University of Colorado Boulder

Water Energy Nexus IRT

2018 Seed Grant Final Report

Title: Application of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) for Environmental Sample Analysis: Development of Internal Expertise

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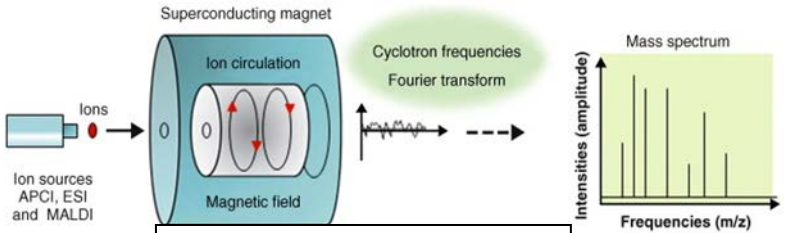
Research Objective(s): FT-ICR MS is a state-of-the-art tool for the characterization of complex organic compound mixtures in environmental studies. Only a few groups in the world are capable of analyzing the FT-ICR MS data, and the main facility is located at the National High Magnetic Field Laboratory (MagLab) in Tallahassee, Florida. This seed grant enabled us to acquire the capability of FT-ICR MS analysis for broader environmental and energy applications.

Research Activities/Methodology: We worked with the MagLab to analyze for the first time the contaminated crude oil and its bioelectrochemical degradation products using the advanced FT-ICR MS instrument, and we obtained and analyzed huge amounts of data to decipher the mechanisms of hydrocarbon transformation and remediation. We obtained in-house capability to conduct complex sample preparasion and data analysis (millions of data points for one sample).



FT-ICR MS working principle

Results: The transformation products containing heteroatoms of oxygen and nitrogen generated from bioelectrochemical remediation of crude oil-contaminated soil were revealed and analyzed by FT-ICR MS for the first time. The main polar compounds were acids O_2 classes species containing aromatic carboxylic acids, and basic N1 class species with the nitrogen-polycyclic aromatic compounds, which were all biodegraded in bioelectrochemical systems.

Accomplishments:

- We obtained a new research grant from Chevron to advance analysis and technology development on hydrocarbon degradation in contaminated sites.
- A manuscript is in preparation on revealing the daughter products generated from bioelectrochemical hydrocarbon degradation (*Characterization of polar compounds in soil bioelectrochemical remediation of petroleum hydrocarbons using negative and positive ion mode ESI FT-ICR MS. To be submitted to ES&T*).

Conclusions/Next Steps:

- More collaborative proposals will be submitted to NSF, DOE, EPA, and other agencies
- Expand the capability for more compound analysis such as natural organic matter, etc.