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Monitoring transformation product formation in the drinking water treatments rapid sand filtration and ozonation

Andrea Mizzi Brunner[1]*, Dennis Vughs[1], Wolter Siegers[1], Cheryl Bertelkamp[1], Roberta Hofman-Caris[1], Annemieke Kolkman[1], Thomas ter Laak [1]

[1] KWR Watercycle Research Institute, P.O. Box 1072, 3430 BB Nieuwegein, The Netherlands

*corresponding author

Abstract

Transformation products (TPs) can be formed from organic micropollutants in the water cycle through both biological and technological processes. Despite the TPs' potentially altered toxicity compared to their parent compounds, transformation processes are not routinely monitored, and in particular those induced by drinking water treatment remain elusive. This lack of information is mainly due to the technical challenges in analyzing TPs, which are often unknown compounds occurring in low concentrations. Their analysis requires sophisticated analytical techniques such as non-target screening (NTS) based on high-resolution tandem mass spectrometry (HRMS/MS) methods combined with novel data analysis approaches. Here, we addressed the challenges of TP analysis and the scarcity of TP research concerning studies in drinking water. We performed lab-scale experiments to monitor TP formation of three organic micropollutants prevalent in drinking water sources, i.e. carbamazepine, clofibric acid and metolachlor, during rapid sand filtration and ozonation, two readily applied biotic and abiotic drinking water treatments, respectively. To facilitate TP identification in the NTS data, halogenated and/or isotopically labeled parent compounds were used, revealing potential TPs through their isotopic patterns. The experimental results showed that degradation of the parent compounds and TP formation were treatment and compound specific. *In silico* TP prediction and literature mining enabled suspect screening of the non-target data and thereby significantly enhanced TP identification. Overall, the developed workflow enables an efficient and more comprehensive assessment of drinking water quality changes during water treatment.