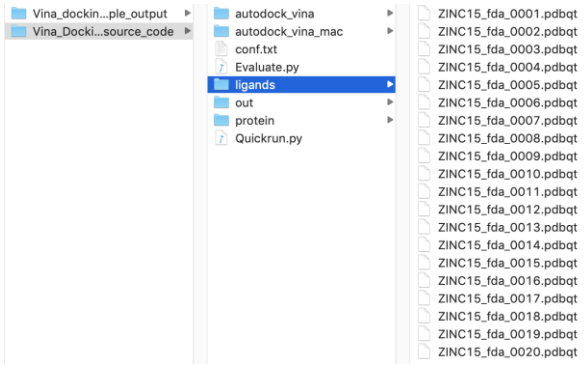
Example output of Autodock Vina batch-mode script

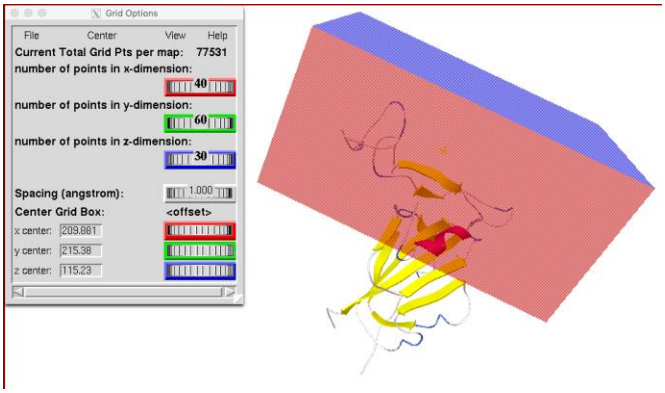
Using 20 random FDA approved drugs from ZINC database (http://zinc15.docking.org/catalogs/dbfda) as an example. For screening studies, ~1600 FDA approved drugs were tested.

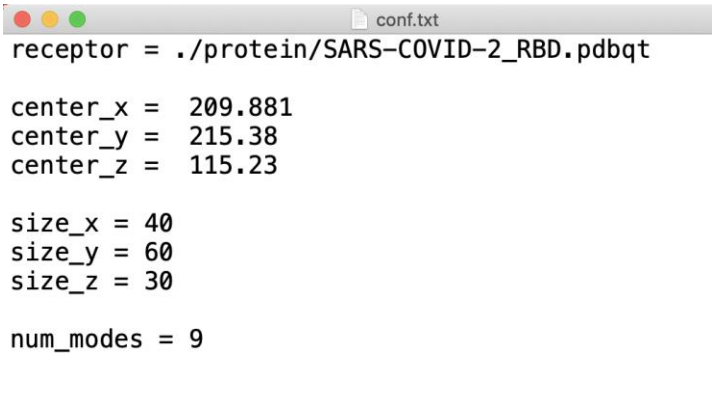
The expected run time for a normal quad-core computer with 8-GB RAM:
This demo of 20 example small molecules on an 8-threaded computer (10 minutes)
A library of 1,500 small molecules on a 16-threaded computer (3-5 hours).
** If the average atomic number of small molecules is greater than **100**, the time of simulation will be very long.*

1. The optimized small molecules were downloaded to the “ligands” folder.



2. The grid space was set using MGLtools.





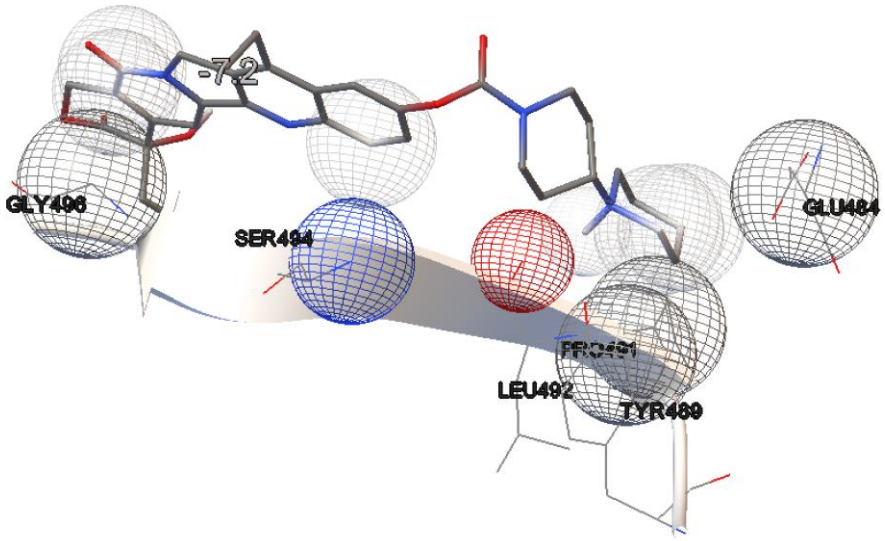
3. Terminal information for script execution is as follows:

```
(base) Wangs-MacBook-Pro:Vina_docking_batch haoqi$ python3 Quickrun.py
Start autodock vina docking
Reading all the existing inhibitors...
>>> ZINC15_fda_0014
>>> ZINC15_fda_0016
>>> ZINC15_fda_0012
>>> ZINC15_fda_0009
>>> ZINC15_fda_0010
>>> ZINC15_fda_0017
>>> ZINC15_fda_0015
>>> ZINC15_fda_0008
>>> ZINC15_fda_0011
>>> ZINC15_fda_0013
>>> ZINC15_fda_0006
>>> ZINC15_fda_0020
>>> ZINC15_fda_0004
>>> ZINC15_fda_0019
>>> ZINC15_fda_0002
>>> ZINC15_fda_0005
>>> ZINC15_fda_0007
>>> ZINC15_fda_0003
>>> ZINC15_fda_0001
>>> ZINC15_fda_0018
Now processing all these inhibitors to autodock vina analysis
Now start to process ZINC15_fda_0014
=================================================
Processing the 1st run on inhibitor ZINC15_fda_0014
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -4.0      0.000      0.000
   2         -3.7      3.188      4.202
   3         -3.7      2.646      3.729
   4         -3.6      3.123      4.107
   5         -3.6      1.746      2.485
   6         -3.5      2.359      3.122
   7         -3.4     13.542     15.203
   8         -3.4      2.731      3.953
   9         -3.3      2.417      2.933
Writing output ... done.
```

4. The binding scores of the 20 sample small molecules were output as follows:

A	B	C	D
Number	BindingScore	Std	Library
10	-7.167	0.047	ZINC15_fda
13	-6.3	0.163	ZINC15_fda
18	-5.967	0.189	ZINC15_fda
6	-5.8	0	ZINC15_fda
17	-5.8	0	ZINC15_fda
16	-5.733	0.094	ZINC15_fda
8	-5.4	0	ZINC15_fda
9	-5.4	0	ZINC15_fda
5	-5.267	0.094	ZINC15_fda
4	-5.233	0.125	ZINC15_fda
20	-5.2	0.082	ZINC15_fda
19	-5.067	0.047	ZINC15_fda
7	-4.433	0.094	ZINC15_fda
12	-4	0	ZINC15_fda
11	-3.967	0.047	ZINC15_fda
14	-3.967	0.047	ZINC15_fda
15	-3.9	0	ZINC15_fda
1	-3.2	0	ZINC15_fda
2	-3.1	0	ZINC15_fda
3	-3.1	0	ZINC15_fda

5. The interactions of the small molecule No.10 (with the highest binding score among the 20 molecules) on the protein receptor can be analyzed via MGLtools. From the figure, this small molecule had -7.2 kcal/mol binding affinity to the receptor. The interaction diagram indicates the existence of non-covalent bonds with amino acids GLY496, SER 494, GLU484, LEU 492, PRO 491 and TYR 489 on the receptor protein.



6. (optional) The docking results and ligand interactions can also be viewed using other visualization programs. An example of the small molecule No.10 interacting with the protein receptor after minimization is depicted below using Schrödinger Maestro.