Identification and quantification of dichloroiodoacetic acid in the chlorinated waters

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ABSTRACT
Due to the high toxicity of iodinated disinfection byproducts (I-DBPs), their discovery becomes crucial for drinking water safety. In this study, we identified and quantified a previously predicted yet analytically unclear I-DBP, dichloroiodoacetic acid (DCIAA), which was overlooked in electrospray ionization because of the in-source fragmentation. The molecular formula of DCIAA was confirmed through high-resolution mass spectrometry full scan analysis after the formation, and its structure was determined by product ion scan characterization. 2-iodophenol was selected as the optimal precursor for DCIAA yield during chlorination at pH 8.0. Following isolation and purification, the synthesized DCIAA was quantified by inductively coupled plasma mass spectrometry, with subsequent employment for calibration standard. DCIAA remained stable for two months across pH 2.0-12.0, suggesting its potential persistence in drinking water distribution systems post-formation. The quantification method was developed using multiple reaction monitoring with the optimized m/z transitions at 208.8/126.9, showing superior selectivity through MS/MS confirmation, and Oasis WAX cartridges exhibited optimal recovery for solid-phase extraction of DCIAA. DCIAA concentrations was detected at 18.4-38.8 ng/L and 129.8- 463.1 ng/L in real tap water samples in Japan and chlorinated raw waters prepared in laboratory, respectively, which revealed the prevalent existence and importance of DCIAA in drinking waters.

KEYWORDS: Iodinated disinfection byproduct; chlorinated water; standard preparation; in-source fragmentation

CONTENTS:
1. This study is the first accurate identification and quantification of a predicted I-DBP in the real drinking waters which collected from different Japanese cities.
2. This study evaluated several key ESI parameters effects on the in-source fragmentation of DCIAA, which provides insight for the discovery of other fragile compound in ESI in the future.
3. This study provides a scheme to quantify a predicted halogenated DBP that was previously challenging to analyze through a simple reaction that produce the target product.