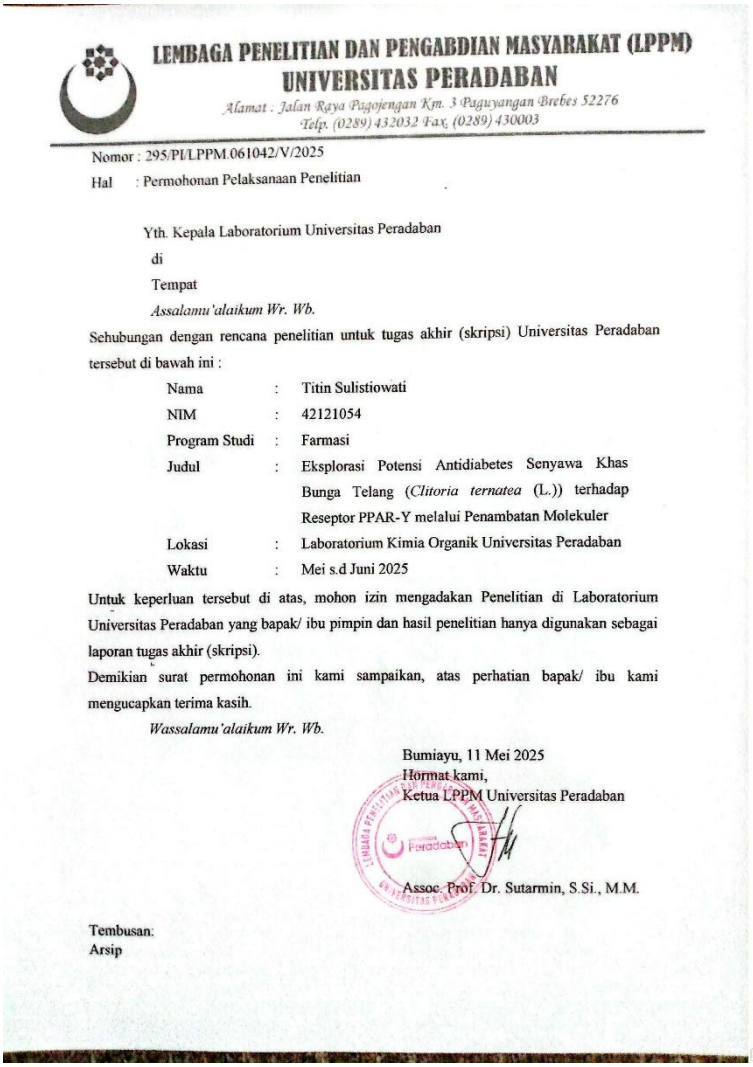
LAMPIRAN-LAMPIRAN

Lampiran 1. Surat Izin Penelitian



LEMBAGA PENELITIAN DAN PENGABDIAN MASYARAKAT (LPPM)
UNIVERSITAS PERADABAN
Alamat : Jalan Raya Pagojengan Km. 3 Paguyangan Brebes 52276
Telp. (0289) 432032 Fax. (0289) 430003

Nomor : 295/PI/LPPM.061042/V/2025
Hal : Permohonan Pelaksanaan Penelitian

Yth. Kepala Laboratorium Universitas Peradaban
di
Tempat
Assalamu'alaikum Wr. Wb.

Sehubungan dengan rencana penelitian untuk tugas akhir (skripsi) Universitas Peradaban tersebut di bawah ini :

Nama	:	Titin Sulistiowati
NIM	:	42121054
Program Studi	:	Farmasi
Judul	:	Eksplorasi Potensi Antidiabetes Senyawa Khas Bunga Telang (*Clitoria ternatea* (L.)) terhadap Reseptor PPAR-Y melalui Penambatan Molekuler
Lokasi	:	Laboratorium Kimia Organik Universitas Peradaban
Waktu	:	Mei s.d Juni 2025

Untuk keperluan tersebut di atas, mohon izin mengadakan Penelitian di Laboratorium Universitas Peradaban yang bapak/ ibu pimpin dan hasil penelitian hanya digunakan sebagai laporan tugas akhir (skripsi).

Demikian surat permohonan ini kami sampaikan, atas perhatian bapak/ ibu kami mengucapkan terima kasih.

Wassalamu'alaikum Wr. Wb.

Bumiayu, 11 Mei 2025
Hormat kami,
Ketua LPPM Universitas Peradaban

Assoc. Prof. Dr. Sutarmin, S.Si., M.M.

Tembusan:
Arsip

Lampiran 2. Surat Keterangan Penelitian

UNIVERSITAS PERADABAN
FAKULTAS SAINS DAN TEKNOLOGI
PROGRAM STUDI FARMASI
Laboratorium Farmasi
(Kimia Farmasi, Farmasetika, Biologi Farmasi, Farmakologi dan Klinis)
Jalan Raya Pagojengan Km. 3 Pagojengan Kab. Brebes 52276, Telp. 0289-432032 Fax. 0289-430003

SURAT KETERANGAN PENELITIAN

NO: 42121054/SKP/LF-UP/VII/2025

Yang bertanda tangan di bawah ini:

Nama : Luthfi Hidayat Maulana, S.KM., M.Si.
Jabatan : Kepala Laboratorium

dengan ini menerangkan bahwa:

Nama : **Titin Sulistiowati**
NIM : 42121054
Tahun Masuk : Data Tidak Ditemukan
Institusi : Prodi Farmasi Universitas Peradaban

benar-benar melakukan penelitian untuk memenuhi tugas Akhir Skripsi yang berjudul:

Ekplorasi Potensi Antidiabetes Senyawa Khas Bunga Telang (Clitoria ternatea (L.)) Terhadap Reseptor PPAR-Y Melalui Penambatan Molekuler

di Laboratorium Farmasi Universitas Peradaban pada tanggal:
05 Mei 2025 dinyatakan telah selesai pada tanggal 05 Juni 2025

Demikian surat keterangan ini dibuat untuk digunakan sebagaimana mestinya.

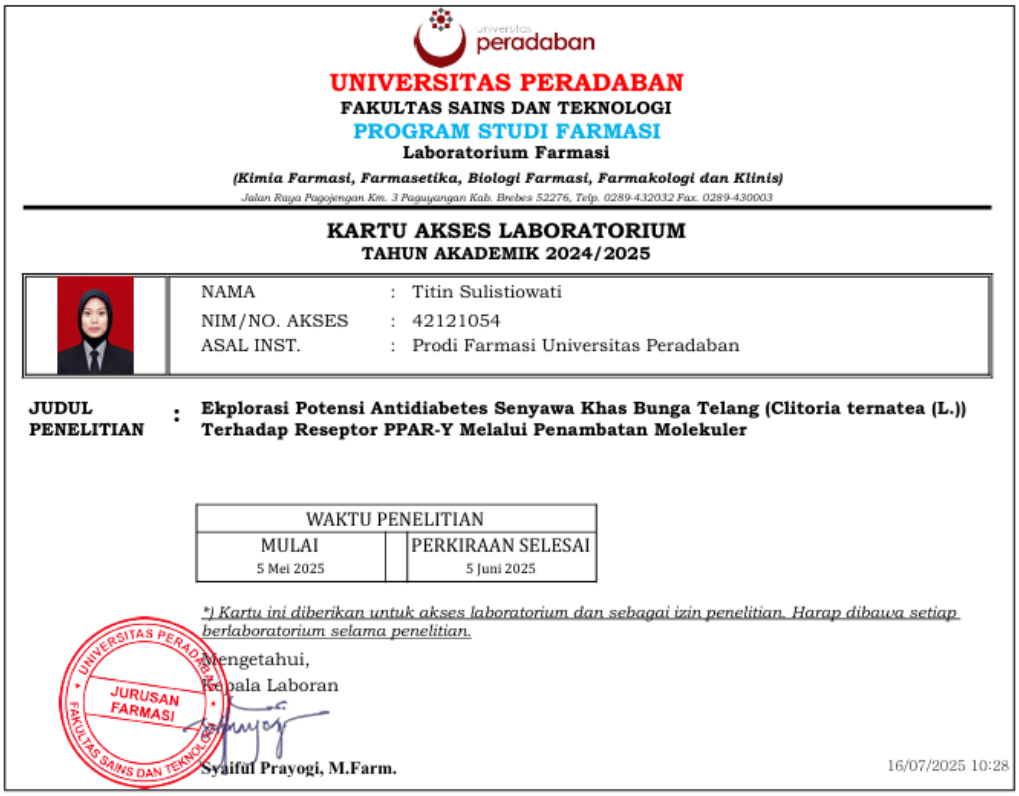
Bumiayu, 16 Juli 2025
Mengetahui,
Kepala Laboratorium

UNIVERSITAS PERADABAN
JURUSAN FARMASI
FAKULTAS SAINS DAN TEKNOLOGI

Luthfi Hidayat Maulana, S.KM., M.Si.

Tanggal permohonan	Tanggal cetak
16/07/2025 11:31:00	16/07/2025 11:31:00

Lampiran 3. Kartu Penelitian



universitas peradaban

UNIVERSITAS PERADABAN
FAKULTAS SAINS DAN TEKNOLOGI
PROGRAM STUDI FARMASI
Laboratorium Farmasi
(Kimia Farmasi, Farmasetika, Biologi Farmasi, Farmakologi dan Klinis)
Jalan Raya Pagojengan Km. 3 Pagujangan Kab. Brebes 52276, Telp. 0289-432032 Fax. 0289-430003

KARTU AKSES LABORATORIUM
TAHUN AKADEMIK 2024/2025

NAMA	:	Titin Sulistiowati
NIM/NO. AKSES	:	42121054
ASAL INST.	:	Prodi Farmasi Universitas Peradaban

JUDUL PENELITIAN : **Ekplorasi Potensi Antidiabetes Senyawa Khas Bunga Telang (Clitoria ternatea (L.)) Terhadap Reseptor PPAR-Y Melalui Penambatan Molekuler**

WAKTU PENELITIAN	
MULAI	PERKIRAAN SELESAI
5 Mei 2025	5 Juni 2025

**) Kartu ini diberikan untuk akses laboratorium dan sebagai izin penelitian. Harap dibawa setiap berlaboratorium selama penelitian.*

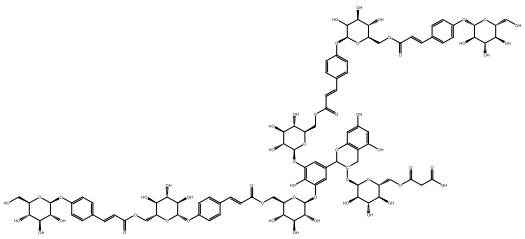
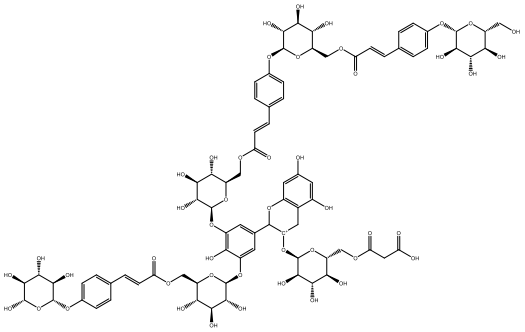
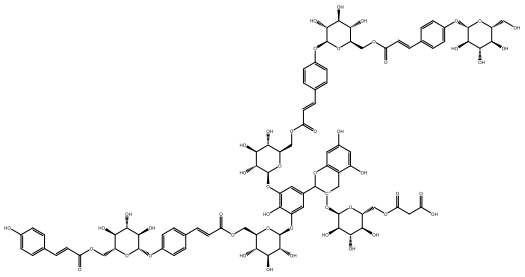
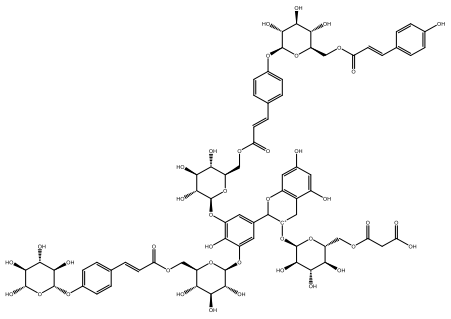
Mengetahui,
Kepala Laboran

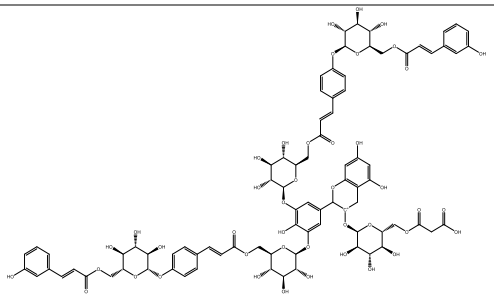
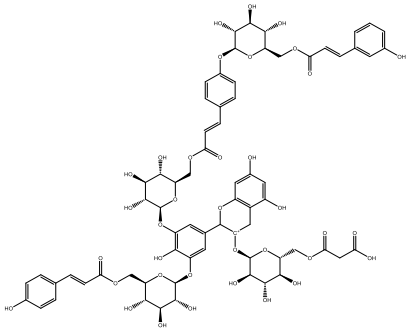
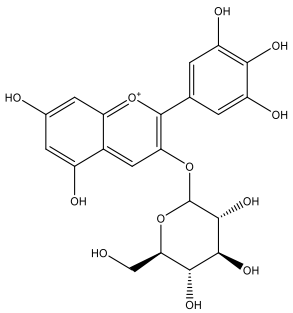
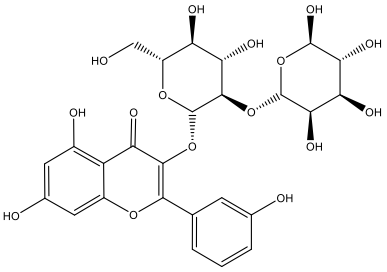
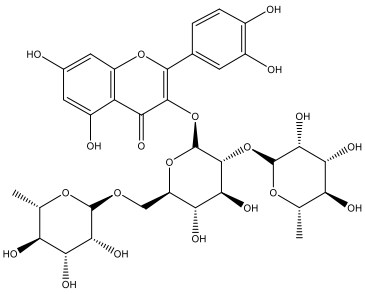
UNIVERSITAS PERADABAN
JURUSAN FARMASI
FAKULTAS SAINS DAN TEKNOLOGI

Syaiful Prayogi, M.Farm.

16/07/2025 10:28

Lampiran 4. Senyawa Uji Bunga Telang dan Hasil Pemodelan Struktur

Struktur	Nama
	Ternatin A1
	Ternatin A2
	Ternatin B1
	Ternatin B2

	Ternatin D1
	Ternatin D2
	Delphinidin 3-Oglucoside
	Kaemferol 3-neohesperidoside
	Quercetin 3-Orutinoside

Lampiran 5. Hasil Penambatan Senyawa Uji dengan Reseptor

Replikasi I

a) Pioglitazone

```
#################################################################
# 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)
Output will be ligan_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -395783872
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        -7.1      3.344     10.059
   3        -7.0      5.193      7.317
   4        -7.0      4.641      7.135
   5        -7.0      8.859     12.058
   6        -6.9      7.536     10.702
   7        -6.9     15.379     17.945
   8        -6.9      7.313     10.219
   9        -6.8      5.001      8.460
  10        -6.7      8.468     11.827
Writing output ... done.
```

b) Ternatin A1

```
#################################################################
# 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)
Output will be ternatina1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 302214376
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        -8.4      3.505     10.874
   3        -7.8      2.262      5.890
   4        -7.7      3.599     10.585
   5        -7.7      2.958     13.231
   6        -7.6      4.438      8.949
   7        -7.6      2.519     12.920
   8        -7.6      3.198      9.795
   9        -7.6      3.363     12.148
  10        -7.6      3.807     11.292
Writing output ... done.
```

c) Ternatin A2

```
#################################################################
# 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)
Output will be terantina2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -758257308
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -11.2      0.000      0.000
   2       -11.1      3.890      6.502
   3       -11.1      4.495     12.124
   4       -11.1      4.714     14.804
   5       -11.0      4.363      9.585
   6       -10.7      5.153     15.165
   7       -10.6      3.892      9.657
   8       -10.5      4.507     12.707
   9       -10.5      3.454     13.493
  10       -10.4      4.916     11.606
```

d) Ternatin B1

```
#################################################################
# 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)
Output will be ternatinb1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 8416316
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        -8.9      2.215      5.397
   3        -8.5      4.261     10.605
   4        -8.3      4.572     12.656
   5        -8.3      2.760      5.705
   6        -8.3      2.282      4.266
   7        -8.2      4.348     13.492
   8        -8.2      2.587      6.709
   9        -8.2      1.590      5.257
  10        -8.1      3.571     12.333
Writing output ... done.
```

e) Ternatin B2

```
#################################################################
# 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)
Output will be ternatinb2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 423266988
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.3      0.000      0.000
   2        -10.2      2.434      7.661
   3        -10.0      2.138      4.943
   4        -10.0      2.094      7.979
   5         -9.9      4.385      9.083
   6         -9.8      3.727     13.451
   7         -9.8      2.718      8.115
   8         -9.8      4.204     10.337
   9         -9.8      3.055     12.749
  10         -9.6      2.364      3.884
Writing output ... done.
```

f) Ternatin D1

```
#################################################################
# 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)
Output will be ternatind1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1837974552
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         -9.9      1.399      2.978
   3         -9.8      3.354     14.198
   4         -9.6      4.313     14.268
   5         -9.6      3.877     11.637
   6         -9.6      4.296     11.340
   7         -9.5      3.530     10.179
   8         -9.4      3.422     10.897
   9         -9.4      3.580     10.247
  10         -9.4      3.233     14.403
Writing output ... done.
```

g) Ternatin D2

```
#################################################################
# 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)
Output will be ternatind2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1883298020
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      2.444      9.467
   3         -7.6      1.448      2.116
   4         -7.5      3.194      6.318
   5         -7.5      3.347      9.293
   6         -7.4      2.683      5.446
   7         -7.4      2.171      9.662
   8         -7.4      1.786      4.447
   9         -7.4      4.954     10.729
  10         -7.4      2.495     10.235
Writing output ... done.
```

h) Delphinidin 3-Oglukoside

```
#################################################################
# 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)
Output will be delphinidin_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1860748556
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      0.967      2.186
   3         -8.6      1.508      5.190
   4         -8.4      3.611      7.927
   5         -8.3      1.498      7.237
   6         -8.3      1.696      5.253
   7         -8.3      1.913      3.192
   8         -8.1      1.508      6.402
   9         -8.0      1.586      5.385
  10         -7.8      2.710      6.141
Writing output ... done.
```

i) Kaemferol 3-neohesperidoside

```
#################################################################
# 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)
Output will be kaemferol_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1161205888
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      1.267      2.301
   3         -9.1      2.278      7.047
   4         -9.0      2.108      6.764
   5         -9.0      2.305      5.472
   6         -8.9      1.686      6.941
   7         -8.8      2.374      7.998
   8         -8.8      2.340      6.863
   9         -8.5      3.137      6.764
  10         -8.4      3.254      7.663
Writing output ... done.
```

j) Quercetin 3 O-rutinoside

```
#################################################################
# 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)
Output will be quercetin3orutinoside_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1717049960
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.5      0.000      0.000
   2        -10.0      1.351      2.070
   3         -9.9      1.366      2.002
   4         -9.8      2.023      8.184
   5         -9.7      1.751      6.641
   6         -9.7      2.069      6.570
   7         -9.6      1.932      8.228
   8         -9.6      2.388      7.845
   9         -9.5      2.368      8.505
  10         -9.5      3.266      8.889
Writing output ... done.
```

Replikasi II

a) Pioglitazon

```
#################################################################
# 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)
Output will be pioglitazone_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 577069252
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         -7.3      3.233      9.963
   3         -7.3      2.496      2.836
   4         -7.1     25.285     27.285
   5         -7.1      5.658      9.702
   6         -7.0      6.740      9.778
   7         -6.9      8.697     11.941
   8         -6.9      5.102      7.084
   9         -6.8      6.977      9.522
  10         -6.8     25.731     27.861
Writing output ... done.
```

b) Ternatin A1

```
#################################################################
# 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)
Output will be ternatina1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 302214376
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         -8.4      3.505     10.874
   3         -7.8      2.262      5.890
   4         -7.7      3.599     10.585
   5         -7.7      2.958     13.231
   6         -7.6      4.438      8.949
   7         -7.6      2.519     12.920
   8         -7.6      3.198      9.795
   9         -7.6      3.363     12.148
  10         -7.6      3.807     11.292
Writing output ... done.
```

c) Ternatin A2

```
#################################################################
# 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)
Output will be terantina2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1643199788
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.3      0.000      0.000
   2        -10.2      4.976     13.398
   3        -10.1      4.178      8.864
   4        -10.0      5.905     12.321
   5        -10.0      3.879      8.578
   6         -9.9      4.684     13.115
   7         -9.9      4.465     14.587
   8         -9.9      3.642      7.661
   9         -9.8      4.934     12.170
  10         -9.7      5.132     11.530
Writing output ... done.
```

d) Ternatin B1

```
#################################################################
# 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)
Output will be ternatinb1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1130211132
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         -9.1      3.873     13.492
   3         -9.1      3.244     14.572
   4         -9.0      3.939      7.571
   5         -8.9      3.364     13.600
   6         -8.9      6.606     13.485
   7         -8.9      3.101     13.967
   8         -8.8      2.883      7.409
   9         -8.8      3.314      8.648
  10         -8.6      2.793      6.033
Writing output ... done.
```

e) Ternatin B2

```
#################################################################
# 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)
Output will be ternatinb2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1966338240
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         -9.1      1.542      2.178
   3         -9.0      3.369     12.462
   4         -9.0      1.187      2.208
   5         -8.9      3.770      9.759
   6         -8.9      3.413     12.414
   7         -8.9      3.326     10.989
   8         -8.8      2.662      7.834
   9         -8.8      3.586      7.006
  10         -8.8      4.139     10.487
Writing output ... done.
```

f) Ternatin D1

```
#################################################################
# 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)
Output will be ternatind1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 346134704
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.2      0.000      0.000
   2         -8.1      2.182     10.108
   3         -8.1      1.976     10.191
   4         -8.0      2.295      6.384
   5         -8.0      2.237      9.910
   6         -7.9      2.464     11.188
   7         -7.9      2.431     11.281
   8         -7.7      2.150      8.868
   9         -7.7      3.407      9.451
  10         -7.5      5.381     12.637
Writing output ... done.
```

g) Ternatin D2

```
#################################################################
# 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)
Output will be ternatind2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1866921824
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         -8.9      4.104      8.998
   3         -8.8      1.326      2.401
   4         -8.8      1.906     10.930
   5         -8.8      2.319      3.874
   6         -8.7      2.859     10.733
   7         -8.7      3.395      8.721
   8         -8.7      2.831      6.915
   9         -8.7      1.488      3.463
  10         -8.7      2.347     11.013
Writing output ... done.
```

h) Delphinidin 3-Oglukoside

```
#################################################################
# 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)
Output will be delphinidin_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 90518032
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      0.967      2.185
   3         -8.6      1.503      6.721
   4         -8.6      1.512      5.192
   5         -8.4      3.631      7.908
   6         -8.3      1.649      7.384
   7         -8.3      1.669      5.371
   8         -8.3      2.321      6.227
   9         -8.3      1.838      7.476
  10         -8.2      3.447      7.605
Writing output ... done.
```

i) Kaemferol 3-neohesperidoside

```
#################################################################
# 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)
Output will be kaemferol_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1635274532
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      1.254      2.294
   3         -9.2      1.442      4.974
   4         -9.1      2.275      7.050
   5         -9.0      2.122      6.790
   6         -8.9      2.289      5.209
   7         -8.8      2.370      7.978
   8         -8.8      3.206      6.772
   9         -8.8      2.353      6.921
  10         -8.8      2.562      7.531
Writing output ... done.
```

j) Quercetin 3 O-rutinoside

```
#################################################################
# 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)
Output will be quercetin3orutinoside_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1072387120
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -10.6      0.000      0.000
   2        -10.4      1.310      1.797
   3         -9.9      1.352      2.001
   4         -9.8      1.758      6.639
   5         -9.5      2.306      7.163
   6         -9.4      2.475      7.813
   7         -9.4      2.304      8.520
   8         -9.4      2.445      7.607
   9         -9.3      1.737      7.410
  10         -9.2      2.925      6.025
Writing output ... done.
```

Replikasi III

a) Pioglitazone

```
#################################################################
# 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)
Output will be pioglitazone_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 767179296
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        -7.5      4.620      5.709
   3        -7.3      3.090     10.123
   4        -7.1      5.147      9.164
   5        -7.0      8.258     11.908
   6        -7.0      7.504     10.260
   7        -6.9      8.106     10.402
   8        -6.8      7.693     10.122
   9        -6.8      7.548      9.616
  10        -6.7      8.515     12.102
Writing output ... done.
```

b) Ternatin A1

```
#################################################################
# 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)
Output will be ternatina1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -971437540
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       -10.0      3.892      8.108
   3       -10.0      1.482      2.073
   4        -9.9      3.812      8.612
   5        -9.9      4.188     13.670
   6        -9.9      4.063     13.765
   7        -9.8      4.344     11.741
   8        -9.8      4.004      8.168
   9        -9.8      2.953      9.295
  10        -9.8      3.165      8.183
Writing output ... done.
```

c) Ternatin A2

```
#################################################################
# 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)
Output will be terantina2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 356160220
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      4.801     12.252
   3        -9.7      4.731     12.368
   4        -9.5      4.013     11.240
   5        -9.4      1.297      2.648
   6        -9.4      4.535     10.728
   7        -9.2      4.490     13.830
   8        -9.2      4.570     11.932
   9        -9.2      4.359     11.059
  10        -9.1      4.263      9.875
Writing output ... done.
```

d) Ternatin B1

```
#################################################################
# 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)
Output will be ternatinb1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 775073888
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      1.489      2.106
   3        -9.7      1.463      5.135
   4        -9.5      3.958      9.870
   5        -9.4      3.795      8.793
   6        -9.4      3.627      9.653
   7        -9.4      2.741      9.460
   8        -9.3      4.244      9.993
   9        -9.3      3.932      9.727
  10        -9.1      4.802     14.683
Writing output ... done.
```

e) Ternatin B2

```
#################################################################
# 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)
Output will be ternatinb2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1303837752
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -11.4      0.000      0.000
   2        -10.8      2.754     12.642
   3        -10.8      4.502      9.813
   4        -10.8      1.386      2.759
   5        -10.7      4.579      9.114
   6        -10.6      4.192     10.234
   7        -10.5      4.570     10.016
   8        -10.5      2.887     12.997
   9        -10.4      3.788      8.635
  10        -10.4      3.993      8.638
Writing output ... done.
```

f) Ternatin D1

```
#################################################################
# 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)
Output will be ternatind1_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 861199440
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         -9.4      3.080     11.394
   3         -9.4      3.297     11.730
   4         -9.3      3.666     12.393
   5         -9.3      3.326     10.142
   6         -9.3      3.359     12.185
   7         -9.2      3.008     11.094
   8         -9.2      2.860     12.005
   9         -9.1      2.882     11.916
  10         -9.1      3.043     10.471
Writing output ... done.
```

g) Ternatin D2

```
#################################################################
# 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)
Output will be ternatind2_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -685269324
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      4.973     13.766
   3         -9.7      4.126     11.059
   4         -9.7      1.360      3.367
   5         -9.7      4.084     10.068
   6         -9.6      4.206      9.417
   7         -9.6      4.483     11.297
   8         -9.5      4.998     10.290
   9         -9.5      3.999      9.224
  10         -9.4      2.175      6.620
Writing output ... done.
```

h) Delphinidin 3-Oglukoside

```
#################################################################
# 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)
Output will be delphinidin_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 636162668
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      0.966      2.186
   3         -8.6      1.503      5.181
   4         -8.6      1.519      6.613
   5         -8.5      3.609      7.899
   6         -8.5      1.719      5.930
   7         -8.2      1.777      3.023
   8         -8.0      3.411      8.003
   9         -7.7     20.598     22.451
  10         -7.7      2.482      6.092
Writing output ... done.
```

i) Kaemferol 3-neohesperidoside

```
#################################################################
# 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)
Output will be kaemferol_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1632414368
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      1.464      4.938
   3        -9.1      2.088      5.045
   4        -9.1      2.267      7.033
   5        -9.0      2.153      6.778
   6        -8.9      2.330      5.542
   7        -8.9      2.348      7.994
   8        -8.8      2.663      7.529
   9        -8.7      2.531      7.031
  10        -8.7      1.623      2.716
Writing output ... done.
```

j) Quercetin 3-Orutinoside

```
#################################################################
# 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)
Output will be quercetin3orutinoside_out.pdbqt
Detected 2 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 403652688
Performing search ... done.
Refining results ... done.
mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -10.6      0.000      0.000
   2        -9.9      1.361      2.018
   3        -9.8      1.762      6.634
   4        -9.7      2.085      6.584
   5        -9.6      2.302      7.156
   6        -9.4      2.362      7.605
   7        -9.4      2.140      7.624
   8        -9.3      2.345      7.839
   9        -9.1      2.272      8.023
  10        -9.1      2.953      7.984
Writing output ... done.
```

RATA-RATA REPLIKASI

***Scoring docking* (Kcal/mol)**

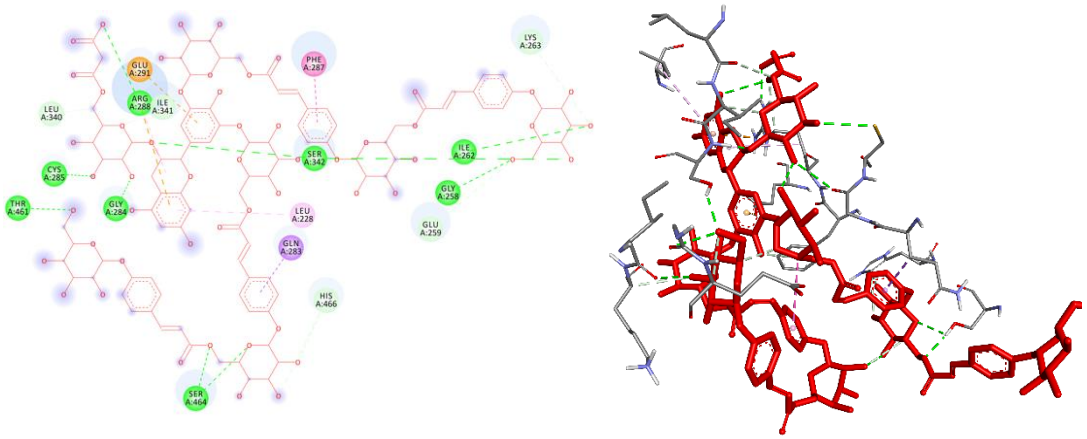
Replikasi	TernatinA1	TernatinA2	TernatinB1	TernatinB2	TernatinD1	TernatinD2	Delphinidin 3-Oglucoside	Kaemferol 3 neohesperidoside	Quercetin 3 - Orutinoside	ligand alami (pioglitazone)
1	-8,5	-11,2	-9	-10,3	-10	-7,9	-8,8	-9,7	-10,5	-7,6
2	-8,5	-10,3	-9,2	-9,2	-8,2	-9,1	-8,8	-9,7	-10,6	-7,6
3	-10	-9,9	-9,9	-11,4	-9,5	-10	-8,8	-9,7	-10,6	-7,5
JUMLAH	-27	-31,4	-28,1	-30,9	-27,7	-27	-26,4	-29,1	-31,7	-22,7
RATA-RATA	-9	-10,466667	-9,36666667	-10,3	-9,2333333	-9	-8,8	-9,7	-10,56667	-7,566666667

Lampiran 6. Hasil Visualisasi Interaksi Ligan-Reseptor

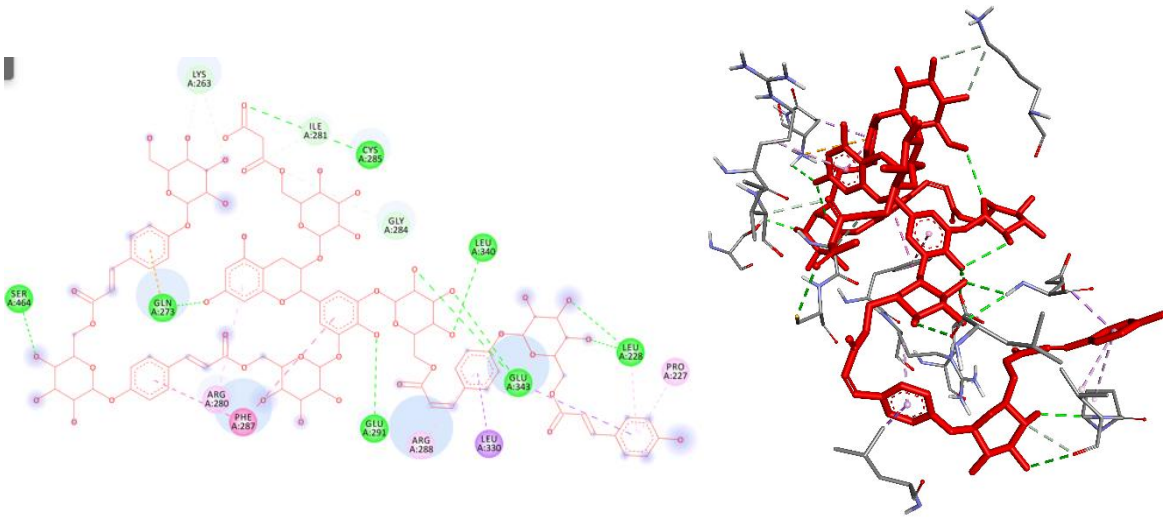
Senyawa	Ikatan yang dihasilkan	
	Ikatan Hidrogen	**Interaksi lain (Ikatan Hidrofobik/ Elektrostatik**
Pioglitazone (Ligand Reference)	**Ser342**, **Cys285**	**Ile341**, **Arg288,** Met464, His449, **Leu330**, Phe363, Gly284
Ternatin A1	**Cys285,** Thr461, Gly284, Leu340, Arg288, Ile341, Ser464, Ser342, His466, Glu259, Gly258, Ile262, Lys263,	Gln283, Phe287, Leu228, Glu291
Ternatin A2	**Cys285**, Lys263, Gln283, Gln286, Ser464, Thr461, Ser274, Asp462, Glu276, His466, Gln294, Glu291, Glu295, Glu343, **Arg288**, Glu259, Lys275	**Ile341**
Ternatin B1	Ser464, Gln273, Glu291, Glu343, Leu228, Leu340, Gly284, **Cys285**, Ile281, Lys263	Arg280, Phe287, **Arg288**, **Leu330**, Pro227
Ternatin B2	Glu259, Lys263, Asp260, Gly284, Gln273, **Cys285**, Met329, **Arg288**, Leu340, **Ser342**, Arg280	Lys275, Phe287, Ile281, Ile341, Met348, Ala292, **Leu330**
Ternatin D1	Leu340, Glu291, **Cys285, Ser342**, His466, Ser464, Gln273, **Arg288**, Glu343, Gln345	Arg280, **Ile341**, Gly284, Phe287
Ternatin D2	Glu460, Thr461, Ser464, Gln273, Gly258, **Ser342**, Glu259, Glu291, Phe287,	Ile279, Arg280, **Ile341,**
Delphinidine 3-Oglukoside	**Cys285, Ser342,** Glu259, Glu291, **Arg288**	**Ile341,** Met364
Kaemferol 3-Neohesperodoside	**Arg288, Cys285**	Val339, **Ile341**, Ile281, Met348
Quercetin 3-Orutinoside	Ser342**, Gln283, Ser274, Gln273,** Arg288**,** Ile341**,** Cys285**, Gly284, Glu259, Ile262**	Phe287

Keterangan: Cetak tebal merupakan asam amino yang mirip dengan ligan referensi, seluruh senyawa antosianin dan flavonoid bunga telang memiliki kesamaan asam amino (Ser342, Cys285, Arg288, Ile341, Leu330) dan tidak ditemukan senyawa yang mengikat reseptor pada asam amino kunci full agonist (Tyr473, His323 His449), oleh karena itu seluruh senyawa bunga telang ini termasuk dalam agonis parsial *selective PPAR modulator* (SPPARMs) dengan resiko efek samping yang ditimbulkan akan kecil, namun harus ada pengujian lanjutan.

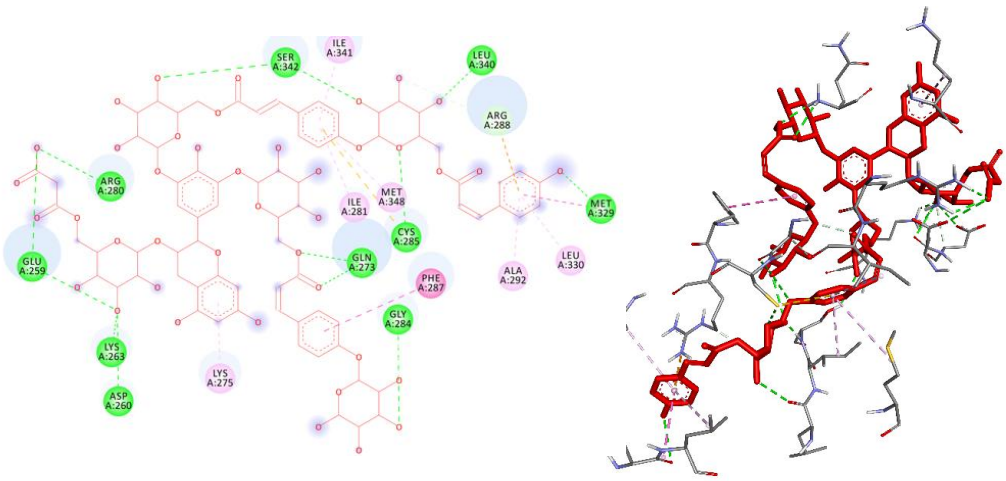
Lampiran 7. Hasil Visualisasi 2D dan 3D Senyawa Uji Bunga Telang



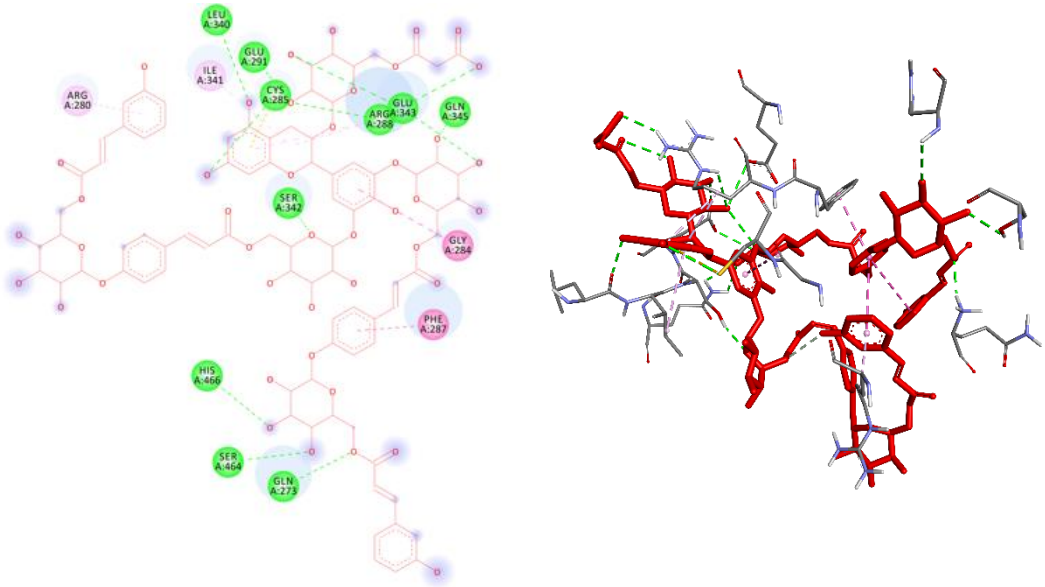
Senyawa Ternatin A1 2D kiri & 3D kanan



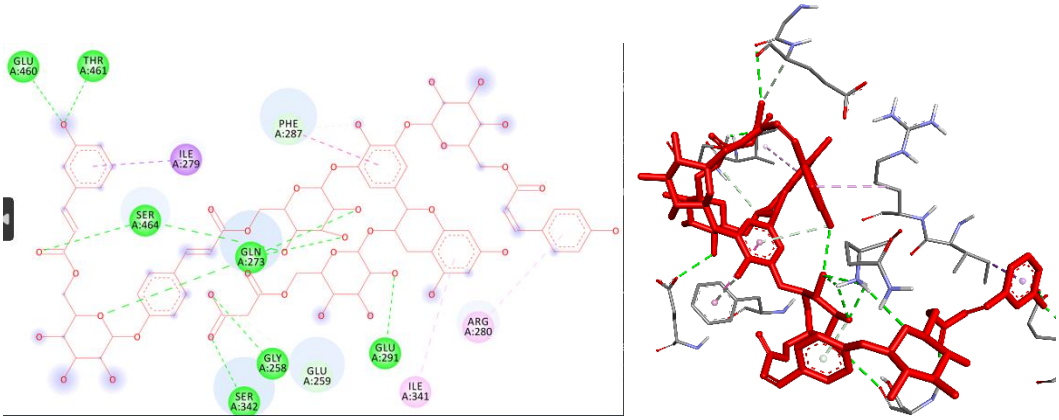
Senyawa Ternatin B1 2D kiri & 3D kanan



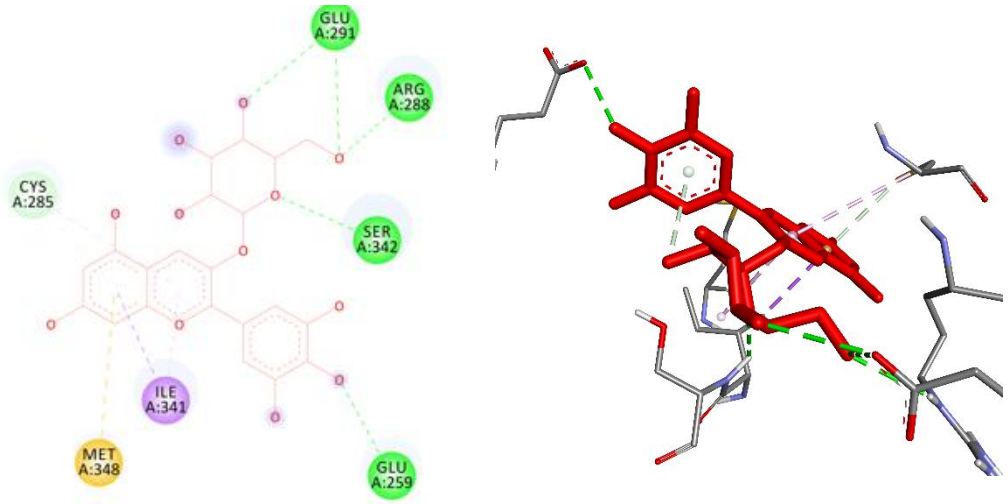
Senyawa Ternatin B2 2D kiri & 3D kanan



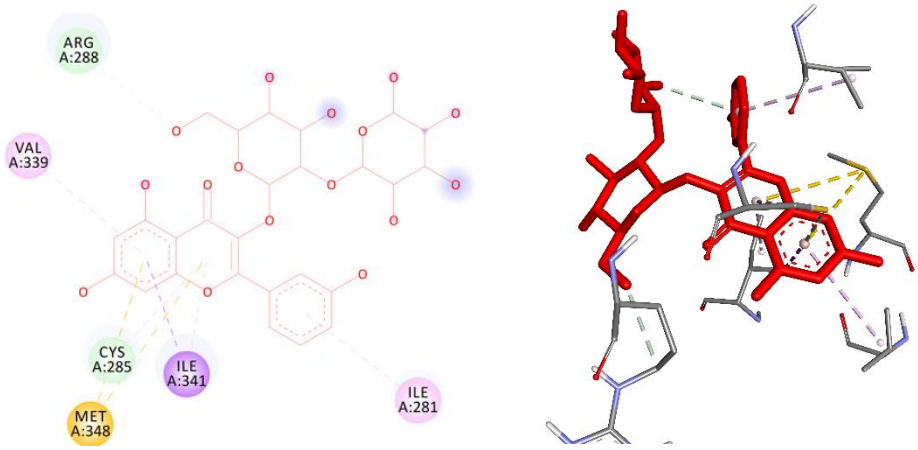
Senyawa Ternatin D1 2D kiri & 3D kanan



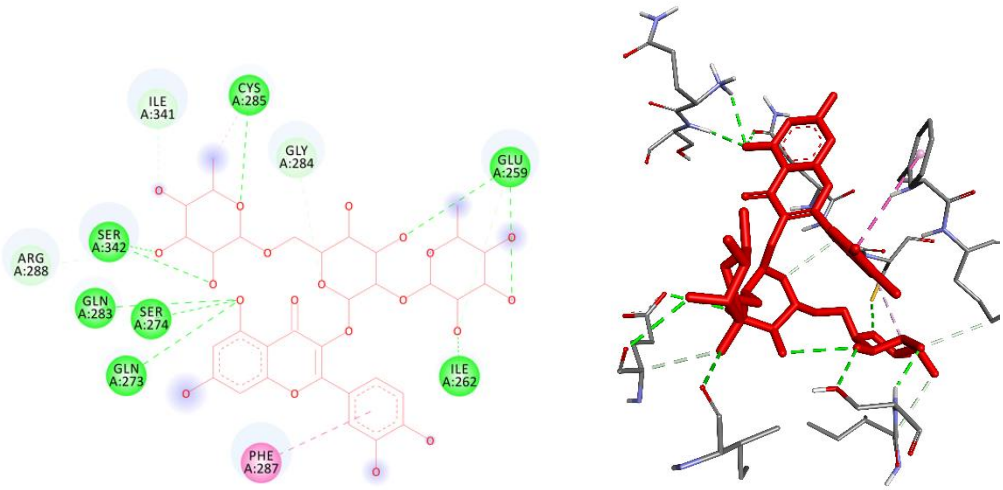
Senyawa Ternatin D2 2D kiri & 3D kanan



Senyawa Delphinidine 3-Oglukoside 2D kiri & 3D kanan



Senyawa Kaemferol 3-neohesperidoside 2D kiri & 3D kanan



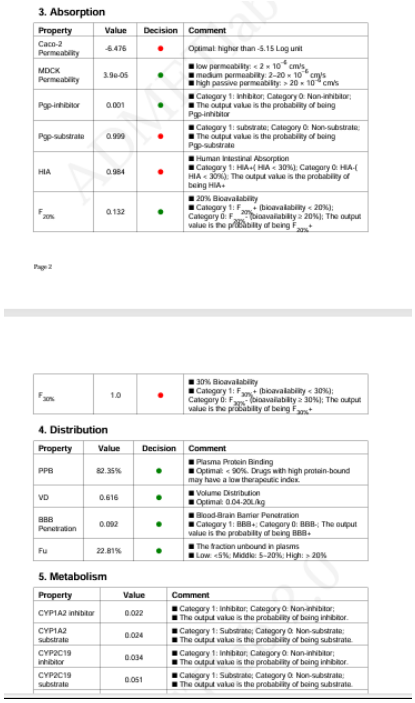
Senyawa Quercetin 3-Orutinoside 2D kiri & 3D kanan

Interactions

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

Lampiran 8. Hasil Prediksi ADME

a) Ternatin A1



3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-6.476	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	3.9e-05	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.001	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.999	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.984	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.132	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$-(bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

Page 2

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$-(bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

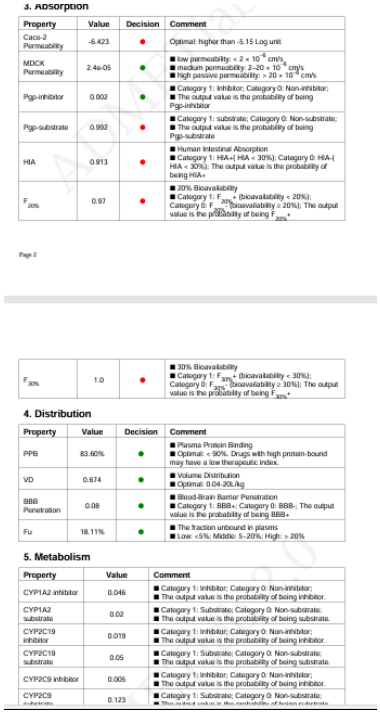
4. Distribution

Property	Value	Decision	Comment
PPB	82.35%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.616	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.092	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	22.81%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.022	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.024	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.034	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.051	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

b) Ternatin A2



3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-6.423	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	2.4e-05	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.002	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.992	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.913	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.97	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$-(bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

Page 2

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$-(bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

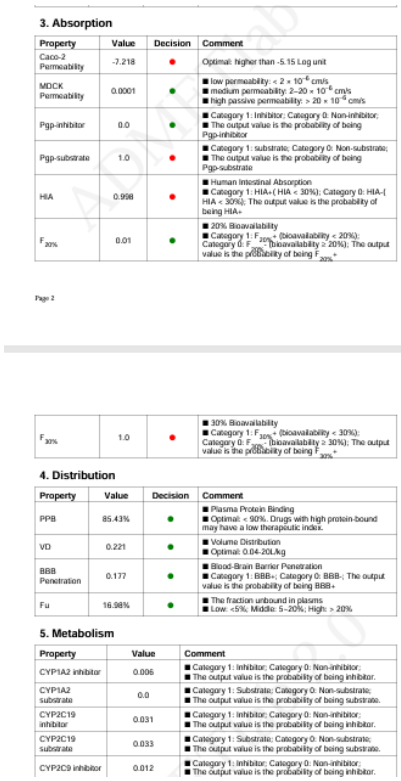
4. Distribution

Property	Value	Decision	Comment
PPB	83.60%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.674	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.08	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	18.11%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.046	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.02	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.019	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.05	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.005	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C9 substrate	0.123	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

c) Ternatin B1



3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.218	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	0.0001	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.998	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{30\%}$	0.01	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$-(bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

Page 2

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$-(bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

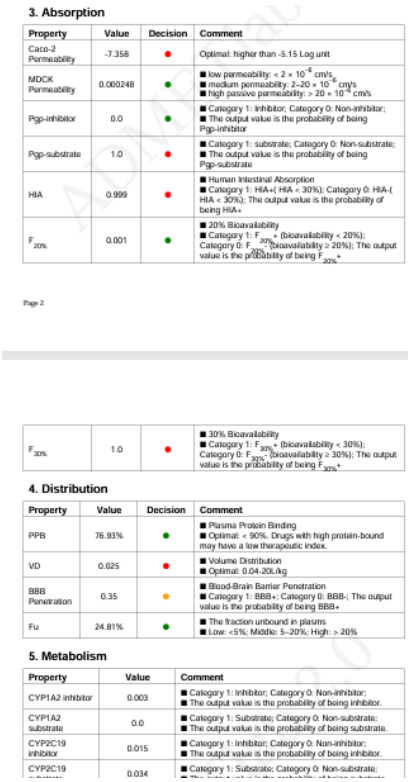
4. Distribution

Property	Value	Decision	Comment
PPB	85.43%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.221	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.177	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	16.98%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.006	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.031	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.033	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.012	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

d) Ternatin B2



3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.358	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	0.000248	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.999	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.001	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$-(bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

Page 2

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$-(bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	76.93%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.025	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.35	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	24.81%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.003	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.015	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.034	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

e) Ternatin D1

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.328	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	0.00012	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	1.0	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.003	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$- (bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$- (bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	86.76%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.001	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.182	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	19.38%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.007	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.022	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.03	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.01	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

f) Ternatin D2

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.173	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	5.7e-05	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.999	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.036	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$- (bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$- (bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	92.79%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.184	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.079	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	10.56%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.011	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.039	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.027	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.105	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

g) Delphinidin 3-Oglukoside

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-6.473	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	5e-06	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.005	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	0.691	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.844	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.993	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$- (bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$- (bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	88.57%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.717	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.019	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	16.59%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.166	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.036	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.013	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.048	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.

h) Kaemferol 3-neohesperidoside

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.461	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	0.000254	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2–20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	1.0	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.0	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$- (bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$- (bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	79.08%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	-0.234	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.37	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	28.20%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5–20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.003	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.01	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.031	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.0	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

i) Quercetin 3-Orutinoside

3. Absorption

Property	Value	Decision	Comment
Caco-2 Permeability	-7.084	●	Optimal: higher than -5.15 Log unit
MDCK Permeability	4e-05	●	■ low permeability: < 2 × 10^{-6} cm/s ■ medium permeability: 2~20 × 10^{-6} cm/s ■ high passive permeability: > 20 × 10^{-6} cm/s
Pgp-inhibitor	0.0	●	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being Pgp-inhibitor
Pgp-substrate	1.0	●	■ Category 1: substrate; Category 0: Non-substrate; ■ The output value is the probability of being Pgp-substrate
HIA	0.991	●	■ Human Intestinal Absorption ■ Category 1: HIA+(HIA < 30%); Category 0: HIA-(HIA < 30%); The output value is the probability of being HIA+
$F_{20\%}$	0.059	●	■ 20% Bioavailability ■ Category 1: $F_{20\%}$+ (bioavailability < 20%); Category 0: $F_{20\%}$-(bioavailability ≥ 20%); The output value is the probability of being $F_{20\%}$+

Page 2

$F_{30\%}$	1.0	●	■ 30% Bioavailability ■ Category 1: $F_{30\%}$+ (bioavailability < 30%); Category 0: $F_{30\%}$-(bioavailability ≥ 30%); The output value is the probability of being $F_{30\%}$+

4. Distribution

Property	Value	Decision	Comment
PPB	89.60%	●	■ Plasma Protein Binding ■ Optimal: < 90%. Drugs with high protein-bound may have a low therapeutic index.
VD	0.414	●	■ Volume Distribution ■ Optimal: 0.04-20L/kg
BBB Penetration	0.082	●	■ Blood-Brain Barrier Penetration ■ Category 1: BBB+; Category 0: BBB-; The output value is the probability of being BBB+
Fu	9.758%	●	■ The fraction unbound in plasms ■ Low: <5%; Middle: 5~20%; High: > 20%

5. Metabolism

Property	Value	Comment
CYP1A2 inhibitor	0.011	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP1A2 substrate	0.0	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C19 inhibitor	0.033	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.
CYP2C19 substrate	0.031	■ Category 1: Substrate; Category 0: Non-substrate; ■ The output value is the probability of being substrate.
CYP2C9 inhibitor	0.104	■ Category 1: Inhibitor; Category 0: Non-inhibitor; ■ The output value is the probability of being inhibitor.

Lampiran 9. Hasil Prediksi Toksisitas

a) Ternatin A1

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

b) Ternatin A2

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

c) Ternatin B1

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

d) Ternatin B2

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

e) Ternatin D1

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

f) Ternatin D2

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

g) Delphinidin 3-Oglukoside

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	YES

h) Kaemferol 3-neohesperidoside

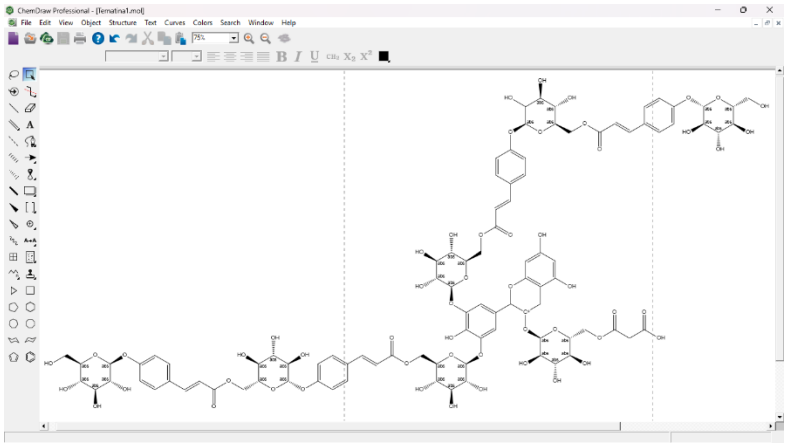
Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	NO

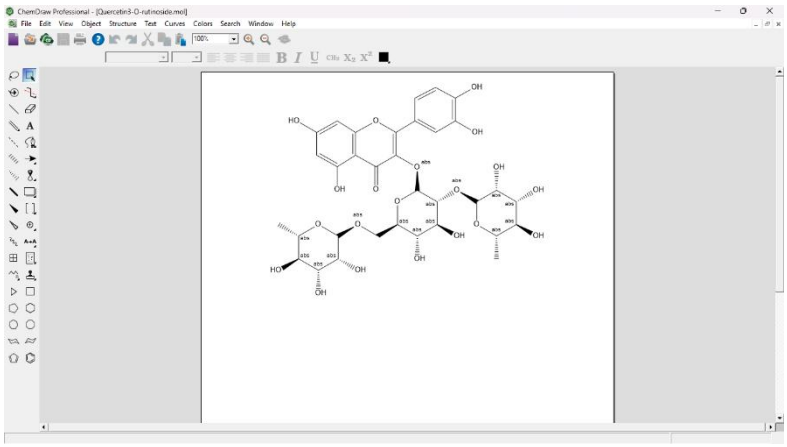
i) Quercetin 3-Orutinoside

Available structure attributes	
Cramer rules	High (Class III)
Error when applying the ...	NO
For a better assessment ...	NO
Negative for genotoxic c...	YES
Negative for nongenoto...	YES
No alerts for S. typhimuri...	NO

Lampiran 10. Dokumentasi Penelitian

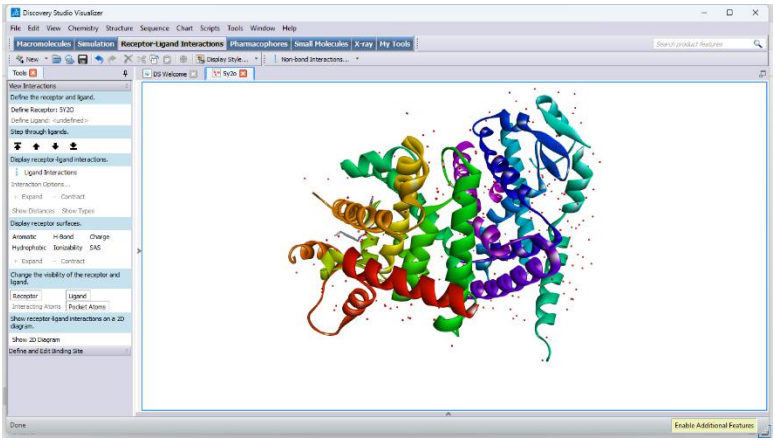
a. Pemodelan Struktur Senyawa Uji Bunga Telang



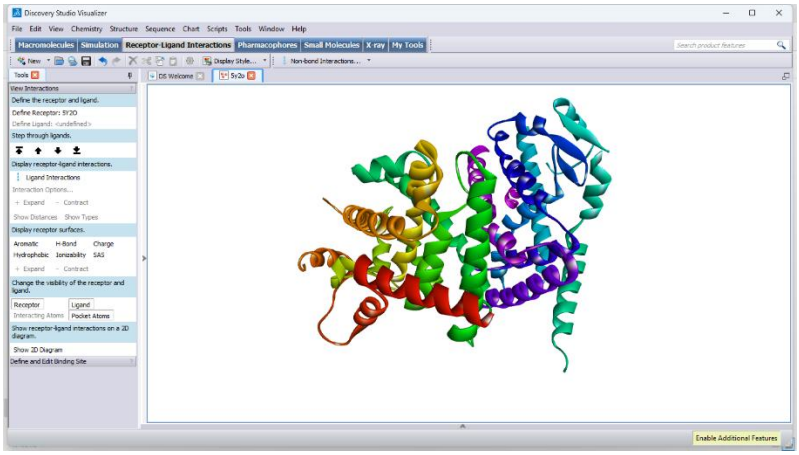


b. Preparasi Reseptor PPAR-γ

Pengunduhan Reseptor PPAR-γ pada laman PDB (https://www.rcsb.org/) dengan ID 5Y2O

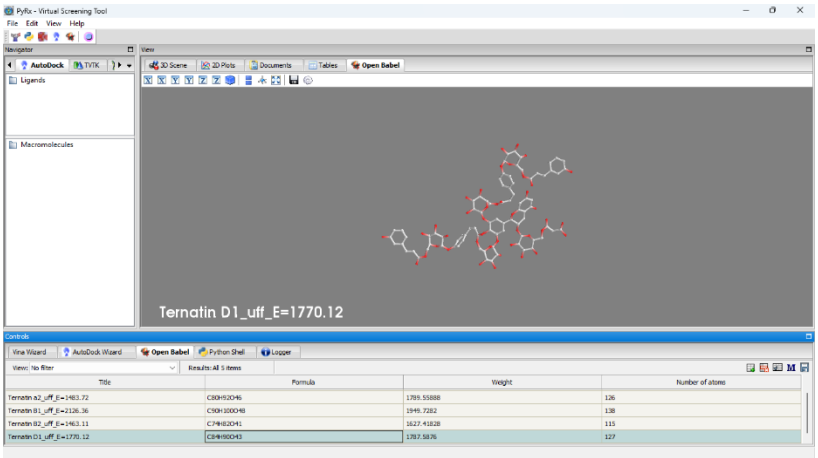


Reseptor sebelum dipreparasi

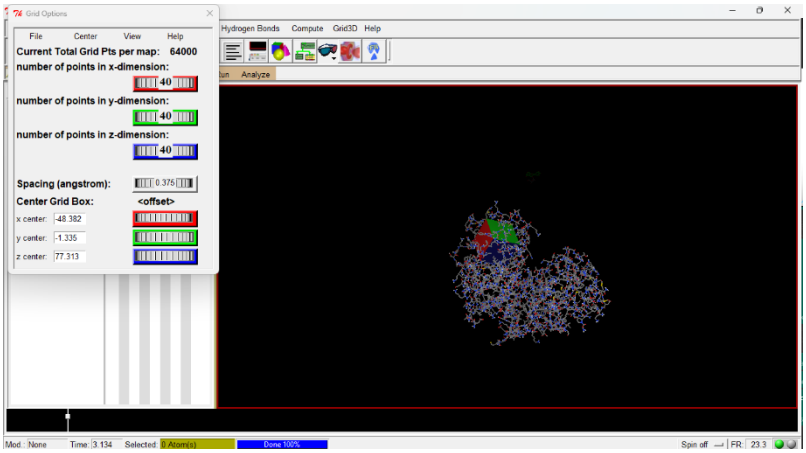


Reseptor setelah dipreparasi

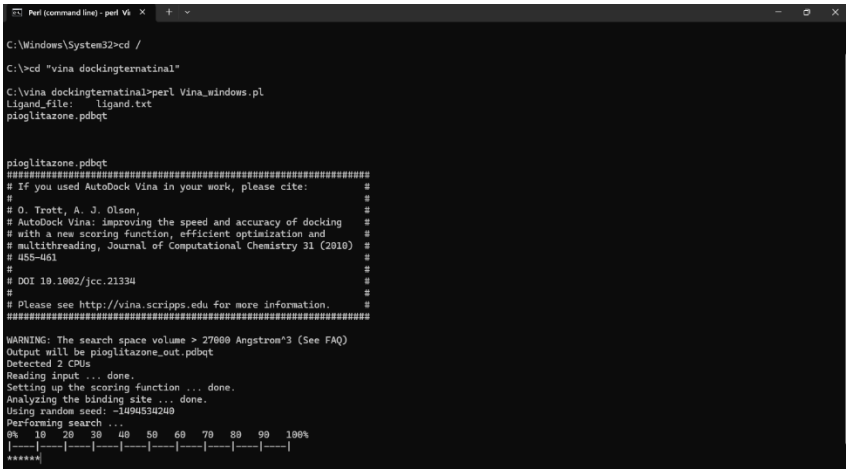
c. Optimasi Senyawa Uji



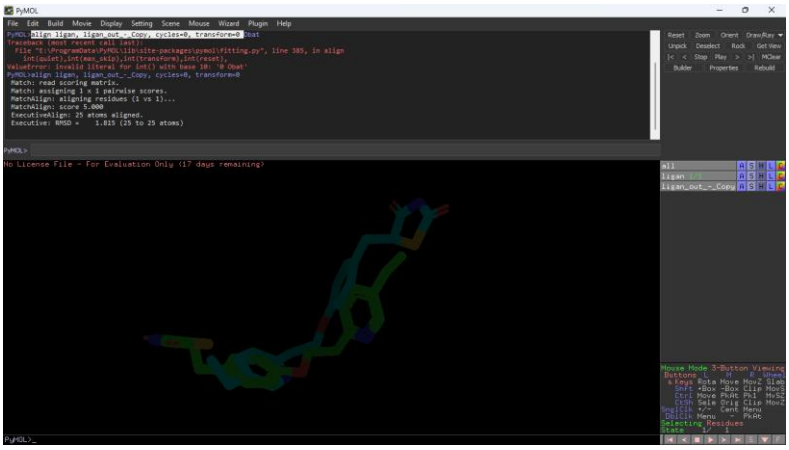
d. Validasi *Docking*



Pengaturan Gridbox Menggunakan Autodock Tools

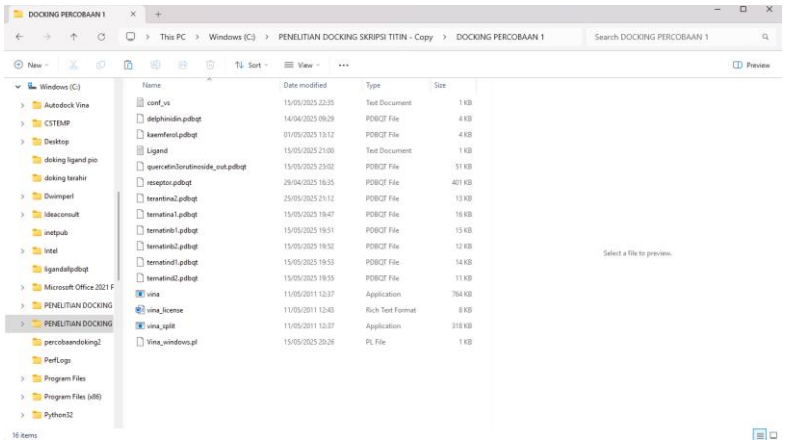


Re-*docking* Ligand Alami

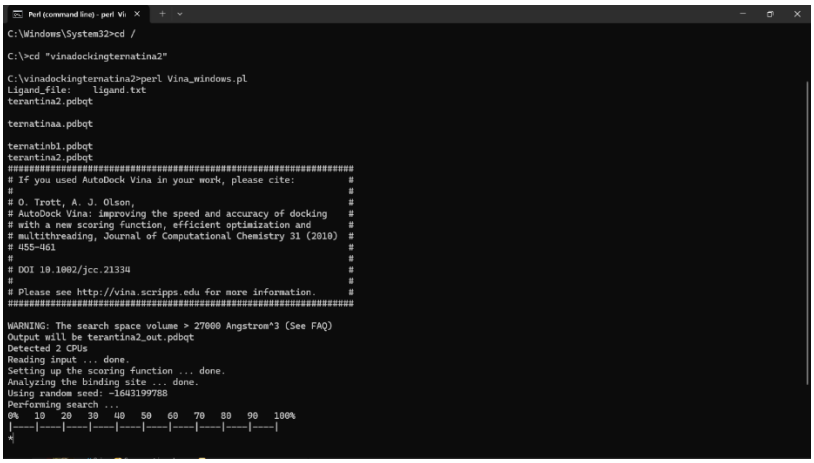


Perhitungan Nilai RMSD Menggunakan PYMOL

e. Penambatan Ligand-Reseptor

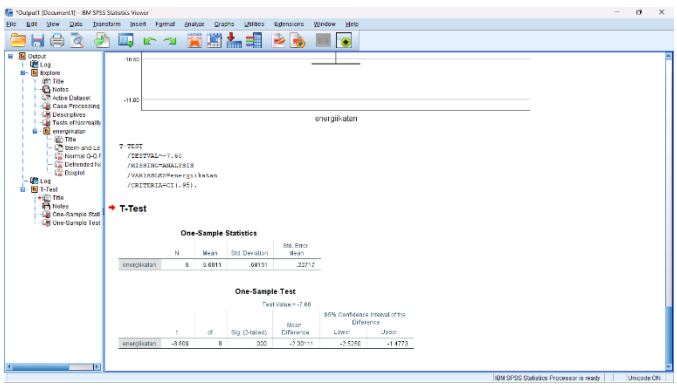


Penyiapan File *Docking*

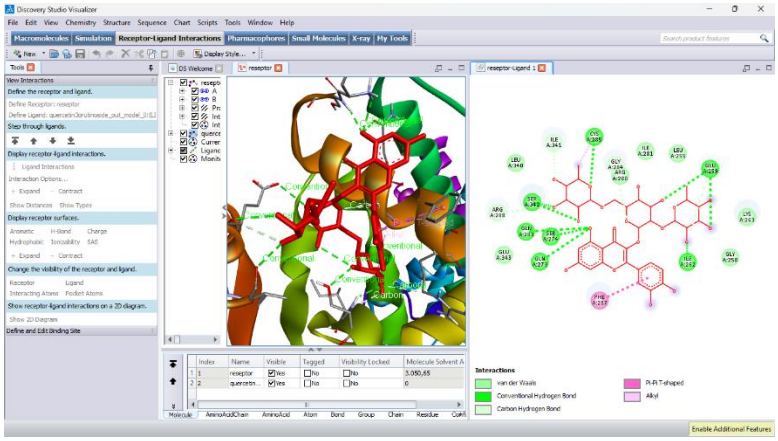


Tampilan cmd Vina Windows perl, ketikan nama file yang sudah disiapkan (“vinadockingternatina2”) kemudian ketikan perintah “Ligand.txt”

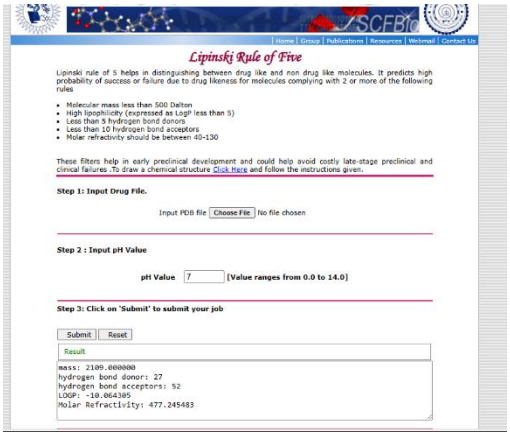
f. Uji *Independent T-Test*



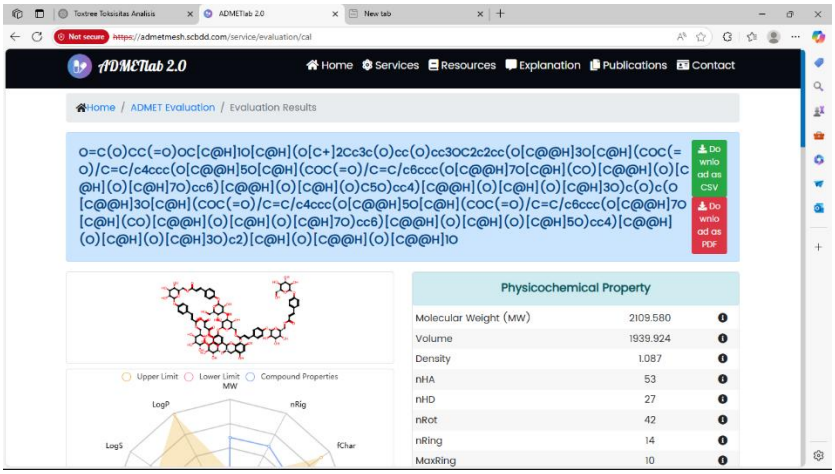
g. Visualisasi hasil



h. Pengujian Aturan *Lipinski Rule of Five*

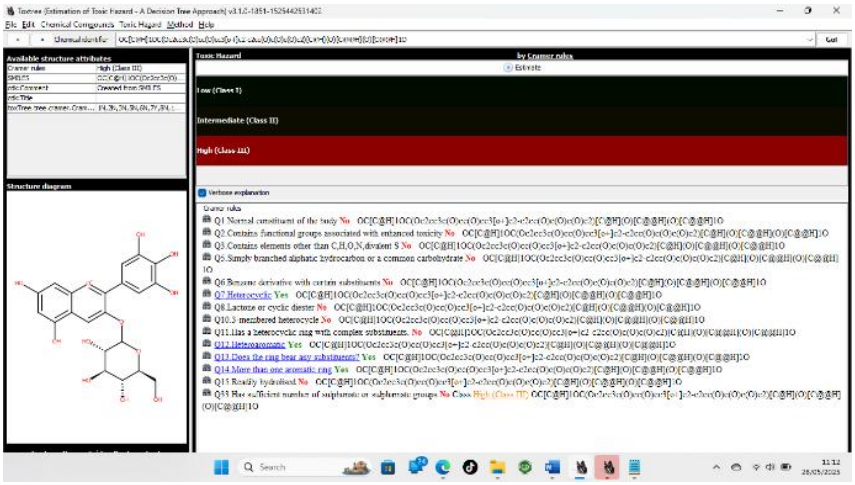


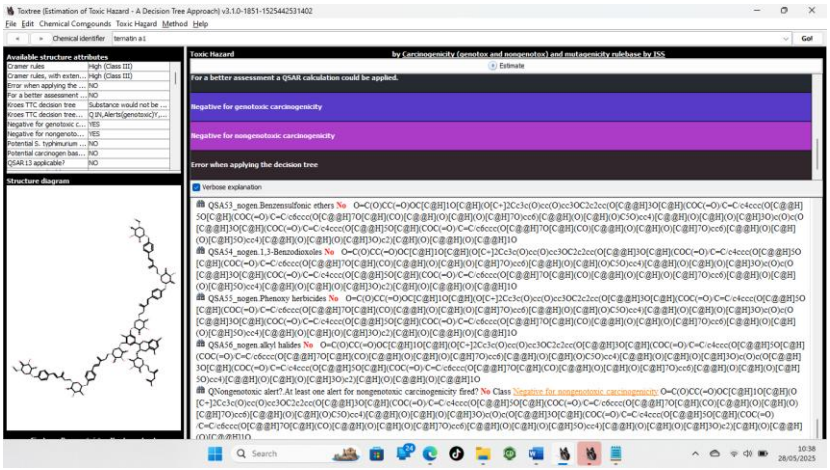
i. Prediksi ADME

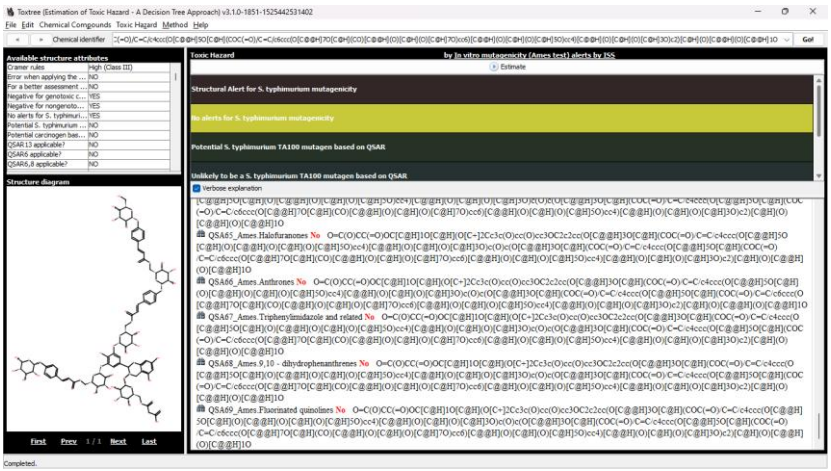


Tampilan Prediksi ADME Menggunakan ADMETlab 2.0 dengan Memasukan Kode SMILES Senyawa dan unduh hasil dalam bentuk pdf

j. Prediksi Toksisitas







Lampiran 11. Biodata Penulis

Nama	: Titin Sulistiowati
Tempat, tanggal lahir	: Brebes, 16 Oktober 2003
Jenis kelamin	: Perempuan
Alamat	: Desa Kaliloka RT 01/ RW 03 Manggis, Kec. Sirampog Kab. Brebes Jawa Tengah 52272
Agama	: Islam
No. WA	: 085727872381
Email	: titinnafsi@gmail.com
Riwayat Pendidikan	: 1. Sekolah Dasar Negeri Kaliloka (2009-2015)
	2. Sekolah Menengah Pertama Al-Hikmah Benda 01 (2015-2018)
	3. Sekolah Menengah Kejuruan Semesta Bumiayu-Jurusan Farmasi (2018-2021)
	4. Universitas Peradaban (2021-2025)
Pengalaman Pekerjaan	: 1. Asisten Apoteker Praktek Kerja Lapangan Puskesmas Sirampog (2019)
	2. Asisten Apoteker Praktek Kerja Lapangan Apotek Barokah (2019)
	3. Pengajar Bimbel UV Course Mendala (2022)
	4. Asisten Laboratorium Farmasi Fisik (2022)
	5. Asisten Laboratorium Mikrobiologi Farmasi (2022)
	6. Asisten Laboratorium Kimia Analisis II (2024)
	7. Asisten Apoteker Praktek Kerja Lapangan Rumah Sakit Harapan Sehat Bumiayu (2024)

Lampiran 12. Keterangan Bebas Plagiasi

universitas peradaban | PERPUSTAKAAN

SURAT KETERANGAN PENGECEKAN *SIMILARITY*
Nomor : 119/CP/E.5/K.BP/061042/VIII/2025

Setelah melalui proses pengecekan dengan menggunakan aplikasi Turnitin, dengan ini menerangkan bahwa skripsi yang ditulis oleh:

Nama Penulis	: TITIN SULISTIOWATI
NIM	: 42121054
Program Studi	: FARMASI
Judul Skripsi	: EKSPLORASI POTENSI ANTIDIABETES SENYAWA KHAS BUNGA TELANG (Clitoria ternatea (L.)) TERHADAP RESEPTOR PPAR-Y MELALUI PENAMBATAN MOLEKULER
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Demikian surat keterangan ini, untuk dipergunakan sebagaimana mestinya.

Paguyangan, 31 Agustus 2025
Kepala Unit Layanan Perpustakaan

Muhamad Nidzomuddin, S.Sos.
NIPY : 11.012.049

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