Project 3. Binding Free Energy Calculations With MM-PB/GBSA

1. **Select a protein system** (Thrombin was used as an example in class)

Protein Class	PDB Code	-logk_d	Resolution
Neuraminidase	2QWG	8.4	1.8
DHFR	1DHF	7.4	2.3
L-arabinose	1ABE	6.52	1.7
Thrombin	1A5G	10.15	2.06
Human oxresin receptor 1	4ZJ8	~10	2.75

2. **Prepare topologies for energy calculations with implicit solvent**
   - Xleap
   - Tleap

3. **Run mmpbsa.py to do the calculation**
   - Input file
   - Output files

4. **Analyze the MM-PB/GBSA results**
   - Igb =1
   - Igb =2
   - Igb =5
   - Pb

   Do the following comparisons:

   1) Performance of different solvent models
   2) Binding affinities of the native ligand and docking hits

Suggestion: copy the command scripts, input files from the 1A5G subdirectories (/home/mmms/project3/1A5G).