COMPUTATIONAL DATA in Supplementary Information

1. *N*-myristoyl Transferase (PDB: 1IYL)

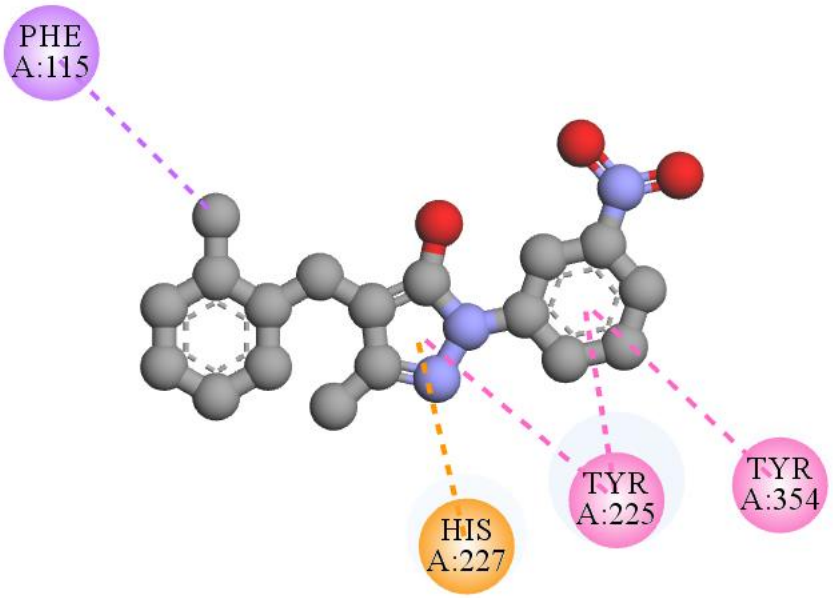
Grid box volume – Autodock Vina

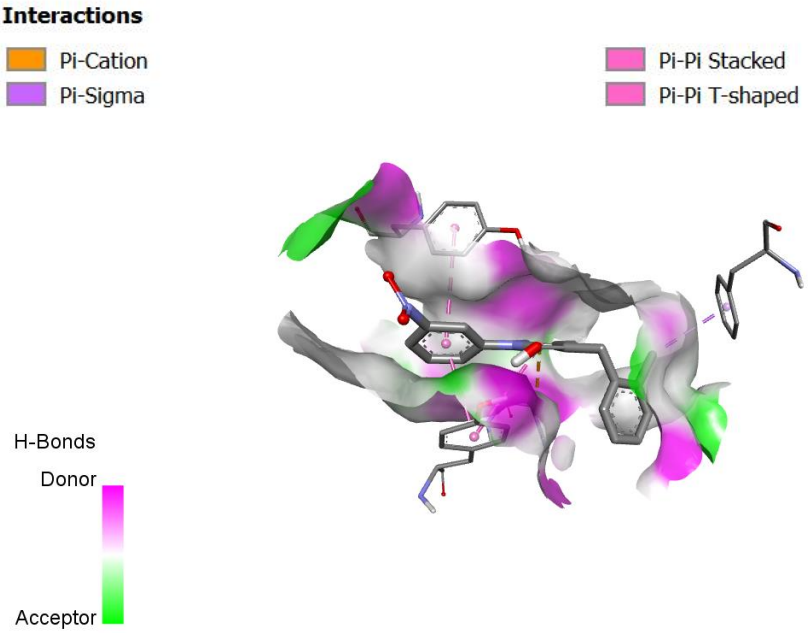
```
receptor = 1iylF.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 12.6146
center_y = 47.7652
center_z = -0.440754

size_x = 25
size_y = 25
size_z = 25

energy_range = 4

exhaustiveness = 8
```

Config.txt File

1.1. Compound 4a

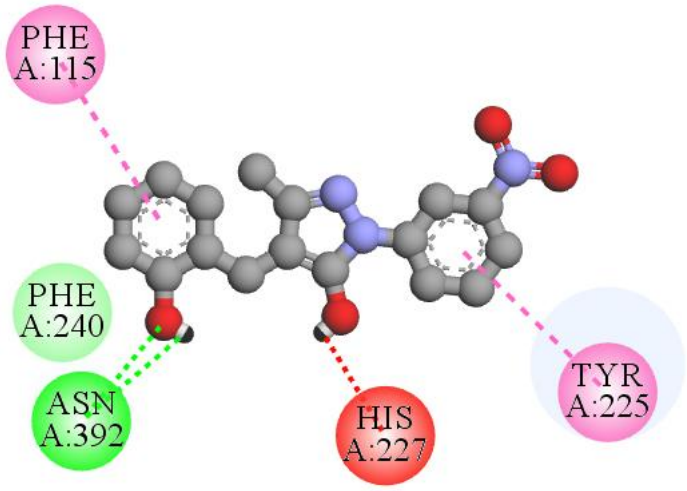
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1981336496
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.4      0.000      0.000
   2         -9.3      3.755      7.467
   3         -9.3      2.174      3.417
   4         -9.1      1.661      1.930
   5         -9.1      1.266      1.778
   6         -9.1      4.364      7.612
   7         -8.9      2.058      3.239
   8         -8.7      3.808      8.159
   9         -8.6      3.653      5.592
Writing output ... done.
```


PHE
A:115
HIS
A:227
TYR
A:225
TYR
A:354


Interactions
Pi-Cation
Pi-Sigma
Pi-Pi Stacked
Pi-Pi T-shaped
H-Bonds
Donor
Acceptor

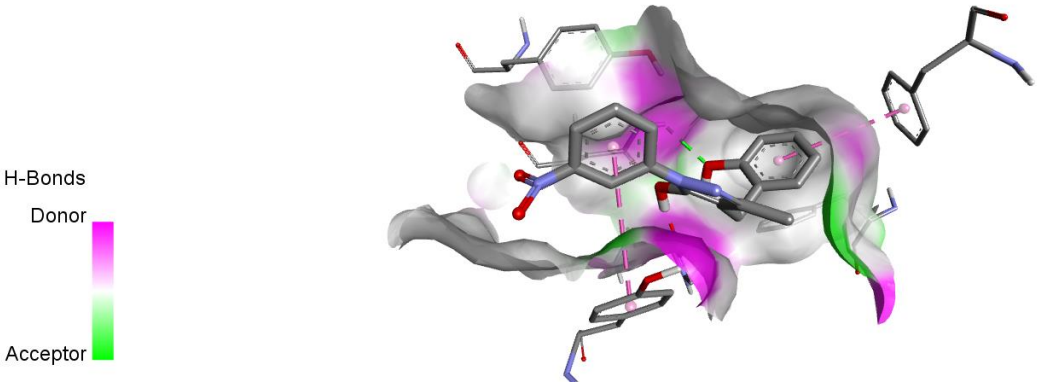
1.2. Compound 4h

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -215951584
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.4      0.000      0.000
   2         -9.4      2.292      3.841
   3         -9.1      3.586      7.436
   4         -9.0      2.997      7.906
   5         -9.0      4.471      8.044
   6         -9.0      2.195      3.170
   7         -9.0      3.279      7.404
   8         -8.6      2.397      3.087
   9         -8.5      3.543      7.807
Writing output ... done.
```



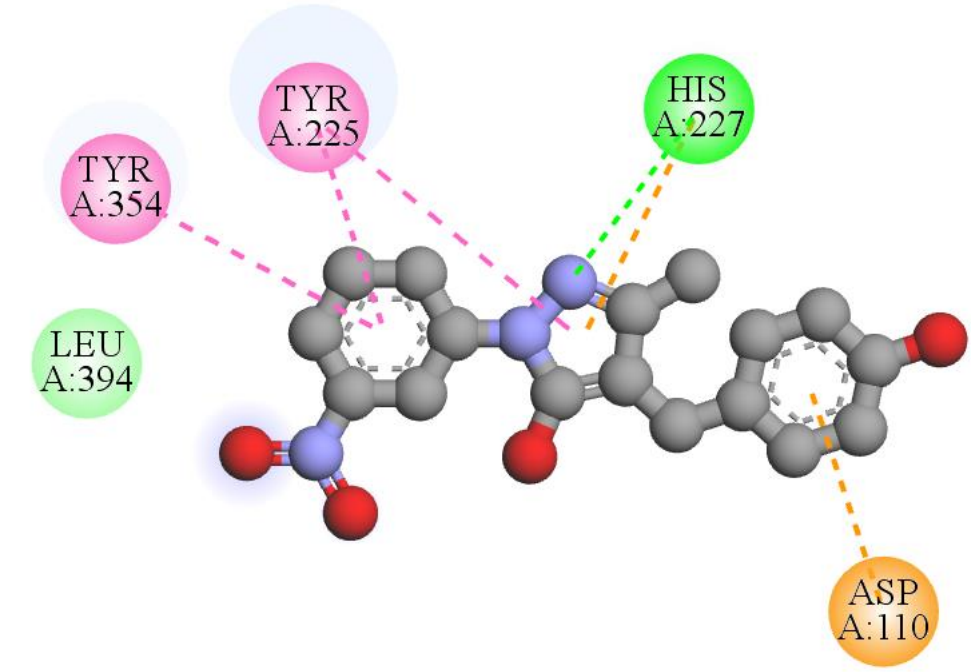
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Pi Stacked
- Pi-Pi T-shaped



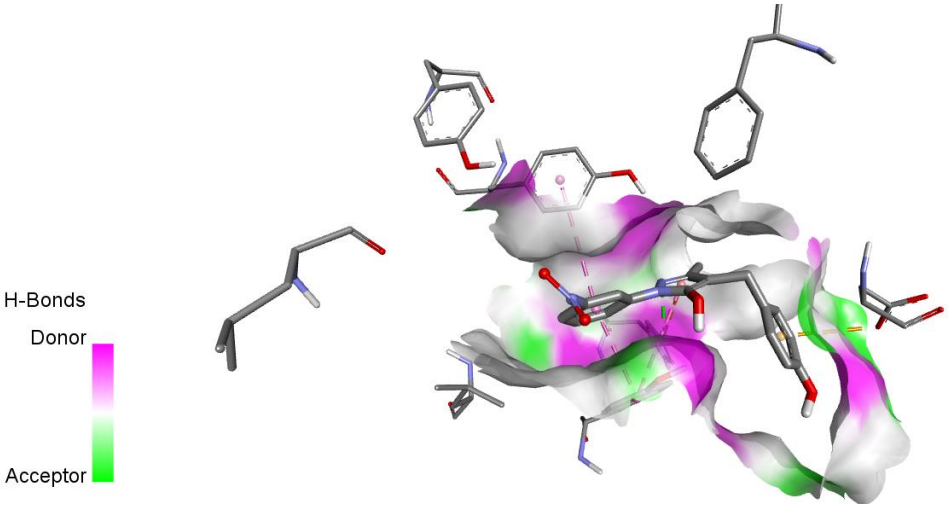
1.3. Compound 4i

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1180915360
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.3      0.000      0.000
   2         -9.1      2.594      7.746
   3         -9.1      5.608      8.946
   4         -9.0      3.920      7.963
   5         -9.0      1.649      2.342
   6         -9.0      5.133      8.262
   7         -8.8      5.635      8.858
   8         -8.7      4.707      8.019
   9         -8.6      5.608      7.874
Writing output ... done.
```



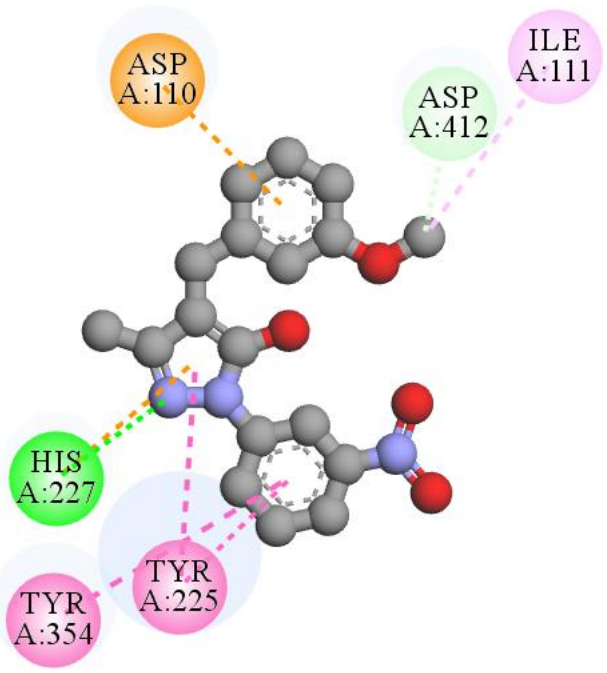
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Pi Stacked
- Pi-Pi T-shaped



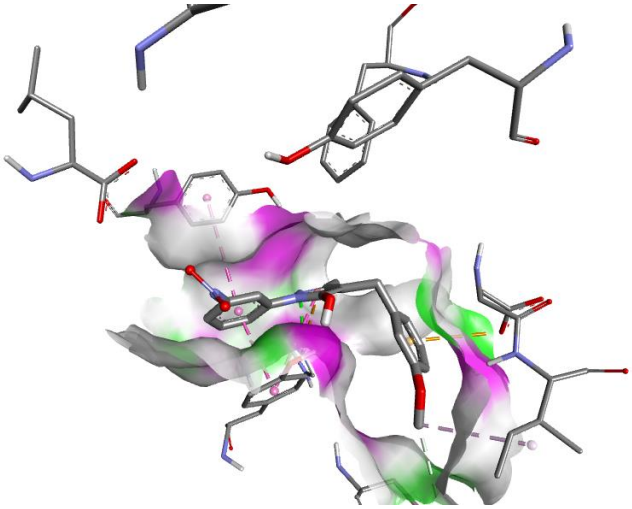
1.4. Compound 4l

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -628191640
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.4      0.000      0.000
   2         -9.3      1.155      1.665
   3         -9.2      2.291      7.390
   4         -9.1      1.753      2.342
   5         -8.9      4.324      8.047
   6         -8.8      1.817      2.445
   7         -8.8      1.540      2.003
   8         -8.7      3.819      8.349
   9         -8.5      2.426      7.346
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl



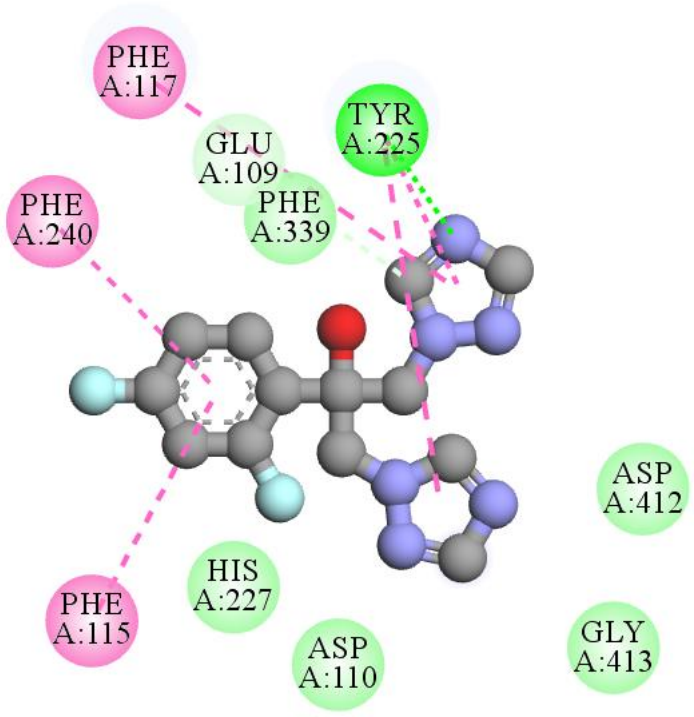
H-Bonds

Donor

Acceptor

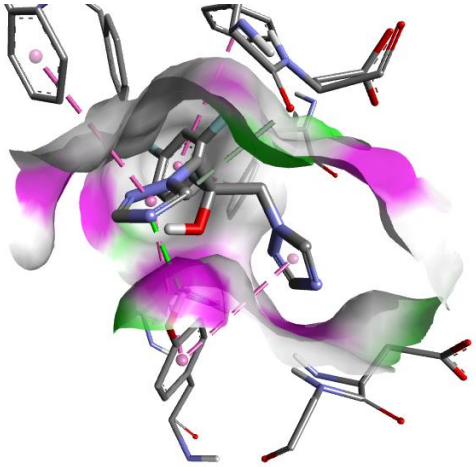
1.5. Fluconazole (Flu)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -155065680
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.9      0.000      0.000
   2         -7.8      1.098      3.969
   3         -7.8      2.173      2.881
   4         -7.4      1.630      4.344
   5         -7.3      5.301      7.018
   6         -7.3      6.035      8.218
   7         -7.2      6.145      8.274
   8         -7.0      5.798      8.368
   9         -7.0      8.894      9.729
Writing output ... done.
```



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Pi Stacked
- Pi-Pi T-shaped



H-Bonds

Donor

Acceptor

2. ***Sortase A (PDB: 2MLM)***

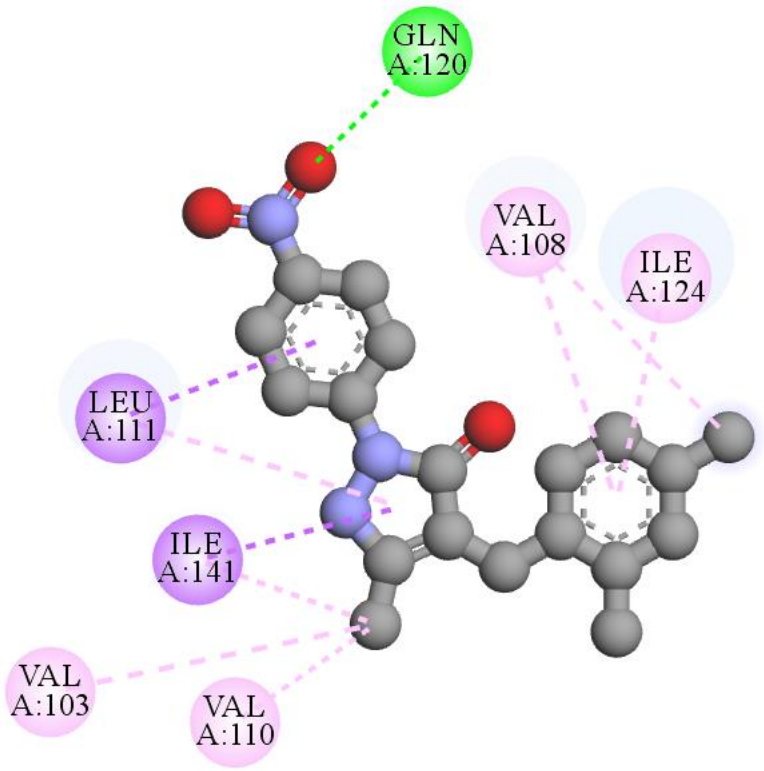
Grid box volume – Autodock Vina

```
receptor = 2mlmB.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 25.1894
center_y = 17.8404
center_z = 10.6867

size_x = 25
size_y = 25
size_z = 25

energy_range = 4

exhaustiveness = 8
```

Config.txt File

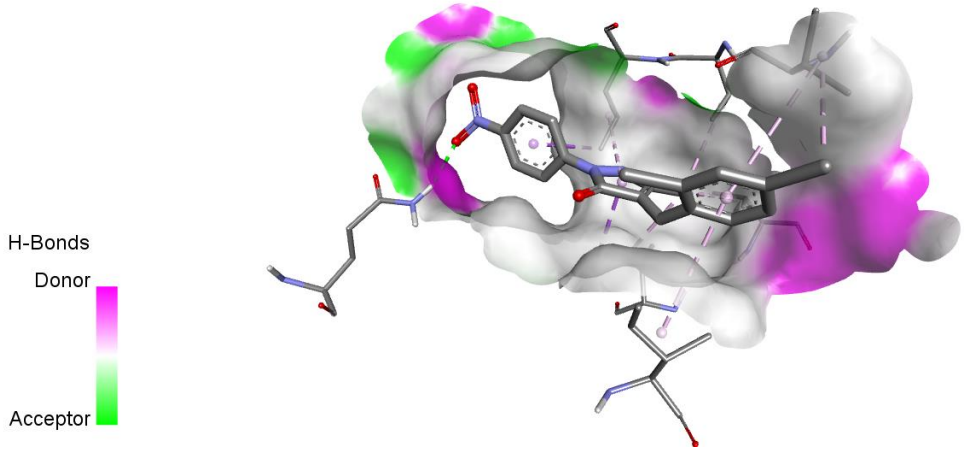
2.1. Compound 3d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 838361216
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.8      0.000      0.000
   2         -7.5      6.356     10.783
   3         -7.3      1.936      2.579
   4         -7.2      5.629      6.627
   5         -7.1     10.188     14.632
   6         -6.9      9.903     14.255
   7         -6.8      5.866     10.199
   8         -6.7      5.122      7.229
   9         -6.7      2.179      3.003
Writing output ... done.
```



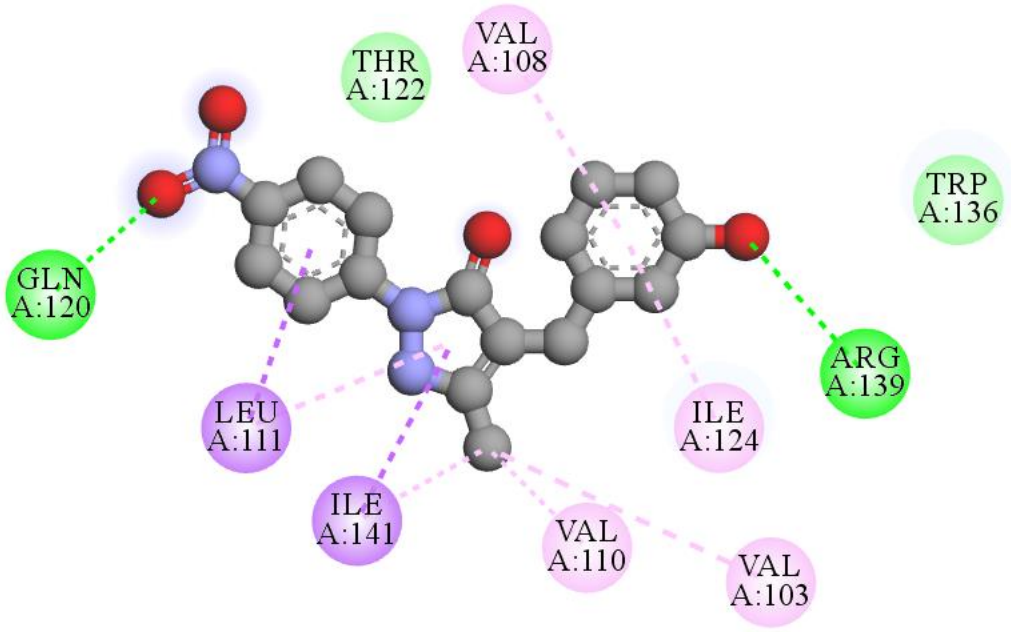
Interactions

Conventional Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl



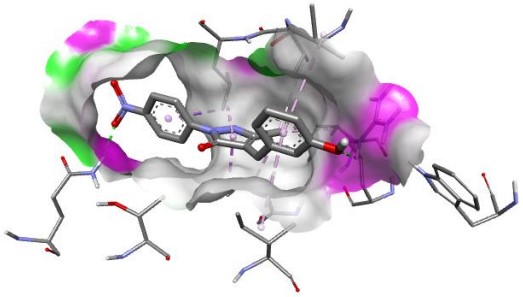
2.2. Compound 3m

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -8089024
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.0      0.000      0.000
   2         -7.4      2.191      8.610
   3         -7.3      5.136     10.587
   4         -7.2      9.309     14.847
   5         -7.0      1.315      2.108
   6         -7.0      2.152      3.386
   7         -6.9      2.786      3.536
   8         -6.9      2.100      8.601
   9         -6.8      9.848     14.792
Writing output ... done.
```



Interactions

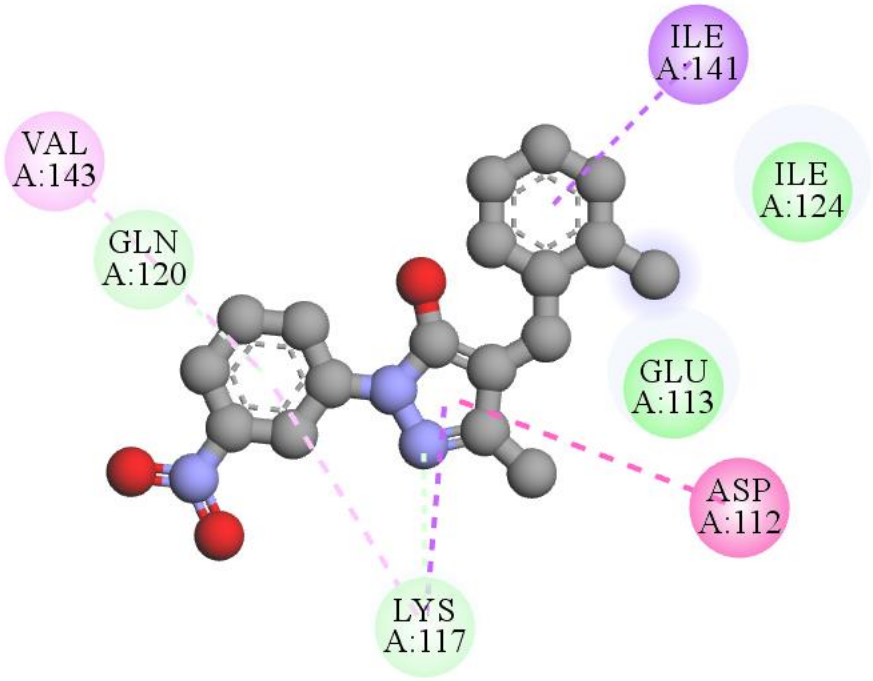
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl



H-Bonds
Donor
Acceptor

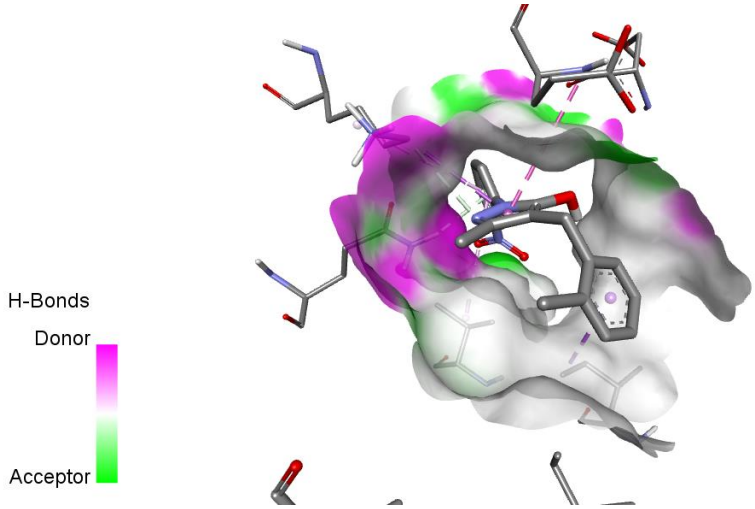
2.3. Compound 4a

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1324194440
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -7.2      4.150      6.036
   3         -7.1     14.761     18.681
   4         -7.0      8.974     12.750
   5         -6.9      2.398      3.374
   6         -6.8      3.363      7.186
   7         -6.6      5.127      7.044
   8         -6.5      5.225      7.310
   9         -6.5      3.802      5.386
Writing output ... done.
```



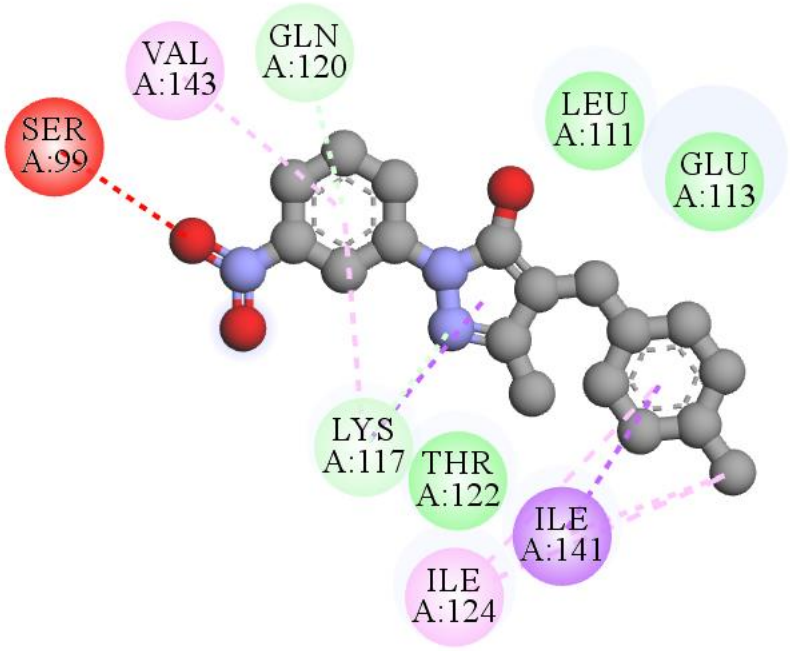
Interactions

- van der Waals
- Carbon Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



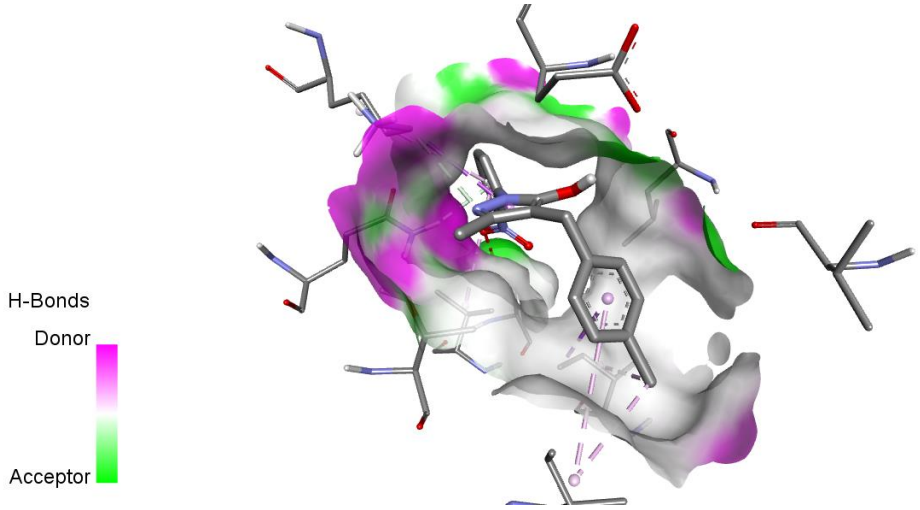
2.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1394022408
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.5      0.000      0.000
   2         -7.2      2.025      2.366
   3         -7.2      4.690      6.690
   4         -7.1      4.441      6.271
   5         -7.1     14.506     18.457
   6         -7.1      3.999      7.350
   7         -6.8      3.586      6.808
   8         -6.8      8.872     12.634
   9         -6.8      4.656      7.080
Writing output ... done.
```



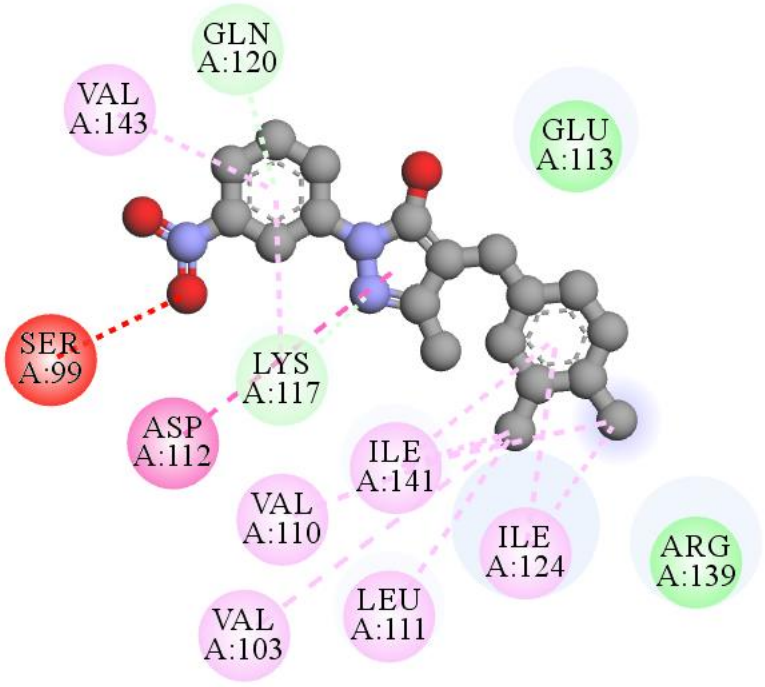
Interactions

- van der Waals
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Alkyl
- Pi-Alkyl



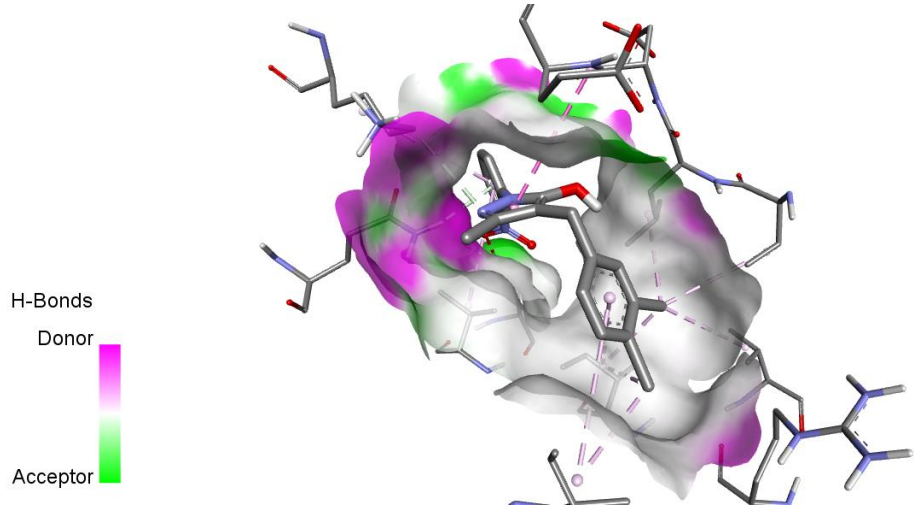
2.5. Compound 4d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1896630904
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.8      0.000      0.000
   2         -7.5      3.493      6.752
   3         -7.4      4.520      8.124
   4         -7.3     14.269     18.215
   5         -7.3      4.403      6.150
   6         -6.9      8.605     12.319
   7         -6.9      5.254      7.434
   8         -6.9      3.212      4.583
   9         -6.8      3.767      6.020
Writing output ... done.
```



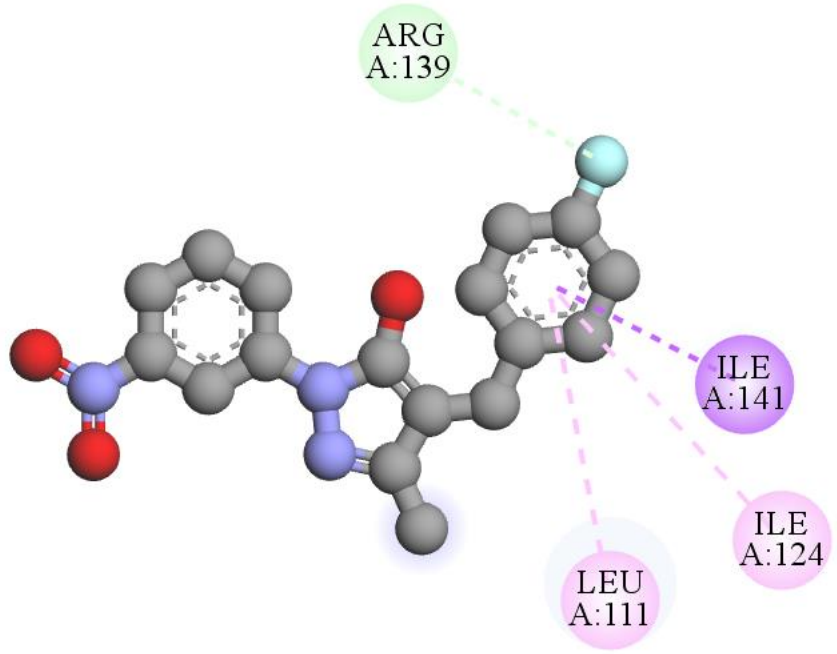
Interactions

- van der Waals
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Donor Hydrogen Bond
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



2.6. Compound 4g

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1319015384
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.4      1.844      2.349
   3         -7.4      3.383      4.898
   4         -7.4     13.296     15.832
   5         -7.3      4.210      6.988
   6         -7.2      4.445      5.662
   7         -7.2      3.548      5.470
   8         -7.0      7.644     10.230
   9         -6.9      4.223      8.033
Writing output ... done.
```

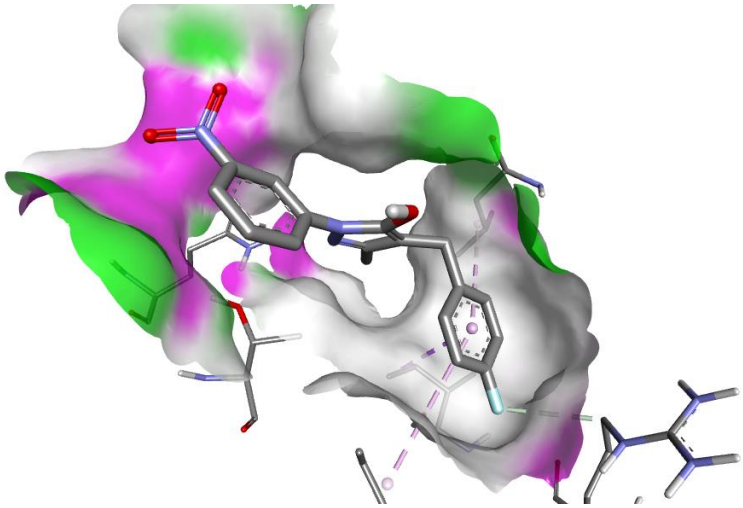


Interactions

Carbon Hydrogen Bond

Pi-Alkyl

Pi-Sigma



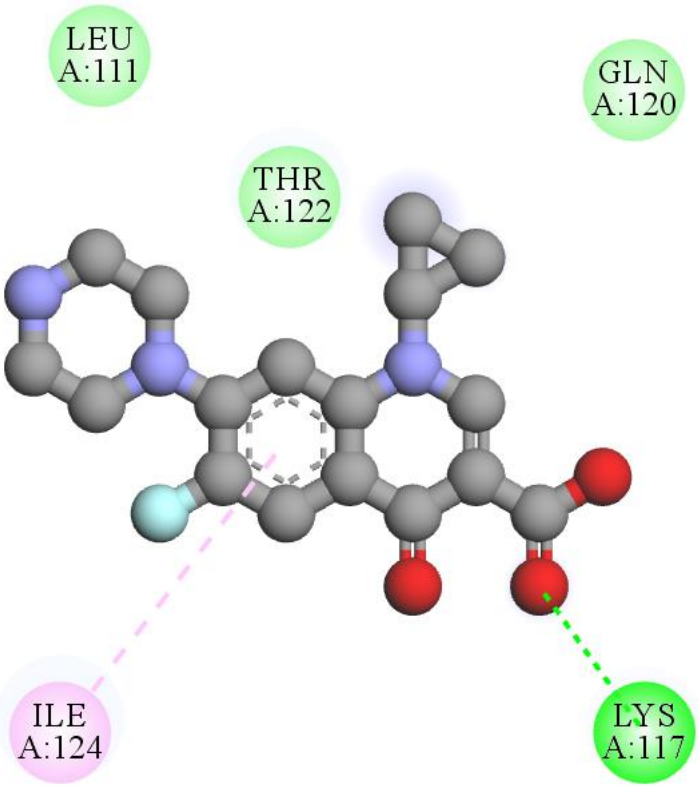
H-Bonds

Donor

Acceptor

2.7. Ciprofloxacin (Cipro)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -12741124
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.8      0.000      0.000
   2         -6.7      3.092      6.526
   3         -6.7      1.985      3.751
   4         -6.6      3.511      5.980
   5         -6.6      3.655      6.091
   6         -6.4      4.167      6.730
   7         -6.3      2.680      5.968
   8         -6.2      3.855      6.639
   9         -6.2      2.518      3.921
Writing output ... done.
```

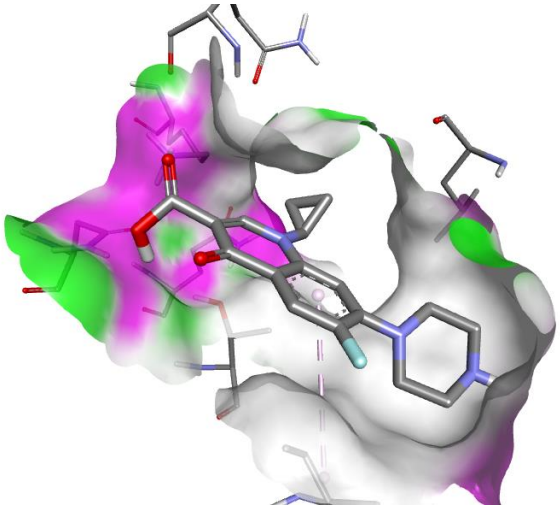


Interactions

van der Waals

Pi-Alkyl

Conventional Hydrogen Bond



H-Bonds

Donor

Acceptor

3. ***Dihydrofolate Reductase – Bacteria (PDB: 3FYV)***

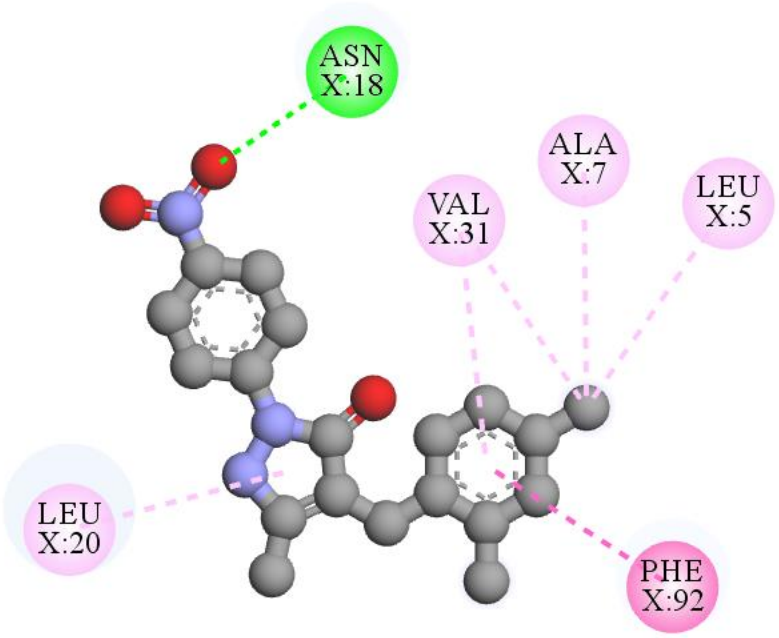
Grid box volume – Autodock Vina

```
receptor = 3fyvB.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 23.972
center_y = 17.083
center_z = 41.528

size_x = 30
size_y = 35
size_z = 30

energy_range = 4

exhaustiveness = 8
```

Config.txt File

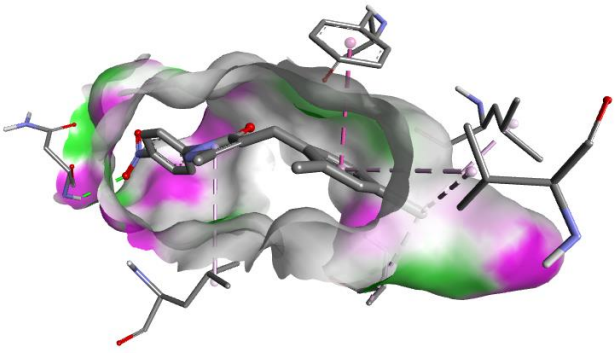
3.1. Compound 3d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 316126712
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.5      0.000      0.000
   2         -9.0      1.968      3.084
   3         -8.9      4.179      8.205
   4         -8.9      2.219      2.978
   5         -8.6      2.328      4.560
   6         -8.5      1.954      3.035
   7         -8.2      2.618      3.950
   8         -8.2      4.820      8.653
   9         -8.1      3.449      5.210
Writing output ... done.
```



Interactions

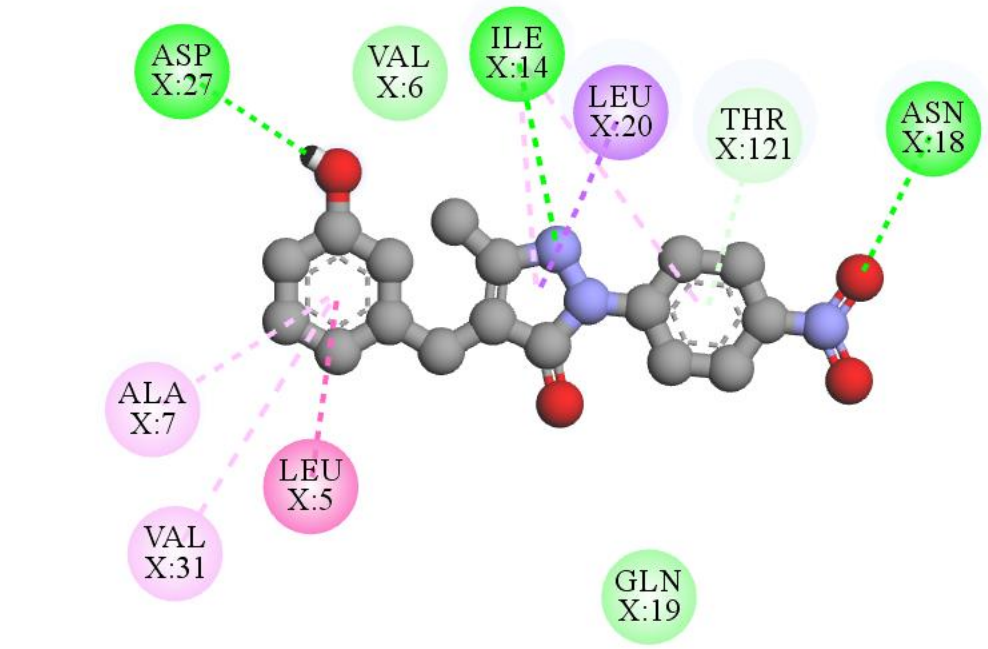
Conventional Hydrogen Bond
Pi-Pi Stacked
Alkyl
Pi-Alkyl



H-Bonds
Donor
Acceptor

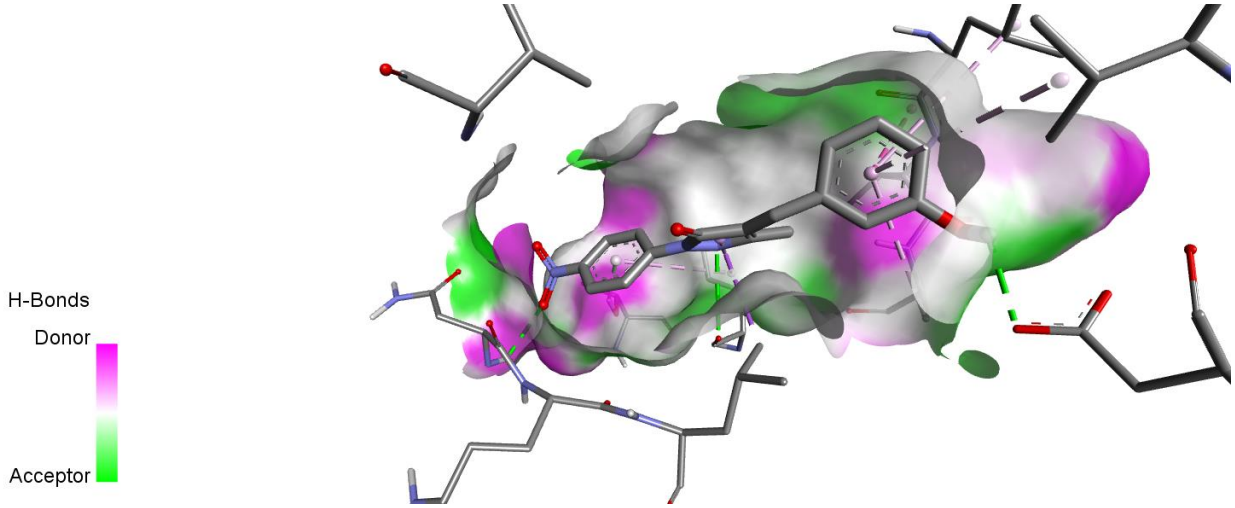
3.2. Compound 3m

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 829764120
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.7      0.000      0.000
   2         -9.3      1.724      2.421
   3         -9.2      1.855      2.645
   4         -9.0      1.903      2.360
   5         -8.8      2.645      4.200
   6         -8.8      2.146      3.068
   7         -8.5      3.198      5.065
   8         -8.4      5.739     10.633
   9         -8.4      3.300      9.258
Writing output ... done.
```



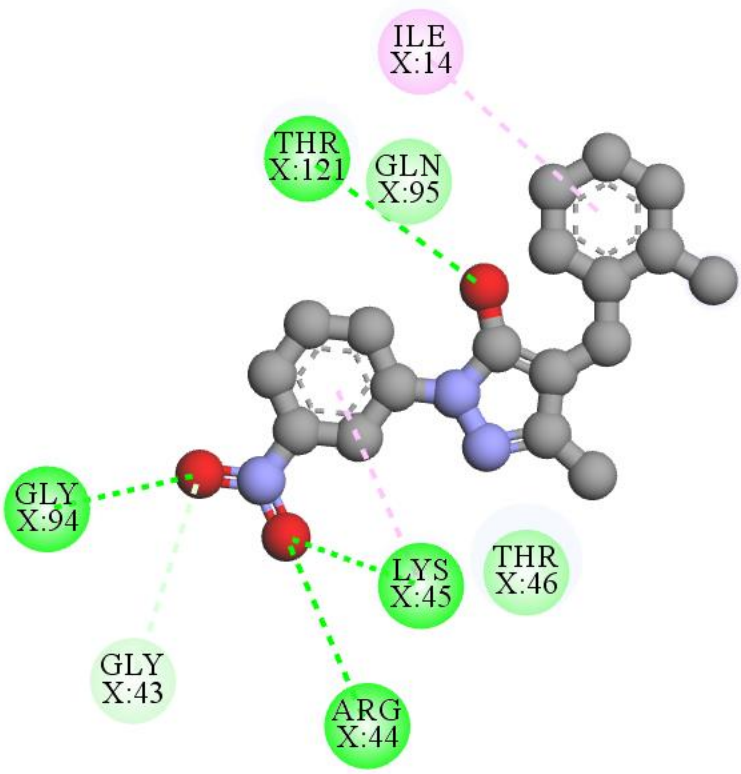
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



3.3. Compound 4a

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2130331144
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.7      0.000      0.000
   2         -9.6      1.502      1.837
   3         -9.0      3.641      5.710
   4         -8.9      3.549      5.694
   5         -8.6      3.478      5.661
   6         -8.3      3.784      5.777
   7         -8.3      4.098      7.589
   8         -8.2      4.474      7.975
   9         -7.9      3.698      5.763
Writing output ... done.
```



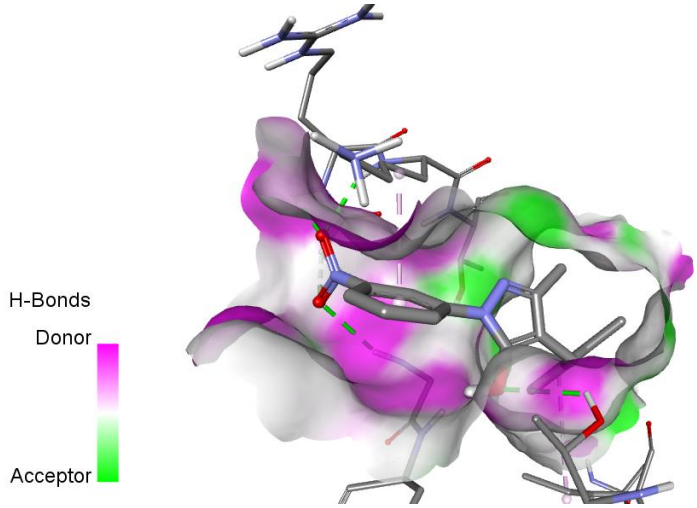
Interactions

van der Waals

Conventional Hydrogen Bond

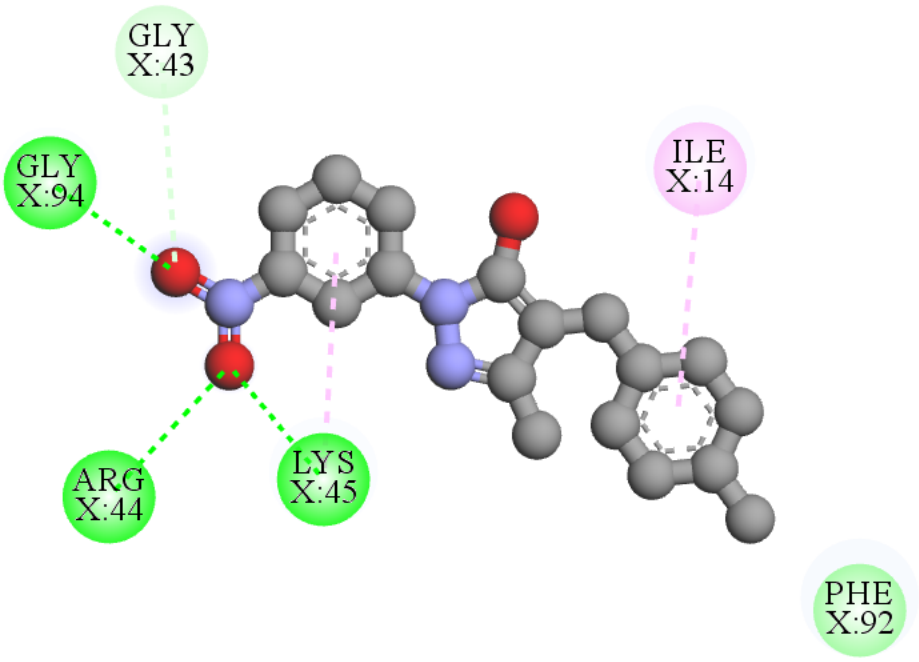
Carbon Hydrogen Bond

Pi-Alkyl



3.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1559833088
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.6      0.000      0.000
   2         -9.2      3.306      5.299
   3         -9.1      1.880      2.579
   4         -8.7      3.403      5.044
   5         -8.6      2.956      5.175
   6         -8.6      4.762      8.261
   7         -8.5      3.414      5.741
   8         -8.2      4.941      8.182
   9         -8.0      5.315      8.447
Writing output ... done.
```



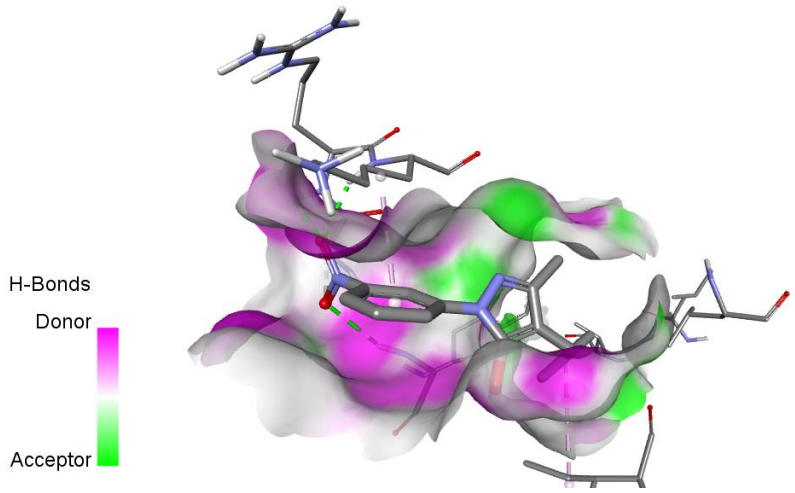
Interactions

van der Waals

Conventional Hydrogen Bond

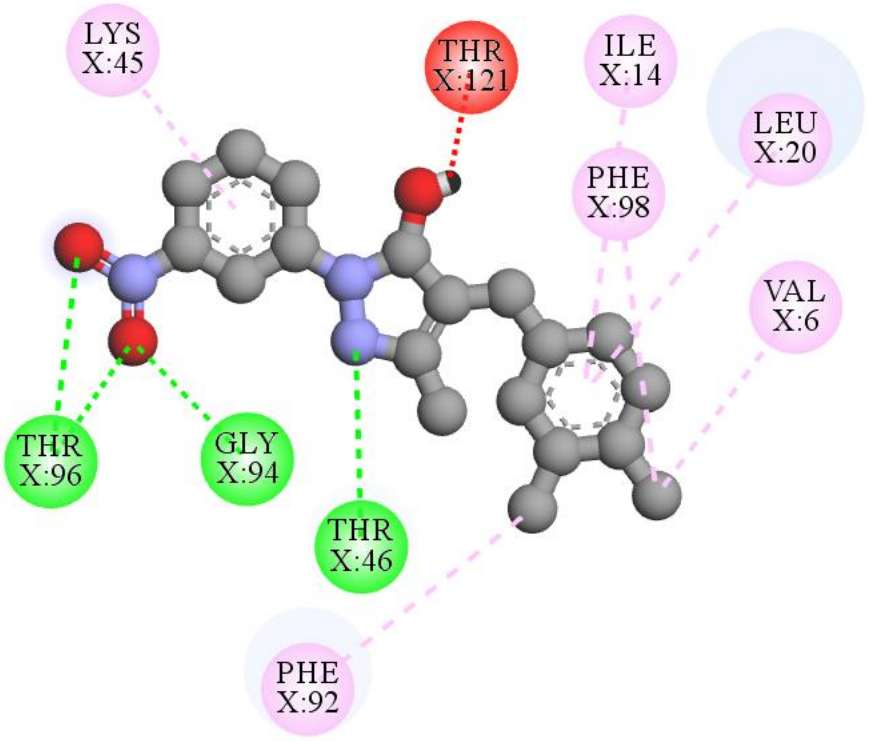
Carbon Hydrogen Bond

Pi-Alkyl



3.5. Compound 4d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1383937920
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.9      0.000      0.000
   2         -9.1      2.941      4.373
   3         -8.9      2.686      3.874
   4         -8.6      4.676      8.145
   5         -8.4      2.628      4.112
   6         -8.3      5.325      8.911
   7         -8.2      4.450      7.694
   8         -8.2      4.363      7.855
   9         -7.8      6.149      8.364
Writing output ... done.
```



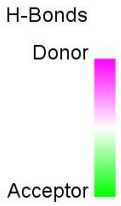
Interactions

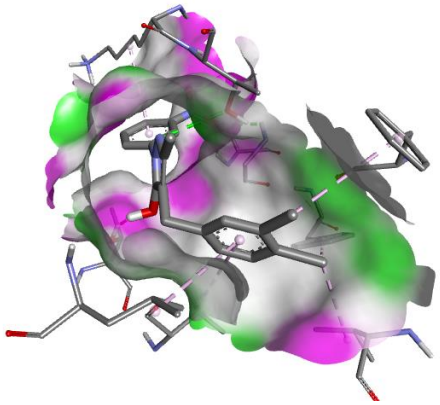
Conventional Hydrogen Bond

Unfavorable Donor-Donor

Alkyl

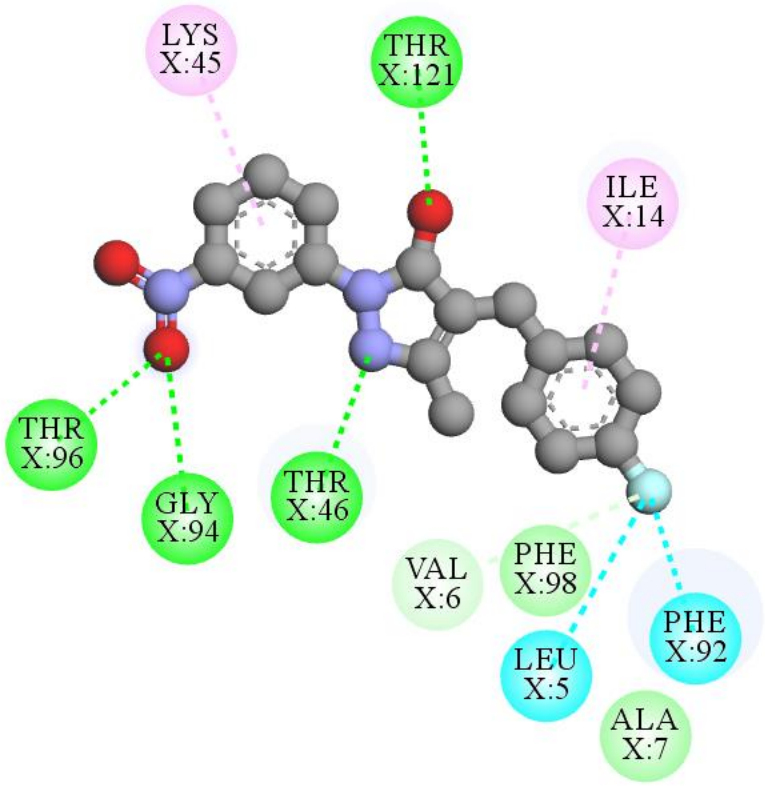
Pi-Alkyl





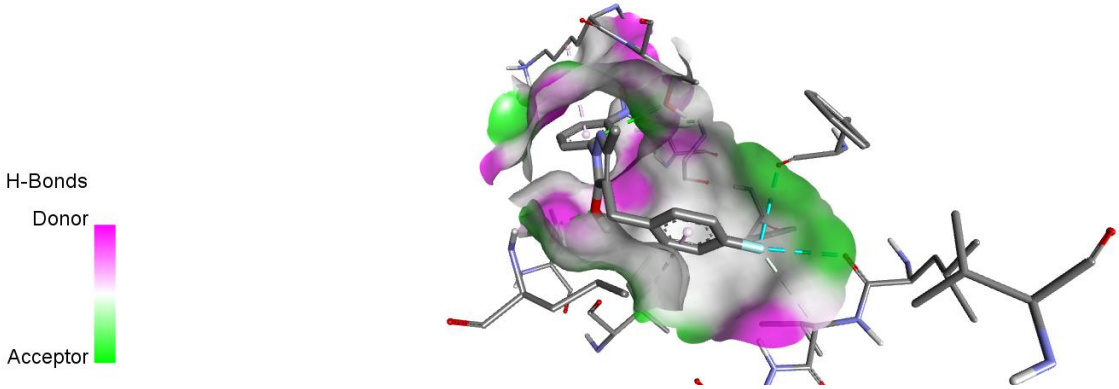
3.6. Compound 4g

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1279408636
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.7      0.000      0.000
   2         -9.2      3.030      4.691
   3         -9.0      3.143      5.004
   4         -9.0      2.537      3.145
   5         -9.0      1.845      2.408
   6         -8.6      4.309      7.938
   7         -8.5      2.793      4.392
   8         -8.3      3.783      7.462
   9         -8.2      4.759      8.215
Writing output ... done.
```



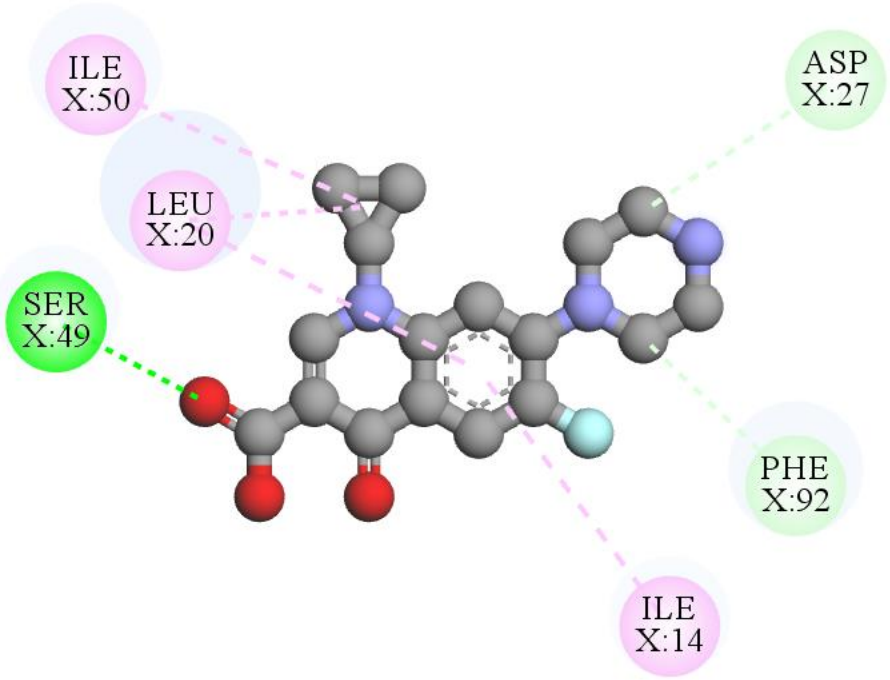
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Halogen (Fluorine)
- Pi-Alkyl



3.7. Ciprofloxacin (Cipro)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -513689680
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -9.1      0.000      0.000
   2         -8.7      3.415      6.648
   3         -8.6      3.981      7.323
   4         -8.3      3.828      6.614
   5         -8.1      2.880      4.605
   6         -8.0      4.056      5.964
   7         -8.0      3.816      6.169
   8         -7.7      4.603      7.303
   9         -7.6      3.342      6.250
Writing output ... done.
```



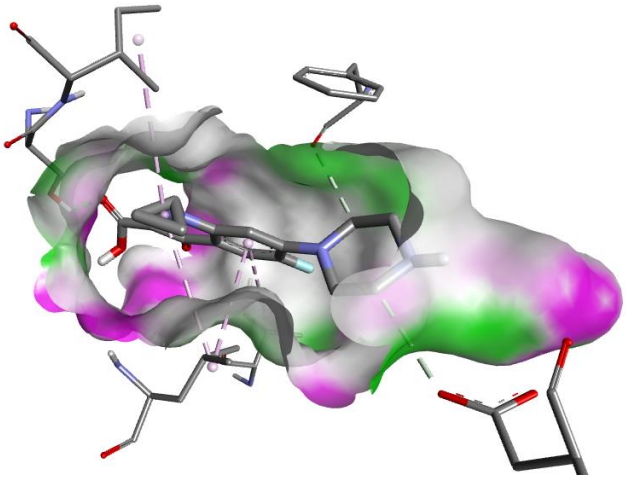
Interactions

Conventional Hydrogen Bond

Carbon Hydrogen Bond

Alkyl

Pi-Alkyl



H-Bonds

Donor

Acceptor

4. Aspartic Protease (PDB: 3Q70)

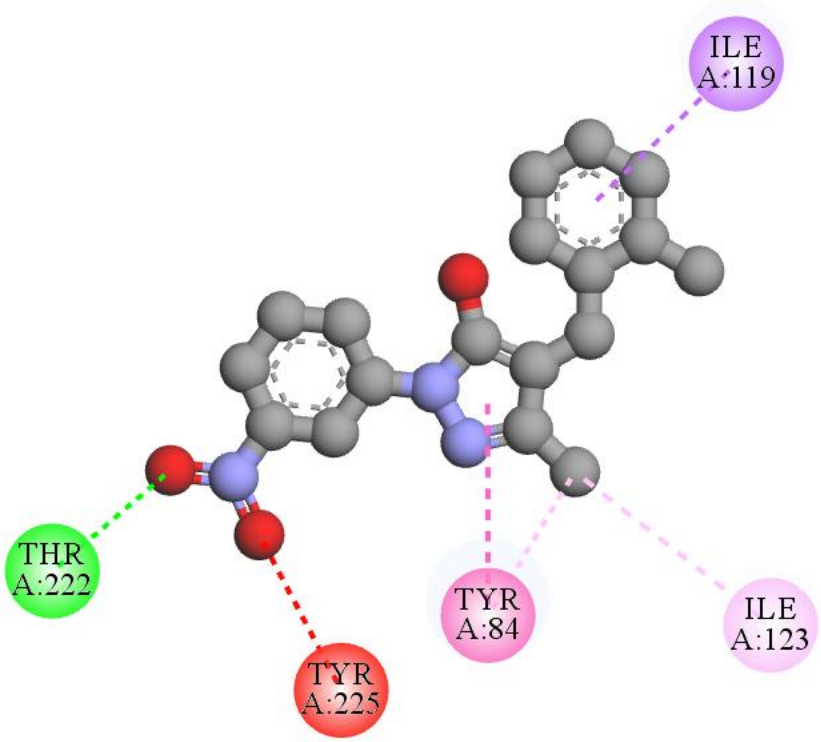
Grid box volume – Autodock Vina

```
receptor = 3q70F.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = -24.1441
center_y = -13.3872
center_z = 21.6952

size_x = 30
size_y = 30
size_z = 30

energy_range = 4

exhaustiveness = 8
```

Config.txt File

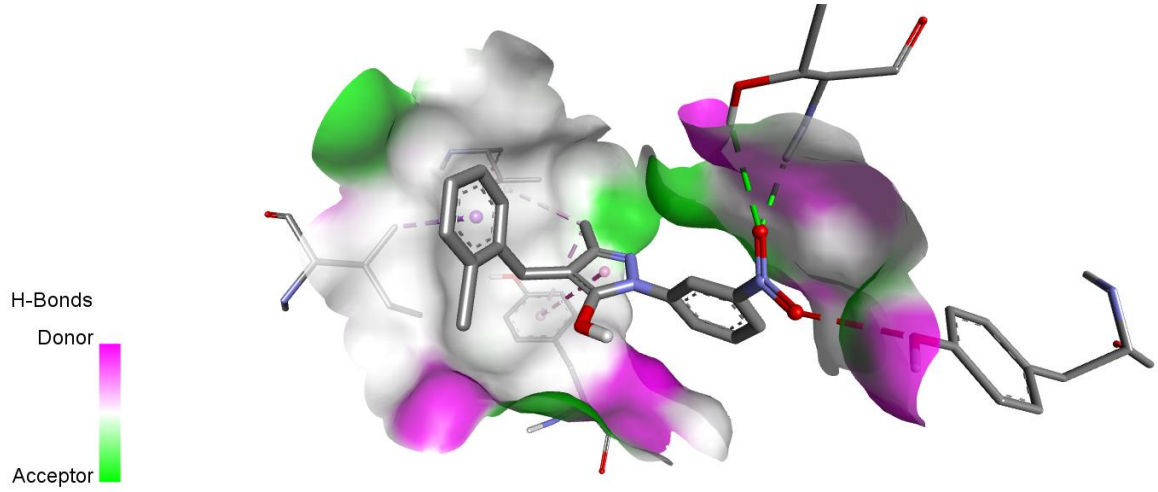
4.1. Compound 4a

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2044458272
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.4      0.000      0.000
   2         -7.3      4.066      7.320
   3         -7.3      3.671      7.614
   4         -7.2      3.295      4.134
   5         -7.2      3.977      5.605
   6         -7.1      2.424      3.118
   7         -7.1      1.878      2.230
   8         -7.1      2.089      2.879
   9         -7.0      1.943      2.244
Writing output ... done.
```



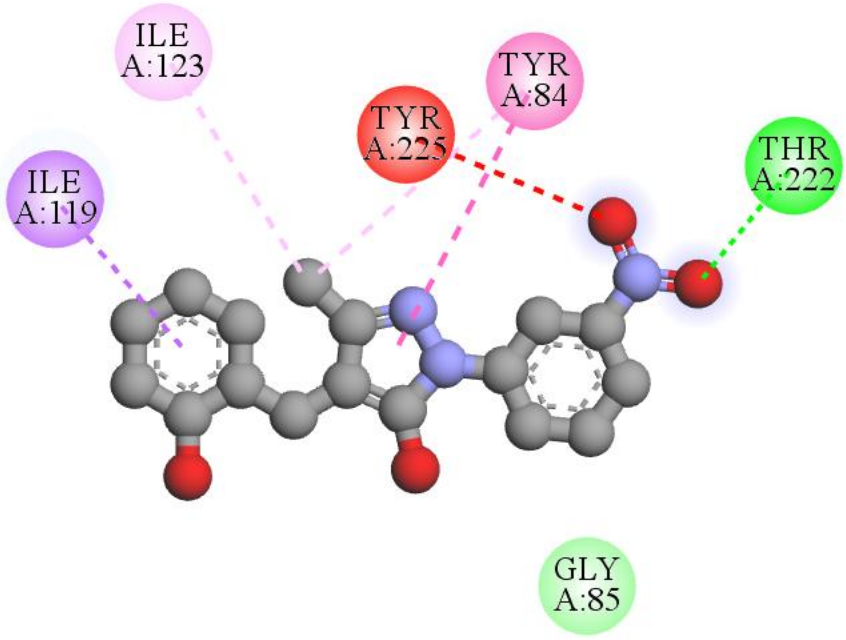
Interactions

- Conventional Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Sigma
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl



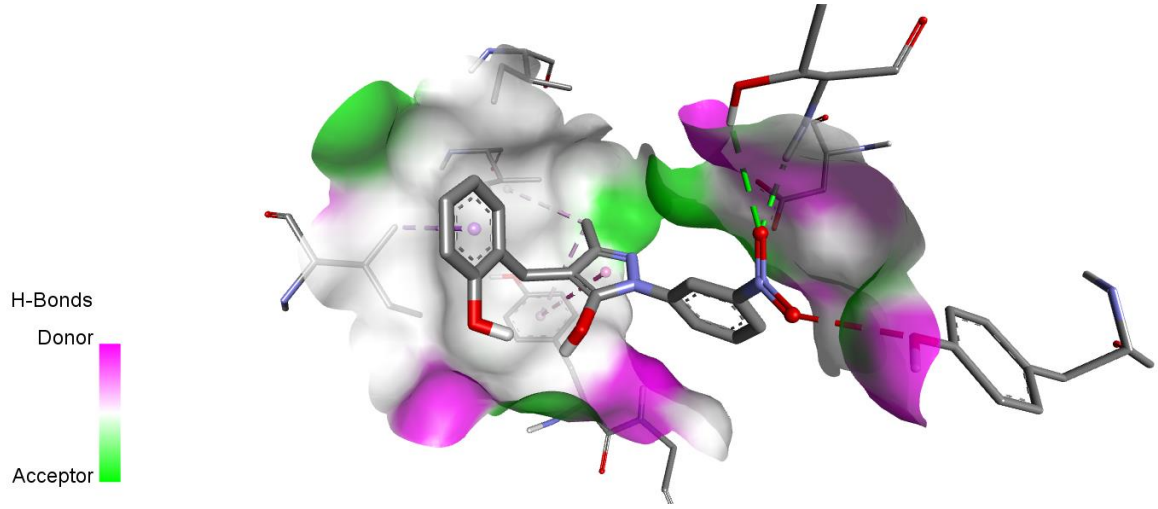
4.2. Compound 4h

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -129789856
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.5      0.000      0.000
   2         -7.4      3.615      7.092
   3         -7.2      1.917      2.205
   4         -7.2      3.172      4.265
   5         -7.1      3.599      6.243
   6         -7.1      3.156      3.913
   7         -6.9      4.277      6.565
   8         -6.8      1.920      2.897
   9         -6.8      4.896      7.145
Writing output ... done.
```



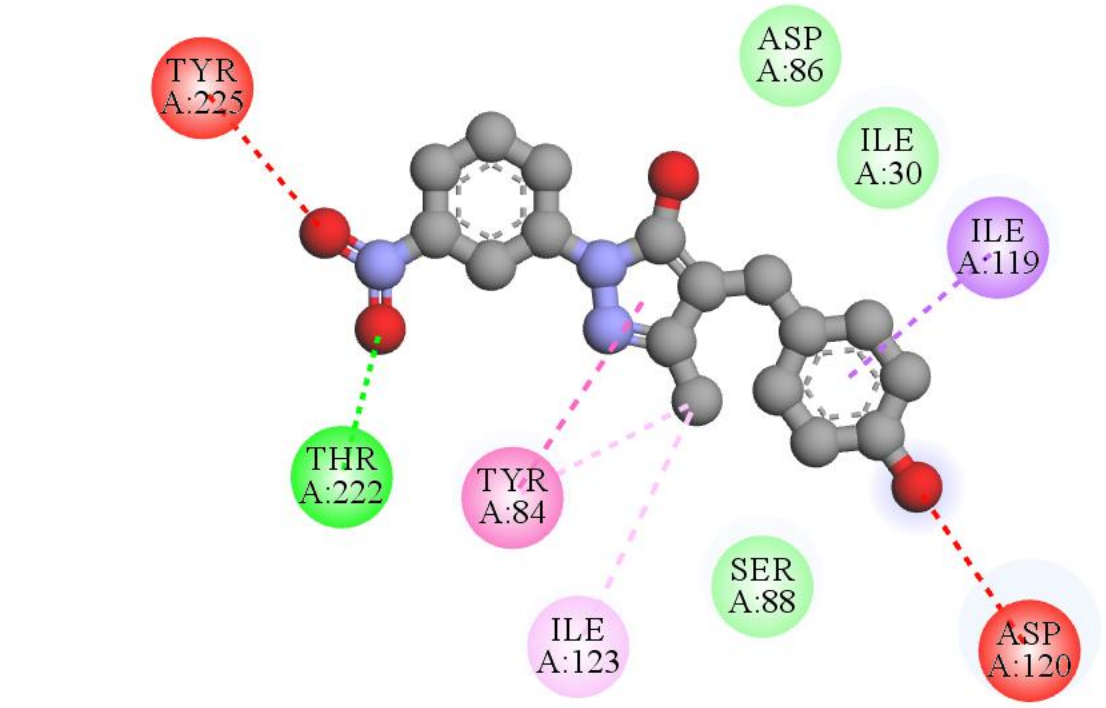
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Sigma
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl



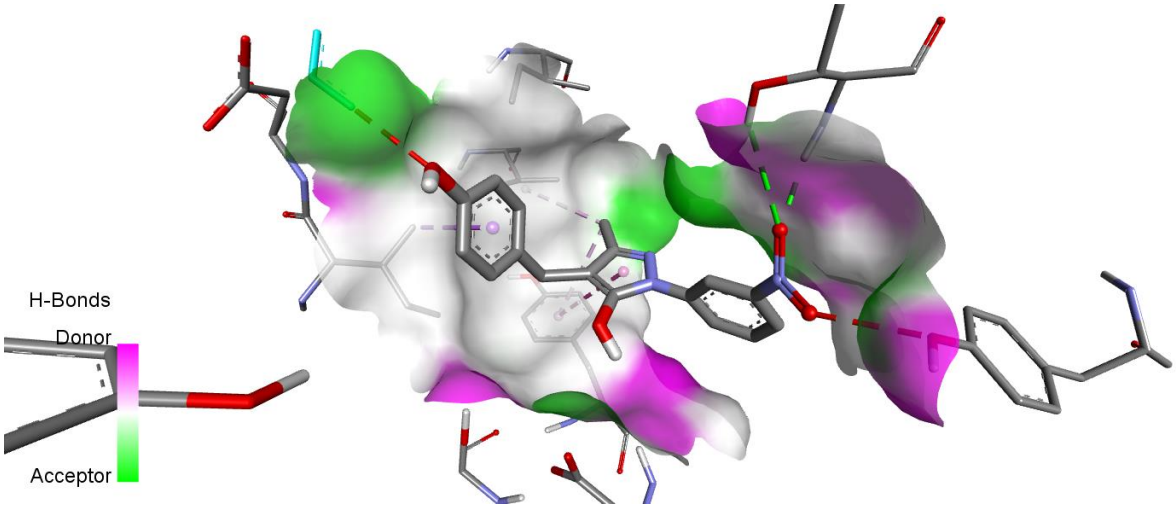
4.3. Compound 4i

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 684019816
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.3      1.780      2.088
   3         -7.2      3.088      7.175
   4         -7.1      4.082      7.655
   5         -7.1      3.643      7.584
   6         -7.1      3.984      7.826
   7         -6.8      2.355      3.087
   8         -6.8      2.759      3.634
   9         -6.8      4.101      6.436
Writing output ... done.
```



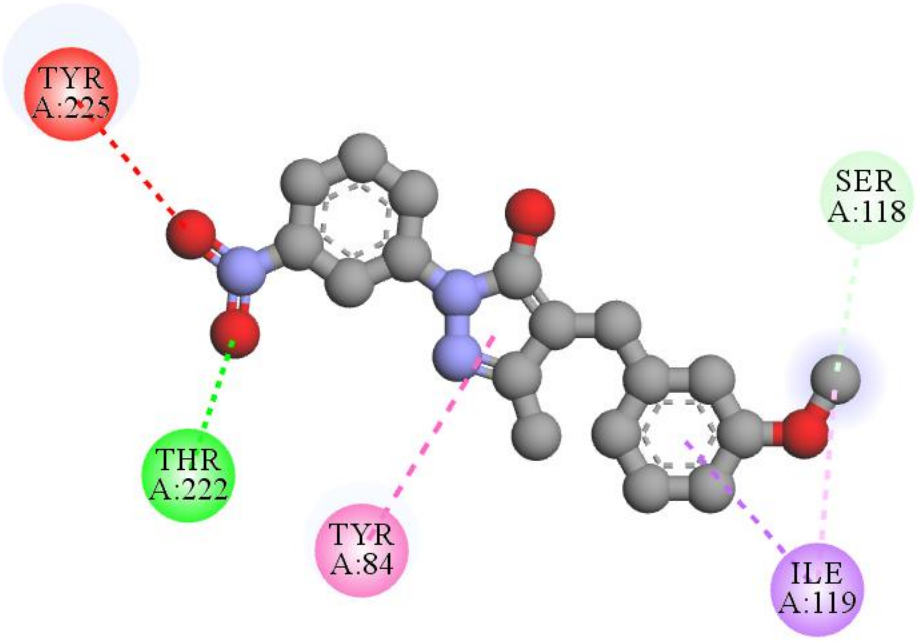
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Sigma
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl



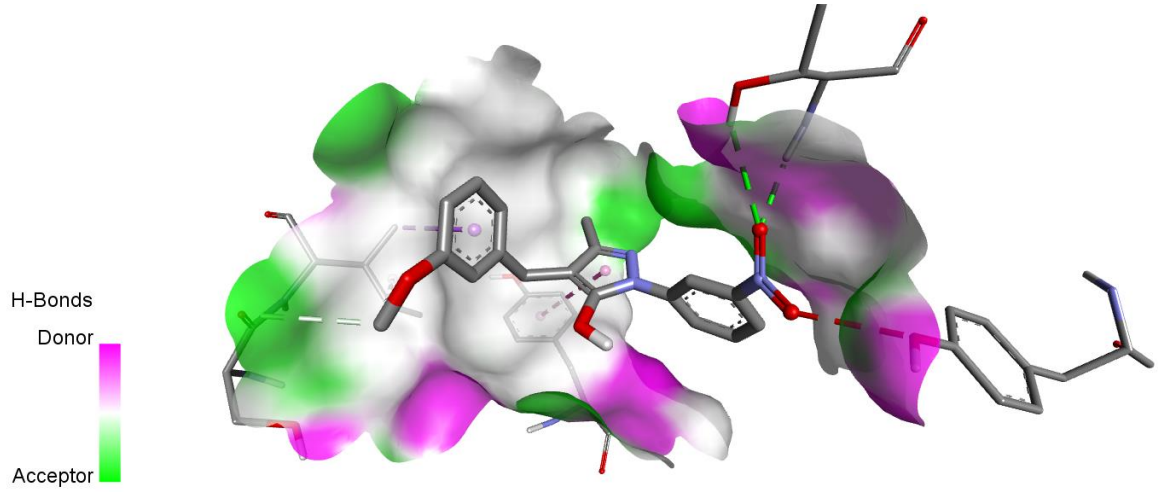
4.4. Compound 4l

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -670916768
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.6      0.000      0.000
   2         -7.6      0.991      1.919
   3         -7.5      2.807      7.021
   4         -7.2      1.742      2.107
   5         -7.2      3.967      7.611
   6         -7.1      3.591      7.741
   7         -7.1      3.844      7.878
   8         -7.0      3.735      5.269
   9         -6.9      2.897      7.857
Writing output ... done.
```



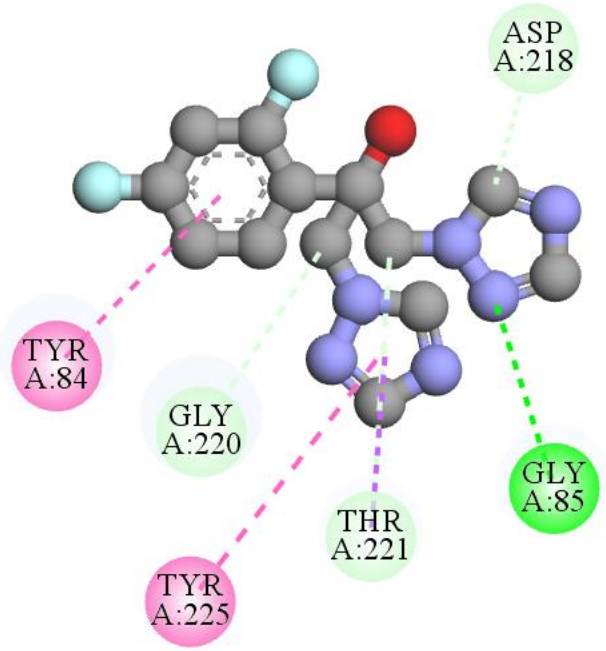
Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Sigma
- Pi-Pi Stacked
- Alkyl



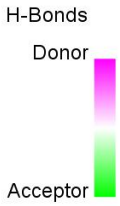
4.5. Fluconazole (Flu)

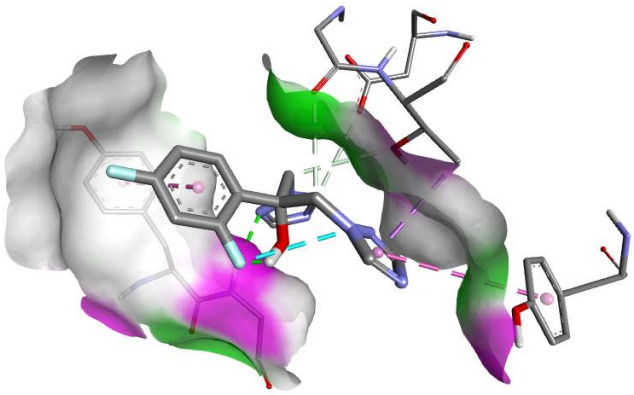
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1767898368
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.4      0.000      0.000
   2         -6.2      7.449      9.640
   3         -6.2      7.241      9.265
   4         -6.1      6.019      8.370
   5         -6.1      3.370      4.799
   6         -6.0      3.229      5.677
   7         -6.0      1.671      4.007
   8         -5.9      3.285      5.609
   9         -5.9      3.853      5.871
Writing output ... done.
```



Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked





5. ***Dihydrofolate Reductase – Fungi (PDB: 4HOF)***

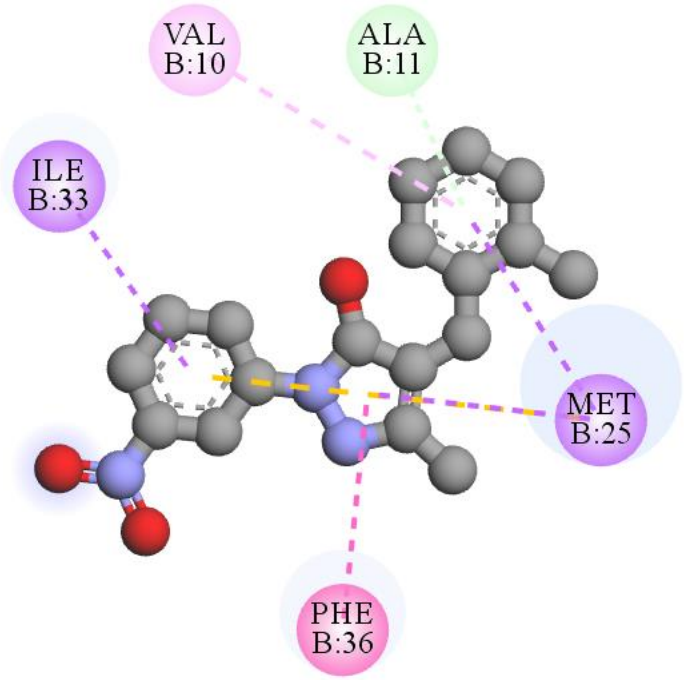
Grid box volume – Autodock Vina

```
receptor = 4hofF.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 11.44
center_y = -32.6283
center_z = 17.3865

size_x = 30
size_y = 30
size_z = 30

energy_range = 4

exhaustiveness = 8
```

Config.txt File

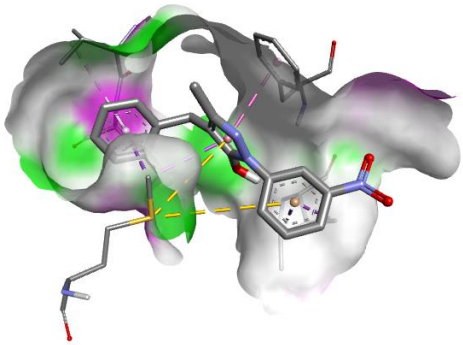
5.1. Compound 4a

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 252792100
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.7      0.000      0.000
   2         -8.6      1.857      2.222
   3         -8.0      3.177      7.830
   4         -7.9     13.242     15.459
   5         -7.6      2.920      7.801
   6         -7.4     10.466     12.727
   7         -7.4     11.588     14.111
   8         -7.4      4.274      6.325
   9         -7.3      5.300      6.650
Writing output ... done.
```



Interactions

- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked
- Pi-Alkyl



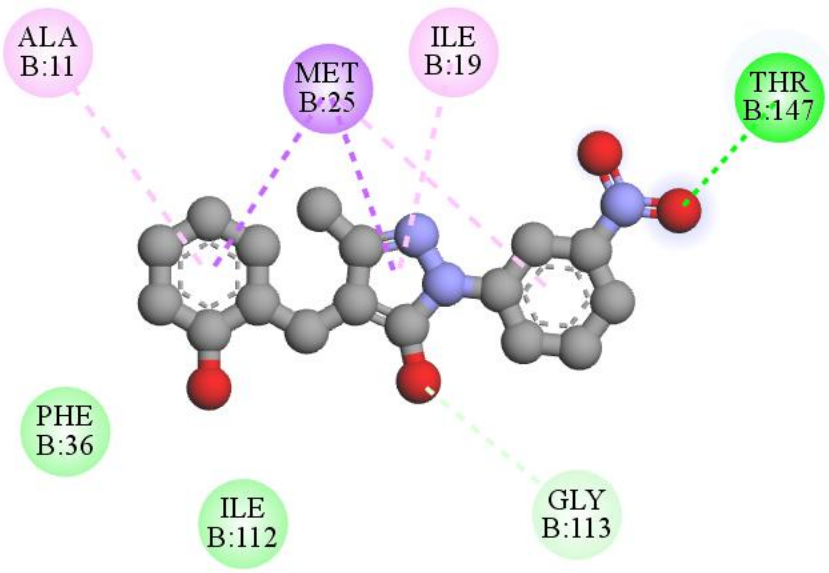
H-Bonds

Donor

Acceptor

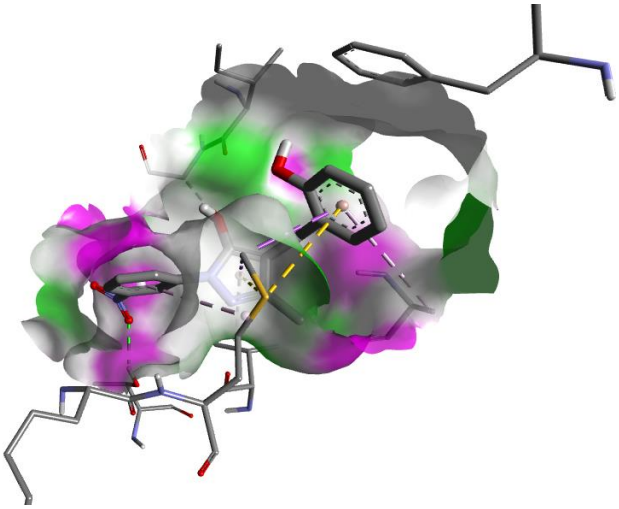
5.2. Compound 4h

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1193428936
Performing search ... 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         -8.4      5.546      8.876
   3         -8.3      5.518      8.274
   4         -8.2      4.490      7.512
   5         -7.5      8.129     10.732
   6         -7.4      5.980      8.946
   7         -7.3      6.431      9.428
   8         -7.2      4.733     10.024
   9         -7.2      8.795     11.815
Writing output ... done.
```



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Alkyl



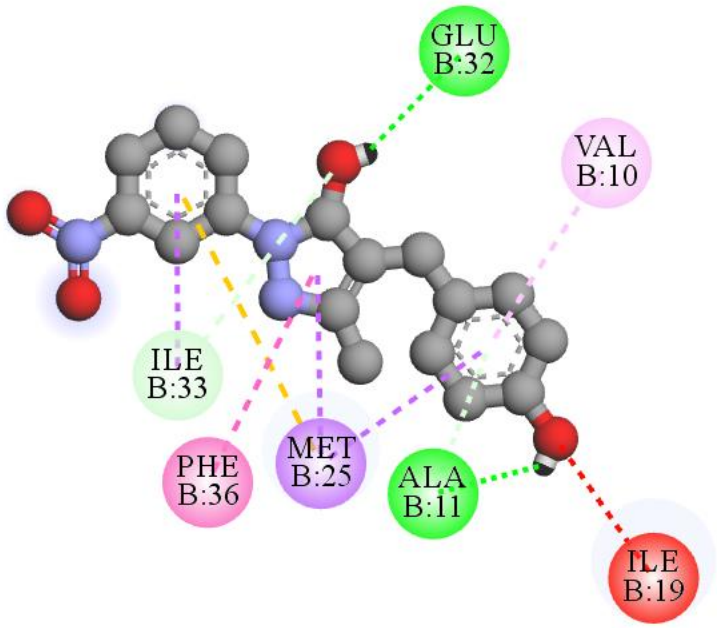
H-Bonds

Donor

Acceptor

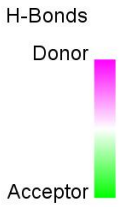
5.3. Compound 4i

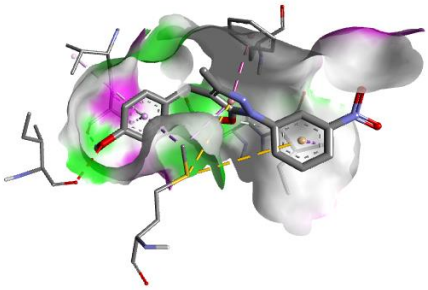
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1506152720
Performing search ... 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         -8.5      1.908      2.197
   3         -8.2      4.911      8.921
   4         -7.5     13.122     15.513
   5         -7.4      1.626      2.449
   6         -7.3     10.923     13.940
   7         -7.2     13.538     16.120
   8         -7.2      2.497      3.077
   9         -7.2      9.225     12.620
Writing output ... done.
```



Interactions

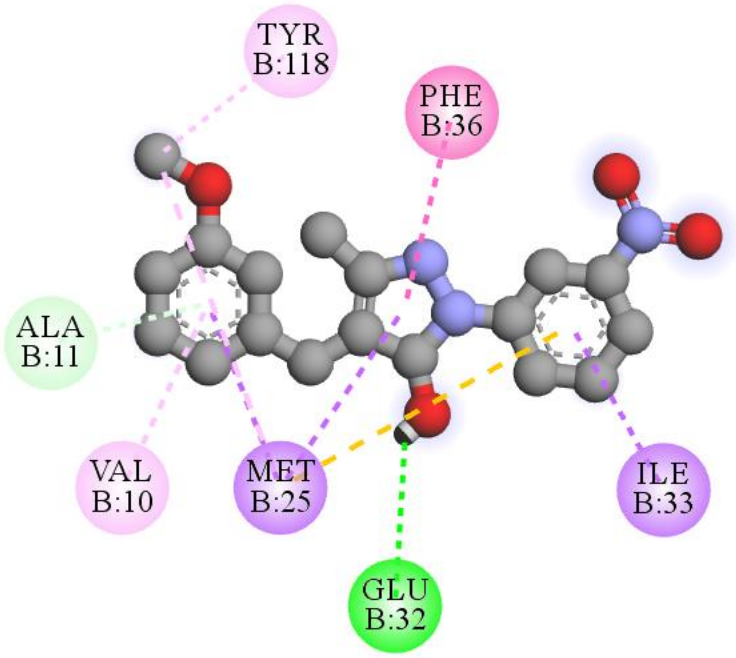
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Unfavorable Acceptor-Acceptor
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked
- Pi-Alkyl





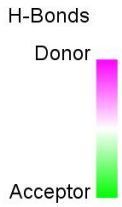
5.4. Compound 4l

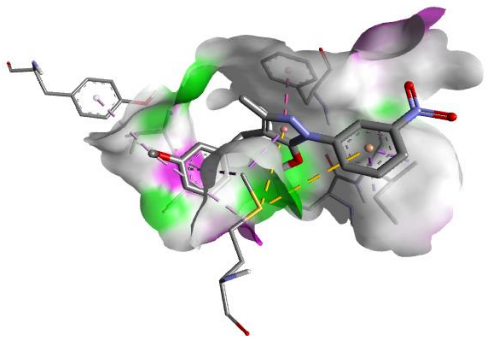
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1287968560
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -8.3      4.428      8.155
   3         -8.3      7.108     11.659
   4         -8.1      2.998      3.554
   5         -7.7     13.760     17.714
   6         -7.4      1.777      1.884
   7         -7.4      8.772     12.628
   8         -7.4     12.702     15.587
   9         -7.3     11.467     15.734
Writing output ... done.
```



Interactions

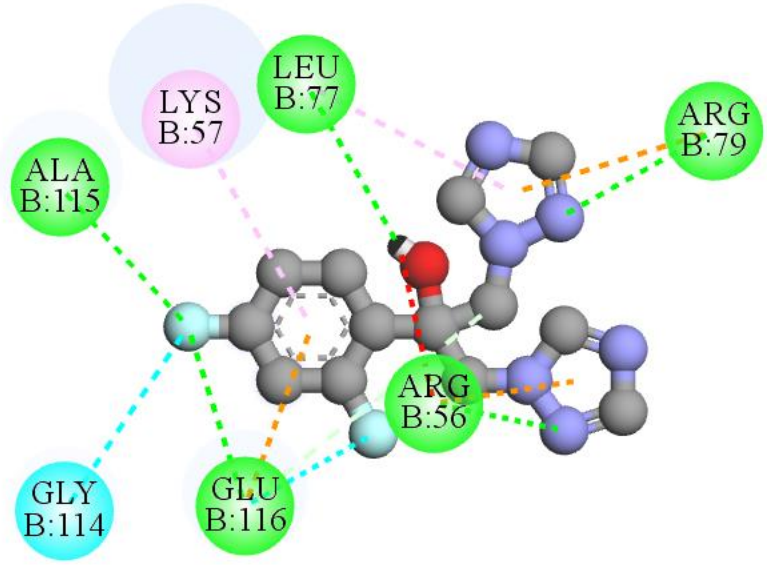
- Conventional Hydrogen Bond
- Pi-Donor Hydrogen Bond
- Pi-Sigma
- Pi-Sulfur
- Pi-Pi Stacked
- Alkyl
- Pi-Alkyl





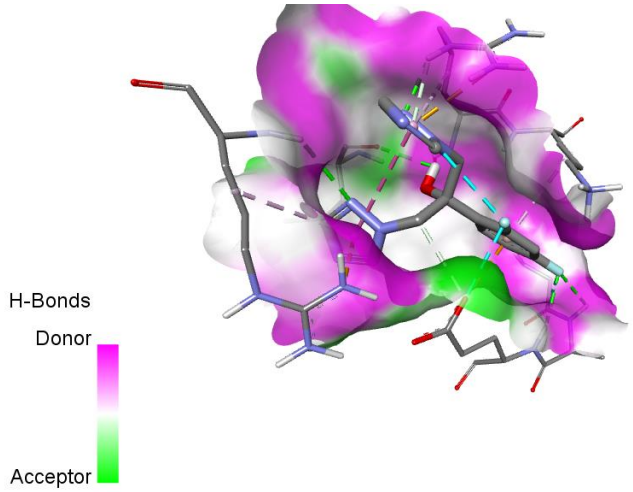
5.5. Fluconazole (Flu)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 354969912
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.1      0.000      0.000
   2         -6.7     15.479     17.571
   3         -6.7      5.965      8.371
   4         -6.6      6.990      9.783
   5         -6.6      6.269      8.190
   6         -6.5     16.115     18.311
   7         -6.5     15.812     17.920
   8         -6.5      6.688      8.914
   9         -6.4      6.307      8.629
Writing output ... done.
```



Interactions

Conventional Hydrogen Bond	Pi-Cation
Carbon Hydrogen Bond	Pi-Anion
Halogen (Fluorine)	Pi-Donor Hydrogen Bond
Unfavorable Donor-Donor	Pi-Alkyl



6. ***Thymidylate Kinase (PDB: 4QGG)***

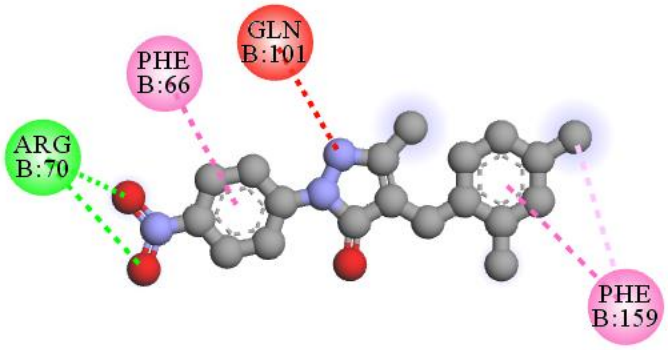
Grid box volume – Autodock Vina

```
receptor = 4qggB.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 34.7925
center_y = 2.75142
center_z = -14.1059

size_x = 30
size_y = 30
size_z = 30

energy_range = 4

exhaustiveness = 8
```

Config.txt File

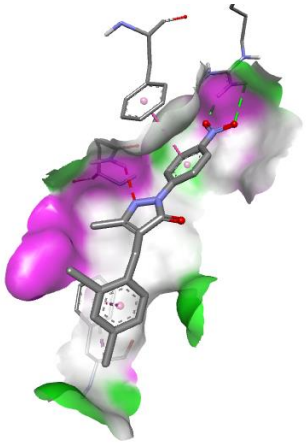
6.1. Compound 3d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1145350832
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.0      0.000      0.000
   2         -7.8      7.304      9.805
   3         -7.8      7.846     10.469
   4         -7.7      8.504     11.064
   5         -7.6      7.425      9.916
   6         -7.4      2.360      3.188
   7         -7.2      1.527      2.549
   8         -7.1      8.015     10.552
   9         -7.1      7.848      8.922
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Pi-Alkyl



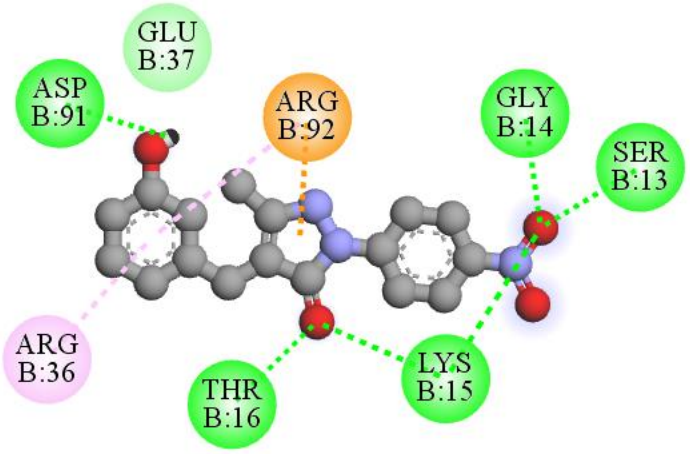
H-Bonds

Donor

Acceptor

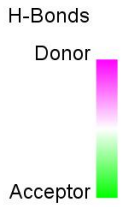
6.2. Compound 3m

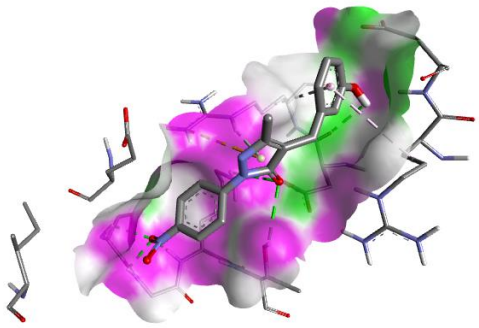
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1693231928
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.0      0.000      0.000
   2         -7.8      3.990      5.521
   3         -7.5      6.411      7.981
   4         -7.1      1.516      2.333
   5         -7.0      2.447      2.916
   6         -7.0      7.184     10.679
   7         -6.9      2.549      8.811
   8         -6.8      2.394      8.756
   9         -6.7      9.522     11.008
Writing output ... done.
```



Interactions

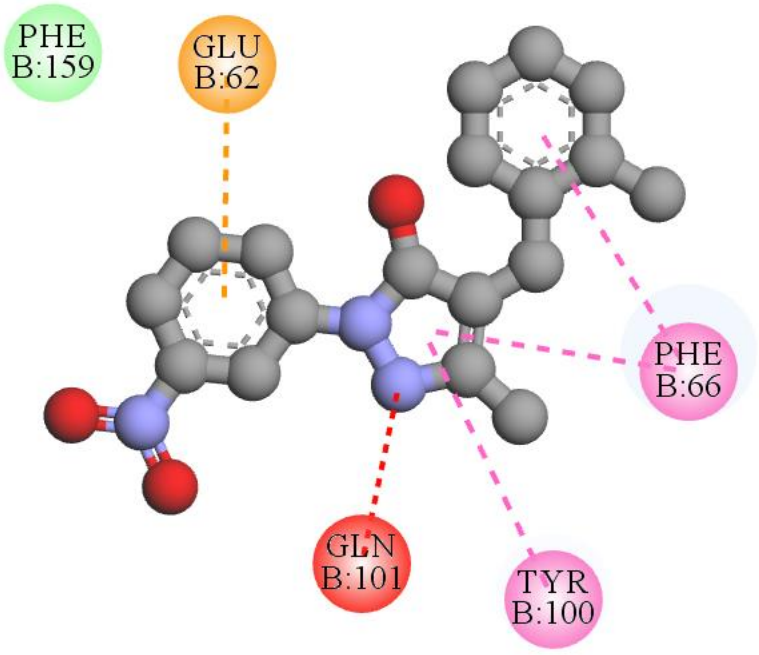
- van der Waals
- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Donor Hydrogen Bond
- Pi-Alkyl

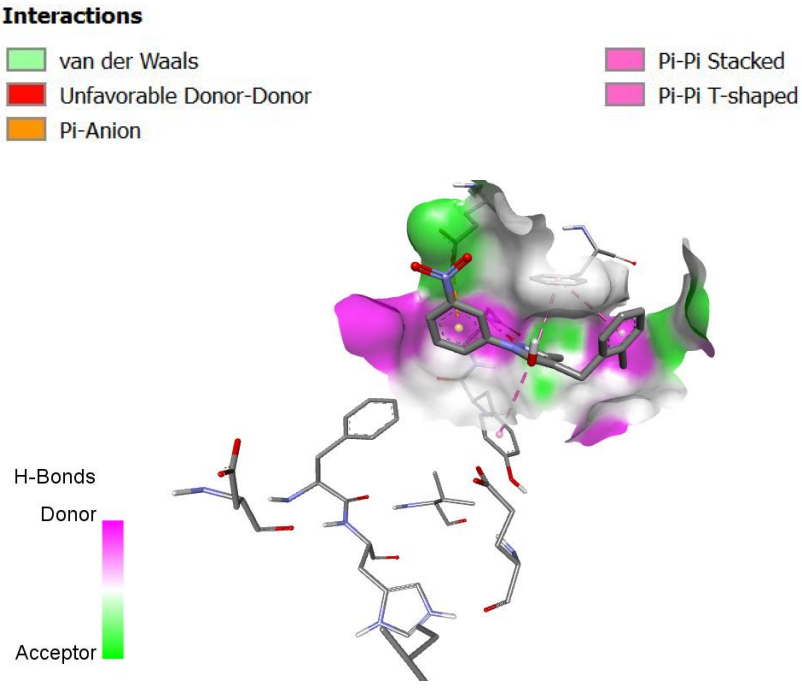




6.3. Compound 4a

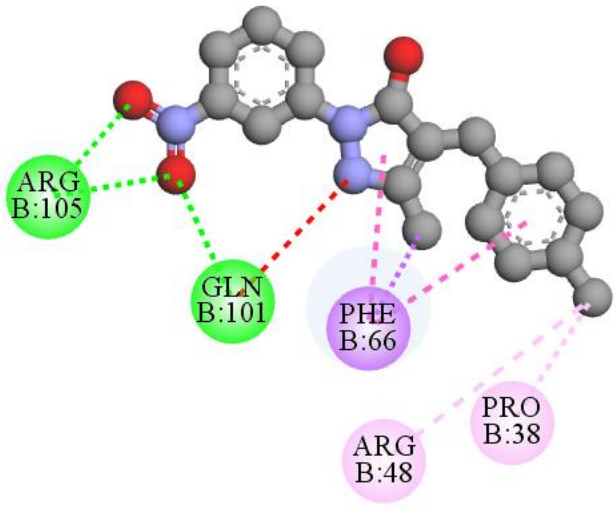
```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -963219588
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.6      0.000      0.000
   2         -7.4      4.227      6.183
   3         -7.4      2.052      2.413
   4         -7.4      3.960      5.905
   5         -7.3      2.412      3.362
   6         -7.2      4.568      5.934
   7         -7.1      3.102      4.452
   8         -7.0      8.114     10.219
   9         -6.9      5.745      8.359
Writing output ... done.
```


PHE
B:159
GLU
B:62
PHE
B:66
GLN
B:101
TYR
B:100


Interactions
van der Waals
Unfavorable Donor-Donor
Pi-Anion
Pi-Pi Stacked
Pi-Pi T-shaped
H-Bonds
Donor
Acceptor

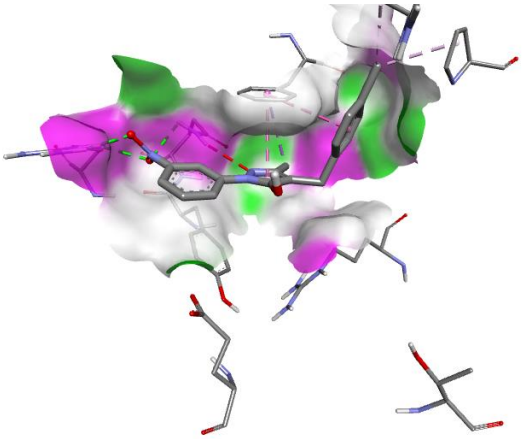
6.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1205324416
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -7.7      2.982      4.502
   3         -7.6      3.764      5.381
   4         -7.5      6.440      7.991
   5         -7.4      7.926      9.543
   6         -7.4      4.612      6.381
   7         -7.3      6.965      8.806
   8         -7.3      7.523      9.068
   9         -7.2      2.604      3.231
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl



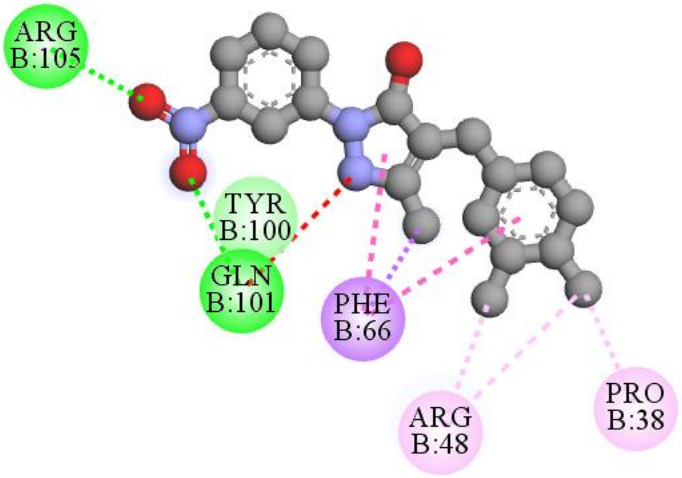
H-Bonds

Donor

Acceptor

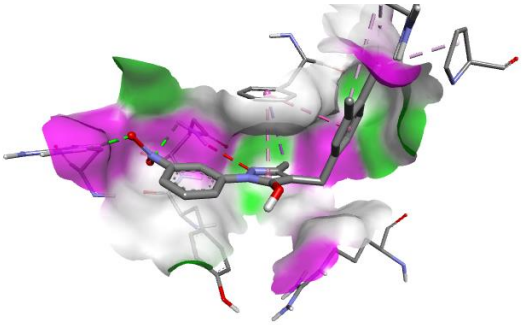
6.5. Compound 4d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2110747456
Performing search ... 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         -8.0      5.299      7.152
   3         -7.9      1.806      2.163
   4         -7.7      4.538      6.391
   5         -7.7      4.717      7.052
   6         -7.7      6.775      8.575
   7         -7.7      3.774      5.403
   8         -7.7      6.281      7.929
   9         -7.7      7.810      9.418
Writing output ... done.
```



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Unfavorable Donor-Donor
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped
- Alkyl



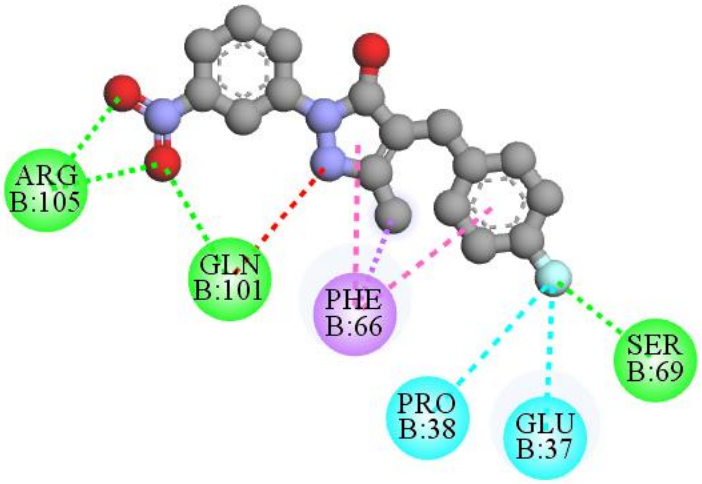
H-Bonds

Donor

Acceptor

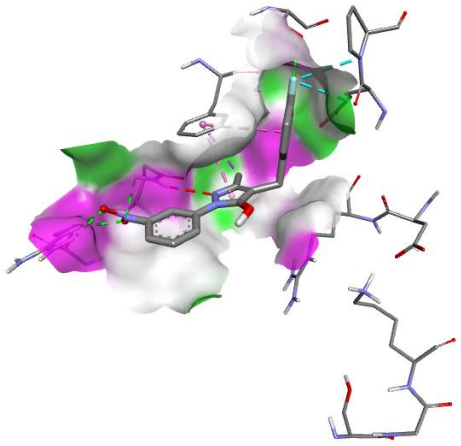
6.6. Compound 4g

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -710671832
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.5      0.000      0.000
   2         -8.2      5.462      7.302
   3         -8.2      2.217      3.163
   4         -7.9      1.816      2.352
   5         -7.8      2.040      2.855
   6         -7.7      3.567      4.990
   7         -7.7      3.895      5.327
   8         -7.6      4.429      6.115
   9         -7.5      6.404      7.931
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Halogen (Fluorine)
- Unfavorable Donor-Donor
- Pi-Sigma
- Pi-Pi Stacked
- Pi-Pi T-shaped



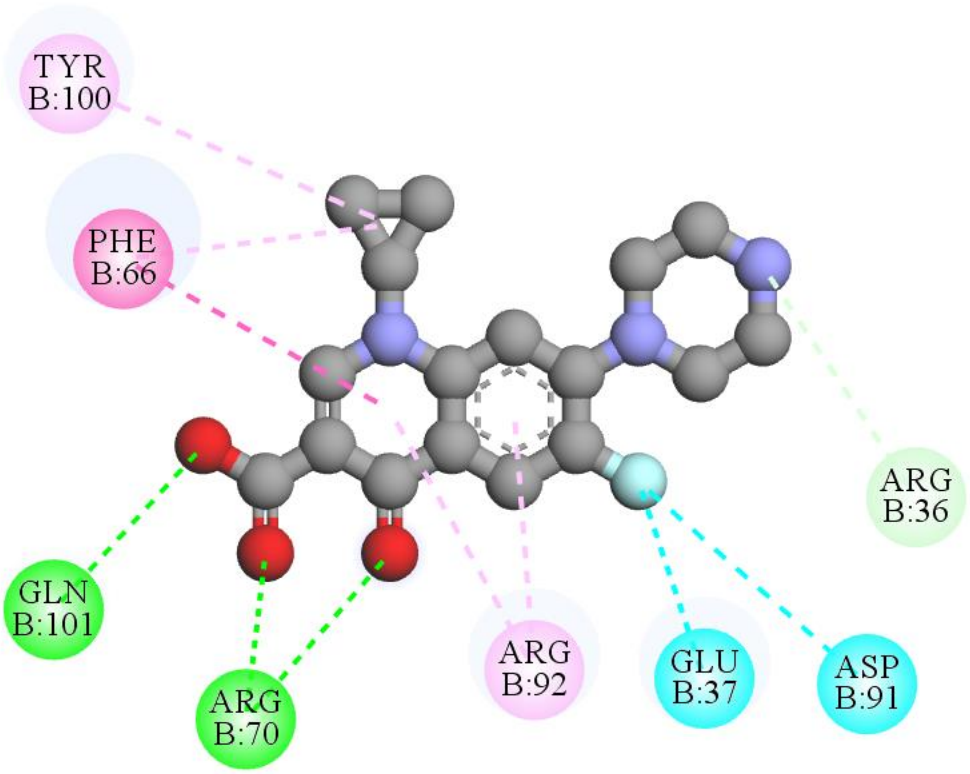
H-Bonds

Donor

Acceptor

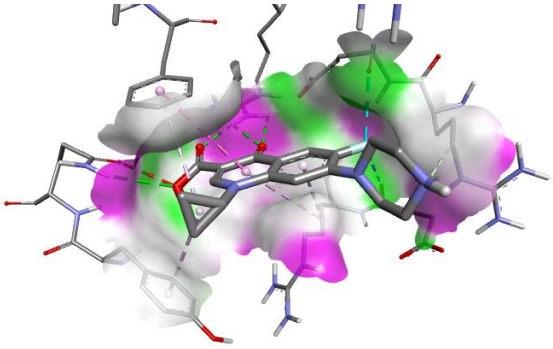
6.7. Ciprofloxacin (Cipro)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1865215276
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.9      0.000      0.000
   2         -7.4      2.822      4.437
   3         -7.2      3.299      6.431
   4         -7.2      2.268      3.420
   5         -7.1      3.153      6.649
   6         -6.9      6.456      8.994
   7         -6.9      4.233      5.818
   8         -6.8      3.553      4.916
   9         -6.7      3.966      6.578
Writing output ... done.
```



Interactions

- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Halogen (Fluorine)
- Unfavorable Acceptor-Acceptor
- Pi-Pi Stacked
- Pi-Alkyl



H-Bonds

Donor

Acceptor

7. Gyrase B (PDB: 4URM)

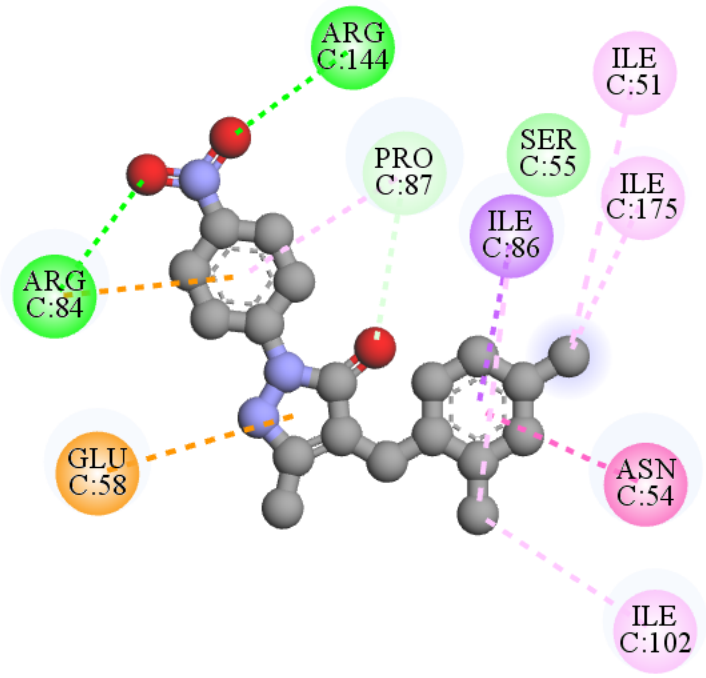
Grid box volume – Autodock Vina

```
receptor = 4urmB.pdbqt
ligand = ligand.pdbqt

out = outlig.pdbqt

center_x = 23.9228
center_y = 7.94566
center_z = 90.4085

size_x = 30
size_y = 30
size_z = 30

energy_range = 4

exhaustiveness = 8
```

Config.txt File

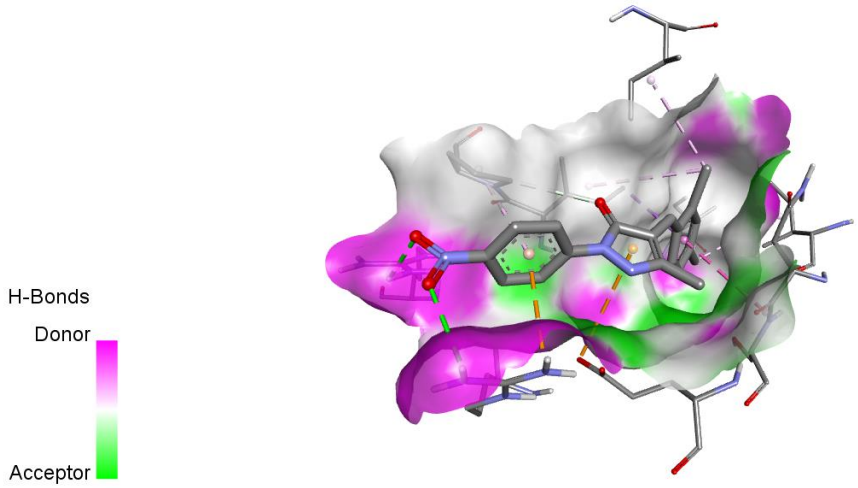
7.1. Compound 3d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1632630336
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -7.8      3.692      4.764
   3         -7.6      4.727      8.154
   4         -7.6      3.222      3.750
   5         -7.6      4.678      8.489
   6         -7.5      4.189      8.329
   7         -7.4      4.164      8.210
   8         -7.3      4.406      8.168
   9         -7.3      4.227      8.531
Writing output ... done.
```



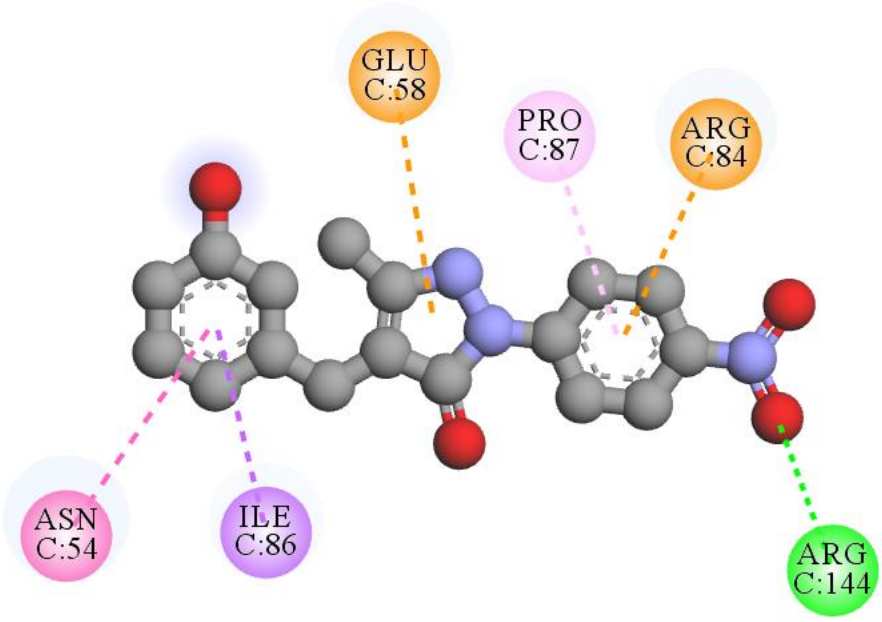
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



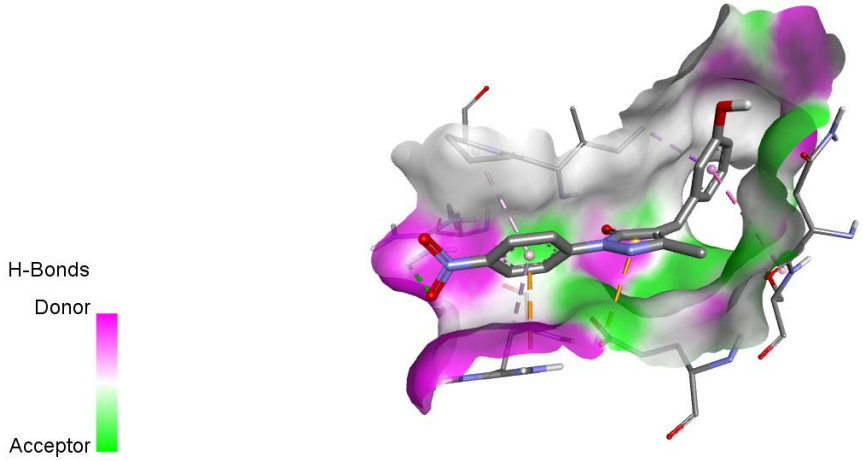
7.2. Compound 3m

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1048647408
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.4      0.000      0.000
   2         -7.7      2.452      8.039
   3         -7.5      4.553      5.690
   4         -7.4      3.836      8.029
   5         -7.3      3.779      7.789
   6         -7.2      3.939      5.202
   7         -7.1      4.345      7.339
   8         -7.0      3.960      8.187
   9         -7.0      3.428      8.215
Writing output ... done.
```



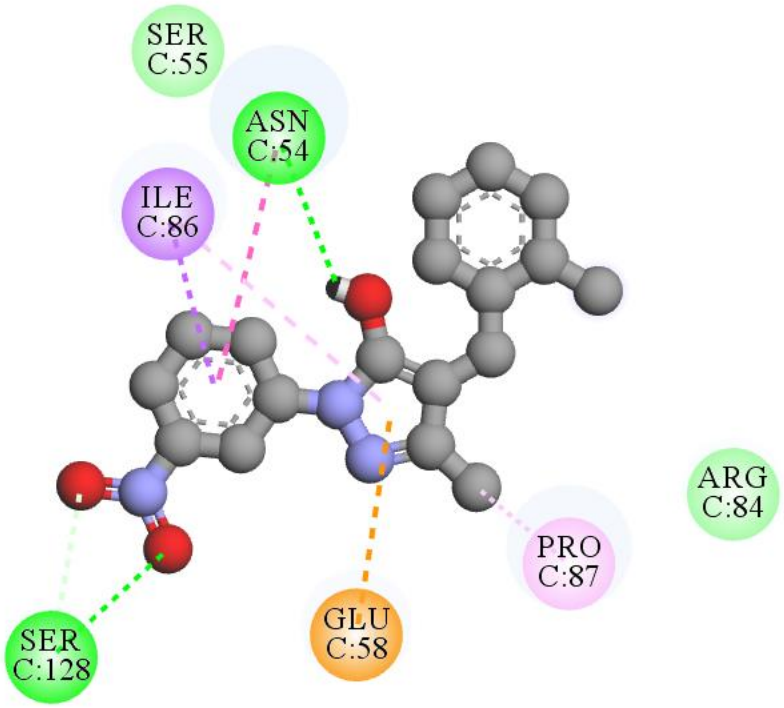
Interactions

- Conventional Hydrogen Bond
- Pi-Cation
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



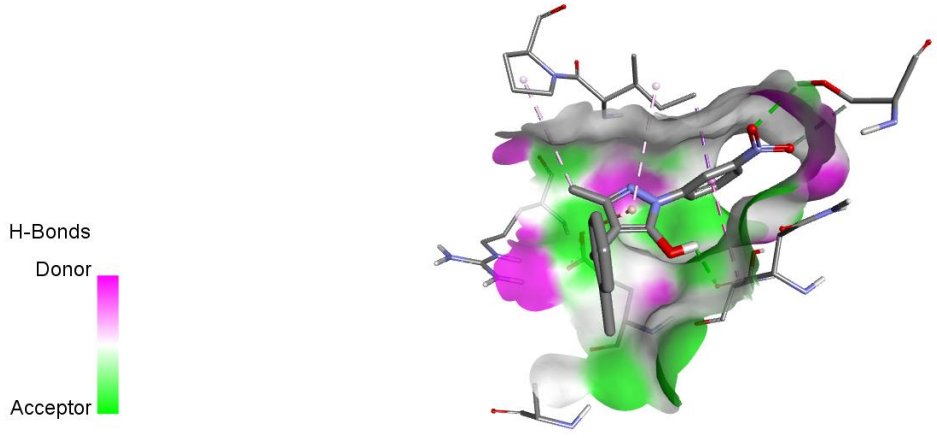
7.3. Compound 4a

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1740973184
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.4      0.000      0.000
   2         -7.2      3.443      4.050
   3         -7.2      1.625      1.952
   4         -7.2      1.706      2.308
   5         -7.1      1.787      2.304
   6         -7.1      2.394      3.532
   7         -7.0      4.608      7.105
   8         -7.0      2.387      3.046
   9         -7.0      2.820      3.583
Writing output ... done.
```



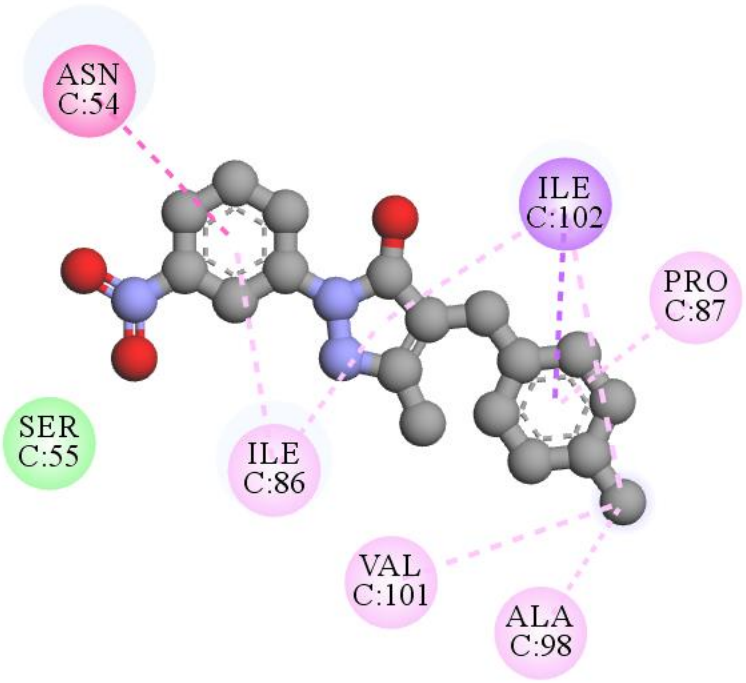
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Carbon Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



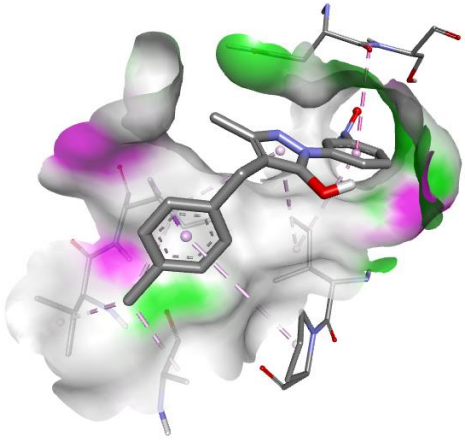
7.4. Compound 4b

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1156560672
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.7      0.000      0.000
   2         -7.5      1.739      2.827
   3         -7.5      1.426      2.200
   4         -7.5      3.454      4.323
   5         -7.4      3.492      4.112
   6         -7.3      3.573      5.113
   7         -7.3      3.043      4.244
   8         -7.1      4.207      7.624
   9         -7.1      3.981      5.101
Writing output ... done.
```



Interactions

- van der Waals
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



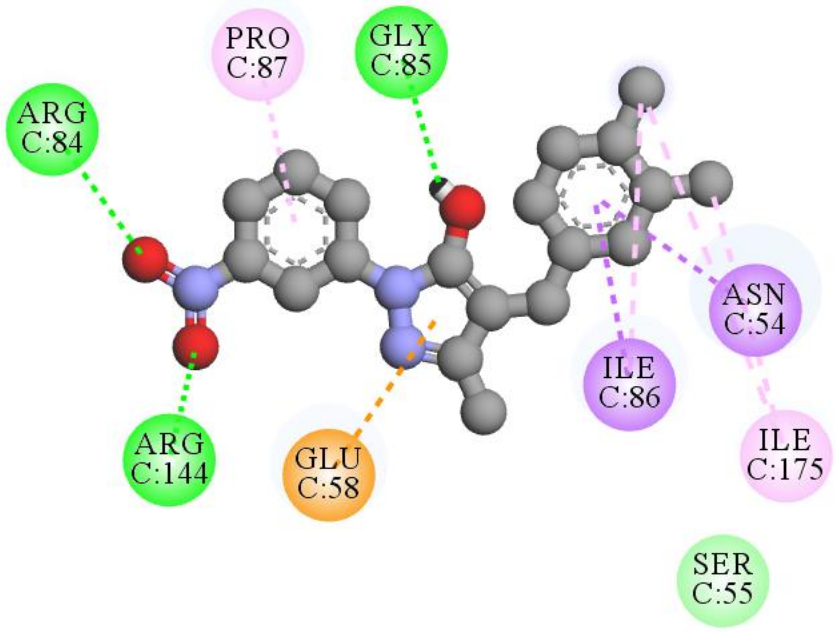
H-Bonds

Donor

Acceptor

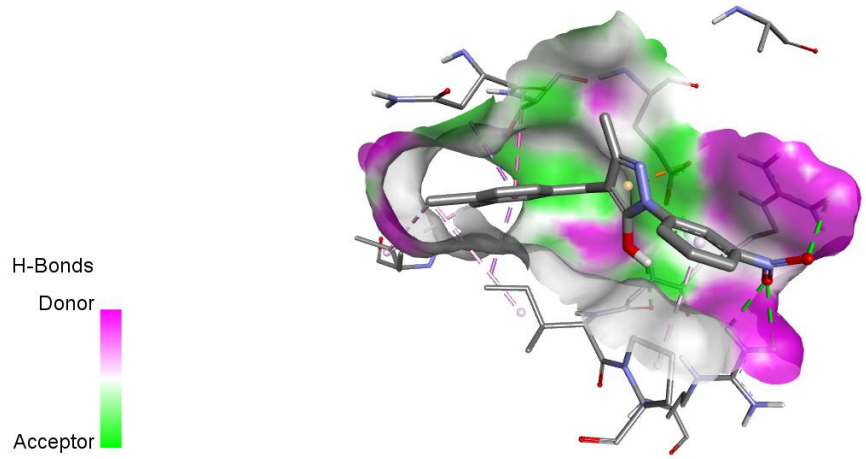
7.5. Compound 4d

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1852671472
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.3      0.000      0.000
   2         -7.8      4.557      7.774
   3         -7.7      1.685      1.986
   4         -7.6      3.830      7.654
   5         -7.5      4.712      8.185
   6         -7.5      4.814      7.860
   7         -7.4      4.852      8.078
   8         -7.4      3.963      4.875
   9         -7.2      4.738      7.873
Writing output ... done.
```



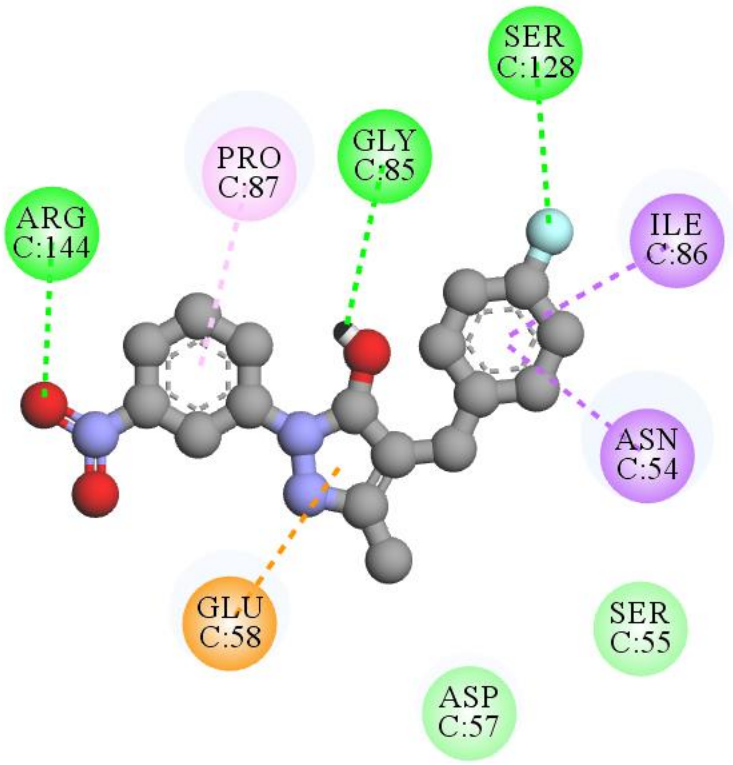
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



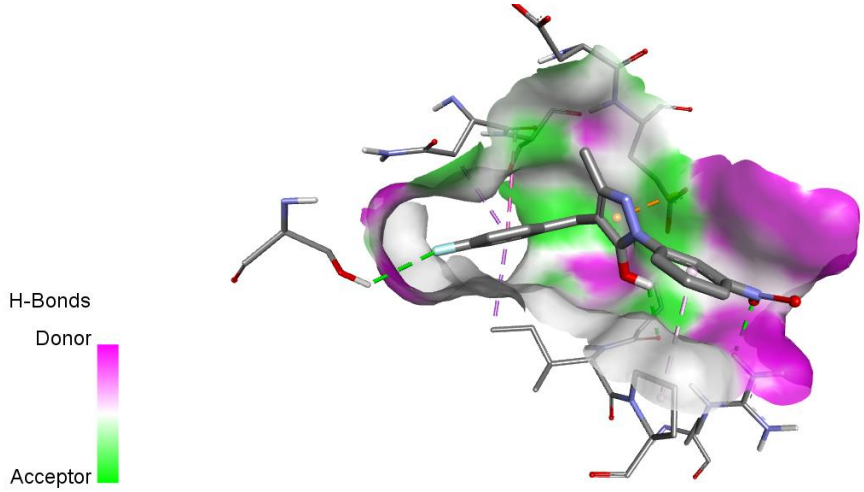
7.6. Compound 4g

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 47954948
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.9      0.000      0.000
   2         -7.8      4.187      7.342
   3         -7.6      4.281      5.255
   4         -7.6      4.074      7.601
   5         -7.6      4.347      7.771
   6         -7.5      4.289      7.745
   7         -7.3      3.382      4.465
   8         -7.3      4.168      4.969
   9         -7.2      2.734      3.452
Writing output ... done.
```



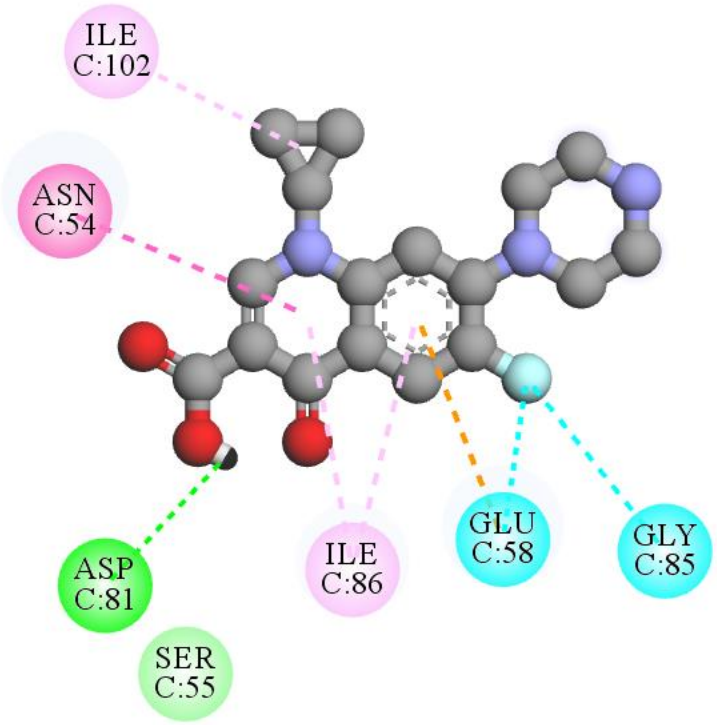
Interactions

- van der Waals
- Conventional Hydrogen Bond
- Pi-Anion
- Pi-Sigma
- Amide-Pi Stacked
- Pi-Alkyl



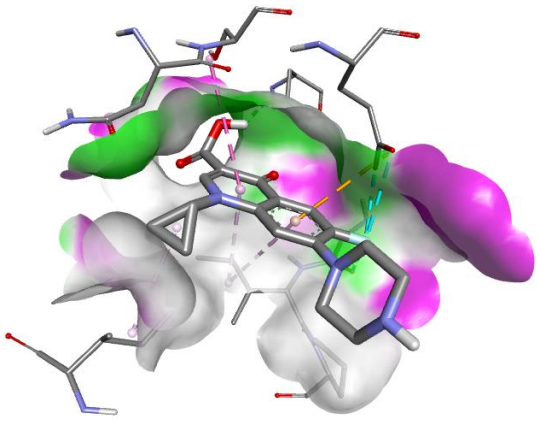
7.7. Ciprofloxacin (Cipro)

```
#################################################################
# If you used AutoDock Vina in your work, please cite:          #
#                                                               #
# O. Trott, A. J. Olson,                                        #
# AutoDock Vina: improving the speed and accuracy of docking    #
# with a new scoring function, efficient optimization and       #
# multithreading, Journal of Computational Chemistry 31 (2010)  #
# 455-461                                                       #
#                                                               #
# DOI 10.1002/jcc.21334                                         #
#                                                               #
# Please see http://vina.scripps.edu for more information.      #
#################################################################

Detected 8 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2086554712
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -6.8      3.636      6.717
   3         -6.8      2.752      4.126
   4         -6.5      3.179      6.720
   5         -6.3      4.616      7.313
   6         -6.3      3.824      7.281
   7         -6.1      5.312      8.134
   8         -6.0      2.119      2.728
   9         -6.0      3.443      4.758
Writing output ... done.
```



Interactions

- van der Waals
- Conventional Hydrogen Bond
- Halogen (Fluorine)
- Pi-Anion
- Amide-Pi Stacked
- Alkyl
- Pi-Alkyl



H-Bonds

Donor

Acceptor