the Molecular Bond

EMSL

SCIENTIFIC INNOVATION THROUGH INTEGRATION

December 2015

Scratching the Surface

Studying Sea Spray Aerosols at EMSL

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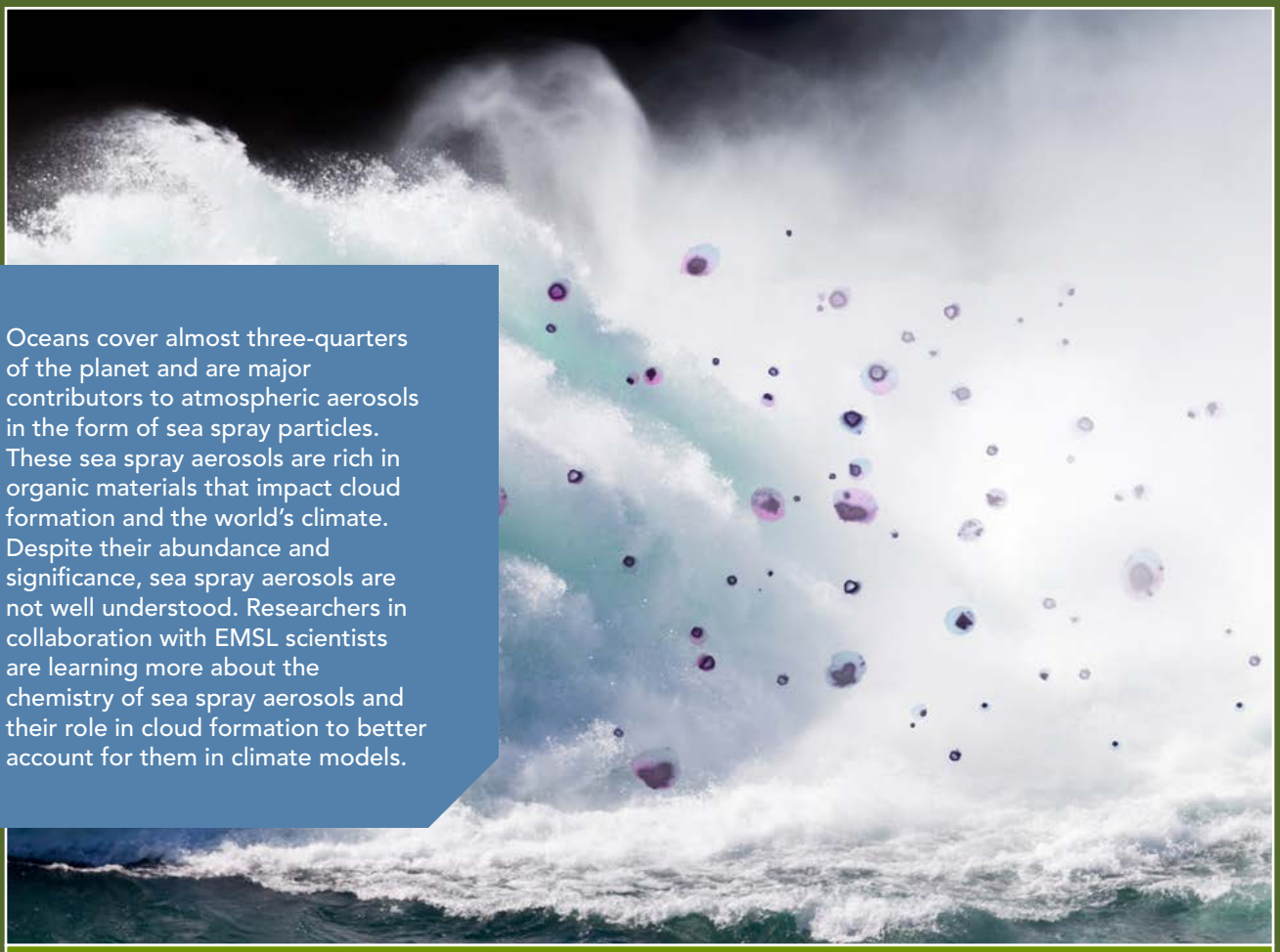
Joint Call Using EMSL & ARM Capabilities Launched

EMSL's R&D 100 Award-Winning Scientists Announced

Lead Named to Support Users' Computational Needs

Harnessing Energy from Microbial Mats

A Deeper Understanding of Cell Growth



Oceans cover almost three-quarters of the planet and are major contributors to atmospheric aerosols in the form of sea spray particles. These sea spray aerosols are rich in organic materials that impact cloud formation and the world's climate. Despite their abundance and significance, sea spray aerosols are not well understood. Researchers in collaboration with EMSL scientists are learning more about the chemistry of sea spray aerosols and their role in cloud formation to better account for them in climate models.

About *The Molecular Bond*

The Molecular Bond is EMSL's bimonthly newsletter for users, potential users and other interested individuals. EMSL Communications oversees the production of *The Molecular Bond*.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research in the Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world.

Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies. More information about EMSL is available at: www.emsl.pnnl.gov

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Scientists looking for better ways to produce biofuels and biochemicals are using metabolomics, or the study of the fundamental metabolic workings of a cell in a changing environment. This vial contains metabolites, lipids and proteins extracted from *Yarrowia lipolytica*, an oil-producing yeast. Scientists analyze each of these layers using specialized instruments to better understand the fungus' cellular metabolism. (EMSL file photo)

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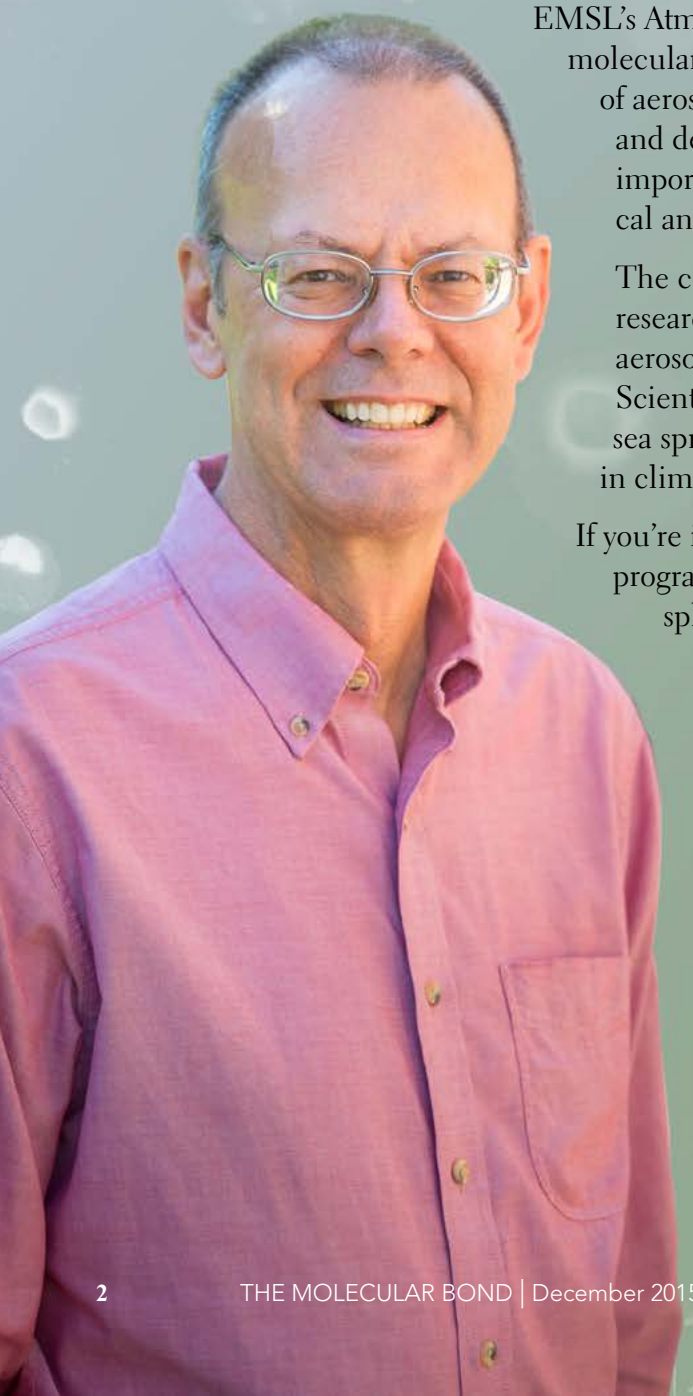
FROM THE DIRECTOR

Harvey Bolton

Over the years, EMSL has developed and honed its research emphasis into four major science themes – Atmospheric Aerosol Systems, Biosystem Dynamics & Design, Energy Materials & Processes, and Terrestrial & Subsurface Ecosystems. These science themes help guide EMSL's research investments and focus our user projects to accelerate scientific innovation and discovery.



EMSL's Atmospheric Aerosol Systems Science Theme focuses on a molecular-scale understanding of key chemical and physical properties of aerosols to improve the accuracy of climate model simulations and develop a predictive understanding of climate, which are of importance to the Department of Energy and its Office of Biological and Environmental Research.

The cover story of this issue of *The Molecular Bond* explores research being conducted at EMSL on sea spray aerosols. These aerosols are generated from ocean waves and become airborne. Scientists are working at EMSL to gain a better understanding how sea spray particles evolve in the atmosphere and their significance in climate models and potential impact on climate.

If you're interested in conducting aerosol research, check out our pilot program for a joint call using capabilities at EMSL and the Atmospheric Radiation Measurement, or ARM, Climate Research Facility. The EMSL and ARM programs are seeking proposals that will demonstrate integration of their capabilities in a single research project. Proposals are due Feb. 1.

Speaking of science themes and calls for proposals, EMSL's annual call solicits proposals on specific topics within the four science themes mentioned above. EMSL's 2016 annual call for proposals will be announced in early January. Look for email announcements after the first of the year on how we can collaborate to advance your research.

—Harvey

Developed to advance carbon cycling, microbial biology and atmospheric aerosol characterization research, EMSL's 21 Tesla Fourier-transform ion cyclotron resonance mass spectrometer, or 21T FTICR MS, will enable a variety of biomolecular and other natural organic compound studies. Ljiljana Paša-Tolić, lead scientist for mass spectrometry at EMSL, is shown with the instrument. Read more about Paša-Tolić's research using the 21T FTICR MS on page 12. (EMSL file photo)

NEWS & KUDOS

Campbell Elected President-Elect of ACS

Allison Campbell

Allison Campbell, acting associate laboratory director and former EMSL director, has been elected the 2016 American Chemical Society president-elect by members of ACS. Campbell will serve as president of the society in 2017 and immediate past-president in 2018; she will also serve on the society's board of directors.

Campbell is currently acting associate laboratory director of the Earth and Biological Sciences Directorate at Pacific Northwest National Laboratory and is responsible for many of the laboratory's Department of Energy's Office of Science research programs. She also oversees two Department of Energy user facilities — EMSL and the Atmospheric Radiation Measurement program. Campbell served as the director of EMSL for more than a decade.

Read the PNNL news release: http://1.usa.gov/21tqR7e.

Joint Call Using EMSL and ARM Capabilities Announced

A pilot call for proposals is now open for research in focused topics in atmospheric aerosol science that takes advantage of both the analytical instrumentation and capabilities at EMSL and the infrastructure and observational capabilities of the Atmospheric Radiation Measurement, or ARM, Climate Research Facility. Proposals may be submitted until Feb. 1 at 11 p.m. PST, and will follow unique proposal guidance and review processes.

The EMSL and ARM programs are seeking proposals that will demonstrate integration of their capabilities in a single research project. Proposals should advance the understanding of the molecular, physical, and/or optical properties of aerosol particles that influence and control macroscopic climate-relevant processes, such as cloud formation, radiation balance and precipitation. Proposals should focus on collection of samples at the surface or near surface ARM's Southern Great Plains site in Oklahoma with subsequent analysis of those samples at EMSL.

Questions about this call may be directed to the EMSL User Support Office at emsl@pnnl.gov, 509-371-6003.

EMSL Scientists on R&D 100 Award-Winning Teams

R&D Magazine honored two technologies developed by researchers at EMSL. Every year, the magazine selects the 100 most innovative scientific and technological breakthroughs of the year.

An award went to the research team of David Hoyt, Jesse Sears, Eric Walter and Hardeep Mehta, all from EMSL; along with Kevin Rosso and Jian Zhi Hu, both from Pacific Northwest National Laboratory, or PNNL; and former PNNL researcher Flaviu Turcu.

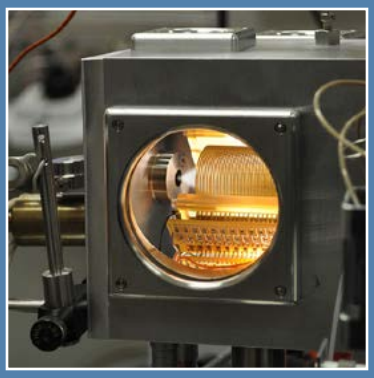
The team developed and applied "pressurized magic angle spinning technology" to nuclear magnetic resonance spectroscopy to allow analysis of complex samples under conditions that mimic real-world environments. The research team has used the technology to study carbon sequestration, recreate conditions deep underground and track the complex chemical reactions in biofuels.

The second award went to the team that includes EMSL's Ryan Kelly; PNNL staff members Keqi Tang, Gordon Anderson and Richard Smith; Randall Pedder of Ardara Technologies, which has licensed the technology; and former PNNL staffers Jason Page, Ioan Marginean and Jonathan Cox.

This team built on a previous PNNL device known as the "electrodynamic ion funnel" that effectively channels charged particles into a small space where they can be measured and manipulated by mass spectrometry. The team's new development, known as "subambient pressure ionization with nanoelectrospray, or SPIN," creates and sends particles to the funnel in a single system under the same atmospheric conditions. Using SPIN, nearly 50 times as many gas-phase ions enter the mass spectrometer for improved accuracy.

Read the PNNL news release: http://1.usa.gov/1RkMEtu.

The pressurized magic-angle spinning technology (right) and its components (left) makes it possible to study samples with NMR under real-world conditions. (Courtesy of Pacific Northwest National Laboratory.)



Technology known as SPIN – subambient pressure ionization with nanoelectrospray – boosts the number of molecules available for mass spectrometry analysis, making more precise measurements possible. (Courtesy of Pacific Northwest National Laboratory.)

Climate-Friendly Rice Named a Top Science Development of 2015

Rice farming is a big source of methane, a potent greenhouse gas. Christer Jansson, director of plant sciences at EMSL, led a team of scientists that developed a new strain of rice that produces nearly zero greenhouse gas emissions during its growth.

Christer Jansson

Popular Science magazine recognized the team's research with a "Best of What's New" award for 2015. *Popular Science* named the research the grand prize winner in the magazine's engineering category, one of 10 categories in which a total of 100 research developments around the globe were recognized. The awards are described in the December issue of the magazine.

For more than a decade, Jansson has worked closely with Chuanxin Sun of the Swedish University of Agricultural Sciences, who has contributed significantly to the research on rice. The two published a research paper about the rice in July in *Nature*, together with other researchers at the Swedish institution and colleagues at China's Fujian Academy of Agricultural Sciences and Hunan Agricultural University.

Read the PNNL news release: http://1.usa.gov/1NKaoYh

Paša-Tolic Part of Initiative Studying Microbiomes

Ljiljana Paša-Tolic

Ljiljana Paša-Tolic, lead scientist for mass spectrometry at EMSL, is a member of the Unified Microbiome Initiative, or UMI, Consortium, comprising 48 scientists from various scientific fields at national labs and universities across the United States. The consortium has proposed an interdisciplinary, unified program to learn more about how the microbiome functions and its properties. The scientists hope to harness these microbial communities to ultimately launch innovations in agriculture, energy, health, the environment and more.

Members of the consortium describe the UMI in the Oct. 28 online edition of *Science*. Pacific Northwest National Laboratory, or PNNL, plays a key role in this new initiative as well as in the consortium. Janet Jansson, chief scientist for biology at PNNL, is one of the consortium's founding members, and a co-author of the *Science* Perspectives article.

Reference: Alivisatos AP, MJ Blaser, EL Brodie, M Chun, JL Dangl, TJ Donohue, PC Dorrestein, JA Gilbert, JL Green, JK Jansson, R Knight, ME Maxon, MJ McFall-Ngai, JF Miller, KS Pollard, EG Ruby, and SA Taha. 2015. "A Unified Initiative to Harness Earth's Microbiomes." *Science* 350(6260):507-508. DOI: 10.1126/science.aac8480.

McCue Named EMSL MSC Capability Lead

Lee Ann McCue

Lee Ann McCue has accepted the position of capability lead for EMSL's Molecular Science Computing, or MSC, Scientific Consulting. McCue started in her new role on Dec. 1.

McCue is a senior research scientist at Pacific Northwest National Laboratory. Her research includes the analysis of microbial populations and metagenomes for microbial ecology studies, and the application of high performance computing techniques for sequencing technologies. McCue has a bachelor's degree from Iowa State University, a Ph.D. from The Ohio State University and post-doctoral studies at the University at Albany - SUNY.

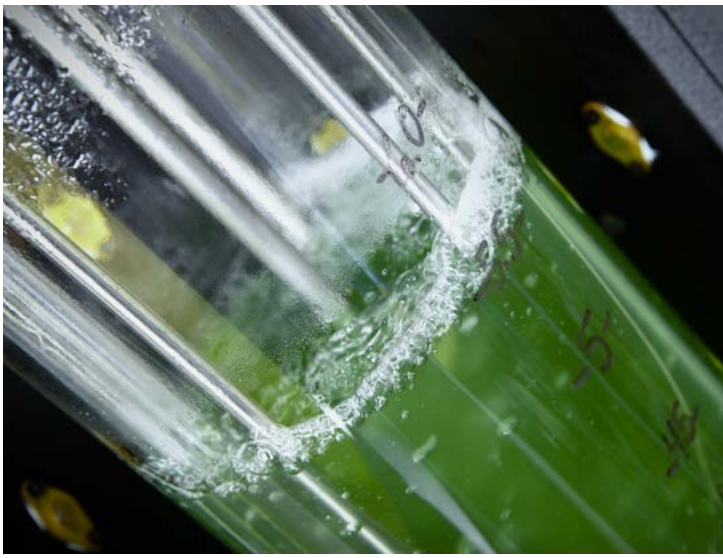
EMSL has two MSC capability leads. As the capability lead for MSC Scientific Consulting, McCue will collaborate with users to help ensure the integration between experimental and computational resources for improved scientific discovery. Dave Cowley is the capability lead for MSC Operations and oversees operations of the Cascade supercomputer and Aurora data file storage.

Microbes Map Path Toward Renewable Energy Future

The goal is to use the sun and water to produce renewable energy. Researchers have known *Cyanothece 51142*, a type of bacteria also called blue-green algae, makes hydrogen by drawing upon sugars it stores during growth. A team of scientists at Pacific Northwest National Laboratory and EMSL using capabilities at EMSL found *Cyanothece* also draws on a second, unexpected source of energy, using sunlight and water directly to make hydrogen. The team's findings were published in *Scientific Reports*.

Reference: Hans C. Bernstein, Moiz A. Charania, Ryan S. McClure, Natalie C. Sadler, Matthew R. Melnicki, Eric A. Hill, Lye Meng Markillie, Carrie D. Nicora, Aaron T. Wright, Margaret F. Romine and Alexander S. Beliaev. "Multi-omic dynamics associate oxygenic photosynthesis with nitrogenase-mediated H_2 production in *Cyanothece* sp. ATCC 51142," *Scientific Reports*, Nov. 3, 2015, DOI: 10.1038/srep16004.

Read the PNNL news release: http://1.usa.gov/1XFqge8.



Cyanothece 51142, **a blue-green algae, is a workhorse for natural hydrogen production in a bioreactor.**

Scratching the Surface

Studying Sea Spray Aerosols at EMSL

The salty tang of ocean spray touches everything within reach of the wind and the waves. But there's more to sea spray than its salty residue; it creates ocean-borne aerosols rich in organic materials, too. With almost three-quarters of the planet covered by oceans, the impact of these aerosols on cloud formation – and, in turn, the world's climate – could be huge. Despite this vast potential, sea spray aerosols are poorly understood. Scientists are using EMSL expertise and specialized instruments to pick apart these ocean-borne particles and better account for these aerosols in climate models.

"Oceans are major contributors to atmospheric aerosols and for a long time they were modeled and studied in laboratories as if they were only made of sodium chloride," said Vicki Grassian, a chemistry professor at the University of Iowa and co-director of the Center for Aerosol Impacts on Climate and the Environment, or CAICE, based at the University of California, San Diego. "But there's a much richer chemistry that we need to understand."

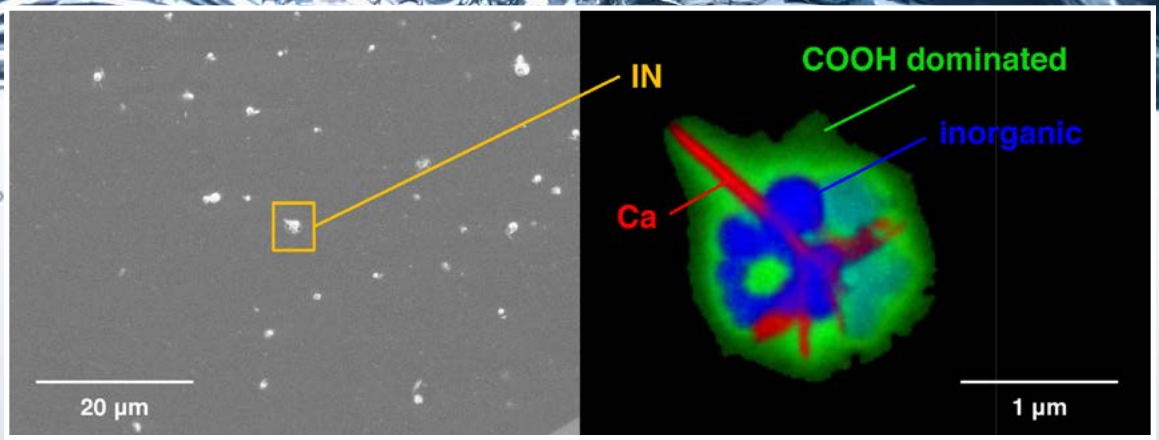
The surface of the sea teems with a mélange of organic material – viruses, bacteria and the detritus of marine life. When bubbles burst upward from the watery depths, organic matter can cling to their surface and rise into the atmosphere as sea spray. Although the particles are within easy reach – within 50 nanometers of the water's surface – parsing out their effect under complex oceanic conditions is a challenge.

DIY Aerosols

To control that complexity, researchers at CAICE make their own aerosols. Funded as part of the National Science Foundation's Centers for Chemical Innovation program, the center is home to a giant flume of ocean water. This simulated ocean setup allows scientists to create sea spray aerosols, or SSAs, and capture them for further study.

"A wide range of molecules come out of seawater, and we sample these particles as a function of size," said Grassian. So far, researchers including University of Iowa student Olga Laskina and postdoctoral associate Richard Cochran have detected more than 280 organic compounds with EMSL's high resolution mass spectrometers.

Beyond chemically cataloguing these compounds, CAICE scientists also want to understand how the ocean's changing biology affects the composition of SSAs. For example, in one experiment they created two plankton blooms and analyzed aerosol particles at time intervals throughout the two events. After analyzing those samples, the scientists found each bloom produced a different outcome depending on the degree of bacterial degradation in the water. These results showed for the first time the



Identification of Individual Ice Nuclei

The left panel shows a highlighted particle, likely of marine origin, identified as ice nuclei. The right panel indicates the highlighted particle exhibits an inorganic core with an organic coating shown in green. (Images provided by Daniel Knopf, State University of New York at Stony Brook.)

role of bacteria on SSAs, said Grassian. Prior to these studies, only chlorophyll was thought to be a measure of biology activity in seawater that could impact SSA.

Figuring out what these SSAs actually look like as they leave the ocean's surface is the work of CAICE researcher Joseph Patterson, an assistant project scientist in Nathan Gianneschi's laboratory at the UC San Diego. With a background in synthetic polymer nanomaterials, Patterson collects lab-made aerosols and views them with a cryogenic electron microscopy technique he developed specifically for aerosols. Unlike other methods that require dehydrating the particles, this electron microscopy technique gets high-resolution images of "wet," intact particles.

"These images provide the most direct observations of what's inside these aerosols and how they exist," said Patterson. One surprise was finding an abundance of complex, multilamellar vesicles that contained small particles. Although the particles have not yet been identified, he suspects the materials are phospholipid membranes containing enzymes and proteins that eventually end up in SSAs.

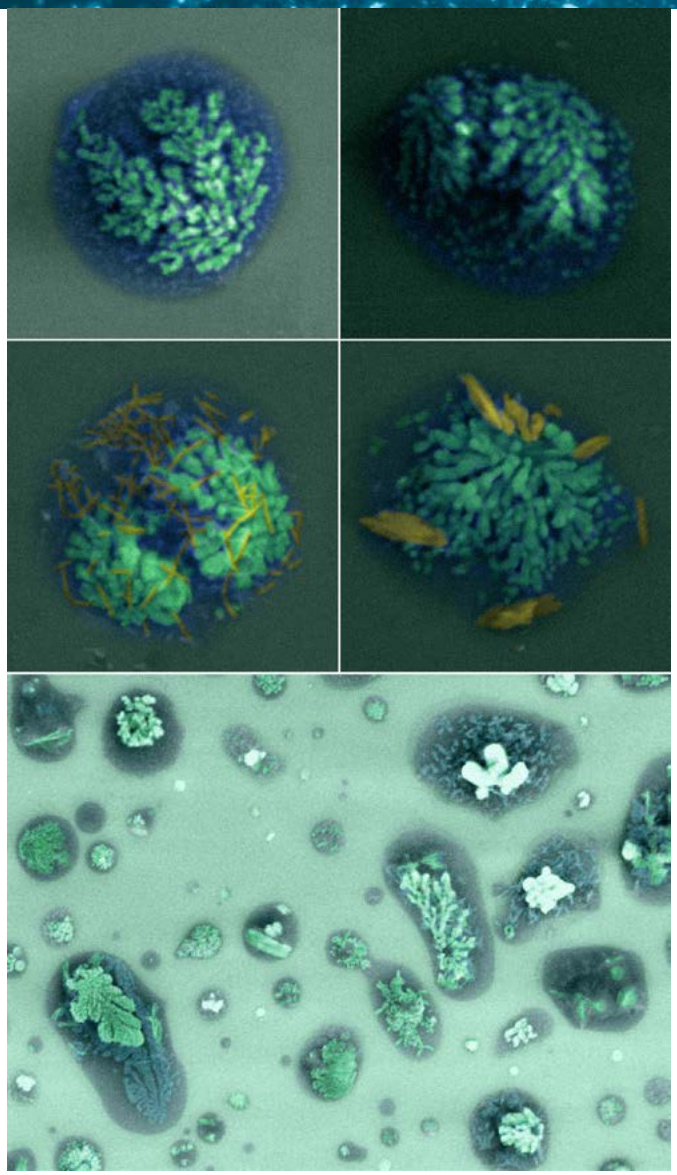
"One big drive behind working at EMSL are the highly specialized microscopes," said Patterson. "With them, we have chemical analysis capabilities and we're able to localize specific bioparticles to measure how they affect the overall elemental composition of aerosols."

Next, he plans to look at aerosols with a transmission electron microscope, which gives high spatial resolution and elemental information, and then go to nanoscale secondary ion mass spectrometry, or nanoSIMS, for more detailed analysis of the surface.

An artificial marine system also helps Daniel Knopf, a professor of atmospheric sciences at the State University of New York at Stony Brook, to study the effects of phytoplankton on aerosols. With his colleague, marine microbiologist Josephine Aller, they create phytoplankton blooms under controlled conditions and measure parameters such as cell counts and amounts of organic carbon produced. In parallel experiments, they interrogate the composition of lab-generated aerosols with single particle microspectroscopy tools to analyze how plankton blooms modulate SSA composition.

In addition, Knopf wants to understand the potential of organic material to become ice nuclei that instigate cold cloud formation. "Ice nucleation represents a big conundrum in atmospheric science because only a few particles have this ability – maybe only one particle in one liter of air – and we don't know why," said Knopf.

Although the ice nuclei capabilities of mineral dust are well known, Knopf – a physicist by training – wondered if marine scientists could help discover other sources of ice formation at the ocean surface. In previous work, fragments of plankton cells were capable of increasing ice formation under atmospheric conditions. More recently, Knopf was part of an international



The lower panel shows aged sea salt particles imaged using scanning electron microscopy. The top panel shows identified aged sea salt particles that nucleated ice. The dark shadow represents organic material. The particles' form and structure are similar to previous studies investigating marine affected particles. (Images provided by Daniel Knopf, State University of New York at Stony Brook.)

collaboration of scientists who sampled sea surfaces from around the world and showed enhanced ice formation with plankton exudate, or emitted fluid, less than 200 nanometers in size.

The identity of this minute amount of "ice active" material lurking at the surface of the sea remains a mystery. Knopf wants its spectral fingerprint; with that he can search for similar features and freezing profiles among the samples collected from the sea or generated in the lab. Beyond getting that identification, analyzing sea spray particles with EMSL's computer-controlled scanning electron microscopy and energy dispersive X-ray spectroscopy could show the surface structures that contribute to this enhanced ice formation.

"The computer-controlled systems let us look at hundreds of particles automatically, which helps us be statistically certain about the elemental compositions in lab-made and field-collected SSAs," said Knopf.

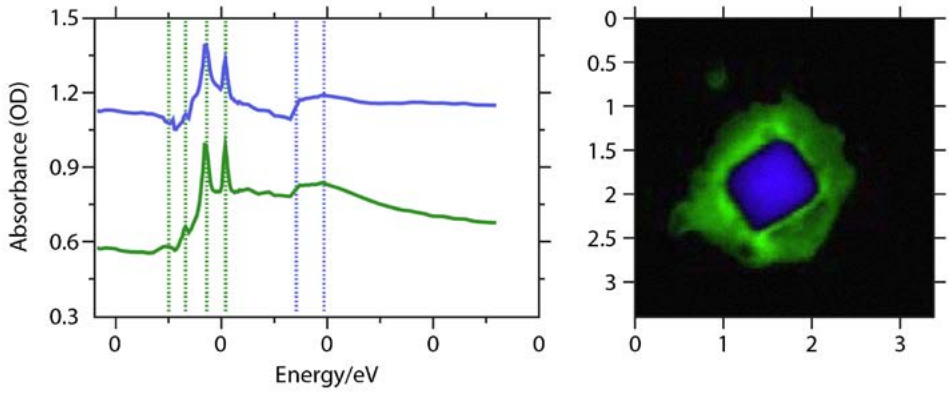
In the Field

A new method developed by Knopf, and colleagues who include EMSL scientists Alex Laskin and Bingbing Wang, allows real-time analysis of ice nucleation in particles. In a Department of Energy-sponsored effort, researchers collected particles from central California to run experiments in this high-resolution ice nuclei environmental scanning electron microscope. With this, they can see where the nucleus forms and then find the particle again to conduct organic functionality investigation or elemental particle position, explained Knopf.

"You have to imagine these particles, about two orders of magnitude smaller than average hair, are deposited on substrates and with this new instrument we can directly – *in situ* – see the ice nucleation as it happens," said Knopf.

This work could answer many questions, such as: What is the nucleation mechanism? Is there liquid water present or not? On which particle did ice preferentially form?

In one case, the research team found aged sea salt particles could nucleate ice, hinting that the ocean could serve as a source of SSAs, which not only affect warm clouds, but also clouds at lower temperatures where ice forms.



These are spectroscopic and morphological features of a sea spray aerosol. The right panel shows compositional analysis of a sea spray aerosol. The blue represents inorganic material, likely NaCl due to cubic shape, and green organic material acting as a coating. (Images provided by Daniel Knopf, State University of New York at Stony Brook.)

"It's amazing to discover there may be ice nucleating material within the top hundred micrometers of the ocean, which affects what's going on up to 10 kilometers in the atmosphere," said Knopf.

By the Sea

The Arctic is another site that may yield key information about the impact of SSAs on cloud formation. From the decks of the Arctic Ocean research vessel, the *CCGS Amundsen*, environmental chemist Allan Bertram takes sea spray aerosols directly from the atmosphere. He also collects samples from the top microlayer of the Arctic Ocean.

The Arctic is an area with a climate that is warming faster than anywhere else on Earth. With naturally low aerosol levels, the region is more sensitive to environmental impacts. Bertram's research, funded by NETCARE, or the Network on Climate and Aerosols: Addressing Key Uncertainties in Remote Canadian Environments, is in the early phases. After obtaining preliminary measurements of ice nucleation properties at the University of British Columbia, he is getting samples ready to go to EMSL for scanning electron microscopy and energy dispersive X-ray spectroscopy analysis to get at particle morphology and chemical composition. Bertram also plans to put the samples through the novel ice nuclei environmental scanning electron microscope analysis.

Already, Bertram's work collecting samples by air from the Northwest Territories shows there are many ice-nucleating particles that may originate from mineral dust in Asia. That is another complication for Arctic climate that needs to be included in our models, he said. If the ocean's microlayers also have ice nuclei capabilities, that could further affect cloud formation and precipitation in these regions.

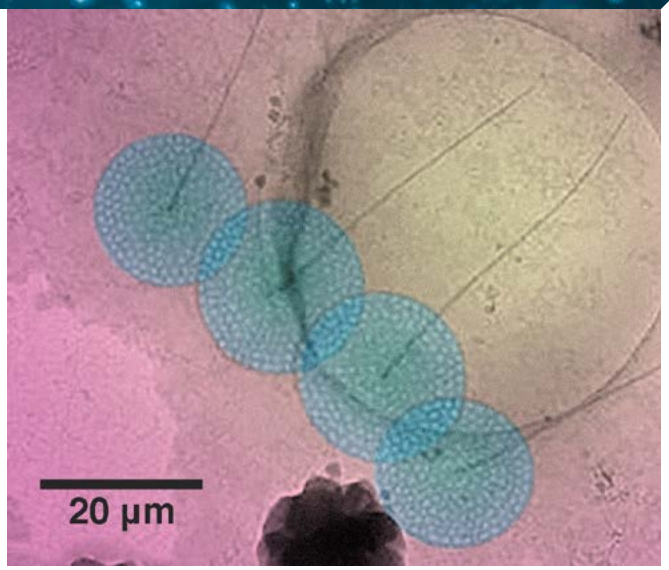
"Both of those are important points," said Bertram. "But we need EMSL's capabilities to help us dig deeper on a molecular level and confirm our hypotheses."

Modeling the "Plausibilities"

Instead of generating aerosols to examine, Pacific Northwest National Laboratory, or PNNL, scientist Susannah Burrows creates models to understand what might happen at the surface of the bubbles traversing the air-water interface.

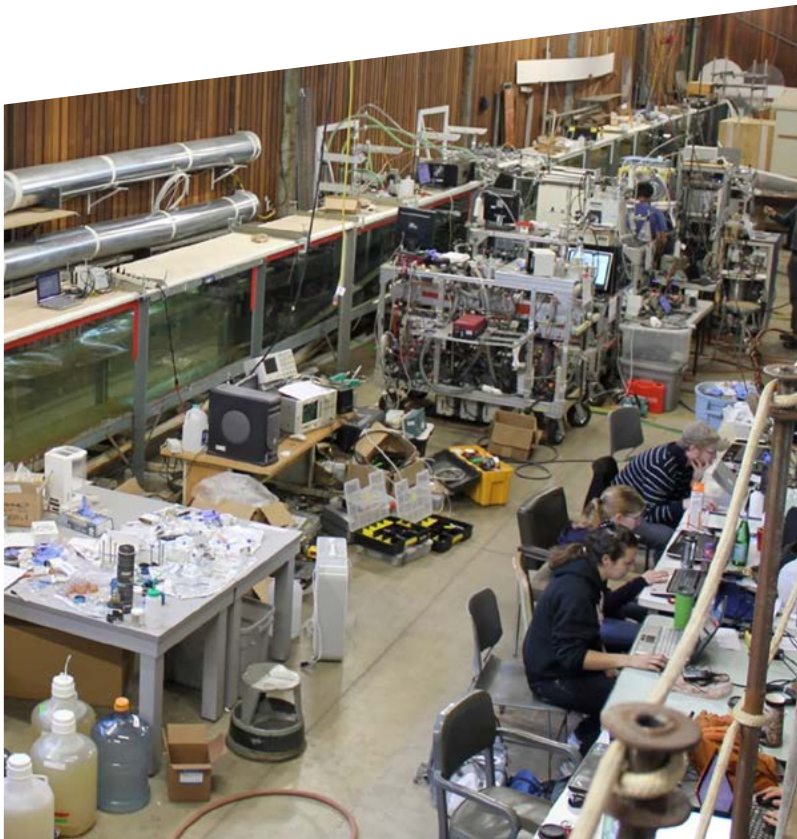
Field samples show that under certain conditions almost 75 percent of SSAs can be coated with organic matter, a finding at odds with models which predicted coatings with only up to 40 percent of organic material. Contributing to that conundrum, most of the coating is made of polysaccharides, compounds which are so water soluble they should not float at the surface like fats or other oils. Further, if the polysaccharides are dissolved in water, then how can they latch onto bubbles at the surface and get launched into the air?

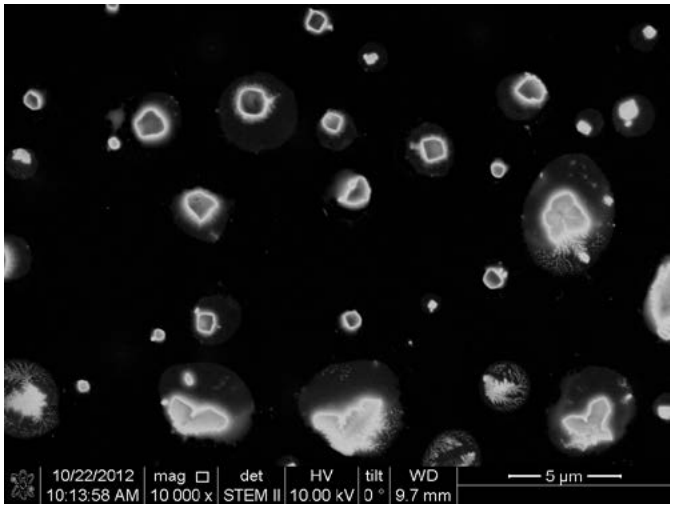
To explain that conflict, Burrows worked with Scott Elliott, an ocean biogeochemist at Los Alamos National Laboratory, and Philip Rasch, the chief scientist for climate science at PNNL, to



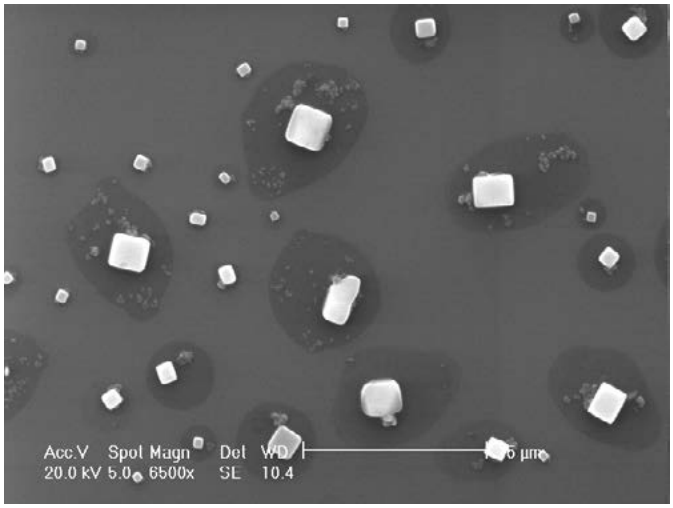
This is a cluster of four diatoms from sea spray aerosols. This cryo-transmission electron microscopy image shows the detail of the diatoms porous silica cell wall. (Image provided by Joseph Patterson, University of California, San Diego.)

The centerpiece of the Center for Aerosol Impacts on Climate and the Environment activities is a 108-foot linear wave channel utilized in understanding the properties of sea spray through spontaneous breaking of waves. It is located at the Hydraulics Laboratory at the Scripps Institution of Oceanography, La Jolla, Calif. (Image provided by Vicki Grassian, University of Iowa.)





Shown are samples of sea spray particles imaged with EMSL's scanning electron microscope. (Image provide by Bingbing Wang, EMSL.)



Shown are samples of sea spray particles composed of NaCl cores (cubic shapes) and organic outer layers. (Image provided by Bingbing Wang, EMSL.)

develop a cooperative adsorption model. This model theorized a thin layer of lipids at the ocean's surface attracted the dissolved polysaccharides. By sticking to the lipids, the polysaccharides could glom onto bubbles when they burst at the surface of the sea.

To test that hypothesis, Burrows turned to Hongfei Wang, a chief scientist at EMSL who developed a high-resolution vibrational sum-frequency generation spectroscopy to improve analysis of complex surface interfaces. In turn, Wang recruited Rob Walker, Montana State University, for his expertise in surface chemistry.

"This idea of organic enrichments was plausible, but there was no experimental basis for knowing whether or not that was true, let alone how powerful that effect could be," said Walker.

In a series of experiments with proxy molecules for sugars and phospholipids, Walker and his students used the high-resolution vibrational sum-frequency generation spectroscopy to reveal that glucosamine, a common sugar in plant cell membranes, could stick to a layer of lipids. Moreover, that interaction modified the interfacial water structure and the organization of lipid molecules at the water's surface.

"Until now, we assumed these molecules didn't interact with each other," said Burrows. "But this mechanism gives us some basis for creating a representation that we can use in our models."

Although the model system worked, "the landscape before us is largely unexplored," Walker cautioned. They initially worked with DPPC, short for the phospholipid dipalmitoylphosphatidylcholine, but in reality there is a heterogeneous mixture of lipids in the ocean. Does a mix of lipids enhance or inhibit cooperative adsorption? We have no idea, said Walker, and there is a long list of other environmental variables.

"We know it can work. Next, we need to know what matters about how it works," said Walker. He is planning more studies at EMSL to test more complex models. To date, this research has been supported by the National Science Foundation and an EMSL user proposal.

Closing the Gap

There remains much to learn about sea spray aerosols and their role in cloud formation. However, the close collaboration among scientists working on fundamental experiments and modeling studies are a unique aspect of research efforts at EMSL, said John Shilling, interim lead for EMSL's Atmospheric Aerosol Systems Science Theme.

"There are no degrees of separation between experimentalists and modelers at our facility," he said. "I think that enhances our research about the effect of these aerosols on our climate." ■

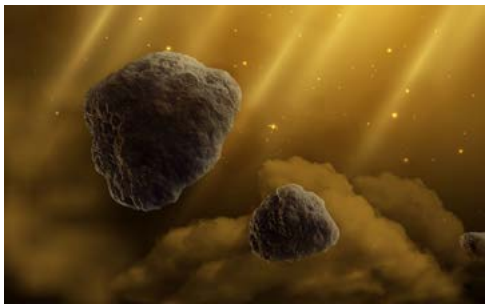
Elizabeth Devitt is a science journalist and freelance writer.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world. Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies.

SCIENCE HIGHLIGHTS

Atmospheric Carbon Chemistry

Improving climate models by understanding brown carbon chemistry



Atmospheric brown carbon is generated from a variety of biogenic and anthropogenic emission sources. The carbon absorbs a significant amount of solar radiation and therefore has a substantial impact on climate. Despite its importance in atmospheric science, it is not clear how brown carbon's chemical composition influences its light-absorption properties. This is because it has been technically challenging to separate light-absorbing organic compounds from other aerosol constituents. A recent study overcame this hurdle by combining advanced chemical separations techniques with state-of-the-art mass spectrometry methods to investigate the optical properties and chemical composition of individual components of brown carbon.

The study significantly improves fundamental understanding of brown carbon chemistry, revealing that overall light absorption by a specific type of brown carbon can be attributed to a set of specific molecules – brown carbon chromophores. By paving the way for more accurate model estimates of light absorption by brown carbon, the findings could have a major impact in the field of atmospheric science.

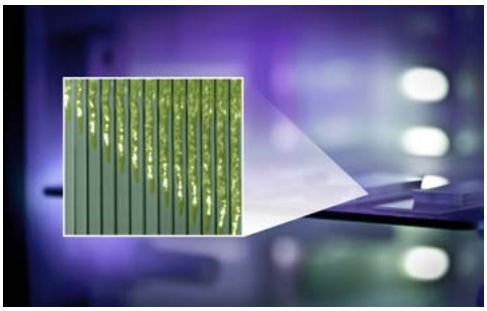
Funding: The research was supported by the Department of Commerce, National Oceanic and 347 Atmospheric Administration through Climate Program Office's AC4 program.

Publication: Lin P, J Laskin, SA Nizkorodov and A Laskin. 2015. "Revealing Brown Carbon Chromophores Produced in Reactions of Methylglyoxal with Ammonium Sulfate." *Environmental Science & Technology*. DOI:10.1021/acs.est.5b03608.

Participating Organizations: EMSL, PNNL and University of California, Irvine.

Visualizing Single Cell Growth Dynamics

Using a robust microfluidic system for visualizing cellular dynamics



Asymmetrical growth is a property of many types of cells in organisms as diverse as algae, fungi, plants and animals. Among the organisms that employ asymmetrical growth are bioenergy-relevant filamentous fungi. Cells from filamentous fungi often resemble a long tube with a slightly tapered tip, where new materials are added during growth. A recent study demonstrated a novel microfluidic system for tracking long-term polarized cell growth, nuclear dynamics and changes in gene expression for filamentous fungi as a way to visualize these highly regulated and environmentally controlled processes with better clarity.

Because fungi produce enzymes that degrade plant cell walls, understanding their growth and how they respond to changes in their environment is critical for developing efficient strategies for breaking up woody material for bioethanol production. Many fungi also have the ability to increase productivity of bioenergy crops such as switchgrass through mutually beneficial relationships. Demonstrating a robust, high-performance microfluidic system for visualizing single cell dynamics could lead to a deeper understanding of cell growth, chemical sensing and communication in fungi and other organisms relevant to bioenergy applications, and pave the way for the development of efficient strategies for biofuel production, bioenergy, biotechnology and medicine.

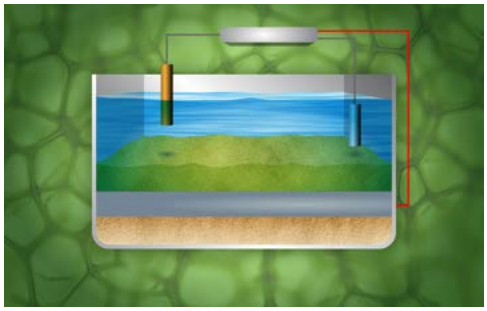
Funding: This research was supported by Mesoscale to Molecules *In-situ* Bioimaging project at Pacific Northwest National Laboratory, or PNNL, sponsored by the Department of Energy's Office of Science, Office of Biological and Environmental Research.

Publication: Geng T, EL Bredeweg, CJ Szymanski, B Liu, SE Baker, G Orr, JE Evans and RT Kelly. 2015. "Compartmentalized microchannel array for high-throughput analysis of single cell polarized growth and dynamics." *Scientific Reports* 5:16111. DOI:10.1038/srep16111.

Participating Organizations: PNNL and EMSL.

Manipulating Microbial Mats

Harnessing energy from microbial mats for biotechnology



Phototrophic microbial mats are among the most diverse ecosystems in nature. These self-sustaining natural ecosystems are composed of highly interactive species that exchange energy and nutrients and catalyze complete biogeochemical cycles over a scale of less than one centimeter. They are an important living system to study because they capture energy from sunlight and convert it to chemical energy that could potentially be converted to high value chemicals and biofuels. A recent study characterized effects of electron transfer processes on the structure, composition and activity of the microbial communities found in these mats.

The findings suggest it is possible to electrochemically regulate the structure, community composition and activities of phototrophic communities in microbial mats. The findings may even represent a new paradigm for designing and manipulating microbial communities. Manipulating these living systems to convert carbon dioxide to specific end products could benefit the biotechnology industry as well as climate science. Moreover, some of these products could potentially be used as chemical feedstocks for energy conversion.

Funding: This research was supported by the Genomic Science Program, Office of Biological and Environmental Research and Pacific Northwest National Laboratory, or PNNL, Foundational Scientific Focus Area. Ryan Renslow was supported by a Linus Pauling Distinguished Postdoctoral Fellowship at PNNL.

Publication: Ha PT, RS Renslow, E Atci, PN Reardon, SR Lindemann, JK Fredrickson, DR Call and H Beyenal. 2015. "Regulation of electron transfer processes affects phototrophic mat structure and activity." *Frontiers in Microbiology* 6:13. DOI:10.3389/fmicb.2015.00909.

Participating Organizations: Washington State University, PNNL and EMSL.

Top-Down Proteomics: Onward and Upward

Characterizing functional proteomes from microbial systems

Achieving a holistic, molecular-level understanding of cellular machinery and communication, microbial community dynamics, and other interactions between organisms and their environments remains a formidable scientific challenge. Realizing this goal would enable more rapid and cost-effective resolution of environmental problems, improve approaches for carbon capture and sequestration, and make large-scale biomass conversion processes more efficient. To this end, new analytical techniques that can provide universal molecular information to inform and guide our understanding of molecular dynamics in complex systems are needed.

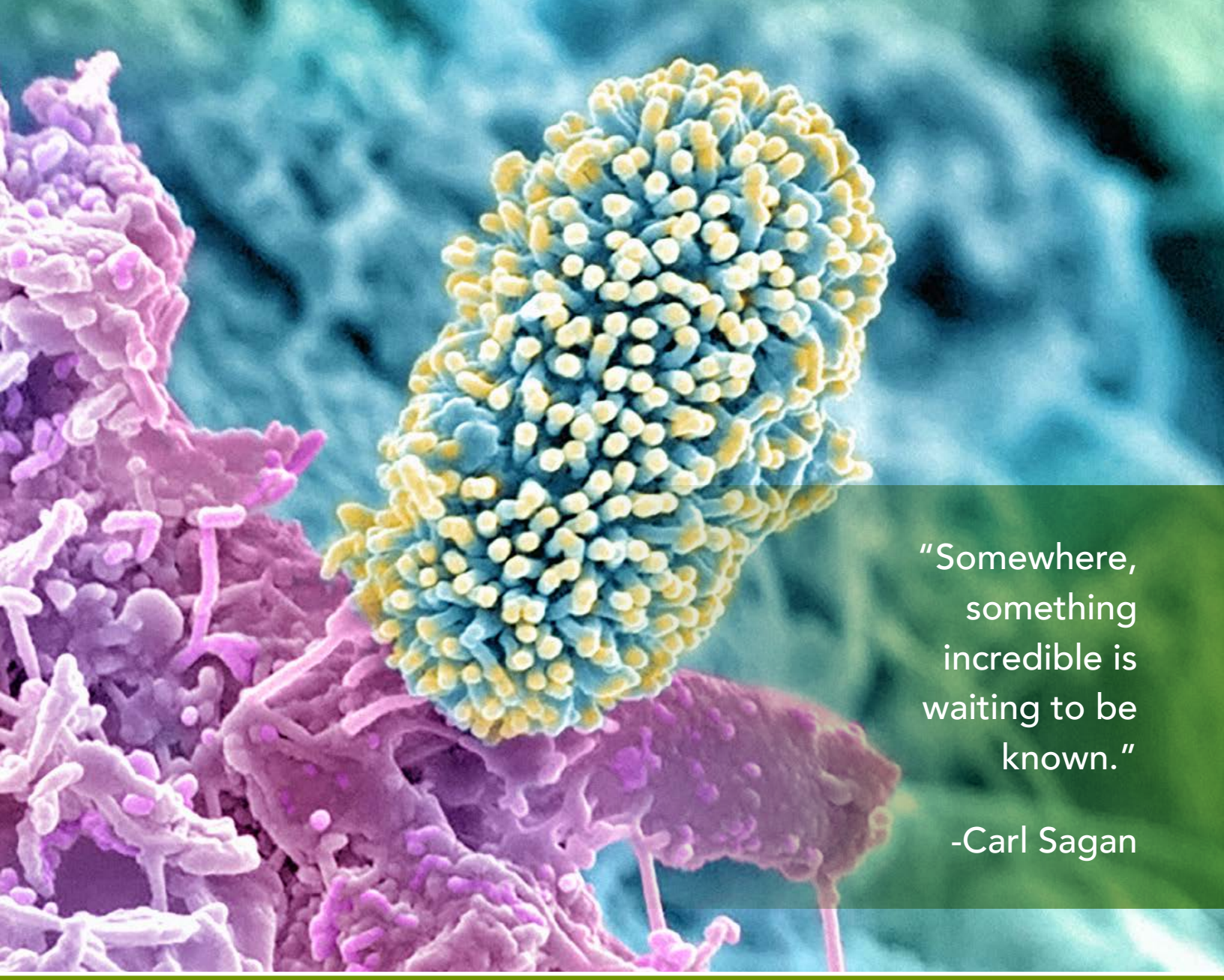
Fourier transform ion cyclotron resonance mass spectrometry, or FTICR MS, offers the highest mass resolution and accuracy of any mass analyzer. One of the world's most powerful FTICR MS systems has recently been developed and is now online at EMSL. The 21 Tesla FTICR MS, which is one of only two in the world with this high of magnetic field strength, will significantly enhance EMSL's overall MS analytical and characterization performance in terms of sensitivity, dynamic range, accuracy, resolution and speed.

The impressive capabilities and promise of this next-generation instrument were highlighted in a feature article published Sept. 11, in *Science*. In the article, Ljiljana Paša-Tolić, EMSL's chief scientist for MS and a technical lead for development of the 21 Tesla FT-ICR MS, explained the potential of using this instrument to characterize complex and heterogeneous glycoforms in fungal secretomes and provide important information for functional studies of glycosylation and their biotechnological applications. Paša-Tolić was one of six scientists featured in the article.

Publications: Perkel JM. 2015. "Top-Down Proteomics: Turning Protein Mass Spec Upside-Down." *Science* 349:1243-1245. DOI:10.1126/science.349.6253.1243.

U.S. DOE. 2015. Office of Biological and Environmental Research Molecular Science Challenges; Workshop Report, DOE/SC-0172. U.S. Department of Energy Office of Science.

Featured Scientist: Ljiljana Paša-Tolić, EMSL.



"Somewhere, something incredible is waiting to be known."

-Carl Sagan

About this Art

The Federation of American Societies for Experimental Biology selected this image by EMSL scientist Alice Dohnalkova as a BioArt winner. The competition showcases the artistic side of cutting-edge science in the biomedical and life sciences fields. Dohnalkova's image was one of 13 award recipients. Winning entries will be exhibited at the National Institutes of Health. View all the winning entries: http://bit.ly/1jzeUuB.

Pictured is a soil bacterium is on the root surface of an *Arabidopsis* plant. The image is from a plant root zone, or rhizosphere, research campaign initiated at EMSL. The campaign, funded by DOE's Office of Biological and Environmental Research, includes scientists from EMSL, Pacific Northwest National Laboratory, the DOE Joint Genome Institute, Brookhaven National Laboratory, the University of Minnesota and the University of Missouri.

Team Members

Ljiljana Paša-Tolić, Alice Dohnalkova, Galya Orr, David Hoyt, Heather Brewer, Meng Markillie and Angela Norbeck, all of EMSL; Kevin Minard and Charles Ansong, both with PNNL; Susannah Green Tringe at DOE JGI; Richard Ferrieri at BNL; Mike Sadowsky and Chanlan Chun, both with the University of Minnesota; and Gary Stacey, Yaya Cui and Lihui Song, all at the University of Missouri. (Image colorized.)