Unravelling Disinfection Byproducts in Chlorinated and Chloraminated Drinking Water

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Funding Grants: Susan D. Richardson (DMR-1644779; ASPIRE); Huiyu Dong (NSFC, 52070184, 52270012); Gregory S. Boebinger (DMR-2128556)

Identification of unknown disinfection byproducts (DBPs), especially unknown drivers of toxicity, is one of the major challenges in the supply of safe drinking water. The ultrahigh mass-resolving power and mass accuracy of the MagLab's 21 tesla Fourier Transform Ion-Cyclotron Resonance Mass Spectrometry (FT-ICR MS) provides confident assignments of elemental compositions to tens of thousands of unique disinfection byproducts.

This collaboration of MagLab users employed an effect-directed analysis protocol based on *in vitro* bioassays to identify unknown DBPs in drinking water. *Using the MagLab's 21T FT-ICR MS, researchers identified 3599 chlorine-containing DBP formulas in the toxic molecular weight fraction (i.e. molecular weights < 1 kiloDalton) of chlorinated and chloraminated water. This represents an increase that is more than tenfold higher than earlier studies that used lower magnetic field (7T to 15T) instruments.* Furthermore, the high resolution of 21T FT-ICR MS enabled the researchers to discern low-abundance ^{37}Cl-containing DBPs, which improves the accuracy of DBP formula assignments through isotope pattern matching (see Figure).

The researchers combined toxicity analysis with the 21T FT-ICR-MS chemical analysis to determine the toxicity drivers within the high-molecular-weight DBPs in drinking water. Future work will target these molecules for structural analysis.

Facilities and instrumentation used: ICR Facility: 21 T hybrid linear ion trap FT-ICR MS.

Citation: Dong, H.; Cuthbertson, A.A.; Plewa, M.; Weisbrod, C.; McKenna, A.M.; Richardson, S.D., *Unravelling High-Molecular-Weight DBP Toxicity Drivers in Chlorinated and Chloraminated Drinking Water: Effect-Directed Analysis of Molecular Weight Fractions,* **Environmental Science and Technology** (2023) doi.org/10.1021/acs.est.3c00771

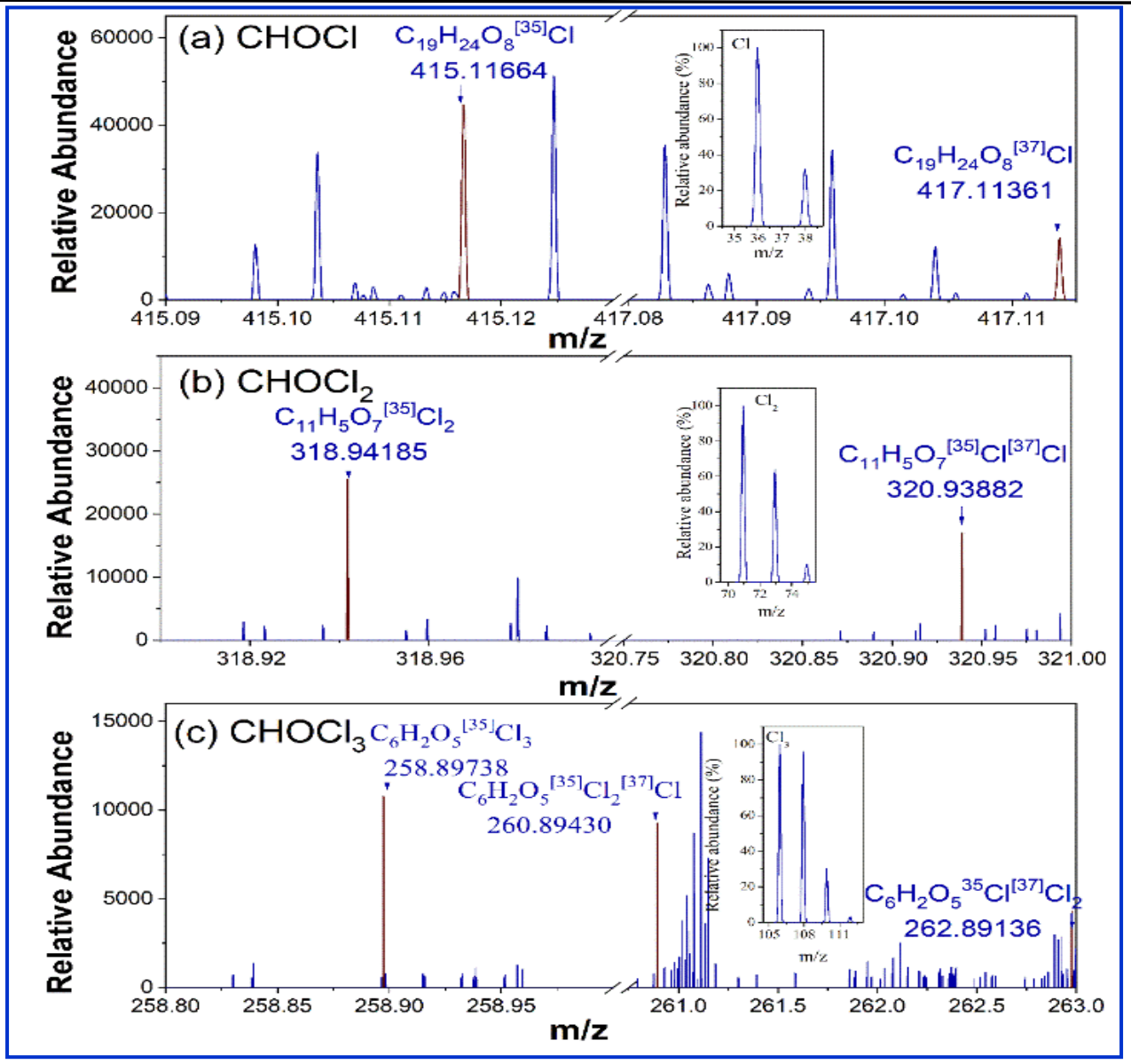

Figure: Representative DBP molecular formula identifications for a molecule that contains (a) one, (b) two, and (c) three chlorine atoms. Confident assignment requires the ultrahigh mass resolving power and mass accuracy provided by 21T FT-ICR MS.

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What is the finding? *MagLab users identified 3599 chlorine-containing disinfection byproducts (DPB's) in the most toxic fraction (i.e. molecular weights < 1 kiloDalton) of drinking water treated by chlorination and chloramination*. These DBPs have empirical formulas that contain one (CHOCl), two ($CHOCl_2$) or three ($CHOCl_3$) chlorine atoms per molecule, with a relative abundance order of Cl_1 > Cl_2 >> Cl_3. Strikingly, chloraminated water contains a higher number of chlorine-containing high-molecular-weight DPBs than chlorinated water.

Why is this important? Disinfection byproducts are associated with adverse health effects, including reproductive and developmental impacts as well as cancer. However, the toxicity-driven unknown DBPs remain poorly understood. Due to lack of chemical standards, it is difficult to assess the toxicity contribution of identified DBPs by high resolution mass spectrometry, as the resolving power requirements to identify these compounds exceeds lower-magnetic-field instruments. Performing *in vitro* bioassays prior to analysis in the MagLab's 21T Fourier Transform – Ion Cyclotron Resonance (FT-ICR) mass spectrometer enabled the discovery of 3599 chlorine-containing DBPs in the toxic fraction of drinking water. *This provides a candidate list for verifying the specific toxicity drivers in disinfected water*.

Why did this research need the MagLab? *The MagLab's unique 21T FT-ICR mass spectrometer leverages the mass measurement accuracy and precision achievable at using 21 tesla magnetic fields to provide world-leading mass-resolving power that enables determination of toxic DPB species in drinking water that contain one, two, or three chlorines per molecule*.

Facilities and instrumentation used: ICR Facility: 21 T hybrid linear ion trap FT-ICR MS.

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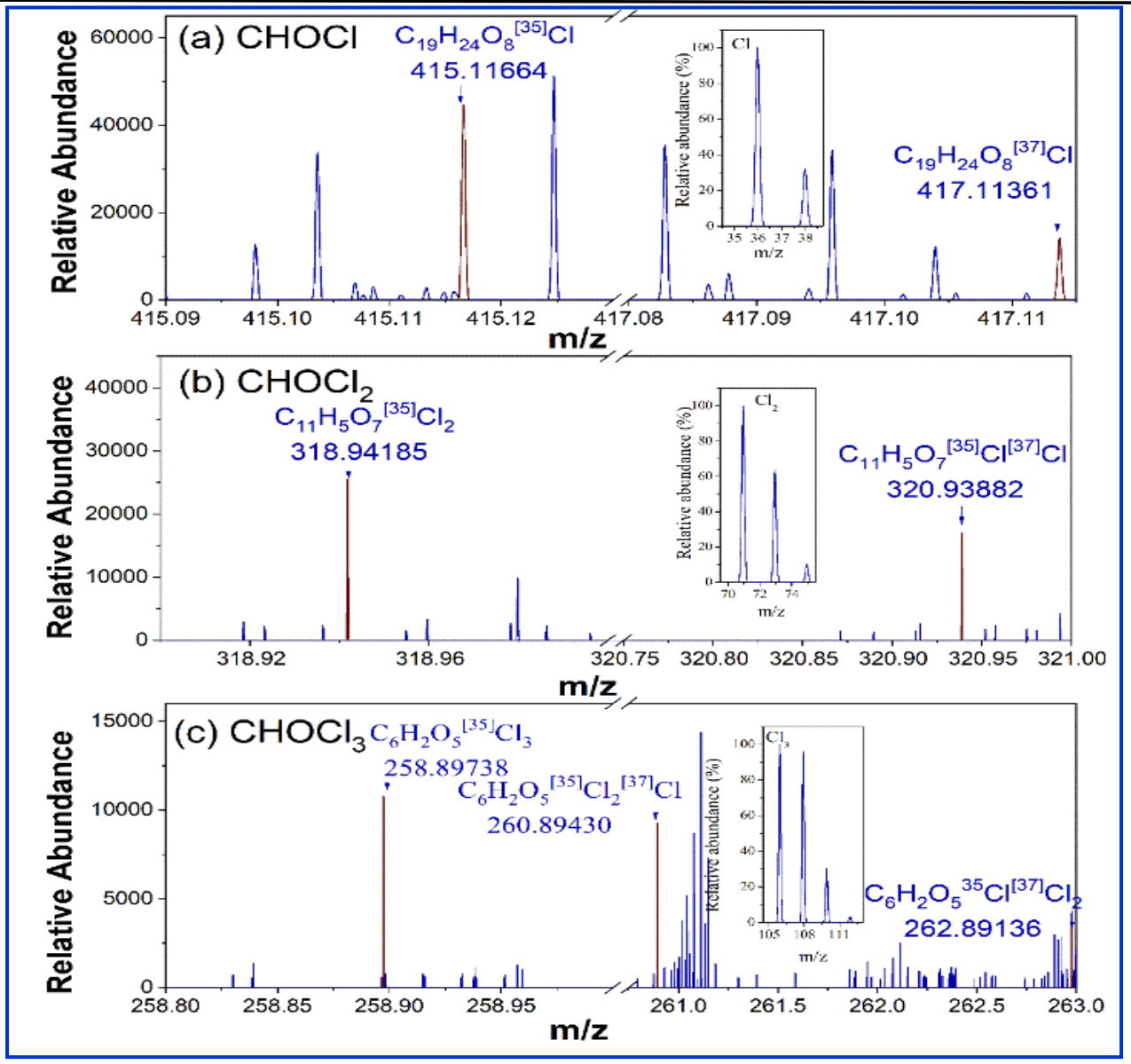

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