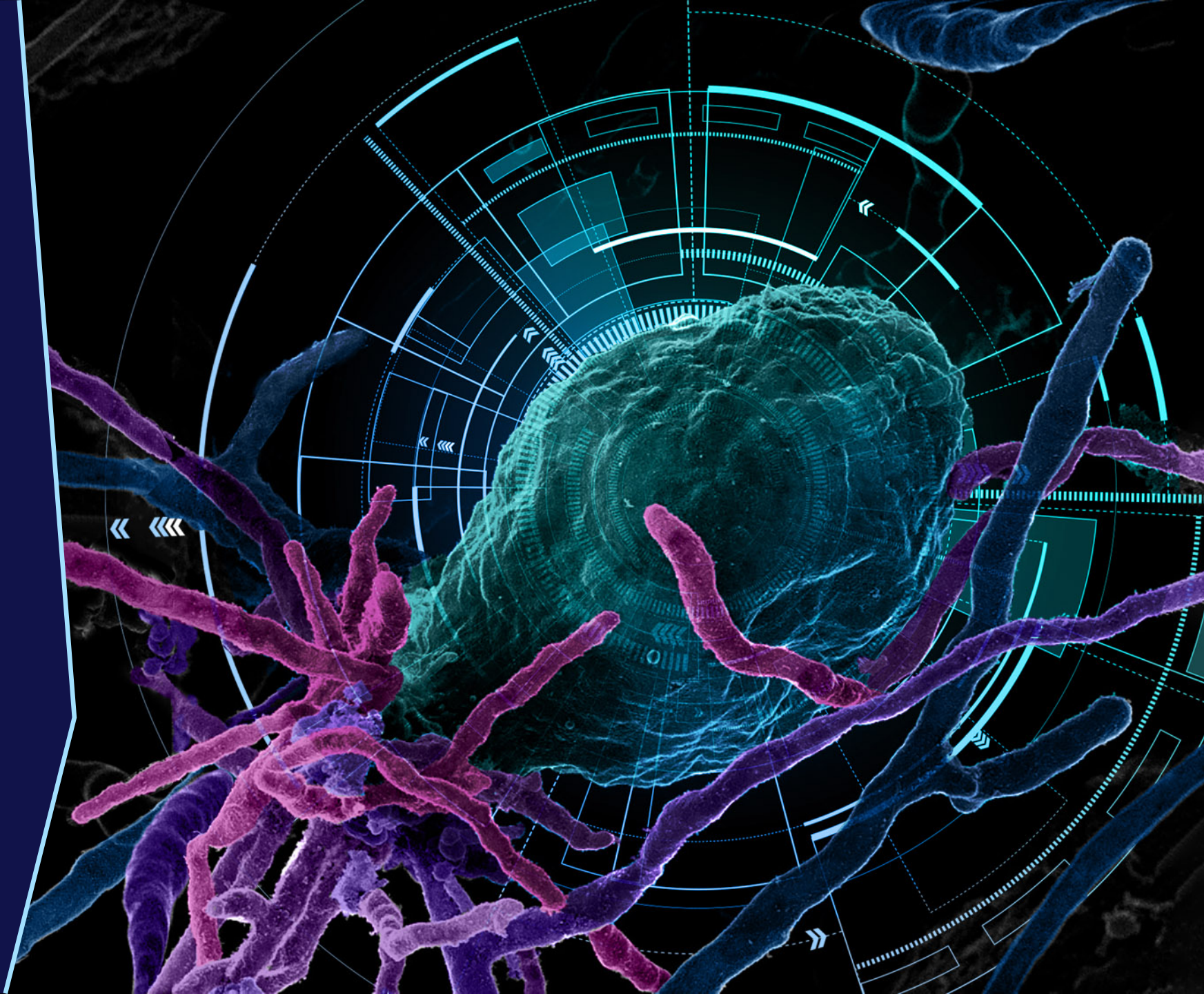




# Environmental Molecular Sciences Laboratory

Nancy Hess  
Environmental  
Transformations and  
Interactions Science Lead







## EMSL at a glance



## Research highlights



## Access

EMSL  
at a  
glance

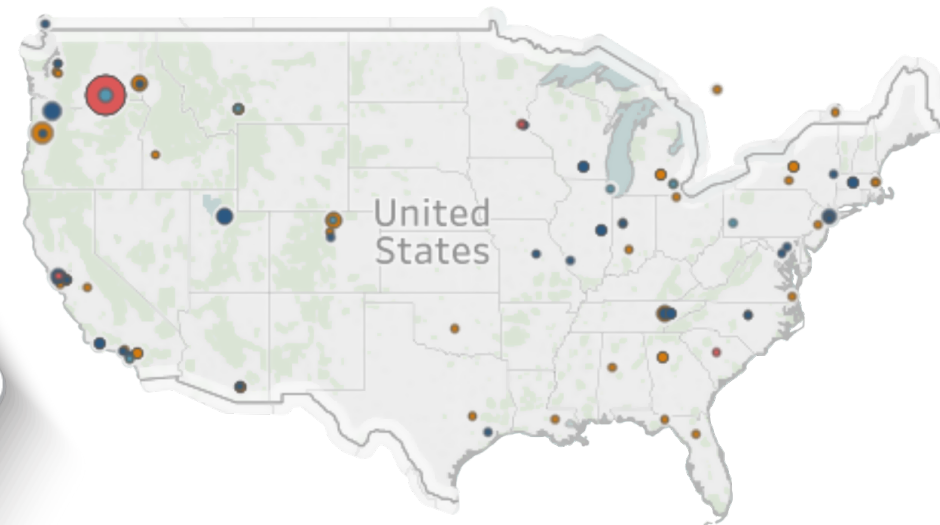
# EMSL is a national user facility with expertise and capabilities in environmental and biological science

- Funded by Office of Science Biological and Environmental Research (DOE SC BER)
- Integrative experimental, modeling, and computational approaches across molecular to ecosystem scale
- User access through peer-reviewed proposal process
- Free for non-proprietary work





# EMSL at a glance

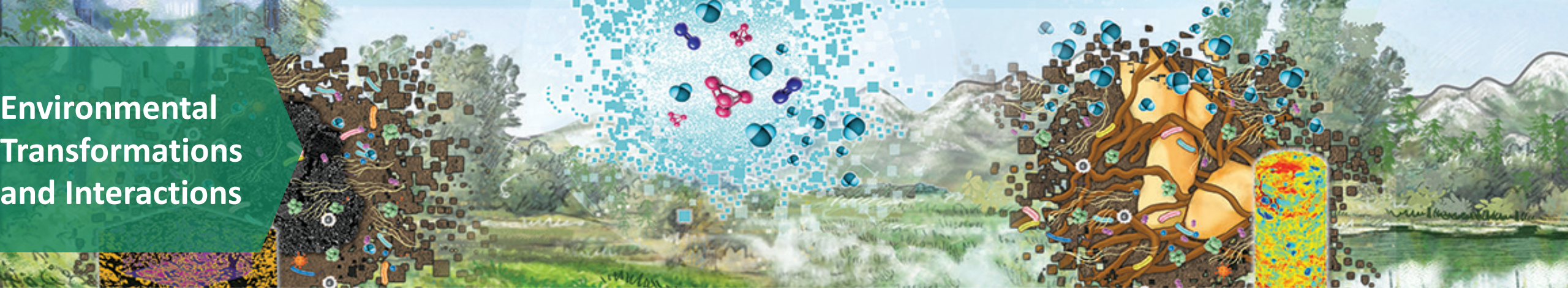


EMSL's global and U.S. user community  
<https://www.emsl.pnl.gov/emslweb/for-users>





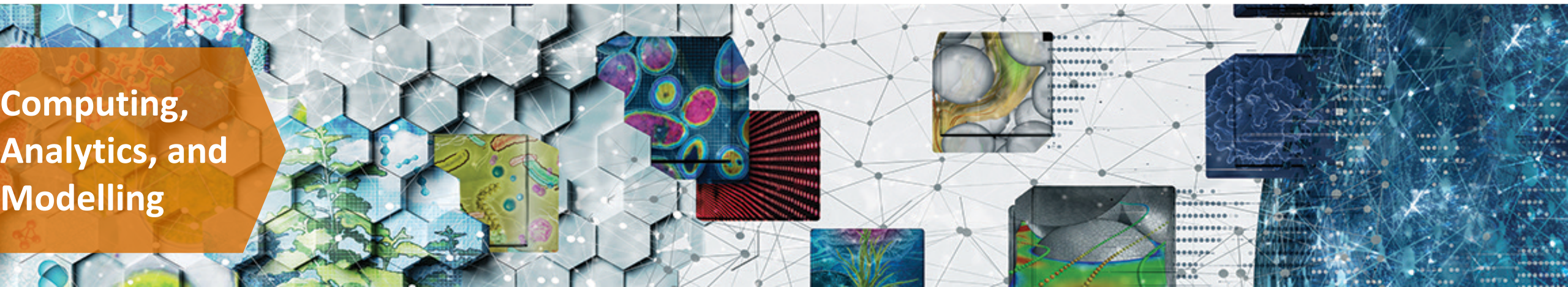
# Environmental Transformations and Interactions



# Functional and Systems Biology



# Computing, Analytics, and Modelling





# EMSL's Science Areas and Integrated Research Platforms

## BIOLOGY IRPS

Structural  
Biology

Biomolecular  
Pathways

Cellular  
Signaling and  
Communications

Cell-cell  
Interactions

In Situ Cellular  
Processes

Global (3D)  
Protein Structure

Protein & Metabolic  
Regulation

Single Cell  
Characterization

## SCIENCE TOPICS

Modeling & Simulation  
of Complex Systems

Data Analysis &  
Visualization

Genotype to  
Phenotype

Metabolic  
Pathways

Microbial  
Community Analysis

Plant-Mineral-  
Microbe Interaction

Stable Isotope  
Probing

## ENVIRONMENT IRPS

Chemical Functional  
Group Reactivity

Subsurface Flow &  
Transport

Environmental  
Nutrient Cycling

Environmental  
Predictive Modeling

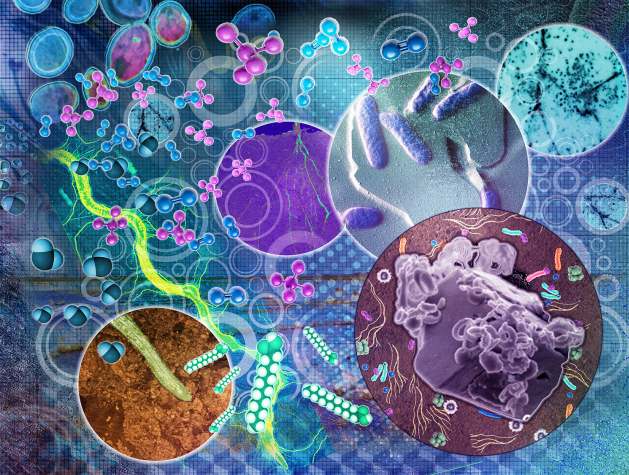
Mineral Associated  
Organic Matter

Plant  
and Ecosystem  
Phenotyping

Biogeochemical  
Transformations

Ecosystem  
Interfaces





**BGT:** Examines the detailed molecular biogeochemistry within microdomains in soils and sediments.

**EI:** Multi-disciplinary expertise focused on studying the transport of nutrients and materials that contribute to enhanced rates of biogeochemical processes at ecosystem interfaces.

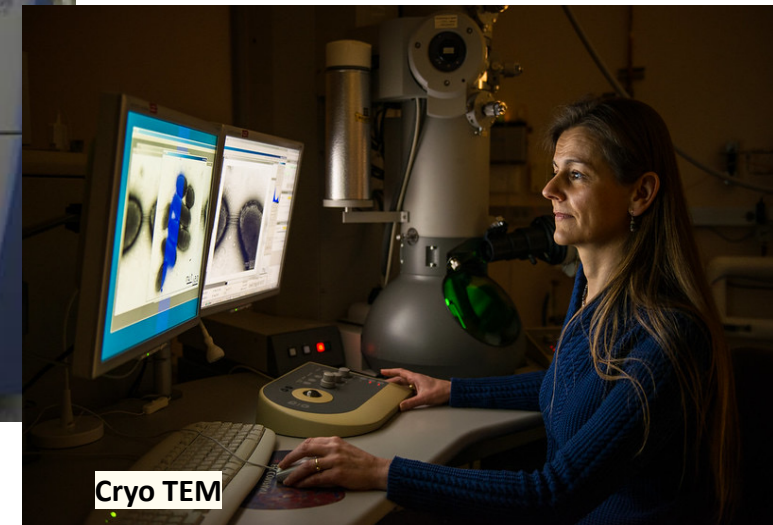
## Biogeochemical Transformations and Ecosystem Interfaces



SOM/DOM characterization



IRMS



Cryo TEM

**IRP Leads**  
**Emily Graham (BGT)**  
[Emily.graham@pnnl.gov](mailto:Emily.graham@pnnl.gov)  
**Jim Moran (EI)**  
[James.moran@pnnl.gov](mailto:James.moran@pnnl.gov)

- MS and NMR based organic matter analysis
- Isotope studies for quantification of stable isotope tracers
- Electron microscopes for chemical imaging

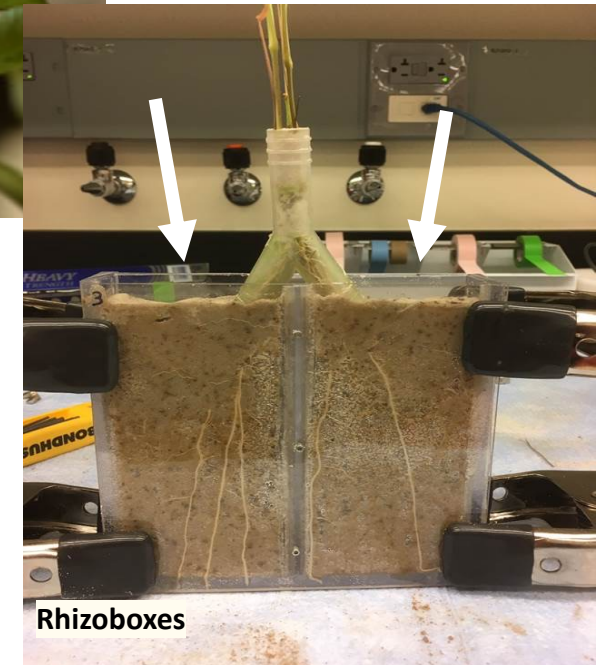


**Aims to dissect plant genotype-environment interactions, including the plant-microbe crosstalk in the rhizosphere region, to establish an advanced understanding of the molecular mechanisms involved in the determination of phenotypic plasticity in a complex multifactorial ecosystem. .**

## Plant and Ecosystem Phenotyping



Plant Growth Chambers

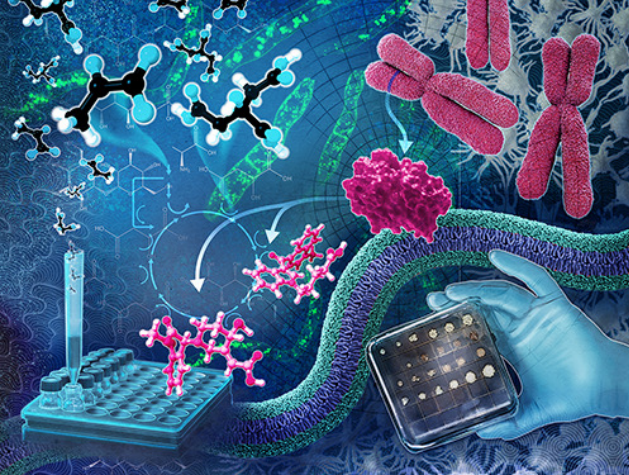


Rhizoboxes

IRP Lead  
**Amir Ahkami**  
[amir.ahkami@pnnl.gov](mailto:amir.ahkami@pnnl.gov)

- Phytotron for controlled plant growth.
- Rhizoboxes and rhizotrons, track plants and their developing roots
- MS and stable isotope tracers to track metabolite and substrate flux



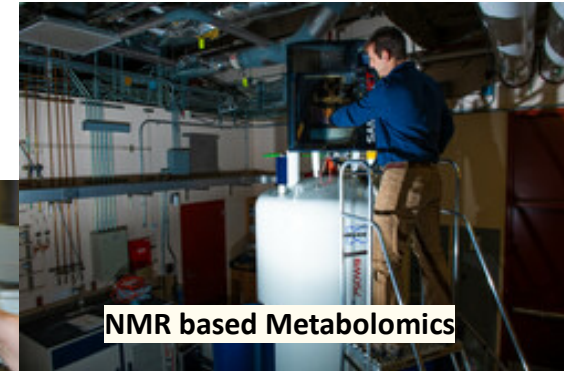


Discovers the principles underlying the translation of genomic information into the metabolic pathways and regulatory networks that determine cellular function.

## Biomolecular Pathways



Proteomics and Lipidomics



NMR based Metabolomics



MS based Metabolomics



Intact Protein Analysis

- Comprehensive and integrated characterization of complex biological and environmental systems
- Multi-omics on the same sample
- In-depth structure and function studies of intact proteins
- MS imaging capabilities for spatial, quantitative molecular information



Pursues an understanding how complex phenotypes arise from individual molecules and their interactions with other molecules within the communication networks that exist between, and across populations and communities of cells.

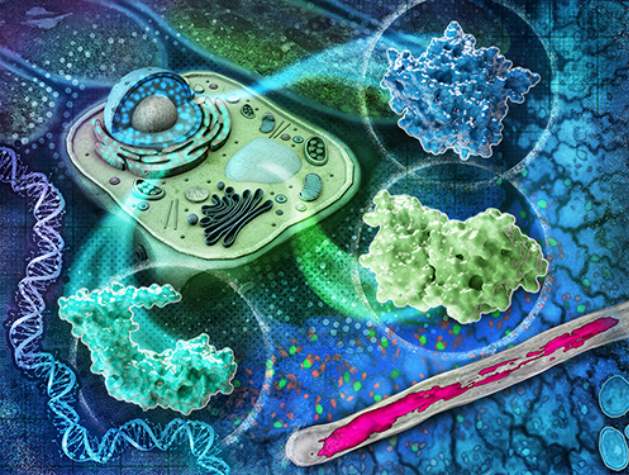
## Cell Signaling and Communication



- Laser capture microdissection microscopes to isolate individual cells or cell types
- Optical microscopy techniques, to understand dynamic processes in live or intact cells.
- Single-molecule fluorescence in situ hybridization (FISH), for quantitative analyses of biomolecules in individual cells within communities or tissues.

IRP Lead  
**Alex Beliaev**  
[Alex.beliaev@pnnl.gov](mailto:Alex.beliaev@pnnl.gov)



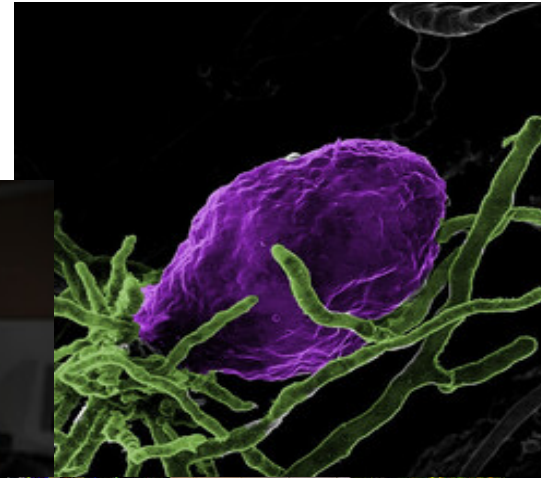


**Generates structural, biochemical, and dynamic information about proteins, protein complexes, and other biomolecules at nanoscale spatial and temporal resolution to determine biological function.**

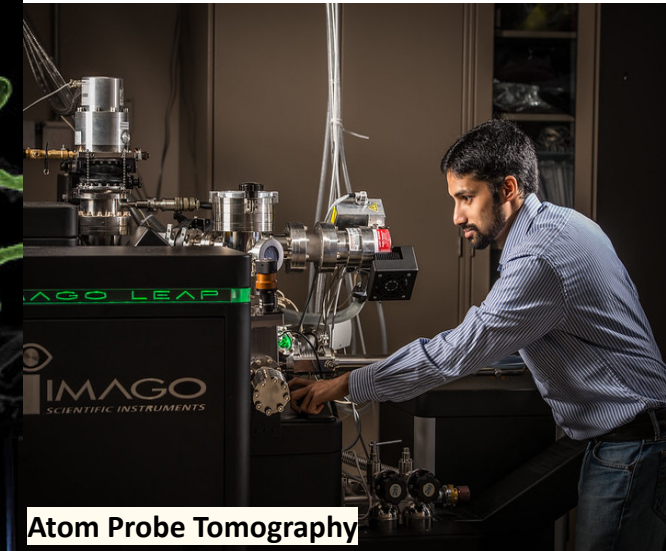
## Structural Biology



Cryo TEM



Tahoma Super Computer



Atom Probe Tomography

- Produce three-dimensional images of elements and molecular fragments—at the atomic scale—within soft biological materials.
- Determine the atomic-scale structure of proteins and protein complexes greater than ~100kDa.
- EMSL's structural biology is expanding to include correlative multi-modal imaging and analyses.

IRP Lead  
**Scott Lea**  
[scott.lea@pnnl.gov](mailto:scott.lea@pnnl.gov)

## Science highlights

**69%**

of user publications  
have EMSL staff co-authors

**45%**

in Top 10 journals

**7.4** avg. impact factor

**40**

High-impact  
journal papers

PNAS (5)

Science (2)

Nature Series (33)

**416**

Publications  
(61% in BER science)

PNAS

Science

nature

nature  
structural &  
molecular biology

nature  
COMMUNICATIONS

nature  
microbiology

nature  
ecology & evolution

nature  
materials

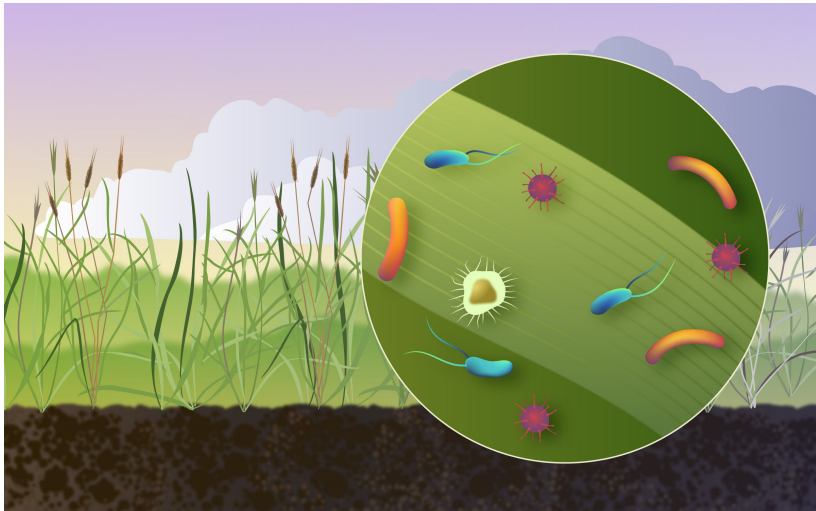




## Self-healing cement for deep CO<sub>2</sub> sequestration

Microscopic and spectroscopic analysis of self-healing polymer-cement composite reveals reduced structural and chemical changes after carbonate formation.

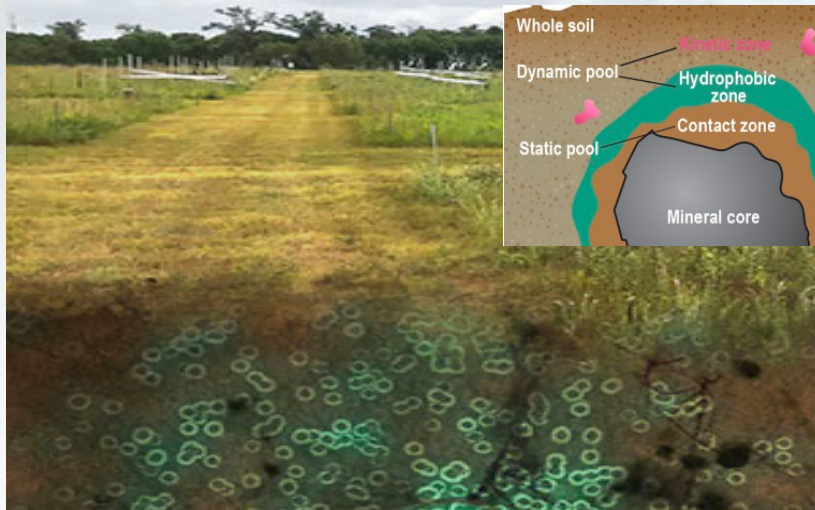
M.S. Elbakhshwan, *et al. Geothermics* (2021)  
DOI:10.1016/j.geothermics.2020.101932



## Wild grass releases a variety of particles into the air over its life cycle

Fungal spores are found to be most abundant during initial growth, while bacteria predominate during flowering and fruit development.

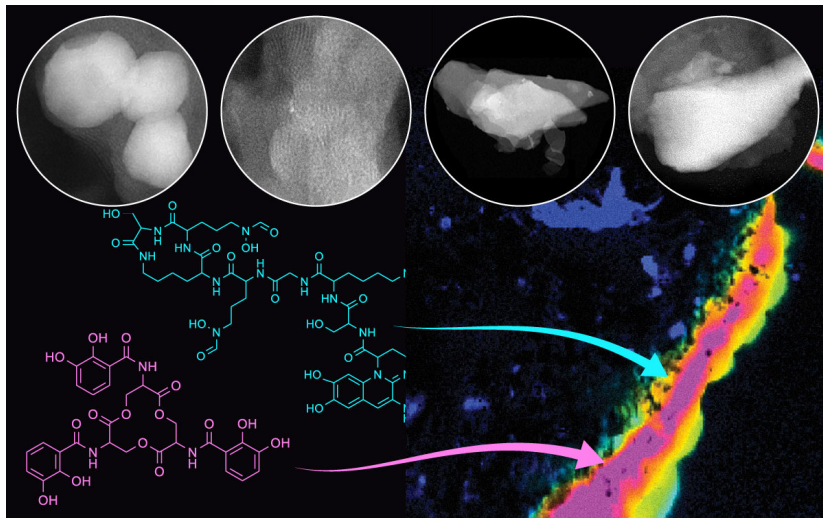
S. China, *et al., ACS Earth and Space Chemistry* (2020).  
DOI: 10.1021/acsearthspacechem.0c00144



## Soil minerals control carbon availability in N fertilized grasslands

Fertilized plots had different assortment of organic molecules associated with soil Fe-minerals than non-fertilized plots.

Q. Zhao, *et al.*, *Science of the Total Environment* (2020)  
DOI: 10.1016/j.scitotenv.2020.137839]



## Ca bridging between OM and minerals in alkaline soil

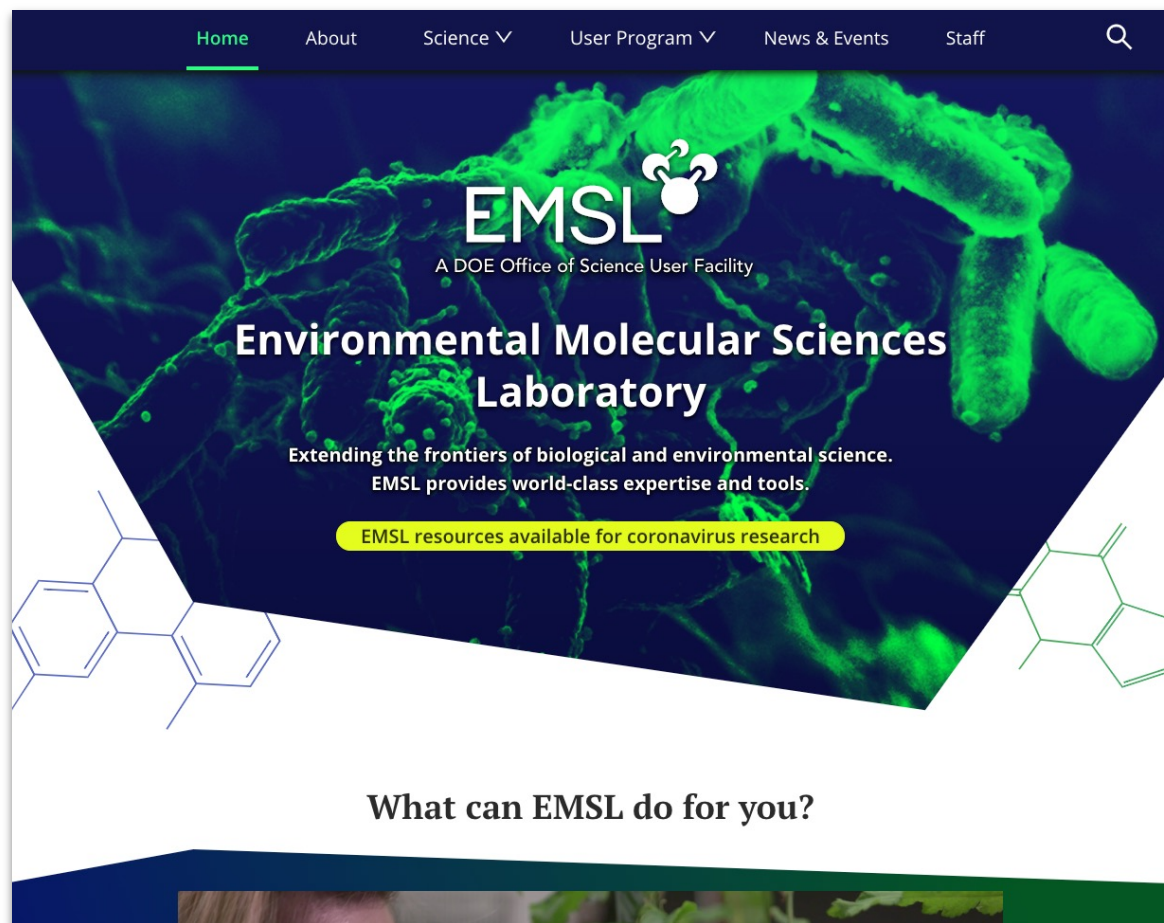
Revealed that organic molecules in which aggregate via cation bridging favoring the stabilization of organic molecule complexes rather than on mineral surfaces.

R.M. Boiteau, *et al.* *Science of the Total Environment* (2020)  
DOI: 10.1016/j.scitotenv.2020.138250



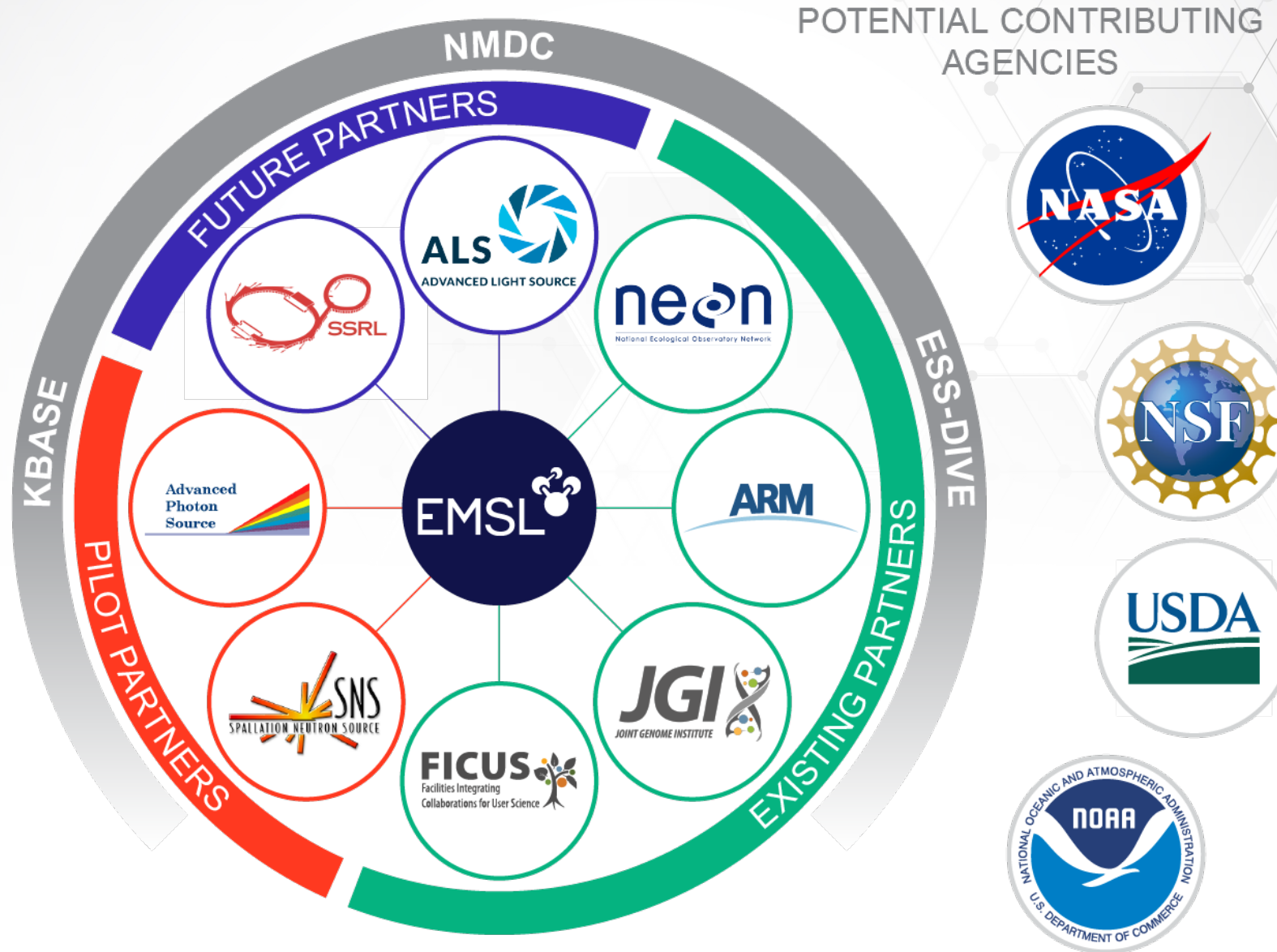
- Large-Scale Research Proposals
- Joint-access FICUS Proposals
- Exploratory Proposals

EMSL offers multiple opportunities for user access



More information at [www.emsl.pnnl.gov](http://www.emsl.pnnl.gov)

# FICUS - Facilities Integrating Collaboration for User Science





# Previous events

Andrea Starr Tim Scheibe Stephanie Nap... Alexander Alle... Amelia Nelson Sarah Hellman

**2020 MULTISCALE MODELING SUMMER SCHOOL**

**Kaitlin Rempfert**  
University of Colorado Boulder

**RPL**  
ROCK POWERED LIFE

- Science Question: How do the mechanisms of low temperature water/rock reactions control the distribution, dynamics, and biosignatures of life in rock-hosted systems?
- Approach/Methods:
  - 16S amplicon and shotgun metagenomic sequencing
  - Lipidomics (HPLC-MS)
  - Context of aqueous geochemistry and mineralogy
    - Including origin of key electron acceptors such as nitrate (dual nitrogen and oxygen isotopic analysis)

Reimpfert et al. 2017, Front. Micro.

**Summer School 2020**  
**July 6-10, 2020**



**2020 EMSL Integration**  
**October 5-8, 2020**

**SHAPING THE FUTURE OF SCIENCE**

**TOWNHALL**

COLLABORATE WITH A DOE USER FACILITY: LEARN ABOUT AVAILABLE EXPERTISE AND RESOURCES, OPEN CALL OPPORTUNITIES, AND IMPORTANT TIPS FOR SUBMITTING SUCCESSFUL PROPOSALS

**AGU FALL MEETING**

**AGU BER User Facility Townhall**  
**December 7, 2020**

**Pacific Northwest National Laboratory**

**X-ray Spectroscopy Studies of Molecules and Materials with Linear-Response TDDFT**

**Niri Govind**  
EMSL-SSRL Workshop  
Jan 2021

**ENERGY BATTTELLE**

**Spectroscopy and Modeling Workshop**  
**January 26, 2021**

**FICUS**  
Facilities Integrating  
Collaborations for User Science

**EMSL**  
**JGI**  
**OAK RIDGE National Laboratory**

**FY 2022 FICUS Call for Proposals**  
EMSL/JGI (including CSMB and NEON)

Webinar for BioSANS instrument

**LSR/FICUS Webinars**  
**February - March 2021**



# UPCOMING EVENTS

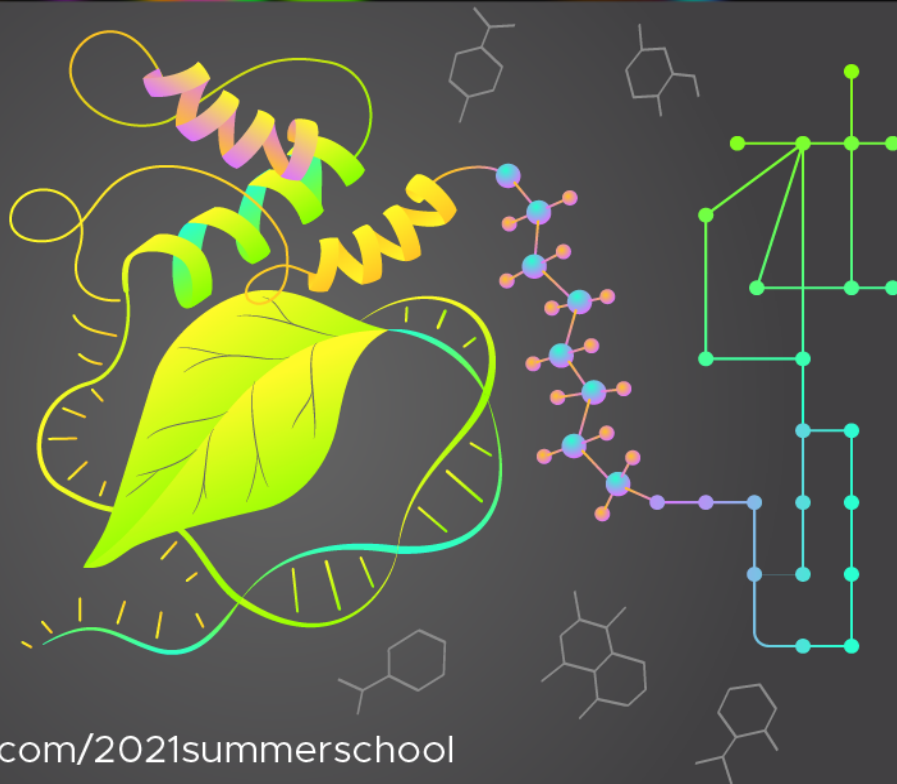
EMSL

## SUMMER SCHOOL

Multi-omics  
Modeling of  
Biochemical  
Pathways

July 12-16, 2021

[pnnl.cventevents.com/2021summerschool](https://pnnl.cventevents.com/2021summerschool)



## 2021 INTEGRATION Meeting

Environmental sensors

October 4-7



EMSL

Free! • Virtual • Engaging speakers • Instructive tutorials • Registration required



# Questions?



Nancy Hess, [nancy.hess@pnnl.gov](mailto:nancy.hess@pnnl.gov)

Environmental Transformations  
and Interactions

Scott Baker, [scott.baker@pnnl.gov](mailto:scott.baker@pnnl.gov)

Functional and Systems Biology

Lee Ann McCue, [leeann.mccue@pnnl.gov](mailto:leeann.mccue@pnnl.gov)

Computation, Analytics, and Modeling