

OFFICE OF ENERGY RESEARCH

Notice 96-03

DEPARTMENT OF ENERGY

OFFICE OF ENERGY RESEARCH

Energy Research Financial Assistance Program Notice 96-03: Computational Structural Biology

Agency: Office of Energy Research, Department of Energy (DOE).

Action: Notice inviting grant applications.

SUMMARY: The Office of Health and Environmental Research (OHER) of the Office of Energy Research (ER), U.S. Department of Energy (DOE), supports a comprehensive research program in the area of environmental sciences, health effects and life sciences, and medical applications. Major program research emphasis is placed on characterization of human and microbial genomes, structural biology, cellular and molecular biology, global climate change, improved technology for cleanup of DOE contaminated sites, advanced imaging technologies, and molecular nuclear medicine. With the explosion of nucleic acid and amino acid sequence data that stems from genome projects, there is an immediate need for greatly improved experimental and computational approaches for protein structure determination. To help meet this need, and in support of diverse missions of DOE, OHER is initiating a new program in computational structural biology. The purpose of this program is to support research that will enhance understanding of structure-function relationships in biological macromolecules. These relationships are very important for diverse applications in biotechnology, including development of drugs for diseases, new and improved biomaterials, design of enzymes for effective and efficient removal of environmental contaminants, and the development and conversion of bio-mass for fuels. In particular, research applications that integrate existing software tools in novel ways and/or develop new computational strategies to exploit databases of macromolecular structural information towards furthering our understanding of the relationships between sequence and structure are of particular interest to the program at this time. This includes the goals of predicting the structure and function of newly discovered gene sequences and the prediction or design of the chemical properties and architectural arrangement of proteins or nucleic acids needed for a particular functional application. Examples of existing approaches that fall into this category are knowledge-based or molecular extension methods (e.g., homology model building or multiple sequence alignment), ab initio folding (finding structures that fit sequences) and the development of tools to assign existing or new sequences to specific structures (e.g., finding sequences that fit structures through threading or inverse folding algorithms). Attention should be also focussed on the problem of negative design, the identification of aspects of a sequence that precludes its fitting a known structure. More generally, the integration and joint utilization of the growing body of sequence, structural and physical information is an area that offers new opportunities that are of interest to the program.

Studies that rigorously compare existing tools and/or exploit the latest advances in multiple approaches (in algorithms, simulation, modeling and graphical representation/visualization) or that include the development of new computational and visualization techniques for application to the prediction of protein and nucleic acid structure and the exploitation of structure to predict function, will also be considered particularly responsive. Collaborative projects with two to five principal investigators, of complementary expertise and each with independent funding, aimed at achieving a synergistic effect in improving structure prediction accuracy through such activities as evaluation of different potential functions, the development of shared code, or an integrated attack on a set of problems in an area of prediction or in testing current modeling techniques are also encouraged. Funds for such projects would be comparable to individual awards, but could be used to nucleate a larger group effort.

DATES: Formal applications submitted in response to this notice must be received by 4:30 p.m., E.D.T., April 25, 1996, to be accepted for a June merit review and to permit timely consideration of award in Fiscal Year 1996.

ADDRESSES: Formal applications referencing Program Notice 96-03 should be forwarded to: U.S. Department of Energy, Office of Energy Research, Grants and Contracts Division, ER-64, 19901 Germantown Road, Germantown, Maryland 20874-1290, ATTN: Program Notice 96-03. The same address as above must be used when submitting applications by U.S. Postal Service Express Mail, any commercial mail delivery service, or hand carried by the applicant.

FOR FURTHER INFORMATION CONTACT: Dr. Matesh N. Varma, Office of Health and Environmental Research, ER-73, U.S. Department of Energy, 19901 Germantown Road, Germantown, Maryland 20874-1290, telephone: (301) 903-3209, Fax: (301) 903-0567, (E-mail: matesh.varma@mailgw.er.doe.gov).

SUPPLEMENTARY INFORMATION: Before preparing a formal application, potential applicants must submit a brief preapplication in accordance with 10 CFR 600.10(d)(2), which consists of two to three pages of narrative describing research objectives and methods of accomplishment. These will be reviewed relative to the scope and research needs for the computational structural biology program. Preapplications referencing Program Notice 96-03 should be received by January 23, 1996, and sent to Dr. Matesh N. Varma, Office of Health and Environmental Research, 19901 Germantown Road, Germantown, Maryland 20874-1290, (301) 903-3209. Telephone and fax numbers and e-mail addresses are required to be part of the preapplication. A response to the preapplication discussing potential relevance of a formal application will be communicated by February 20, 1996. It is anticipated that approximately \$2.0 million will be available for grant awards during Fiscal Year 1996 contingent upon availability of funds. We expect to award several grants in this area of research up to a few hundred thousand dollars per year. Information about development, submission, and the selection process, and other policies and procedures may be found in 10 CFR Part 605, and in the Application Guide for the Office of Energy Research Financial Assistance Program. The Application Guide is available from the U.S. Department of Energy, Office of Health and Environmental, ER-73, 19901 Germantown Road, Germantown, Maryland 20874-1290. Telephone requests may be made by calling (301) 903-5349. Electronic access to ER's Financial Assistance Guide is possible via the Internet using the following E-mail address: <http://www.er.doe.gov/>

The Catalog of Federal Domestic Assistance Number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Issued in Washington, D.C. on December 11, 1995.

D. D. Mayhew
Associate Director
Office of Resource Management
Office of Energy Research

Published in the Federal Register, December 19, 1995 (Vol. 60, No. 243,
pages 65320-65321.