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Florida International University
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Doctoral Dissertation Defense

Abstract

Molecular Level Characterization of Dissolved Organic Matter integrating Trapped Ion Mobility Spectrometry and Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

by

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Dissolved organic matter (DOM) is an extremely complex mixture of organic molecules ubiquitous in aquatic systems and a critical component of the global carbon cycle. Little is known about DOM structural composition at the molecular level. The work presented in this dissertation summarizes the development of a novel analytical toolbox based on trapped ion mobility spectrometry and Fourier transform ion cyclotron resonance mass spectrometry (TIMS-FT-ICR MS) that has significantly contributed to expand our knowledge of DOM molecular complexity and diversity. The TIMS-FT-ICR MS/MS analysis provided for the first-time lower and upper estimation of the molecular isomeric diversity. The TIMS-FT-ICR MS/MS methodology was further developed to allow for chemical formula-based isomeric and neutral loss fragmentation structural description and database validation. This novel procedure enabled the unambiguous assignment of candidate isomeric structures based on accurate mass, database MS/MS matching scores, and ion mobility. A fast and routine structural characterization DOM workflow method was developed: GraphDOM. The method utilizes neutral loss fragmentation patterns acquired using continuous accumulation of selected ions (CASI)-collision induced dissociation (CID) FT-ICR MS/MS. The neutral mass loss patterns are used to define structural families leading to the identification and visualization of the DOM transformational processes. The GraphDOM methodology was successfully applied to the characterization of DOM along a salinity transect of the Harney River, Florida Everglades. The GraphDOM method was further implemented with isomeric content description at the molecular level and applied to four common aquatic systems. The application of the GraphDOM methodology allowed for the first time identification of common and unique DOM transformational networks across aquatic ecosystems.

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Place: CP 320   **Major Professor**: Dr. Francisco Fernandez Lima
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