Tandem MS Focus Topic
Room: 5 & 6 - Session TM-MoA

Applications in Mass Spectrometry Imaging using Tandem MS

Moderators: Gregory L. Fisher, Physical Electronics, Alexander Pirkl, ION-TOF GmbH, Germany

2:40pm **TM-MoA4 Utilization of Complementary Multimodal Techniques for *in situ* Identification of Soybean Root Nodule Metabolites**, *S. Stopka*, The George Washington University, *D. Veličković*, Pacific Northwest National Laboratory, *B. Agtuca*, University of Missouri, *D.W. Koppenaal, L. Paša-Tolić*, Pacific Northwest National Laboratory, *G. Stacey*, University of Missouri, *A. Vertes*, The George Washington University, ***Christopher R. Anderton***, Pacific Northwest National Laboratory

In an effort to attain more sustainable agricultural practices, there is a great interest in understanding metabolic processes within plant systems known to acquire nitrogen through biological nitrogen fixation. The symbiotic association between nitrogen-fixing soil bacteria (*Rhizobiaceae*) and plants of the family *Leguminosae* are one such system of interest. This symbiosis generates specialized organs, called root nodules, where rhizobia reduce N_2 into bioavailable products accessible to the host plant, and in exchange the plant provides a carbon source to the bacteria to ensure (among other things) sufficient energy for nitrogen fixation. Using both laser ablation electrospray ionization (LAESI) and matrix-assisted laser desorption/ionization (MALDI) mass spectrometry (MS) methods, we explored the array of metabolites involved, and their spatial distribution, that influence the rhizobia-legume association of *Bradyrhizobium japonicum* and soybean (*Glycine max* Williams 82). While these MS-based spatial metabolomics approaches provided insight into the heterogeneous distribution of analytes within soybean root nodules, orthogonal measurements were required for increased levels of confidence in the molecular identifications of the detected species. Here, we will describe how tandem MS, pre-mass analysis ion mobility separations, and high mass resolution and mass accuracy measurements of the isotopic envelope were utilized to provide confidence in the identity and localization of metabolites within soybean root nodules. We further applied this information to elucidate active metabolic pathways within different compartments of the nodules.

3:00pm **TM-MoA5 Coupling Front-end Electron Transfer Dissociation to Ultra-High Field FTICR-MS**, ***Chad Weisbrod***, *D.F. Smith*, *L.C. Anderson*, *L. He*, *A.G. Marshall*, *C.L. Hendrickson*, The National High Magnetic Field Laboratory **INVITED**

Tandem MS is an indispensable tool of the mass spectrometrist. It enables structural elucidation and aides in unambiguous identification of precursor ions. Many means of performing tandem MS exist and can largely be categorized into three distinct groups: collision-, electron-, and photon-based. Each group has its own set of analytical merits and must be considered carefully when choosing which will best suit the analytical demand. Further, tandem MS can occur in-space or in-time which are unique to specific mass spectrometer configurations. A brief discussion of these categories of tandem MS will be given along with their relative strengths and weaknesses. A justification for our incorporation of front-end electron transfer dissociation (FETD) within the 21 T FTICR-MS at NHMFL will also be discussed. The 21T FT ICR-MS at NHMFL was constructed to achieve extraordinary performance with respect to top-down analysis. This is achieved by the increased field strength and the culmination of several technologies included during its construction. Here we focus on the inclusion of front-end electron transfer dissociation (FETD) coupled with an external multipole storage device (MSD), which allows for analysis of larger cumulative ion targets than ever before and lessens the need transient summing. We demonstrate linear operational range in terms of cumulative ion target (<5.0E4-3E7 total charges) and mass spectra with very high sequence coverage, in-spectrum dynamic range, and mass measurement accuracy despite the large cumulative injection targets. We show performance of FETD applied to standard proteins (3-30 kDa), human cell lysate samples, and monoclonal antibodies.

Authors Index

Bold page numbers indicate the presenter