



## EMSL Update: Strategy, Science, Capabilities

Allison A. Campbell  
Acting Associate Laboratory Director  
Earth & Biological Sciences Directorate



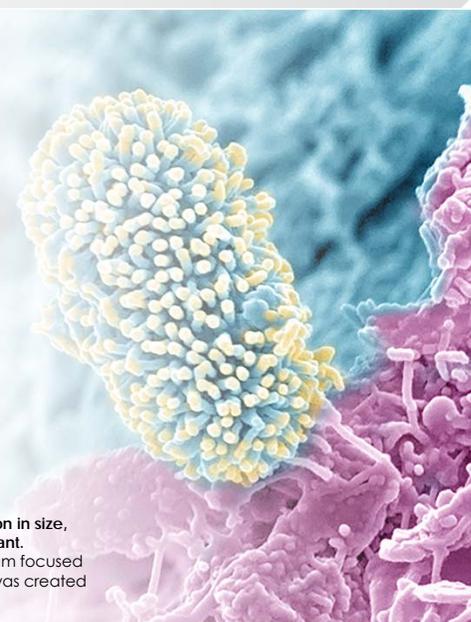
Scientific Innovation Through Integration ■ [www.emsl.pnnl.gov](http://www.emsl.pnnl.gov)

### 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.





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

EMSL

Strategic Plan 2014

Implementation

TSE Implementation Plan Timeline

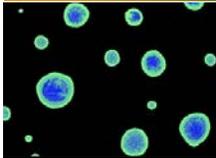
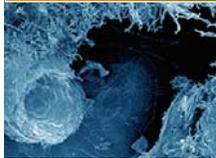
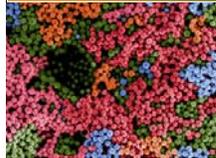
| Current Status   | 2014-2016  | 2017-2020  | 2021-2024  |
|--|--|--|--|
| <p>Established leadership</p> <ul style="list-style-type: none"> <li>EMSL is a BER/DOE program</li> <li>EMSL is a DOE program</li> <li>EMSL is a BER program</li> <li>EMSL is a DOE program</li> <li>EMSL is a BER program</li> <li>EMSL is a DOE program</li> </ul>             | <p>Develop a vision and strategy</p> <ul style="list-style-type: none"> <li>Develop a vision and strategy</li> </ul> | <p>Develop a vision and strategy</p> <ul style="list-style-type: none"> <li>Develop a vision and strategy</li> </ul> | <p>Develop a vision and strategy</p> <ul style="list-style-type: none"> <li>Develop a vision and strategy</li> </ul> |
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- 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.

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EMSL ENVIRONMENTAL MOLECULAR SCIENCE LABORATORY

### 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 ( $\mu$ sec-psec) TEM

High performance mass spectrometry for characterization of complex Earth systems EMSL

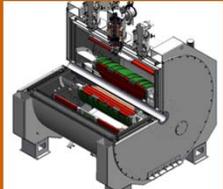
Secondary Organic Aerosols

Soil-Microbe-Plant-Atmosphere Interactions

Dissolved/Soil Organic Matter

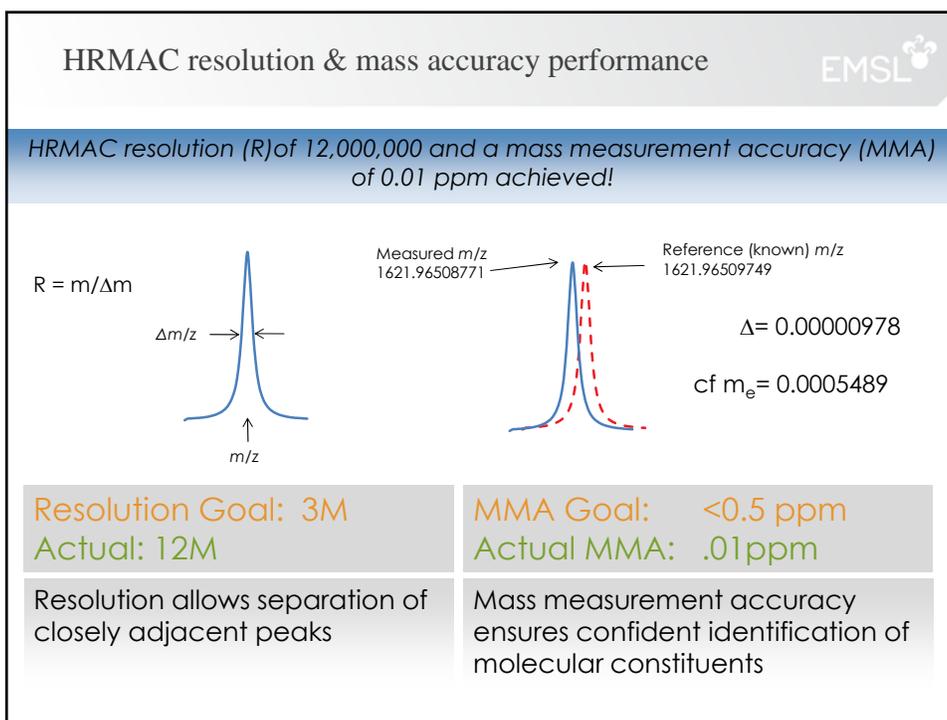
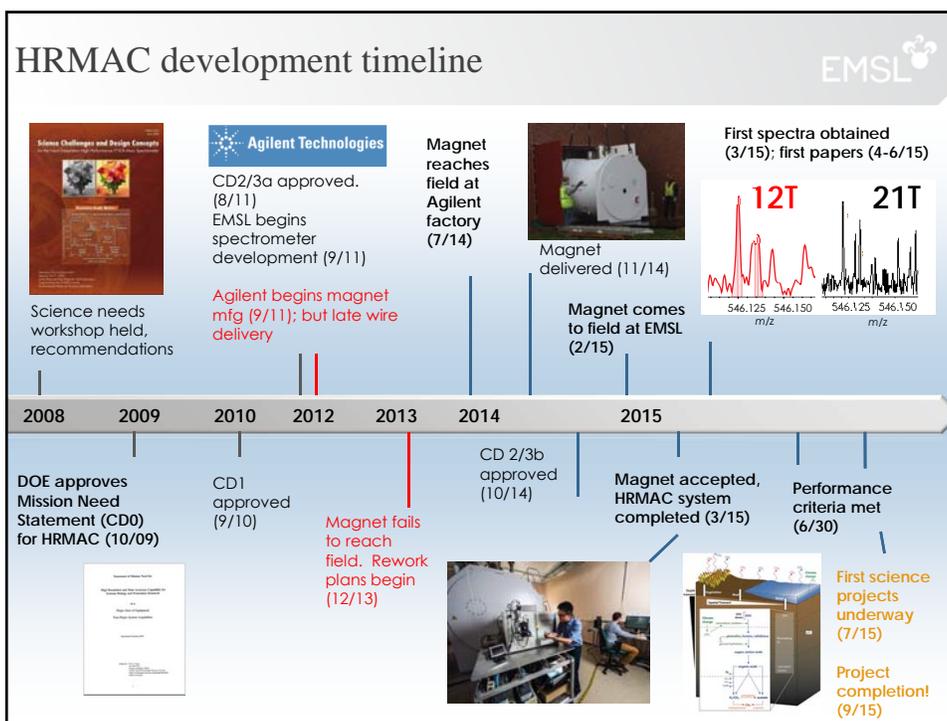
HRMAC – what is it? EMSL

Ultra-high resolution mass spectrometer

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

\$17.5 M budget, 2009-2015 project period

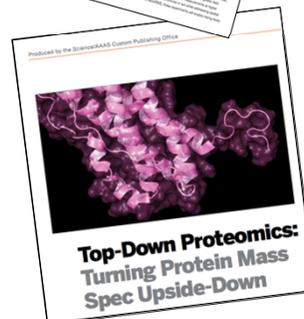
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## HRMAC – first science and outreach



- 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>

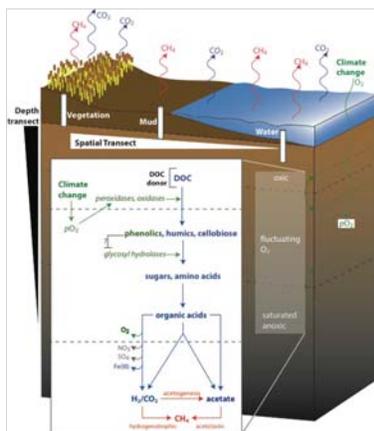


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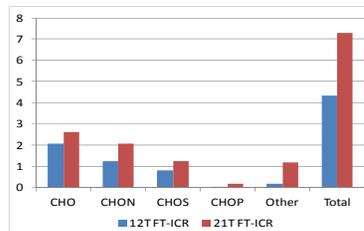
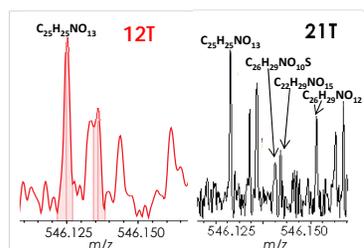
## Characterization of dissolved organic carbon in wetland sediments



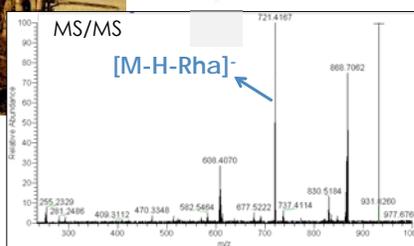
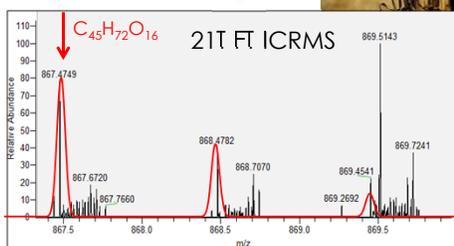
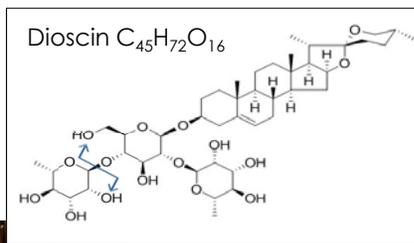
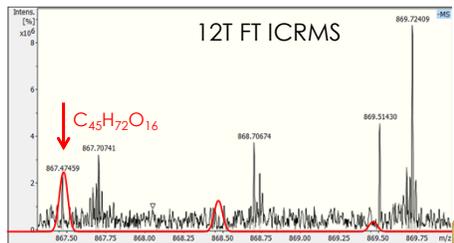
High-resolution, parallel measurements of wetland organic C and microbial community metabolism under changing redox conditions. *Kelly Wrighton, Ohio State University*



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



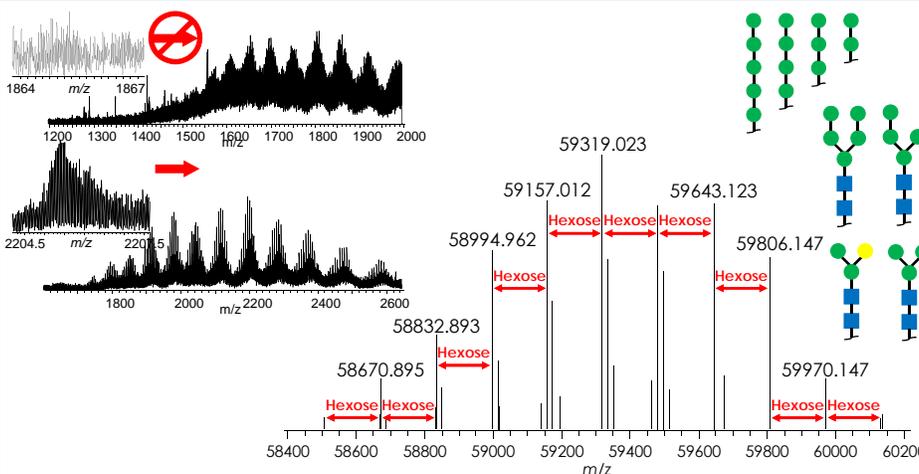
Switchgrass root exudates indentified in rhizosphere soil organic matter (Jim Tiedje, Michigan State Univ.)



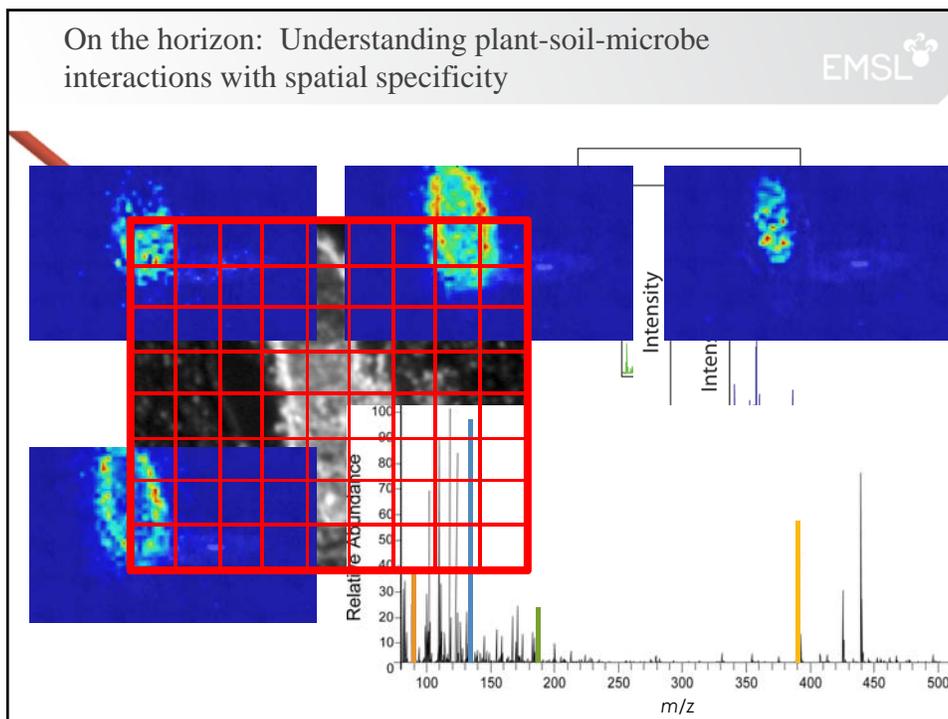
Using top-down proteomics to correlate protein modifications and microbial activity



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

(A) (B)

10 μm

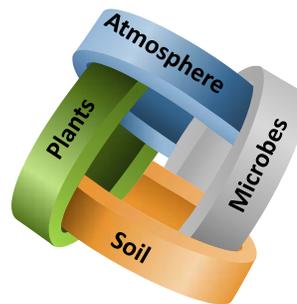
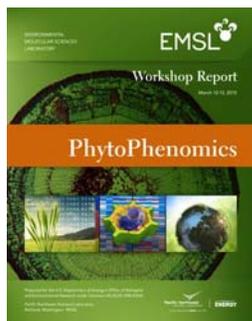
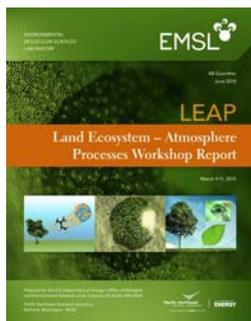
Combines laser ablation with secondary electron spray ionization with 21T FTICRMS



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)



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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

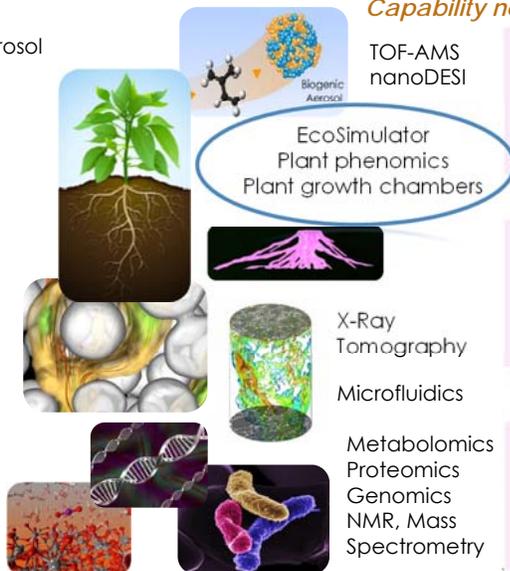
TSE

X-Ray  
Tomography

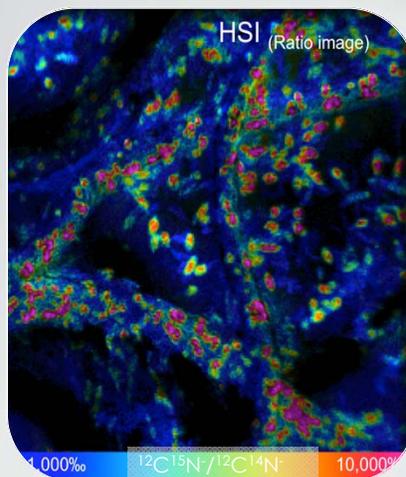
Microfluidics

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