財團法人國家實驗研究院
國家高速網路與計算中心
National Center for High-Performance Computing

Molecular Simulations Workshop:
Proteins (protein drugs) simulations: (3)

Applied Scientific Computing Division, National Center for High-Performance Computing

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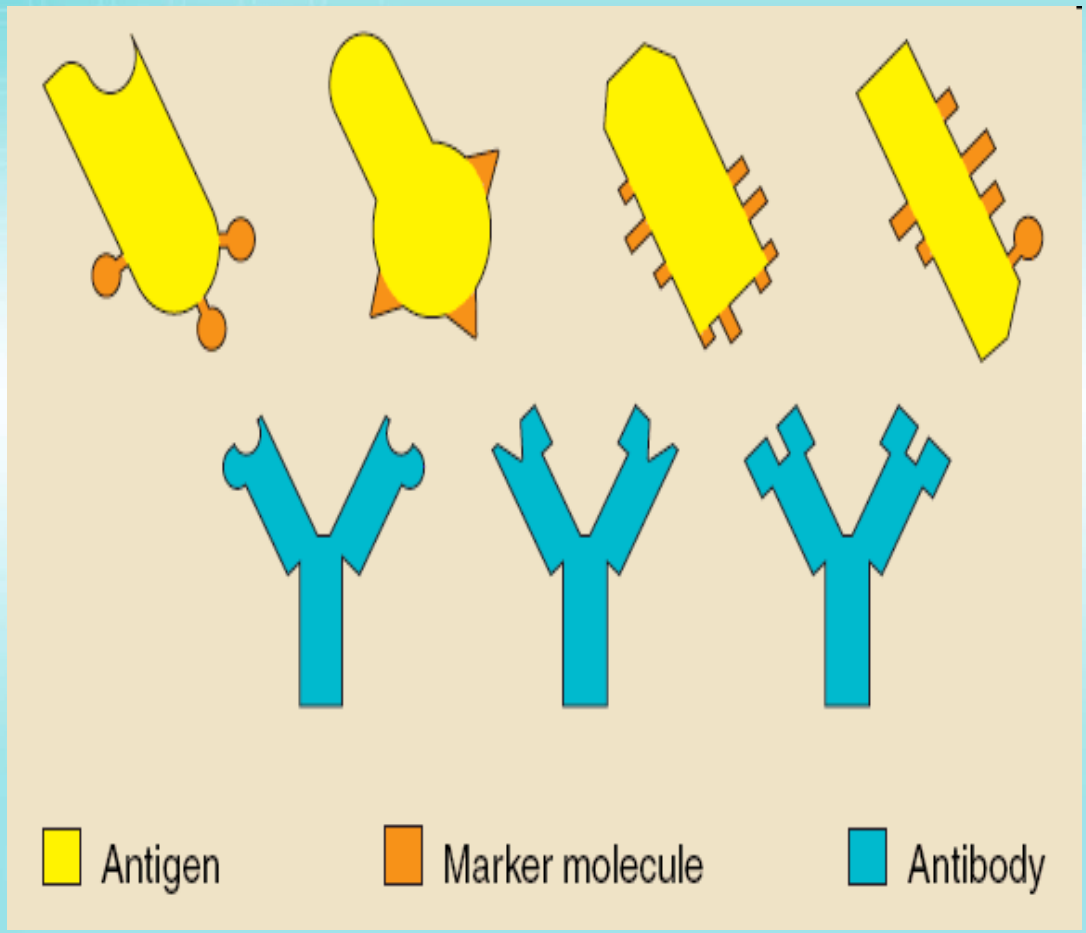
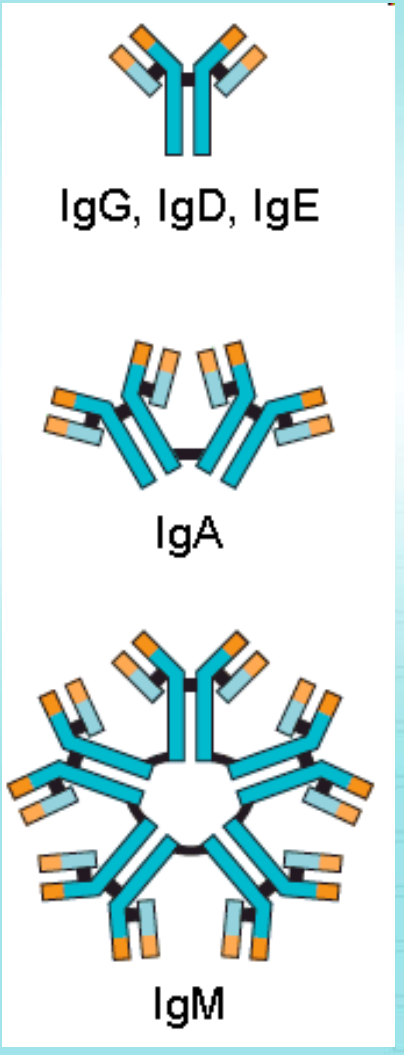
Binding hot spots: Antibody-antigen





Binding hot spots: Antibody-antigen

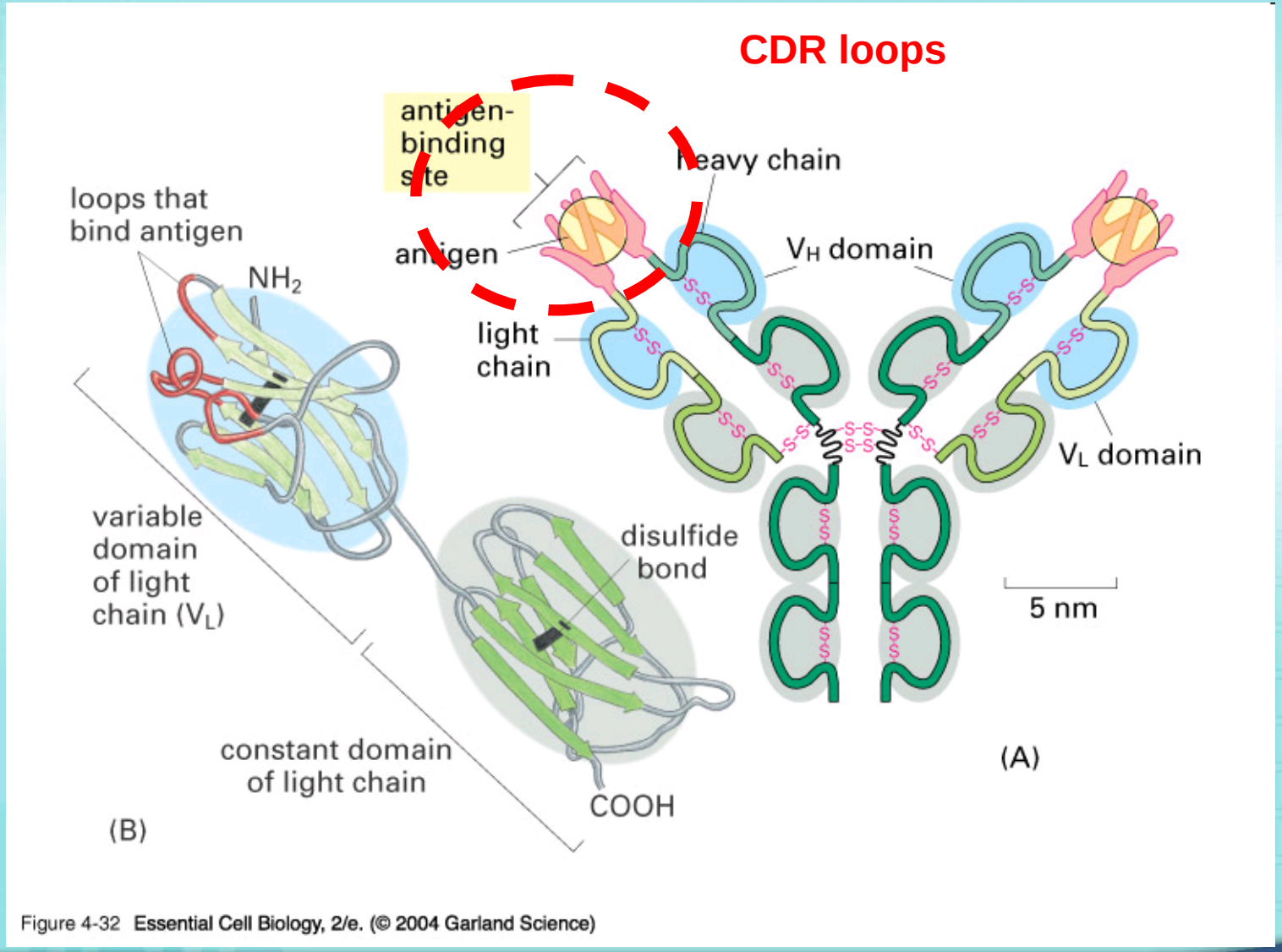
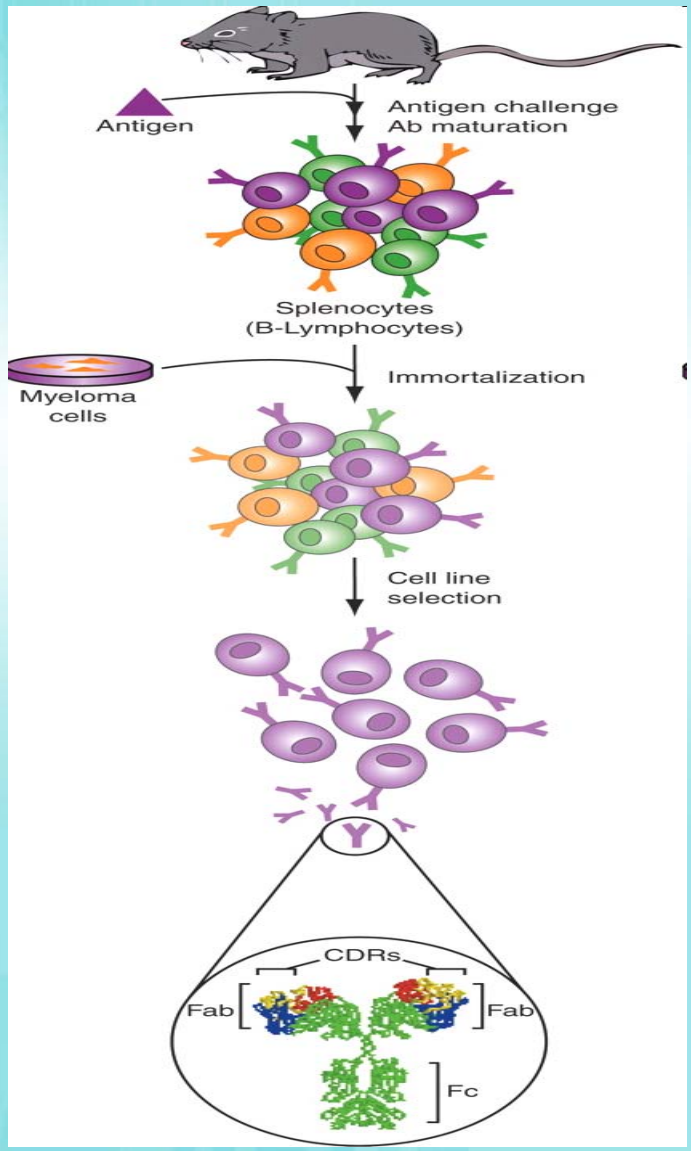
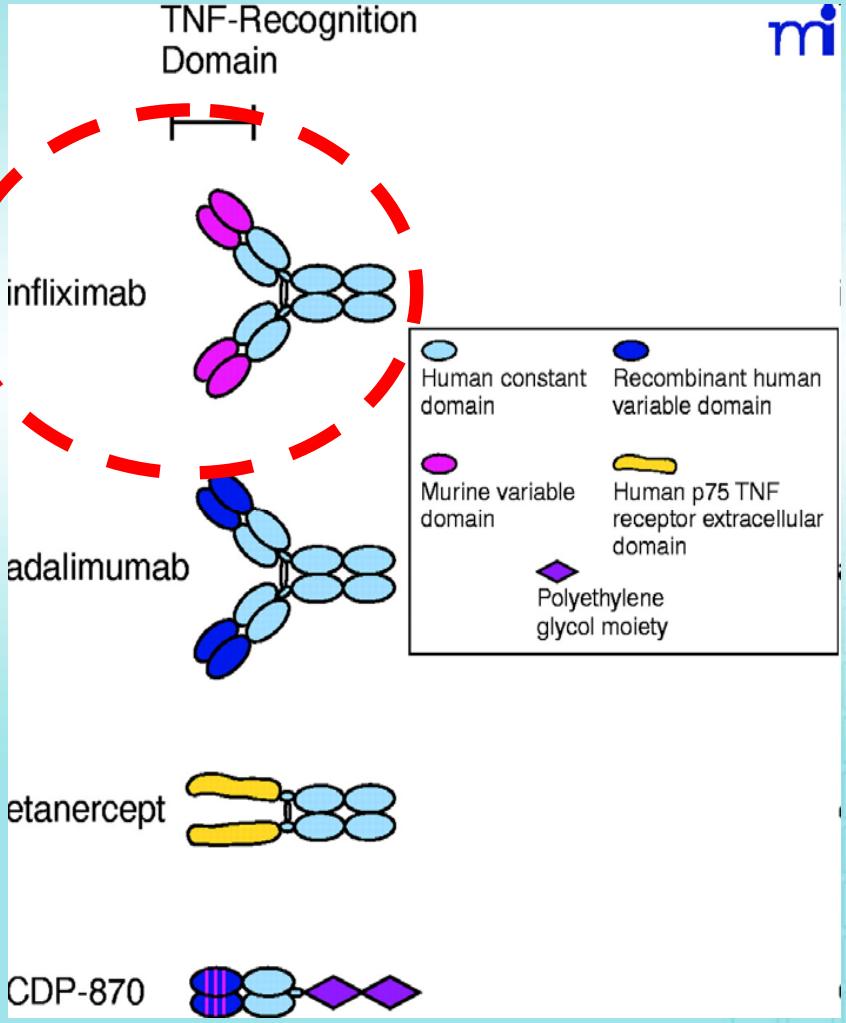


Figure 4-32 Essential Cell Biology, 2/e. (© 2004 Garland Science)

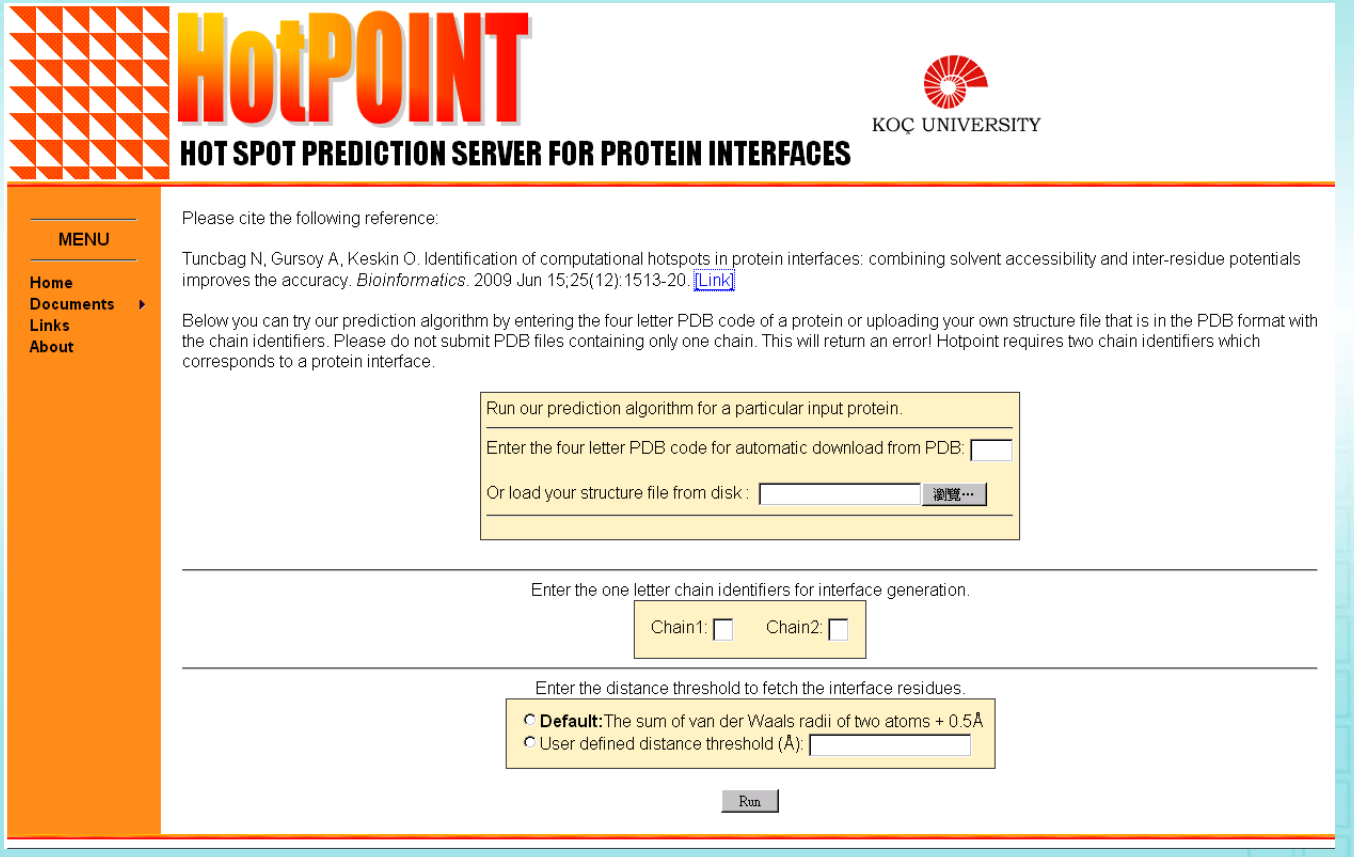
Binding hot spots: Antibody-antigen



Rheumatoid arthritis

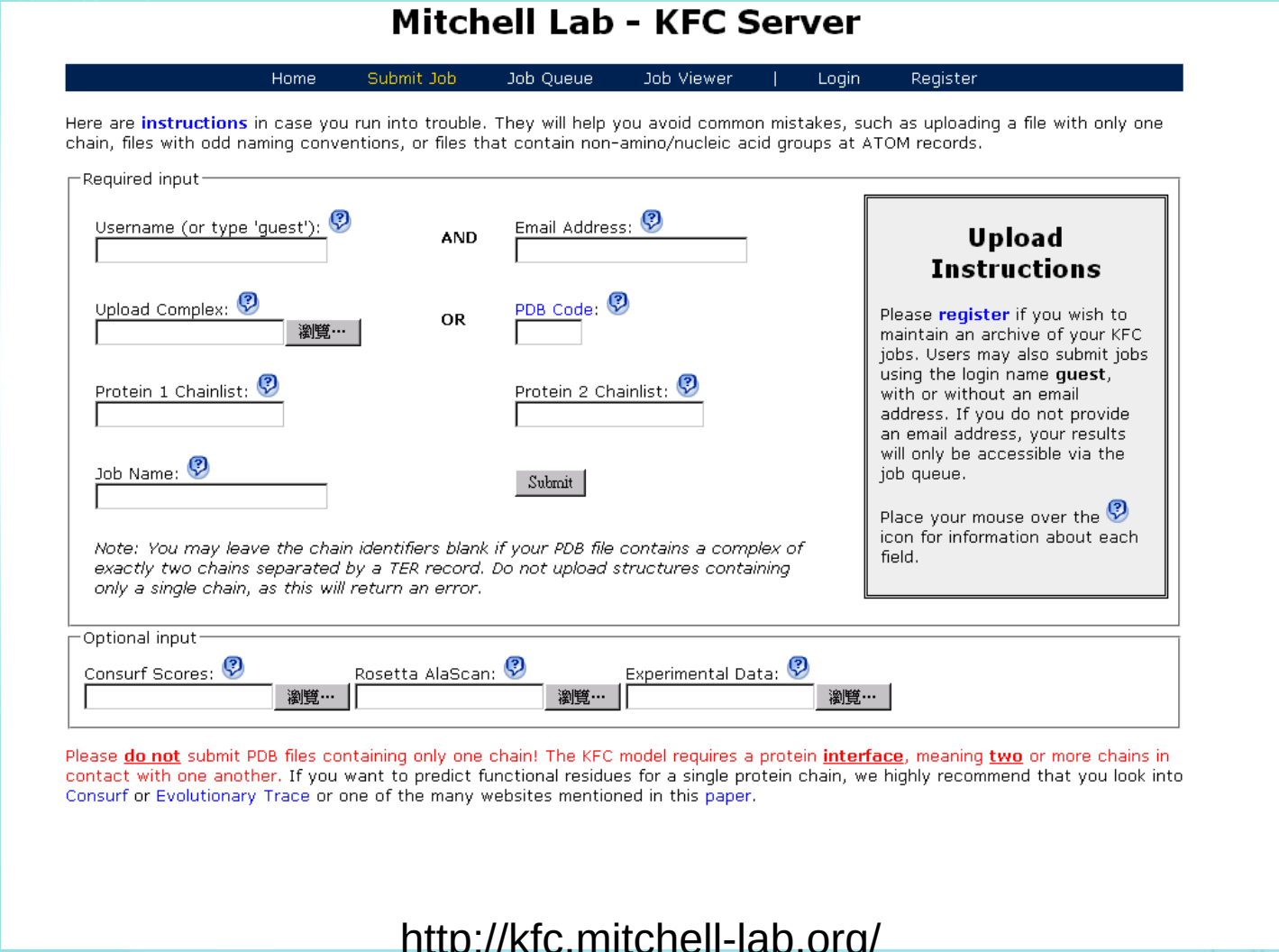


Binding hot spots: Antibody-antigen



http://prism.ccbb.ku.edu.tr/hotpoint/

Binding hot spots: Antibody-antigen



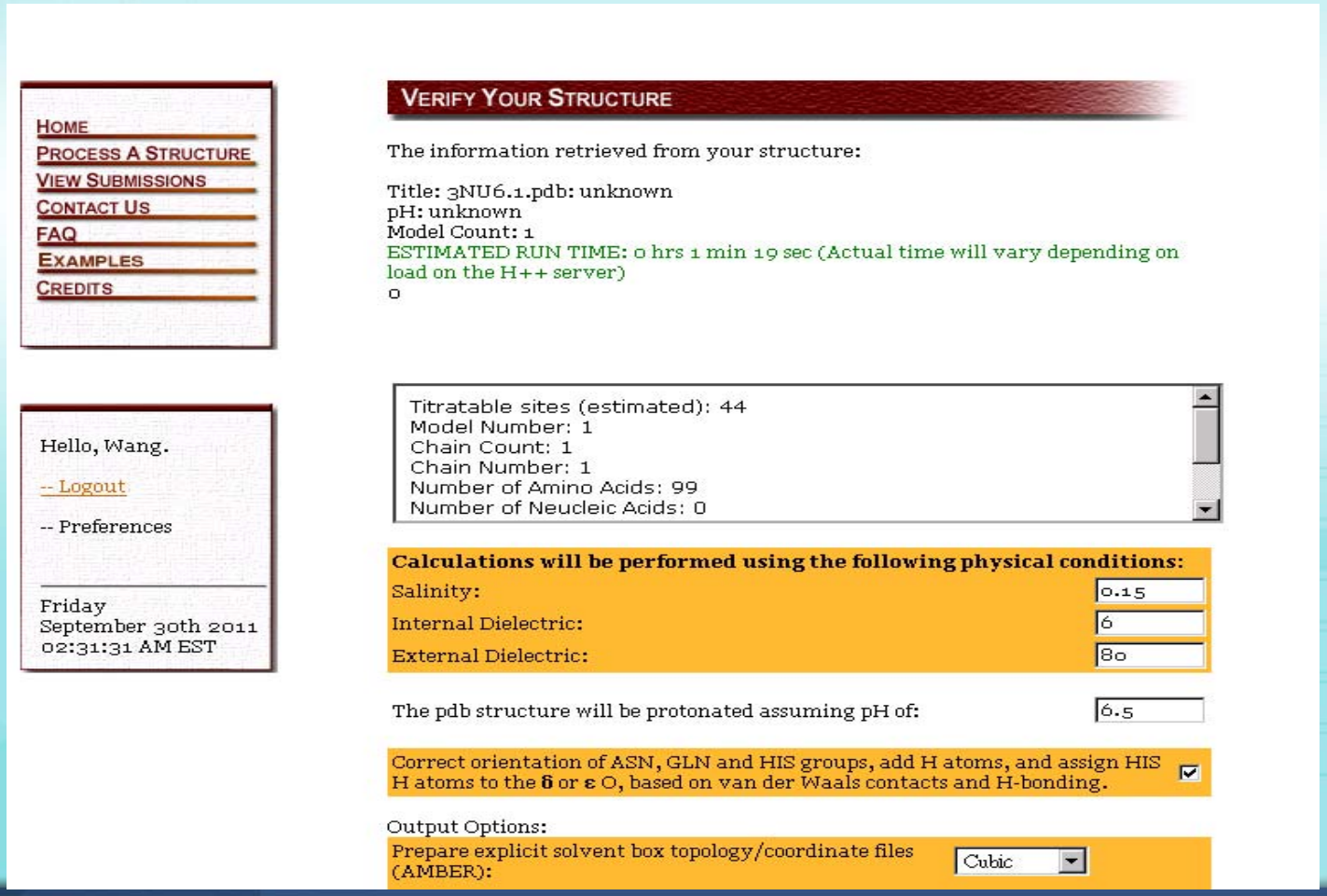
http://kfc.mitchell-lab.org/

Tutorial 3: Ibalizumab

Creating proteins structure:

1.Pdb ID: 3O2D (TMB355)

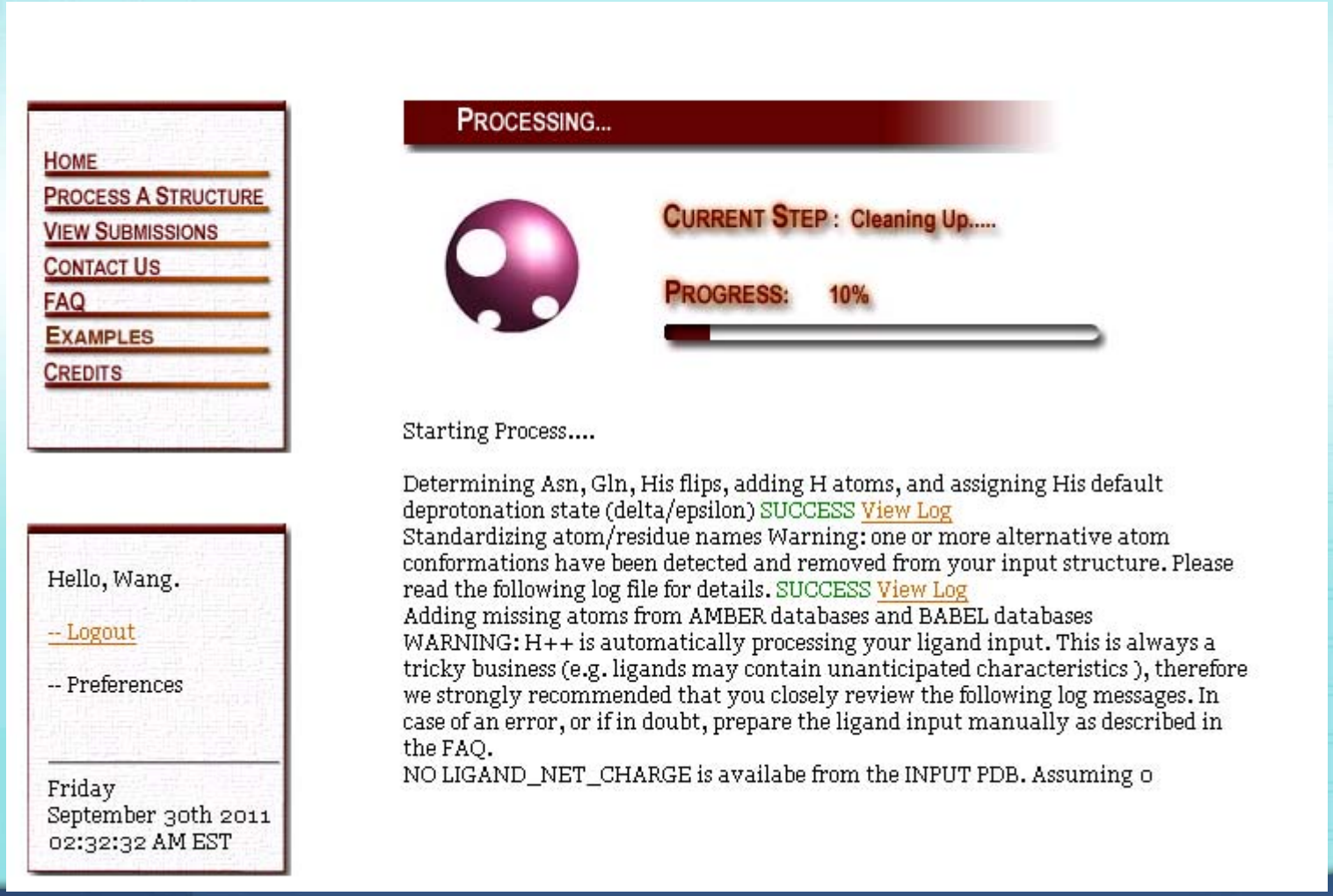
2.Submitting 3O2D file to H++ server



Tutorial 3: Ibalizumab

Creating proteins structure:

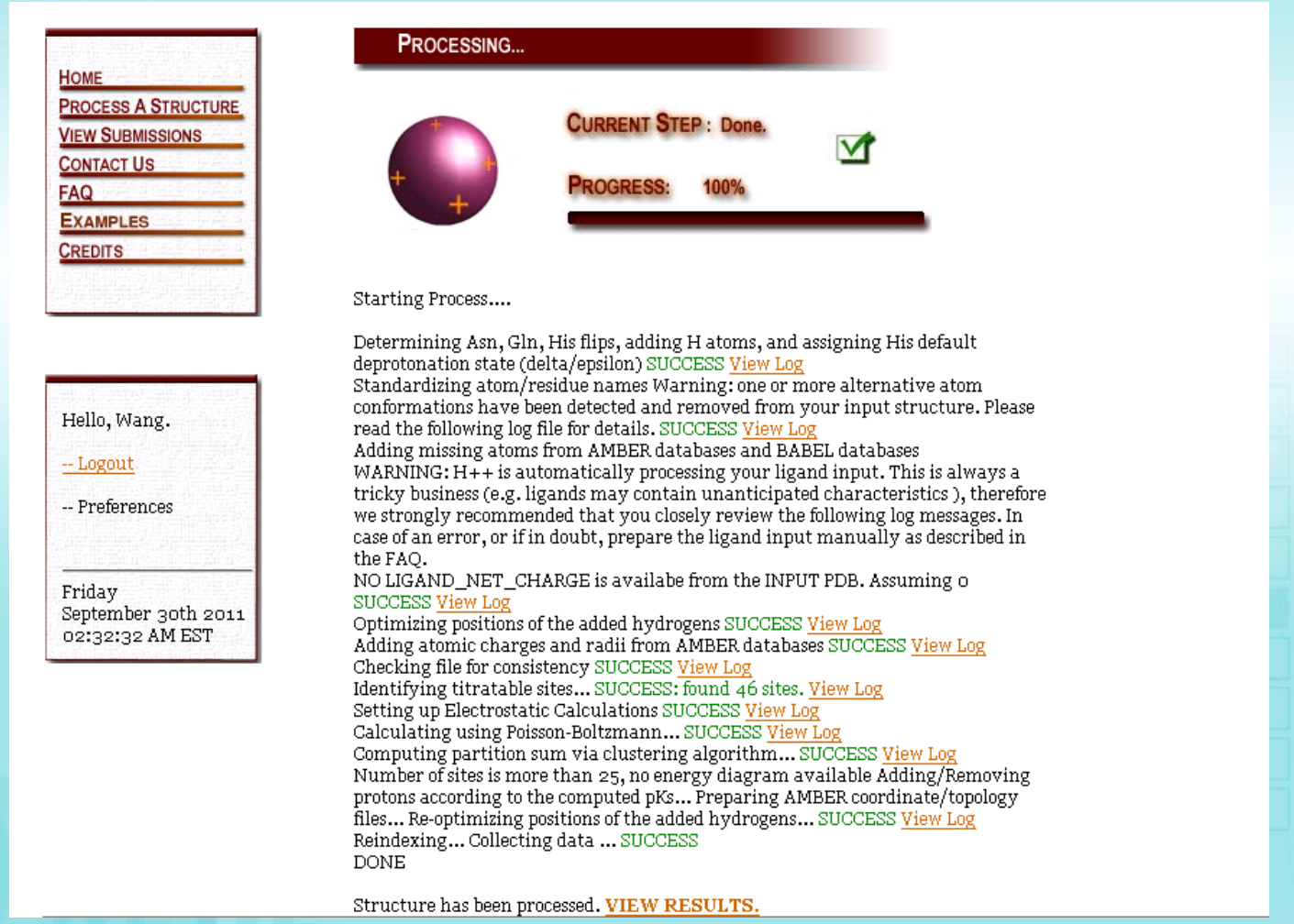
3. Waiting for the H++ server ~10 min



Tutorial 3: Ibalizumab

Creating proteins structure:

4. Downloading GB and TIP3 files



Tutorial 3: Ibalizumab

Creating proteins structure:

4. GB and Tip3 water box simulations (the same as before)

Reference to the files

(gb.md.in gb.min.in polyAT_wat_md1.in polyAT_wat_md2.in polyAT_wat_min1.in polyAT_wat_min2.in 3O2D.sh 3O2D.TIP3.sh)

5. $BRIMM_ROOT/bin/sietraj -pt 3O2D.top -trj 3O2D.md.x -sf 1 -ef 100 -inc 10 -tr 1-6633 -lr 6634-9434 -o gb.sie.out -sie

6. $BRIMM_ROOT/bin/sietraj -ave gb.sie.out

```
Energies in kcal/mol:

                Average  StdErr    Stdev
     Inter vdW -127.27     2.31     7.31
 Inter Coulomb   13.13     3.77    11.92
Reaction Field   -0.40     2.83     8.94
        Cavity  -24.51     0.31     0.97
      Constant   -2.89     0.00     0.00
               ------------------------
       Delta G  -17.46     0.35     1.11
```

Tutorial 3: Ibalizumab

further study

1.Mutating the residues of CDR loops/ binding-hot spots residues and running MD simulations.

2.Using the same methods to analyze the potential energies and RMSD profiles.