EMSL

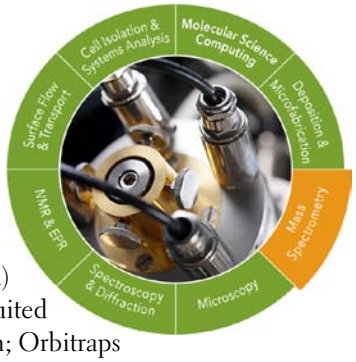
Capabilities Series

Mass Spectrometry

EMSL's expansive mass spectrometry capability group enables high-throughput, high-resolution analysis of complex mixtures of many sample types. These world-class instruments and techniques are part of an unparalleled collection of capabilities designed for research that integrates experimental and computational tools. In particular, mass spectrometry at EMSL facilitates advanced global proteomics research, aerosol particle characterization, the study of ion-surface collisions, and materials characterization. These tools enable novel, fundamental research in EMSL's Science Themes of Biological Interactions and Dynamics, Geochemistry/Biogeochemistry and Subsurface Science, and Science of Interfacial Phenomena. Specific research topics include:

- Proteomics – studying protein signatures in human, animal, plant, and microbial cells and cell communities to uncover fundamental processes within whole organisms
- Environmental remediation and clean energy – understanding and tailoring biological systems to return contaminated areas to their natural state; making strides toward alternative energy sources based on microbial and plant biology systems
- Biomarkers and disease – defining and detecting specific protein signatures that indicate the health status of a system
- Aerosols and pollution – obtaining chemical makeup of aerosols to understand the processes that control the atmospheric aerosol life cycle; helping model the relationship between aerosols and climate
- Surface Science – conducting highly specific surface modification, cluster ion-solid interactions, trace element characterization in materials, and three-dimensional distribution of small functional molecules in biological samples.

CAPABILITY DETAIL



Proteomics

- Fourier transform (FT) mass spectrometry, including high-field (up to 15 Tesla as of summer 2010) Fourier transform ion cyclotron resonance (FTICR) spectrometers particularly well-suited for top-down proteomics research; Orbitraps and LTQ-Orbitraps for global (quantitative) proteomics, phosphoproteomics, metablomics, and lipidomics research
- A set of triple-quadrupole spectrometers for targeted proteomics and metabolomics, including multi-reaction monitoring
- Several ion mobility spectrometry (IMS) time-of-flight (TOF) spectrometers for ultra-high throughput applications
- Custom high-performance (multi-dimensional) liquid chromatography systems (HPLC)

Aerosol and Ion-Surface Collisions

- LTQ-Orbitrap for environmental research
- Field-deployable, second-generation single-particle TOF mass spectrometer (SPLAT II)
- 6-Tesla FTICR specially configured for studying ion-surface interactions
- Ion deposition instrument for selective preparation of novel materials using ion soft-landing
- Time-of-flight secondary ion mass spectrometry (TOF-SIMS) capabilities for materials characterization

WHY MASS SPECTROMETRY AT EMSL?

- EMSL provides mass spectrometry tools within an integrated problem-solving environment that combines custom instrumentation and techniques with world-class staff expertise.
- A highly integrated LC, IMS and mass spectrometry (FTMS, TOF, triple-quadrupole) platform is constantly being upgraded for enhanced sensitivity, better resolution, and higher throughput analysis of biological systems, including proteomics, metabolomics, and lipidomics.
- In-house bioinformatics tools lead to meaningful interpretation of 'omics datasets using effective and novel data storage, assimilation, and visualization.
- Specially configured instruments allow researchers to uncover the fundamental aspects of activation, dissociation, and deposition (soft-landing) of complex molecular ions following collision with specially prepared surfaces.

ABOUT EMSL

EMSL, a U.S. Department of Energy national scientific user facility located at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.

EMSL's distinctive focus on integrating computational and experimental capabilities as well as collaborating among disciplines yields a strong, synergistic scientific environment. Bringing together experts and an unparalleled collection of state-of-the-art instruments under one roof, EMSL has helped thousands of researchers use a multidisciplinary, collaborative approach to solve some of the most important and complex national scientific challenges in energy and environmental sciences.

To learn more about EMSL, the science conducted at EMSL, as well as the instruments and expertise available to users, visit www.emsl.pnl.gov.

BECOME AN EMSL USER

Researchers are invited to access the world-class capabilities and collaborate with the internationally recognized experts at EMSL via its peer-reviewed proposal process. To submit a proposal, follow the five steps outlined on the EMSL website (www.emsl.pnl.gov) under User Access. Current and potential EMSL users are encouraged to respond to Calls for Proposals, which are announced each spring. However, unique research proposals that fall outside the Calls for Proposal focus may be submitted at any time.

Applicants are encouraged to submit proposals for use of EMSL's capabilities with an emphasis on integrating computational and experimental tools. In general, most users whose open research proposals are accepted may use EMSL resources free of charge. Open research is loosely defined as science and engineering research for which the resulting information is published and shared broadly within the scientific community.

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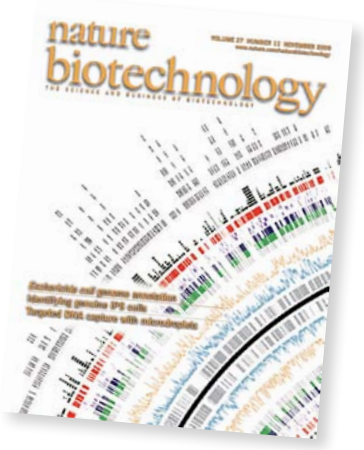
MASS SPECTROMETRY RESEARCH HIGHLIGHTS

Understanding Genome Structure to Unlock its Function



Cover Story A graphical representation of part of the *E. coli* genome, the organization of which was elucidated by EMSL users.

To augment current knowledge of how genetic information is controlled at the molecular level, researchers have developed and applied a new systems-level approach for generating the comprehensive transcription unit architecture of *Escherichia coli* K-12 MG1655.

Integrating multiple 'omics measurements, including proteomics data obtained at the EMSL, a team of researchers from the University of California San Diego and Virginia Commonwealth University identified roughly five times more transcription units of *E. coli* than were previously known, and improved translation start site mapping over earlier annotations. The team's research was featured on the November 2009 cover of *Nature Biotechnology*.

EMSL Users: University of California San Diego, Virginia Commonwealth University

Cho et al. 2009. *Nature Biotechnology* 27(11):1043-1051.

A Better Way to Measure Particles

SPLAT II and its companion software package exemplify EMSL's ability to not only yield vast and varied mass spectrometry data, but also move from data to discovery.

Tiny particles are pivotal to climate change, public health, and nanotechnology. A significant fraction of these particles are aspherical, yet scientists must routinely assume the particles are spherical to interpret many measurements of particle properties. To determine the true shape of particles, expert scientists devised SPLAT II, a single particle mass spectrometer housed in EMSL that provides extremely precise multi-dimensional particle measurement and characterization.

The 2006 paper that details SPLAT II's ability to determine dynamic shape factors is the second most cited article in *Aerosol Science and Technology*, the official journal of the American Association for Aerosol Research. Other SPLAT-related publications include special features and invited papers in the *Proceedings of the National Academy of Sciences* and *International Reviews in Physical Chemistry*.

EMSL Users: Pacific Northwest National Laboratory, Imre Consulting

Zelenyuk et al. 2006. *Aerosol Science and Technology* 40(3):197-217.

Zelenyuk et al. 2009. *International Reviews in Physical Chemistry* 28(2):309-358.

Vaden et al. 2010. *Proceedings of the National Academy of Sciences* 107 (15) 6658-6663, early edition published March 1, 2010.

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