



Advanced Analytical Technologies and Water Research

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Disinfection of drinking water effectively prevents waterborne disease, but an unintended consequence of the chemical disinfection process is the formation of disinfection byproducts (DBPs). Epidemiological studies have indicated potential chronic adverse health effects of DBPs. However, it remains unclear which DBPs cause the observed effects and to date, the majority of DBPs remain unidentified. Reactive organic nitrogen in source water can produce both toxic and odorous DBPs. Odor and off taste of drinking water are additional challenges for the water industry. Therefore, we aim to develop innovative analytical approaches to address water quality issues. Our current research focuses on the development of advanced separation and mass spectrometry techniques with machine-learning-assisted data processing for rapid identification of reactive nitrogenous organics in source water and their odorous DBPs in treated drinking water. Here we will present the integration of machine learning with hydrogen/deuterium (H/D) stable isotopic methyl labeling high-performance liquid chromatography–high resolution mass spectrometry technology (HPLC-HRMS) for comprehensive analysis of chemicals in water. The H/D-HPLC-HRMS nontargeted analysis provides high sensitivity detection of chemicals, while machine learning provides rapid data processing and tentative identification. We will present the development and application of the automated data processing platform HDPairFinder with H/D-HPLC-HRMS in water research.