Autodock Automation Instruction:

**Step 1.** Make 8 folders for 8 proteins (with/without water)

**Step 2.** In each folder, create 1 folder for each ligand. The ligand folder name needs to be the same name as your *ligand.pdbqt* file. For example, if your ligand is *baicalein.pdbqt*, then your folder needs to be called *baicalein*.

**Step 4.** Set up your docking parameters in the config.txt file, as they are different for each site:

For example, for site 1:

center\_x = 6.428

center\_y = 0.502

center\_z = 20.708

size\_x = 42

size\_y = 26

size\_z = 28

energy\_range = 4

exhaustiveness = 8

num\_modes = 10

Reminder:

Site 1 docking grid: xyz = 6.428, 0.502, 20.708; Size (x\*y\*z) = 42\*26\*28

Site 2 docking grid: xyz = -58.057, -22.175, -1.827; Size (x\*y\*z) = 40\*40\*40

Site 3d docking grid: xyz = -46.656, -6.683, 20.394; Size (x\*y\*z) = 32\*36\*32

Site 3m docking grid: xyz = -46.189, -0.586, 12.875; Size (x\*y\*z) = 34\*24\*26

**Step 4.** Put your ligand.pdbqt, protein.pdbqt and config.txt files in each folder with the ligand name. The docking will not run if any of these is missing.

**Step 5.** Open 8 command line windows (one for each protein), and,

#Change directory to the folder containing your ligand folders:

For example.

cd /Users/ianyang/Desktop/Autodock\_Vina/docking\_results/Site1/with\_water/

**Step 6:** Automated way to run docking for all ligands. You will need to create a shell script (ending with .sh) using containing the following code:

#!/bin/bash

for dir in \*/

do

cd $dir

lig=${dir%/}

printf "Start docking for ligand $lig."

printf "\n"

#You will need to change the following line to: "FileLocation/vina" --receptor protein.pdbqt --ligand $lig.pdbqt --config config.txt –log log.txt --out output.pdbqt

“/Users/ianyang/Desktop/Autodock\_Vina/autodock\_vina\_1\_1\_2\_mac\_catalina\_64bit/bin/vina” --receptor Site1\_with\_water.pdbqt --ligand $lig.pdbqt --config config.txt –log log.txt --out output.pdbqt

printf "Docking for ligand $lig complete."

printf "\n\n"

cd ..

done

**Step 7:** Repeat docking analysis using the same docking parameters, but you will need to change the names of your log file and output file so that the results don’t overwrite your first repeat.

For example, with my ligand, notice I have changed log.txt to log2.txt and output.pdbqt to output2pdbqt:

“/Users/ianyang/Desktop/Autodock\_Vina/autodock\_vina\_1\_1\_2\_mac\_catalina\_64bit/bin/vina” --receptor Site1\_with\_water.pdbqt --ligand $lig.pdbqt --config config.txt –log log2.txt --out output2.pdbqt