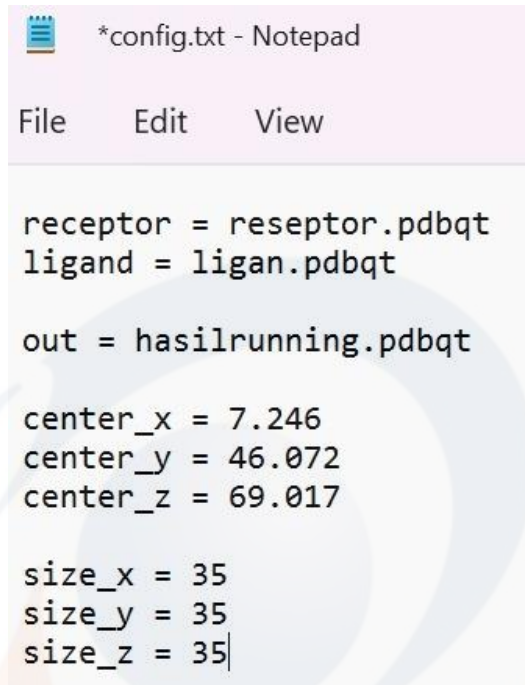


LAMPIRAN

Lampiran 1. Konfigurasi vina pada notepad



```
*config.txt - Notepad
File Edit View

receptor = reseptor.pdbqt
ligand = ligan.pdbqt

out = hasilrunning.pdbqt

center_x = 7.246
center_y = 46.072
center_z = 69.017

size_x = 35
size_y = 35
size_z = 35|
```

Lampiran 2. Data hasil penambatan *Autodock vina*

Aliskiren

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1177749944
Performing search ... done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b. |
-----+-----+-----+-----+
  1   |   -9.0   |    0.000   |    0.000   |
  2   |   -8.6   |    4.363   |   11.035   |
  3   |   -8.6   |    2.755   |    3.292   |
  4   |   -8.5   |    4.447   |   10.360   |
  5   |   -8.4   |    2.160   |    3.034   |
  6   |   -8.3   |    1.832   |    2.284   |
  7   |   -8.2   |    2.017   |    3.350   |
  8   |   -8.0   |    3.832   |    9.958   |
  9   |   -7.9   |    3.311   |   11.025   |
Writing output ... done.
    
```

Luteolin

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2138026096
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   |    -8.9   |    3.852   |    7.968
  3   |    -8.6   |    3.721   |    9.205
  4   |    -8.4   |    2.927   |    4.178
  5   |    -8.3   |   10.872   |   15.190
  6   |    -8.3   |    1.257   |    4.639
  7   |    -8.3   |    3.494   |    8.782
  8   |    -8.2   |    1.479   |    2.150
  9   |    -8.1   |    3.373   |    6.749

Writing output ... done.

```

Kuersetin

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1922822620
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   |   -9.3   |   4.815   |  11.007
  3   |   -9.2   |   3.010   |   4.828
  4   |   -9.1   |   3.482   |   6.131
  5   |   -8.9   |   3.668   |   7.721
  6   |   -8.9   |   4.125   |   6.147
  7   |   -8.7   |   3.837   |   5.086
  8   |   -8.6   |   3.623   |   7.619
  9   |   -8.6   |   3.579   |   5.448

Writing output ... done.

```

Kaempferol

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -759144064
Performing search ... done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1   |   -10.0   |    0.000   |    0.000
  2   |    -9.8   |    1.179   |    2.213
  3   |    -9.5   |    4.575   |    8.780
  4   |    -9.5   |    1.244   |    2.762
  5   |    -9.3   |    4.747   |    9.015
  6   |    -9.1   |    1.070   |    2.166
  7   |    -9.0   |    4.755   |    8.829
  8   |    -8.7   |    4.752   |    8.961
  9   |    -8.7   |    4.592   |    8.814

Writing output ... done.

```

Mirisetin

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 337892360
Performing search ... done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1   |   -9.2   |    0.000   |    0.000
  2   |   -8.2   |    1.848   |    6.204
  3   |   -8.1   |    3.471   |    8.451
  4   |   -7.8   |    2.459   |    6.218
  5   |   -7.7   |    2.198   |    8.083
  6   |   -7.7   |   12.264   |   16.767
  7   |   -7.6   |    1.821   |    4.563
  8   |   -7.6   |   11.530   |   17.002
  9   |   -7.5   |    2.125   |    8.602
Writing output ... done.

```

Naringenin

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1048958128
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      -9.8      1.188      2.197
3      -9.5      4.811      8.904
4      -9.4      4.961     12.268
5      -9.3      5.183     12.766
6      -9.2      4.754      9.116
7      -9.0      6.319     10.203
8      -8.8      4.580      8.841
9      -8.7      4.444      8.762
Writing output ... done.

```

Hesperitin

```
*log.txt - Notepad
File Edit View

-#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1202140032
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   |   -9.0   |   3.239   |  10.793
  3   |   -9.0   |   1.839   |  11.419
  4   |   -9.0   |   2.952   |  11.230
  5   |   -8.9   |   5.043   |  10.589
  6   |   -8.9   |   6.788   |  10.743
  7   |   -8.5   |   2.869   |   6.074
  8   |   -8.5   |   4.002   |   9.263
  9   |   -8.4   |   3.358   |   6.665
Writing output ... done.
```


Epikatekin

```

log.txt - Notepad
File Edit View

#####
# 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 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 602936112
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   |   -8.8   |    2.358   |    8.119
  3   |   -8.8   |    2.047   |    2.672
  4   |   -8.5   |    2.860   |    3.886
  5   |   -8.4   |   14.749   |   18.303
  6   |   -8.1   |    5.036   |    9.656
  7   |   -8.0   |   15.182   |   18.812
  8   |   -8.0   |   14.296   |   17.761
  9   |   -8.0   |   15.585   |   19.220

Writing output ... done.

```