Empirical Force Fields & Quantum Mechanics

Molecular Mechanics Energy Functions
Electrostatics and Polarization for MM
Potential Surfaces and Optimization Methods
Basics of Molecular Orbital Theory

Monte Carlo & Molecular Dynamics Simulations

Monte Carlo Techniques
Molecular Dynamics Techniques
Computation of Properties from Simulation
Path Methods for Navigating Potential Surfaces

Free Energy Methods, Docking & Binding

Free Energy Methods I
Free Energy Methods II
Docking & Binding

Cheminformatics & Drug Discovery

QSAR and 3-D QSAR
Pharmacophore Active Site Modeling
Structure-Based Drug Design
Chemoinformatics

Homology Modeling, Structure Prediction & Design

Template-Based Modeling of Protein Structure

Molecular Recognition

Structure Prediction: Homology Modeling

Structure Prediction: Threading Methods & ab Initio

Structure Prediction: Design & Engineering