

Challenges in the Identification of New Toxic Iodinated Disinfection By-Products Using Mass Spectrometry

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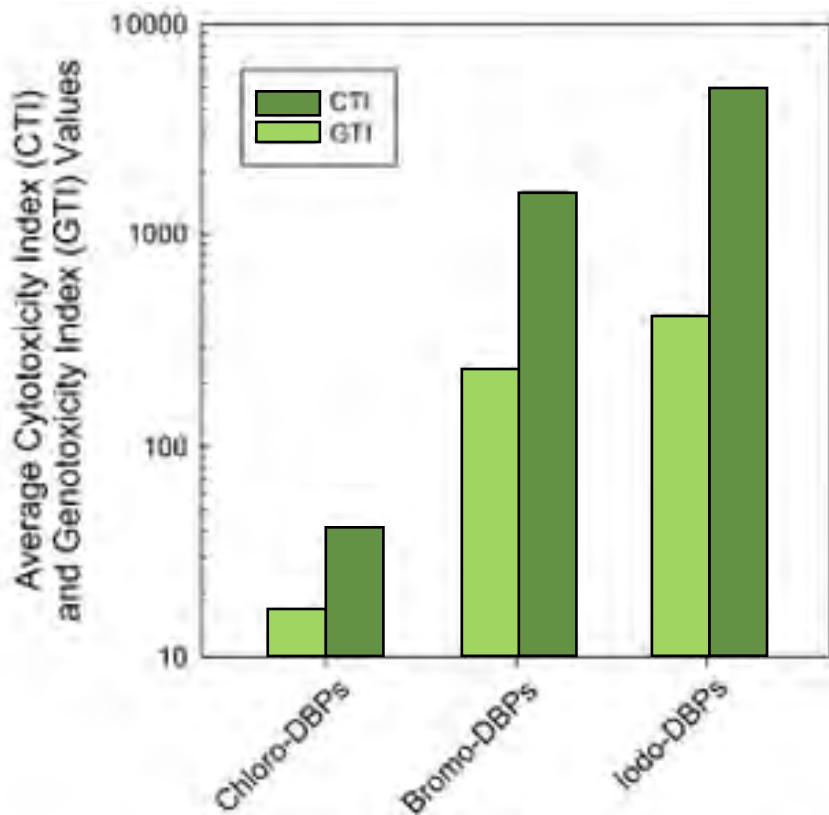
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Disinfection By-Products (DBPs)

NOM
+ Br⁻/I⁻

DISINFECTANT

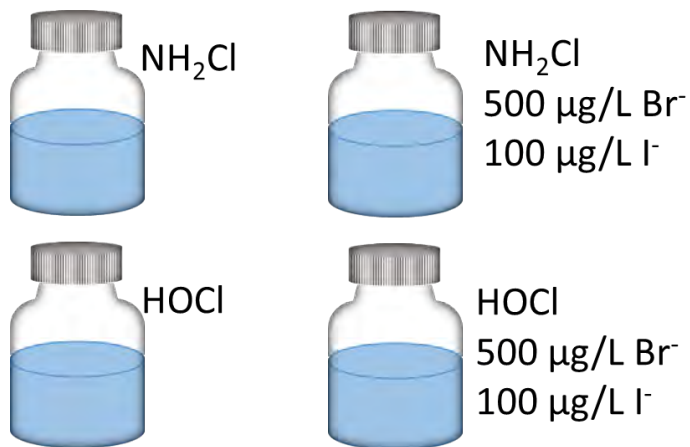
Bromo/Iodo-
DBPs



Halogenated DBP
Relative Toxicity:

I > Br >> Cl

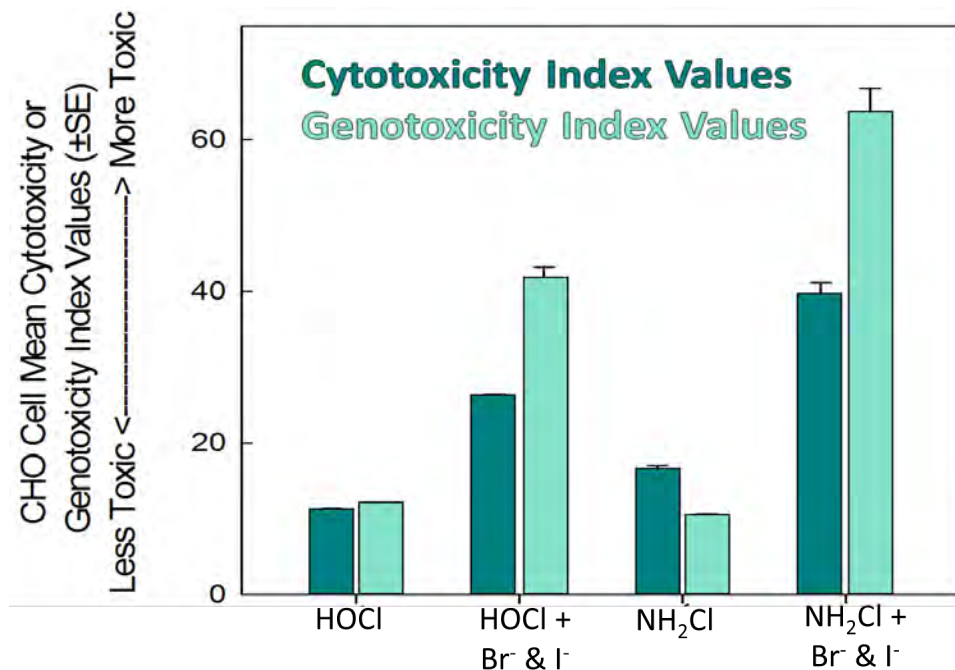
Disinfection Scenarios Investigated:



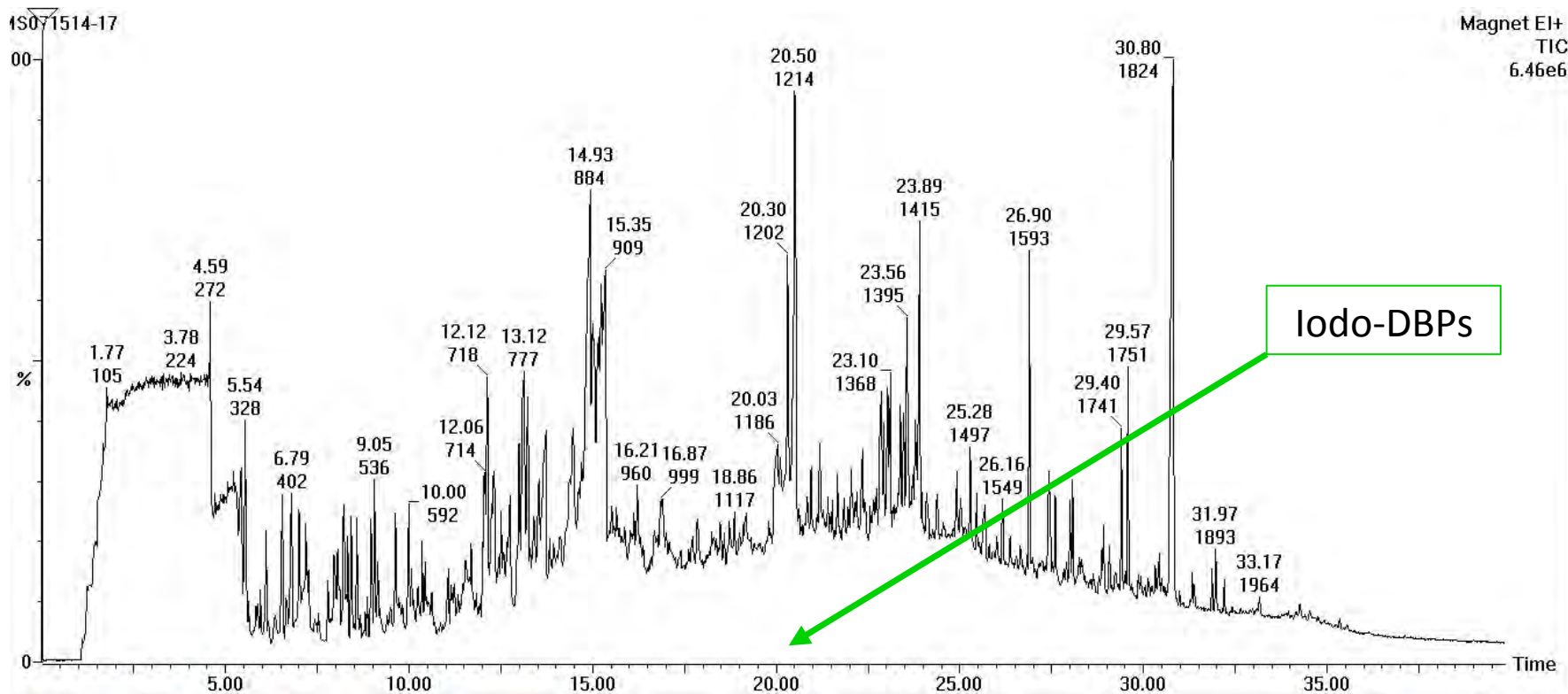
Toxicity of both disinfection processes increased with the addition of bromide and iodide

Chloraminated water with **Br⁻** and **I⁻** spike was the most toxic of the scenarios tested

High and low resolution GC/MS used to identify DBPs contributing to this elevated toxicity



Finding a Needle in a Haystack: DBP Identification By GC/MS



> 1000 compounds per sample – most unidentified

Toxic Iodo-DBPs of particular concern

Challenges of Iodo-DBP Identification

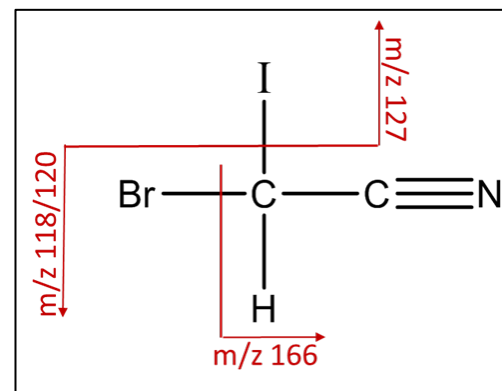
- Not many iodo-DBPs have been identified
- No telltale isotopic patterns indicating iodine
- XIC m/z 127 – I^+ fragment
- 127 not unique to I-containing compounds

Solution: High resolution & accurate mass

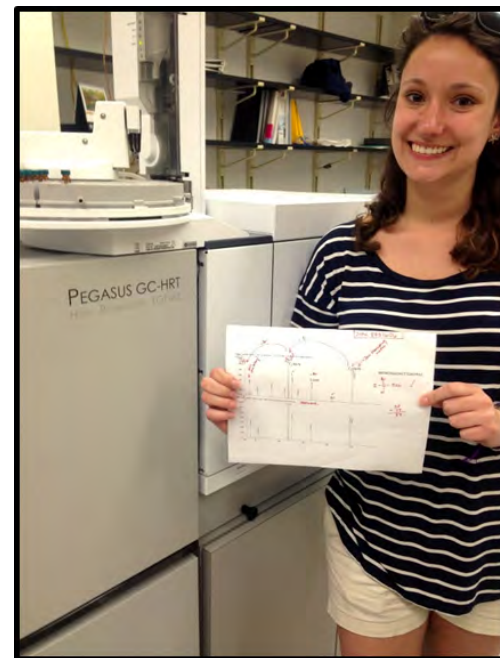
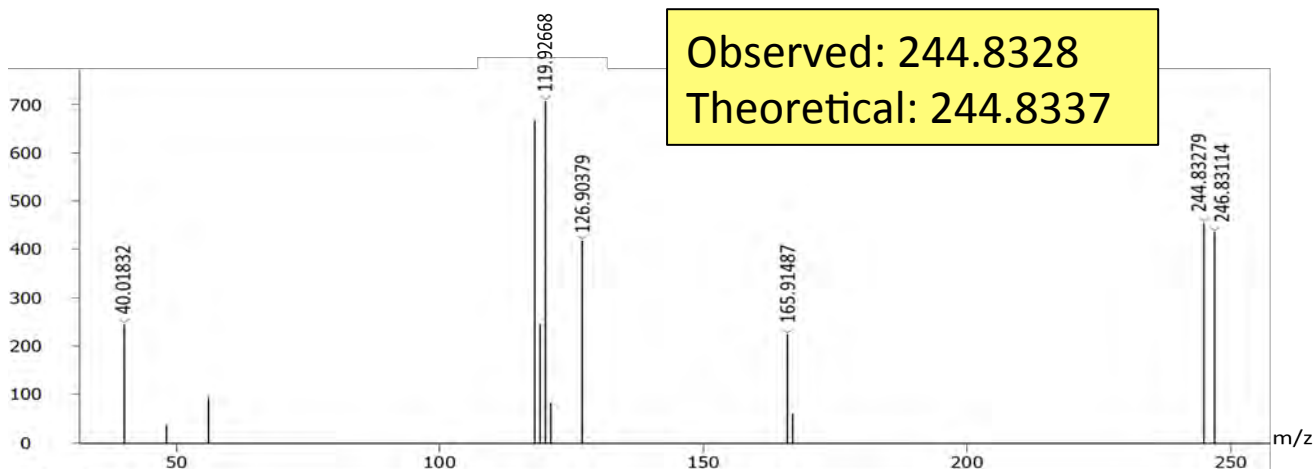
Fragment	Exact Mass	Resolution Needed
$CHClBr^+$	126.8950	13,421
I^+	126.9045	
$C_9H_{19}^+$	127.1487	520

Discovery of New Iodo-DBP

- LECO Pegasus GC-HRT time-of-flight mass spectrometer
- High resolution: 25,000
 - Maximum: 50,000
- Accurate mass
- XIC m/z 126.904
- Continuing data analysis for iodoacetonitriles and other new iodo-DBPs

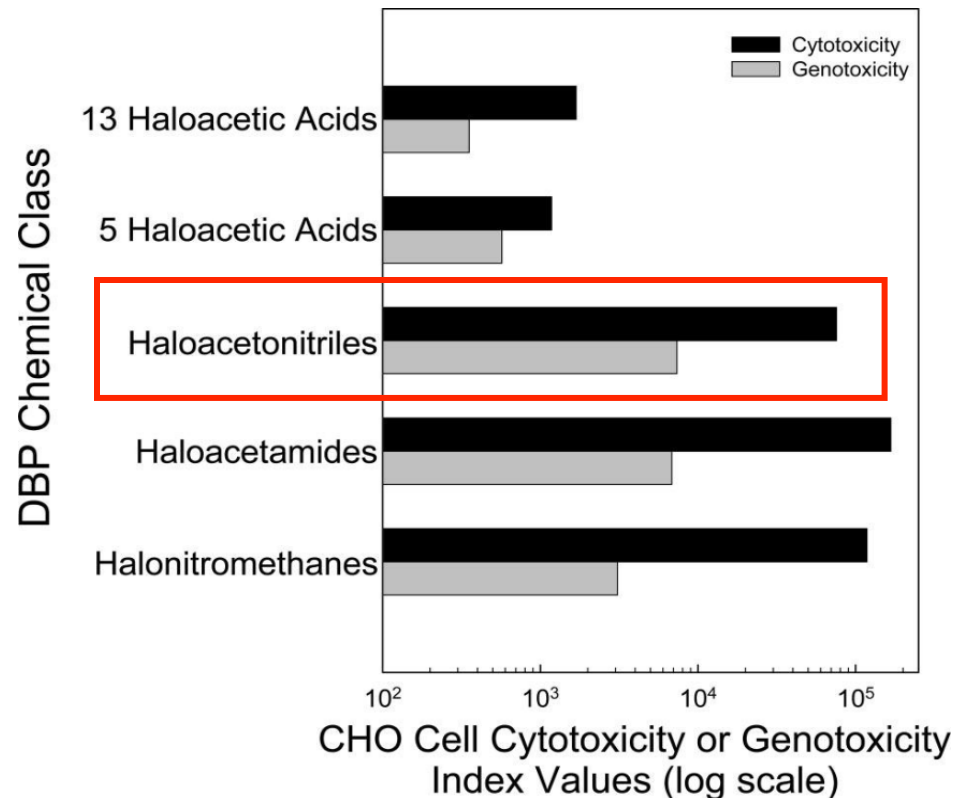


Bromoiodoacetonitrile



Haloacetonitriles are one of the most toxic classes of DBPs

Bromoiodoacetonitrile is likely to be the ***most toxic*** haloacetonitrile identified to date



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- NSF WaterCAMPWS (Award CTS-0120978)
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