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Maolida Nihemaiti (EAC): Novel highly polar sulfonated disinfection by-products in drinking water: identification and formation mechanisms

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Abstract:
"Disinfection is a critical step during drinking water production and distribution to prevent waterborne disease. However, the chemical disinfectants (e.g., chlorine) can react with water matrices (organic matter, halides) to produce disinfection by-products (DBPs), which can cause adverse health effects like birth defect and bladder cancer. A small number of DBPs are regulated (e.g., trihalomethanes). However, the majority of them, especially the main toxicity drivers in disinfected water still remain unknown. The importance of drinking water disinfection is expected to increase with degrading surface water quality due to climate change.
High resolution mass spectrometry (HRMS) coupled to either gas chromatography (GC) or reversed-phase liquid chromatography (RPLC) is the generic method to identify unknown DBPs. But highly polar contaminates cannot be separated and detected by classical GC-MS or RPLC-MS methods. In this study, we applied supercritical fluid chromatography (SFC) coupled to HRMS to characterize DBPs in disinfected water from drinking water treatment plants and distribution network. We successfully identified 15 novel extremely polar DBPs as the sulfonic acid derivatives of haloacetonitriles, haloacetamides, and haloacetaldehydes. Despite the lack of analytical standards, we were able to conduct the structural confirmation and quantification of these newly identified DBPs by preparing their mixture via chlorination of a precursor compound and by combining nuclear magnetic resonance spectroscopy (NMR) analysis with SFC-HRMS. Various lab-scale chlorination experiments on different water matrices were conducted to investigate the precursors and formation mechanisms of sulfonated DBPs. The results indicate that the formation potential of sulfonated DBPs does not follow the trend observed for regulated DBPs, possibly due to their distinct precursors. In accordance with this, the ultrahigh-resolution MS (FT-ICR-MS) analysis suggests that sulfonated DBP formation is likely influenced by other precursors in the source water than those of regulated DBPs.
This study shows how innovative analytical approaches can broaden our understanding of the human health burden, which may escalate with climate change."

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