Burnham Institute for Medical Research and UCSD Researchers Establish Joint Center For Molecular Modeling

$2.1 Million Grant from National Institutes of Health Seeds Collaboration to Expedite Applications from Human Genome Project

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A team of researchers, led by Dr. Adam Godzik at the Burnham Institute for Medical Research and including UCSD computer scientist Pavel Pevzner, is designing tools to accelerate the interpretation, and potential use of, information gleaned from the human genome project.

Armed with $2.1 million over the next three years, this consortium, known as the Joint Center for Molecular Modeling (JCMM), will support scientists from Burnham and UCSD's Computer Science and Engineering department as they collaborate to develop innovative software for improving the quality of predictions of three-dimensional protein structures from raw genetic code. These new tools will be made available to researchers worldwide through open-source databases and may be applied ultimately in the design of smarter drugs.

Researchers are sequencing millions of genes per year in different genomic projects. Solving the structures of the protein products of these genes is proceeding at a slower pace -- between 3,000 and 5,000 per year. Using the structures of proteins that have already been solved, Dr. Godzik and co-principal investigators Drs. Pavel Pevzner, Yuzhen Ye and Piotr Cieplak will develop novel ways to extract rules and trends of how structures change and evolve. They will use these tools to predict how, for instance, a human protein would differ from its counterpart in mice or bacteria.

"Protein structures can be solved experimentally in a couple of months, sometimes weeks," said Dr. Godzik, who is also affiliated with the California Institute for Telecommunications and Information Technology (Calit2) at UCSD. "Scientists around the world have already solved tens of thousands of them. Structures of many proteins can also be predicted on a computer in a matter of minutes, but the quality of such models is generally so poor that they are not useful in many applications, such as drug design. We have developed tools that allow us to learn from structures already solved and apply that knowledge to improve predicted structures of new proteins. This funding from the National Institutes of Health makes it possible for us to prove our concept and make our tools available to scientists worldwide."

According to UCSD's Pevzner, predicting protein structures represents a rich source of new algorithmic challenges. "In recent years new mathematical tools have revolutionized the way we describe rearrangements of genomic elements and domain reshuffling in multi-domain proteins," said Pevzner, the Ronald R. Taylor Professor of Computer Science in the Jacobs School of Engineering. "We believe that they can also be used to recognize and describe the movements of micro-domains in protein structures, and that will be the focus of the Computer Science and Engineering department's participation in this collaboration with the Burnham Institute."

"Dr. Godzik brings together an interdisciplinary team with an impressive track record," said Dr. Jerry Li, Program Director of the National Institute of General Medical Sciences at the National Institutes of Health, which funded the new project. "By developing and using new computational approaches, the group will improve our

ability to accurately model the three-dimensional structures of proteins, which are invaluable to functional studies and rational drug design."

Adam Godzik, Ph.D., is Professor and Director of the Bioinformatics and Systems Biology Program at the Burnham Institute for Medical Research. Yuzhen Ye, Ph.D., and Piotr Cieplak, Ph.D., are Research Assistant Professor and Staff Scientist, respectively, at the Burnham Institute.

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