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A temporal graph to predict chemical transformations in complex dissolved organic matter

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Dissolved organic matter (DOM) is a complex mixture of thousands of natural molecules that undergo constant transformation in the environment, such as sunlight induced, photochemical reactions. Despite molecular level resolution obtained by ultra-high resolution mass spectrometry, the mechanistic understanding of DOM transformations is still hampered due to a multitude of simultaneous reactions. Temporal trends of mass peak intensities are currently the only way to follow photochemical induced molecular changes in DOM, but are often limited by low temporal resolution or the necessity to apply monotonic regression models. Here, we present a novel computational approach using a temporal graph (a temporal molecular network) to model the transformation of DOM molecules in a photolysis experiment by employing a predefined set of basic molecular transformation units (like oxidation, decarboxylation, etc.). The new algorithm focuses on the temporal changes of mass peak intensities of molecular formulas by simultaneously considering educt removal and product formation for molecules linked by a transformation unit (e.g. -CO2). The transformations and molecules are further weighted by the extent of intensity change and grouped by unsupervised machine learning algorithms to find clusters of similar reactivity. The temporal graph thus allows to simultaneously identify relevant molecules subject to similar reactions and to study their time course. The graph can be constructed for low and high temporal resolution data without presumptions on reaction kinetics and with different sets of transformation units according to the experimental design. Our approach overcomes previous data evaluation limitations for mechanistic studies of DOM transformation and leverages the potential of temporal graphs to study the reactivity of complex DOM by means of ultra-high resolution mass spectrometry.