19th Annual Workshop on Emerging HRMS & LC-MS/MS Applications in Environmental Analysis & Food Safety

Sept 24-25, 2023 Center for Tomorrow, University at Buffalo Buffalo, NY

KEYNOTE SPEAKERS

Elin Ulrich
U.S. Environmental Protection Agency
Taming the wild west of NTA: Advancement of Tools & Applications

Rainer Lohmann
University of Rhode Island
Chasing the elusive POPs in water and air

INVITED SPEAKERS

Erin Baker
UNC at Chapel Hill

Damià Barceló Cullerès
ICRA & IDAEA-CSIC Barcelona

Karl Jobst
Mem. University of Newfoundland

Sébastien Sauvé
University of Montréal

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To attend, PLEASE REGISTER BY AUGUST 18.

https://www.buffalo.edu/renew/2023-LCMS-Workshop.html.

University at Buffalo
Research and Education in eNergy, Environment and Water (RENEW)

WORKSHOP AGENDA

Saturday, Sept 23

Preconference trip: Shuttle service to Niagara Falls State Park
Shuttle departs at 11 am or 1 pm from the Center for Tomorrow

Sunday, Sept 24

8:00 am–8:30 am	Registration and refreshments	
8:30 am–8:40 am	Introductory remarks	**Diana Aga, Ph.D.** Scientific Committee Chair

Session 1a: Advancing non-target analysis through cheminformatics

8:40 am–9:10 am	**Keynote-**Taming the wild west of NTA: Advancement of tools & applications	**Elin Ulrich, Ph.D.** U.S Environmental Protection Agency
9:10 am–9:30 am	Applications of recent NTS approaches for PFAS in environmental samples	**Christian Zweiner, Ph.D.** University of Tübingen
9:30 am–9:50 am	Using quantum chemical calculations to estimate physicochemical properties of PFAS	**Scott Simpson, Ph.D.** St. Bonaventure University
9:50 am–10:10 am	Toward quantification without standards: impacts of environmental matrices on the solubilities and ionization efficiencies of per- and polyfluoroalkyl substances (PFAS)	**Shirley Pu** U.S Environmental Protection Agency
10:10 am–10:30 am	Refreshment break	

Session 1b: HRMS and LC-MS/MS applications in wastewater and drinking water-related research

10:30 am–11:00 am	LC-Orbitrap and MALDI TOF-HRMS in wastewater-based epidemiology for the determination of small and large molecules as biomarkers of exposure	**Damià Barceló Cullerès, Ph.D.** ICRA & IDAEA-CSIC Barcelona
11:00 am–11:20 am	Analytical challenges and alternatives for monitoring opioid consumption in communities using wastewater-based epidemiology	**Arjun Venkatesan, Ph.D.** New Jersey Institute of Technology
11:20 am–11:40 am	Tandem mass tag-based quantitative proteomic analysis of viral protein reactivities with free chlorine	**Chonglin Zhu** University at Buffalo
11:40 am–12:00 pm	Viral nucleic acid research: a mass spectrometry approach	**Alex Szczuka, Ph.D.** University of Michigan
12:00 pm–1:10 pm	Lunch break	

WORKSHOP AGENDA

Sunday, Sept 24 (cont.)

Session 1c: More about PFAS

1:10 pm–1:40 pm	PFAS – where are we now?	**Sébastien Sauvé, Ph.D.** University of Montréal
1:40 pm–2:00 pm	Overview of PFAS in South Florida aquatic environments: what we know so far and major gaps	**Natalia Soares Quinete, Ph.D.** Florida International University
2:00 pm–2:20 pm	The future of PFAS analysis: what advances are we making to support routine LC-MS/MS?	**Frank Dorman, Ph.D.** Waters Corporation, Penn State University
2:20 pm–2:40 pm	Understanding and troubleshooting the front end of PFAS analysis	**Charles Powley, Ph.D.** Center for PFAS Solutions
2:40 pm–3:00 pm	Refreshment break	

Session 1d: Applications in food analysis and more!

3:00 pm–3:20 pm	Identification of chemical markers for honey botanical origin analysis	**Tian Lei** McGill University
3:20 pm–3:40 pm	Targeted and nontargeted screening of per- and polyfluoroalkyl substances (PFAS) in food contact materials using the X500R QTOF system	**Holly Lee, Ph.D.** SCIEX, Canada
3:40 pm–4:00 pm	Comparison of different strategies based on LC-MS/MS analysis to establish the chemical profiles of floral nectars and support honey authenticity testing	**Stéphane Bayen, Ph.D.** McGill University
4:00 pm–4:20 pm	Instrumentation for environmental analysis	**William Flannery** GenTech Scientific, LCC
4:30 pm–6:30 pm	Wine & cheese reception and poster session Sponsored by GENTECH SCIENTIFIC	

WORKSHOP AGENDA

Monday, Sept 25

8:00 am–8:25 am	Registration and refreshments	
8:25 am–8:30 am	Introductory remarks	**Diana Aga, Ph.D.** Scientific Committee Chair

Session 2a: Advances in sample preparation and analysis

8:30 am–9:00 am	**Keynote-**Chasing the elusive POPs in water and air	**Rainer Lohman, Ph.D.** University of Rhode Island
9:00 am–9:20 am	High performance direct MS facilitated by SPME probe	**Janusz Pawliszyn** University of Waterloo
9:20 am–9:40 am	Analysis of complex samples via biocompatible solid-phase microextraction and laminar flow tandem mass spectrometry	**Emanuela Gionfriddo, Ph.D.** The University of Toledo
9:40 am–10:00 am	High throughput and automated solid-phase microextraction blades system and its application in environmental water analysis	**Wei Zhou, Ph.D.** University of Waterloo
10:00 am–10:20 am	Refreshment break	

Session 2b: Applications of ion mobility spectrometry and HRMS in non-target analysis

10:20 am–10:50 am	Using ion mobility spectrometry to identify unknowns in non-targeted analyses	**Erin Baker, Ph.D.** UNC at Chapel Hill
10:50 am–11:10 am	Ion mobility filtering for non-targeted analysis of PFAS from environmental samples collected at a ski resort	**Sarah Dowd, Ph.D.** Waters Corporation
11:10 am–11:30 am	From PFAS dark matter to cannabis conundrums: A 13-meter high-resolution ion mobility journey to revealing the unseen	**Frederick Strathmann, Ph.D.** MOBILion Systems
11:30 am–11:50 am	Formation of N-nitroso derivatives from secondary-amine containing pharmaceuticals upon chloramination	**Changcheng Pu** Syracuse University
11:50 am–1:00 pm	Lunch break	

WORKSHOP AGENDA

Monday, Sept 25 (cont.)

Session 2c: Analysis and treatment of emerging contaminants

1:00 pm-1:30 pm	Cyclic ion mobility mass spectrometry: a novel platform that can reveal emerging pollutants	**Karl Jobst, Ph.D.** Memorial University of Newfoundland and Labrador
1:30 pm-1:50 pm	The unusual suspects: screening for persistent, mobile, and toxic plastic additives in common plastic products	**Eric Fries** Toronto Metropolitan University
1:50 pm-2:10 pm	Detection of PFAS using LC-HRMS with ^{19}F-NMR and their capture using a self-assembling zirconium-based metal-organic cage	**Dino Camdzic** University at Buffalo
2:10 pm-2:30 pm	Designing ultraporous mesostructured silica nanoparticles for the remediation of per- and polyfluoroalkyl substances	**Cheng-Hsin Huang** University of Minnesota
2:30 pm–2:50 pm	Refreshment break	

Session 2d: Beyond typical applications of LC-MS/MS

2:50 pm-3:10 pm	Microwave-enabled ionization and chemistries for mass spectrometry analysis	**Steven Ray, Ph.D.** University at Buffalo
3:10 pm-3:30 pm	Monitoring spatial and temporal variation in the chemical composition of the Ohio River using non-target analysis	**Stefanie Landeweer** Florida International University
3:30 pm-3:50 pm	In-depth chemical analysis and exposure assessment of crumb rubbers in artificial turf	**Madison McMinn** Northeastern University
3:50 pm-4:10 pm	Analysis of bisphenol A and other related contaminants in human milk using LC-Q-ToF-MS	**Zhi Hao Chi** McGill University
4:10 pm-4:30 pm	Closing remarks and presentation awards	**Diana Aga, Ph.D.** Scientific Committee Chair
5:30 pm-8:30 pm	**Group dinner and networking event:** location to be announced (Paid by individual; RSVP here)	

POSTERS

P1: Direct photoreactions in extracellular antibiotic resistance genes on surfaces

Asad Aziz

P2: Assessing antibiotic occurrence and environmental dissemination in manures and surrounding agroecosystems

Damalka Balasuriya

P3: Comparison of quantitation of total PFAS including trifluoroacetic acid with total oxidizable precursor assay, LC-HRMS, and 19F-NMR

Dino Camdzic

P4: In vitro effects of per- and polyfluorinated alkyl substances (PFAS) on the cellular lipidome in retinoic acid (RA)-induced differentiated SH-SY5Y neuroblastoma cells

Michelle Camdzic

P5: Assessment of emerging organic contaminants in soil samples from Miami-FL

Luciana Cappelini, Ph.D.

P6: Investigating potential sources of phosphorous to the groundwater in Miami-Dade County using specific chemical tracers and non-target analysis

Milena Ceccopieri

P7: Assessment of per- and polyfluoroalkyl substances (PFAS) in tap waters from Miami-Dade, South Florida

Carolina Cuchimaque

P8: Passive sampling for the detection of persistent, mobile, and toxic (PMT) substances in Canadian waters

Ericka De Oliveira

P9: Complementary targeted, suspect screening, and total analysis for per- and polyfluoroalkyl substances (PFAS) in source and receptor samples using LC-MS/MS, SFC-MS, CIC, and 19F-NMR

Dulan Edirinsinghe, Karla Ríos Bonilla

P10: Monitoring of poly- and perfluoroalkyls substances (PFAS) in rainwater from Miami-Dade, South Florida

Maria Guerra de Navarro

POSTERS

P11: Target analysis of per- and polyfluoroalkyl substances (PFAS) in surface water from Biscayne Bay canals and the Everglades
Courtney Heath

P12: Anilines are Potent Precursors to Haloacetonitriles and other small-molecule disinfection byproducts
Zachary Kralles

P13: First-time report on elasmobranch contamination by per- and polyfluoroalkyl substances in the Southeastern Atlantic
Leila S. Lemos, Ph.D.

P14: Non-targeted screening of novel Per-and polyfluoroalkyl substances (PFAS) in recreational fish and crustaceans using High resolution mass spectrometry (HRMS)
Olutobi Ogunbiyi

P15: Development of sample extraction and cleanup methods for targeted PFAS analysis in environmental and biological matrices
Arundhati Tewari

P16: Quantification of PFAS in phytoremediation studies
Sara Thomas, Ph.D.

P17: Using chemical tracers for phosphorus source apportioning in the tributaries of Biscayne Bay, Florida
Kassidy Troxell

P18: Inclusion of montmorillonite clays in barrier cream formulations to reduce skin exposure to water-soluble chemicals from polluted water
Meichen Wang

P19: Assessing PFAS levels in treated municipal biosolids and human blood: an analytical approach
Mindula Wijayahena

P20: Characterization of wastewater effluents by liquid chromatography-high resolution mass spectrometry and evaluation of wastewater reuse for plant growth
Jingyi Zhou, Ph.D.

SPEAKER BIOS

Baker, Erin

https://chem.unc.edu

Dr. Baker is associate professor at the Chemistry Department at University of North Carolina, Chapel Hill, with research focusing on how the environment affects human health. Her group is developing new analytical and computational approaches for measurements of xenobiotics and endogenous metabolites. This work uses various combinations of separation methods including automated solid-phase extractions, liquid chromatography, supercritical fluid chromatography, ion mobility spectrometry and mass spectrometry.

Barceló Cullerès, Damià

https://www.idaea.csic.es

Dr. Barceló is a Professor at IDAEA-CSIC, Spain, and has been the Director of the Catalan Institute for Water Research (ICRA) since 2008. His expertise is in the analysis, fate, risk, and removal of emerging contaminants and microplastics from water. Barceló serves as co-Editor-in-Chief of the Science of the Total Environment, Editor-in-Chief of Current Opinion in Environmental Science and Health, and Co-Editor-in-Chief of Case Studies of Chemical and Environmental Engineering, Elsevier.

Jobst, Karl

https://www.mun.ca

Dr. Jobst is an Assistant Professor in the Department of Chemistry at Memorial University of Newfoundland and Labrador. He holds a Ph.D. in gas-phase ion chemistry from McMaster University. His current research focuses on identifying emerging contaminants and their environmental and human health impacts using advanced mass spectrometry and computational methods. Dr. Jobst currently serves on the editorial board of Current Opinion in Environmental Science & Health.

Lohmann, Rainer

https://web.uri.edu

Dr. Lohmann is a Professor of Oceanography at the University of Rhode Island's Graduate School of Oceanography. His research focuses on transport, fate, and bioavailability of recalcitrant organic compounds, such as PFAS and other persistent organic pollutants. He is involved in the development and application of passive sampling of organic compounds in the environment, and is studying the biogeochemistry of black carbon in atmosphere, oceans and sediment, and effects on the carbon cycle.

SPEAKER BIOS

Sauvé, Sébastien

https://chimie.umontreal.ca

Dr. Sauvé is an Associate Dean of Research and Creation and a full professor in Environmental Chemistry at the Université de Montréal. His expertise is in water and soil science, environmental chemistry, analytical techniques of mass spectrometry, and the impacts of emerging contaminants on health and the environment. He is also interested in studying the mobility and bioavailability of "traditional" contaminants like lead and cadmium, and compounds of emerging interest, like drugs and cyanotoxins.

Ulrich, Elin

https://www.researchgate.net

Dr. Ulrich is a Research Chemist at the EPA's National Exposure Research Laboratory. Her research interests focuses on developing methods and tools for non-targeted analysis to more rapidly sequence the exposome. In 2018, she organized a workshop with participants from "EPA's Non-Targeted Collaborative Trial (ENTACT)", which lead to the creation of the Best Practices for Non-Targeted Analysis (BP4NTA) working group, which addresses challenges in non-targeted analysis using mass spectrometry.

SCIENTIFIC COMMITTEE

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Joshua Wallace, Ph.D., J.D.
University at Buffalo, USA

Andrzej Wnorowski, Ph.D.
Environment and Climate Change Canada, Canada

DIRECTIONS

Driving Directions from Buffalo Niagara Airport (~12-minute drive)

- Exit the airport following the signs leading to Route 33 West toward Buffalo.
- Take Route 33 West to the I-90 East I-290 West, Niagara Falls Albany exit.
- Take the I-290 West toward Niagara Falls, exit 50.
- Take Exit 5B (Millersport Highway North, Route 263).
- Merge to the left lane. Make left onto Flint Road (by the Marriott Hotel).
- Continue on Flint Road to Service Center Road. Make left onto Service Center Road.
- The entrance for the Center for Tomorrow is on the left and free parking is on the right.

Directions from DoubleTree Hotel (< 10-minute walk)

- From the main hotel entrance turn left and head east to Flint Road.
- Turn left (north) on to Flint Road and cross Maple Road.
- Continue on Flint Road to Service Center Road. Make left onto Service Center Road.
- The entrance for the Center for Tomorrow is on the left and free parking is on the right.

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