Unravelling Disinfection Byproducts in Chlorinated and Chloraminated Drinking Water

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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.

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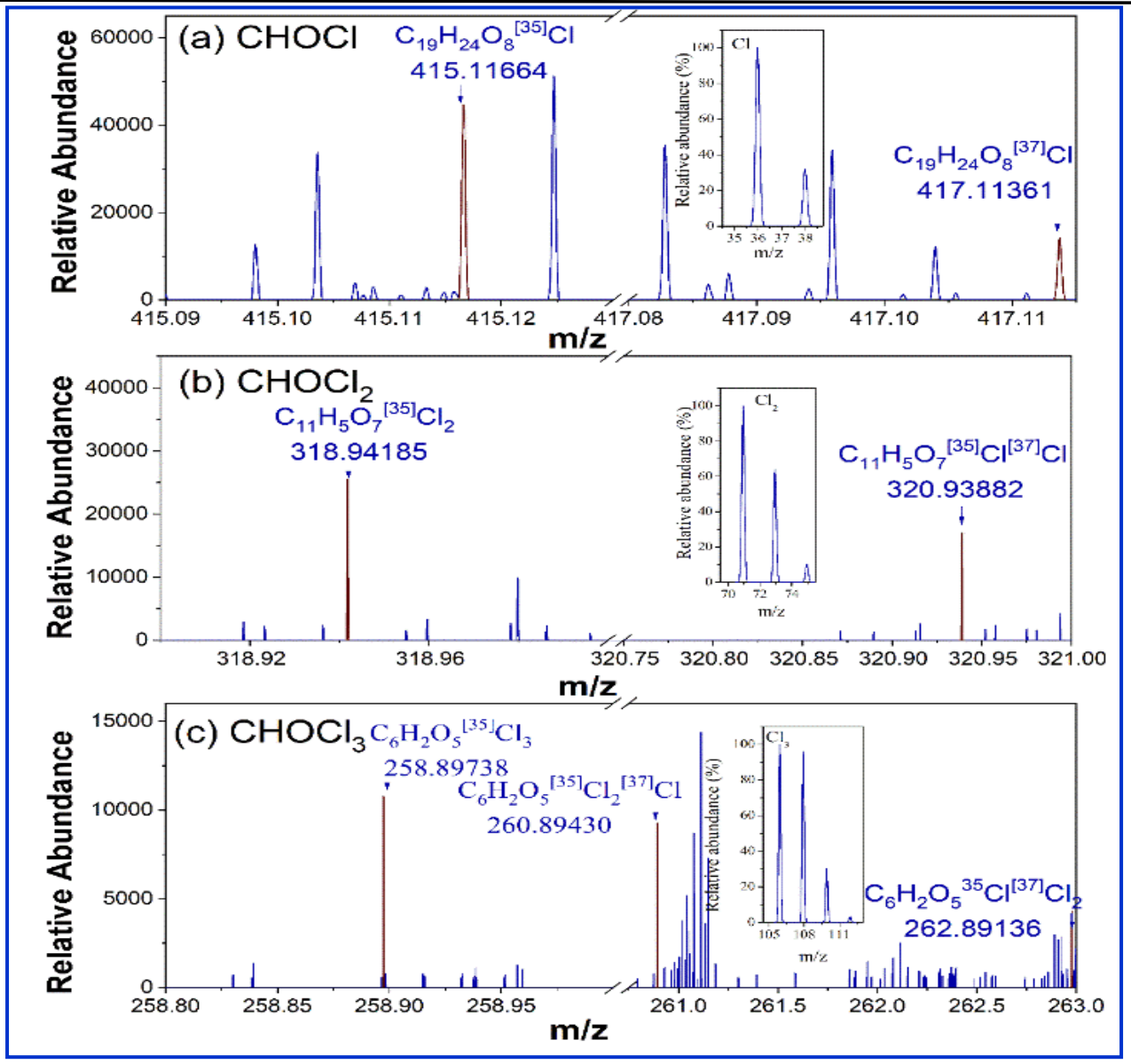

Figure: Representative DBP molecular formula identifications for a molecule that contains (a) one, (b) two, and (c) three chlorine atoms. Confident assignment requires the ultrahigh mass resolving power and mass accuracy provided by 21T FT-ICR MS.