

EMSL Report
July/August 2003

The W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research. At one location, EMSL offers a comprehensive array of leading-edge resources in six research facilities.

Access to the capabilities and instrumentation in EMSL facilities is obtained on a peer-reviewed proposal basis. Users are participants on accepted proposals. Staff members work with users to expedite access to the facilities and scientific expertise. The EMSL Report documents research and activities of EMSL staff and users.

Research Highlights

Identification of Bacterial Spores Using Statistical Analysis of Fourier Transform Infrared Photoacoustic Spectroscopy Data

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Research at PNNL has led to a new technique for identifying strains of bacterial spores that requires a minimum of test sample preparation and provides highly accurate results. This new technique is based on the combination of Fourier transform infrared (FTIR) spectroscopy and photoacoustic spectroscopy (PAS). FTIR offers good differentiation among highly similar substances, while PAS enables the technique to be used on solid samples without the need for extensive pretreatment. The research group developed new algorithms for classification of samples based on FTIR-PAS experimental results. With this spectroscopic/statistical approach, it was proven possible to differentiate bacterial from non-bacterial materials, determine which bacterial samples corresponded to ones in the FTIR-PAS reference library, and identify the exact strain of those bacterial spores. An accuracy of better than 90 percent was obtained at each stage. Further research is planned to expand the range

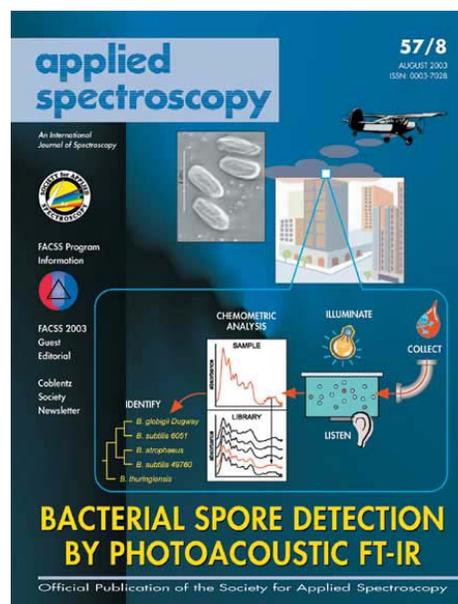


Figure 1. Cover of the August issue of Applied Spectroscopy featuring the research on the photoacoustic FTIR detection of bacterial spores.

of bacteria in the library, to determine the effect of varying growth conditions, and to test the applicability of the technique to mixtures of spores. The instrumentation has the potential to be made portable for testing samples in the field. An article on the research is featured on the cover of the August 2003 issue of the journal *Applied Spectroscopy* (Figure 1).

Citation

Thompson SE, NS Foster, TJ Johnson, NB Valentine, and JE Amonette. 2003. "Identification of Bacterial Spores Using Statistical Analysis of Fourier Transform Infrared Photoacoustic Spectroscopy Data." *Applied Spectroscopy* 57(8):893-899.

Surface Protein Isolation and Identification of *Geobacter*

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(b) University of Massachusetts, Amherst, Massachusetts

The *Geobacter* family of bacteria is known for its ability to reduce groundwater contaminants such as uranium, technetium, and other heavy metals into solid form to prevent their motility. To understand the mechanisms involved in bioremediation of this organism, further investigation is necessary of the surface-exposed proteins using sample preparation techniques and instrumentation within EMSL's High-Performance Mass Spectrometry Facility. As part of this research, biomass was produced for two different *Geobacter* species grown under three different environmental conditions. The surface-exposed proteins of the cells were then labeled and extracted from the remainder of the cells. Portions of labeled proteins will be separated and analyzed via high-pressure liquid chromatography and high-performance mass spectrometry, with the resulting data expected to help identify molecular targets (proteins) involved in bioremediation.

Synthesis, Characterization, and Manipulation of Helical SiO₂ Nanosprings

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(c) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

Researchers have discovered a method for making helical silica nanosprings, which could have applications in composites and nanomechanical and nanoelectromagnetic devices. Zhang et al. have produced unique helical silica nanotubes via a reaction carried out in a tube furnace. Using a dual flow-tube furnace, the researchers placed a silicon wafer substrate in the inner tube, and iron and silicon/SiO₂ powders inside the outer flow tube. Synthesis of the springs took about two hours at 1160°C in the presence of methane.

The helical fibers terminated in straight segments, and nanoparticles were present where the straight and helical segments joined. Silica is generally a highly brittle material, but the silica helices were shown to be flexible and capable of storing energy—thus, the name nanosprings. In this way, the researchers made amorphous helical SiO₂ nanosprings up to 8 μm long with diameters of 80 to 140 nm. The nanosprings, which resembled coiled telephone cords, were joined at either end to straight amorphous SiO₂ nanowires. The ribbon comprising the nanosprings was rectangular, rather than cylindrical, in cross-section.

The team tested the spring-like qualities of the helical wires by focusing the electron beam of a transmission electron microscope (TEM) onto various points along their length (Figure 2). This caused local heating and expansion of the spring, with corresponding contraction of the spring away from the heating point. The researchers also applied pressure to the nanosprings using the tip of an atomic force microscope (AFM), an experience that bent and slightly stretched the nanosprings. The TEM heating experiment and the AFM manipulation suggest that the helical nanosprings possess the same characteristics as micro/macro springs.

Citation

Zhang HF, CM Wang, EC Buck, and LS Wang. 2003. "Synthesis, Characterization, and Manipulation of Helical SiO₂ Nanosprings." *Nano Letters* 3(5):577-580.

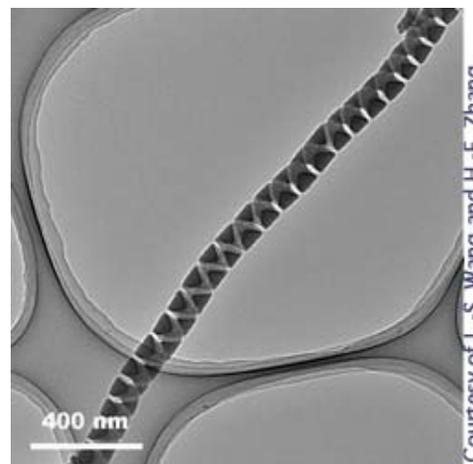


Figure 2. A TEM image of SiO₂ of the helical nanosprings.

Full-Color Emission and Temperature Dependence of the Luminescence in Poly-*P*-phenylene ethynylene-ZnS/Mn²⁺ Composite Particles

W Chen,^(a) AG Joly,^(b) JO Malm,^(c) JO Bovin,^(c) and S Wang^(a)

(a) *Nomadics, Inc., Stillwater, Oklahoma*

(b) *Pacific Northwest National Laboratory, Richland, Washington*

(c) *University of Lund, Lund, Sweden*

Chen et al. have synthesized a composite material composed of anionic poly(phenylene ethynylene) (aPPE) polymer particles and ZnS/Mn²⁺ nanoparticles. The composite material has several unique physical and luminescence properties, including blue (460-nm), green (490-nm), orange (596-nm), and red (706-nm) spectral emissions (Figure 3). In addition, the relative intensities of the spectral emissions change with the excitation energy.

Temperature studies from room temperature to 90°C show that the luminescence at 596 nm increases in intensity with increasing temperature. This interesting result is attributed to thermoluminescence and thermal curing of the particle surface upon heating.

The luminescence properties of this nanocomposite material make it a potential candidate for use in full-color displays. The temperature dependence behavior may have applications for temperature measurement in laser cooling systems where temperature detection is still an unsolved problem.

The characterization of the material's luminescence properties was performed in the EMSL Chemistry and Physics of Complex System (CPCS) Facility's laser spectroscopy laboratory. Understanding the optical properties of composites and nanomaterials has important applications in lasers, laser cooling, optical communications, storage, displays, and imaging techniques.

Citation

Chen W, AG Joly, JO Malm, JO Bovin, and S Wang. 2003. "Full-Color Emission and Temperature Dependence of the Luminescence in Poly-*P*-phenylene ethynylene-ZnS/Mn²⁺ Composite Particles." *Journal of Physical Chemistry B* 107(27):6554-6551.

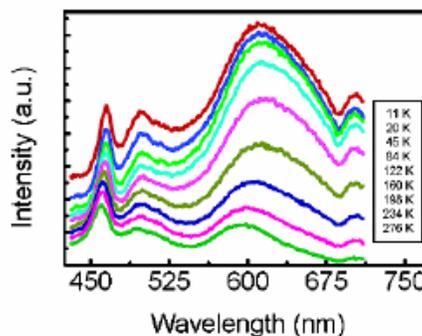


Figure 3. Luminescence spectra of the aPPE-ZnS/Mn²⁺ nanocomposite at different temperatures ranging from 11 to 276 K.

Investigating Molecular Recognition and Biological Function at Interfaces Using Antimicrobial and Biomineralization Peptides

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(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

Many peptides and proteins, such as membrane proteins, antimicrobial molecules, and biomineralization proteins, perform biological functions at interfaces. Understanding molecular recognition at interfaces can provide important knowledge needed to fight many diseases and design new biomaterials and drugs, including broad-spectrum drugs. This research reflects fundamental interest in the principles underlying the biological function and mechanisms of action of peptides and proteins active at interfaces. Much remains to be discovered about the structures and mechanisms of action of such biomolecules at the molecular level. Understanding their function requires analysis of three-dimensional structures of physiologically relevant samples. Using various high-resolution nuclear magnetic resonance (NMR) techniques in the bound states of these biomolecules provides insightful structural and dynamic knowledge. Traditionally, this work has been performed on uniformly labeled proteins in solution; however, many important systems are not suitable for this approach. This includes the peptides and proteins incorporated into membranes.

Possible emerging solid-state NMR techniques can be used on site-specific isotopically labeled peptides to gain structural and dynamic information through distance measurements and relaxation studies on membrane bound proteins and peptides. Cotten et al. are studying the mechanisms of action of antimicrobial peptides from mast cells of fish. These peptides, named piscidins, are cationic antimicrobial peptides found in fish that are believed to interact with microbial lipid membranes as part of their mechanism to kill a broad variety of bacteria. The research team is attempting to learn more about their mechanism of action and more precisely how they interact with lipid membranes by focusing on the peptide backbone structure. The team's strategy includes performing distance measurements using a number of solid-state NMR experiments, especially ^{13}C - ^{15}N REDOR (Rotational Echo Double Resonance). Initially, the team will probe the secondary structure along the peptide by observing several positions along its backbone. Subsequently, they will test various pH conditions and lipid types to determine parameters that regulate the specificity and activity of these peculiar peptides. Initial distance measurements have been carried out at low temperature (i.e. about 20°C), quenching some dynamics problematic at room temperature in the hydrated (physiologically relevant) peptide/lipid samples of interest.

The instrumentation at EMSL, including the Varian solid-state 500-MHz wide bore NMR spectrometer with triple-resonant probes and high-sensitivity, and low-temperature capacity, has been essential for the team's progress.

Surface Decontamination of Simulated Chemical Warfare Agents Using a Nonequilibrium Plasma with Off-Gas Monitoring

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(a) *InnovaTek, Inc., Richland, Washington*

(b) *Pacific Northwest National Laboratory, Richland, Washington*

(c) *W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington*

An effective, near-real-time decontamination system for toxic chemical and biological materials on surfaces would address a range of concerns within military and industrial sectors, including the protection of troops and civilians against warfare agents and other toxic substances in battlefield and terrorist situations. Recent concerns regarding food safety could also be addressed by the development of surface decontamination technology. InnovaTek is developing a surface decontamination technology that uses active species generated in a nonequilibrium corona plasma. This work used a variety of instrumental methods available at EMSL to verify the efficacy of the plasma technology. These methods included gas chromatograph-mass spectrometry (GC-MS), X-ray photoelectron spectroscopy (XPS), and secondary ionization mass spectrometry (SIMS). In addition, ion trap mass spectrometry (ITMS) with direct atmospheric sampling was used as a real-time monitor of the decontamination process.

The plasma technology was tested against dimethyl methylphosphonate (DMMP), a simulant for the chemical agent Sarin. Test coupons, flat pieces of aluminum with an area of approximately 4 cm², were thoroughly cleaned and then inoculated with 5 μ l droplets of DMMP at a minimum concentration of 0.5 g/m². Immediately after inoculation, the test coupons were exposed to the plasma for periods from one to 20 minutes. The quantity of DMMP remaining on the surface of the coupon was determined versus plasma treatment times by rinsing the coupons with acetone and analyzing the solution with GC-MS. The data shown in Figure 4 indicate that greater than a four log₁₀ destruction of the DMMP on an aluminum surface was achieved in a 10-minute plasma treatment.

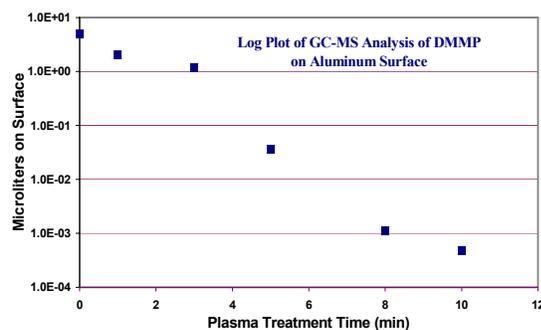


Figure 4. Chemical agent decontamination efficiency for DMMP, a Sarin simulant, on an aluminum surface treated with a 20-watt plasma flare prototype.

Additional information about the plasma decontamination process was obtained by real-time monitoring of the gas-phase products using an ITMS with a direct air-sampling interface. Figure 5 shows the relative concentration versus exposure time for the primary peaks observed in the mass spectrum, PO_3 and PO . The relative concentration of the DMMP breakdown products from plasma exposure shows a range of approximately two orders of magnitude. These data are consistent with the GC-MS results, although the dynamic range is reduced on the low end by signal-to-noise limitations and on the high end by the time response of the system. The apparent induction time of two minutes is a convolution of the actual induction time for the DMMP on the surface to react with the plasma and the delay and broadening due to the capillary interface. This has the effect of spreading the intensity in time and reducing the maximum observed signal. It is significant that the off-gas mass spectrum differs significantly from the pure DMMP mass spectrum, as this demonstrates unequivocally that the cold plasma decontamination is not simply volatilizing the DMMP, but breaking it down into harmless components.

GC-MS analysis showed that a greater than four \log_{10} destruction of the DMMP on an aluminum surface was achieved in a 10-minute treatment. XPS and SIMS were used to detect any trace levels of DMMP. The resulting data were consistent with that from the GC-MS, indicating that less than a monolayer of DMMP remained after plasma treatment. Figure 6 shows SIMS data that demonstrate the changes in surface chemistry produced by exposure to the plasma. The technology is being further refined to develop a product that will not only decontaminate surfaces, but will also sense when decontamination is complete.

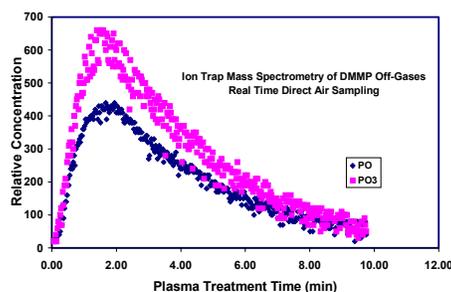


Figure 5. Analysis of off-gases during the decontamination of DMMP, a Sarin simulant, on an aluminum surface treated with a 20-watt plasma.

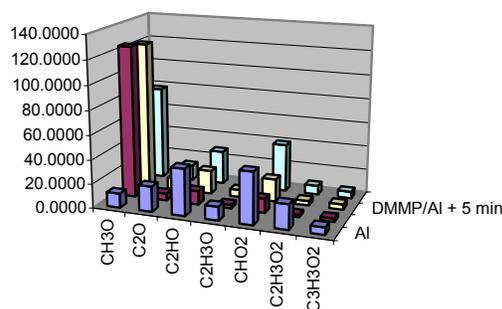


Figure 6. SIMS results for selected chemical fragments resulting from plasma treatment of a test coupon and an aluminum control coupon.

Professional/Community Service

PNNL hosted the Lustre Users Group during the week of July 28, 2003 at EMSL (Figure 7). The meeting was coordinated by Scott Studham, Technical Lead for the Molecular Science Computing Facility's operations group. Fifty attendees from 15 high-performance computing sites were represented, including DOE, academic, and commercial organizations. Presentations covered current Lustre deployments, future directions, configuration, administration, and storage technology.



Figure 7. The first Lustre Users Group meeting was held in Richland, Washington, with fifty attendees from across the U.S.

The Lustre User Group promotes the use of the open source Lustre file system for high performance technical computing and scalable IO. The group is working to develop a community knowledge base of best practices that make Lustre implementations successful and provide feedback to the development community on current issues and future needs.

Major Facility Upgrades

The new Phase 2 Supercomputer (MPP2, Figure 8) became operational on July 31, 2003. MPP2 is completely composed of Intel's 64-bit, 1.5-Gigahertz "Madison" processors. The Phase 1 system was upgraded and integrated with the MPP2 system, and users have since been migrated to the new system. This new system has a theoretical peak performance of more than 11 trillion calculations per second, making it one of the five fastest systems in the world.

The process of re-archiving EMSL's proteomics data to the Molecular Science Computing Facility's (MSCF) NorthWest file system (NWfs) was also completed successfully in July. At the end of August, NWfs contained 13.7 terabytes (one terabyte equals 1000 gigabytes) of data, 10.6 terabytes of which were proteomics data. NWfs' predecessor, the Scientific Archive Management system, stored approximately 5 terabytes when NWfs replaced it in May 2003, nearly



Figure 8. Nathan Tenney, Timothy Witteveen, and Evan Felix working on the MPP2 supercomputer.

tripling the quantity of data stored in MSCF storage servers between May and August, and representing the first time that all of EMSL's proteomics data has been stored on MSCF servers.

News Coverage

On July 15, 2003, The Register printed the article, "HP claims HPTC bragging rights," (<http://www.theregister.co.uk/content/61/31755.html>) that discussed the new Top 500 Supercomputers list released in July. It mentions that Hewlett Packard (HP) is still in the lead with the largest share of the High-Performance Technical Computing market. The article also mentions the PNNL HP Itanium2 cluster (MPP2) and states that it is interesting that HP chooses to highlight this cluster rather than a larger 20-teraflop supercomputer named "ASCI Q" at Los Alamos National Laboratory.

At the end of August, numerous articles about the updated MPP2 system appeared in several newspapers, including a story on the front page of the Tri-City Herald (<http://www.tricityherald.com/tch/local/story/3768900p-3795194c.html>). On August 28, the headline for HPCwire, an online e-zine (email type magazine) was "PNNL SUPERCOMPUTER FASTEST OPEN SYSTEM IN U.S." Other headlines such as "PNNL fastest open supercomputer in U.S." and "HP Unveils World's Fastest Linux Supercomputer Based on HP Integrity Servers" were featured in several other publications, including the Associated Press, Seattle Times, Seattle Post-Intelligencer, USA Today, The Register, Network World, TechNews World, IDG News, Computerworld, ITWorld, InfoWorld, LinuxWorld, and PC World. The release was also covered on several radio and TV stations, including KATU Portland and KIRO AM Seattle, as well as on the World Wide Web at OAKRIDGER.com and Slashdot.com.

Visitors and Users

Chemistry and Physics of Complex Systems Facility

- David Laman and students Zack Jacobson and Seth Miller, Central Washington University, Ellensburg, Washington, worked with Ken Beck to study triplet decay pathways of a specific electrically conducting polymer in an effort to determine how to maximize the efficiencies of photocells based on that polymer.
- Stephen J. Lockett, National Cancer Institute, Frederick, Maryland, visited with staff and toured the facilities in the CPCS and Molecular Science Computing facilities to discuss the potential for a collaborative research program in image processing.
- In July, George Nieman, Monmouth College, Monmouth, Illinois, completed a year-long sabbatical at EMSL. During his sabbatical, he collaborated with Jim Cowin,

conducting scanning mass spectroscopy of aerosols to allow for the better characterization of diesel exhaust particles.

- This summer, several high school and graduate students performed hands-on research or worked along-side researchers at the CPCS Facility to gain a new understanding and greater interest in the sciences:
 - Jormarie Alvarez, Purdue University, West Lafayette, Indiana, studied the dissociative charge inversion of peptides by surface-induced dissociation under the guidance of Julia Laskin and Anil Shukla.
 - A Bridges Post High School Fellowship recipient, Benjamin Arthurs, Richland High School, Richland, Washington, worked with Gary Holtom to study fluorescence microscopy of cells and particles.
 - Aubrey Espana, Washington State University, Pullman, Washington, worked with Wayne Hess on the use of scanning microscopy capabilities to study soil mineral weathering.
 - Ben Elliott, Utah State University, Logan Utah, worked with Lai-Sheng Wang to investigate aromatic and other novel gas-phase atomic clusters and molecules.
 - Brook Holben, Washington State University, Pullman, Washington, and Emily Ashjian, Southridge High School, Kennewick, Washington, worked with Marianne Resat using the electron microbeam to study electron induced genomic instability.
 - Amy Williams, Gonzaga University, Spokane, Washington, worked with Katye Judd and Robert Disselkamp on the ultrasonic catalysis of chemical reactions.
 - In conjunction with the Interfacial and Nanoscale Science Facility and Robert Disselkamp, Bilal Zuberi and Kirsten Johnson, graduate students at the Massachusetts Institute of Technology, Cambridge, Massachusetts, assisted with elemental analysis of bulk aerosol samples collected with a drum impactor during a 2003 field study conducted in Mexico City, Mexico. This research is part of a study involving Jim Cowin and Alex Laskin.

Environmental Spectroscopy & Biogeochemistry Facility

- Sue Clark, Washington State University, Pullman, Washington, will spend part of her one-year sabbatical at EMSL working with Andy Felmy and Odeta Qafoku to collect initial experimental data and develop thermodynamic models in order to predict the binding of metal ions (e.g., calcium) and actinide analogs (e.g., europium) in the microbial outer membrane.
- Colleen Hansel and Jim Neiss, graduate students at Stanford University, Stanford, California, visited EMSL to use the high-resolution transmission electron microscope and energy dispersive spectroscopy capability. Hansel's investigations are focused on the theory of the mechanism of iron biomineralization induced by dissimilatory iron-reducing bacteria. As a part of a well-established collaboration with Stanford professor Scott Fendorf's laboratory, she is interested in further (nanoscale) analyses of previously identified iron-reduction products. Neiss introduced a new project following pathways of bioreduction of U(VI) into U(IV), and its redox competition and secondary mineral formation in columns simulating soil conditions.

Interfacial & Nanoscale Science Facility

- Steven Emory and Haley Pugsley, Western Washington University, Bellingham, Washington, visited the I&NS Facility in connection with characterizing metal nanoparticle nanoassemblies.
- Karl Hibbitts, Tom McCord, and Gary Hansen, University of Washington, Seattle, Washington, are working to irradiate select non-ice materials with MeV ions of oxygen, sulfur, and carbon.
- Yong Joo Kim, Hanbat National University, Vancouver, Canada, continues to work on investigations related to the growth and characterization of oxide nanostructures.
- Michael Nakles, National Aeronautics and Space Administration Glenn Research Center, Cleveland, Ohio, conducted experiments related to low-energy sputtering experiments using Rutherford backscattering.
- Vladimir Petrovsky, University of Missouri-Rolla, Rolla, Missouri, gave the seminar “Nanocrystalline Materials: Preparation, Investigation, and Possible Applications in SOFC.”

High Performance Mass Spectrometry Facility

- David Gibb Camp II, Pacific Northwest National Laboratory, Richland, Washington, collected initial protein identifications from homogenized mouse brain samples as part of “Preliminary Work on the Proteomes of Brains and Dissected Brains Obtained from Control Mice and Treated Mice Simulating Parkinson’s Disease.”
- Mary Lipton, Pacific Northwest National Laboratory, Richland, Washington, is continuing studies of the proteome *Deinococcus* under different stress conditions.
- Anil J. Patwardhan, University of California-San Francisco, San Francisco, California, is working on “Identification and Relative Expression of Membrane Proteins in Breast Cancer Lines.”
- Desmond Smith, University of California, Los Angeles, California, and David Gibb Camp II, Pacific Northwest National Laboratory, Richland, Washington, are working on “High throughput FTICR strategies for the molecular analysis of cancer.” Additional FTICR analyses were completed on cultured human mammary epithelial cells. These analyses will contribute to building a database of proteome biomarkers for human cell lines. Completion of this database will allow studies of proteomics to characterize the onset and development of breast cancer.
- As part of “Functional Genomics and Proteomics of Mitochondria,” Wenzhong Xiao, Stanford University, Stanford, California, collected relative abundance data for mitochondria in yeast.

High Field Magnetic Resonance Facility

- Cheryl Arrowsmith, University of Toronto, Toronto, Ontario, Canada, used the 750- and 600-MHz spectrometers as part of the study “Structural Proteomics: Annotating the Genome Using 3D Structure.”
- Peter Brzovic, University of Washington, Seattle, Washington, used the 800- and 600-MHz spectrometers for “NMR Structural Investigations of BRCA1.”
- Herman Cho, Andrew Felmy, Odeta Qafoku, and Yuanxian Xia, Pacific Northwest National Laboratory, Richland, Washington, used the 500-MHz spectrometer to study “Interaction of Solution-State Silicates with Trivalent Cations.”
- Myriam Cotten, Kenneth Daugherty, and McKenna Manion, Pacific Lutheran University, Tacoma, Washington, used the 500-MHz WB spectrometer to study “Investigating Molecular Recognition and Biological Function at Interfaces Using Antimicrobial and Biomineralization Peptides.”
- Youjun Deng, Washington State University, Pullman, Washington, used the 500-MHz spectrometer to study “Variable-Temperature MAS NMR Spectroscopic Study of Incorporated and Sorbed ^{13}C s and ^{23}Na in Zeolitic Minerals.”
- Kathryn Ely and Klara Briknarova, The Burnham Institute, La Jolla, California, used the 600- and 750-MHz spectrometers as part of the study “Structure of the PR Domain of RIZ1 Tumor Suppressor.”
- Nancy W. Hinman, University of Montana, Missoula, Montana, remotely used the 300-MHz spectrometer to study “Atomic-Level Investigations of Thermal Spring Deposits: S-NMR of Natural Siliceous Sinters.”
- Stephen R. Holbrook, Lawrence Berkeley National Laboratory, Berkeley, California, used the 500-MHz magnet as part of the study “Structural Biology of DNA Repair Proteins: The Nudix Protein Family from the Extremely Radiation-Resistant Bacterium *Deinococcus radiodurans*.”
- John Holladay and Michael Lilga, Pacific Northwest National Laboratory, Richland, Washington, used the 300-MHz spectrometer to study “NMR Analysis of Pyrrolidinone Precursors and Derivatives.”
- Cynthia K. Larive and William H. Otto, University of Kansas, Lawrence, Kansas, recently worked remotely on the 300-MHz spectrometer as part of the study “Solid-State NMR Studies of Rhamnolipid Metal Complexes.”
- Flemming H. Larsen, University of Copenhagen, Copenhagen, Denmark, and Ian Farnan, University of Cambridge, Cambridge, United Kingdom, used the 800-MHz spectrometer as part of the study “Separation of ^{47}Ti and ^{49}Ti Solid-State NMR Lineshapes from Crystalline and Glassy Materials by Static QCPMG Experiments.”

- David Lindquist and Gaylen Burnside, University of Arkansas, Little Rock, Arkansas, used the 300-MHz spectrometer as part of the study “Aluminum Coordination Environments in Lanthanum Stabilized Alumina and in Hydrotalcite.”
- Robert A. Mantz, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, used the 500- and 300-MHz spectrometers to study “Solid-State NMR Investigation of Coating Materials Prepared Using the SNAP Methodology” and “NMR Characterization of Spider Silk Proteins and the Effect of Processing on Spider Silk Films.”
- Gaetano Montelione, Rutgers University, Camden, New Jersey, used the 800- and 600-MHz spectrometers as part of the study “Structural Genomics of Eukaryotic Model Organisms.”
- Kristopher J. Ooms and Michelle Forgeron, University of Alberta, Edmonton, Alberta, Canada, used the 800- and 750-MHz spectrometers to study “High-Field Solid-State ^{99}Ru NMR Spectroscopy in Inorganic and Organometallic Ruthenium Compounds” and “An Extended Study of Solid Molybdenum and Organometallic Magnesium Compounds Using ^{95}Mo and ^{25}Mg Nuclear Magnetic Resonance Spectroscopy.”
- Joseph Quinn, Oregon Health and Science University, Portland, Oregon, used the 500-MHz spectrometer as part of the study “Imaging Beta Amyloid Plaques in a Transgenic Mouse Model of Alzheimer’s Disease.”
- Celine Schneider, University of British Columbia, Vancouver, British Columbia, Canada, used the 750-MHz spectrometer for “Structural Investigations of Solid Materials by High Resolution Solid State NMR at Very High Field.”
- Louis P. Silks, Los Alamos National Laboratory, Los Alamos, New Mexico, used the 500-MHz spectrometer as part of the study “Ultra-High Field NMR Studies of Stable Isotope Applications.”
- Michael J. Smerdon, Washington State University, Pullman, Washington, sent used the 600-MHz spectrometer as part of the study “Structural Biology of Mammalian Chromatin High Mobility Group Protein HMGA1 and UV-Damaged DNA.”
- Frank Soennichsen and Kiattawee Choowongkamon, Case Western Reserve University, Cleveland, Ohio, used the 800-MHz spectrometer to study “Structure Determination of Membrane Proteins.”
- Susan Wallace, University of Vermont, Burlington, Vermont, used the 600- and 500-MHz spectrometers as part of “Structural Studies of *Escherichia coli* Formamidopyrimidine DNA N-Glycosylase and Its Main Biological Substrate 8-Oxoguanine.”
- Brian Wood, Oregon State University, Corvallis, Oregon, and Harold Trease, Pacific Northwest National Laboratory, Richland, Washington, used the 500-MHz spectrometer to study “Continuing Exploration of NMR Imaging of Microorganisms in Porous Media Using NMR Microscopy.”

Molecular Science Computing Facility

- On July 17, 2003, several visitors from Hewlett-Packard visited with members of the MSCF operations team to discuss future plans for high-performance computing. The operations team was able to communicate some of its needs and gain insights into the direction of processors and architectures for next-generation high-performance computers. The team was also able to discuss issues about the current development direction and anticipated needs.
- Representatives from Light Fleet, Vancouver, Washington, held discussions with MSCF staff members about new technologies around free-space optics being developed that may be useful for next-generation supercomputers.
- Don Tilton, SprayCool, Clarkston, Washington, visited to discuss his company's current work using evaporative cooling in electronic applications, including computers. This technology allows computers to be smaller with reduced airflow needs.

New EMSL Staff

Mathew McKinley, Richland High School, Richland, Washington, began working with Shuttha Shutthanandan to analyze particle-induced x-ray emission spectra.

Casey Stratton, Hanford High School, Richland, Washington, began working with the I&NS Facility group in vacuum technology.

Publications

Amonette JE, CK Russell, KA Carosino, NL Robinson, and JT Ho. 2003. "Toxicity of Al to *Desulfovibrio desulfuricans*." *Applied and Environmental Microbiology* 69(7):4057-4066.

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