Molecular Docking (Binding Affinity):

We used this documentation to develop our workflow:
http://autodock.scripps.edu/faqs-help/tutorial/using-autodock-4-with-autodocktools/2012_ADTtut.pdf
Additionally, we found that you can use a python script to run this process automatically:
http://autodock.scripps.edu/faqs-help/how-to/how-to-prepare-a-docking-parameter-file-for-autodock4-1?searchterm=genetic+algorithm

Before using Autodock:

We used autodock4 because we needed to add lanthanide parameters into the program. Do this by pasting the following into the AD4.1_bound.dat file in C:\Program Files (x86)\The Scripps Research Institute\Autodock\4.2.6:

```
atom_par R      5.70  0.843  97.4049  -0.00110  0.0  0.0  0  -1  -1  4  # Lanthanide
```

Or

```
atom_par Y      5.90  0.900  107.5362  -0.00110  0.0  0.0  0  -1  -1  4  # Neodymium
```

When creating a pdb for the ligands, we used Pymol:

1. imported lanmodulin (fetch 6mi5)
2. Import mutant protein
3. On the 6mi5 tab, click “A” > Align > to molecule > “mutant protein”
4. Display > sequence
5. Highlight and delete all the amino acids except for the ligands
6. File > Export Molecule
    a. Selection > 6mi5
    b. Save.. “ligands.pdb”
    c.
7. Go into autodock tools
    a. file>Read Molecule> “Open ligand”
    b. Ligand > Torsion Tree > Detect Root
    c. Ligand > Torsion Tree > Choose Torsions > Done
    d. Ligand > Output > output as .pdbqt
    e. Delete ligand model

When the pdbqt is made,

1. open the file
2. Make sure that all the ligands are present (u should see 3 lines of HETATM)
3. If theyre missing copy and paste the format then change the coordinates to the desired from the .pdb.
4. Change values to the highlighted with ur desired atom:

HETATM 1 R YT3 X 200 43.457 27.032 43.346 1.00 0.00 3.000 R
HETATM 2 R YT3 X 201 29.878 38.075 19.025 1.00 0.00 3.000 R
HETATM 3 R YT3 X 202 26.208 44.050 28.196 1.00 0.00 3.000 R

NOTE: I think you can ignore the errors it gives you when uploading the pdbqt into autodock tools. But let me know if you come across any other problems later on..

Our Documentation:

1. **Autodock 4 Steps:**
2. **Open Autodock Tools**
3. **Open Protein**
    a. Edit > Delete water
    b. Edit > Hydrogens > add > "Polar only" > Ok
4. **Grid > Macromolecules > Choose.. > "select protein" > save it as "protein".pdbqt**
    a. Grid > Set Map Type > Open Ligand > "Import ligand as .pdbqt"
    b. Grid > Grid Box … > "fit protein or interactions into box" > File > close saving current
    c. Grid > Other Options > Parameter Library Filename > Choose file name
    d. Grid > Output > Save gpf > "save as .gpf" (Need to add .gpf)
5. **Docking > Macromolecule > Set Rigid Filename… > "Choose protein .pdbqt"**
    a. Docking > Ligand > Choose > "ligand" > select > accept
    b. Docking > Search Parameters > genetic algorithm > accept
    c. Docking > Docking Parameters > Accept
    d. Docking > Other Options > AutoDock4 2 Parameters > Accept
    e. Docking > Output > Lamarckian > "Save as .dpf" (Need to add .dpf)
6. **Go into folder location type "cmd" in search bar**
    a. **Paste:** "C:\Program Files (x86)\The Scripps Research Institute\Autodock\4.2.6\autogrid4.exe" -p [file name].gpf -l [file name].glg
    b. **Paste:** "C:\Program Files (x86)\The Scripps Research Institute\Autodock\4.2.6\autodock4.exe" -p [file name].dpf -l [file name].dlg