

Computational Postdoctoral Fellow: A position in molecular modeling and drug design is open immediately. The successful candidate will have a Ph.D. in chemistry, biochemistry, medicinal chemistry, physical chemistry or a related field. The postdoctoral position involves carrying out various projects involving designing/identifying of new biologically active molecules through docking and screening, MD/free energy simulations to study protein dynamics, and QM or QM/MM calculations to elucidate biological reaction pathways. Experience in using Amber, Gaussian, Sybyl, Schrödinger packages, Dock, GOLD, or similar programs, is highly desired. Programming/scripting knowledge with Perl/Python/C/Fortran, and experience with using and maintaining UNIX/LINUX workstations are also desirable.

The laboratory is equipped with state-of-the-art workstations with 3D visualization capabilities, a 60-core in-house linux cluster, a 128-core cluster housed at Notre Dame CRC, data storage, and has direct access to Notre Dame's 5000-core main computing facility. Additional computing power is available through XSEDES (formerly known as TeraGrid) clusters. All computers are equipped with established programs and software packages that are necessary to carry out the computational tasks listed above.

The successful candidate will have the opportunity for interactions with synthetic chemists, biochemists, and molecular biologists within the Mobashery group, or with collaborating groups (usually crystallographers). A period of training will be provided, but ability to perform independently in the lab is highly valued.

The research carried out in the laboratory employs a multidisciplinary approach to solving problems of biochemical significance. The research interests encompass investigations of mechanisms of resistance to antibacterials, design of novel antibiotics, bacterial cell wall and its recycling, studies of tumor metastasis and the means to prevent it. The group members have backgrounds in organic chemistry, enzymology, molecular modeling, computational sciences, and molecular biology.

Interested candidates should e-mail their resumes to:

Professor Shahriar Mobashery
Navari Family Chair in Life Sciences
Department of Chemistry and Biochemistry
251 Nieuwland Science Center
University of Notre Dame
Notre Dame, IN 46556 USA
phone: (574) 631-2933
fax: (574) 631-6652
email: mobashery@nd.edu
<http://www.chemistry.nd.edu/faculty/detail/smobashe/>