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Modeling position-specific isotope fractionation of organic micropollutants degradation via different reaction pathways

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Organic compounds are produced in vast quantities for industrial and agricultural use, as well as for human and animal healthcare [1]. These chemicals and their metabolites are frequently detected at trace levels in fresh water environments, such as groundwater systems, and are referred to as organic micropollutants. Degradation of various organic micropollutants occurs via different reaction pathways. Compound specific stable isotope analysis (CSIA) is a valuable tool to characterize different degradation pathways of these contaminants in different aquatic systems and under different environmental conditions. Recent advances in analytical techniques have promoted the fast development and implementation of multi-element CSIA. However, quantitative frameworks to evaluate multi-element stable isotope data and incorporating mechanistic information on the transformation of different organic contaminants [2,3] are still lacking.

In this study we propose an integrated modeling approach to simultaneously predict concentration as well as bulk and position-specific multi-element isotope evolution during the transformation of organic micropollutants [4]. The model simulates position-specific isotopologues explicitly incorporating the atoms that experience isotope effects. Thus, it provides a mechanistic description of isotope fractionation occurring at specific molecular positions. We apply the proposed approach to interpret the data available for three selected organic micropollutants: dichlorobenzamide (BAM), isoproturon (IPU) and diclofenac (DCF). The model successfully reproduces the multi-element isotope data, and precisely captures the dual element isotope trends, characterizing the different degradation pathways. Besides illustrating the model capability of mechanistic evaluation of experimental observations, we also show its potential as a predictive and design tool to explore transformation pathways in micropollutants degradation scenarios for which position-specific isotope data are not (yet) available.

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