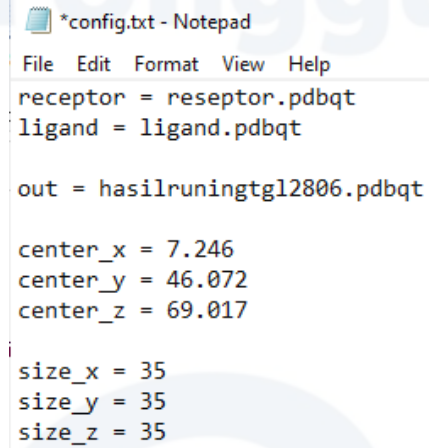


LAMPIRAN**Lampiran 1. Konfigurasi vina pada notepad**

```
*config.txt - Notepad
File Edit Format View Help
receptor = reseptor.pdbqt
ligand = ligand.pdbqt

out = hasilruningtgl2806.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 Format View Help
#
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1781259096
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   |    -9.0   |    2.987   |    6.617
  3   |    -8.8   |    2.350   |    9.944
  4   |    -8.8   |    1.811   |    2.979
  5   |    -8.7   |    2.217   |   10.065
  6   |    -8.7   |    4.340   |   11.573
  7   |    -8.7   |    3.187   |   10.886
  8   |    -8.6   |    4.133   |    7.953
  9   |    -8.6   |    3.444   |    7.664
Writing output ... done.

```

Asam asiatika

```

log.txt - Notepad
File Edit Format View Help
#####
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1222792736
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   |   -8.8   |   3.508   |   7.782
  3   |   -8.2   |   1.677   |   8.291
  4   |   -8.2   |   2.298   |   8.566
  5   |   -8.1   |   3.052   |   8.960
  6   |   -8.0   |   2.667   |   8.241
  7   |   -8.0   |   2.855   |   4.257
  8   |   -7.8   |   4.582   |   8.084
  9   |   -7.8   |   4.771   |   8.814

Writing output ... done.

```

Asiatikosida

```

logasiaticoside.txt - Notepad
File Edit Format View Help
#####
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2005077672
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   |   -9.6   |   6.250   |   9.857
  3   |   -9.6   |   4.041   |   7.574
  4   |   -9.5   |   7.352   |  13.931
  5   |   -9.4   |   4.635   |  14.991
  6   |   -9.3   |   4.518   |   9.504
  7   |   -9.1   |   7.091   |  11.946
  8   |   -9.0   |   3.992   |   7.947
  9   |   -8.9   |   7.638   |  14.015

Writing output ... done.

```

Asam Madasiatik

```

log.txt - Notepad
File Edit Format View Help
#####
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 2010669144
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      -8.4      3.007      5.290
3      -8.2      3.561      6.487
4      -8.1      5.392     10.663
5      -7.8      2.150      8.424
6      -7.7      5.508      8.820
7      -7.5      6.520     10.087
8      -7.5      5.768      9.589
9      -7.5      3.267      9.794

Writing output ... done.

```

Madekasossida

```

logmadeccasoside.txt - Notepad
File Edit Format View Help
#####
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1935593344
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1   |   -10.4   |    0.000   |    0.000
  2   |    -9.7   |    3.620   |    9.588
  3   |    -9.6   |    3.395   |    6.942
  4   |    -9.5   |    3.064   |    9.258
  5   |    -9.4   |    3.240   |    6.180
  6   |    -9.4   |    2.844   |    9.621
  7   |    -9.4   |    5.096   |    7.708
  8   |    -9.1   |    4.294   |    8.886
  9   |    -9.0   |    3.478   |    8.484

Writing output ... done.

```

Asam Madekkasik

```

log.txt - Notepad
File Edit Format View Help
#####
# 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 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1032997808
Performing search ... done.
Refining results ... done.

mode | affinity | dist from best mode
      | (kcal/mol) | rmsd l.b. | rmsd u.b.
-----+-----+-----+-----
  1   |   -8.8   |    0.000   |    0.000
  2   |   -8.7   |    2.955   |    5.314
  3   |   -8.5   |    3.250   |    7.561
  4   |   -8.1   |    3.687   |    5.717
  5   |   -8.0   |    2.417   |    3.704
  6   |   -8.0   |    4.851   |    8.782
  7   |   -7.7   |    3.947   |    6.612
  8   |   -7.6   |    4.945   |    9.568
  9   |   -7.4   |    4.682   |    6.793

Writing output ... done.

```