

Contact: Eleanor Taylor
(630) 252-5510
etaylor@anl.gov
For immediate release

Argonne's Leadership Computing Facility helps researcher win Sackler Prize

ARGONNE, Ill. (Dec. 17, 2008) — David Baker, University of Washington (UW) professor of biochemistry and an investigator at the Howard Hughes Medical Research Institute, has been awarded the 2008 Raymond & Beverly Sackler International Prize in Biophysics.

Baker is being honored for his significant contributions to computer-based studies of the manner and the speed in which chains of amino acids fold into protein molecules. Creating computer models of protein folding is essential for figuring out how genetic information directs protein formation, how proteins work and how misfolded, misshapen and malfunctioning proteins might underlie serious degenerative diseases.

“Dr. Baker’s work is a significant advance towards developing novel therapeutics that will improve our everyday life as well as have positive impacts on our environment,” said Pete Beckman, director of Argonne’s Leadership Computing Facility. “His breakthroughs in predicting and simulating protein structures are invaluable to the community and to accelerating discoveries into practical benefits for society.”

Baker conducted his work on the IBM Blue Gene/P at the Argonne Leadership Computing Facility using 12 million computer processor hours awarded by the U.S. Department of Energy’s (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. INCITE supports computationally intensive, large-scale research projects that can make high-impact scientific advances through the use of substantial allocations of computer time, resources, and data storage at DOE’s global flagship facilities for unclassified supercomputing.

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Sackler Prize – add one

Baker developed computer programs to predict protein structures from amino acid sequences in DNA. His program, Rosetta, is among the most accurate. He has combined data from nuclear magnetic resonance imaging and X-ray diffraction imaging with his computer modeling to more quickly delineate protein molecule structures. He also researches the ways that molecular configurations of proteins determine their functions in biochemical reactions.

"DOE's INCITE program has been critical to the progress made in protein structure modeling using Rosetta," said Baker.

The Rosetta method has been tested on several proteins of known structure up to 189 amino acids in length. In many cases, the accuracy of the prediction was within a remarkable one angstrom of the experimentally solved high-resolution crystal structure.

In addition, Baker and his team have developed new protein folds and have designed and built functional enzymes, and engineered protein interactions that previously did not exist in nature. His group has also contributed new ways of studying proteins in membranes – the thin fatty covering that separates the inside of the cell from the external environment. These transmembrane proteins include molecular channels that permit the flow of calcium into and out of the cell and that are responsible for the passage of neural impulses and communication between cells. The Baker group was able to apply the Rosetta program to these unusual proteins by treating the membranes as a series of layers with different protein folding requirements.

The international Sackler prize was established by arts and sciences philanthropists Raymond R. Sackler and his wife, Beverly Sackler. Raymond Sackler is a psychiatrist and co-founder of a multinational pharmaceutical company. The field for this year's prize was the physics of structure formation and self-assembly of proteins and nucleic acids.

The award was presented to Baker today at Israel's Tel Aviv University. Also recognized were Martin Gruebele of the University of Illinois, Urbana-Champaign, and Jonathan Weissman of the University of California, San Francisco.

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Sackler Prize – add two

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