University of Puerto Rico
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Departmental Seminar

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Friday, January 22nd, 2016
11:30 AM
Q 123
Abbott Seminar Room

Using High Resolution Mass Spectrometry (HRMS) as an environmental protection tool: from the needle in the haystack to a haystack made of needles.

One of the key issues restricting human growth is water availability. Usually water scarcity is described as restriction of volume but lately the pressure has shifted to availability of good quality water rather than simply volume. Having polluted water is equally bad as not having water if treatment is not available. Analytical chemistry technology, in particular mass spectrometry has seen incredible improvements that have outpaced environmental regulations. In the past, the most common task was to do selective quantitation of "target" chemicals using specific molecular information designed to detect compounds above a specific and usually low regulatory benchmark. Whit that in mind, water treatment technologies concentrated on the removal of those "problem chemicals" that are considered toxic, accumulative or persistent. Target analysis was often defined as looking for a needle in a haystack and the challenge was to get rid of the hay. High Resolution Mass Spectrometry (HRMS), in combination with chromatography separations, gave us the opportunity to acquire enough information to characterize both the needle and the hay at the same time. We have employed both Orbitrap and Ion Cyclotron Resonance (ICR) mass spectrometers to measure target compounds, metabolites and transformation products and even unknowns in complex environmental matrices such as raw sewage and crude oils. In one case we detected previously unreported metabolites of drugs of abuse that were used to estimate per capita consumption. In another we characterized recalcitrant compounds that persisted through a river influenced by domestic wastewater and were still present in the finalized drinking water. In every case, use of HRMS to generate molecular formulae followed by statistical analyses resulted on detailed characterization of environmental processes that have been difficult to study with more traditional techniques.