Next Generation Solutions

'Omic' and chemical fingerprinting methodologies using ultrahigh-resolution mass spectrometry for geochemistry and healthy waters.

The Opportunity

Advanced Mass Spectrometry systems are now offering unprecedented opportunities in the field of small molecule chemical analysis as well as large molecule characterization and quantification. The GWF program has invested in state of the art, ultra-high resolution mass spectrometry (UHRMS) systems to quantify both natural and synthetic chemicals in water as well as perform various types of 'omic' investigations of responses of individual organisms, populations and communities of organisms to multiple stressors, including agriculture, resource extraction, urban activities and climate change

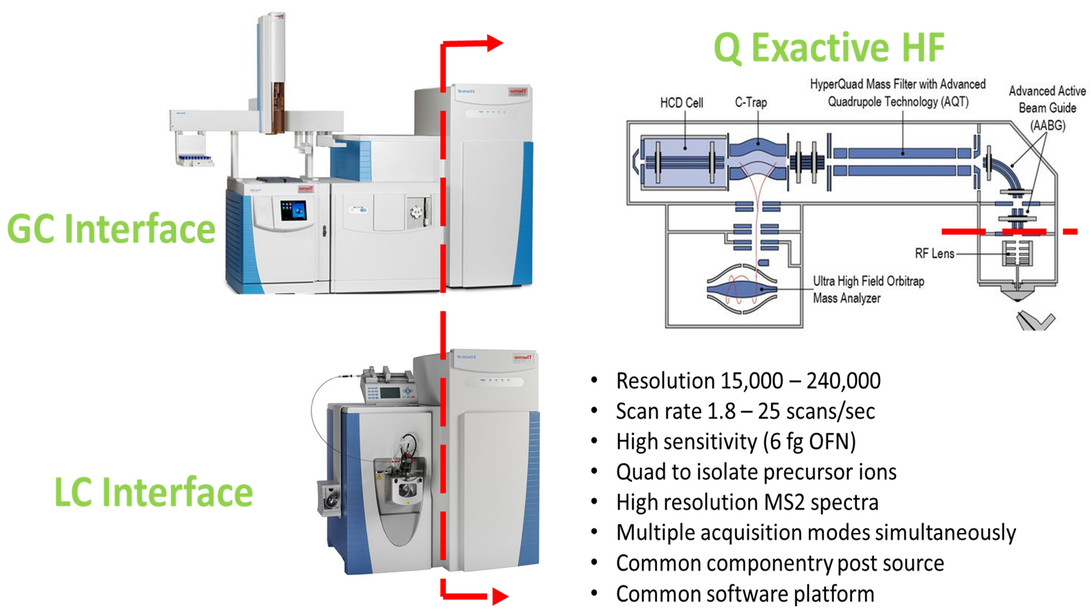


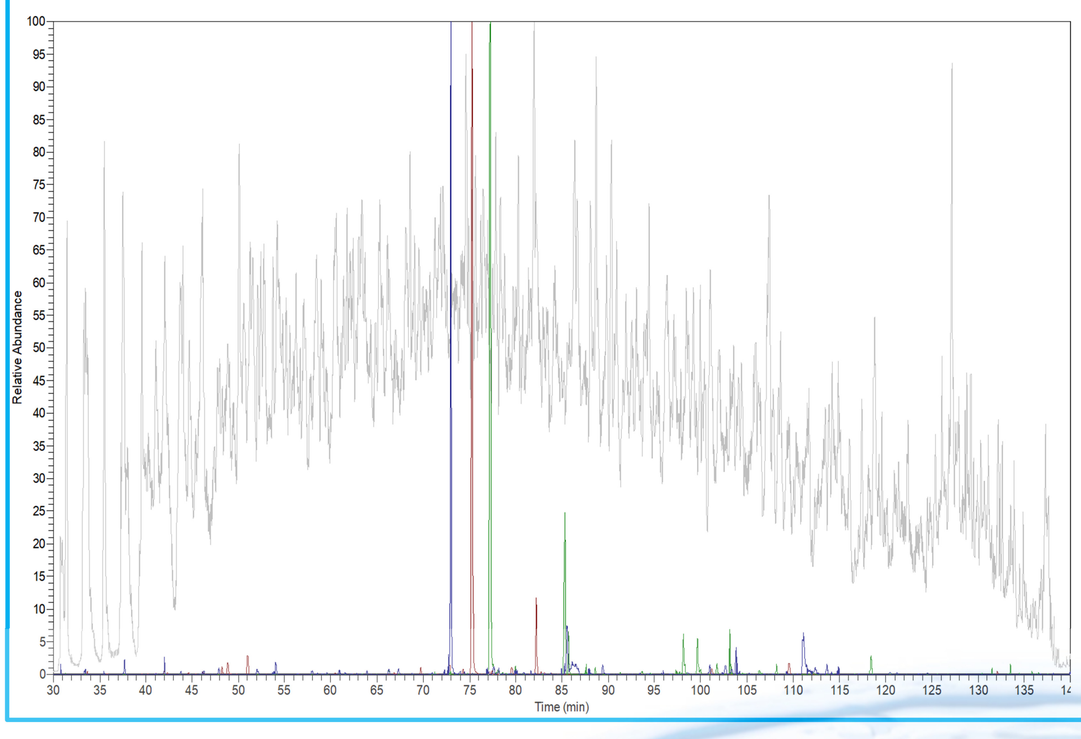
Figure 1 *GWF has purchased 2 state-of-the-art OrbiTrap mass spectrometry instruments, one interfaced to a gas chromatography system and one interfaced to a liquid chromatography system.*

Objective

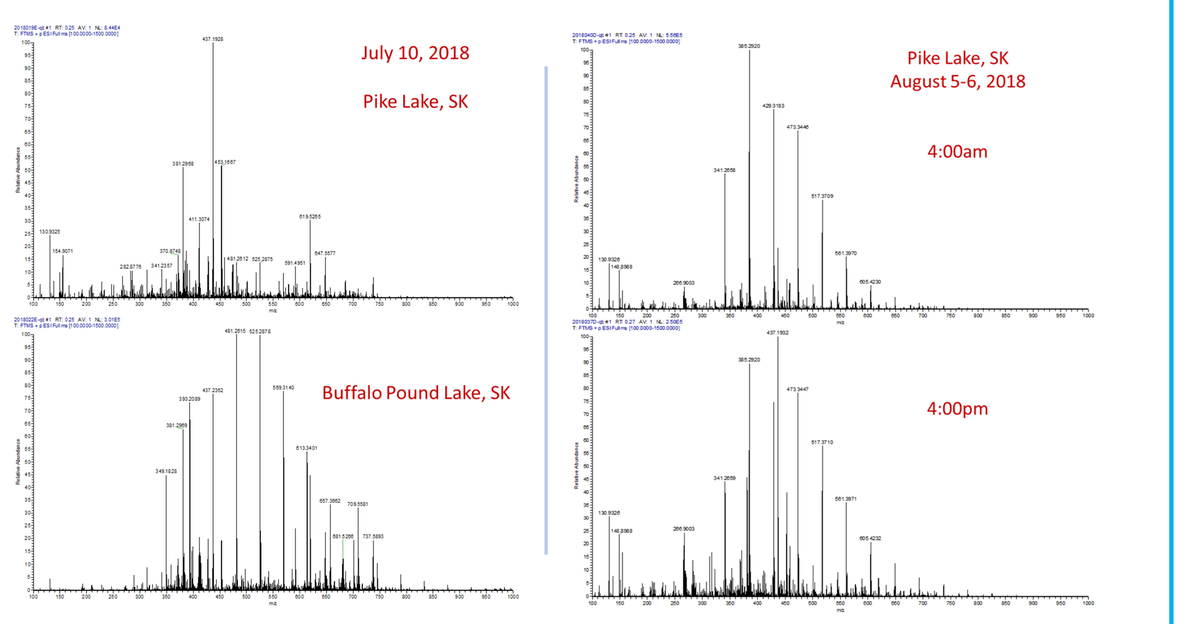
This research program applies emerging and transformative technologies in mass spectrometry and chemometrics to facilitate the development of new analytical paradigms for the protection of water resources. Specifically, advanced mass spectrometry techniques will be used to develop transformative techniques for the measurement of aquatic contaminants and investigating new paradigms for monitoring aquatic environments.

Progress Toward GWF Goals

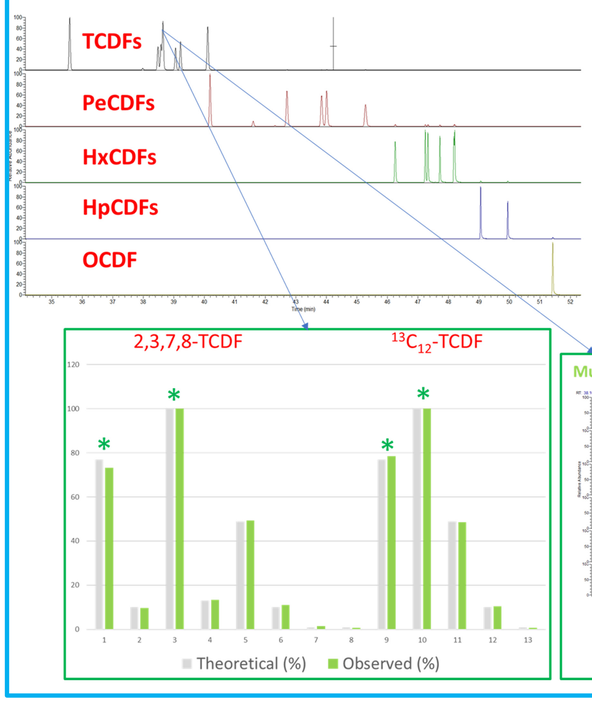
Proteomics *Analysis of a cell digest containing over 19,000 peptides representing 4,200 individual proteins. OrbiTrap mass spectrometry can identify individual peptides (colored traces) in this extremely complex mixture (grey background trace).*



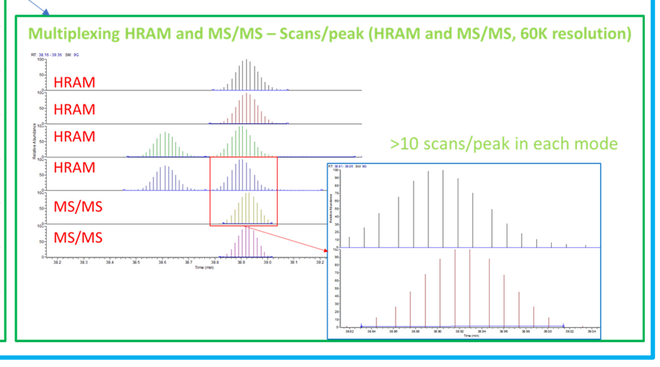
Chemical Fingerprinting *Ultra-High resolution mass spectrometry (UHRMS) has been used to characterize spatial and temporal differences in the chemical profiles of several surface waters. Each fingerprint represents 5,000-10,000 individual chemical compounds. Spatial differences in fingerprints are large (left panel) but short term temporal changes are also detected (right panel).*



Next Generation Dioxin Analysis *Current dioxin analysis methods rely on the use of magnetic sector mass spectrometers that must be operated near the very edge of their capability windows. UHRMS represents a major paradigm shift in dioxin analysis by using a technology with far greater capabilities than current instruments, in terms of resolution, scan rates, data density, and the ability to simultaneously scan in multiple analysis modes.*



The ability to carry out high resolution accurate mass analysis and MS/MS analysis simultaneously at >60,000 mass resolution represents the single greatest technology advance in dioxin analysis in the last 40 years. Also, image current detection means the entire ion cluster can be used for analyte confirmation instead of using just 2 ions as in current methods (* - the 2 ions currently used).



Supporting GWF Investigators

- eDNA project – **Giesy**, **Servos**, **Hecker**, **Jardine, Jones** *et al*
- PAH analyses in support of projects funded by the Department of Fisheries and Oceans – **Jardine, Giesy, Jones**
- Veterinary pharmaceuticals and antibiotics in cattle feed lots funded by the Beef Cattle Research Council Agriculture and Agri-Food Canada – **Giesy, Jones**
- Various GIWS funded projects on PAHs and DOM - **Doig**

Relevance

This program will exploit rapidly emerging technologies in mass spectrometry and chemo-informatics to provide managers with rapid and reliable new approaches to monitor changing aquatic ecosystems. Tools are being developed and validated that will create opportunities to better assess and predict changes in the Canadian environment. These emerging technologies have implications for contributing to international efforts to improve water quality, promote better management of our aquatic resources globally and to "protect and restore water-related ecosystems, including mountains, forests, wetlands, rivers, aquifers and lakes" (UN Sustainable Development Goal 6).

Publications

Jones, PD and Giesy, JP (2017) Quantification of Dioxins by GC-Orbitrap MS. Organohalogen Compounds 79, 589-592.

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