover metabolites/TPs that may be present in real environmental samples.

The use of HRMS allowed to tentatively identify the metabolites/TPs, later to be confirmed by the injection of standards, thanks to the accurate-mass full-spectrum acquisition measurements provided by this potent analytical technique.

Nombre del estudiante

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