

Preface to the Special Issue: Disinfection Byproducts

Analysis of water disinfection byproducts – advances and challenges

The provision of safe potable water is a basic human right, and is directly related to a number of the United Nations Sustainable Development Goals (UN SDGs), specifically SDG 6: Clean Water and Sanitation, but it also relates to others such as SDG 3 focusing on Good Health and Well-being, as well as Sustainable Cities and Communities (SDG 11). Effective treatment of water prior to its distribution for use as drinking water is critical to avoid potential negative human health effects incurred by the presence of pathogens or chemical pollutants which may be present in the source water. Water treatment may, however, generate unwanted disinfection byproducts (DBPs), the analysis of which is the focus of this Special Issue. An example is the formation of halogenated DBPs, which are formed during the treatment of water containing precursors, including natural organic matter which is invariably present in surface water such as rivers. Upon the chlorination or chloramination of such source water, a wide range of chlorinated DBPs may form, whilst brominated DBPs are of concern in salt mining areas.

Disinfection processes may cause odor in drinking water, due to the presence of residual disinfectants as well as odor active DBPs, as reviewed in DOI: 10.1016/j.trac.2023.117224. A range of analytical methods have been developed for both qualitative and quantitative monitoring thereof. These need to be highly sensitive due to the very low odor threshold concentrations for most of these compounds. Aside from being odor-causing, many DBPs have been confirmed to incur negative human health effects, or are suspected to do so. The advances in the assessment of toxicity of drinking water DBPs has thus been reviewed in this Special Issue (DOI: 10.1016/j.trac.2024.117545). It is clear that the toxicity of DBPs is complex in terms of toxicological mechanisms and effects (including those at individual, cellular and genetic levels), but also as a result of the vast number of DBPs which may be present in water contributing to additive, synergistic or antagonistic toxic effects.

The effective monitoring of drinking water for DBPs is therefore critical. This Special Issue comprises reviews on the advances in analytical methods for the sampling, sample preparation, and analysis of disinfection byproducts, as well as that of the precursors to their formation. This is a globally relevant topic, with considerable research being conducted to advance our understanding of the formation of these compounds and their prevalence in drinking water around the world. Detection and identification of these analytes is challenging however, due to the very low concentrations at which they may be present in water, as well as the structural similarity of many of these compounds. Moreover, a complex mixture of disinfection byproducts may be produced during water treatment and distribution. The regulatory framework regarding DBPs, which typically guides analytical method development, varies widely globally, and it should be noted that in some cases there are limits for groups of DBPs, such as total trihalomethane (THM) DBPs, rather than for individual compounds.

Efficient sample preparation methods are generally needed in order to pre-concentrate DBPs present at low levels in drinking water and thereby enable their detection. Functional materials, such as carbon-based nanomaterials, metal-organic frameworks and molecularly imprinted polymers, have been synthesized for use in solid phase extraction (SPE) of DBPs, as reviewed in DOI: 10.1016/j.trac.2023.117296. These materials are designed to offer selectivity, high adsorption capacities as well as re-use possibilities after regeneration, in line with green chemistry principles. Enrichment of DBPs present in samples may also be required prior to the toxicity assessment thereof (<https://doi.org/10.1016/j.trac.2024.117892>). This is complicated by the need to efficiently extract the target analytes (i.e. DBPs) into biologically compatible solvents without incurring losses thereof. Membrane inlet mass spectrometry (MIMS) provides an alternative analytical approach in which the

volatile DBPs in a water sample pervaporate through a membrane into the mass spectrometer, avoiding the need for sample preparation, as described in DOI: 10.1016/j.trac.2023.117141. Here the continuous flow of sample provides for potential on-line process monitoring and the investigation of formation kinetics in real time, if identification and quantification challenges due to peak overlap are suitably addressed. Aside from analytical challenges in the monitoring of DBPs in drinking water as a result of their low concentrations, the physicochemical properties of these compounds such as hydrophilicity, non-volatility and acidity, may present further challenges. This is the case for the haloacetic acids (HAAs), for which numerous pre-treatment methods have been attempted primarily focusing on the extraction and derivatization thereof (reviewed in DOI: 10.1016/j.trac.2024.117617).

The identification and quantification of emerging and new (currently unknown) DBPs is an area of active analytical chemistry research, requiring an expansion from target to non-target workflows and suspect screening approaches utilizing a range of different sample preparation techniques, as reviewed in DOI: 10.1016/j.trac.2024.117621. Both liquid-liquid extraction and solid phase extraction sample preparation methods have been explored in conjunction with gas or liquid chromatography and a number of different mass spectrometry options, each with inherent advantages and disadvantages. The data analysis software needed to correctly identify emerging DBPs may not be readily available, requiring in-house development. Mass spectrometry is a vital analytical tool in the identification of unknown DBPs, particularly those with toxic relevance. In this regard a range of approaches have been employed and are being further developed for DBP characterization. These include selected ion monitoring and multiple reaction monitoring in both low, high and ultra-high resolution mass spectrometry, as reviewed in DOI: 10.1016/j.trac.2023.117209, which highlights the potential influence of extraction method and the need to address noise and artifact formation in order to achieve valid analytical results. Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) can be employed to provide compositional information on non-volatile, high molecular mass DBPs and provides a powerful tool in the identification of unknowns, as discussed in DOI: 10.1016/j.trac.2023.117264. This review emphasises the potential impact of the addition of disinfection quenching agents (such as ascorbic acid) in the decomposition of DBPs or the formation of DBP adducts, as well as the need for the development of systematic verification procedures to ensure that non-target analyses are reliable.

It is important to note that although the presence of DBPs in drinking water is of global concern, very little information on the occurrence of these compounds is available for the African continent, as reviewed with respect to N-nitrosamine DBPs in a status report in this Special Issue (DOI: 10.1016/j.trac.2022.116873). This is an aspect that requires research attention to enable protection of human health via the development of facile and cost-effective analytical methods, appropriate for implementation in developing countries with limited resources.

It is anticipated that the analysis of DBPs will continue to receive attention in terms of analytical method development, as analytical technologies continue to advance enabling the identification of new byproducts. Thanks to the contributions made by experts in the field of DBP monitoring, this Special Issue provides a consolidated yet rigorous review of the current state-of-the-art, and thereby provides a basis for these future developments. Further, robust analytical methods are essential in informing the development of new water treatment processes which minimize the formation of DBPs and/or effectively remove them prior to distribution should they be present in the treated water. Analytical chemistry thus provides essential contributions towards the achievement of clean water for all as enshrined in the SDGs.

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