Introduction to Computational Biophysics
Fall, 2007
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Tuesday & Thursdays 3:30-4:45 pm
SCS First Floor Classroom

Objective

This course aims to expose graduate students and senior undergraduates to the physical bases of biological systems and biological processes. Basic theories of thermodynamics and kinetics will be introduced. Key experimental techniques will be described. For a selection of properties of proteins and nucleic acids, simple physical models will be developed to gain qualitative understanding. In a few cases, realistic molecular modeling will be introduced.

Text

The lecture notes of this course will be published as a book titled "Molecular Biophysics: protein folding and biomolecular interactions" by Oxford University Press (hopefully in 2008). The table of contents is listed below.

Contents

Chap 1. Energy function and Boltzmann distribution
1.1 Discrete and continuous energy
1.2 Energy barrier and thermodynamic state
1.3 Potential of mean force
1.4 Concentration, multiple components, and reactions

Chap 2. Rate processes and rate theories
2.1 Rate constant and relaxation time
2.2 Transition-state theory
2.3 Kramers theory
2.4 Validity of rate description
2.5 Diffusion-controlled binding

Chap 3. Models of polymer chains
3.1 Statistics of long polymer chains
3.2 Chain stiffness and inextensibility
3.3 Dynamic properties
3.4 Contact formation
3.5 Intramolecular binding

Chap 4. Simulation techniques
4.1 Energy functions
4.2 Molecular dynamics

4.3 Monte Carlo simulations
4.4 Brownian dynamics
4.5 Free energy calculations

Chap 5. Protein structures
5.1 Amino acids
5.2 Secondary structures
5.3 Tertiary structures
5.4 Stabilizing interactions
5.5 Distributions of amino acids in folded structures
5.6 Determination of protein structures

Chap 6. Protein folding free energy
6.1 Characterization of the unfolded state
6.2 Measurement of the folding free energy
6.3 Perturbations of protein stability: environmental variables
6.4 Perturbations of protein stability: amino acid mutations

Chap 7. Protein dynamics
7.1 Functional importance of protein dynamics
7.2 Dynamics and function of acetylcholinesterase
7.3 Characterization of protein dynamics by NMR relaxation

Chap 8. Protein folding
8.1 Theoretical models of protein folding
8.2 Experimental and theoretical determination of the transition-state ensemble
8.3 Chaperonin-assisted protein folding

Chap 9. Protein-protein interactions
9.1 Binding affinity
9.2 Binding rate
9.3 Protein-protein interactions constrained by peptide linkers

Chap 10. Motor proteins
10.1 Transduction of chemical energy into mechanical energy
10.2 Linear motors
10.3 Rotary motors

Chap 11. Membranes and membrane proteins
11.1 Lipids and lipid-protein interactions
11.2 Signal transduction across the membrane
11.3 Ion conduction through membrane channels

Chap 12. RNA/DNA conformations and dynamics
12.1 Nucleic acids
12.2 RNA

12.3 DNA

Chap 13. RNA/DNA-protein interactions
13.1 RNA-protein interactions
13.2 DNA-protein interactions

Chap 14. Modern biophysical techniques
14.1 Single molecule techniques
14.2 Electron microscopy
14.3 Quantum dots

Other references:

1. Biophysical Chemistry. Charles R. Cantor and Paul R. Schimmel, W. H. Freeman and Company, 1980. (three volumes)
2. Proteins: Structures and Molecular Properties. Thomas E. Creighton, 2nd edition, W. H. Freeman and Company, 1993.
3. Biochemistry. Donald Voet and Judith G. Voet, 3nd edition, John Wiley & Sons, Inc., 2004.