

# Department of Food Science & Agricultural Chemistry

## Mass Spectrometry Seminar

December 3<sup>rd</sup> 2019, 12-1 PM

Raymond Building 3-045

***Non-targeted screening of halogenated contaminants in environmental and food matrices based on isotopic pattern and mass defect provided by high resolution mass spectrometry profiling: application of the user-friendly HaloSeeker software***

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**ABSTRACT:** Identifying environmental chemical contaminant mixtures in environmental and food matrixes is a major scientific undertaking supporting environmental and health risk assessment. Halogenated contaminants are of particular concern due to their persistence in environment and their potential of bioaccumulation and toxicity. A wide range of halogenated chemicals may be present in environment and food including historical and emerging chemicals, alternatives to legacy contaminants, degradation products, non-intentionally produced compounds. The current targeted analytical methods for characterizing trace contaminants in complex matrixes are highly selective and sensitive but do not cover the full range of existing substances, particularly unknown chemicals. Over the last two decades, non-targeted screening strategies based on High Resolution Mass Spectrometry (HRMS) profiling have been developed to extend the chemical characterization to unsuspected and unknown chemicals. However, since HRMS full-scan mode generate huge data sets, post-acquisition steps are challenging and require specific and complex bioinformatics tools for rapid and efficient review of the signals of interest. In this seminar, I will present a recent all-in-one user-friendly application, HaloSeeker 1.0, developed to promote the accessibility of associated in-house bioinformatics tools to a large audience. This software aims to facilitate the identification of chlorinated and brominated halogenated chemicals in non-targeted HRMS data sets based on isotopic profile and mass defect. Three major applications will be presented to highlight the strengths of this approach.



**BIO:** Caroline Simonnet-Laprade received her Ph.D. in environmental and analytical chemistry from the University of Bordeaux (Talence, France) in 2017. Her PhD studies aimed to investigate the origin, the fate and the trophic transfer of poly- and perfluoroalkyl substances (PFASs) in aquatic ecosystems. She is currently doing an international post-doc at LABERCA (Nantes, France), the French National Reference Laboratory for the analysis of chemicals in food, in collaboration with Dr Bayen from McGill University (Food Science department). Her current research focuses on the characterization of chemical contamination of fish samples using complementary targeted and non-targeted analytical methods based on chromatography-mass spectrometry analysis.