# EMSL<sup>®</sup> INTEGRATION Meeting 2019

# **PLANTS, SOIL AND AEROSOLS:**

Interactions that tell stories of Ecosystems, Climate and National Security

**Christer Jansson** Laboratory Fellow

October 8-10, 2019 Discovery Hall, PNNL



Pacific Northwest

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# **2019 EMSL Integration Meeting Report**

C. Jansson

May 2020

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Pacific Northwest National Laboratory Richland, Washington 99352

### Summary

Community. At the Environmental Molecular Sciences Laboratory (EMSL), community is a word that describes the plant scientists, climatologists, and atmospheric chemists who gathered for the user facility's 2019 Integration Meeting October 8–10, 2019.

World-renowned speakers from Europe, Asia, and the United States met with this scientific community to focus on biogenic volatile organic compounds responsible for ecosystem signaling and biological warfare, primary and secondary aerosol involvement in ecosystem and climate feedbacks, and "carbon on the move"—how photosynthates, the products of photosynthesis, are allocated between plants and the soil.

The guests represented academia, national laboratories, and other institutions, and included representatives from the Office of Biological and Environmental Research and the EMSL User Executive Committee.



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### Introduction

EMSL hosts an annual meeting to bring together scientists from academia, national laboratories, federal agencies, and other institutions. It is an opportunity for scientists at EMSL to share the directions in which its science is heading, answer questions about what the user facility can do for users, and welcome suggestions for new capabilities that the EMSL Leadership Team might explore.

The meeting is also an opportunity for invited speakers to share their research findings during plenary and session presentations, and other speakers to do the same during contributed talks and poster sessions.

Every year, announcements about the upcoming meeting inform the scientific community about the year's topics and dates. Early announcements ask the community to save the date on their calendars. Other announcements invite scientists to submit abstracts for contributed talks and posters. Several methods are used to promote the meeting, including EMSL scientists telling people at other meetings, and making multiple announcements in emails and on social media, on the EMSL website and in the EMSL newsletter.

The 2019 Integration Meeting titled "Plants, Soil and Aerosols:



Registration is now open for EMSL Integration 2019 – Plants, Soil and Aerosols to be held October 8–10 at PNNL. More

Interactions that Tell Stories of Ecosystems, Climate and National Security," took place in Discovery Hall at Pacific Northwest National Laboratory (PNNL), October 8–10, 2019. The timely topics, engaging speakers, and promotional efforts resulted in the largest attendance in the meeting's history.

EMSL scientists and staff, along with support staff, organized the meeting and hosted the scientific community.

Christer Jansson, Laboratory Fellow, Biologist, Lead meeting organizer	Eva Baroni, Project Coordinator
Pubudu Handakumbura, <i>Biologist</i>	Mary McGown, Lead Administrator
Amir Ahkami, <i>Biologist</i>	Haylie Kimball, Administrator
Chris Anderton, <i>Chemist</i>	Linda Isakson, Communications Partner
Libor Kovarik, Materials Scientist	Shalonne Luke, Communications Specialist
Swarup China, <i>Chemist</i>	John Nicksich, Communications Specialist
Teresa Palazzo, Post Doctorate Research Associate	Beth Norris, Community Affairs Specialist

Special thanks to Thermo Fisher Scientific who helped sponsor the meeting.



#### **1.0 Science Sessions**

#### **1.0 Science Sessions**

Christer Jansson, Laboratory Fellow, and lead organizer for the meeting, started Day 1 by welcoming the guests and making opening remarks. Douglas Mans, EMSL Director, followed with his welcome and a brief presentation about EMSL.

Days 1 and 2 were dedicated to science sessions organized around three themes:

- Biogenic volatile organic compounds (BVOC) responsible for ecosystem signaling and biological warfare
- Primary and secondary aerosol involvement in ecosystem and climate feedbacks
- Carbon on the move—how photosynthates, the products of photosynthesis, are allocated between plants and the soil.

Each theme had two sessions that started with one plenary speaker, followed by session speakers, plus contributed talks. The agenda was organized to spread the sessions for each theme across two days. This section of the report summarizes the presentations by the invited plenary and session speakers.



Christer Jansson

# **BVOCs: Ecosystem Signaling and Biological Warfare**

Session Ecosystem chats: Why do plants and microbes send out VOCs and what do they do?

**Plenary Speaker:** Jörg-Peter Schnitzler, Helmholtz Zentrum, Munich, Germany

**Session Speakers:** Christiane Werner, University of Freiburg, Germany; Paulina Garbeva, Netherlands Institute of Ecology, Wageningen, the Netherlands



Douglas Mans

Discovery Hall at PNNL



Jörg-Peter Schnitzler

In his talk, titled Deciphering the volatile vocabulary in plant-microbe interactions - the smell of fungi, Schnitzler described the role of volatile organic compounds (VOC) in mediating biotic interactions between plants, fungi, and bacteria. All partners involved in these interactions emit broad and complex spectra of VOCs. The ecological significance of these volatile substances is currently being intensively investigated. Despite the scientific gaps, it is clear that volatile compounds play a central role in communication between organisms and are essential for the adaptation of plants to changing biotic and abiotic environmental factors. Schnitzler gave an overview of the current state of knowledge and described the role of volatile terpenoids from plants and fungi in the development of induced systemic resistance and growth processes. Schnitzler pointed out conceivable possibilities for the application of these compounds in modern agriculture.

Werner's talk was titled Tracing ecosystem-scale interactions of volatile organic compounds and CO emissions from plants, roots, and soils by isotope labeling. She described research within the European Research Council Project VOCO, where they developed a novel technological approach to couple CO<sub>2</sub> fluxes with VOC emissions based on simultaneous real-time measurements of a stable carbon isotope composition of branch, root, and soil respired CO2 and VOC fluxes. Position-specific <sup>13</sup>C-labeled pyruvate feeding experiments are used to trace carbon partitioning within the metabolic branching points of BVOCs and CO<sub>2</sub> emissions, thereby bridging scales from submolecular to whole-plant and ecosystem processes. To understand ecosystem-scale interactions, they are running a whole-ecosystem labeling experiment in the tropical rainforest biome of the Biosphere 2 experimental facility near Tucson, Arizona. The overarching goal of the Biosphere 2 Water, Atmosphere, and Life Dynamics (B2 WALD) experiment is to track biological mechanisms controlling the fate of CO<sub>2</sub>, BVOCs, and water cycling in a controlled ecosystem under drought and recovery conditions using an interdisciplinary, holistic approach.

In her talk, *The role of volatiles in belowground microbe-microbe and plant-microbe chemical interactions*, Garbeva described how chemical interactions and communication contribute greatly to ecosystem functioning and stability. Hence, the understanding of belowground inter-kingdom (bacteria, protists, fungi, and plants) chemical interactions is crucial for assessing the functioning of



Christiane Werner

#### **1.0 Science Sessions**



Paulina Garbeva

a soil ecosystem. Plant- and microbe-derived compounds play an important role in belowground interactions, e.g., as signaling compounds for communication or as suppressive agents in interference competition. Both plants and microorganisms produce and secrete a wide variety of primary and secondary metabolites, including

volatile and nonvolatile compounds. Garbeva presented their recent discovery of the ecological role of volatile compounds in long-distance belowground plant-microbe and microbe-microbe interactions.

Session Plant sentinels: Detection and decoding of VOCs as bio-threat signatures

**Plenary Speaker:** Cristina Davis, University of California, Davis (UC, Davis)

Session Speaker: Wayne Curtis, Pennsylvania State University

Davis' talk was titled Volatile organic compound as indicators of plant health. She discussed how VOCs are generated by almost all biological systems and are thought to represent end products associated with organism physiology and cellular metabolism. VOC generation applies to many different types of systems across humans, animals, bacteria, trees, and plants. Plants are known to off-gas a plethora of VOCs, some of which may also be associated with the plant's health status and are deeply involved in plant-insect signaling. Because of the potential to exploit this signal, plant VOC monitoring provides a wide range of opportunities for diagnosis of pathophysiological conditions in a noninvasive and potentially inexpensive way. Evidence is mounting that specific odor profile shifts are associated with bacterial or viral infections. Davis' group has demonstrated that VOCs are altered in citrus plants after infection with specific bacteria and viruses. By monitoring emitted chemicals, they can develop tools for early-stage asymptomatic diagnostics that can lead to early therapy and treatment.



Christina Davis

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#### **1.0 Science Sessions**



Wayne Curtis

Curtis gave a presentation on *Plant-sensing activation viral vector-encoded genes*. He described how his lab, nearly 20 years ago, assisted in plant "volatile" signaling with measurements of methyljasmonate (MeJA) vapor pressure. MeJA is not volatile; it is sensed at extremely low concentrations. In his talk, Curtis connected such plant volatile sensing to transactivation of plant virus genes that complement deconstructed viral vectors. This represents an extension of technology being developed to protect plants using insect-delivered "gene therapy."

#### Primary and Secondary Aerosols: Ecosystem and Climate Feedbacks

Session Primary biological particle emissions: Ecosystem-atmosphere interactions

Plenary Speaker: J. Alex Huffman, University of Denver Session Speaker: Alexander Laskin, Purdue University

Huffman presented an overview of bioaerosol types, emission processes, and detection techniques in his talk *Bioaerosols in the atmosphere, their measurement, and gaps of understanding*. He summarized observations of bioaerosols made in a variety of environments and as ice nucleating particles. He also discussed primary biological aerosol particles, a subset of biogenic particles often referred to as bioaerosols. They consist of biological material such as bacteria, fungal spores, pollen, and vegetative detritus, and their fragments and excretions emit directly from terrestrial or marine surfaces into the atmosphere. Huffman explained that bioaerosols are crucial to the reproductive processes of many



J. Alex Huffman

organisms and can spread genetic material over long distances. They can also negatively affect agricultural and public health as pathogenic agents. Furthermore, bioaerosols can be used as agents of biological warfare, can affect atmospheric systems by acting as nuclei on which cloud water droplets or ice particles may form, and may influence cloud properties on regional scales. Unfortunately, direct measurement of the sources, concentrations, and emission properties of bioaerosols presents analytical challenges that have limited well-constrained understanding of their effects. This challenge with detection technologies and improvements serves as a significant motivation for increased cross-disciplinary interaction.

In his presentation about Chemical Imaging of Atmospheric Particles, Laskin explained that airborne particles are very dynamic and highly reactive components of the Earth's atmosphere. Accurate descriptions of particles and their effects in the atmosphere require comprehensive information not only about the particle-type populations, their size distributions, and concentrations, but also about the diversity and the spatial heterogeneity of chemical components within individual particles. Developments and applications of modern chemical imaging approaches for off-line characterization of atmospheric particles have been at the forefront of modern experimental studies. These studies have had a transformative impact on aerosol chemistry and physics. Laskin's presentation highlighted a number of chemical imaging studies that provide unique experimental insights into the nature and sources of previously unrecognized particles, understanding their physical properties, atmospheric reactivity, and transformations.



Alexander Laskin

**Session BioAtmo:** The role of biosphere-atmosphere interactions in climate dynamics

**Plenary Speaker:** Alex Guenther, University of California, Irvine (UC Irvine)

Session Speakers: John Shilling, PNNL; Celia Faiola, UC Irvine

Guenther's talk, *Biogenic volatiles fluxes and interactions in managed landscapes*, described how the land and atmosphere exchange BVOCs originating from plants and soils within terrestrial ecosystems, and drive atmospheric distributions of ozone, particles, and other constituents related to air quality and climate. BVOC emissions are highly sensitive to air quality and climate, which creates the potential for significant interactions and feedbacks. A quantitative understanding of these interactions, and their implications for air quality and climate, requires accurate estimates suitable for input to numerical models of regional to global atmospheric chemistry and transport. BVOC emissions can



Alex Guenther

vary more than an order of magnitude over spatial scales of meters to kilometers, and time scales of minutes to years. Estimating BVOC emissions from urban and agricultural landscapes is especially challenging due to heterogeneity, rapidly changing distributions, and relatively open canopies which modify the light environment. BVOC emission models have primarily focused on natural landscapes and relatively few efforts have been made to characterize urban, agricultural, and other managed landscapes, thereby resulting in relatively high uncertainties in BVOC emission estimates for these areas. Guenther presented an observational approach for quantifying BVOC emissions from urban and other managed landscapes as well as recent results for several regions and compared this strategy with standard emission model simulation approaches. He discussed the implementation of these advances for regional atmospheric chemistry, including interactions and feedbacks, in the latest version of the Model of Emission of Gases and Aerosols from Nature (MEGAN version 3.1) developed by Guenther. He also pointed out the remaining gaps and priorities for future progress in BVOC emission modeling.

Shilling gave a presentation titled Photolysis is a substantial control of atmospheric budgets of biogenic SOA. He explained that secondary organic aerosol (SOA) accounts for a large fraction of tropospheric particulate matter. Accurate modeling of the SOA life cycle is needed to quantify its effects on radiative forcing, cloud formation, and air



John Shilling

quality. While SOA production rates and mechanisms have been extensively investigated, loss pathways remain uncertain. Most large-scale chemistry and transport models account for wet and dry deposition of SOA, but chemical losses, such as photolysis, are rarely included. The Shilling lab has shown, through a combined experimental and modeling approach, that photolytic loss of SOA mass has the potential to significantly alter SOA predictions in models. Using environmental chamber experiments, they found that SOA produced from several representative BVOCs undergoes photolysis-induced mass loss at rates between 0 and 2.2 percent ± 0.4 percent of nitrogen dioxide (NO<sub>2</sub>) photolysis, equivalent to 24-hour average SOA atmospheric lifetimes as short as 10 hours. Photolysis of biogenic SOA has significant implications for interpreting chamber yield measurements and extrapolating the atmospherically relevant conditions. By incorporating the SOA photolysis rates into a high-resolution regional chemical transport model, they are testing the sensitivity of predicted biogenic SOA mass concentrations to photolytic losses. The addition of photolysis at rates consistent with their experimental conditions causes a 50 percent reduction in biogenic SOA loadings over the Amazon, indicating photolysis can exert substantial control over the lifetime of atmospheric SOA, with a likely dependence on SOA molecular composition and thus production mechanisms.



In her talk, Secondary organic aerosol formation from herbivore-stressed plant emissions, Faiola discussed how plant stress in a changing climate will alter the mixture of volatile biogenic compounds emitted by plants into the atmosphere. Biogenic volatiles contribute to SOA production, so these strong perturbations to the types of

Celia Faiola

compounds emitted could have significant impacts on SOA production. Many of these compounds have not been traditionally studied for their aerosol formation potential, but they could play a larger role in future climate regimes. In her presentation, Faiola summarized changes in SOA formation from Scots pine and *Baccharis salicifolia* emissions resulting from two types of insect herbivory stress: bark boring pine weevils and aphids. The herbivore-stressed emissions vary depending on the herbivore-plant combination and have corresponding and varying effects on SOA formation. Faiola proposed that the SOA formation potential of the emissions can be explained by the molecular structures of the major stress emission compounds.

# Carbon on the move: Allocation of photosynthate in the plant-soil system

Session Source-sink communication: Sugar signaling and negative feedback loops

**Plenary Speakers:** Xinguang Zhu, Center of Excellence in Molecular Plant Sciences, Chinese Academy of Sciences, Shanghai, China

Session Speakers: Diane M. Beckles, UC, Davis; Astrid Wingler, University College Cork, Ireland; Eric Hoppe, PNNL

Zhu's talk was titled Multiscale Systems Modeling of Plant Source-Sink Interactions to Guide Improvement of Light Use Efficiency and Crop Yield Potential. As Zhu pointed out, photosynthesis provides the food, energy, fiber, and ecological services for humankind. Though photosynthesis has been on Earth for billions of years, evidence increasingly shows that the current photosynthetic apparatus is far from optimal in terms of its efficiency in converting light energy into chemical energy. How to identify molecular targets to improve photosynthetic efficiency and hence the potential crop yield is a major challenge facing contemporary plant biologists. Identifying molecular targets is especially important now because, due to the rapid advances in genomics and genome editing technologies, any identified engineering options can be rapidly implemented in plants. To tackle this challenge, the Zhu lab has been focusing on developing multiscale, multi-physics models of photosystems, which span from the molecular



Xinguang Zhu

scale—through metabolism, cell, leaf, canopy—to the whole plant system scale. These models enabled the identification of a series of engineering targets that can improve photosynthetic efficiency, many of which have been tested and successfully validated in both model plants and crop species. In his talk, Zhu discussed the rationale behind this new approach, the models that have been developed, and the recent advances in applying this approach to guide photosynthesis improvement and crop yield enhancement.

Beckles' talk, Starch-to-sugar and back again: a critical role for starch metabolism in plant sugar signaling, explained how sugars act as metabolites, sources of energy, and carbon building blocks for all plant growth processes. Sugars are also among the most powerful signals in plants, because their levels regulate multiple feedforward and feedback regulatory processes in diverse tissues. These regulatory processes collectively calibrate appropriate plant growth responses and biomass accumulations in relation to the carbon acquired through photosynthesis. Beckles argued that sugar signaling could also be viewed in the context of starch metabolism. Starch is a metabolically inert sugar polymer. One starch granule contains millions of glucose molecules that plants may access, as needed. Emerging evidence shows that the sugarstarch flux has broad implications for balancing plant carbon usage under abiotic stress, and for the normal developmental partitioning of carbon between source and sink tissues. Beckles proposed that this starch-to-sugar interconversion influences the concentration of the intermediate sugar signaling molecules that play a central role in mediating plant



Diane M. Beckles

growth in response to developmental and external cues. Consequently, the Beckles lab has undertaken a holistic and integrative assessment of the starch-sugar dynamic, both at the cellular and the whole-plant level, to develop an overarching view of how starch metabolism may support plant metabolic flexibility. In her talk, Beckles established a framework for such processes, and showed that the accumulation of starch itself, as well as its role in balancing sugar levels, should be considered as a central part of sugar signaling essential for plant growth and productivity.

Wingler gave a presentation titled Regulation of resource allocation in annual and perennial plants – implications for growth, yield and carbon sequestration. She discussed how the allocation of carbon and nitrogen in plants is tightly regulated in response to environmental factors, such as light conditions, temperature, atmospheric  $CO_2$ , and soil nitrogen



Astrid Wingler

availability. Sugar signaling plays an important role in integrating environmental and developmental factors, thereby regulating the allocation of carbon and nitrogen between different organs. For example, scientists have identified trehalose-6-phosphate as a key signaling component for carbon availability, regulating processes such as growth, stress responses, grain filling, and senescence-dependent nutrient recycling. While the role of sugar signaling pathways in resource allocation has been explored in detail in annual plants, the scientific community knows less about sugar signaling in perennial species. Perennial plants typically allocate a higher proportion of biomass to the root system than annual plants. In addition to improving the potential for soil carbon sequestration, this increases the stress resilience of perennials. There is, therefore, considerable interest in breeding perennial grain crops. However, the grain yield of perennials is usually lower than that of related annual species. In her talk, Wingler explored how differences in the regulation of resource allocation determine annual and perennial life histories through controlling senescence. She discussed trade-offs between carbon and nitrogen allocation to the root system versus the grains, as well as the question—is it possible to breed perennial grain crops that combine high soil carbon sequestration and stress resilience with high yield?

#### **1.0 Science Sessions**

#### **1.0 Science Sessions**



Eric Hoppe

Hoppe, a scientist at PNNL and local vintner, poured wine, and talked about The importance of terroir. During a short wine tasting session, he discussed the influence terroir (natural environments) has on the characteristic flavors of finished wine and which factors, such as soil chemistry, topography, or climate conditions, affect the wine most significantly. Everyone got the chance to taste three wines, all produced by the same winemaker and from the same varietal grape using an identical clone. Two of the wines were from the same vineyard but different vintages. Another wine was from one of the same vintages but from a different vineyard experiencing very similar climate conditions only miles away. This session talk aimed to illustrate the importance and impact of soil properties from plant cultivation to the bottled product.

Session The soil dilemma: Balancing soil health and carbon storage

Plenary Speaker: Shannon Cappellazzi, The Soil Health Institute, OR

Session Speakers: Janet Jansson, PNNL; Kirsten Hofmockel, PNNL

In her talk, Soil Health Framework, from functions of microbes to a functioning Earth, Cappellazzi pointed out that, at the core, soil health is about quantifying the ability of the soil to function to its potential. The Soil Health Institute is working to determine the best suites of measurements to interpret and describe how well the soil is performing vital individual ecosystem services. Each of these services or functions is dependent on the activities of living organisms, which are largely dependent on soil carbon, and both are subject to the inherent nature of the place where the specific soil develops. Cappellazzi discussed the challenge of building a measurement system and interpretation framework that use rigorous science to demonstrate and encourage producers to value and enhance the life-giving carbon in their system. This task requires a proper accounting of the limitations and variability that an individual producer encounters to have a fair system that is flexible enough to be applicable in any environment.



Shannon Cappellazzi

Jansson gave a talk titled *Climate change impacts on carbon cycling by soil microbiomes.* She described how soil microorganisms cycle carbon and contribute to the flux of greenhouse gases. She pointed out that climate models vary widely in their predictions of the fate of soil carbon, with soil either serving as a source or a sink of greenhouse gases in the future as climate changes. Part of the discrepancy in climate models lies in a lack of understanding



Janet Jansson

of the biochemical pathways underlying soil organic carbon transformations. Also, different soil environments are expected to change with anticipated changes in climate, making sweeping claims about the global fate of soil carbon difficult. Recent advances in multi-omics technologies are filling some knowledge gaps regarding the impact of environmental changes on soil microbial functions. For example, Jansson's group used a combination of metagenomics, metatranscriptomics, and metaproteomics to determine the response of permafrost soil microbiomes to thaw. In another study, the group combined targeted gene sequencing with metatranscriptomics and metabolomics to determine how soil microbiomes respond to changes in soil moisture. To determine the details of carbon transformations between members of soil microbial communities during organic carbon decomposition, Jansson's team recently derived a model soil consortium with 20 members, six of which were obtained as isolates and genome sequenced. This model system enabled the scientists to start teasing out positive and negative interactions between community members during growth on different carbon substrates. They also derived a soil microfluidics chip and soil box that allowed them to determine spatial interactions between soil microbial community members during carbon transformation. Finally, they established a system for on-line monitoring of soil respiration that allowed them to determine the metabolic response of the soil microbiome to changes in soil moisture. Together, these studies are providing new knowledge of the soil

microbiome response to environmental perturbation. Ultimately, this knowledge will help improve predictions of how a changing climate will affect soil microbial cycling of carbon.

Hofmockel gave a presentation titled Mineral-OM relationships across the Nutrient Network grassland *experiment*. She started with the multifaceted nature of biochemical-mineral interactions that make it hard to identify unifying factors that govern organic matter (OM) persistence in soil. Using a multi-site study, the Hofmockel group has demonstrated how the composition of sorbed OM is a function of the mineral components in the soils. Across six different grassland locations, the abundance of ferrihydrite positively correlated with lipid- and protein-like molecules in sorbed soil OM pools and lignin-like molecules in water-extractable OM. These relationships provide field evidence that supports the conceptual model of the zonal mineral-OM association. The addition of experimental nitrogen disrupted the accumulation of proteinlike molecules, as well as the positive correlation of water-extractable lignin-like molecules with ferrihydrite content. If these kinds of relationships are prevalent over larger spatial and temporal scales, there is a foundation for understanding soil OM persistence under a variety of environmental contexts.



Kirsten Hofmockel

#### 2.0 Additional Activities

### 2.0 Additional Activities

Beyond the science sessions, guests had additional opportunities to learn and participate. A brief account, along with photos, of some of their experiences follows.

#### **Flash Talks**

Guests ate their lunches during flash talks given by EMSL scientists who shared some of the exciting research happening at EMSL. The talks included FREDA, a web application for data analysis and interactive visualization; machine learning to analyze primary biological aerosol and soil particles; plant growth-promoting bacteria and seed interactions; high-throughput single-cell proteomics; visualizing molecular interactions in the rhizosphere; aerosolmicrobe-plant interactions in the phyllosphere; drought-induced proteome and metabolome changes in sorghum; and the national microbiome data collaborative.



Allison Thompson



Tamas Varga



Lili Paša-Tolić and M.T. Thomas Award winner Ying Zhu

#### M.T. Thomas Award

Ying Zhu, a biological scientist at EMSL, received EMSL's 2018 M.T. Thomas Award for Outstanding Postdoctoral Achievement at the meeting. EMSL's User Executive Committee selected Zhu for his creativity in microfluidics and scientific productivity. Laboratory Fellow and EMSL Deputy of Technology Lili Paša-Tolić introduced Zhu and presented him with a plaque celebrating his achievement. Zhu also presented his research on microfluidic nano droplets that push the boundary of proteomics to single cells and tissue mapping.



Sarai Williams @SaraiWi21371511 · Oct 8, 2019 Congratulations to @YingZhu\_pnnl for receiving the MT Thomas Award at the EMSL Integration 2019 Conference! @PNNLab @EMSLscience



#### **2.0 Additional Activities**



Poster Session

#### **Poster Session**

Research posters filled the lobby at PNNL's Discovery Hall offering scientists the opportunity to learn more about their colleagues' research and sparking conversations for future collaborations.

#### **2.0 Additional Activities**



Teresa Palazzo

#### **Tutorials**

Two-hour tutorials on the third day of the meeting showcased techniques and capabilities for probing atmospheric aerosol using advanced analytical platforms, stable isotope tracers and probes in plant and soil biology, and data visualization.

#### **EMSL Tour**

The many networking opportunities notwithstanding, a tour of EMSL at the end of Day 3 was a welcome change after sitting for two and a-half days. The guided tour gave guests the opportunity to connect with other guests, see several capabilities that EMSL has to offer, and ask questions along the way.



Jim Moran

#### **2019 EMSL Integration Meeting Report**

# Conclusion

The 2019 Integration Meeting was sponsored by EMSL and Thermo Fisher Scientific and held at PNNL October 8–10. The guests from the scientific community along with representatives from the Office of Biological and Environmental Research and the EMSL User Executive Committee shared three days of great science, connections, and a sense of belonging. Christer Jansson, along with several collaborators, are developing a paper as one of the outcomes of the meeting.

#### 2019 Integration Meeting Numbers



#### Looking Ahead to 2020

Plans are under way for the 2020 EMSL Integration Meeting, titled "Visualizing the Proteome," October 6–8. This engaging meeting will encompass the following topics:

- Pushing the frontier of structural biology
- Understanding subcellular compartmentalization and ultrastructure
- Annotating protein function and modifications via native and top-down proteomics
- Revealing cellular complexity and dynamics with single- to few-cell proteomics
- Advancing cellular models and protein design with high-performance computing.



# Appendix A: Agenda

#### EMSL Integration 2019

Plant, Soil and Aerosols: Interactions that tell stories of Ecosystems, Climate and National Security October 8-10, 2019 #EMSLINTEGRATION2019

Tuesday, O	ctober 8, 2019			Location
7:30 am	Registration and Badging			Discovery Hall
8:30 am	Opening Remarks	Christer Jansson	PNNL	Horizon
8:35 am	Welcome	Douglas Mans, EMSL Director	EMSL	Horizon
Biogenic V	OCs: Ecosystem	Signaling & Biological Warfare		
Session: Ec	osystem chats: V	Why do plants and microbes send out VOCs and what	do they do?	
Session Cha	air: Pubudu Hand	lakumbura		
8:45 am	Plenary #1	Jörg-Peter Schnitzler - Deciphering the volatile vocabulary in plant-microbe interactions - the smell of fungi	Helmholtz Center, Munich, Germany	Horizon
9:30 am	Session Speaker #1	Christiane Werner - Tracing ecosystem-scale interactions of volatile organic compound (BVOC) and CO2 emissions from plants, roots, and soils by isotope labelling	University of Freiburg, Germany	Horizon
10:00 am	Networking (Break)			Discovery Hall Lobby
10:15 am	Session Speaker #2	Paolina Garbeva - The role of volatiles in belowground microbe-microbe and plant-microbe chemical interactions	Netherlands Institute of Ecology, Wageningen, Netherlands	Horizon-ZOOM
10:35 am	Christer Jansson – Discussion of EMSL Ecotron Vision PN		PNNL	Horizon
10:55 am	MT Thomas Award Speaker	Ying Zhu - Microfluidic nanodroplets pushed the boundary of proteomics to single cells and tissue mapping	PNNL	Horizon
11:40 am	Group Photo			Horizon
11:45 am	Working Lunch - Capability Flash Talks/Virtual Tour		Horizon	
	Allison Thompson – FREDA: A web application for analysis and interactive visualization of FT-MS data			
	Tamas Varga - Analysis of internally mixed primary biological aerosol and soil particles using machine learning approaches			
	Xiao-Ying Yu - Revealing plant growth-promoting bacteria and seed interactions using time-of-flight secondary ion mass spectrometry			

Primary & Secondary Aerosols: Ecosystem & Climate Feedbacks				
Session: Primary biological particle emissions: Ecosystem-atmosphere interactions				
Session Cha	air: China Swarup	)		
1:00 pm	Plenary #2	Alex Huffman - Bioaerosols in the atmosphere, their measurement, and gaps of understanding	University of Denver	Horizon
1:45 pm	Session Speaker #4	Alex Laskin - Chemical imaging of atmospheric particles	Purdue University	Horizon
2:05 pm	Contributed Talk #1	Manish Shrivastava - Urban pollution greatly enhances formation of natural aerosols over the pristine Amazon	PNNL	Horizon
2:25 pm	Contributed Talk #2	Jun Liu - Arctic atmospheric particle sources, morphology, and elemental composition	University of Michigan	Horizon
2:45 pm Networking (Break)			Discovery Hall Lobby	
Carbon on	the move: Alloca	tion of photosynthate in the plant-soil system		
Session: So	urce-sink commu	inication: Sugar signaling and negative feedback loops		
Session Cha	air: Amir Ahkami			
3:00 pm	Plenary #3	Xinguang Zhu - Multiscale systems modeling of plant source sink interactions to guide improvement of light use efficiency and crop yield potential	Shanghai Institutes for Biological Sciences, Shanghai, China	Horizon
3:45 pm	Session Speaker #7	Diane Beckles - Starch-to-sugar and back again: a critical role for starch metabolism in plant sugar signaling	UC Davis	Horizon
4:05 pm	Session Speaker #8	Astrid Wingler - Regulation of resource allocation in annual and perennial plants – implications for growth, yield and carbon sequestration	University College, Cork, Ireland	Horizon
4:30 pm	Session Speaker #9	Eric Hoppe – Abbreviated wine tasting: the importance of terroir	PNNL	Horizon
4:45 pm Poster Session & Reception			Discovery Hall Lobby	
6:00 pm	Dinner on your own			

Wednesday, October 9, 2019			Location	
Biogenic VOCs: Ecosystem Signaling & Biological Warfare				
Session: Pla	nt sentinels: Det	ection and decoding of VOCs as bio-threat signatures		
Session Cha	air: Christer Janss	son		
7:45 am	Discussion Outo	come Opinion Paper (for Invited Speakers)		Frontier
8:30 am	Plenary #4	Cristina Davis - Volatile organic compound (VOC) indicators of citrus plant health	UC Davis	Horizon
9:15 am	Session Speaker #10	Wayne Curtis - Plant-sensing activation viral vector encoded genes	Penn State University	Horizon
9:35 am	Contributed Talk #3	Claire Moffett - Influences on the composition of biogenic aerosol on the north slope of Alaska	Baylor University	Horizon
9:55 am	Networking (Bre	eak)		Discovery Hall Lobby
10:10 am	Contributed Talk #4	Jerome Fast - Implications of biogenic volatile organic compounds observed during the HI-SCALE campaign	PNNL	Horizon
Primary & S	econdary Aeros	ols: Ecosystem & Climate Feedbacks		
Session: Bic	Atmo: The role o	of biosphere-atmosphere interactions in climate dynam	nics	
Session Cha	air: Libor Kovarik			
10:30 am	Plenary #5	Alex Guenther - Biogenic volatiles fluxes and interactions in managed landscapes	UC Irvine	Horizon
11:15 am	Working Lunch - Capability Flash Talks/Virtual Tour			Discovery Hall
	Ying Zhu – High	throughput single cell proteomics		Lobby
	Dusan Velickovic – Unlocking the ability to visualize molecular interactions occurring within the rhizosphere			
	Albert Rivas-Ubach – Understanding the aerosol-microbe-plant interactions in the phyllosphere using "–omics" techniques			
	Kim Hixson – Drought induced proteome and metabolome changes in sorghum			
	Lee Ann McCue & Mary Lipton - National microbiome data collaborative			
1:30 pm	Session Speaker #13	John Shilling - Photolysis is a substantial control of atmospheric budgets of biogenic SOA	PNNL	Horizon
1:50 pm	Session Speaker #14	Celia Faiola - Secondary organic aerosol formation from herbivore-stressed plant emissions	UC Irvine	Horizon
Carbon on the move: Allocation of photosynthate in the plant-soil system				
Session: The soil dilemma: Balancing soil health and carbon storage				
Session Chair: Chris Anderton				
2:10 pm	Plenary #6	Shannon Cappellazzi - Soil health framework: from functions of microbes to a functioning earth	Soil Health Institute	Horizon
2:55 pm	Session Speaker #15	Janet Jansson - Climate change impacts on carbon cycling by soil microbiomes	PNNL	Horizon
3:15 pm	m Networking (Break)			Discovery Hall Lobby
3:30 pm	Session Speaker #16	Kirsten Hofmockel - Mineral-OM relationships across the nutrient network grassland experiment	PNNL	Horizon

#### **2019 EMSL Integration Meeting Report**

#### Appendix A

3:50 pm	Contributed Talk #5	Marie-Anne de Graaff - Plant genotype impacts on soil biochemical profiles and microbial community structure: implications for soil C storage	Boise State University	Horizon
4:10 pm	Closing Remarks	Christer Jansson	PNNL	Horizon
Thursday, C	October 10, 2019			Location
8:00 am – 10:00 am	Tutorial: Probin	g Atmospheric Aerosol Using Advanced Analytical Pla	tforms	EMSL/1077
8:00 am – 10:00 am	Tutorial: Using Stable Isotope Tracers and Probes in Plant and Soil Biology			EMSL Boardroom
				(Meet in EMSL Lobby)
8:00 am – 10:00 am	Tutorial: Data V Horizon	isualization Tutorial		
10:00 am	Networking (Break)			Discovery Hall Lobby
10:15 am – 12:15 pm	Tutorial: Probing Atmospheric Aerosol Using Advanced Analytical Platforms			EMSL/1077
10:15 am – 12:15 pm	Tutorial: Using Stable Isotope Tracers and Probes in Plant and Soil Biology			EMSL Boardroom
				(Meet in EMSL Lobby)
10:15 am – 12:15 pm	Tutorial: Data Visualization Tutorial			Horizon
12:15 pm	Working Lunch/Round Table Discussion Outcome Opinion Paper (open to everyone)			Discovery Hall
2:00 pm	Organize for EMSL Tour			EMSL Lobby
2:15 pm – 3:15 pm	EMSL Tour			EMSL
3:15 pm	Networking (Br	eak)		EMSL Lobby
3:30 pm – 4:30 pm	Panel Discussion: How to write a successful EMSL user proposal			EMSL Auditorium
Poster Sess	sion – Tuesday 1	0/8/19		
Number	Title		Name	
1	Healthy and ap metabolomics i aerosol	hid-stressed shrubby plant (Baccharis Salicifolia) mpact on produced biogenic secondary organic	Fatemeh Khalaj	
2	Direct interspec	ies electron transfer (DIET) in syntrophic microbes	Xiao-Ying Yu	
3	Exploratory dat	a analysis and interactive visualization of FT-MS data	Allison Thompson	
4	Interactions bet	ween synthetic bilgewater emulsion and biofilms	Jiyoung Son	
5	Carbon on the microbe-soil co	nove – carbon uptake and distribution in the plant- ntinuum	Pubudu Handakumbura	
6	Regeneration o platform for ass spectrometry	f dormant soil communities by hydration: a new sessing soil activity by direct real-time mass	Karl Weitz	
7	Urban pollution the pristine Am	greatly enhances formation of natural aerosols over azon	Manish Shrivast	ava

8	Arctic atmospheric particle sources, morphology, and elemental composition	Jun Liu
9	Starch metabolism in relation to early growth under abiotic stress	Emma Shipman
10	Spatial evaluation of carbon flow and microbial function through the root-rhizosphere-soil continuum	Jim Moran
11	Understanding the aerosol-microbe-plant interactions in the phyllosphere using "–omics" techniques.	Albert Rivas-Ubach
12	PSpecteR: A proteomics data analysis application in R	David Degnan
13	Time-dependent gene expression and metabolic mapping of Brachypodium root development	Amir Ahkami
14	Analysis of internally mixed primary biological aerosol and soil particles using machine learning approaches	Tamas Varga
15	High-throughput single cell proteomics enabled by multiplex isobaric labeling in a nanodroplet sample preparation platform	Ying Zhu
16	Molecular phenotyping of Setaria and Brachypodium in elevated $\mathrm{CO}_{_2}$	Kim Hixson
17	PECTIN – Poplar esterified cell wall transformation and metabolic integration study; integration of cell wall esterification with methanol and acetic acid volatile emissions	Rebecca Dewhirst
18	Research needs for bridging the measurement-to-models gap in representation of atmospheric ice-nucleating particles	Susannah Burrows
19	The influence of Setaria genotype on rhizosphere phenotype within a marginal soil	Stephen Callister
20	Understanding green rust formation in ionic liquids by liquid ToF-SIMS and SALVI	Yanjie Shen
21	Unlocking the ability to visualize molecular interactions occurring within the rhizosphere	Dusan Velickovic
22	pmartR: Software for quality control and statistics robust to missing data for mass spectrometry-based biological data	Lisa Bramer
23	Toward understanding the effect of gas-phase polycyclic aromatic hydrocarbons on the formation and properties of biogenic secondary organic aerosol particles	Alla Zelenyuk-Imre
24	Observation of biomass burning aerosol particles at high-altitude mountain station	Kuo-Pin Tseng
25	Sorghum root microbiome dynamics under nutrient-limited and drought conditions	Susannah Tringe
26	Chemical speciation information using <b>q</b> -XRF imaging at SSRL: examples from Plant and Soil Science	Jocelyn Richardson
27	ToF-SIMS imaging of plant seed interactions with plant-growth promoting bacteria	Yuchen Zhang
28	Artificial soils as a tool to understand the interactions between microbes and the soil matrix	llenne Del Valle
29	Visualization of large biological mass spectrometry datasets via integration of pmartR and trelliscopejs	Rachel Richardson
30	Regulatory mechanisms of source-to-sink carbon partitioning in poplar	Vimal Balasubramanian
31	Computational modeling of metabolic and regulatory networks of Yarrowia Lypolytica	Neeraj Kumar

# **Appendix B: EMSL Integration 2019 Meeting Tutorials**

# The 2019 Integration Meeting organizer thanks everyone who led tutorials.

#### **Data Visualization**

- Allison Thompson
- Daniel Claborne
- Chaevien Clendinen
- Lisa Bramer

#### Probing Atmospheric Aerosol Using Advanced Analytical Platforms

- Swarup China
- Libor Kovarik
- Albert Rivas Ubach
- Rosey Chu

# Using Stable Isotope Tracers and Probes in Plant and Soil Biology

- Jim Moran
- Pubudu Handakumbura
- Karl Weitz

#### How to Write a Successful EMSL User Proposal

- Nancy Washton
- Scott Baker
- Terry Law
- Celia Faiola