BT 610 Frontiers in Bimolecular Simulation (3 0 0 6)

Introduction to computational structural biology; review of protein structure; basic thermodynamics; quantum mechanics; molecular mechanics; computer simulation; free energy calculations; protein structure prediction; protein-ligand interaction; enzyme catalysis; molecular docking: large scale screening of ligands against a target; advanced sampling techniques; molecular modeling software.

Texts:

1. Andrew Leach, *Molecular Modeling; Principles and Applications,* 2nd Edition Addison-Wesley Publications. 2001

2. D. Frenkel and B. Smit, *Understanding Molecular Simulation,* 2nd Edition, Academic Press, 2001

References:

1. K. A. Dill and S. Bromberg, *Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology,* Garland Science, 2003