FAIR Data: Reuse of MagLab Data Enhances the Processing of Dissolved Organic Matter Mass Spectra

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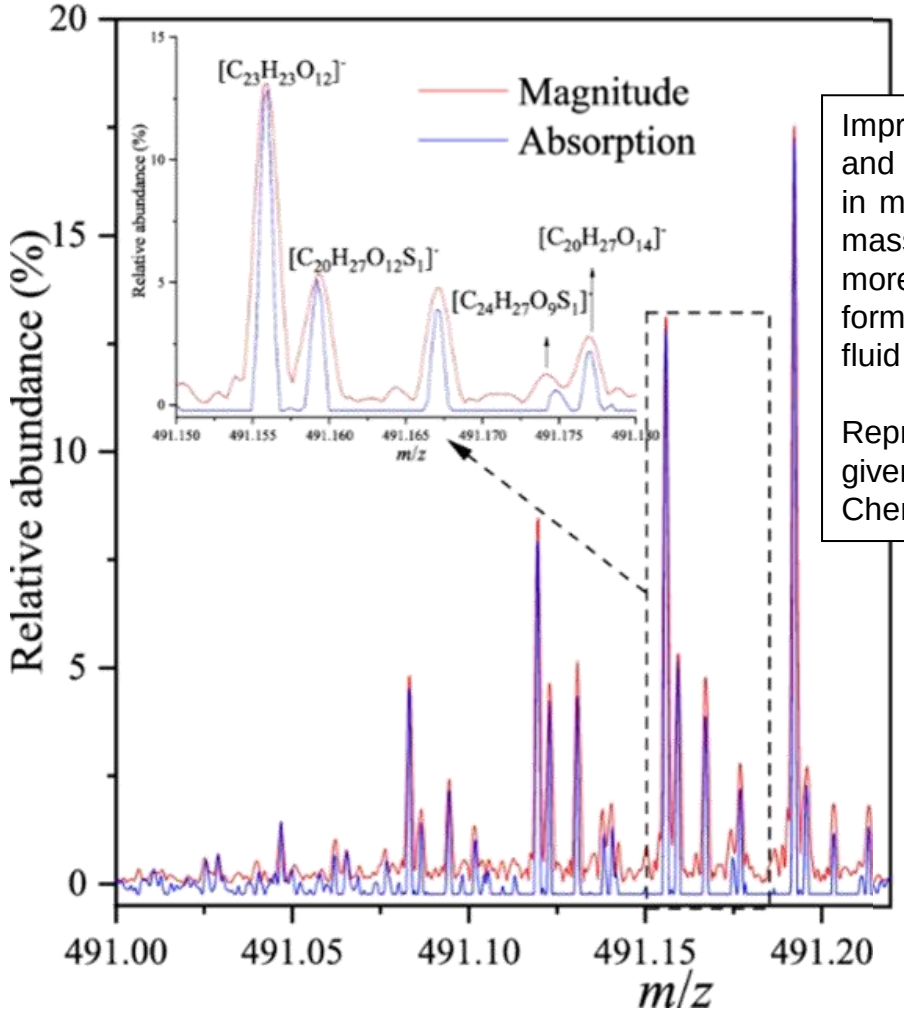
Rivers and lakes can contain many millions of unique chemical compounds, including toxic chemicals produced by human activity as well as natural compounds created from the breakdown of plant material. These natural compounds are referred to as Dissolved Organic Matter. *Techniques like Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) are necessary to characterize these highly complex mixtures and understand how man-made pollutants impact our natural environment. In this study, the authors reused data originally collected in 2022 at the MagLab in order to validate their approach to processing FT-ICR MS data.*

Raw FT-ICR MS data must be processed and calibrated to produce an interpretable mass spectrum. *Broadband absorption mode processing (BAMP), a technique originally developed at the MagLab, can greatly improve the mass error, mass resolving power, and signal-to-noise ratio of peaks in a mass spectrum* (see **Figure**). BAMP can theoretically increase the signal-to-noise ratio by a factor of $\sqrt{2}$, an improvement that would otherwise require much higher magnetic fields to achieve. This can allow for the assignment of a far greater number of unique chemical formulas from a given complex fluid sample, particularly those formulas corresponding to very low-abundance compounds. The authors were able to demonstrate the value of BAMP for analyzing Dissolved Organic Matter samples by achieving improvements to all figures of merit for positively-charged- and negatively -harged-mode mass spectra.

The authors of this new study were "FAIR data users", that is, they reused archived MagLab data to strengthen their analysis and validate their new data. The dataset used for this study was originally generated and made publicly available by MagLab researcher Amy McKenna in 2022. *As such, this research demonstrates the utility of BAMP for Dissolved Organic Matter sample analysis as well as the value of reuse of MagLab datasets under the MagLab's FAIR data protocols.*



Improved mass resolution and signal-to-noise ratio in mass absorption mode mass spectra leads to more assigned chemical formulas within a complex fluid sample.

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Facilities and instrumentation used: Ion Cyclotron Resonance User Facility, 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer

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