





EMSL Update: Strategy, Science, Capabilities

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Scientific Innovation Through Integration ■ www.emsl.pnnl.gov

Outline



- EMSL strategy
- Science themes
- New capabilities
- On the horizon

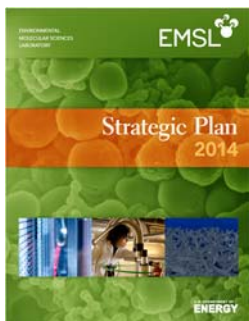


An intricately structured soil bacterium, less than a micron in size, makes its home on the root surface of an Arabidopsis plant.
*Image was captured with the Helios Nanolab dual-beam focused ion beam/scanning electron microscope at EMSL and was created by Alice Dohnalkova.

Our focus is on challenges where molecular-level understanding will have an impact



EMSL's strategic plan sets out 10-year vision and outlines our roadmap for success




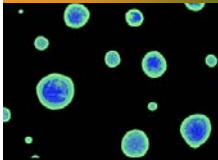
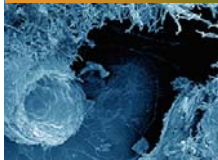
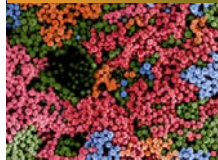
Implementation

TSE Implementation Plan Timeline

Current Status	As assessed by	2014-2016	2017-2020
Energy Efficiency Leadership	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL
Leadership in the field	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL
High quality and award winning research	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL
Leadership in the field	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL	DOE, BER, and DOE-EMSL

- Describes BER and DOE challenges where EMSL can have a sustained scientific impact
- Provides science lens for capability investments
- Developed and peer review with advisory committees, BER, the user community, and EMSL Triennial Review.

EMSL ENVIRONMENTAL MOLECULAR SCIENCE THEMES

Biosystem Dynamics & Design	Atmospheric Aerosol Systems	Terrestrial & Subsurface Ecosystems	Energy Materials & Processes
			
Understanding and optimizing biological pathways in plants and microbes that are central to biofuel production and the global carbon cycle	Molecular-scale understanding of key chemical and physical properties of aerosols to improve the prediction of climate models	Understanding the dynamics of nutrients, metabolites, and contaminants at biogeochemical interfaces to improve their representation in Earth system models	Understanding the physical and chemical properties of interfaces needed to design new materials and systems for sustainable energy applications

EMSL has worked to develop two new instruments to enable new science



- **H**igh **R**esolution **M**ass **A**ccuracy **C**apability (**HRMAC**) is an ultra-high resolution 21T FTICR mass spectrometer
- **D**ynamic **T**ransmission **E**lectron **M**icroscope (**DTEM**) is a near-atomic resolution time-resolved (μ sec-psec) TEM

High performance mass spectrometry for characterization of complex Earth systems EMSL


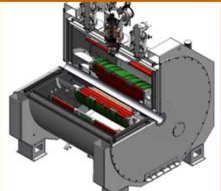

Secondary Organic Aerosols

Soil-Microbe-Plant-Atmosphere Interactions

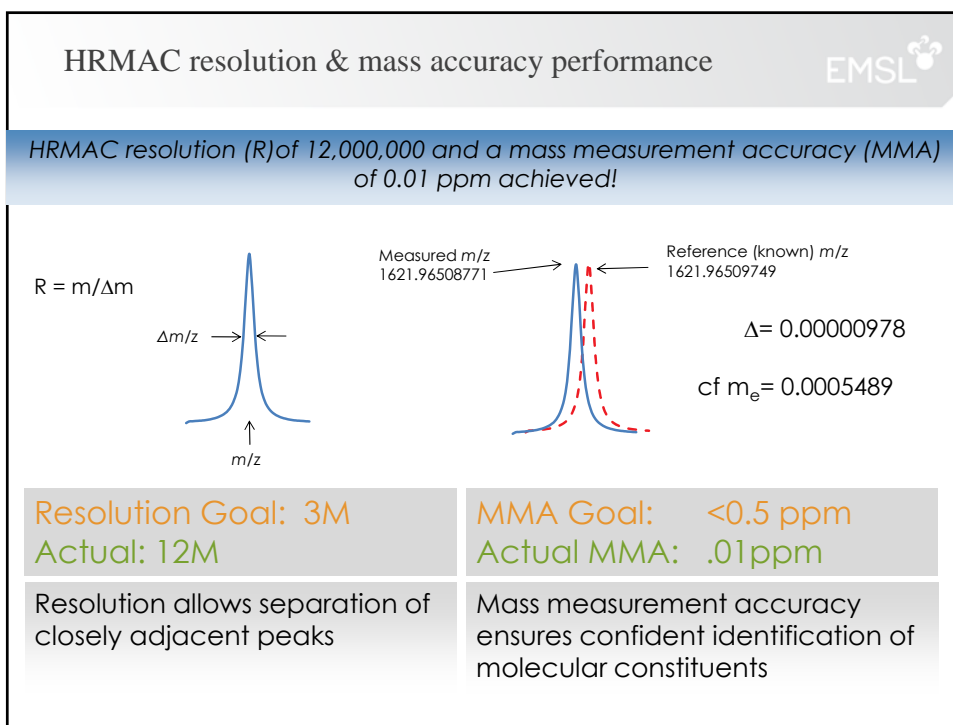
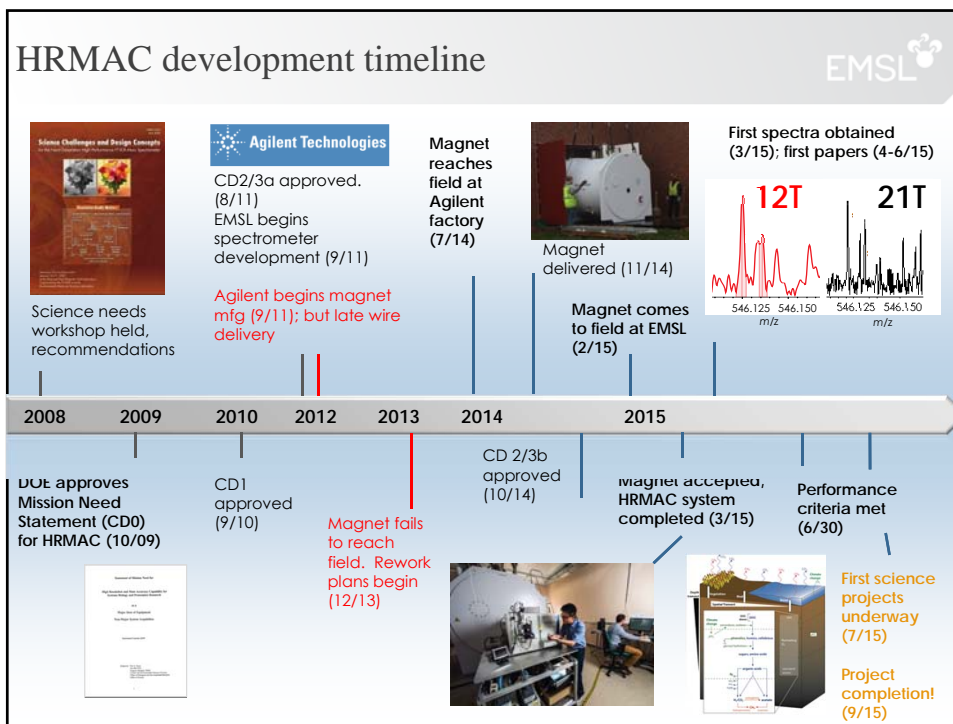
Dissolved/Soil Organic Matter

HRMAC – what is it? EMSL

Ultra-high resolution mass spectrometer

<p>Spectrometer</p>  <ul style="list-style-type: none"> • Sample ionization and transfer, with compositional integrity • Detect, measure ion cyclotron frequencies 	<p>21 T magnet</p>  <ul style="list-style-type: none"> • Induce ion motion in cyclotron field 	<p>Data/control system</p>  <ul style="list-style-type: none"> • Instrument control • Data acquisition, frequency, m/z conversion
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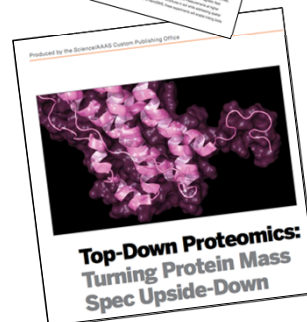
8



HRMAC – first science and outreach



- EMSL issued Special Science Call for HRMAC in April, 2014
 - 11 proposals received; 6 projects selected
- Highlighted in Top-down Proteomics Science article (Sept 11, 2015)
- ~15 technical papers
- 3-4 publications
- <http://www.emsl.pnnl.gov/emslweb/21t-high-resolution-mass-accuracy-capability>

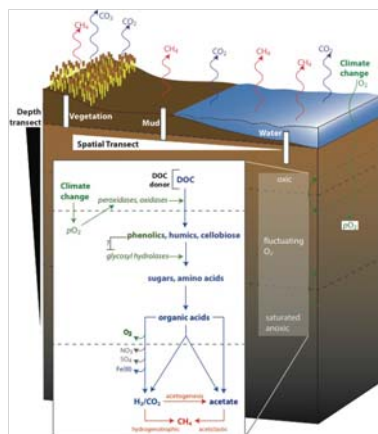


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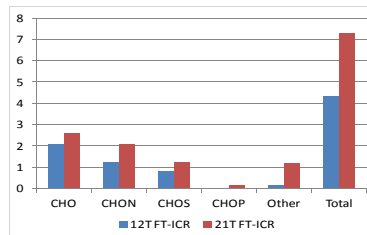
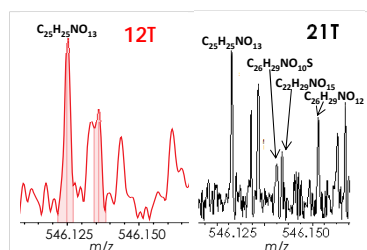
Characterization of dissolved organic carbon in wetland sediments



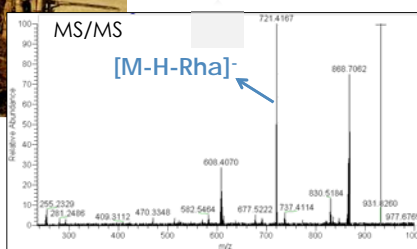
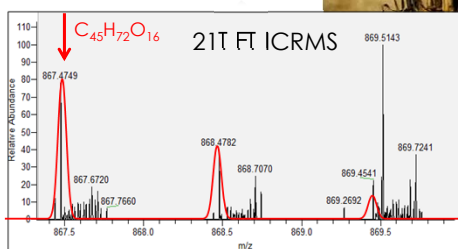
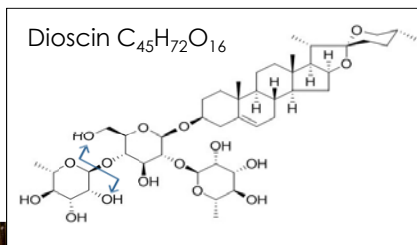
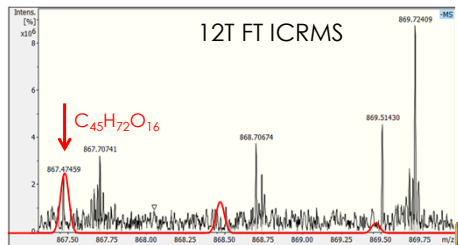
High-resolution, parallel measurements of wetland organic C and microbial community metabolism under changing redox conditions. *Kelly Wrighton, Ohio State University*



Old Woman Creek National Estuarine Research Reserve, Lake Erie (operated by NOAA)



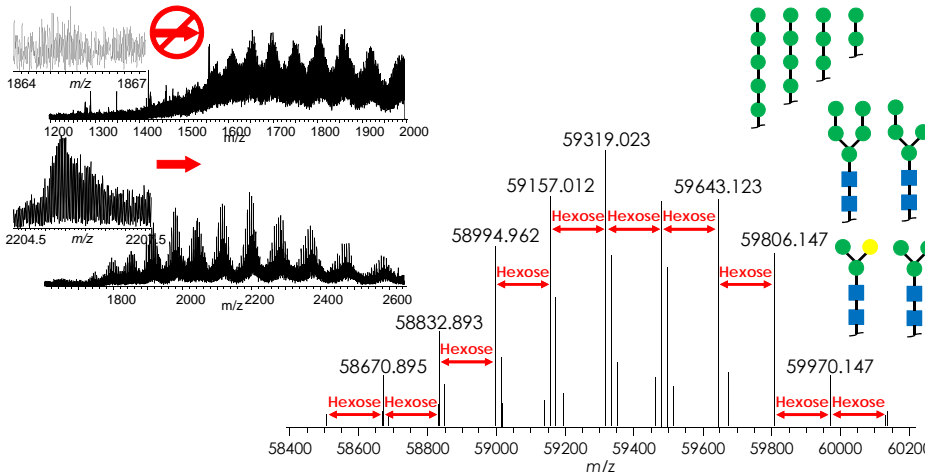
Switchgrass root exudates indentified in rhizosphere soil organic matter (Jim Tiedje, Michigan State Univ.)



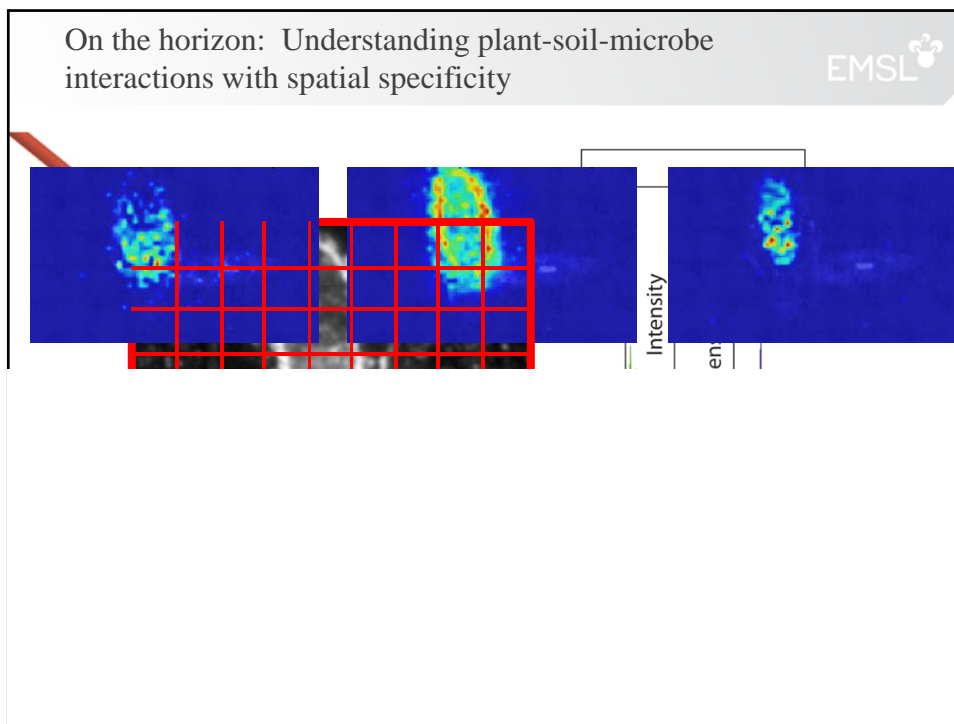
Using top-down proteomics to correlate protein modifications and microbial activity




Glycoproteome analysis of the secretome of the lignocellulose degrading fungus *Neurospora crassa*, Chris R. Somerville, U California, Berkeley



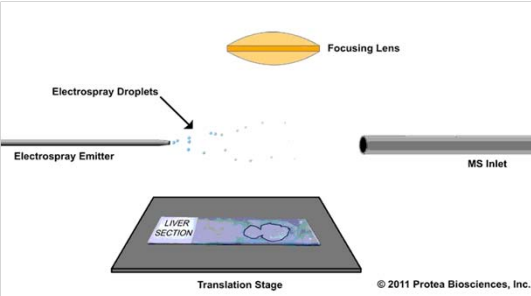
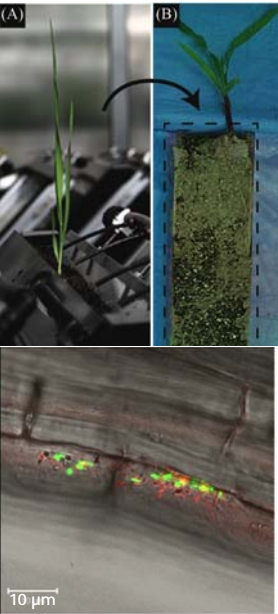
21T FTICR MS lets us not only see large proteins but identify ~ dozen glycoforms



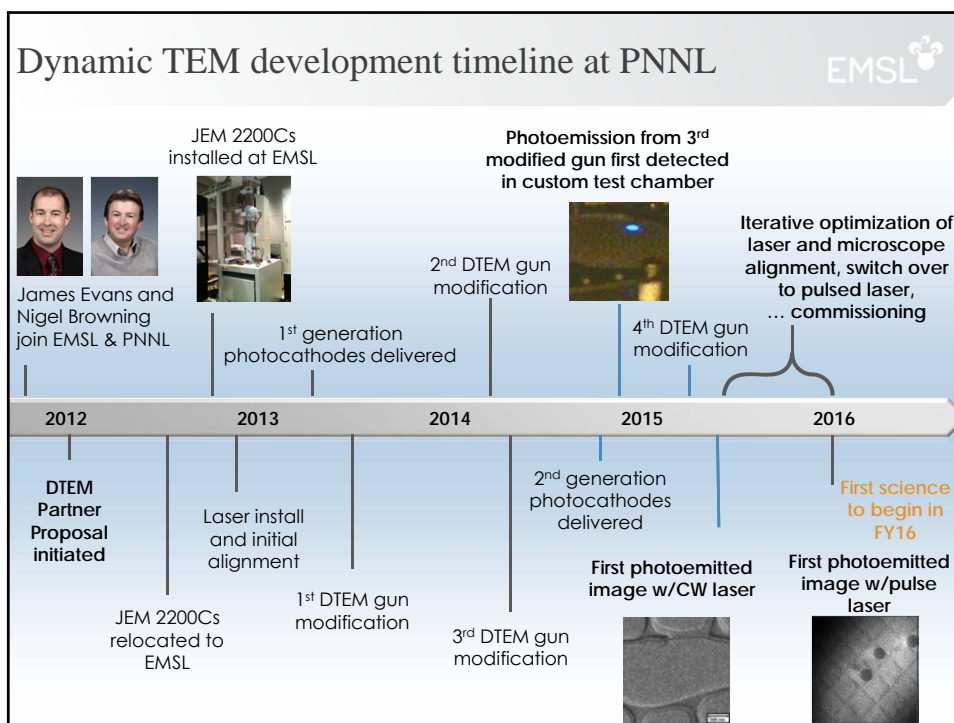
On the Horizon: *In situ* molecular imaging of the soil/rhizosphere



Development and refinement of a molecular microscope capability based on ultra-high resolution mass spectrometry.
 BER Mesoscale Imaging Pilot Project
 Gary Stacey, U Missouri
 George Vertes, George Washington U
 Pasa-Tolic & Koppenaal, PNNL

Combines laser ablation with secondary electron spray ionization with 21T FTICRMS



On the horizon: Visualizing conformational changes of soluble protein complexes Understanding nitrogen fixation

Understanding nitrogen fixation

PDBs: 2AFH, 2AFI, 2AFK

Reaction can be initiated by flash photolysis of NPE-caged ATP

PI: Rauaei
Co-PIs Seefeldt and Evans

Current structures for nucleotide free, Mg-AMPPCP bound and Mg-ADP bound solved using static X-ray crystallography

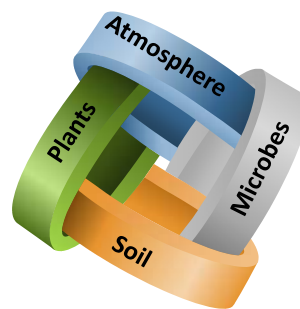
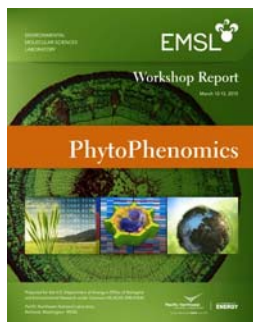
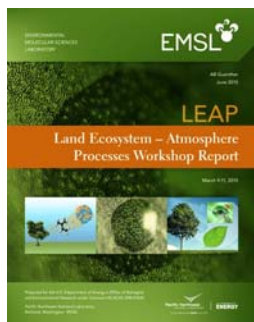
Real-time *in situ* observations with Dynamic TEM to probe structures of non-stabilized and transient conformations...
Will be extensible to cellulosome and other large complexes

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On the horizon: Exploring integrated plant-aerosol-soil sciences capability/facility



Advance our understanding of plant ecosystem dynamics by exploring interactions among plants, microbes, atmosphere, and soil in integrated Plant-Atmosphere-Soil Systems (iPASS)



19

Building upon a strong foundation



Science needs

VOC Emission and Aerosol Formation, Cloud Interactions

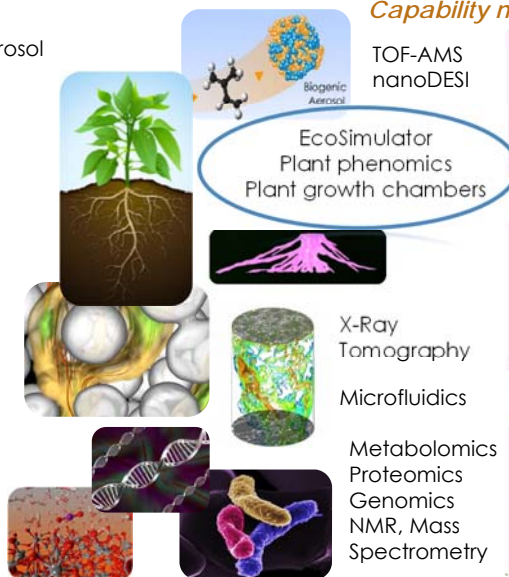
Plant Photosynthesis and Respiration

Root Morphology and Flow

Porous Media Flow and Transport

Genome-Based Metabolic Models

Free Energy Calculations



Capability needs

TOF-AMS
nanoDESI

AAS

EcoSimulator
Plant phenomics
Plant growth chambers

TSE

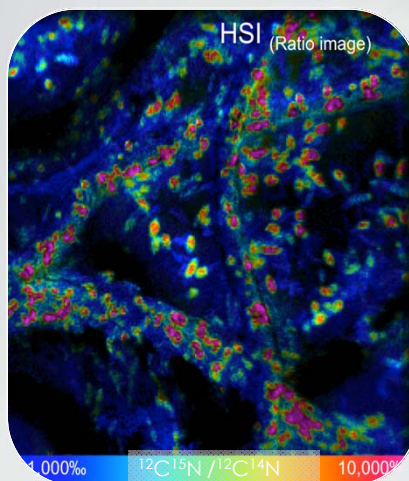
X-Ray
Tomography

Microfluidics

Metabolomics
Proteomics
Genomics
NMR, Mass Spectrometry

BDD

Questions?



NanoSIMS ratio image of $^{12}\text{C}^{15}\text{N}/^{12}\text{C}^{14}\text{N}$ in uncyanobacterial consortia measured using a CAMECA NanoSIMS by John Cliff