Development of New Soft Ionization Mass Spectrometry Approaches for Spatial Imaging of Complex Chemical and Biological Systems

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Purpose

Development of a new suite of MS-based chemical imaging capabilities, which will be broadly applicable to multiple chemical and biological systems, and their application to **multimodal chemical characterization of microbial biofilms**.

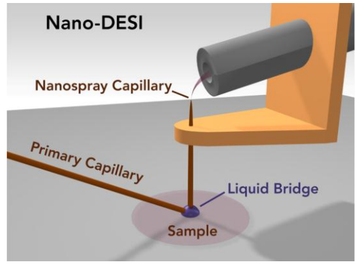
Expected Outcomes

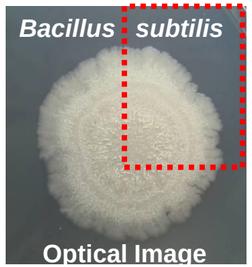
Development of novel MS imaging approaches – a new signature strength at PNNL

Multimodal MS imaging of microbial communities

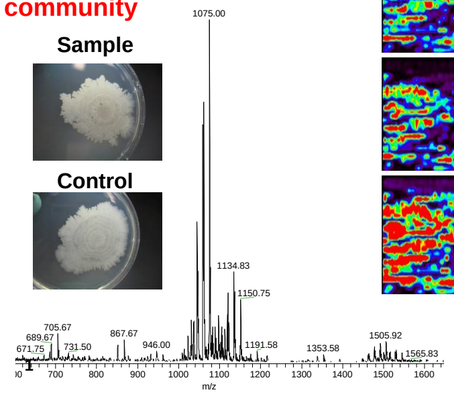
Understanding extracellular electron transport mechanisms in metal transforming organisms of interest to bioremediation and cleanup of DOE nuclear sites

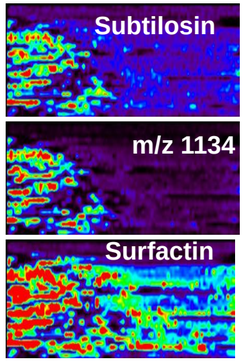
Nanospray Desorption Electrospray Ionization (nanoDESI) Imaging





nanoDESI spectrum and images of a living microbial community





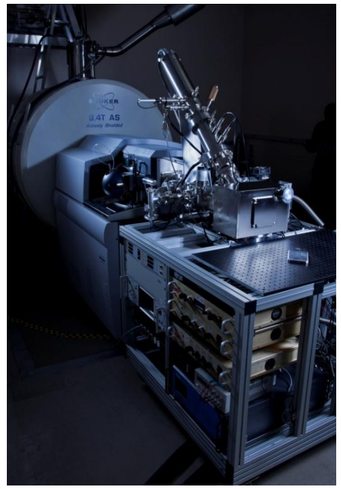
First demonstration of direct sampling of bacterial colonies from agar without loss of viability

First demonstration of ambient nanoDESI imaging

- Spatial profiling of metabolites
- High spatial resolution
- High sensitivity
- No sample pretreatment

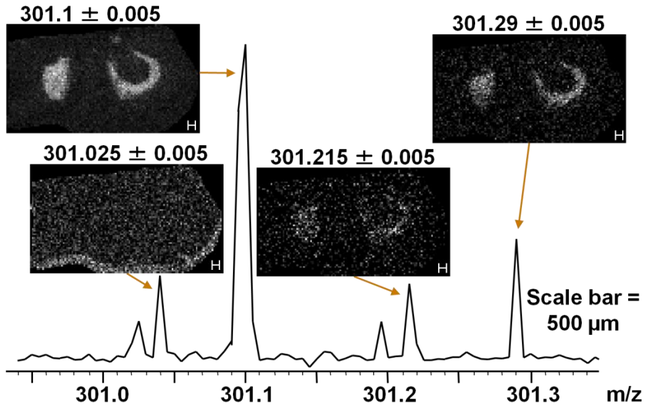
MALDI FT-ICR MS Imaging

Designed and built world's first SIMS FT-ICR MS by interfacing 40 keV C_{60} primary-ion gun (Ionoptika) to 9.4T (12T) solariX FT-ICR spectrometer (Bruker). Demonstrated high mass accuracy (<1 ppm), high mass resolving power (m/Δm50% >200,000), tandem MS capabilities and applied to biological samples.



World's first C_{60} SIMS FT-ICR MS Images

C_{60} SIMS FT-ICR MS Images of a mouse brain tissue



Why It Matters

Multimodal imaging of microbial communities enables applications in bioremediation, understanding and mitigating biological threats, drug discovery, and clinical research.

PJ Roach, BS Heath, L Cazares, OJ Semmes, J Laskin, "Tissue Imaging Using Nanospray Desorption Electrospray Ionization Mass Spectrometry," *Angew. Chem. Intl. Ed.*, submitted

Talks at ASMS meeting

DF Smith et al., "High Performance Chemical Imaging: C_{60} SIMS FT-ICR Mass Spectrometry"

B Heath et al., "Identification of Mechanisms of Extracellular Respiration by *Shewanella oneidensis* MR-1 Using Imaging Mass Spectrometry"

J Laskin et al., "Nanospray Desorption Electrospray Ionization: a New Technique for Ambient Imaging Mass Spectrometry"

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