Computer simulations of folding and mis-folding of proteins.

A key component in the molecular machinery of cells are proteins, but despite the remarkable progress in experimental machinery and techniques for producing and characterizing proteins, a detailed understanding of folding and interaction of proteins is still missing. Computer simulations can complement experiments in unveiling these processes. We are looking for a highly motivated student that will help us in developing more efficient algorithms for this purpose. Our new techniques will be tested by investigating the folding mechanism of wild type and various mutants of A and B domain of protein G. The student will learn to perform Monte Carlo and molecular dynamics simulations (using the GROMACS and SMMP program suites) and to use graphic visualization programs. This project is suited for students interested in the cross section between chemistry and computer science, math, biophysics, biochemistry or bioinformatics. Programming skills in C, C++, or FORTRAN95 are required.

Assembly and stability of amyloid structures.

Understanding the pathology of various diseases such as cancer or Alzheimer's requires insight into the workings of cells on a molecular level. However, cellular processes are often controlled by transient interactions between proteins that are difficult to determine by experiments. Simulations can help to trace such interactions. We are looking for a highly motivated student to investigate the assembly and stability of small amyloid structures by Monte Carlo and molecular dynamics. The student will also learn graphic visualization programs and other analyzing techniques. Simulations will rely on the GROMACS programing suite. This project is suited for students interested in the cross section between chemistry and computer science, math, biophysics, biochemistry or bioinformatics. Some programming experience in Python and/or C/C++ is required.