



## **Molecular-level characterization of fluorescent dissolved organic matter in 120 boreal lakes using ultrahigh resolution mass spectrometry**

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Dissolved organic matter (DOM) is a highly diverse composite of degradation products, with its reactivity and composition central to the role inland waters play in the global carbon cycle. Thus characterizing DOM is of great interest; however, a major challenge in DOM characterization is its inherent heterogeneity. Absorbance and fluorescence spectroscopy are accessible and time-efficient characterization techniques, thus the use of such techniques continues to increase. Despite the pervasive use of these methods, the molecular basis of many commonly used indices remains a subject of great interest. We analyzed 120 lakes across Sweden using 15 Tesla ultrahigh resolution electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS). This method allows for precise molecular formula assignment of thousands of molecules in each sample. These data were then compared to absorbance and fluorescence properties including a six-component model derived from parallel factor analysis (PARAFAC). We found that aliphatic compounds were most highly associated with microbially derived components and vascular plant-derived polyphenols were most highly associated with terrestrial components. This state of the art analysis reveals the specific chemistry behind widely used absorbance and fluorescence fingerprinting techniques and serves as a basis for future studies looking to understand the molecular characteristics of optical parameters.