

# Notes about Autodock vina

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## 1. Get the vina package

```
wget http://vina.scripps.edu/download/autodock_vina_1_1_2_linux_x86.tgz
tar xf autodock_vina_1_1_2_linux_x86.tgz
cd autodock_vina_1_1_2_linux_x86/bin
mv vina /Applications/
```

## 2. Prepare the system

```
# Prepare receptor for docking
./pythonsh prepare_receptor4.py -r pocket.pdb
./pythonsh prepare_ligand4.py -l ligand-b.pdb

# Above codes would generate pdbqt files:
#    pocket.pdbqt, ligand-b.pdbqt
```

## 3. Configure and run Autodock Vina

```
/Applications/vina --config conf.txt --out out-10modes.pdbqt --log log.txt

# Content of conf.txt:
receptor = pocket.pdbqt
ligand = ligand-b.pdbqt

center_x = 139
center_y = 145
center_z = 171

size_x = 25
size_y = 25
size_z = 25

num_modes = 10
```

The results PDB file for ligand poses are in "out-10modes.pdbqt" and the docking summary is like follows:

```
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 838757149
Performing search ...
0%   10   20   30   40   50   60   70   80   90  100%
|----|----|----|----|----|----|----|----|----|
*****
done.
Refining results ... done.

mode |   affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1      -8.6      0.000      0.000
  2      -7.7      0.926      3.279
  3      -6.7      1.970      7.796
  4      -6.6      2.001      7.587
  5      -6.5      2.610      8.036
  6      -6.4      2.782      8.434
  7      -6.2      6.909      8.542
  8      -6.2      8.815     11.453
  9      -6.1      3.495      6.656
 10      -6.1      6.202     10.949
Writing output ... done.
```

#### 4. MGLtools

This is for selecting the coordinates and the box for Vina. We can do this directly in PyMOL or VMD.

## Appendix

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Files under this folder:

```
archive/
├─ conf.txt                # Configuration file
├─ ligand-b.pdb            # ligand PDB
├─ ligand-b.pdbqt          # ligand PDBQT file for vina
├─ pocket.pdb             # receptor PDB
├─ pocket.pdbqt           # receptor PDBQT file for vina
├─ prepare_ligand4.py      # Prepare ligand PDBQT file
├─ prepare_receptor4.py    # Prepare protein PDBQT file
├─ log.txt                 # Vina log file
├─ out-10modes.pdbqt       # Ligand poses file
└─ pythonsh                # Executable python file
```