

Prof. William A. Goddard III at Caltech (Pasadena CA) is seeking for an exceptional postdoctoral scholar to join our team to work in the area of protein modeling and drug discovery using molecular dynamics simulations. The project mainly involves predicting and modeling structures of G-protein coupled receptors (GPCR), prediction of binding free energies of various ligands acting on the GPCRs, and finding the activation pathway for the GPCR to activate the G-Protein (GP). The project is centered on taste receptors where it is expected that many factors in addition to activation of the GP by the GPCR may play important roles in taste perception (competition with other ligands, role of allosteric modulators, transport into the cell and to the GPCR). Thus to understand dose-response an important component will be to use chemometrics involving descriptors for the ligand and other aspects of the cells to supplement binding and activation barriers from the MD.

This position is now available to be filled.

Qualified candidates must hold a Ph.D. in Chemistry, Physics, Biological Science, Materials Science, Chemical Engineering, or a related area, with a strong track record of productivity. Candidates are expected to have demonstrated capabilities in several of the following areas:

- 1) Experience with protein-ligand docking and in homology predictions of membrane bound proteins
- 2) classical molecular dynamics (MD) simulations with a variety of force fields.
- 3) Proficiency in using well-established MD software package such as GROMACS and NAMD.
- 4) Expertise in enhanced sampling methods and free energy calculations.
- 5) Experience with chemometrics
- 6) Strong skills in biological sequence analysis, building proteins, homology modeling, or other protein structure prediction techniques.
- 7) Proficient in scripting languages such as Python and Perl
- 8) Excellent communication in spoken and written English.

And they should be very smart, resourceful, and unafraid to tackle impossible problems.

Qualified applicants should send:

1. *CV with contact information and list of publications*
2. *Visa status if not a US citizen*
3. *Three personal references familiar with your background and accomplishments. Include phone numbers, fax numbers, and e-mail addresses, so we can contact them.*
4. *One paragraph description of how your background is appropriate for our projects*
5. *Two paragraph description of your career goals and how this position would be consistent with your goals.*
6. *Pdf for your best 3 publications*

These materials should be sent in a single PDF file via e-mail to wag@caltech.edu with a copy to davism@caltech.edu.

Put as the subject title: Application for GPCR PD with Goddard, your name, your institution

Salary is commensurate with demonstrated capabilities and experience. Caltech offers an attractive benefits package and a comfortable living environment in the San Gabriel Valley near Los Angeles. Caltech is an equal opportunity employer.