The Department of Chemistry is pleased to offer the following research project for the summer of 2007. Interested students are urged to contact the faculty member(s) directing the project that most interests them. By contacting the faculty member, you can discover more about the project, learn what your responsibilities will be and if possible, develop a timetable for the twelve-week research period.

Computational modeling of substrate protein recognition by the eukaryotic chaperonins

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Project Description

The research focus in my group is on the development and application of computational methods for modeling systems of biomedical interest. In particular, I am interested in computational molecular modeling of chaperonin molecules. Chaperonins are biological nanomachines that employ a spectacular mechanism to assist protein folding. During the chaperonin cycle, concerted, large scale, rigid body conformational changes, ultimately driven by ATP hydrolysis, result in a dramatically expanded chaperonin cavity serving as folding chamber. Chaperonins are essential for cell survival and chaperonin mutations lead to serious diseases. From a therapeutic point of view, chaperonins are being considered for use against protein aggregation diseases such as polyglutamine diseases. Currently, very little is known about the annealing action of eukaryotic chaperonins. My proposed project for the REWU program would be "Computational modeling of substrate protein recognition by the eukaryotic chaperonins". In this project, we are aiming to pinpoint the eukaryotic chaperonin binding sites. To this end, we will employ structural analysis and bioinformatics methods that will suggest putative binding sites. This is an opportunity to acquire a diverse set of computational skills and apply them to problems of biomedical interest. In addition, our soon-to-be-built supercomputer cluster provides a chance to learn about designing and maintaining high-performance computers for data intensive applications.