

SafeCREW Final Conference, 26 - 27 March 2026, Brussels



Occurrence of novel highly polar sulfonated disinfection by-products in drinking water

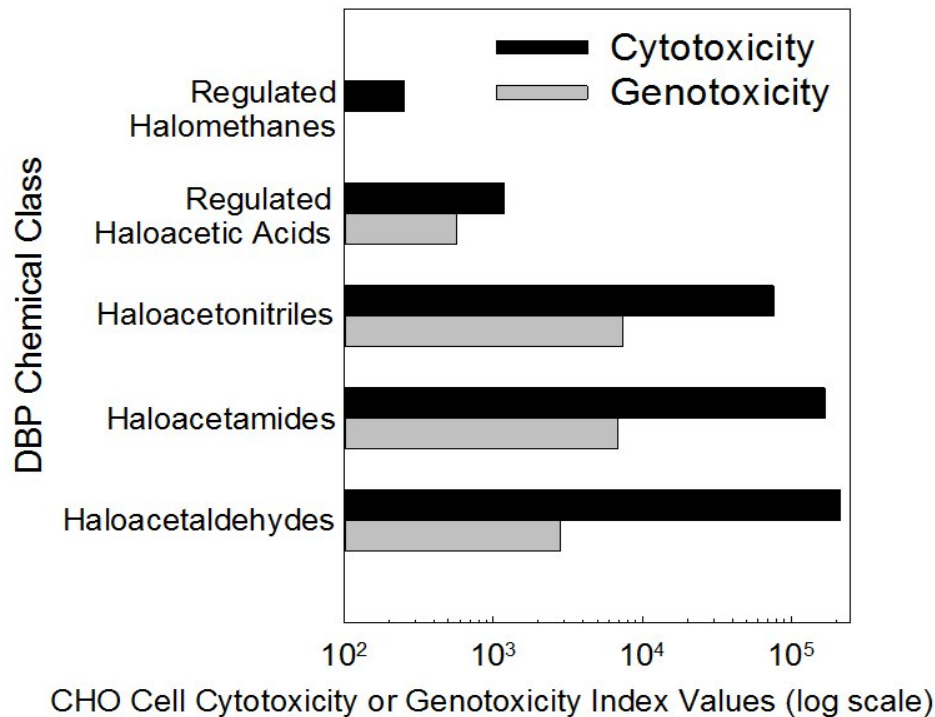
Maolida Nihemaiti

(Helmholtz Centre for Environmental Research - UFZ)

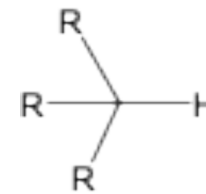


Funded by
the European Union

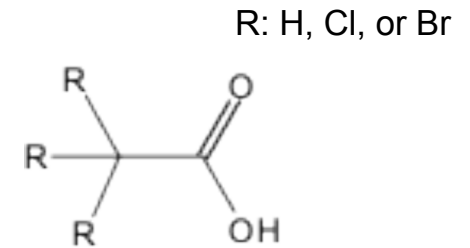
- Cyto- and genotoxicity of DBPs (Plewa et al., 2008; Plewa and Wagner, 2009)



- Regulated DBPs

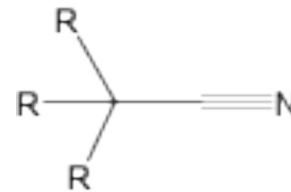


Trihalomethanes (THMs)

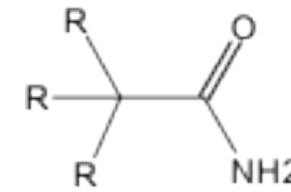


Haloacetic acids (HAAs)

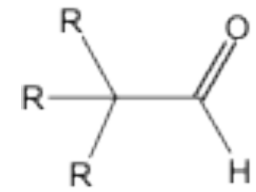
- (some of the) unregulated DBPs



Haloacetonitriles



Haloacetamides

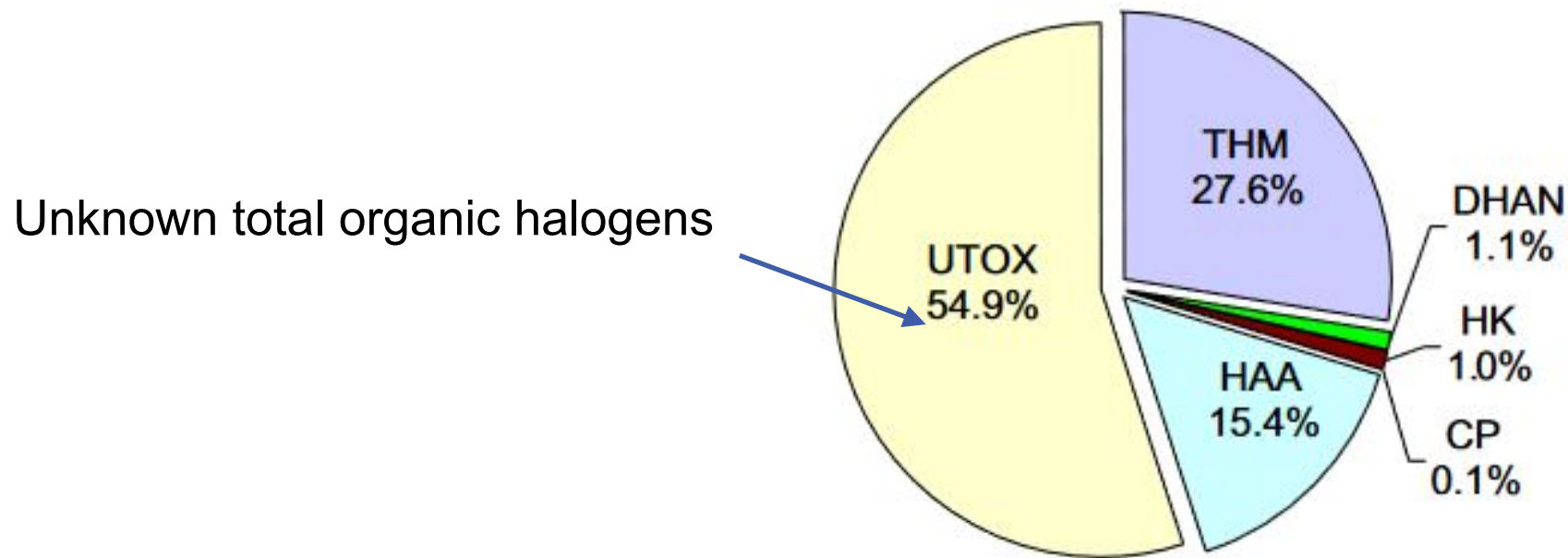


Haloacetaldehydes

Many unregulated DBPs are more toxic than the regulated THMs and HAAs



- Over 1000 DBPs have been characterized so far.
- However, more than 50% of total organic halogens (TOX) produced during chlorination are still unknown.



TOX distribution from chlorination of a surface water
conditions: pH=7, reaction time= 48 h

[1] Hua and Reckhow (2007) Water Res.41, 1667-1678.
[2] Li and Richardson (2026) TrAC. 198, 118668.



- Gas chromatography-mass spectrometry (GC-MS)



- Reversed-phase liquid chromatography MS (RPLC-MS)



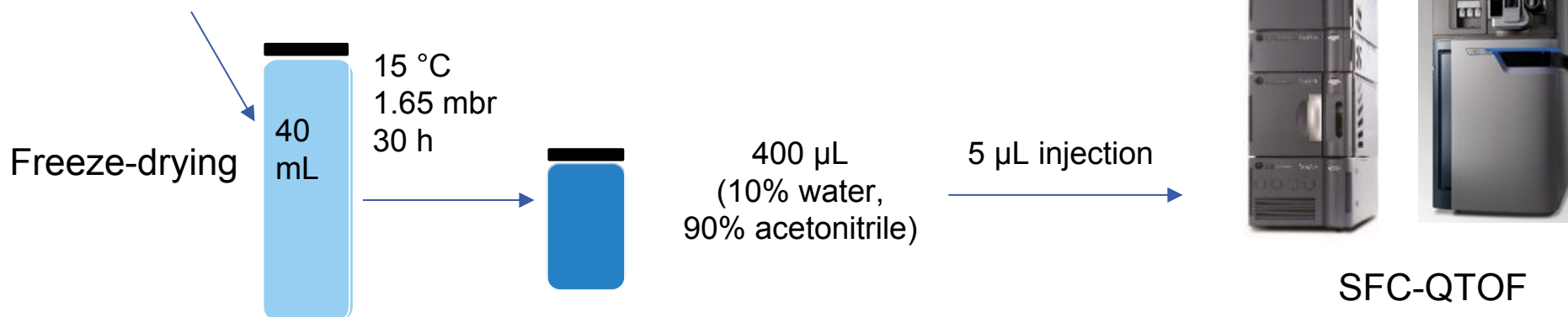
- GC-MS and LC-MS can overlook the very polar fractions of DBPs
 - nonvolatile for GC analysis and hardly retainable in RPLC (e.g., C18 column)

➔ SFC-MS for polar DBP analysis

SafeCREW Approach for Characterizing Highly Polar DBPs

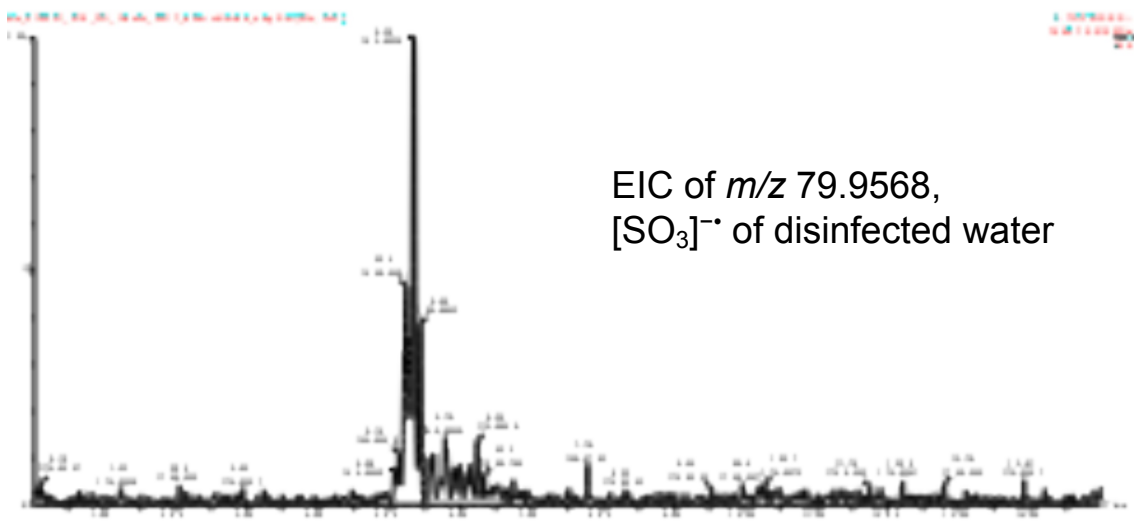
- Sample enrichment (if needed): freeze-drying
- An alternative analytical platform: supercritical-fluid chromatography–mass spectrometry (SFC-MS)
 - SFC-QTOF: non-target screening
 - SFC-MS/MS: targeted quantification

40 mL of drinking water sample



Identification of Novel Sulfonated DBPs by SFC-Q-TOF-MS

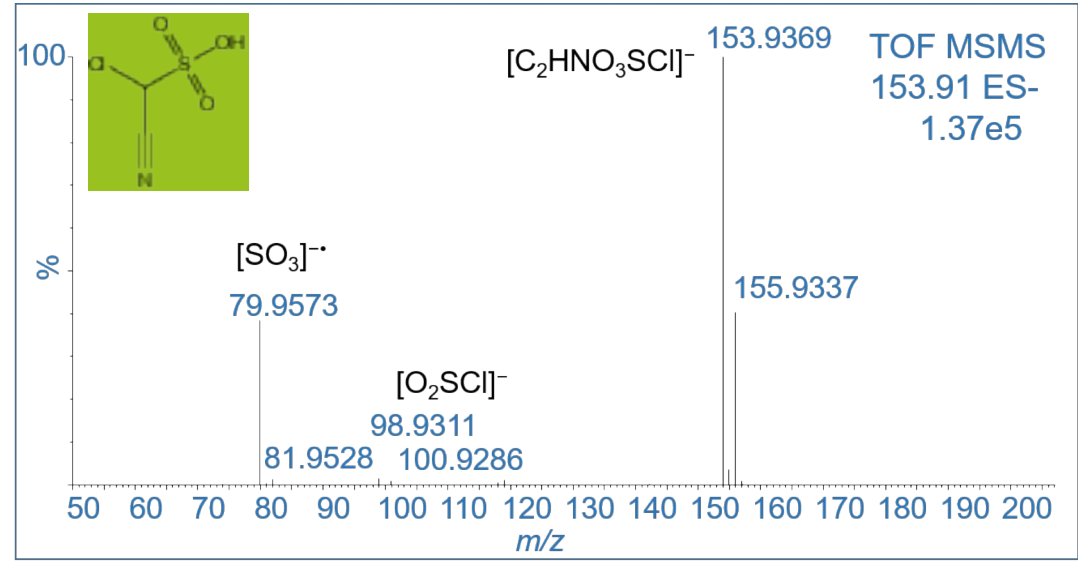
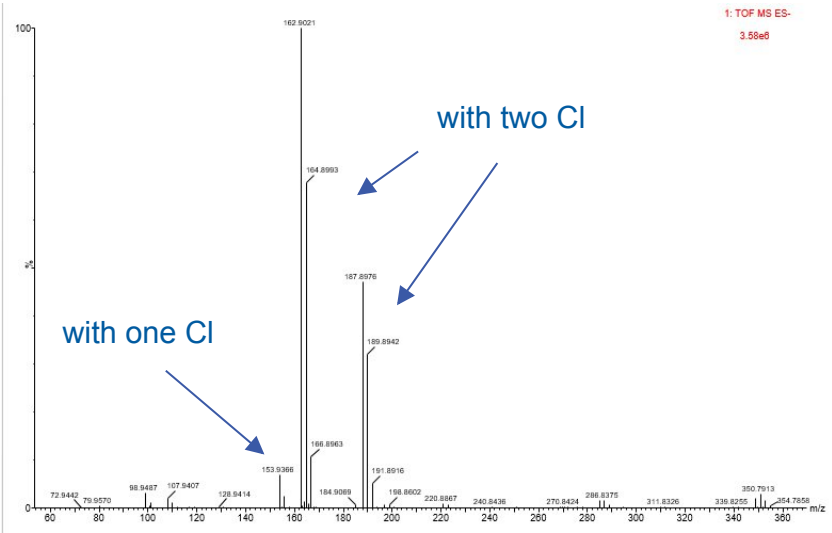
In Leipzig drinking water



EIC of m/z 79.9568, $[\text{SO}_3]^-$ of disinfected water

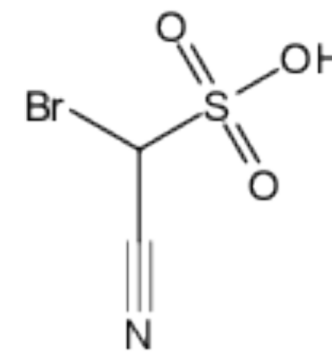
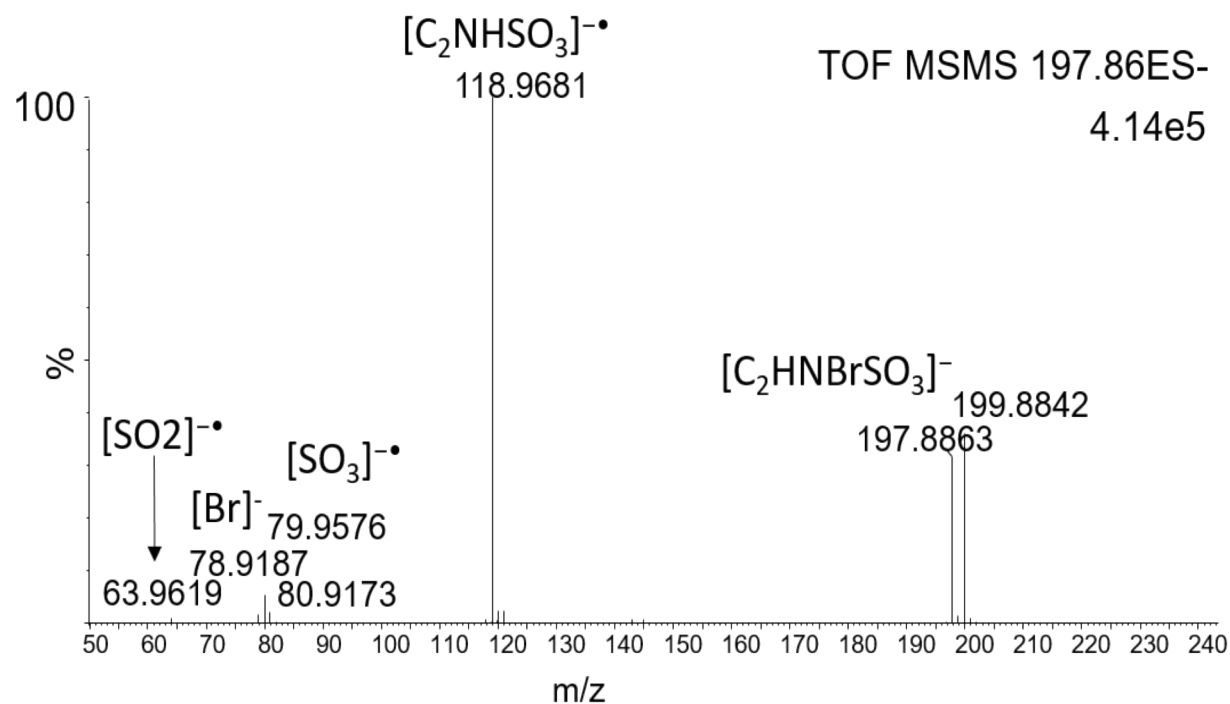
- Identification of m/z 153.9369
 - Structures were proposed based on the exact mass and fragmentation patterns obtained from HRMS data
 - Monochloroacetonitrile sulfonic acid

Mass spectrum at RT 5.35 min



Funded by the European Union

- Brominated analogues were also observed



- Chlorine reacts with Br⁻ in water to produce secondary oxidant: HOBr



Hua et al. (2006) Environ. Sci Technol. 40 (9), 3050-3056



Cl

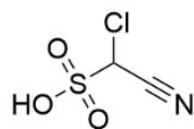
Cl₂

BrCl

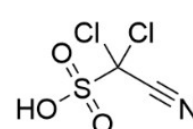
Br

Br₂

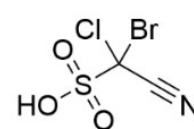
Haloacetonitrile sulfonic acids



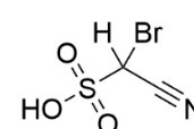
ClANSA



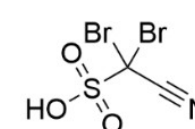
Cl₂ANSA



BrClANSA

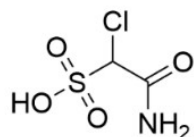


BrANSA

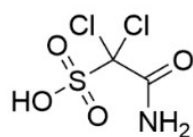


Br₂ANSA

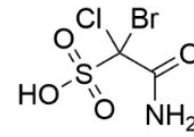
Haloacetamide sulfonic acids



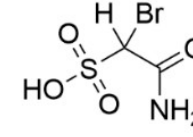
ClAcAmSA



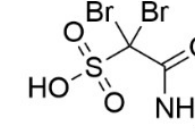
Cl₂AcAmSA



BrClAcAmSA

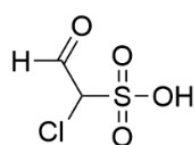


BrAcAmSA

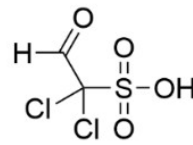


Br₂AcAmSA

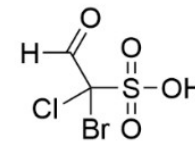
Haloacetaldehyde sulfonic acids



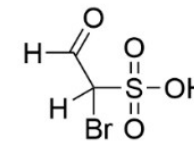
ClAcAISA



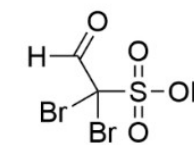
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BrClAcAISA



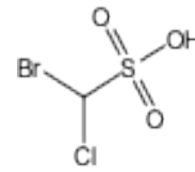
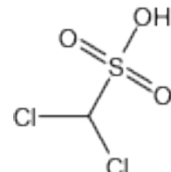
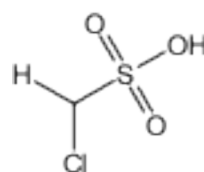
BrAcAISA



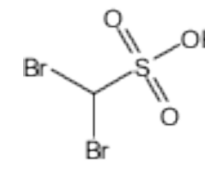
Br₂AcAISA

Halomethane sulfonic acids

(Zahn et al., 2016, 2019; HILIC-MS)



Br



Questions Related to Novel Sulfonated DBPs

• Q1: Occurrence across different water samples (isolated case in Leipzig water or more widespread?)

• Q2: Factors affecting formation (drinking water source, type of disinfectant, seasonal variations, etc.)

- In collaboration with



• Q3: Relationship to regulated DBPs

- In collaboration with



• Q4: Identification of precursors

- In collaboration with



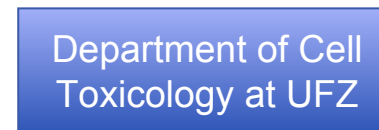
• Q5: Efficiency of water treatment processes in remote areas

- In collaboration with



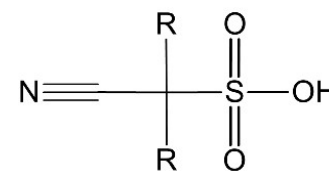
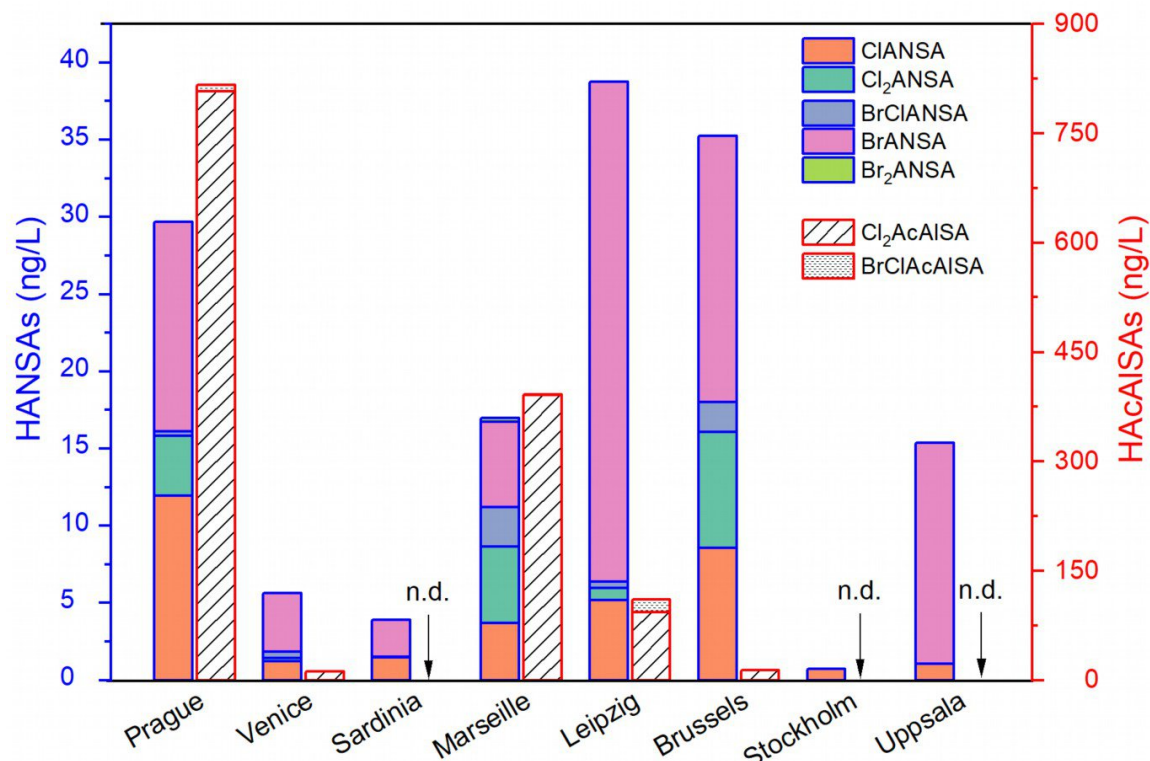
• Q6: Toxicity and Risk

- In collaboration with

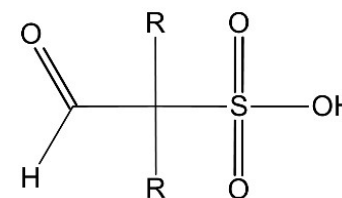


Q1: Occurrence across different water samples

- tap water samples from 8 European cities



up to 40 ng/L



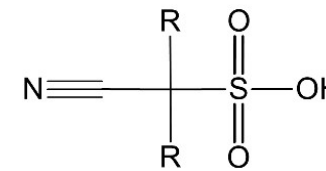
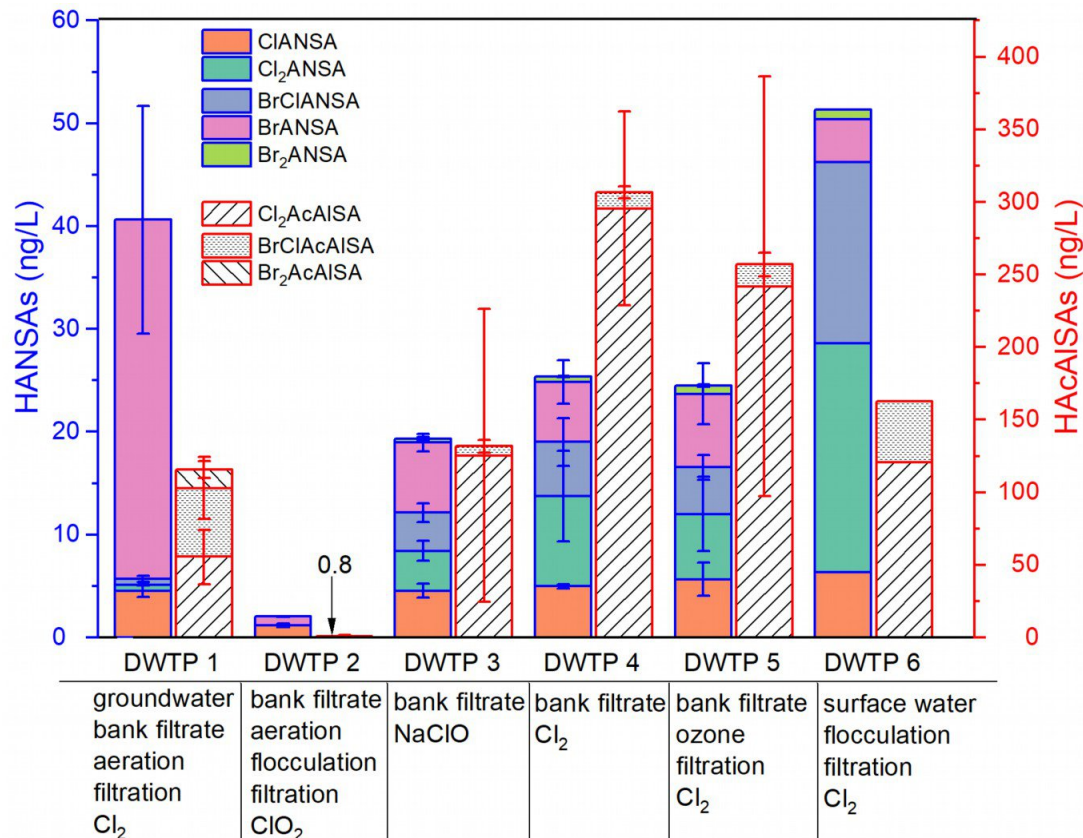
up to 800 ng/L

- widespread occurrence with varying concentrations

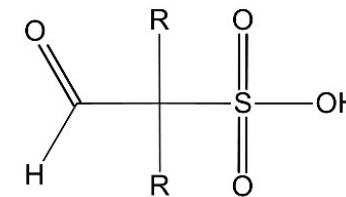


Q2: Factors affecting formation: drinking water source & type of disinfectant

- Finished water from 6 drinking water treatment plants



up to 50 ng/L



up to 300 ng/L

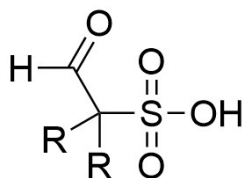
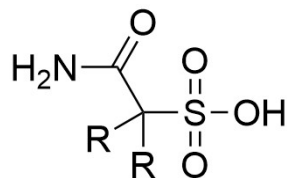
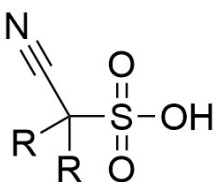
- formed in all treatment plants regardless of the source water type and treatment trains

→ precursors in groundwater, river bank filtrate, surface water.

- ClO₂ disinfection produces less than chlorination (confirmed with lab-scale studies)

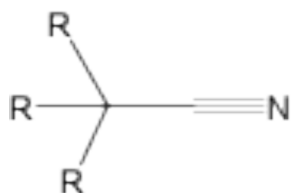


Q6: Toxicity and Risk

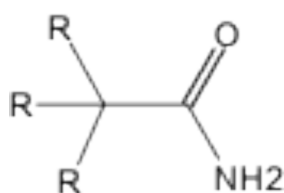


R: H, Cl, or Br

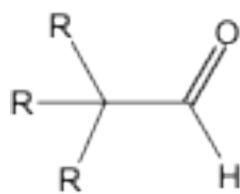
structurally similar to toxic DBPs



Haloacetonitriles

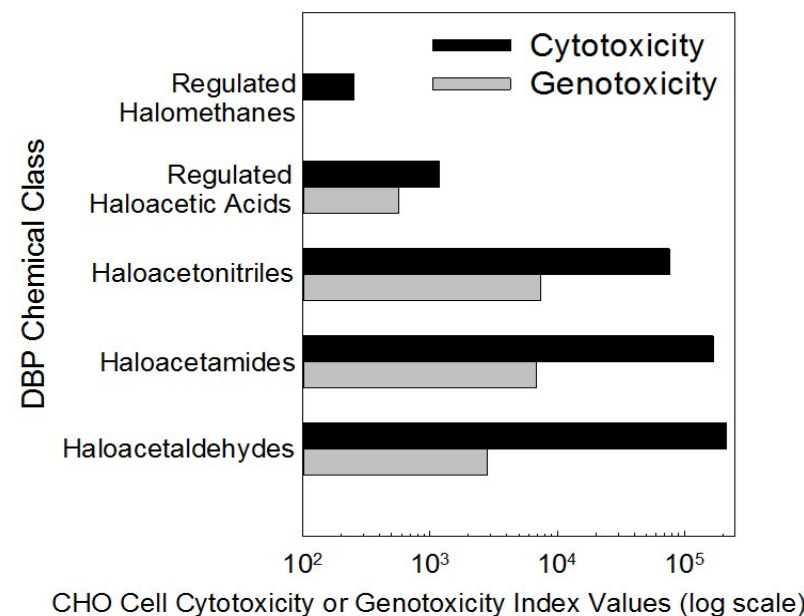


Haloacetamides



Haloacetaldehydes

Cyto- and genotoxicity of DBPs
(Plewa et al., 2008; Plewa and Wagner, 2009)



- **Occurrence:** Sulfonic acid derivatives of all regulated and regularly monitored DBPs are present in disinfected water regardless of water source or treatment methods.
- **Influencing Factors:** The type of disinfectant, seasonal variations in water quality, and temperature can influence the formation potential of sulfonated DBPs.
- **Research Needs:** Considering their structural similarity to toxic DBPs, further studies are required to assess the toxicity and risk of the other 15 sulfonated DBPs.



Cooperation

- Univ. of Leipzig
 - Maik Icker
- SafeCREW project partners, namely
 - Hamburg University of Technology
 - Jon Wullenweber, Mathias Ernst
 - Consorci d'Aigües de Tarragona
 - Noemí Benavente Calderón, Josepa Fargas-Cerdà, Andreu Fargas-Marquès
 - Eurecat, Centre Tecnològic de Catalunya
 - Laura Vinardell, Irene Jubany



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Thanks for your attention!

