Postdoctoral Research Associates in Protein/Ligands Interactions and Dynamics

Biosciences Division
Biological and Environmental Sciences Directorate
Oak Ridge National Laboratory
Oak Ridge, Tennessee

ORNL08–114–BESD

Project Description:
The Biosciences Division at the Oak Ridge National Laboratory is seeking to fill a postdoctoral research position in protein/ligands interactions and dynamics, coupled with experimental neutron scattering experiments and solution NMR.

The dynamics of protein play a key role in their function, and in particular in their capacity to bind biologically important ligands. The research here will provide a framework for understanding the energetics and dynamics of protein/ligand interactions, combining high-performance simulation with experiments on a next-generation neutron source, the new Spallation Neutron Source at Oak Ridge National Laboratory. This project will be done in collaboration with research groups at the University of Tennessee, Knoxville, for molecular biology and solution NMR experiments.

Specifically, we aim to (i) Perform molecular modeling simulations to investigate the dynamics and thermodynamics of protein/ligand interactions, in particular the dynamics of opening/closing of substrate access channels and product release channels. (ii) Perform neutron scattering experiments aimed at identifying the protein residues that undergo dynamical change during ligand access/release. (iii) Interface with collaborators for specific labeling experiments and solution NMR experiments.

Several crystal structures exist for apo- and bound- species of proteins and protein/ligand complexes. In several cases, the apo- and bound- species do not exhibit major changes outside the very binding site domain. However, transient structural changes are needed to allow the ligand to move from the cytoplasmic environment to the inside of the protein. Molecular simulations of the ligand entry and exit pathways can be performed to identify protein domains involved and the corresponding dynamics. Neutron spectroscopy experiments can be used to investigate and verify that residues suggested by the simulation as important are indeed experiencing modified structural environment and dynamics upon ligand binding. Solution NMR will provide complementary results and will be included in the design of the simulations.

Qualifications:
A Ph.D. in chemistry, physics, biophysics or closely related field. Applicants cannot have received the most recent degree more than five years prior to the date of application appointment and must complete all degree requirements before starting their appointment.

Technical Information:
For additional information contact Jerome Baudry, Ph.D. (baudryjy@ornl.gov, 865-576-0930)

How to Apply:
Qualified applicants must apply online at https://www2.orau.gov/ORNL_POST/. All applicants will need to register before they can begin the online application. For complete instructions, on how to apply, please see the instructions at http://www.orau.gov/orise/edu/ornl/ornl-pdpm/application.htm. When applying for this position, please reference the position title and number.

This appointment is offered through the ORNL Postgraduate Research Participation Program and is administered by the Oak Ridge Institute for Science and Education (ORISE). The position is open to citizens or legal permanent residents of the US without regard to race, color, age, religion, sex, national origin, physical or mental disability, or status as a Vietnam-era veteran or disabled veteran.