

We've configured colab to use a GPU (Runtime->Change runtime type->Hardware Accelerator=GPU)

```
!nvidia-smi
```

```
Wed Apr 24 02:49:03 2024
+-----+
| NVIDIA-SMI 535.104.05      Driver Version: 535.104.05    CUDA Version: 12.2 |
+-----+
| GPU  Name        Persistence-M | Bus-Id     Disp.A  | Volatile Uncorr. ECC | | |
| Fan  Temp     Perf  Pwr:Usage/Cap | Memory-Usage | GPU-Util  Compute M. |
|          |          |              |               | MIG M.   |
+-----+
| 0  Tesla T4           Off  00000000:00:04.0 Off |           0%      Default |
| N/A   37C   P8          9W /  70W |    0MiB / 15360MiB |           0%      N/A   |
+-----+
+-----+
| Processes:                               GPU Memory |
| GPU  GI CI      PID  Type  Process name        Usage  |
| ID  ID          |
+-----+
| No running processes found            |
+-----+
```

```
!apt install openbabel
```

```
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following additional packages will be installed:
  libinchi1 libmaeparser1 libopenbabel7
The following NEW packages will be installed:
  libinchi1 libmaeparser1 libopenbabel7 openbabel
0 upgraded, 4 newly installed, 0 to remove and 45 not upgraded.
Need to get 3,903 kB of archives.
After this operation, 16.9 MB of additional disk space will be used.
Get:1 http://archive.ubuntu.com/ubuntu jammy/universe amd64 libinchi1 amd64 1.03+dfsg-4 [455 kB]
Get:2 http://archive.ubuntu.com/ubuntu jammy/universe amd64 libmaeparser1 amd64 1.2.4-1build1 [81 kB]
Get:3 http://archive.ubuntu.com/ubuntu jammy/universe amd64 libopenbabel7 amd64 3.1.1+dfsg-6ubuntu5 [104 kB]
Get:4 http://archive.ubuntu.com/ubuntu jammy/universe amd64 openbabel amd64 3.1.1+dfsg-6ubuntu5 [104 kB]
Fetched 3,903 kB in 1s (2,612 kB/s)
Selecting previously unselected package libinchi1.
(Reading database ... 121752 files and directories currently installed.)
Preparing to unpack .../libinchi1_1.03+dfsg-4_amd64.deb ...
Unpacking libinchi1 (1.03+dfsg-4) ...
Selecting previously unselected package libmaeparser1:amd64.
Preparing to unpack .../libmaeparser1_1.2.4-1build1_amd64.deb ...
Unpacking libmaeparser1:amd64 (1.2.4-1build1) ...
Selecting previously unselected package libopenbabel7.
Preparing to unpack .../libopenbabel7_3.1.1+dfsg-6ubuntu5_amd64.deb ...
Unpacking libopenbabel7 (3.1.1+dfsg-6ubuntu5) ...
Selecting previously unselected package openbabel.
Preparing to unpack .../openbabel_3.1.1+dfsg-6ubuntu5_amd64.deb ...
Unpacking openbabel (3.1.1+dfsg-6ubuntu5) ...
Setting up libmaeparser1:amd64 (1.2.4-1build1) ...
Setting up libinchi1 (1.03+dfsg-4) ...
Setting up libopenbabel7 (3.1.1+dfsg-6ubuntu5) ...
Setting up openbabel (3.1.1+dfsg-6ubuntu5) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
/sbin/ldconfig.real: /usr/local/lib/libtbbbind.so.3 is not a symbolic link
/sbin/ldconfig.real: /usr/local/lib/libtbbbind_2_0.so.3 is not a symbolic link
/sbin/ldconfig.real: /usr/local/lib/libtbbbind_2_5.so.3 is not a symbolic link
/sbin/ldconfig.real: /usr/local/lib/libtbbmalloc.so.2 is not a symbolic link
/sbin/ldconfig.real: /usr/local/lib/libtbbmalloc_proxy.so.2 is not a symbolic link
```

24/04/2024, 11:12

2-docking\_small\_molecule\_to\_receptor.ipynb - Colab

/sbin/ldconfig.real: /usr/local/lib/libtbb.so.12 is not a symbolic link

Processing triggers for man-db (2.10.2-1) ...

```
# !cat /etc/*release  
# !nvcc --version
```

```
# !apt-get install build-essential git cmake wget libboost-all-dev libeigen3-dev libgoogle-glog-dev
```

```
# %%bash -v  
# git clone https://github.com/openbabel/openbabel.git  
# cd openbabel  
# mkdir build  
# cd build  
# cmake -DWITH_MAEParser=OFF -DWITH_CoORDgen=OFF -DPYTHON_BINDINGS=ON -DRUN_SWIG=ON ..  
# make  
# make install
```

```
# git clone https://github.com/gnina/gnina.git  
# cd gnina  
# mkdir build  
# cd build  
# cmake ..  
# make  
# make install
```

```
# !rm -r gnina  
# !rm -r openbabel
```

**Download** the linux binary and make it executable.

```
!wget https://github.com/gnina/gnina/releases/download/v1.1/gnina
```

```
--2024-04-24 02:49:14-- https://github.com/gnina/gnina/releases/download/v1.1/gnina  
Resolving github.com (github.com)... 140.82.114.3  
Connecting to github.com (github.com)|140.82.114.3|:443... connected.  
HTTP request sent, awaiting response... 302 Found  
Location: https://objects.githubusercontent.com/github-production-release-asset-2e65be/45548146/  
--2024-04-24 02:49:14-- https://objects.githubusercontent.com/github-production-release-asset-2e65be/45548146/  
Resolving objects.githubusercontent.com (objects.githubusercontent.com)... 185.199.110.133, 185.199.110.134  
Connecting to objects.githubusercontent.com (objects.githubusercontent.com)|185.199.110.133|:443  
HTTP request sent, awaiting response... 200 OK  
Length: 306470832 (292M) [application/octet-stream]  
Saving to: 'gnina'
```

```
gnina          100%[=====] 292.27M   203MB/s   in 1.4s
```

```
2024-04-24 02:49:15 (203 MB/s) - 'gnina' saved [306470832/306470832]
```

```
!chmod +x gnina
```

```
./gnina --version
```

```
gnina v1.1 master:e4cb380+ Built Dec 18 2023.
```

Get a pdb and extract the receptor and ligand.

```
!wget http://files.rcsb.org/download/3ERK.pdb
```

```
--2024-04-24 02:49:20-- http://files.rcsb.org/download/3ERK.pdb
Resolving files.rcsb.org (files.rcsb.org)... 128.6.159.157
Connecting to files.rcsb.org (files.rcsb.org)|128.6.159.157|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: '3ERK.pdb'
```

3ERK.pdb [ => ] 270.21K --.-KB/s in 0.1s

2024-04-24 02:49:22 (2.40 MB/s) - '3ERK.pdb' saved [276696]

```
# !grep SB4 3ERK.pdb
```

```
# !grep ATOM 3ERK.pdb
```

```
!wget http://files.rcsb.org/download/6CYT.pdb
```

```
--2024-04-24 02:49:23-- http://files.rcsb.org/download/6CYT.pdb
Resolving files.rcsb.org (files.rcsb.org)... 128.6.159.157
Connecting to files.rcsb.org (files.rcsb.org)|128.6.159.157|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: '6CYT.pdb'
```

6CYT.pdb [ => ] 958.71K 5.78MB/s in 0.2s

2024-04-24 02:49:23 (5.78 MB/s) - '6CYT.pdb' saved [981720]

```
# !wget https://go.drugbank.com/structures/small_molecule_drugs/DB04542.pdb -O lig.pdb
```

```
!wget https://go.drugbank.com/structures/small_molecule_drugs/DB04542.sdf?type=3d -O DB04542.sdf
```

```
--2024-04-24 02:49:30-- https://go.drugbank.com/structures/small\_molecule\_drugs/DB04542.sdf?type=3d
Resolving go.drugbank.com (go.drugbank.com)... 172.66.42.250, 172.66.41.6, 2606:4700:3108::ac42::1
Connecting to go.drugbank.com (go.drugbank.com)|172.66.42.250|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [text/plain]
Saving to: 'DB04542.sdf'
```

DB04542.sdf [ => ] 5.53K --.-KB/s in 0s

2024-04-24 02:49:30 (30.6 MB/s) - 'DB04542.sdf' saved [5662]

```
!obabel DB04542.sdf -O DB04542.pdb
```

1 molecule converted

```
!grep UNL DB04542.pdb > lig.pdb
```

```
!grep ATOM 6CYT.pdb > rec.pdb
```

```
!cat lig.pdb
```

HETATM	1	P	UNL	1	-2.911	1.345	1.001	1.00	0.00	P
HETATM	2	P	UNL	1	-4.302	-0.558	-0.758	1.00	0.00	P
HETATM	3	0	UNL	1	1.367	0.860	1.085	1.00	0.00	O
HETATM	4	0	UNL	1	-1.322	1.612	1.154	1.00	0.00	O
HETATM	5	0	UNL	1	4.380	-1.771	0.062	1.00	0.00	O
HETATM	6	0	UNL	1	-3.018	0.124	-0.053	1.00	0.00	O
HETATM	7	0	UNL	1	-3.453	2.613	0.156	1.00	0.00	O
HETATM	8	0	UNL	1	1.234	-5.123	-0.051	1.00	0.00	O
HETATM	9	0	UNL	1	-3.636	1.107	2.294	1.00	0.00	O

HETATM	10	0	UNL	1	-4.877	0.618	-1.706	1.00	0.00	0
HETATM	11	0	UNL	1	-3.638	-1.597	-1.804	1.00	0.00	0
HETATM	12	0	UNL	1	-5.295	-1.157	0.194	1.00	0.00	0
HETATM	13	N	UNL	1	2.129	-1.162	0.187	1.00	0.00	N
HETATM	14	N	UNL	1	2.985	3.132	-0.271	1.00	0.00	N
HETATM	15	N	UNL	1	2.800	-3.433	0.006	1.00	0.00	N
HETATM	16	N	UNL	1	2.867	4.358	-0.429	1.00	0.00	N1+
HETATM	17	N	UNL	1	2.769	5.486	-0.569	1.00	0.00	N1-
HETATM	18	C	UNL	1	1.851	2.320	-0.730	1.00	0.00	C
HETATM	19	C	UNL	1	0.914	2.066	0.444	1.00	0.00	C
HETATM	20	C	UNL	1	2.340	0.934	-1.079	1.00	0.00	C
HETATM	21	C	UNL	1	2.378	0.247	0.274	1.00	0.00	C
HETATM	22	C	UNL	1	-0.529	1.849	0.004	1.00	0.00	C
HETATM	23	C	UNL	1	0.811	-1.608	0.205	1.00	0.00	C
HETATM	24	C	UNL	1	3.189	-2.091	0.084	1.00	0.00	C
HETATM	25	C	UNL	1	0.442	-2.893	0.130	1.00	0.00	C
HETATM	26	C	UNL	1	1.505	-3.928	0.020	1.00	0.00	C
HETATM	27	C	UNL	1	-0.982	-3.347	0.151	1.00	0.00	C
HETATM	28	H	UNL	1	1.358	2.801	-1.583	1.00	0.00	H
HETATM	29	H	UNL	1	0.947	2.864	1.194	1.00	0.00	H
HETATM	30	H	UNL	1	3.313	0.912	-1.581	1.00	0.00	H
HETATM	31	H	UNL	1	1.617	0.449	-1.747	1.00	0.00	H
HETATM	32	H	UNL	1	3.344	0.423	0.763	1.00	0.00	H
HETATM	33	H	UNL	1	-0.901	2.745	-0.504	1.00	0.00	H
HETATM	34	H	UNL	1	-0.625	1.002	-0.680	1.00	0.00	H
HETATM	35	H	UNL	1	0.036	-0.858	0.279	1.00	0.00	H
HETATM	36	H	UNL	1	3.547	-4.117	-0.069	1.00	0.00	H
HETATM	37	H	UNL	1	-1.234	-3.859	-0.783	1.00	0.00	H
HETATM	38	H	UNL	1	-1.677	-2.510	0.272	1.00	0.00	H
HETATM	39	H	UNL	1	-1.151	-4.038	0.984	1.00	0.00	H
HETATM	40	H	UNL	1	-3.615	3.460	0.624	1.00	0.00	H
HETATM	41	H	UNL	1	-5.718	0.470	-2.189	1.00	0.00	H
HETATM	42	H	UNL	1	-4.221	-2.207	-2.302	1.00	0.00	H

```
!ls -alh
```

```
total 294M
drwxr-xr-x 1 root root 4.0K Apr 24 02:49 .
drwxr-xr-x 1 root root 4.0K Apr 24 02:45 ..
-rw-r--r-- 1 root root 271K Apr 24 02:49 3ERK.pdb
-rw-r--r-- 1 root root 959K Apr 24 02:49 6CYT.pdb
drwxr-xr-x 4 root root 4.0K Apr 22 13:25 .config
-rw-r--r-- 1 root root 6.6K Apr 24 02:49 DB04542.pdb
-rw-r--r-- 1 root root 5.6K Apr 24 02:49 DB04542.sdf
-rwxr-xr-x 1 root root 293M Dec 18 21:22 gnina
-rw-r--r-- 1 root root 3.4K Apr 24 02:49 lig.pdb
-rw-r--r-- 1 root root 444K Apr 24 02:49 rec.pdb
drwxr-xr-x 1 root root 4.0K Apr 22 13:25 sample_data
```

Redock the cognate ligand. Set random seed for reproducibility.

Affinity is the Vina score of the pose. CNN pose score is a probability calculated by a convolutional neural network that the pose is a low RMSD pose. CNN affinity is the CNN's prediction of the pK (higher is better, e.g. 9 is nanomolar, 6 is micromolar).

This particular ligand has an experimental affinity of 18μM so the prediction is pretty close.

```
!./gnina -r rec.pdb -l lig.pdb --autobox_ligand rec.pdb -o docked.sdf --seed 0 --device 0 --verbosit
```

```
total energy after refinement: -9.47150
```

```
energy after refinement: -9.21563
ical energy after refinement: -9.21663
```

```
energy after refinement: -9.21496
ical energy after refinement: -9.21444
```

```
energy after refinement: -9.13627
ical energy after refinement: -9.13905
```

```
energy after refinement: -9.09616
ical energy after refinement: -9.09653
```

```
energy after refinement: -9.13509
ical energy after refinement: -9.13710
```

```
energy after refinement: -8.79156
ical energy after refinement: -8.79339
```

```
energy after refinement: -8.63850
ical energy after refinement: -8.63520
```

```
energy after refinement: -8.78609
ical energy after refinement: -8.77916
```

```
energy after refinement: -8.69041
ical energy after refinement: -8.69263
```

```
energy after refinement: -8.52908
ical energy after refinement: -8.52873
```

affinity (kcal/mol)	intramol (kcal/mol)	CNN pose score	CNN affinity
-7.84	-1.27	0.7215	6.675
-7.69	-0.48	0.6588	6.735
-8.77	-1.36	0.5767	6.009
-7.26	-1.08	0.4946	6.850
-7.66	-0.34	0.4691	6.524
-8.37	-1.19	0.4594	6.947
-8.51	-0.33	0.4206	6.990
-8.25	-0.93	0.4096	6.875
-7.93	-0.13	0.3994	6.732

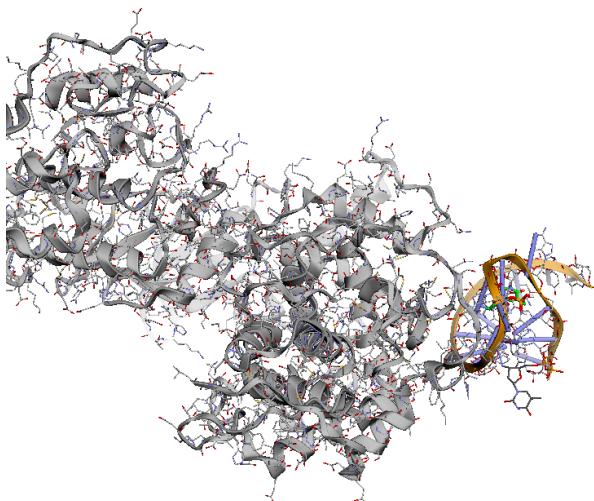
```
emory usage: 1999 MB
```

```
# !./gnina -r rec.pdb -l lig.pdb --autobox_ligand lig.pdb -o docked.sdf --seed 0
```

```
!pip install py3Dmol
```

```
Collecting py3Dmol
  Downloading py3Dmol-2.1.0-py2.py3-none-any.whl (12 kB)
Installing collected packages: py3Dmol
Successfully installed py3Dmol-2.1.0
```

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':4000})
```



```
<py3Dmol.view at 0x7897dd327700>
```

The top ranked pose is <2A from the crystal pose

```
!obrms -f lig.pdb docked.sdf
```

```
RMSD lig.pdb: 45.7373
RMSD lig.pdb: 46.157
RMSD lig.pdb: 88.4307
RMSD lig.pdb: 52.4566
RMSD lig.pdb: 46.5465
RMSD lig.pdb: 47.281
RMSD lig.pdb: 46.8989
RMSD lig.pdb: 47.7493
RMSD lig.pdb: 47.7907
```

Fostemsavir is an antiretroviral medication for adults living with HIV/AIDS who have tried multiple HIV medications and whose HIV infection cannot be successfully treated with other therapies because of resistance, intolerance or safety considerations.

Fostemsavir is an HIV entry inhibitor and is a human immunodeficiency virus type 1 (HIV-1) **gp120-directed attachment inhibitor**.

Here, we are trying to check if the above mentioned drug binds to gp120 protein. It will help in determining the accuracy of the model.

The molecule has 10 conformers. I am trying first one.

More information about the medication can be found at: <https://www.drugs.com/monograph/fostemsavir.html>

2D and 3D structure of the molecule can be found at: <https://pubchem.ncbi.nlm.nih.gov/compound/Fostemsavir>

I will be using the molecule structure from the above source. The structure used here will be 3 D structure of the molecule.

Source: <https://en.wikipedia.org/wiki/Fostemsavir>

gp120 protein structure:

<https://www.rcsb.org/structure/5F4R>

Drugbank: [https://go.drugbank.com/structures/small\\_molecule\\_drugs/DB11796.sdf?type=3d](https://go.drugbank.com/structures/small_molecule_drugs/DB11796.sdf?type=3d)

More about HIV Virus: <https://www.youtube.com/watch?v=XP8tMBm8zbY>

Mechanism of Action for HIV-1: <https://www.youtube.com/watch?v=xzWaw9T7XD8>

```
!wget http://files.rcsb.org/download/5F4R.pdb
```

```
--2024-04-24 02:52:17-- http://files.rcsb.org/download/5F4R.pdb
Resolving files.rcsb.org (files.rcsb.org)... 128.6.159.100
Connecting to files.rcsb.org (files.rcsb.org)|128.6.159.100|:80... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [application/octet-stream]
Saving to: '5F4R.pdb.1'

5F4R.pdb.1 [=>] 502.77K --.-KB/s in 0.1s

2024-04-24 02:52:18 (3.59 MB/s) - '5F4R.pdb.1' saved [514836]
```

```
# !cat 5F4R.pdb
```

```
!wget https://go.drugbank.com/structures/small_molecule_drugs/DB11796.sdf?type=3d -O Fostemsavir.sdf
```

```
--2024-04-24 02:52:26-- https://go.drugbank.com/structures/small\_molecule\_drugs/DB11796.sdf?type=3d
Resolving go.drugbank.com (go.drugbank.com)... 172.66.41.6, 172.66.42.250, 2606:4700:3108::ac42::
Connecting to go.drugbank.com (go.drugbank.com)|172.66.41.6|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: unspecified [text/plain]
Saving to: 'Fostemsavir.sdf'

Fostemsavir.sdf [=>] 7.92K --.-KB/s in 0s

2024-04-24 02:52:27 (78.5 MB/s) - 'Fostemsavir.sdf' saved [8110]
```

```
!ls -alh
```

```
total 295M
drwxr-xr-x 1 root root 4.0K Apr 24 02:52 .
drwxr-xr-x 1 root root 4.0K Apr 24 02:45 ..
-rw-r--r-- 1 root root 271K Apr 24 02:49 3ERK.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:51 5F4R.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:52 5F4R.pdb.1
-rw-r--r-- 1 root root 959K Apr 24 02:49 6CYT.pdb
drwxr-xr-x 4 root root 4.0K Apr 22 13:25 .config
-rw-r--r-- 1 root root 6.6K Apr 24 02:49 DB04542.pdb
-rw-r--r-- 1 root root 5.6K Apr 24 02:49 DB04542.sdf
-rw-r--r-- 1 root root 25K Apr 24 02:51 docked.sdf
-rw-r--r-- 1 root root 8.0K Apr 24 02:52 Fostemsavir.sdf
-rwxr-xr-x 1 root root 293M Dec 18 21:22 gnina
-rw-r--r-- 1 root root 3.4K Apr 24 02:49 lig.pdb
-rw-r--r-- 1 root root 444K Apr 24 02:49 rec.pdb
drwxr-xr-x 1 root root 4.0K Apr 22 13:25 sample_data
```

```
!obabel Fostemsavir.sdf -O Fostemsavir.pdb
```

```
1 molecule converted
```

```
# !cat Fostemsavir.pdb
```

```
!grep UNL Fostemsavir.pdb > lig.pdb
```

```
!grep ATOM 5F4R.pdb > rec.pdb
```

```
!cat lig.pdb
```

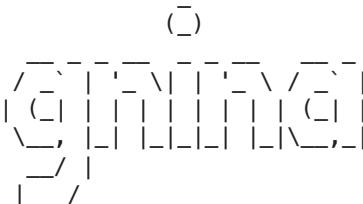
HETATM	1	P	UNL	1	-1.906	3.611	1.176	1.00	0.00	P
HETATM	2	O	UNL	1	1.091	-3.097	3.024	1.00	0.00	O
HETATM	3	O	UNL	1	6.415	0.898	1.386	1.00	0.00	O
HETATM	4	O	UNL	1	0.406	-3.983	0.280	1.00	0.00	O
HETATM	5	O	UNL	1	-1.578	-4.190	-1.446	1.00	0.00	O
HETATM	6	O	UNL	1	-1.986	2.100	0.607	1.00	0.00	O
HETATM	7	O	UNL	1	-3.258	3.792	2.046	1.00	0.00	O
HETATM	8	O	UNL	1	-0.746	3.563	2.303	1.00	0.00	O
HETATM	9	O	UNL	1	-1.703	4.672	0.134	1.00	0.00	O
HETATM	10	N	UNL	1	2.443	-1.983	1.457	1.00	0.00	N
HETATM	11	N	UNL	1	4.242	0.141	0.976	1.00	0.00	N
HETATM	12	N	UNL	1	-2.108	-0.191	0.889	1.00	0.00	N
HETATM	13	N	UNL	1	-4.625	0.391	-0.704	1.00	0.00	N
HETATM	14	N	UNL	1	-4.200	-1.655	-1.776	1.00	0.00	N
HETATM	15	N	UNL	1	-4.234	1.662	-0.878	1.00	0.00	N
HETATM	16	N	UNL	1	-6.340	1.856	-0.327	1.00	0.00	N
HETATM	17	C	UNL	1	3.572	-1.770	2.364	1.00	0.00	C
HETATM	18	C	UNL	1	2.644	-1.504	0.083	1.00	0.00	C
HETATM	19	C	UNL	1	4.017	-0.311	2.350	1.00	0.00	C
HETATM	20	C	UNL	1	3.091	-0.044	0.082	1.00	0.00	C
HETATM	21	C	UNL	1	1.323	-2.670	1.901	1.00	0.00	C
HETATM	22	C	UNL	1	-0.825	-1.989	0.666	1.00	0.00	C
HETATM	23	C	UNL	1	-1.901	-2.094	-0.258	1.00	0.00	C
HETATM	24	C	UNL	1	-2.689	-0.954	-0.097	1.00	0.00	C
HETATM	25	C	UNL	1	5.453	0.745	0.634	1.00	0.00	C
HETATM	26	C	UNL	1	0.271	-2.926	0.890	1.00	0.00	C
HETATM	27	C	UNL	1	-0.979	-0.809	1.357	1.00	0.00	C
HETATM	28	C	UNL	1	-3.834	-0.736	-0.853	1.00	0.00	C
HETATM	29	C	UNL	1	-2.283	-3.045	-1.216	1.00	0.00	C
HETATM	30	C	UNL	1	-2.583	1.081	1.390	1.00	0.00	C
HETATM	31	C	UNL	1	5.617	1.234	-0.740	1.00	0.00	C
HETATM	32	C	UNL	1	-3.437	-2.761	-1.934	1.00	0.00	C
HETATM	33	C	UNL	1	5.253	2.542	-1.062	1.00	0.00	C
HETATM	34	C	UNL	1	6.138	0.393	-1.723	1.00	0.00	C
HETATM	35	C	UNL	1	-5.906	0.562	-0.372	1.00	0.00	C
HETATM	36	C	UNL	1	5.409	3.007	-2.368	1.00	0.00	C
HETATM	37	C	UNL	1	6.295	0.859	-3.028	1.00	0.00	C
HETATM	38	C	UNL	1	-5.259	2.527	-0.652	1.00	0.00	C
HETATM	39	C	UNL	1	5.930	2.166	-3.351	1.00	0.00	C
HETATM	40	C	UNL	1	-2.081	-5.068	-2.449	1.00	0.00	C
HETATM	41	C	UNL	1	-5.150	3.979	-0.760	1.00	0.00	C
HETATM	42	H	UNL	1	4.385	-2.420	2.018	1.00	0.00	H
HETATM	43	H	UNL	1	3.313	-2.077	3.383	1.00	0.00	H
HETATM	44	H	UNL	1	3.422	-2.137	-0.360	1.00	0.00	H
HETATM	45	H	UNL	1	1.746	-1.613	-0.528	1.00	0.00	H
HETATM	46	H	UNL	1	3.237	0.331	2.777	1.00	0.00	H
HETATM	47	H	UNL	1	4.920	-0.187	2.957	1.00	0.00	H
HETATM	48	H	UNL	1	3.311	0.271	-0.940	1.00	0.00	H
HETATM	49	H	UNL	1	2.287	0.601	0.459	1.00	0.00	H
HETATM	50	H	UNL	1	-0.382	-0.355	2.137	1.00	0.00	H
HETATM	51	H	UNL	1	-2.220	1.171	2.421	1.00	0.00	H
HETATM	52	H	UNL	1	-3.668	1.125	1.450	1.00	0.00	H
HETATM	53	H	UNL	1	-3.838	-3.413	-2.702	1.00	0.00	H
HETATM	54	H	UNL	1	4.846	3.206	-0.304	1.00	0.00	H
HETATM	55	H	UNL	1	6.424	-0.628	-1.482	1.00	0.00	H
HETATM	56	H	UNL	1	-6.566	-0.268	-0.150	1.00	0.00	H
HETATM	57	H	UNL	1	5.125	4.025	-2.619	1.00	0.00	H
HETATM	58	H	UNL	1	6.700	0.203	-3.794	1.00	0.00	H

```
!ls -alh
```

```
total 295M
drwxr-xr-x 1 root root 4.0K Apr 24 02:52 .
drwxr-xr-x 1 root root 4.0K Apr 24 02:45 ..
-rw-r--r-- 1 root root 271K Apr 24 02:49 3ERK.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:51 5F4R.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:52 5F4R.pdb.1
-rw-r--r-- 1 root root 959K Apr 24 02:49 6CYT.pdb
drwxr-xr-x 4 root root 4.0K Apr 22 13:25 .config
-rw-r--r-- 1 root root 6.6K Apr 24 02:49 DB04542.pdb
-rw-r--r-- 1 root root 5.6K Apr 24 02:49 DB04542.sdf
```

```
-rw-r--r-- 1 root root 25K Apr 24 02:51 docked.sdf
-rw-r--r-- 1 root root 11K Apr 24 02:52 Fostemsavir.pdb
-rw-r--r-- 1 root root 8.0K Apr 24 02:52 Fostemsavir.sdf
-rwxr-xr-x 1 root root 293M Dec 18 21:22 gnina
-rw-r--r-- 1 root root 5.3K Apr 24 02:52 lig.pdb
-rw-r--r-- 1 root root 416K Apr 24 02:52 rec.pdb
drwxr-xr-x 1 root root 4.0K Apr 22 13:25 sample_data
```

```
!./gnina -r rec.pdb -l lig.pdb --autobox_ligand rec.pdb -o docked.sdf --seed 0 --device 0 --verbosit
```



```
gnina v1.1 master:e4cb380+ Built Dec 18 2023.
gnina is based on smina and AutoDock Vina.
Please cite appropriately.
```

```
Commandline: ./gnina -r rec.pdb -l lig.pdb --autobox_ligand rec.pdb -o docked.sdf --seed 0 --dev:
=====
=====
```

```
*** Open Babel Warning in PerceiveBondOrders
Failed to kekulize aromatic bonds in OBMol::PerceiveBondOrders
```

```
=====
*** Open Babel Warning in PerceiveBondOrders
Failed to kekulize aromatic bonds in OBMol::PerceiveBondOrders
```

Weights	Terms
-0.035579	gauss(o=0,_w=0.5,_c=8)
-0.005156	gauss(o=3,_w=2,_c=8)
0.840245	repulsion(o=0,_c=8)
-0.035069	hydrophobic(g=0.5,_b=1.5,_c=8)
-0.587439	non_dir_h_bond(g=-0.7,_b=0,_c=8)
1.923	num_tors_div

```
Using search box with center -17.605,-32.0835,26.846 and size 78.292,89.209,74.364
```

```
Detected 2 CPUs
```

```
Reading input ... done.
```

```
Setting up the scoring function ... done.
```

```
Analyzing the binding site ... done.
```

```
Using random seed: 0
```

```
Performing search ...
```

```
0% 10 20 30 40 50 60 70 80 90 100%
|---|---|---|---|---|---|---|---|---|
```

```
*****
```

```
done.
```

```
Refining results ...
```

```
Total energy after refinement: -13.52535
```

```
Empirical energy after refinement: -13.52772
```

```
Total energy after refinement: -12.49665
```

```
Empirical energy after refinement: -12.49843
```

```
Total energy after refinement: -12.44858
```

```
Empirical energy after refinement: -12.44968
```

```
Total energy after refinement: -12.34549
```

```
Empirical energy after refinement: -12.34322
```

```
Total energy after refinement: -12.40310
```

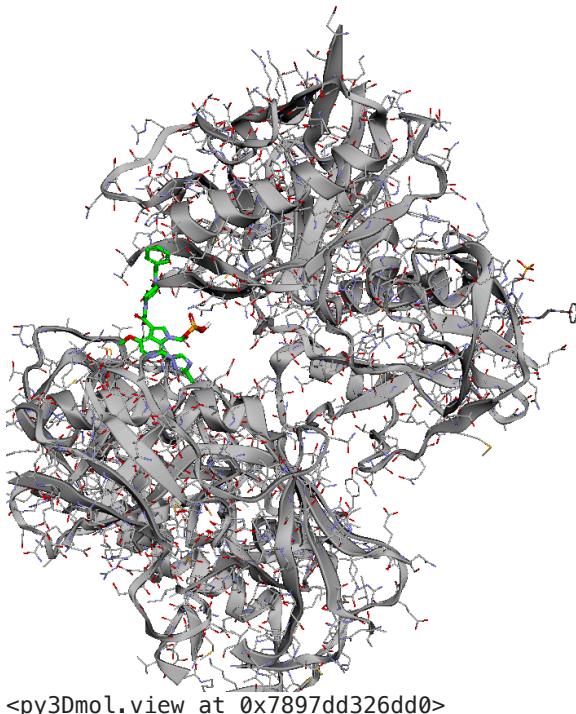
```
Empirical energy after refinement: -12.40795
```

```
Total energy after refinement: -12.22878
```

```

import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})

```



```
!obrms -f lig.pdb docked.sdf
```

```

RMSD lig.pdb: 52.6495
RMSD lig.pdb: 51.1808
RMSD lig.pdb: 43.7758
RMSD lig.pdb: 66.0157
RMSD lig.pdb: 48.512
RMSD lig.pdb: 53.542
RMSD lig.pdb: 30.5009
RMSD lig.pdb: 52.0133
RMSD lig.pdb: 66.9166

```

```
# !cat docked.sdf
```

```

%%bash
for i in {1..10}
do
    obabel Conformer3D_COMPOUND_CID_11319217_${i}.sdf -O Fostemsavir_${i}.pdb -o pdb
    grep UNL Fostemsavir_${i}.pdb > lig_${i}.pdb
done

1 molecule converted

```

```
1 molecule converted
1 molecule converted
1 molecule converted
```

```
!ls -alh
```

```
total 296M
drwxr-xr-x 1 root root 4.0K Apr 24 04:27 .
drwxr-xr-x 1 root root 4.0K Apr 24 02:45 ..
-rw-r--r-- 1 root root 271K Apr 24 02:49 3ERK.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:51 5F4R.pdb
-rw-r--r-- 1 root root 503K Apr 24 02:52 5F4R.pdb.1
-rw-r--r-- 1 root root 959K Apr 24 02:49 6CYT.pdb
drwxr-xr-x 4 root root 4.0K Apr 22 13:25 .config
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_10.sdf
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_1.sdf
-rw-r--r-- 1 root root 8.5K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_2.sdf
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_3.sdf
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_4.sdf
-rw-r--r-- 1 root root 8.8K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_5.sdf
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_6.sdf
-rw-r--r-- 1 root root 8.8K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_7.sdf
-rw-r--r-- 1 root root 8.7K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_8.sdf
-rw-r--r-- 1 root root 8.8K Apr 24 03:46 Conformer3D_COMPOUND_CID_11319217_9.sdf
-rw-r--r-- 1 root root 6.6K Apr 24 02:49 DB04542.pdb
-rw-r--r-- 1 root root 5.6K Apr 24 02:49 DB04542.sdf
-rw-r--r-- 1 root root 0 Apr 24 04:24 docked_{i}.sdf
-rw-r--r-- 1 root root 34K Apr 24 02:56 docked.sdf
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_10.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_1.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_2.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_3.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_4.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_5.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_6.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_7.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_8.pdb
-rw-r--r-- 1 root root 11K Apr 24 04:27 Fostemsavir_9.pdb
-rw-r--r-- 1 root root 11K Apr 24 02:52 Fostemsavir.pdb
-rw-r--r-- 1 root root 8.0K Apr 24 02:52 Fostemsavir.sdf
-rwxr-xr-x 1 root root 293M Dec 18 21:22 gnina
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_10.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_1.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_2.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_3.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_4.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_5.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_6.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_7.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_8.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 04:27 lig_9.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 03:57 lig_{i}.pdb
-rw-r--r-- 1 root root 5.3K Apr 24 02:52 lig.pdb
-rw-r--r-- 1 root root 416K Apr 24 02:52 rec.pdb
drwxr-xr-x 1 root root 4.0K Apr 22 13:25 sample_data
```

```
!./gnina -r rec.pdb -l lig_1.pdb --autobox_ligand rec.pdb -o docked_1.sdf --seed 0 --device 0 --verb
```

```
Empirical energy after refinement: -9.82220
```

Total energy after refinement: -9.60765

Empirical energy after refinement: -9.60041

Total energy after refinement: -9.62671

Empirical energy after refinement: -9.62808

Total energy after refinement: -9.53293

Empirical energy after refinement: -9.53381

Total energy after refinement: -9.55837

Empirical energy after refinement: -9.55598

Total energy after refinement: -9.44071

Empirical energy after refinement: -9.43856

Total energy after refinement: -9.48674

Empirical energy after refinement: -9.48977

Total energy after refinement: -9.44197

Empirical energy after refinement: -9.43716

Total energy after refinement: -9.46487

Empirical energy after refinement: -9.46496

Total energy after refinement: -9.41769

Empirical energy after refinement: -9.41663

done.

mode	affinity   (kcal/mol)	intramol   (kcal/mol)	CNN   pose score	CNN   affinity
1	-7.63	0.95	0.6808	5.617
2	-6.86	0.77	0.3814	5.311
3	-7.02	-1.14	0.3283	4.973
4	-7.90	-0.31	0.3135	5.251
5	-7.23	-0.33	0.3004	5.361
6	-7.69	-0.53	0.2589	5.046
7	-9.22	0.55	0.2237	5.272
8	-7.43	0.24	0.1999	5.066
9	-6.91	-1.31	0.1580	5.151

done.

GPU memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_2.pdb --autobox_ligand rec.pdb -o docked_2.sdf --seed 0 --device 0 --verb
```

```
Empirical energy after refinement: -9.02494
```

Total energy after refinement: -9.33581

Empirical energy after refinement: -9.33670

Total energy after refinement: -9.04043

Empirical energy after refinement: -9.03993

Total energy after refinement: -9.19849

Empirical energy after refinement: -9.19755

Total energy after refinement: -8.99282

Empirical energy after refinement: -8.99321

Total energy after refinement: -9.10916

Empirical energy after refinement: -9.11223

done.

mode	affinity (kcal/mol)	intramol (kcal/mol)	CNN pose score	CNN affinity
1	-7.08	-0.38	0.6888	5.726
2	-6.13	-0.95	0.4177	5.452
3	-6.16	-1.28	0.4175	5.666
4	-7.87	0.52	0.4161	5.957
5	-6.41	-0.95	0.4088	5.607
6	-6.36	0.64	0.3263	5.138
7	-7.52	1.39	0.3218	5.496
8	-6.72	-1.02	0.2405	5.002
9	-8.10	-1.01	0.2352	4.880

done.

GPU memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_3.pdb --autobox_ligand rec.pdb -o docked_3.sdf --seed 0 --device 0 --verb
```

Total energy after refinement: -9.12676  
Empirical energy after refinement: -9.12403  
done.

mode	affinity	intramol	CNN	CNN
	(kcal/mol)	(kcal/mol)	pose score	affinity
1	-7.65	-0.77	0.3883	5.604
2	-7.02	-0.05	0.3794	5.680
3	-7.77	-0.62	0.3703	5.536
4	-6.81	-1.67	0.3114	5.633
5	-7.39	-0.97	0.2844	5.476
6	-7.31	-1.03	0.2698	5.734
7	-6.32	-1.59	0.2246	5.270
8	-6.59	-1.73	0.2043	5.433
9	-7.38	0.21	0.1991	5.422

done.

GPU memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_4.pdb --autobox_ligand rec.pdb -o docked_4.sdf --seed 0 --device 0 --verb
```

24/04/2024, 11:12

2-docking\_small\_molecule\_to\_receptor.ipynb - Colab

o	-0.49	-0.44	0.2128	0.309
7	-7.01	-0.33	0.2710	5.585
8	-6.40	-1.51	0.2635	5.503
9	-6.96	-1.86	0.2324	5.394

done.

GPU memory usage: 1999 MB

!./gnina -r rec.pdb -l lig\_5.pdb --autobox\_ligand rec.pdb -o docked\_5.sdf --seed 0 --device 0 --verb

Total energy after refinement: -10.54988

Empirical energy after refinement: -10.54987

Total energy after refinement: -9.84426

Empirical energy after refinement: -9.84276

Total energy after refinement: -10.55258

Empirical energy after refinement: -10.55760

Total energy after refinement: -10.06669

Empirical energy after refinement: -10.07403

Total energy after refinement: -10.49755

Empirical energy after refinement: -10.49882

Total energy after refinement: -10.22070

Empirical energy after refinement: -10.22560

Total energy after refinement: -10.27356

Empirical energy after refinement: -10.27340

Total energy after refinement: -10.26876

Empirical energy after refinement: -10.26807

Total energy after refinement: -9.50175

Empirical energy after refinement: -9.49744

Total energy after refinement: -9.93533

Empirical energy after refinement: -9.93842

Total energy after refinement: -10.46622

Empirical energy after refinement: -10.46606

Total energy after refinement: -10.26467

Empirical energy after refinement: -10.26855

Total energy after refinement: -10.08068

Empirical energy after refinement: -10.08248

Total energy after refinement: -9.87235

Empirical energy after refinement: -9.87078

done.

mode	affinity (kcal/mol)	intramol (kcal/mol)	CNN pose score	CNN affinity
1	-7.13	-1.00	0.6116	5.773
2	-6.77	-0.28	0.5031	5.722
3	-8.16	1.66	0.3350	6.242
4	-7.15	-1.01	0.3160	5.359
5	-7.51	0.09	0.3045	5.719
6	-7.73	-0.59	0.2962	5.355
7	-7.47	-1.33	0.2662	5.441
8	-8.68	0.40	0.2592	5.271
9	-6.87	-0.79	0.2457	5.414

done.

GPU memory usage: 1999 MB

!./gnina -r rec.pdb -l lig\_6.pdb --autobox\_ligand rec.pdb -o docked\_6.sdf --seed 0 --device 0 --verb

Total energy after refinement: -10.34655  
 Empirical energy after refinement: -10.34917

Total energy after refinement: -11.21687  
 Empirical energy after refinement: -11.21827

Total energy after refinement: -10.58140  
 Empirical energy after refinement: -10.57795

Total energy after refinement: -10.57525  
 Empirical energy after refinement: -10.57361

Total energy after refinement: -10.62153  
 Empirical energy after refinement: -10.61936

Total energy after refinement: -10.26879  
 Empirical energy after refinement: -10.26799

Total energy after refinement: -10.38220  
 Empirical energy after refinement: -10.38218

Total energy after refinement: -10.43906  
 Empirical energy after refinement: -10.44139

Total energy after refinement: -9.92923  
 Empirical energy after refinement: -9.93104

Total energy after refinement: -10.32548  
 Empirical energy after refinement: -10.32526

Total energy after refinement: -10.37916  
 Empirical energy after refinement: -10.37867

Total energy after refinement: -10.30325  
 Empirical energy after refinement: -10.30468

Total energy after refinement: -10.14612  
 Empirical energy after refinement: -10.14734  
 done.

mode	affinity   (kcal/mol)	intramol   (kcal/mol)	CNN pose score	CNN affinity
1	-6.77	-0.84	0.5706	5.297
2	-7.75	0.08	0.5186	5.557
3	-8.38	0.85	0.3096	6.038
4	-7.20	-0.38	0.2942	5.264
5	-7.29	-0.62	0.1893	5.286
6	-7.89	-1.64	0.1788	5.120
7	-7.71	-0.51	0.1412	5.056
8	-7.11	-0.68	0.1291	4.811
9	-7.36	-1.36	0.1206	5.400

done.

GPU memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_7.pdb --autobox_ligand rec.pdb -o docked_7.sdf --seed 0 --device 0 --verb
```

Total energy after refinement: -9.78420  
Empirical energy after refinement: -9.78403

Total energy after refinement: -9.65604  
Empirical energy after refinement: -9.65768

Total energy after refinement: -9.45198  
Empirical energy after refinement: -9.44852

Total energy after refinement: -9.42854  
Empirical energy after refinement: -9.42454

Total energy after refinement: -9.22738  
Empirical energy after refinement: -9.22646

Total energy after refinement: -9.40164  
Empirical energy after refinement: -9.40125

Total energy after refinement: -9.26456  
Empirical energy after refinement: -9.26311

Total energy after refinement: -9.03490  
Empirical energy after refinement: -9.03480

Total energy after refinement: -9.00558  
Empirical energy after refinement: -9.00750  
done.

mode	affinity	intramol	CNN	CNN
	(kcal/mol)	(kcal/mol)	pose score	affinity
1	-6.67	-0.58	0.5199	5.369
2	-6.14	-0.85	0.4651	5.735
3	-7.27	-0.03	0.3943	5.439
4	-6.78	-1.31	0.3828	5.485
5	-6.77	-1.50	0.3483	5.579
6	-7.47	-1.41	0.3330	5.683
7	-6.98	-0.58	0.3290	5.462
8	-6.16	-1.12	0.3100	5.640
9	-6.42	-0.26	0.2779	5.422

done.

GPU memory usage: 1999 MB

!./gnina -r rec.pdb -l lig\_8.pdb --autobox\_ligand rec.pdb -o docked\_8.sdf --seed 0 --device 0 --verb

```
total energy after refinement: -8.980/0
Empirical energy after refinement: -8.98975
```

```
Total energy after refinement: -9.03682
Empirical energy after refinement: -9.03147
```

```
Total energy after refinement: -9.18828
Empirical energy after refinement: -9.18943
```

```
Total energy after refinement: -9.08840
Empirical energy after refinement: -9.09269
```

```
Total energy after refinement: -8.87274
Empirical energy after refinement: -8.87210
done.
```

mode	affinity	intramol	CNN	CNN
	(kcal/mol)	(kcal/mol)	pose score	affinity
1	-6.64	-0.15	0.6217	5.564
2	-6.93	-0.55	0.5749	5.977
3	-6.83	0.28	0.5246	5.331
4	-6.24	-1.30	0.4248	5.672
5	-6.19	-0.84	0.3763	5.596
6	-6.70	-1.08	0.3716	5.610
7	-6.77	-1.16	0.3608	5.520
8	-7.50	-0.93	0.3561	5.385
9	-6.73	-1.53	0.3372	5.735

done.

GPU memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_9.pdb --autobox_ligand rec.pdb -o docked_9.sdf --seed 0 --device 0 --verb
```

total energy after refinement: -9.65890  
 Empirical energy after refinement: -9.64155  
 done.

mode	affinity	intramol	CNN	CNN
	(kcal/mol)	(kcal/mol)	pose score	affinity
1	-7.49	-1.27	0.5215	5.908
2	-6.87	-1.52	0.4484	5.796
3	-7.17	-0.74	0.4221	5.630
4	-6.53	-0.86	0.4062	5.499
5	-6.57	-1.13	0.3876	5.588
6	-7.55	-1.10	0.3567	5.518
7	-6.76	-0.81	0.3124	5.299
8	-6.73	-1.25	0.2013	5.458
9	-6.71	-1.27	0.1938	5.468

done.

GPII memory usage: 1999 MB

```
!./gnina -r rec.pdb -l lig_10.pdb --autobox_ligand rec.pdb -o docked_10.sdf --seed 0 --device 0 --ve
```

```
0.840245      repulsion(o=0,_c=8)
-0.035069     hydrophobic(g=0.5,_b=1.5,_c=8)
-0.587439     non_dir_h_bond(g=-0.7,_b=0,_c=8)
1.923         num_tors_div
```

Using search box with center -17.605,-32.0835,26.846 and size 78.292,89.209,74.364

Detected 2 CPUs

Reading input ... done.

Setting up the scoring function ... done.

Analyzing the binding site ... done.

Using random seed: 0

Performing search ...

```
0%   10   20   30   40   50   60   70   80   90   100%
|---|---|---|---|---|---|---|---|---|---|
```

```
*****
```

done.

Refining results ...

Total energy after refinement: -12.81862

Empirical energy after refinement: -12.81992

Total energy after refinement: -12.43734

Empirical energy after refinement: -12.43077

Total energy after refinement: -12.51578

Empirical energy after refinement: -12.51323

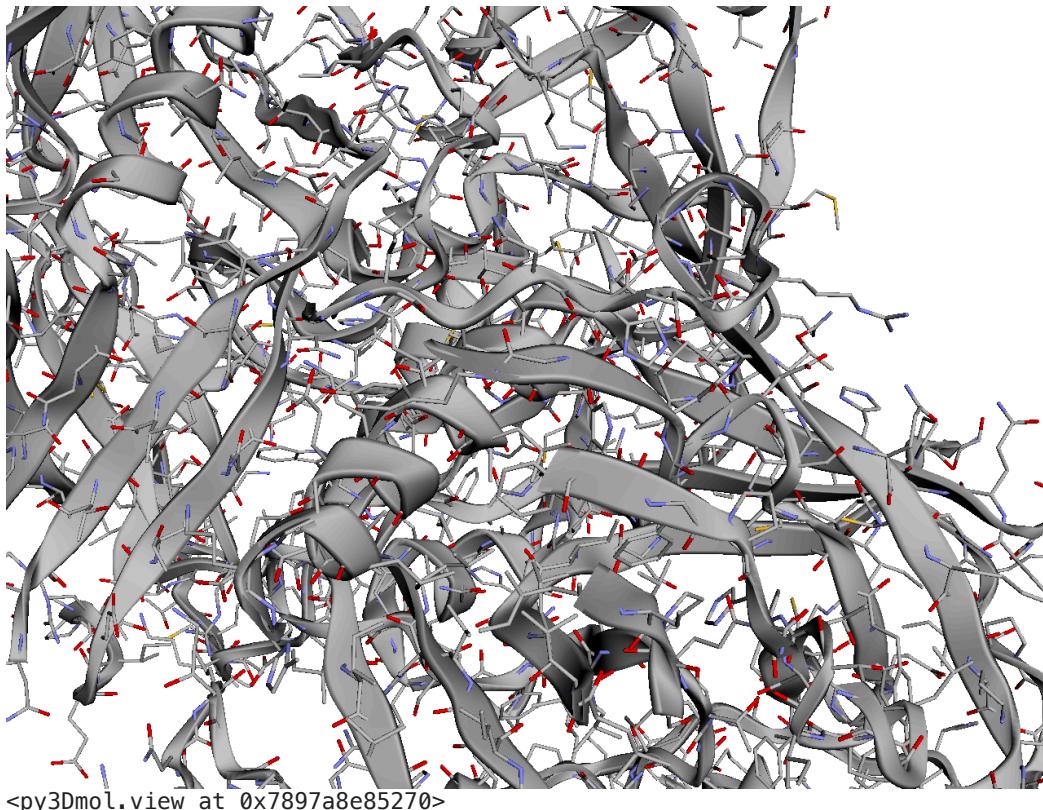
Total energy after refinement: -12.51682

Empirical energy after refinement: -12.52210

Total energy after refinement: -11.70398  
Empirical energy after refinement: -11.70296

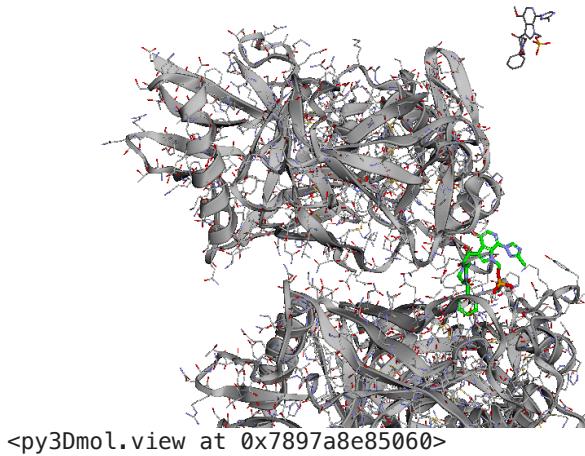
Total energy after refinement: -11.70398  
Empirical energy after refinement: -11.70296

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_1.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_1.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



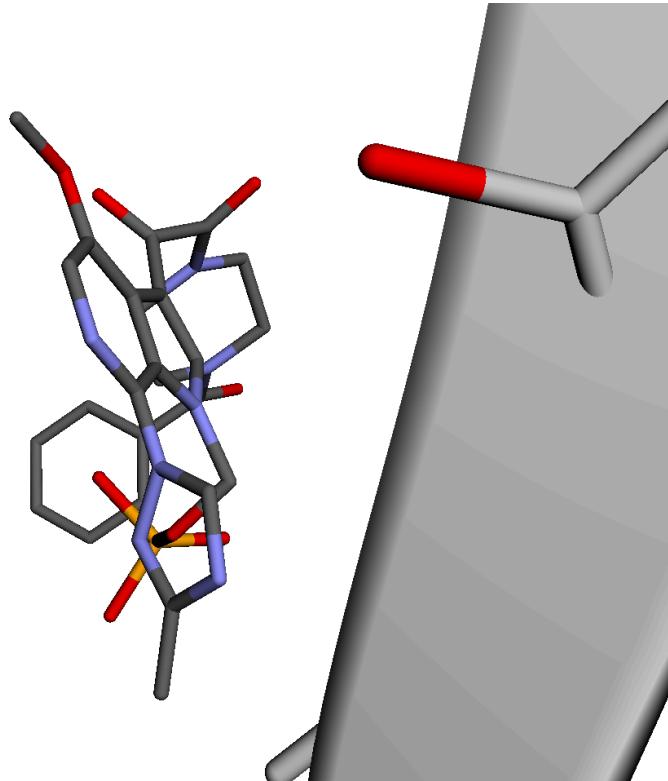
<py3Dmol.view at 0x7897a8e85270>

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_2.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_2.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



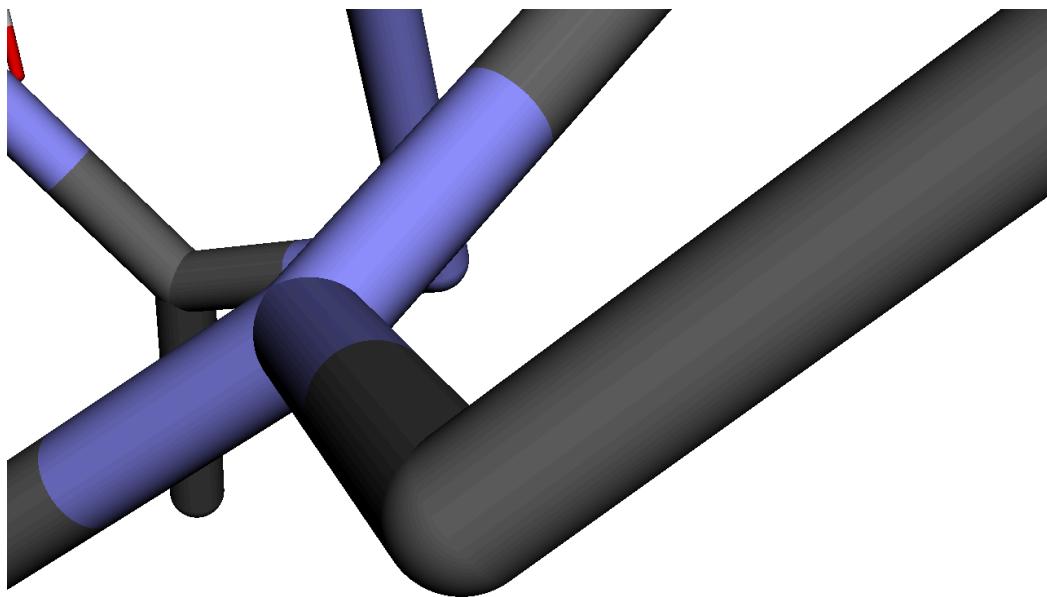
```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_3.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_3.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_4.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_4.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



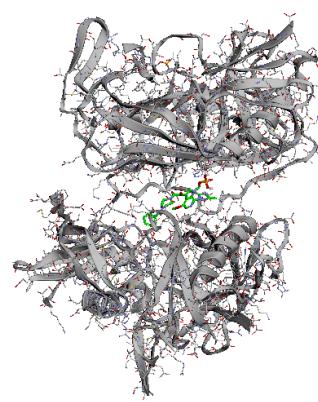
<py3Dmol.view at 0x7897a8e84280>

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_5.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_5.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



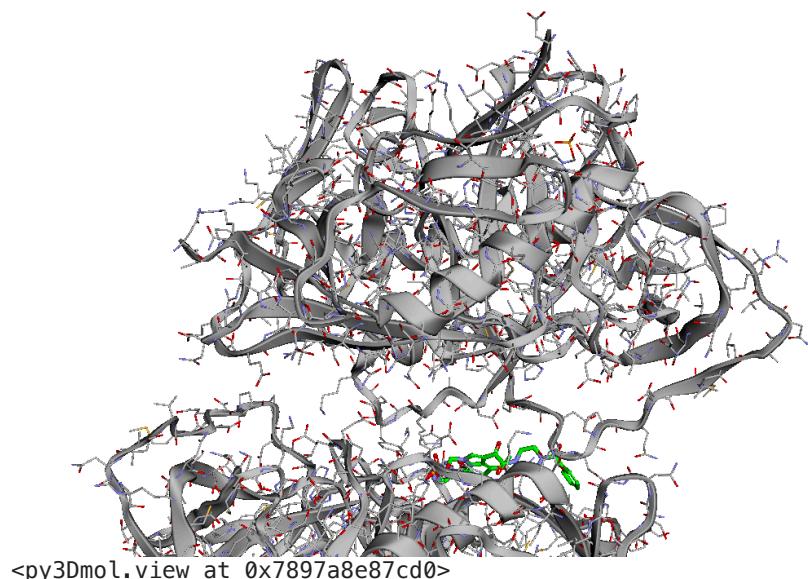
```
<py3Dmol.view at 0x7897a8e84220>
```

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_6.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_6.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



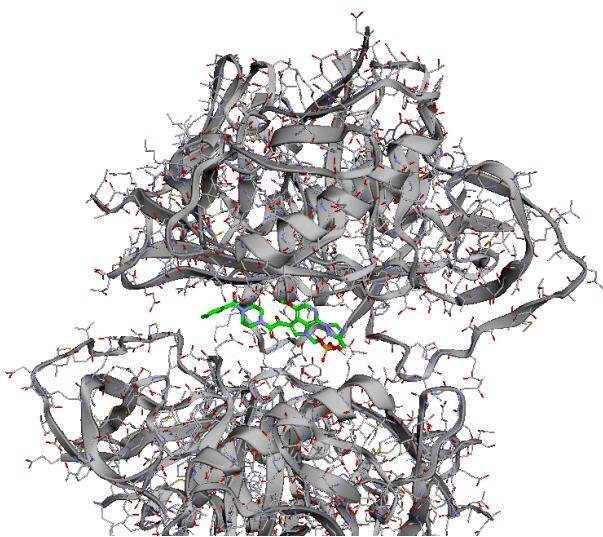
```
<py3Dmol.view at 0x7897a8e868f0>
```

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_7.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_7.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



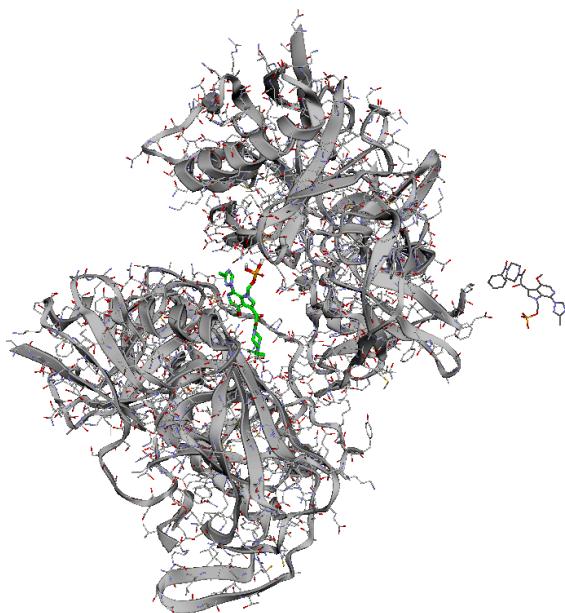
<py3Dmol.view at 0x7897a8e87cd0>

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_8.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_8.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



<py3Dmol.view at 0x7897a8e846a0>

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{},'stick':{'radius':.1}})
v.addModel(open('lig_9.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_9.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```



<py3Dmol.view at 0x7897a8e85210>

```
import py3Dmol
v = py3Dmol.view()
v.addModel(open('rec.pdb').read())
v.setStyle({'cartoon':{}},{'stick':{'radius':.1}})
v.addModel(open('lig_10.pdb').read())
v.setStyle({'model':1},{'stick':{'colorscheme':'dimgrayCarbon','radius':.125}})
v.addModelsAsFrames(open('docked_10.sdf').read())
v.setStyle({'model':2},{'stick':{'colorscheme':'greenCarbon'}})
v.zoomTo({'model':1})
v.rotate(90)
v.animate({'interval':2000})
```