

# ADVANCING ANALYSIS OF HALOGENATED AND NITROGENOUS CONTAMINANTS IN WATER

Speaker

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## Abstract

Water disinfection effectively prevents microbial infections, but it inevitably produces disinfection byproducts (DBPs). To date, halogenated DBPs largely remain unidentified, although 50 years of research has significantly improved water quality. Nontargeted high-resolution mass spectrometry (HRMS) analysis of water detects large datasets of chemical features, but structural annotation is a bottleneck in advancing DBP identification. To address this challenge, we have developed two machine learning-guided platforms, HalogenFinder and IodoFinder, to automatically recognize Cl-, Br-, and I-containing compounds in LC-HRMS nontargeted analysis datasets. HalogenFinder employs hierarchical Random Forest models trained on simulated isotope patterns from 1.3 million PubChem molecular formulas, achieving 95% accuracy in identification of Cl/Br-compounds and number of halogen atoms in a chemical feature. IodoFinder leverages diagnostic fragmentation features from 6,000 MS/MS spectra of 381 iodinated compounds, reaching 96.5% and 100% accuracy in positive and negative ionization modes, respectively. HalogenFinder and IodoFinder were validated using authentic standards (277 Cl/Br-compounds; 161 I-compounds) and applied to real water samples and DBP mixtures. These tools revealed novel halogenated DBPs. Additionally, isotope labeling combined with HDPairFinder enabled identification of reactive nitrogenous precursors in source water. Together, these platforms offer high-throughput, accurate, and accessible solutions for comprehensively identifying halogenated contaminants and reactive precursors in water, enabling exposomic studies of water contaminants.

## Biography

Dr. Xing-Fang Li is Professor in the Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry at the University of Alberta. She is Canada Research Chair (Tier 1) in Analytical and Environmental Toxicology and an elected Fellow of the Royal Society of Canada, Academy of Science.

Dr. Li's research group develops innovative analytical and molecular techniques that enable ultrasensitive detection of environmental contaminants, microbial pathogens, and biomolecular interactions. Dr. Li is the recipient of the 2020 Ricardo Aroca Award for "a distinguished contribution to the field of analytical chemistry", the 2017 Environment Research & Development Dima Award for "distinguished contributions to research and/or development in the fields of environmental chemistry", and the 2010 W.A.E. McBryde Medal for "a significant achievement in pure or applied analytical chemistry", from the Canadian Society for Chemistry and the Chemical Institute of Canada. Dr. Li has also received the Excellence in Mentoring Award (2014) and Killam Annual Professorship (2013) from the University of Alberta.

Dr. Li currently serves as an Associate Editor for ACS Environmental Au (American Chemical Society) and Editorial Board Member for ACS journals Analytical Chemistry, Environmental Science and Technology, Environment and Health, ACS ES&T Water.



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**Room 3574 (Lift 27/28)  
Civil Engineering  
Conference Room**

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