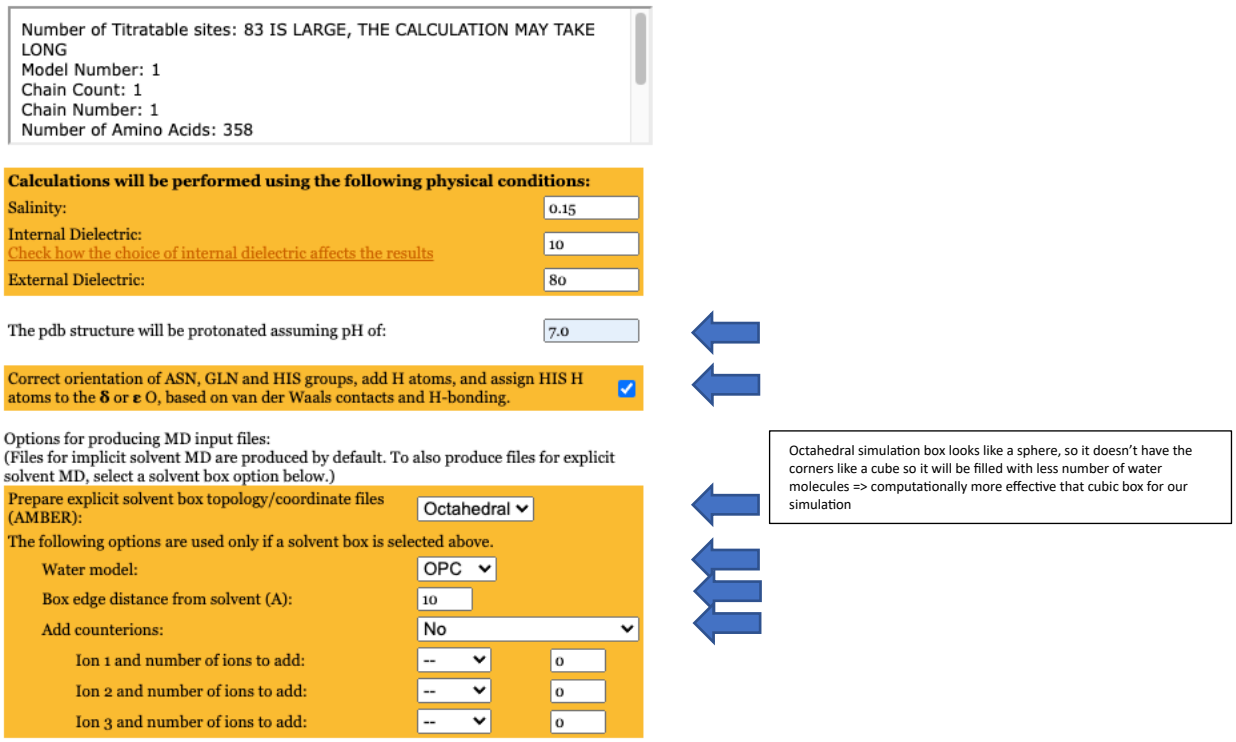
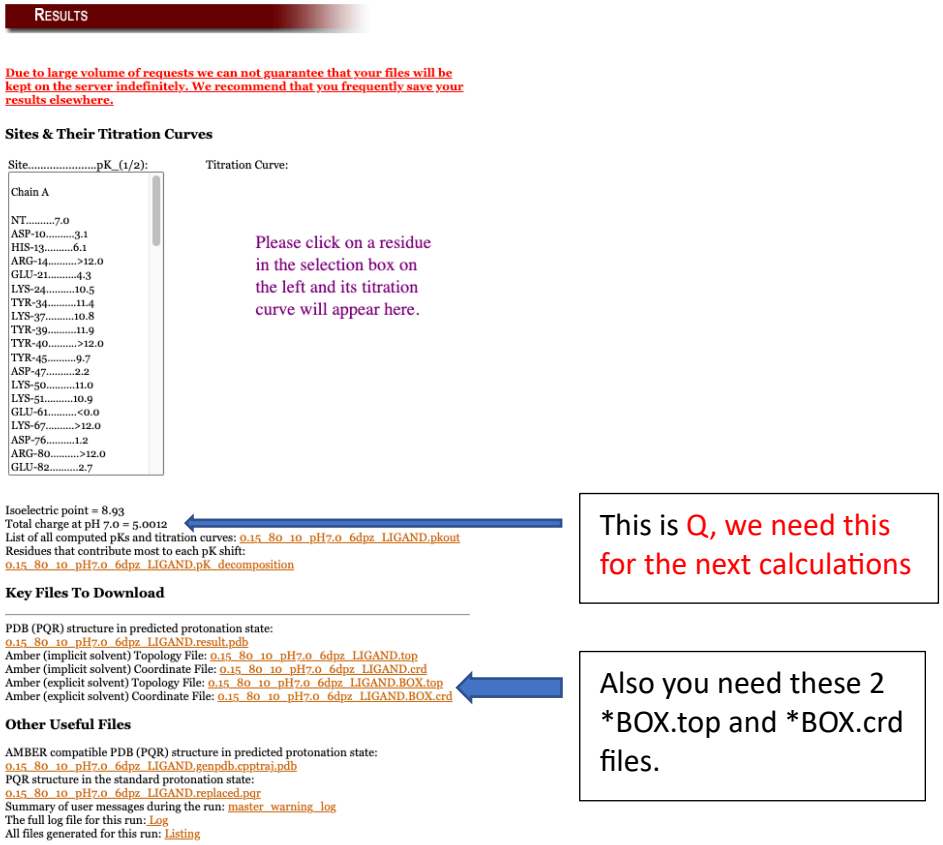
H++ Tutorial for Tim

At first we run the complex.pdb (protein_LIGAND.pdb) file through H++ without adding any ions. But we put this adjustment as follow:



Once it processed, we need to get 2 informations:

1) Total charge of the complex (Q)
2) Number of the water molecules inside the box



To count the number of WATER molecules inside the simulation box we need to make a .pdb file from those *BOX.top and *BOX.crd files using AMBER.

Here is the command that we use:
ambpdb -p 0.15_80_10_pH7.0_6dpz_LIGAND.BOX.top <0.15_80_10_pH7.0_6dpz_LIGAND.BOX.crd> complex.pdb

```
[fatemeh@strugatsky HHH]$ ls
0.15_80_10_pH7.0_6dpz_LIGAND.BOX.crd  0.15_80_10_pH7.0_6dpz_LIGAND.BOX.top
[fatemeh@strugatsky HHH]$ ambpdb -p 0.15_80_10_pH7.0_6dpz_LIGAND.BOX.top <0.15_80_10_pH7.0_6dpz_LIGAND.BOX.crd> complex.pdb
[fatemeh@strugatsky HHH]$ ls
0.15_80_10_pH7.0_6dpz_LIGAND.BOX.crd  0.15_80_10_pH7.0_6dpz_LIGAND.BOX.top  complex.pdb
```

Using the generated .pdb file, you can calculate the number of water molecules.
Here in this example is = 936 WAT molecules

Then we use the equations of the previously sent paper:

$$N_0 = \frac{N_w M_w c_0}{\rho_w} \sim \frac{N_w c_0}{56}$$

N_0 = 936*0.15/56 = 2.5
** 0.15 is the salt concentration that we usually use in explicit solvent simulations **

Where Nw is the number of water molecules, c0 is the salt concentration in Molar units and 1/56 is the conversion factor.

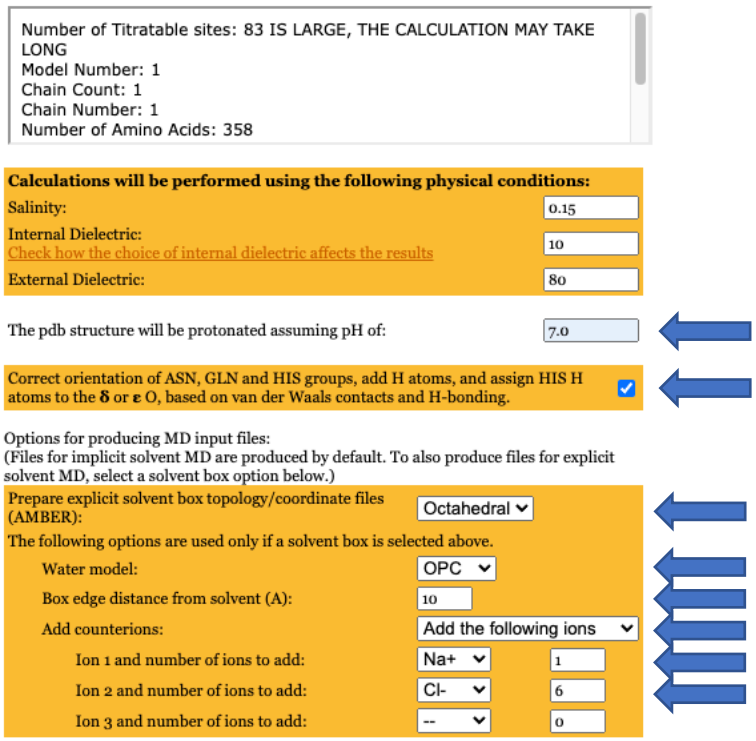
Then:

$$N_{\pm} = N_0 \sqrt{1 + \left(\frac{Q}{2N_0}\right)^2} \mp \frac{Q}{2}$$

Cl- = 2.5 $\sqrt{1 + (\frac{5}{2*2.5})}$ + 5/2 = 3.5+2.5=**6**

Na+ = 3.5 – 2.5 = **1**

Now we go back to the H++ for the final set up:



We need these 2 new files to start Molecular Dynamics Simulation:

0.15_80_10_pH7.0_6dpz_LIGAND.BOX.top
0.15_80_10_pH7.0_6dpz_LIGAND.BOX.crd

If you open .top file, you'll see the desired ions are added correctly.

-Done, Let me know if you have any questions.
Fatemeh22@vt.edu
(540)558-3061