Syllabus for Molecular Structure Visualization and Prediction - I

1. Basic structural principles
   - Building blocks of life
   - Chemical properties of polypeptides
   - PDB Database

2. Intermolecular forces
   - Types of intermolecular forces
   - Entropy and temperature
   - Protein folding
   - Levinthal Paradox

3. Levels of protein structure
   - Primary structure
   - Secondary structure
   - Tertiary structure
   - Quaternary structure

4. Motifs of protein structure
   - Hydrophobic and hydrophilic regions
   - Ramachandran plot
   - Alpha-helix
   - Beta sheets
   - Loops
   - Topology diagrams
   - Various structural motifs

5. Protein structure prediction
   - Impediments
   - Sequence considerations
   - Structural considerations
   - Energy consideration
   - Energy landscape
   - Validation

6. Structure prediction of small proteins using *ab initio* stochastic models
   - Lattice simulation
   - Random-walk model
   - Self-avoiding model
   - HP-models

7. Structure prediction of small proteins using *ab initio* deterministic models
   - Ergodic hypothesis
   - Use of Newtonian equations of motion
   - Optimization techniques: Steepest descent, GA, simulated annealing
   - Force fields (Amber, CHARMM)

8. X-Ray crystallography and NMR
   - Structure determination methods
   - Structure evaluation methods

9. Nucleic acid structures
   - DNA structures
   - RNA structures
   - Secondary structure prediction in RNA

10. Useful tools
    - Visualization using VMD
    - PROCHECK
    - WHATIF
    - Simulation using Amber

Books:

1. Molecular Modelling: Principles and Applications (2nd Edition)
   Andrew R. Leach (Prentice Hall)

2. Introduction to Protein Structure
   Carl Branden, John Tooze (Garland)

3. Proteins: Structures and Molecular Properties
   Thomas E. Creighton (Freeman)

4. Principles of Nucleic Acid Structure
   Stephen Neidle (Academic Press)