

## Molecular Modeling and Molecular Dynamics Simulation Workshop

November 6 - 9, 2006

## **SPONSORS:**

- National Center for Research Resources
- <u>University of Pittsburgh</u>
  Department of Structural Biology

## SITE:

Department of Structural Biology Biomedical Science Tower 3, Pittsburgh, PA



**APPLICATION**: Register Online

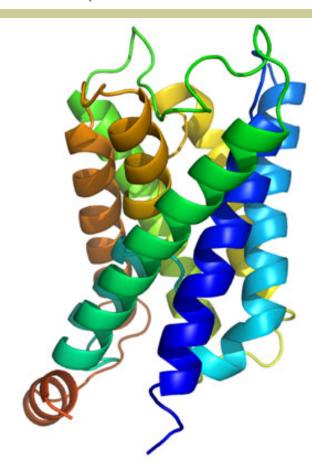
APPLICATION DEADLINE: October 4, 2006

## **DESCRIPTION:**

The workshop will explore physical models and computational approaches used for the simulation of biological systems and the investigation of their function at an atomic level. The course will be based on case studies including the properties of membranes and membrane proteins, mechanisms of molecular motors, trafficking in the living cell through water and ion channels, and signaling pathways. Relevant physical concepts, mathematical techniques, and computational methods will be introduced, including force fields and algorithms used in molecular modeling, molecular dynamics simulations on parallel computers and steered molecular dynamics simulations.

The workshop is designed for graduate students and postdoctoral researchers in biophysics, structural and computational biology who seek to extend their research skills to include computational and theoretical expertise, as well as other researchers interested in these fields. Theory sessions in the morning will be followed by hands-on computer labs in the afternoon in which students will be able to set up and run simulations.

Enrollment limited to 20 participants.



**TOPICS** 

<u>AGENDA</u>

**INSTRUCTORS** 

**ONLINE APPLICATION** 

**READINGS** 

**SOFTWARE** 

PARTICIPANT INFORMATION