

**THE SCRIPPS RESEARCH INSTITUTE  
Kellogg School of Science and Technology**

**Theoretical and Computational Statistical Biophysics Course Outline  
Spring 2008**

**Class Times: Tuesday/Thursday 8:15 to 9:45 a.m.**

**Location: Suite 110, Building 3377**

**Course Director: Dr. David A. Case**

**Fundamentals:**

- Introduction to classical and statistical thermodynamics. Allostery. (4 lectures)
- Force fields, molecular dynamics, Monte Carlo methods, and free energy simulations. (4 lectures)
- Kinetic processes: transition state theory and master equations. (2 lectures)

**More advanced topics:**

- Electrostatics and implicit solvent models (3 lectures)
- Practical free energy simulations: umbrellas, acceptance ratios, non-equilibrium sampling. (3 lectures)
- Connections to spectroscopy: NMR and vibrational probes of structure and dynamics (2 lectures)

Textbook: *Computational Biochemistry and Biophysics*, Becker, MacKerell, Roux and Watanabe, editors. (Marcel Dekker, 201)

Homework: Course grade will be based on four homework assignments.