



VANCOUVER 2013

48TH ANNUAL WESTERN CANADA TRACE ORGANIC WORKSHOP

WESTERN CANADA TRACE ORGANIC WORKSHOP – 2013 AGENDA

EMPIRE LANDMARK HOTEL

1400 Robson Street
Vancouver, BC V6G 1B9
(604) 687 0511

SUNDAY, MAY 12, 2013

7:00 pm to 10:00 pm	Poster & Exhibitor Setup	Coal Harbour Room
7:00 pm to 8:00 pm	Registration	Cloud 9 Revolving restaurant
7:00pm to 10:00 pm	Reception & Mixer	Cloud 9 Revolving restaurant

MONDAY, MAY 13, 2013

8:00 am to 9:00 am	Registration	Coal Harbour Room
8:00 am to 9:00 am	Continental Breakfast Session Chair: Dave Hope	Courtesy of Canadian Life Science
9:00 am	Opening Remarks and Welcome	
9:05 am	Keynote Address: Ultrasensitive, automated capillary electrophoresis mass spectrometry for the analysis of organic molecules in complex samples	David Chen – UBC Chemistry
9:55 am	Analysis of Neonicotinoid Pesticides in Water and Sediments	Jonathan Bailey – Environment Canada
10:25 am	Coffee Break: Posters & Exhibits	Courtesy of Chromatographic Specialties
11:00 am	Disposition of Per- and Polyfluoroalkyl Substances During Wastewater Treatment	Jonathan Benskin - AXYS Analytical Services
11:30 am	Analysis of Complex Samples by Liquid Chromatography High Resolution Accurate Mass Spectrometry	Jonathan Beck – ThermoFisher Scientific
12:00 pm	Lunch	Courtesy of PerkinElmer Inc.
	Session Chair: Angelo Di Cicco	

1:00 pm	High Throughput Analysis of Contaminants in Drinking Water or Waste Water with integrated Sample Clean-up and Spectral Confirmation	Julie Marr – Agilent Technologies
1:30 pm	Fluorescent Detection of Trace Amounts of Bioorganic Molecules using a Nanobioarray (NBA) Chip	Paul Li - Simon Fraser University
2:00 pm	A Rapid Screening of Naphthenic Acids in Surface Water using LC/MS	Maxine Haberl – Environment Canada
2:30 pm	Mass spectral study of anti-cancer polyactylenes in Devil's Club (<i>Oplopanax Horridus</i>); an important medicinal plant of the Pacific Northwest	David Hasman – BCIT Forensic Science and Technology
3:00 pm	Coffee Break: Posters & Exhibits	Courtesy of AB Sciex
3:30 pm	Analysis of Low Concentrations of PAH and Alkyl PAH in Environmental Samples	Dale Hoover – AXYS Analytical
4:00 pm	A New, Single-pass, Automated Solid Phase Extraction Approach for Troublesome Waste Water Samples for Semi-Volatile Compounds	Marc Hamel – Horizon Technology Inc.
4:30 pm	Interactions of Transition Metal Ions with Organophosphorus Pesticides Probed by Electrospray Ionisation Mass Spectrometry	Bernd O. Keller – UBC Pathology and Laboratory Medicine

TUESDAY, MAY 14, 2013

8:00 to 9:00 am	Continental Breakfast Session Chair: Dayue Shang	Courtesy of Metrohm
9:00 am	Keynote Address: Trace Organic Analysis in Seconds Without Sample Prep	Charlie Schmidt – PerkinElmer Inc.
9:40 am	Applied Ion Analysis of various water matrices in Hydraulic Fracturing Process	Jay Gandhi – Metrohm Inc.

10:10 am	Coffee Break: Posters & Exhibits	Courtesy of MasSpec Consulting
10:30 am	High Definition Mass Spectrometry (HDMS) application of ion mobility in oil and petroleum analysis	Patrice Lemire – Waters Ltd.
11:00 am	Preventing Protein Adsorption on Liquid-Solid Interface for Trace Proteomics Analysis	Gilbert Lee – Simon Fraser University
11:30 pm	HRMS Analysis of PBDE	Dave Hope – Pacific Rim Laboratories
12:00 pm	Lunch	Courtesy of ThermoFisher Scientific
	Session Chair: Brent Coates	
1:00 pm	Stability of Reactive Sulfur Species in Air Post Sampling	Brittany Orfino – Alberta Innovates - Technology Futures
1:30 pm	Some Highlights of the Recent Trace Organics Literature	Gerry Reimer
2:00 pm	Determination of POEA in Environmental Samples by LC-MS/MS	Andrew Ross - Fisheries and Oceans Canada
2:30 pm	Coffee Break: Posters & Exhibits	Courtesy of PromochromTechnologies
3:00 pm	Migrating from Helium to Hydrogen Carrier Gas in GC-MS Analysis of Volatile and Semi-Volatile Organic Compounds in Water	Alexander Semyonov – ThermoFisher Scientific
3:30 pm	Rapid general environmental unknown trace organic chemical detection and determination without method development - using single generic operating mode	Dayue Shang – Environment Canada
4:00 pm	Solvent-Free Sample Preparation for API and MALDI Mass Spectrometry	Yun Ling - UBC Chemistry
4:30 pm	Automated Aflatoxin and Ochratoxin Sample Clean-up and Analysis	David Mazawa – Pickering Laboratories

6:30 pm	Transportation to Vancouver Aquarium	Empire Landmark lobby
7:00 to 10:00 pm	Reception, Caledon Award Presentation and Dinner – Courtesy of WCTOW 2013 & Sponsors	Vancouver Aquarium
10:00 pm	Transportation available to Hotel	Vancouver Aquarium

WEDNESDAY, MAY 15, 2013

8:00 am to 9:00 am	Continental Breakfast	Courtesy of <i>Waters Ltd.</i>
Session Chair: Sime Buric		
9:00 am	Analysis of Oil Sands Processing Water Extracts by High Resolution MS	Nian Sun – University of Alberta
9:30 am	The fate of emerging contaminants in wastewater treatment plants	Michel Simhon - UBC Civil Engineering
10:00 am	Evaluation of Water Quality in Alberta's Irrigation Districts: Pesticides	Claudia Sheedy – Agriculture and Agri-food Canada
10:30 am	Coffee Break	Courtesy of <i>K'(Prime)Technologies</i>
11:00 am	Analysis of Naphthenic Acids in Water, Solids, and Tissues	Million Woudneh – AXYS Analytical Services
11:30 am	Automation from sample extraction to clean-up	Haibin Wan – Promochrom Technologies Ltd.
12:00 pm	Closing Remarks & 49 th WCTOW	Dave Hope
1:30 pm	<u>Special Presentation:</u> Applied Ion Analysis of various water matrices in Hydraulic Fracturing Process - Extended	Jay Gandhi Location To Be Determined

POSTER SESSION

POSTER SESSION

*Please note: It is requested that posters are removed from the hall at the end of **Day 2***

Francois Breton	A Method for the Analysis of Brominated Flame Retardants in Human Milk	Health Canada
Hongwen Chen & Colin Zhang	Chemical Characterization using NMR and MS at SFU	SFU Chemistry
Jaimie Duddridge	To Be Determined	CARO Analytical Services
Daniel Gaudet	Development of an iPCR methodology for the sensitive determination of livestock estrogens in water	Agriculture and Agri-food Canada
Blair Surridge	Determination of Pesticides in Fruits and Vegetables: A Comparison of Sample Preparation Techniques SPME and QuEChERS	Camosun College
Robert Taylor	To Be Determined	Waters Ltd
Haibin Wan	Benefits and challenges in reduction of particle size of SPE columns	PromoChrom Technologies Ltd.

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PRESENTATION ABSTRACTS

KEYNOTE PRESENTATIONS

David Chen – *Ultrasensitive, Automated Capillary Electrophoresis Mass Spectrometry for the Analysis of Organic Molecules in Complex Samples*

Charlie Schmidt – *Trace Organic Analysis in Seconds without Sample Prep*

The Direct Sample Analysis (DSA) ion source was developed for the analysis of solid, liquid and gas samples using PerkinElmer's patented "field free" Atmospheric Pressure Chemical Ionization-like (APCI) design. Coupling the DSA with the AxION 2 Time of Flight (TOF) mass spectrometer system enables a streamlined and simplified alternative workflow for a broad range of applications in the fields of environmental, forensics, food safety and pharmaceuticals. This state-of-the-art technology is used to provide elemental composition for unknowns and provides results of targeted analytes in seconds with without lengthy sample preparation, no expensive chromatography, nor complicated method development.

This presentation will cover how the integration of both DSA and TOF technologies provides a more productive and cost effective workflow in the trace organic laboratory. Applications covering the screening of pesticides and other trace level residues at low ppb concentrations in a number of food matrices, such as olive oil, orange juice and other food products will be discussed. Typical measurements performed with DSA/TOF took less than 30 seconds. Similar analyses with an LC/MS system would take 15-30 minutes. Screening with the DSA/TOF can increase sample throughput by a factor of 50-100 in comparison to other LC/MS systems. In addition, no (or limited) glassware, organic solvents, extraction devices were used with DSA and this greatly reduces the cost per sample when compared to a traditional LC/MS approach.

PRESENTATIONS

Jonathan Bailey – *Analysis of Neonicotinoid Pesticides in Water and Sediments*

Jonathan Beck – *Analysis of Complex Samples by Liquid Chromatography High Resolution Accurate Mass Spectrometry*

Jonathan Benskin – *Disposition of Per- and Polyfluoroalkyl Substances During Wastewater Treatment*

Jay Gandhi – *Applied Ion Analysis of Various Water Matrices in Hydraulic Fracturing Processes*

Hydraulic fracturing is the use of fluid and material to create or restore small fractures in a formation in order to stimulate production from new and existing oil and gas wells. This creates paths that increase the rate at which fluids can be produced from the reservoir formations.

The process includes steps to protect water supplies. To ensure that neither the fluid that will eventually be pumped through the well, nor the oil (or gas) that will eventually be collected enters the water supply, steel surface or intermediate casings are inserted into the well to depths of between 1,000 and 4,000 feet. Once the cement has set, then the drilling continues from the bottom of the surface or intermediate cemented steel casing to the next depth. This process is repeated, using smaller steel casings each time, until the oil and gas-bearing reservoir is reached (generally 6,000 to 10,000 ft).

Water and sand make up 98 - 99.5% of the fluid used in hydraulic fracturing. In addition, chemical additives such as acid solutions, scale inhibitors, stabilizing agents, corrosion inhibitors, friction reducing agents, gelling agents, etc. are used - exact formulation will vary depending on the well.

In this presentation, collaborative approach with USEPA to perform chemical analysis methodologies using ion analytical instruments will be discussed.

Maxine Haberl – *A Rapid Screening of Naphthenic Acids in Surface Water*

Marc Hamel – *A New, Single-pass, Automated Solid Phase Extraction Approach for Troublesome Waste Water Samples for Semi-Volatile Compounds*

Using solid phase extraction (SPE) for the broad range of semi-volatile organic compounds over conventional continuous liquid-liquid extraction (CLLE) and liquid-liquid extraction (LLE) techniques offers a substantial reduction in user interaction time, consumption of organic solvents as well as sample extraction time. Using a SPE disk with hydrophilic and hydrophobic interaction sites along with a carbon cartridge, a 1 liter sample containing various acidic basic and neutral SVOC compounds can be extracted in as little as 1.5 hours as compared to CLLE which can take up to 48 hours (24 hours for the acidified sample and 24 hours for the basified sample). LLE can be inconsistent due to human interactions along with troublesome emulsions.

In this presentation we introduce a novel SPE disk with multi-modal functionality for the automated processing of both high and low pH samples simultaneously. The precision data and percent recoveries of this method for complex water samples will be presented, along with how it is compared with traditional extraction techniques.

Coreen Hamilton – *Analysis of Low Concentrations of PAH and Alkyl PAH in Environmental Samples*

Davis Hasman – *Mass Spectral Study of Anti-cancer Polyactylenes in Devil's Club (Oplopanax Horridus); an important medicinal plant of the Pacific Northwest*

Allan Hendry – *Flexible Machined for Laboratory Automation*

Bernd O. Keller – *Interactions of Transition Metal Ions with Organophosphorus Pesticides Probed by Electropray Ionisation Mass Spectrometry*

Patrice Lemire – *To Be Determined*

Andrew Lewis – *Chemical Characterization using NMR and MS at SFU*

Yun Ling – *Solvent-Free Sample Preparation for API and MALDI Mass Spectrometry*

Julie Marr – *High Throughput Analysis of Contaminants in Drinking Water or Waste Water with Integrated Sample Clean-up and Spectral Confirmation*

Brittany Orfino – *Stability of Reactive Sulfur Species in Air Post Sampling*

Gerry Reimer – *Some Highlights of the Recent Trace Organics Literature*

This talk will present a brief review of the recent trace organics literature with a focus on chromatographic GC and LC methods. The talk will focus on advances in solid-phase microextraction (SPME), direct-inject LC-MS methods and online-SPE-LC-MS methods.

Andrew Ross – *Determination of POEA in Environmental Samples by LC/MS-MS*

Alexander Semyonov – *To Be Determined*

Dayue Shang – *Rapid General Environmental Unknown Trace Organic Chemical Detection and Determination without Method Development – using Single Generic Operating Mode*

Claudia Sheedy – *Evaluation of Water Quality in Alberta's Irrigation Districts: Pesticides*

Michel Simhon – *The Fate of Emerging Contaminants in Wastewater Treatment Plants*

Nian Sun – *Analysis of Oil Sands Processing Water Extracts by High Resolution MS*

Oil sand industry in Alberta has been one of the fast growing industries in the past decade in Canada. To extract crude oil from the oil sand, huge amount of water is needed and thus the process results in the production of oil sands process-affected water (OSPW). OSPW is considered to be dangerous to local environmental and ecological system due to its high content of toxic constituents such as naphthenic acids (NAs) and polycyclic aromatic hydrocarbons (PAHs). It is desirable to be able to degrade the toxic constituents and monitor the degradation process by estimating the level of NAs or PAHs in OSPW, which has raised analytical challenges since OSPW is a very complex matrix that often associates with suspended solids, high concentration of inorganic salts and carbonates. Extraction and fractionation of OSPW can sufficiently reduce its complexity by separating organic species into different portions based on their physical and structural properties. In the work presented here various organic solvents were used to extract OSPW at different pH values. Each organic fraction and its counterpart water residue were analyzed by SYNAPT G2 High Resolution Mass Spectrometer (HRMS) and the concentrations (mg/L) of both classic NAs and oxydized NAs were estimated for each sample. Fluorescence spectrometry was used to check the presence of PAHs. It was found out that both solvent polarity and sample pH values have significant impacts on how the analytes were extracted from raw OSPW and fractioned into small portions.

Haibin Wan – *Automation from Sample Extraction to Clean-up*

Xiaomeng Wang – *Determination of Thermodynamic and Transport Parameters of Naphthenic Acids and Organic Process Chemicals in Oil Sand Tailing Pond Water*

Oil sand tailings pond water contains naphthenic acids and process chemicals. These chemicals are toxic and can seep through the foundation of the tailings pond to the subsurface, potentially affecting the quality of groundwater. As a result, it is important to measure the thermodynamic and transport parameters of these chemicals in order to study the transport behavior of contaminants through the foundation as well as underground. In this study, batch adsorption studies and column experiments were performed. It was found that the transport parameters of these chemicals are related to their molecular structures and other properties. The computer program (CXTFIT) was used to further evaluate the transport process in the column experiments. The results from this study show that the transport of naphthenic acids in a glass column is an equilibrium process while the transport of process chemicals seems to be a non-equilibrium process.

Million Woudneh – *Analysis of Naphthenic Acids in Water, Solids, and Tissues*