2012 ASMS Workshop

Interest Group Name: **Environmental MS Interest Group**

Workshop Title: **Challenges and Opportunity in Water and Health Research**

Presiding: **Susan Richardson (US EPA) and Xing-Fang Li (University of Alberta)**

Date: **May 23, 5:45-7:00 pm**

Summary of Program and Discussion

The 2012 Environmental Interest Group workshop discussed the global challenges of sustainable water source and quality from rivers, lakes, and groundwater to our tap water and human health and opportunities for research and development of mass spectrometry technologies and applications. The workshop highlighted three areas of water issues and research opportunities, including (1) emerging water disinfection byproducts and human health effects, (2) oil sand produced water and ecotoxicology, and (3) emerging environmental contaminants and mass spectrometry. The workshop was a success with about 200 participants who had extensive discussion and provided suggestions and comments for the future research on water and health.

Susan Richardson opened up the workshop presentations by providing an overview of emerging environmental contaminants in water, including perfluorinated chemicals (PFCs), pharmaceuticals, nanomaterials, disinfection by-products (DBPs), pesticide transformation products, brominated flame retardants, algal toxins, hormones, naphthenic acids, and pathogens. She provided information on issues regarding exposure, toxicity, and bioaccumulation, and closed with a slide of challenges and opportunities for mass spectrometry, outlining many ongoing issues and data gaps that mass spectrometry could help to solve. These issues and data gaps included understanding precursors and transformation/degradation products for PFCs, confirming tentative identifications for pharmaceutical transformation products (is there a better way than pre-LC with NMR?), real-world measurement of nanomaterials in the environment, improving the ability of LC/MS/MS to identify unknown DBPs in drinking water, incorporating new direct technologies (such as Leaf Spray-MS) into routine testing, understanding advanced oxidation reaction products/intermediates for algal toxins, and finally, the ongoing need for a unified LC/MS/MS library to help with identification of contaminants in environmental waters.

Kerry Peru of Environment Canada presented background information and significant analytical challenges with respect to the characterization and monitoring of environmentally important polar organic compounds (naphthenic acids and related components) derived from the oil sands produced water from northern Alberta. Advances using high resolution mass spectrometry and data analysis were presented as part of the solution to such challenges.

The Athabasca oils sands region of Alberta, Canada constitute the one of world's largest bitumen reserves with a proven 170 billion barrels of crude oil. Approximately 3 barrels of river water are used during the alkaline/hot water extraction process of the mined oil sand for every barrel of oil produced. During the extraction process, acidic bitumen components (including naphthenic acids) are solubilized in the water. This oil sands process water (OSPW) is then stored in massive tailings ponds due to a zero discharge policy. Acidic components of bitumen are highly toxic to aquatic organisms, possible pond leakage is a growing concern. Development of analytical methods that can distinguish between compounds found within industrially derived OSPW from those derived from natural weathering of oil

sands deposits is required. This is a difficult challenge as possible leakage beyond tailings ponds containments will likely be in the form of a mixture of water soluble organic acids that are similar to those leaching naturally to aquatic environments. An overview was given on the progress of such analytical developments and the current state of analysis. The potential for high resolution mass spectrometry and accurate mass for chemical fingerprinting of oil sands acids from tailing ponds, interceptor wells, groundwater and reference river surface waters is evaluated. Principal component analysis was performed for all species observed using negative-ion electrospray ionization. Using high resolution mass spectrometry data, PCA clustering is clearly observed indicating that this technique may be a useful tool in analytical forensics relating to oils sands related environmental monitoring.

Recognizing that the oil sands acid fraction contains many more components that the traditionally defined O2 species, as published from past work from our group and others, further studies have been conducted to determine the influence of extraction procedure on what is being measured. Significant differences were observed depending on the extraction procedure and/or extraction solvent of choice. These observations were only evident with the use of high resolution data as the differences observed were most significant in the non-O2 species. Depending on the intended use and purpose of the data, careful selection of extraction procedure is required. In addition, a standardized extraction technique is advised in order to obtain cross lab comparative data sets.

Imma Ferrer of University of Colorado Boulder gave a brief presentation and led the discussion on the following aspects:

- Accurate mass, using time-of-flight (TOF) mass spectrometry instruments, has been recently the method of choice for many scientists in the environmental field in order to identify and detect organic contaminants, such as pharmaceutical and pesticides, in complex matrices.

- Several tools, using accurate mass, have been used to identify new and emerging contaminants in water samples. Some of these tools include the following: the use of molecular feature extraction based software, accurate mass databases, isotope filters, mass defect, use of accurate MS-MS and mass profiling.

- The increase in resolving power in the last few years has been one of the main achievements, thus opening up a wide range of possibilities for unequivocal identification and interference discrimination of environmental relevant compounds in complex samples. Accurate mass using TOF was shown to discriminate between several isobaric/isomeric pairs of compounds.

- Reported in the presentation was a set of new pharmaceuticals and metabolites not identified to date.