An Overview of EMSL Science and an Example from Recent Structural Studies of the Major Pilin Protein from *Geobacter Sulfurreducens*

Karl Mueller (karl.mueller@pnnl.gov) - EMSL/PNNL (PI), Patrick Reardon, EMSL/PNNL (Co-PIs).

EMSL, a DOE national user facility in Richland WA, provides integrated experimental and computational resources and expertise for scientific research and discovery, generating foundational scientific knowledge needed to address climate, bioenergy, and environmental challenges of importance to BER, DOE, and the nation. EMSL users and staff address science gaps that limit the translation of fundamental molecular-scale science into solutions for DOE's most pressing challenges.

Through the integration of field, experimental, and computational approaches, EMSL users gain new knowledge of molecular-scale phenomena that can be parameterized and integrated into the types of local, regional, and global scale models designed to predict the impact of life on earth's climate and environment. To enhance EMSL's scientific impact and unique capabilities, user proposal calls focus on four BER- and DOE-aligned science themes in atmospheric aerosol chemistry, biosystems dynamics and design, terrestrial and subsurface ecosystems, and energy materials and processes. EMSL is also active in leveraging its capabilities with other DOE user facilities to provide maximal scientific advantage to DOE and the scientific community. As an example, EMSL and the DOE Joint Genome Institute (JGI) have recently sponsored joint user calls to take best advantage of DOE's genomic/transcriptomic and other bio-omic capabilities for systems biology advances.

As an example of current research carried out at EMSL and of interest to researchers in the SBR and TES programs, we have recently determined the atomic resolution structure in detergent micelles of the major pilin protein from Geobacter sulfurreducens, PilA, using high resolution NMR spectroscopy. Geobacter sulfurreducens and related species of proteobacteria can utilize a wide range of insoluble extracellular electron acceptors, such as metal oxides, during respiration; and the transport of electrons by G. sulfurreducens is thought to be facilitated by filamentous type IV pili, often referred to as bacterial nanowires. We have determined that the PilA protein is greater than 85% Î±-helical and is structurally similar to the N-terminal region of other non-conductive type IVa pilins. Modeling of the PilA NMR structure onto the type IVa pilus fiber model from Neisseria gonorrhoeae provides insight into the organization of aromatic amino acids that have been suggested to play a role in electrical conduction.