Wednesday	4/7	Free energies from simulations (PMFs, direct estimates)
Friday	4/9	Free energy perturbation and thermodynamic integration
Monday	4/12	Umbrella sampling and weighted histogram analysis
Wednesday	4/14	Replica exchange and generalized ensemble methods
Friday	4/16	Multiscale modeling I: Implicit solvent representations
Monday	4/19	Practical applications of implicit solvent
Wednesday	4/21	Multiscale modeling II: Coarse-grained molecular representations
Friday	4/23	Practical applications of coarse-grained methods

During the first lab, on Wednesday I plan on having the students run simple MD simulations of solvated molecules with CHARMM as a follow up on Professor Cukier's lectures.
The labs during the following two Wednesdays will mostly involve free energy calculations with explicit and implicit solvent, also using CHARMM and the MMTSB Tool Set.