

## Comprehensive analysis of oil-sands-processed-water by direct-infusion offline-UHPLC FTICR-MS

Adrien Nyakas<sup>1</sup>, Jun Han<sup>1</sup>, Kerry M Peru<sup>2</sup>, John V Headley<sup>2</sup> and Christoph H Borchers<sup>1</sup>

<sup>1</sup>University of Victoria, Canada

<sup>2</sup>Environment Canada, Canada

The constantly growing mining activity in the Athabasca oil sands region (Alberta, Canada) has generated vast amounts of oil-sands-processed water (OSPW), which are stored in large tailings ponds in direct proximity to the Athabasca river.

In this study, OSPW was investigated by extraction-only (EO) direct infusion (DI) negative-ion electrospray ionization (ESI) fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS), as well as by offline ultra-high performance liquid chromatography (UHPLC) and subsequent DI-FTICR-MS. A comparison of these two approaches revealed that a preliminary offline UHPLC separation led to approximately twice as many identified compounds compared to EO-DI-FTICR-MS analysis of the unfractionated sample. With the EO approach, 856 compounds were found, whereas offline UHPLC resulted in the identification of 1734 compounds. To overcome sample loading limitations pooling of corresponding fractions from two consecutive offline UHPLC runs prior to the MS analysis was performed, resulting in approximately 50% more compound assignments (2511) than did the analysis of a single injection of the low-pH organic OSPW extract. Ultimately, pooling of identical fractions increased the number of identifications by a factor of three compared to EO-DI-FTICR MS using the same amount of starting material. Most of the identified molecules corresponded to the group of naphthenic-(C<sub>n</sub>H<sub>2n+z</sub>O<sub>2</sub>) and oxy-naphthenic (C<sub>n</sub>H<sub>2n+z</sub>O<sub>x</sub>) acids (NAs and ONAs) (64%), followed by sulfur-containing compounds (23%), nitrogen-containing compounds (8%), and others (5%).

Liquid-liquid extraction followed by offline UHPLC fractionation thus holds enormous potential for a more comprehensive profiling of OSPW, resulting in a deeper understanding of its chemical nature and environmental impact.

[adrien@proteincentre.com](mailto:adrien@proteincentre.com)