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Factors controlling composition of lake DOM across Sweden using ultrahigh-resolution mass spectrometry combined with fluorescence.

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Dissolved organic matter (DOM) is a heterogeneous mixture of decomposition products. The character and reactivity of DOM, as well as what controls the molecular composition of this dynamic community of compounds, is not well understood. Furthermore, there is growing evidence that lake DOM contributes substantially to the global carbon cycle. Thus we attempt to gain further insight into controls on the structural composition of DOM in boreal lakes by combining information from multiple analytical approaches. Mass spectra of DOM were analyzed for 150 Swedish lakes using a 15 Tesla ultrahigh-resolution electrospray ionization Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS). The high resolution provided by this method allows for molecular formula assignment and is an integral step in understanding the reactivity and character of DOM. From the mass spectra, we calculated the relative intensity of each peak, aromaticity index, and H:C and O:C ratios. Fluorescence spectra were analyzed using parallel factor analysis where we derived 6 fluorescence components. In addition, we derived several common spectral indices related to percent aromaticity, level of humification and information on DOM source. Our study compares the results generated from FT-ICR-MS and optical methods to establish if these methods are complementary or merely redundant. Finally, to determine factors explaining the variability in DOM composition among lakes across Sweden, we collected data on a suite of water chemistry parameters, and extracted land cover data for lake catchments to gain insight on the terrestrial sources of DOM.