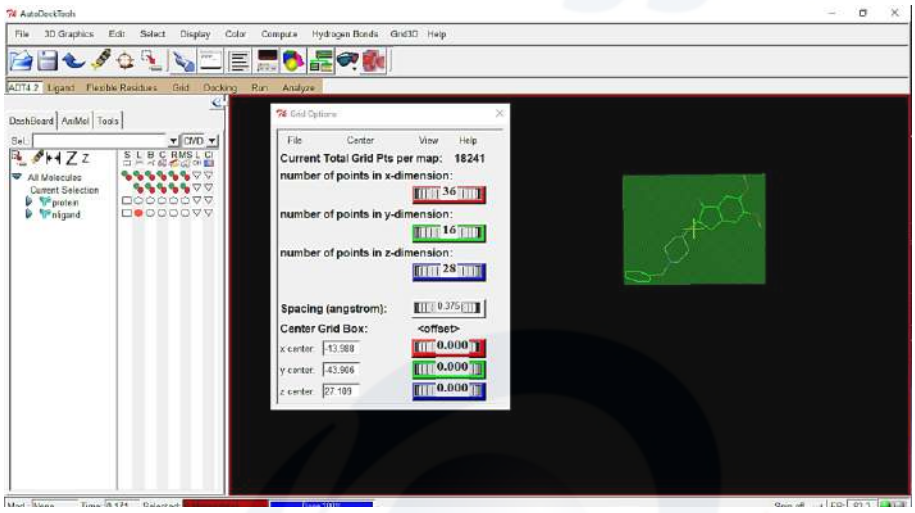
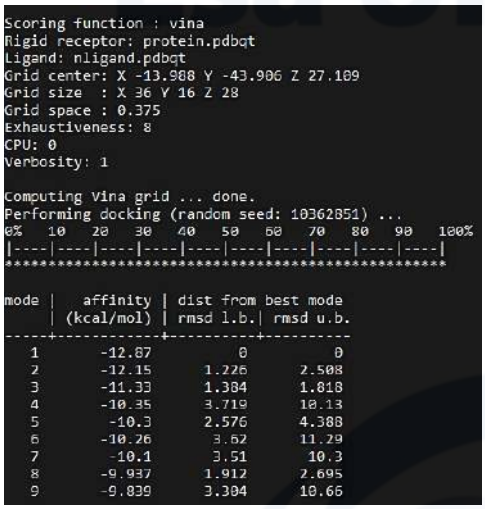
LAMPIRAN

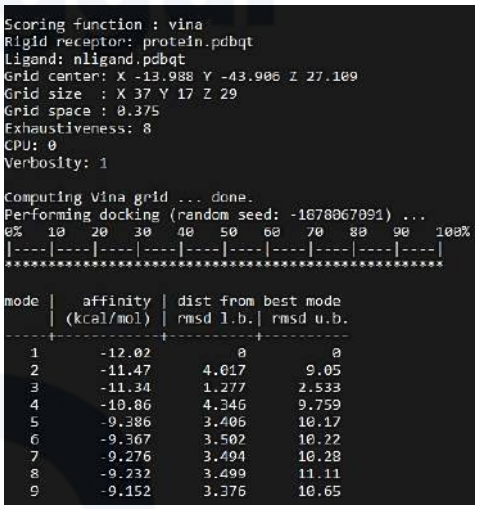
Lampiran 1. *Grid box* ligan asli



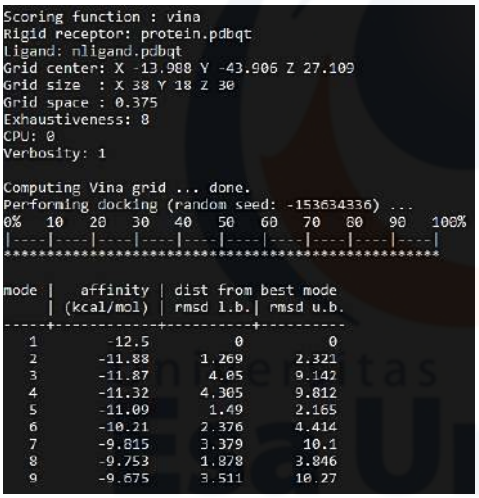
Lampiran 2. Energi afinitas ligan asli dari *command prompt* dengan tiap pengaturan ukuran *grid box* yang dinaikan 1 poin



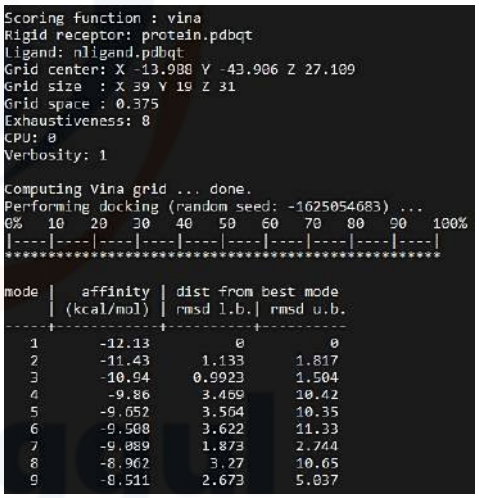
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: 10362851) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -12.87          0          0
   2       -12.15      1.226      2.508
   3       -11.33      1.384      1.818
   4       -10.35      3.719      10.13
   5        -10.3      2.576      4.388
   6       -10.26       3.62      11.29
   7        -10.1       3.51       10.3
   8       -9.937      1.912      2.695
   9       -9.839      3.304      10.66
```



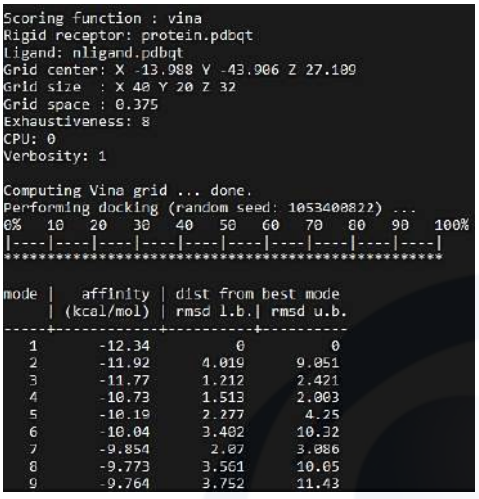
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 37 Y 17 Z 29
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1878067091) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -12.02          0          0
   2       -11.47      4.017       9.05
   3       -11.34      1.277      2.533
   4       -10.86      4.346      9.759
   5       -9.386      3.406      10.17
   6       -9.367      3.502      10.22
   7       -9.276      3.494      10.28
   8       -9.232      3.499      11.11
   9       -9.152      3.376      10.65
```



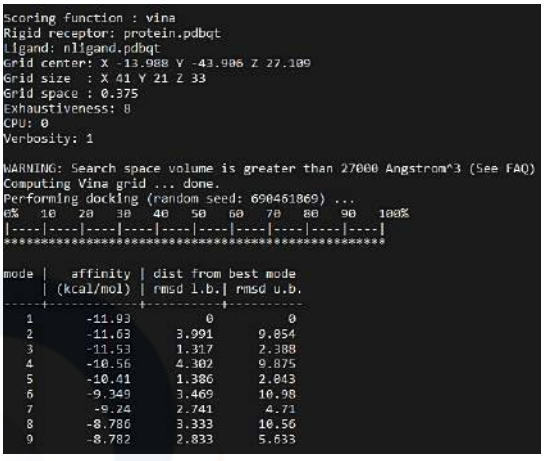
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 38 Y 18 Z 30
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -153634336) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -12.5          0          0
   2       -11.88      1.269      2.321
   3       -11.87       4.05      9.142
   4       -11.32      4.305      9.812
   5       -11.09       1.49      2.165
   6       -10.21      2.376      4.414
   7       -9.815      3.379       10.1
   8       -9.753      1.878      3.846
   9       -9.675      3.511      10.27
```



```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 39 Y 19 Z 31
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1625054683) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -12.13          0          0
   2       -11.43      1.133      1.817
   3       -10.94     0.9923      1.504
   4        -9.86      3.469      10.42
   5       -9.652      3.564      10.35
   6       -9.508      3.622      11.33
   7       -9.089      1.873      2.744
   8       -8.962       3.27      10.65
   9       -8.511      2.673      5.037
```

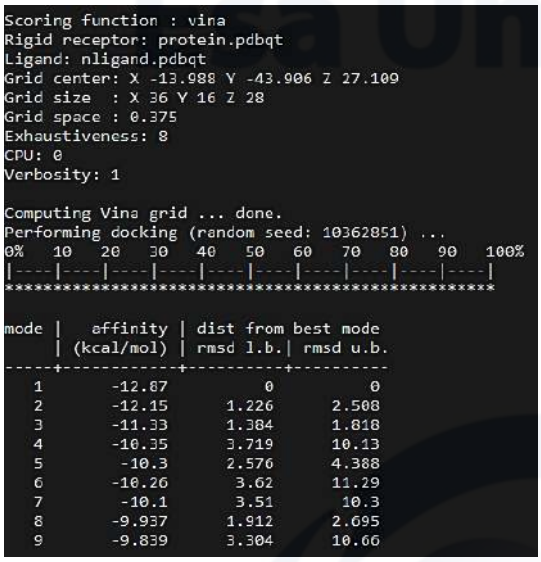


```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 40 Y 20 Z 32
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: 1053400822) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -12.34          0          0
   2       -11.92      4.019      9.051
   3       -11.77      1.212      2.421
   4       -10.73      1.513      2.003
   5       -10.19      2.277       4.25
   6       -10.04      3.402      10.32
   7       -9.854       2.07      3.086
   8       -9.773      3.561      10.05
   9       -9.764      3.752      11.43
```



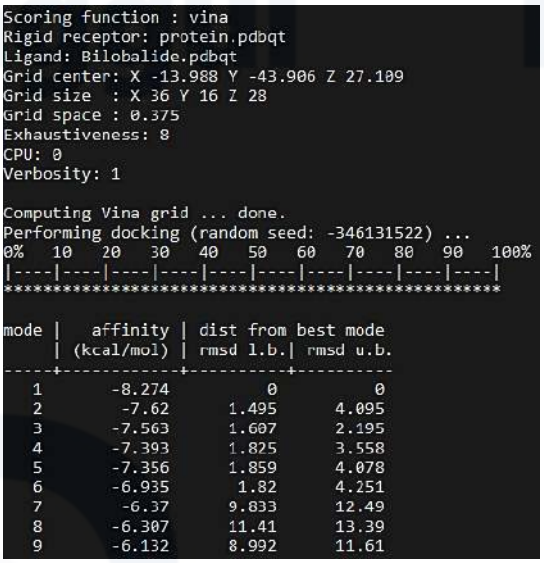
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 41 Y 21 Z 33
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

WARNING: Search space volume is greater than 27000 Angstrom^3 (See FAQ)
Computing Vina grid ... done.
Performing docking (random seed: 690461869) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -11.93          0          0
   2       -11.63      3.991      9.854
   3       -11.53      1.317      2.388
   4       -10.56      4.302      9.875
   5       -10.41      1.386      2.043
   6       -9.349      3.469      10.98
   7        -9.24      2.741       4.71
   8       -8.786      3.333      10.56
   9       -8.782      2.833      5.633
```

Lampiran 3. Energi afinitas ligan asli dan ligan uji dari *command prompt*



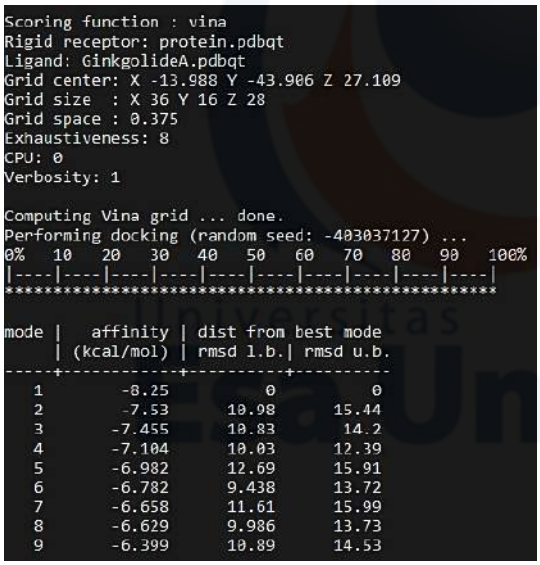
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: nligand.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: 10362851) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -12.87          0          0
   2       -12.15      1.226      2.508
   3       -11.33      1.384      1.818
   4       -10.35      3.719      10.13
   5        -10.3      2.576      4.388
   6       -10.26       3.62      11.29
   7        -10.1       3.51       10.3
   8       -9.937      1.912      2.695
   9       -9.839      3.304      10.66
```

Ligan asli (donepezil)



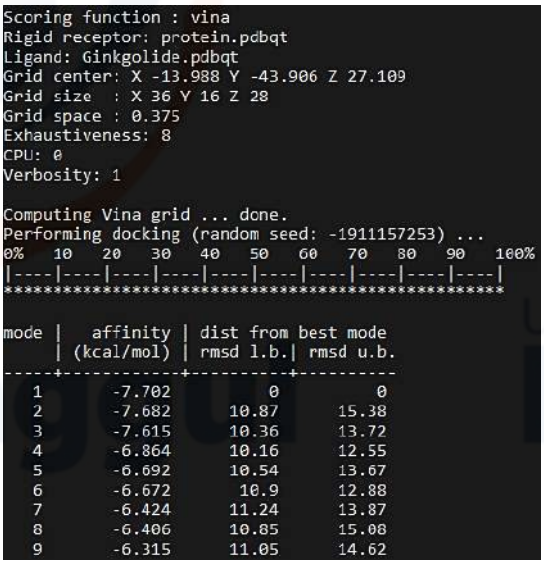
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Bilobalide.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -346131522) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -8.274          0          0
   2        -7.62      1.495      4.095
   3       -7.563      1.607      2.195
   4       -7.393      1.825      3.558
   5       -7.356      1.859      4.078
   6       -6.935       1.82      4.251
   7        -6.37      9.833      12.49
   8       -6.307      11.41      13.39
   9       -6.132      8.992      11.61
```

Bilobalida



```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: GinkgolideA.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -403037127) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -8.25          0          0
   2       -7.53      10.98      15.44
   3      -7.455      10.83       14.2
   4      -7.104      10.03      12.39
   5      -6.982      12.69      15.91
   6      -6.782      9.438      13.72
   7      -6.658      11.61      15.99
   8      -6.629      9.986      13.73
   9      -6.399      10.89      14.53
```

Ginkgolida A



```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Ginkgolide.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1911157253) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -7.702          0          0
   2       -7.682      10.87      15.38
   3       -7.615      10.36      13.72
   4       -6.864      10.16      12.55
   5       -6.692      10.54      13.67
   6       -6.672       10.9      12.88
   7       -6.424      11.24      13.87
   8       -6.406      10.85      15.08
   9       -6.315      11.05      14.62
```

Ginkgolida B

(lanjutan)

```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: GinkgolideC.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1314907336) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -8.032          0          0
   2       -7.815      1.836      6.325
   3       -7.597      10.97       14.1
   4       -7.539      1.323      5.994
   5       -7.352      1.753      5.674
   6       -7.234      1.591      3.956
   7       -7.061       1.93      2.903
   8       -6.887      1.708      2.241
   9       -6.817      1.914      3.831
```

Ginkgolida C

```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Isorhamnetin.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -592983521) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -9.358          0          0
   2       -9.311      2.301      3.464
   3       -9.192      1.984      7.669
   4       -9.066      5.187      9.794
   5       -8.712      4.315       8.98
   6       -8.359      4.173       7.75
   7       -8.127      2.757      4.853
   8       -8.113      1.794      7.425
   9       -7.504      2.592      7.222
```

Isorhamnetin

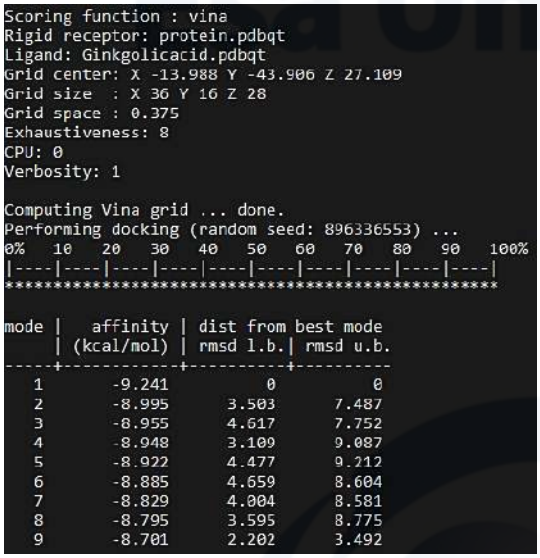
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Kaempferol.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1572294819) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -9.978          0          0
   2       -9.958      2.948      4.863
   3       -9.807        7.4      11.66
   4       -9.742      5.257      9.377
   5       -9.664      3.553      4.936
   6        -9.48      1.688      3.262
   7       -8.633      1.646      6.985
   8       -8.575      8.347         12
   9       -8.431      2.548      4.486
```

Kaempferol

```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Quercetin.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -2044877184) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -10.37          0          0
   2       -9.746      6.916      10.19
   3       -9.659      2.667      5.174
   4       -9.658      9.192      12.05
   5       -9.427      6.656      8.503
   6       -9.344      1.189      2.886
   7       -9.287       5.94      9.384
   8       -8.932      2.568      5.613
   9       -8.902      3.144      5.958
```

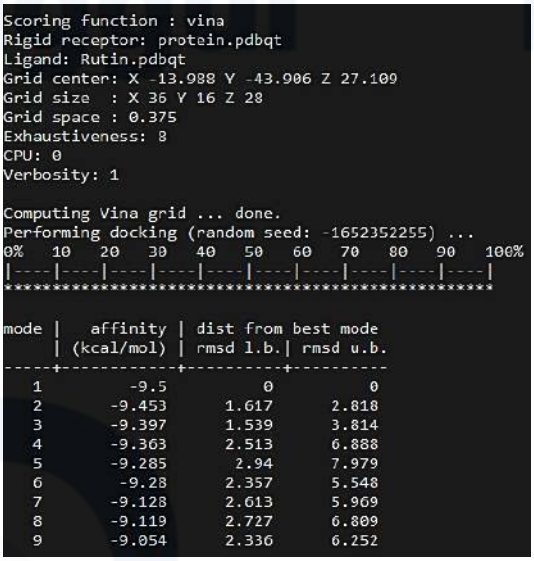
Kuersetin

(lanjutan)



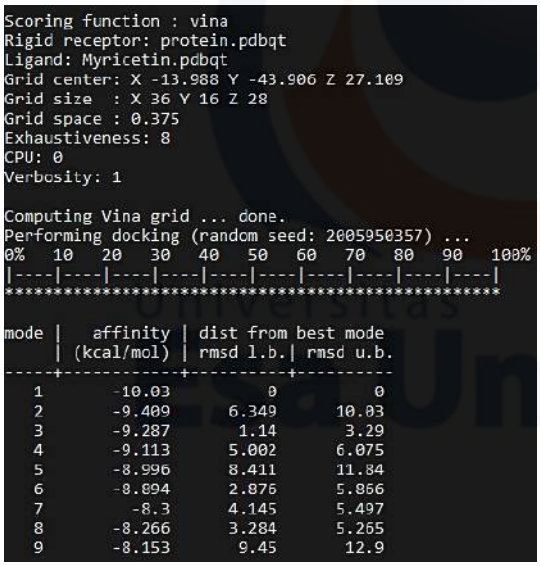
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Ginkgolicacid.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: 896336553) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -9.241          0          0
   2       -8.995      3.503      7.487
   3       -8.955      4.617      7.752
   4       -8.948      3.109      9.087
   5       -8.922      4.477      9.212
   6       -8.885      4.659      8.604
   7       -8.829      4.004      8.581
   8       -8.795      3.595      8.775
   9       -8.701      2.202      3.492
```

Asam ginkgolik



```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Rutin.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: -1652352255) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -9.5          0          0
   2      -9.453      1.617      2.818
   3      -9.397      1.539      3.814
   4      -9.363      2.513      6.888
   5      -9.285       2.94      7.979
   6       -9.28      2.357      5.548
   7      -9.128      2.613      5.969
   8      -9.119      2.727      6.809
   9      -9.054      2.336      6.252
```

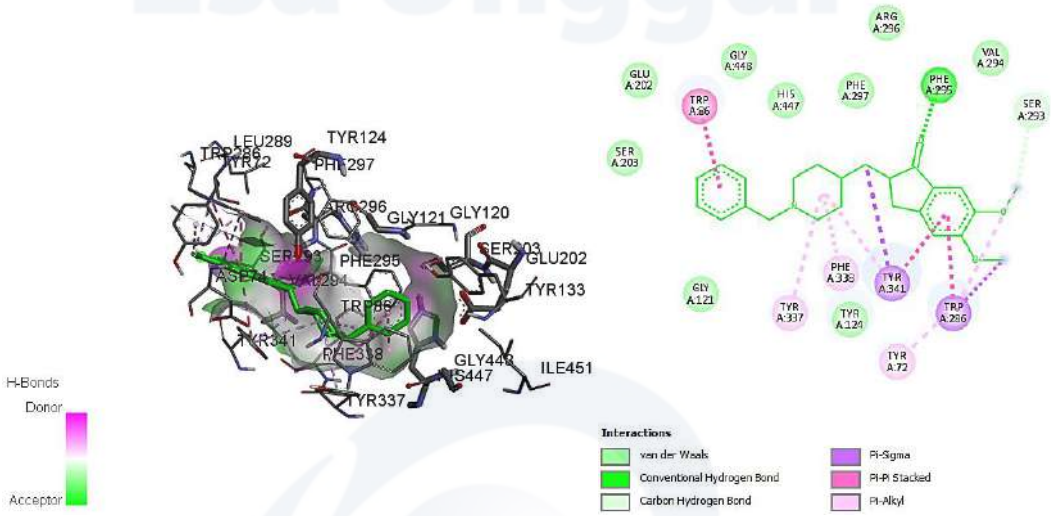
Rutin



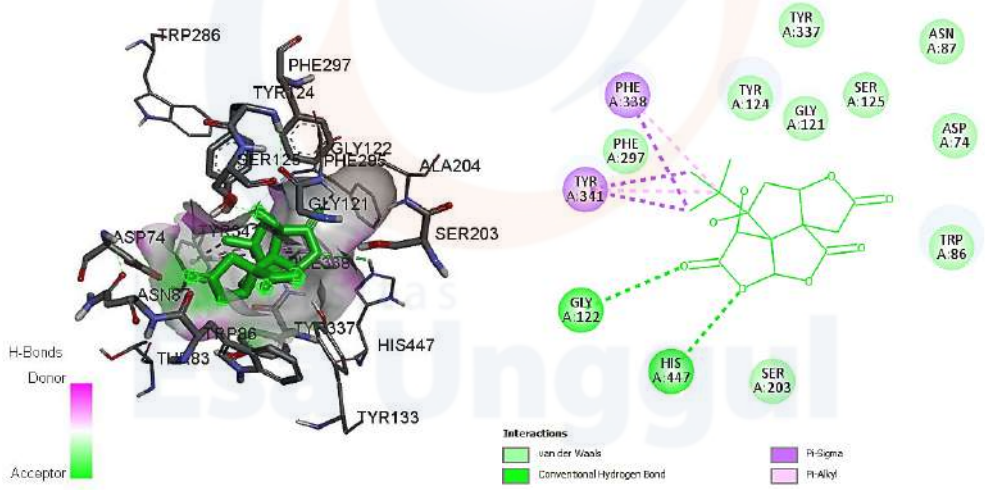
```
Scoring function : vina
Rigid receptor: protein.pdbqt
Ligand: Myricetin.pdbqt
Grid center: X -13.988 Y -43.906 Z 27.109
Grid size  : X 36 Y 16 Z 28
Grid space : 0.375
Exhaustiveness: 8
CPU: 0
Verbosity: 1

Computing Vina grid ... done.
Performing docking (random seed: 2005950357) ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1       -10.03          0          0
   2       -9.409      6.349      10.03
   3       -9.287       1.14       3.29
   4       -9.113      5.002      6.075
   5       -8.996      8.411      11.84
   6       -8.894      2.876      5.866
   7         -8.3      4.145      5.497
   8       -8.266      3.284      5.265
   9       -8.153       9.45       12.9
```

Mirisetin

Lampiran 4. Visualisasi interaksi molekuler dan residu asam amino untuk ligan asli dan ligan uji dalam bentuk 3D dan 2D

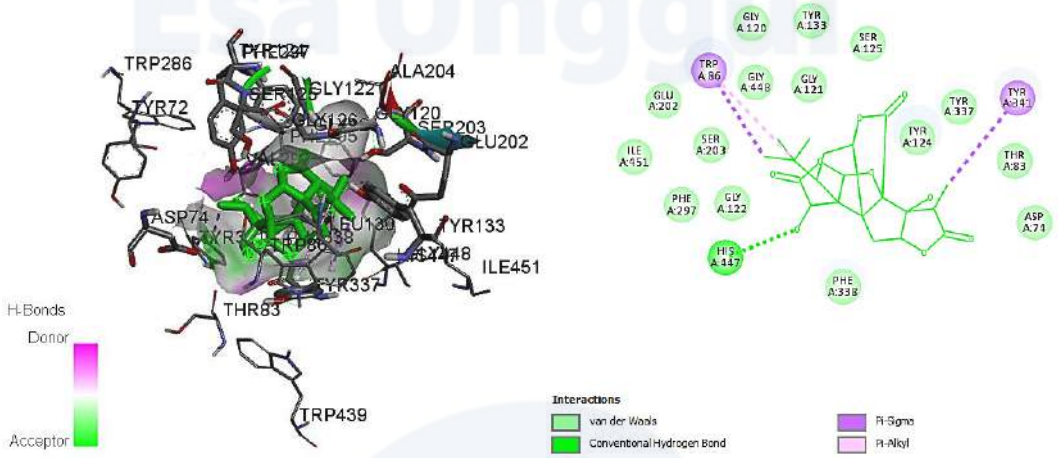


Donepezil (ligan asli) dengan protein

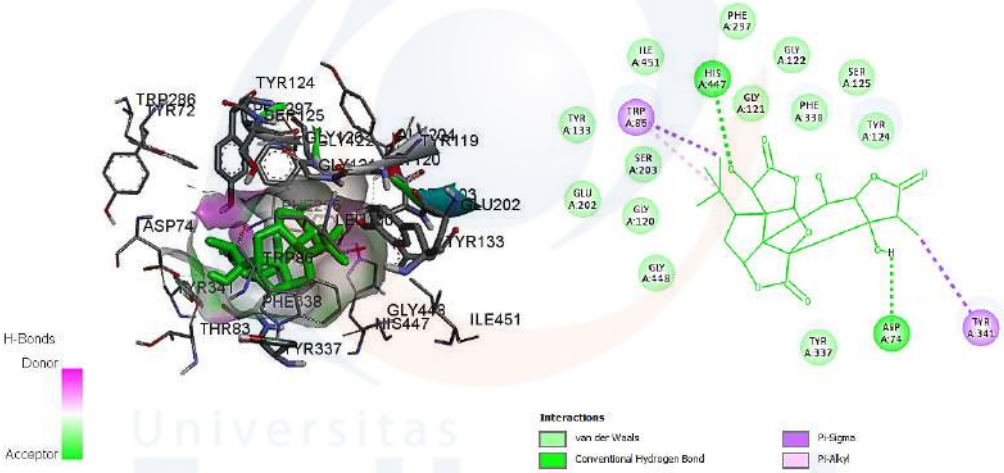


Bilobalida (ligan uji 1) dan protein

(lanjutan)

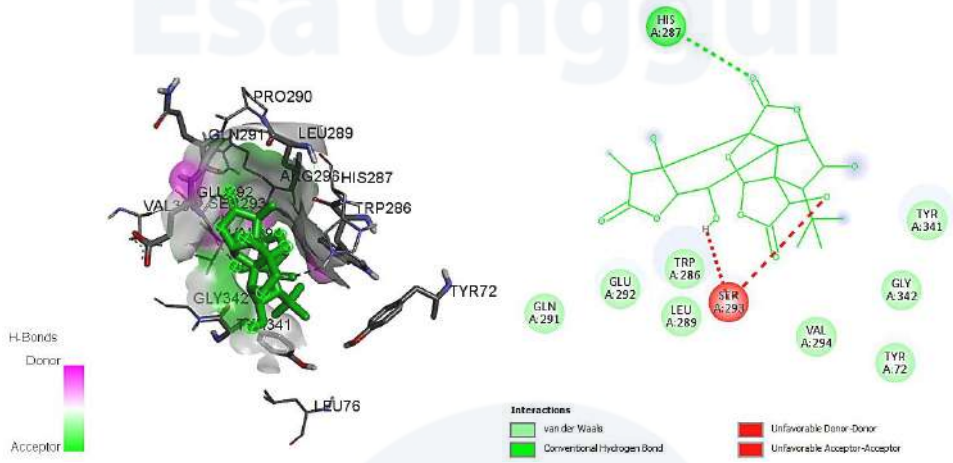


Ginkgolida A (ligan uji 2) dan protein

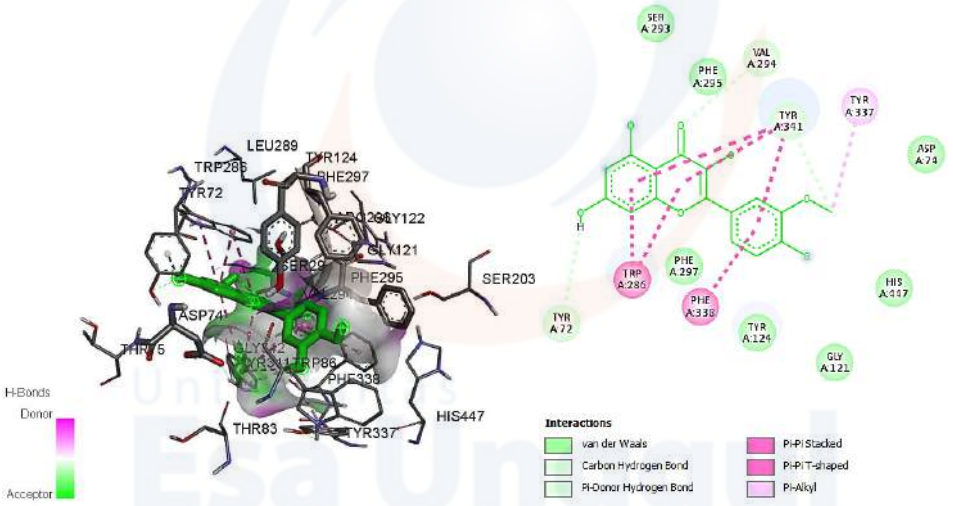


Ginkgolida B (ligan uji 3) dan protein

(lanjutan)

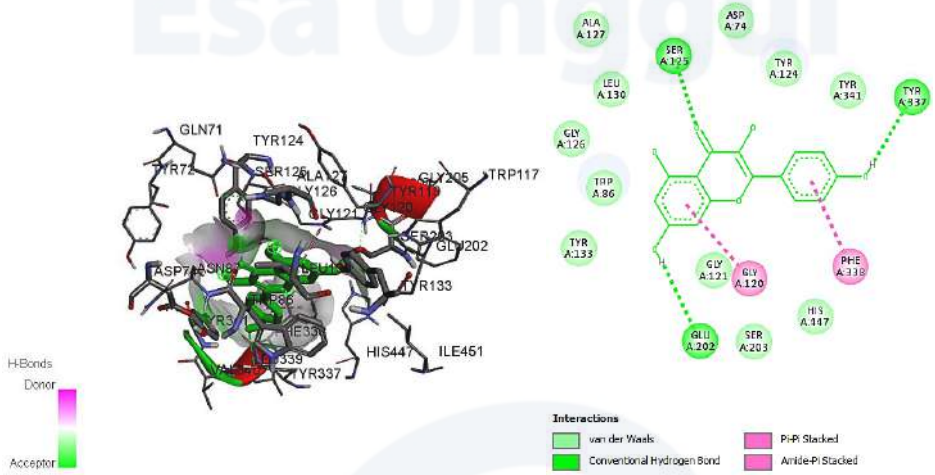


Ginkgolida C (ligan uji 4) dan protein

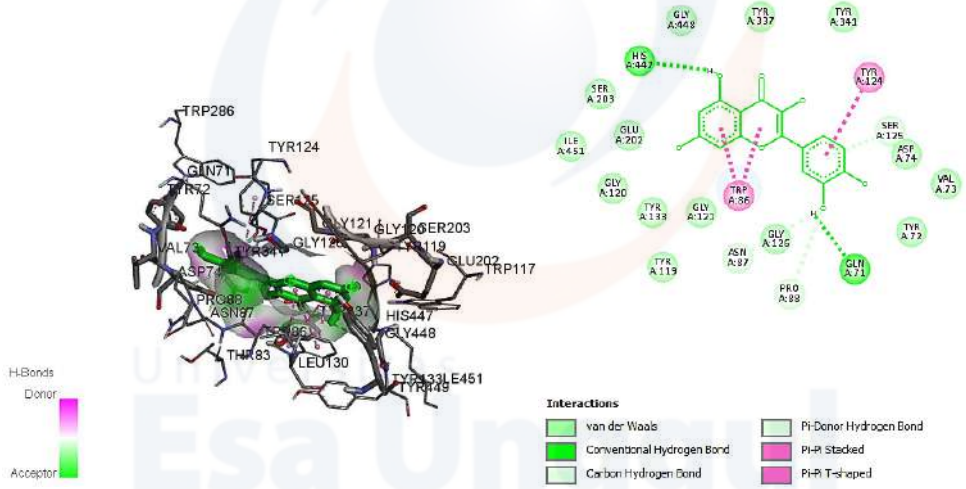


Isorhamnetin (ligan uji 5) dan protein

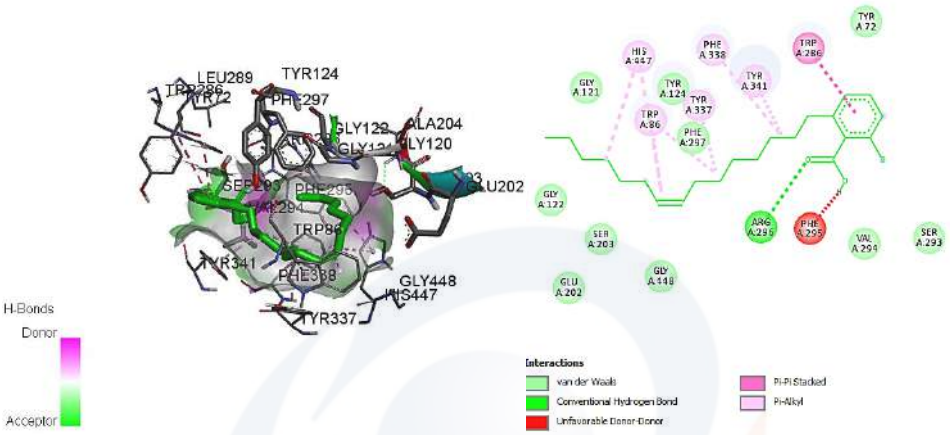
(lanjutan)



Kaempferol (ligan uji 6) dan protein

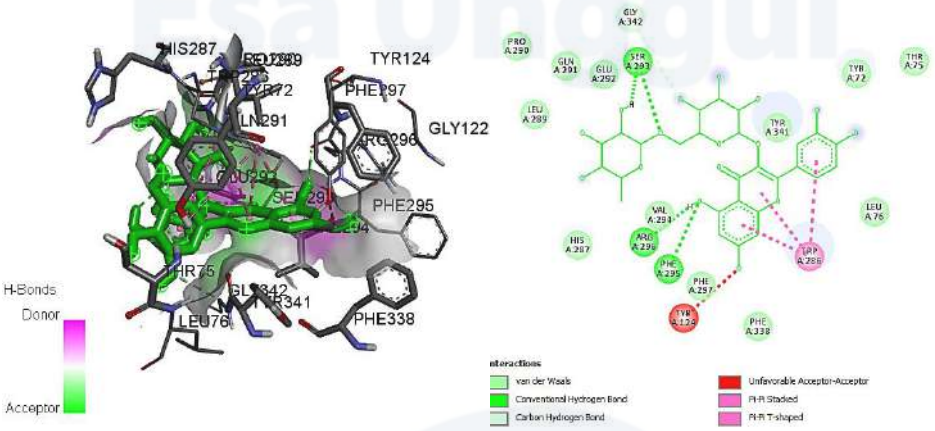


Kuersetin (ligan uji 7) dan protein

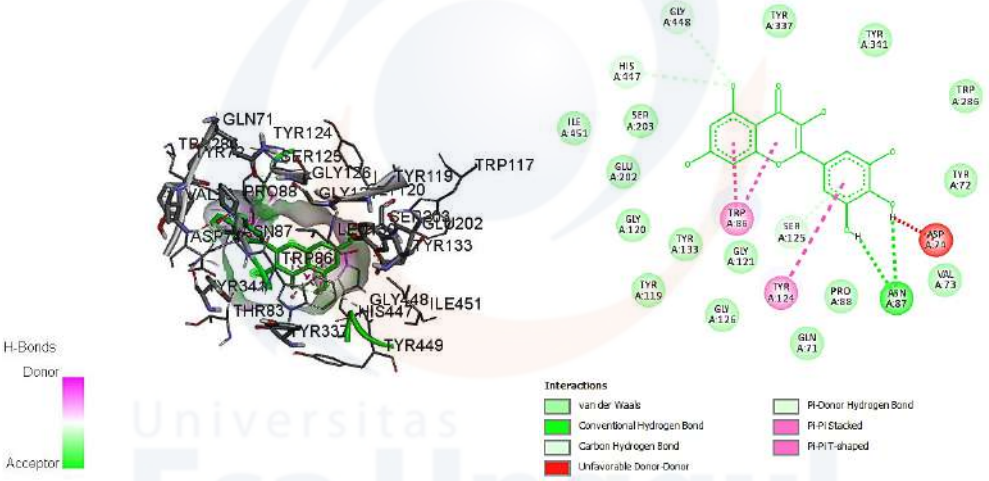


Asam ginkgolik (ligan uji 8) dan protein

(lanjutan)

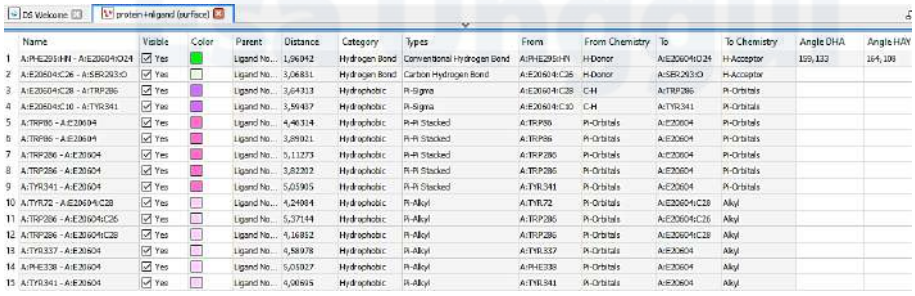


Rutin (ligan uji 9) dan protein



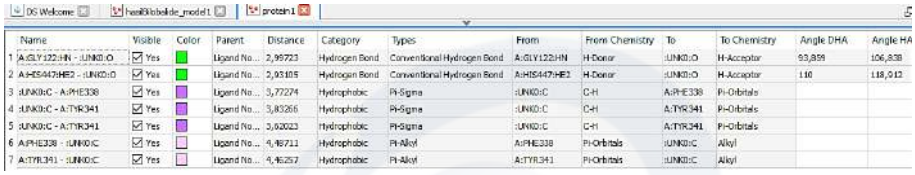
Mirisetin (ligan uji 10) dan protein

Lampiran 5. Ikatan ligan asli dan ligan uji



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HAY
1	A:PHE295:HN - A:E20604:O24	Yes		Ligand No...	1,96942	Hydrogen Bond	Conventional Hydrogen Bond	A:PHE295:HN	H-Donor	A:E20604:O24	H-Acceptor	159,133	164,198
2	A:E20604:C26 - A:SER293:O	Yes		Ligand No...	3,06831	Hydrogen Bond	Carbon Hydrogen Bond	A:E20604:C26	H-Donor	A:SER293:O	H-Acceptor		
3	A:E20604:C28 - A:TRP286	Yes		Ligand No...	3,64313	Hydrophobic	Pi-Sigma	A:E20604:C28	C-H	A:TRP286	Pi-Orbitals		
4	A:E20604:C10 - A:TYR341	Yes		Ligand No...	3,59437	Hydrophobic	Pi-Sigma	A:E20604:C10	C-H	A:TYR341	Pi-Orbitals		
5	A:TRP86 - A:E20604	Yes		Ligand No...	4,46314	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	A:E20604	Pi-Orbitals		
6	A:TRP86 - A:E20604	Yes		Ligand No...	3,89021	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	A:E20604	Pi-Orbitals		
7	A:TRP286 - A:E20604	Yes		Ligand No...	5,11273	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	A:E20604	Pi-Orbitals		
8	A:TRP286 - A:E20604	Yes		Ligand No...	3,82202	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	A:E20604	Pi-Orbitals		
9	A:TYR341 - A:E20604	Yes		Ligand No...	5,05905	Hydrophobic	Pi-Pi Stacked	A:TYR341	Pi-Orbitals	A:E20604	Pi-Orbitals		
10	A:TYR72 - A:E20604:C28	Yes		Ligand No...	4,24964	Hydrophobic	Pi-Alkyl	A:TYR72	Pi-Orbitals	A:E20604:C28	Alkyl		
11	A:TRP286 - A:E20604:C26	Yes		Ligand No...	5,37144	Hydrophobic	Pi-Alkyl	A:TRP286	Pi-Orbitals	A:E20604:C26	Alkyl		
12	A:TRP286 - A:E20604:C28	Yes		Ligand No...	4,16852	Hydrophobic	Pi-Alkyl	A:TRP286	Pi-Orbitals	A:E20604:C28	Alkyl		
13	A:TYR337 - A:E20604	Yes		Ligand No...	4,58978	Hydrophobic	Pi-Alkyl	A:TYR337	Pi-Orbitals	A:E20604	Alkyl		
14	A:PHE338 - A:E20604	Yes		Ligand No...	5,05927	Hydrophobic	Pi-Alkyl	A:PHE338	Pi-Orbitals	A:E20604	Alkyl		
15	A:TYR341 - A:E20604	Yes		Ligand No...	4,08695	Hydrophobic	Pi-Alkyl	A:TYR341	Pi-Orbitals	A:E20604	Alkyl		

Ligan asli (donepezil)



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HA
1	A:GLY122:HN - :UNK0:O	Yes		Ligand No...	2,95723	Hydrogen Bond	Conventional Hydrogen Bond	A:GLY122:HN	H-Donor	:UNK0:O	H-Acceptor	93,859	106,838
2	A:HIS447:HE2 - :UNK0:O	Yes		Ligand No...	2,93105	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS447:HE2	H-Donor	:UNK0:O	H-Acceptor	110	118,012
3	:UNK0:C - A:PHE338	Yes		Ligand No...	3,77274	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:PHE338	Pi-Orbitals		
4	:UNK0:C - A:TYR341	Yes		Ligand No...	3,83266	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TYR341	Pi-Orbitals		
5	:UNK0:C - A:TYR341	Yes		Ligand No...	3,62023	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TYR341	Pi-Orbitals		
6	A:PHE338 - :UNK0:C	Yes		Ligand No...	4,48711	Hydrophobic	Pi-Alkyl	A:PHE338	Pi-Orbitals	:UNK0:C	Alkyl		
7	A:TYR341 - :UNK0:C	Yes		Ligand No...	4,46257	Hydrophobic	Pi-Alkyl	A:TYR341	Pi-Orbitals	:UNK0:C	Alkyl		

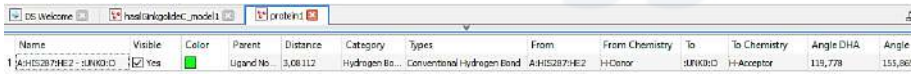
Bilobalida

	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HAY
1	A:HIS447:HE2 - :UNK0:O	Yes		Ligand No...	2,3132	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS447:HE2	H-Donor	:UNK0:O	H-Acceptor	99,899	110,476
2	:UNK0:C - A:TYR341	Yes		Ligand No...	3,96665	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TYR341	Pi-Orbitals		
3	:UNK0:C - A:TRP86	Yes		Ligand No...	3,46696	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TRP86	Pi-Orbitals		
4	A:TRP86 - :UNK0:C	Yes		Ligand No...	5,12735	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0:C	Alkyl		
5	A:TRP86 - :UNK0:C	Yes		Ligand No...	4,33982	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0:C	Alkyl		

Ginkgolida A

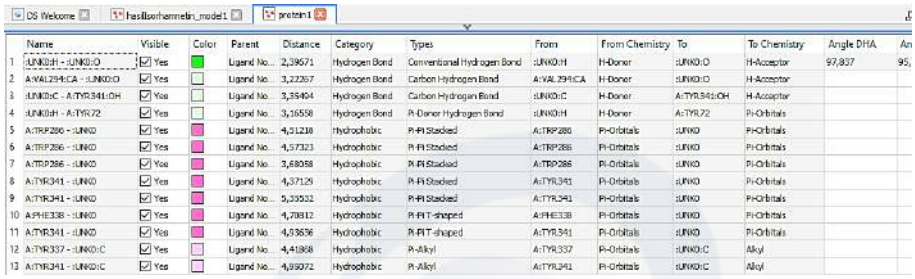
	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle
1	A:HIS447:HE2 - :UNK0:O	Yes		Ligand No...	2,34244	Hydrogen Bond	Conventional Hydrogen Bond	A:HIS447:HE2	H-Donor	:UNK0:O	H-Acceptor	99,53	118,2
2	:UNK0:H - A:ASP74:OD2	Yes		Ligand No...	2,45876	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASP74:OD2	H-Acceptor	130,67	142,2
3	:UNK0:C - A:TYR341	Yes		Ligand No...	3,98008	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TYR341	Pi-Orbitals		
4	:UNK0:C - A:TRP86	Yes		Ligand No...	3,45251	Hydrophobic	Pi-Sigma	:UNK0:C	C-H	A:TRP86	Pi-Orbitals		
5	A:TRP86 - :UNK0:C	Yes		Ligand No...	5,0181	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0:C	Alkyl		
6	A:TRP86 - :UNK0:C	Yes		Ligand No...	4,18952	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0:C	Alkyl		

Ginkgolida B



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle
1	A:HIS287:HE2 - :UNK0:O	Yes		Ligand No...	3,08112	Hydrogen Bo...	Conventional Hydrogen Bond	A:HIS287:HE2	H-Donor	:UNK0:O	H-Acceptor	119,778	155,86

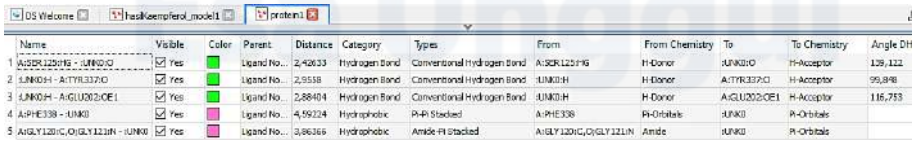
Ginkgolida C



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	An
1	:UNK0:H - :UNK0:O	Yes		Ligand No...	2,39571	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor	97,837	95,
2	A:VAL294:CA - :UNK0:O	Yes		Ligand No...	3,22267	Hydrogen Bond	Carbon Hydrogen Bond	A:VAL294:CA	H-Donor	:UNK0:O	H-Acceptor		
3	:UNK0:C - A:TYR341:OH	Yes		Ligand No...	3,35404	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	A:TYR341:OH	H-Acceptor		
4	:UNK0:H - A:TYR72	Yes		Ligand No...	3,16558	Hydrogen Bond	Pi-Donor Hydrogen Bond	:UNK0:H	H-Donor	A:TYR72	Pi-Orbitals		
5	A:TRP286 - :UNK0	Yes		Ligand No...	4,51218	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
6	A:TRP286 - :UNK0	Yes		Ligand No...	4,57323	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
7	A:TRP286 - :UNK0	Yes		Ligand No...	3,68058	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
8	A:TYR341 - :UNK0	Yes		Ligand No...	4,37129	Hydrophobic	Pi-Pi Stacked	A:TYR341	Pi-Orbitals	:UNK0	Pi-Orbitals		
9	A:TYR341 - :UNK0	Yes		Ligand No...	5,33532	Hydrophobic	Pi-Pi Stacked	A:TYR341	Pi-Orbitals	:UNK0	Pi-Orbitals		
10	A:PHE338 - :UNK0	Yes		Ligand No...	4,70812	Hydrophobic	Pi-Pi T-shaped	A:PHE338	Pi-Orbitals	:UNK0	Pi-Orbitals		
11	A:TYR341 - :UNK0	Yes		Ligand No...	4,93656	Hydrophobic	Pi-Pi T-shaped	A:TYR341	Pi-Orbitals	:UNK0	Pi-Orbitals		
12	A:TYR337 - :UNK0:C	Yes		Ligand No...	4,41868	Hydrophobic	Pi-Alkyl	A:TYR337	Pi-Orbitals	:UNK0:C	Alkyl		
13	A:TYR341 - :UNK0:C	Yes		Ligand No...	4,89072	Hydrophobic	Pi-Alkyl	A:TYR341	Pi-Orbitals	:UNK0:C	Alkyl		

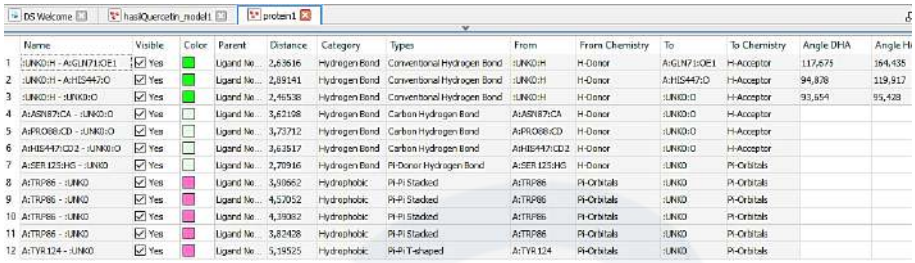
Isorhamnetin

(lanjutan)



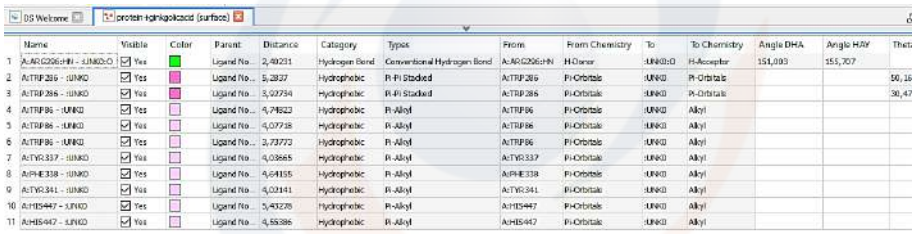
	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DH
1	A:SER125:HG - :UNK0:O	Yes		Ligand No...	2,42633	Hydrogen Bond	Conventional Hydrogen Bond	A:SER125:HG	H-Donor	:UNK0:O	H-Acceptor	139,122
2	:UNK0:H - A:TYR337:O	Yes		Ligand No...	2,9558	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:TYR337:O	H-Acceptor	99,848
3	:UNK0:H - A:GLU202:OE1	Yes		Ligand No...	2,88404	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLU202:OE1	H-Acceptor	116,753
4	A:PHE338 - :UNK0	Yes		Ligand No...	4,59224	Hydrophobic	Pi-Pi Stacked	A:PHE338	Pi-Orbitals	:UNK0	Pi-Orbitals	
5	A:GLY120:C,O:GLY121:N - :UNK0	Yes		Ligand No...	3,86366	Hydrophobic	Amide-Pi Stacked	A:GLY120:C,O:GLY121:N	Amide	:UNK0	Pi-Orbitals	

Kaempferol



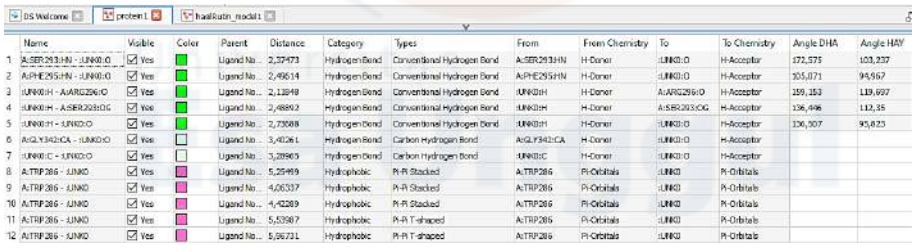
	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle H
1	:UNK0:H - A:GLN71:OE1	Yes		Ligand No...	2,63616	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:GLN71:OE1	H-Acceptor	117,675	164,435
2	:UNK0:H - A:HIS447:O	Yes		Ligand No...	2,89141	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:HIS447:O	H-Acceptor	94,878	119,917
3	:UNK0:H - :UNK0:O	Yes		Ligand No...	2,46538	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor	93,654	95,428
4	A:ASN87:CA - :UNK0:O	Yes		Ligand No...	3,62108	Hydrogen Bond	Carbon Hydrogen Bond	A:ASN87:CA	H-Donor	:UNK0:O	H-Acceptor		
5	A:PRO88:CD - :UNK0:O	Yes		Ligand No...	3,73712	Hydrogen Bond	Carbon Hydrogen Bond	A:PRO88:CD	H-Donor	:UNK0:O	H-Acceptor		
6	A:HIS447:CD2 - :UNK0:O	Yes		Ligand No...	3,63517	Hydrogen Bond	Carbon Hydrogen Bond	A:HIS447:CD2	H-Donor	:UNK0:O	H-Acceptor		
7	A:SER125:HG - :UNK0	Yes		Ligand No...	2,70916	Hydrogen Bond	Pi-Donor Hydrogen Bond	A:SER125:HG	H-Donor	:UNK0	Pi-Orbitals		
8	A:TRP86 - :UNK0	Yes		Ligand No...	3,90662	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
9	A:TRP86 - :UNK0	Yes		Ligand No...	4,57052	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
10	A:TRP86 - :UNK0	Yes		Ligand No...	4,39082	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
11	A:TRP86 - :UNK0	Yes		Ligand No...	3,82428	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
12	A:TYR124 - :UNK0	Yes		Ligand No...	5,19525	Hydrophobic	Pi-Pi T-shaped	A:TYR124	Pi-Orbitals	:UNK0	Pi-Orbitals		

Kuersetin



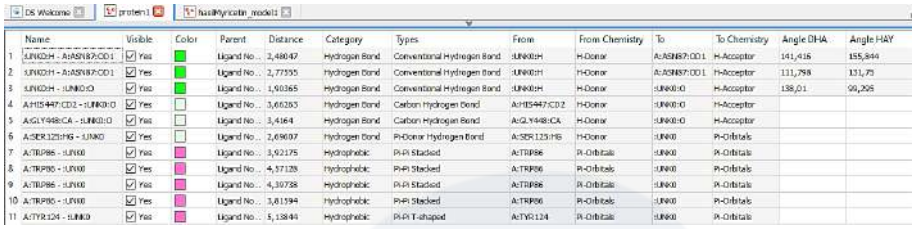
	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HAY	Thet
1	A:ARG296:HN - :UNK0:O	Yes		Ligand No...	2,40231	Hydrogen Bond	Conventional Hydrogen Bond	A:ARG296:HN	H-Donor	:UNK0:O	H-Acceptor	151,093	155,707	
2	A:TRP286 - :UNK0	Yes		Ligand No...	5,2837	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals			90,16
3	A:TRP286 - :UNK0	Yes		Ligand No...	5,02734	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals			90,47
4	A:TRP86 - :UNK0	Yes		Ligand No...	4,74823	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0	Alkyl			
5	A:TRP86 - :UNK0	Yes		Ligand No...	4,07718	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0	Alkyl			
6	A:TRP86 - :UNK0	Yes		Ligand No...	3,73772	Hydrophobic	Pi-Alkyl	A:TRP86	Pi-Orbitals	:UNK0	Alkyl			
7	A:TYR337 - :UNK0	Yes		Ligand No...	4,03665	Hydrophobic	Pi-Alkyl	A:TYR337	Pi-Orbitals	:UNK0	Alkyl			
8	A:PHE338 - :UNK0	Yes		Ligand No...	4,64155	Hydrophobic	Pi-Alkyl	A:PHE338	Pi-Orbitals	:UNK0	Alkyl			
9	A:TYR341 - :UNK0	Yes		Ligand No...	4,02141	Hydrophobic	Pi-Alkyl	A:TYR341	Pi-Orbitals	:UNK0	Alkyl			
10	A:HIS447 - :UNK0	Yes		Ligand No...	5,43276	Hydrophobic	Pi-Alkyl	A:HIS447	Pi-Orbitals	:UNK0	Alkyl			
11	A:HIS447 - :UNK0	Yes		Ligand No...	4,65386	Hydrophobic	Pi-Alkyl	A:HIS447	Pi-Orbitals	:UNK0	Alkyl			

Asam ginkgolik



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HAY
1	A:SER293:HN - :UNK0:O	Yes		Ligand No...	2,37473	Hydrogen Bond	Conventional Hydrogen Bond	A:SER293:HN	H-Donor	:UNK0:O	H-Acceptor	172,575	103,237
2	A:PHE295:HN - :UNK0:O	Yes		Ligand No...	2,49614	Hydrogen Bond	Conventional Hydrogen Bond	A:PHE295:HN	H-Donor	:UNK0:O	H-Acceptor	105,071	94,967
3	:UNK0:H - A:ARG296:O	Yes		Ligand No...	2,13848	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ARG296:O	H-Acceptor	159,153	119,697
4	:UNK0:H - A:SER203:OG	Yes		Ligand No...	2,48892	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:SER203:OG	H-Acceptor	136,446	112,35
5	:UNK0:H - :UNK0:O	Yes		Ligand No...	2,73008	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor	136,907	95,823
6	A:GLY342:CA - :UNK0:O	Yes		Ligand No...	3,40261	Hydrogen Bond	Carbon Hydrogen Bond	A:GLY342:CA	H-Donor	:UNK0:O	H-Acceptor		
7	:UNK0:C - :UNK0:O	Yes		Ligand No...	3,28965	Hydrogen Bond	Carbon Hydrogen Bond	:UNK0:C	H-Donor	:UNK0:O	H-Acceptor		
8	A:TRP286 - :UNK0	Yes		Ligand No...	5,25499	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
9	A:TRP286 - :UNK0	Yes		Ligand No...	4,06537	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
10	A:TRP286 - :UNK0	Yes		Ligand No...	4,42289	Hydrophobic	Pi-Pi Stacked	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
11	A:TRP286 - :UNK0	Yes		Ligand No...	5,53987	Hydrophobic	Pi-Pi T-shaped	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		
12	A:TRP286 - :UNK0	Yes		Ligand No...	5,66731	Hydrophobic	Pi-Pi T-shaped	A:TRP286	Pi-Orbitals	:UNK0	Pi-Orbitals		

Rutin



	Name	Visible	Color	Parent	Distance	Category	Types	From	From Chemistry	To	To Chemistry	Angle DHA	Angle HAY
1	:UNK0:H - A:ASN87:OD1	Yes		Ligand No...	2,48047	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASN87:OD1	H-Acceptor	141,416	155,844
2	:UNK0:H - A:ASN87:OD1	Yes		Ligand No...	2,77555	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	A:ASN87:OD1	H-Acceptor	111,798	131,73
3	:UNK0:H - :UNK0:O	Yes		Ligand No...	1,90365	Hydrogen Bond	Conventional Hydrogen Bond	:UNK0:H	H-Donor	:UNK0:O	H-Acceptor	138,01	99,295
4	A:HIS447:CD2 - :UNK0:O	Yes		Ligand No...	3,66263	Hydrogen Bond	Carbon Hydrogen Bond	A:HIS447:CD2	H-Donor	:UNK0:O	H-Acceptor		
5	A:GLY448:CA - :UNK0:O	Yes		Ligand No...	3,4164	Hydrogen Bond	Carbon Hydrogen Bond	A:GLY448:CA	H-Donor	:UNK0:O	H-Acceptor		
6	A:SER125:HG - :UNK0	Yes		Ligand No...	2,69607	Hydrogen Bond	Pi-Donor Hydrogen Bond	A:SER125:HG	H-Donor	:UNK0	Pi-Orbitals		
7	A:TRP86 - :UNK0	Yes		Ligand No...	3,92175	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
8	A:TRP86 - :UNK0	Yes		Ligand No...	4,57128	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
9	A:TRP86 - :UNK0	Yes		Ligand No...	4,39738	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
10	A:TRP86 - :UNK0	Yes		Ligand No...	3,81594	Hydrophobic	Pi-Pi Stacked	A:TRP86	Pi-Orbitals	:UNK0	Pi-Orbitals		
11	A:TYR124 - :UNK0	Yes		Ligand No...	5,13844	Hydrophobic	Pi-Pi T-shaped	A:TYR124	Pi-Orbitals	:UNK0	Pi-Orbitals		

Mirisetin

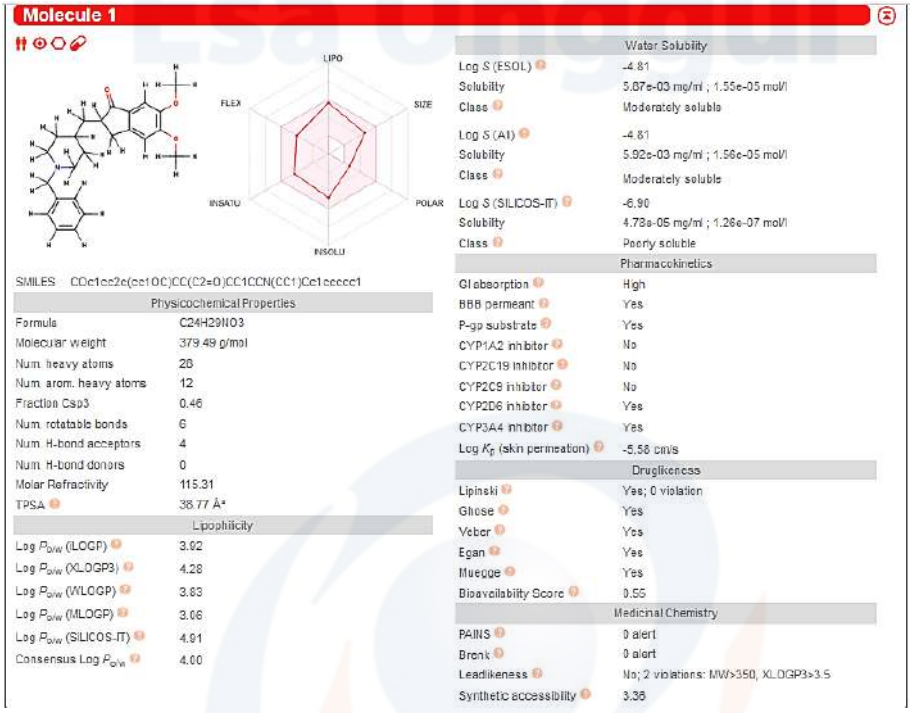
Lampiran 6. Kode SMILES dari ligan asli dan ligan uji

No.	Senyawa	Kode SMILES
1.	Donepezil (ligan asli)	COC1=C(OC)C=C2C(=O)C(CC3CCN(CC4=CC=CC=C4)CC3)CC2=C1
2.	Bilobalida (ligan uji 1)	[H]O[C@@]1([H])C(=O)O[C@@]2([H])OC(=O)[C@]34C([H])([H])C(=O)O[C@@]3([H])C([H])([H])[C@@](O[H])(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@]124
3.	Ginkgolida A (ligan uji 2)	[H]O[C@@]1([H])C(=O)O[C@@]2([H])O[C@]34C(=O)O[C@]5([H])C([H])([H])[C@@]([H])(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])[C@]12[C@]35C([H])([H])[C@]1([H])OC(=O)[C@@]([H])(C([H])([H])[H])[H])[C@]41O[H]
4.	Ginkgolida B (ligan uji 3)	C[C@@H]1C(=O)O[C@H]2[C@@H](O)[C@@]34[C@H]5C[C@@H](C(C)(C)C)[C@@]33[C@@H](O)C(=O)O[C@H]3O[C@@]4(C(=O)O5)[C@@]12O
5.	Ginkgolida C (ligan uji 4)	C[C@@H]1C(=O)O[C@H]2[C@@H](O)[C@]34[C@@H]5OC(=O)[C@]3(O[C@@H]3OC(=O)[C@H](O)[C@]43[C@@H]([C@H]5O)C(C)(C)C)[C@@]12O
6.	Isorhamnetin (ligan uji 5)	[H]OC1=C([H])C(O[H])=C2C(=O)C(O[H])=C(OC2=C1[H])C1=C([H])C(OC([H])([H])[H])=C(O[H])C([H])=C1[H]
7.	Kaempferol (ligan uji 6)	[H]OC1=C([H])C([H])=C(C([H])=C1[H])C1=C(O[H])C(=O)C2=C(O[H])C([H])=C(O[H])C([H])=C2O1
8.	Kuersetin (ligan uji 7)	[H]OC1=C([H])C(O[H])=C2C(=O)C(O[H])=C(OC2=C1[H])C1=C([H])C(O[H])=C(O[H])C([H])=C1[H]
9.	Asam ginkgolik (ligan uji 8)	CCCCCC\C=C/CCCCCCCC1=C(C(O)=O)C(O)=CC=C1
10.	Rutin (ligan uji 9)	C[C@@H]1O[C@@H](OC[C@H]2O[C@@H](OC3=C(OC4=CC(O)=CC(O)=C4C3=O)C3=CC(O)=C(O)C=C3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O

(lanjutan)

11.	Mirisetin (ligan uji 10)	[H]OC1=C([H])C(O[H])=C2C(=O)C(O[H])=C(OC2=C1[H])C1=C([H])C(O[H])=C(O[H])C(O[H])=C1[H]

Lampiran 7. SwissADME pada ligan asli dan ligan uji



Molecule 1

SMILES: COc1cc2c(cc1OC)CC(C2=O)CC1CCN(CC1)Cc1ccccc1

Physicochemical Properties	
Formula	C24H29NO3
Molecular weight	379.49 g/mol
Num. heavy atoms	28
Num. arom. heavy atoms	12
Fraction Csp3	0.46
Num. rotatable bonds	6
Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	115.31
TPSA	38.77 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.92
Log $P_{o/w}$ (XLOGP3)	4.28
Log $P_{o/w}$ (WLOGP)	3.83
Log $P_{o/w}$ (MLOGP)	3.06
Log $P_{o/w}$ (SILICOS-IT)	4.91
Consensus Log $P_{o/w}$	4.00

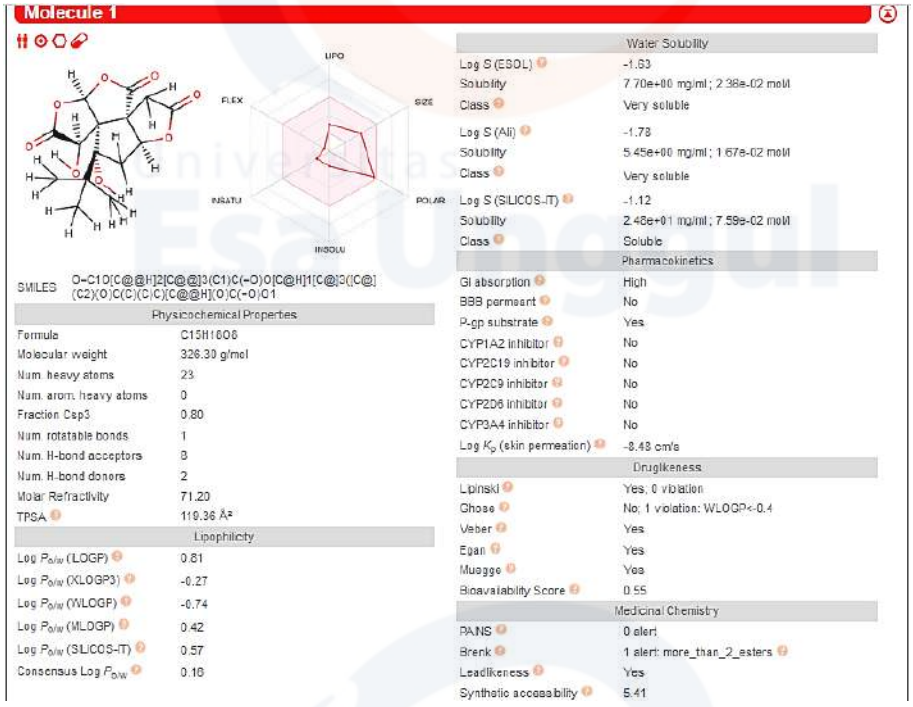
Water Solubility	
Log S (ESOL)	-4.81
Solubility	5.87e-03 mg/ml ; 1.55e-05 mol/l
Class	Moderately soluble
Log S (Ali)	-4.61
Solubility	5.92e-03 mg/ml ; 1.56e-05 mol/l
Class	Moderately soluble
Log S (SILICOS-IT)	-6.90
Solubility	4.78e-05 mg/ml ; 1.26e-07 mol/l
Class	Poorly soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-5.56 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 2 violations: MW>350, XLOGP3>3.5
Synthetic accessibility	3.36

Ligan asli (donepezil)



Molecule 1

SMILES: O=C1O[C@@H]2[C@@]3(C1)C(=O)O[C@H]1[C@]3([C@](C2)(O)C(C)(C)C)[C@@H](O)C(=O)O1

Physicochemical Properties	
Formula	C15H18O8
Molecular weight	326.30 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	1
Num. H-bond acceptors	8
Num. H-bond donors	2
Molar Refractivity	71.20
TPSA	119.36 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	0.61
Log $P_{o/w}$ (XLOGP3)	-0.27
Log $P_{o/w}$ (WLOGP)	-0.74
Log $P_{o/w}$ (MLOGP)	0.42
Log $P_{o/w}$ (SILICOS-IT)	0.57
Consensus Log $P_{o/w}$	0.10

Water Solubility	
Log S (ESOL)	-1.63
Solubility	7.70e+00 mg/ml ; 2.36e-02 mol/l
Class	Very soluble
Log S (Ali)	-1.78
Solubility	5.45e+00 mg/ml ; 1.67e-02 mol/l
Class	Very soluble
Log S (SILICOS-IT)	-1.12
Solubility	2.48e+01 mg/ml ; 7.59e-02 mol/l
Class	Soluble

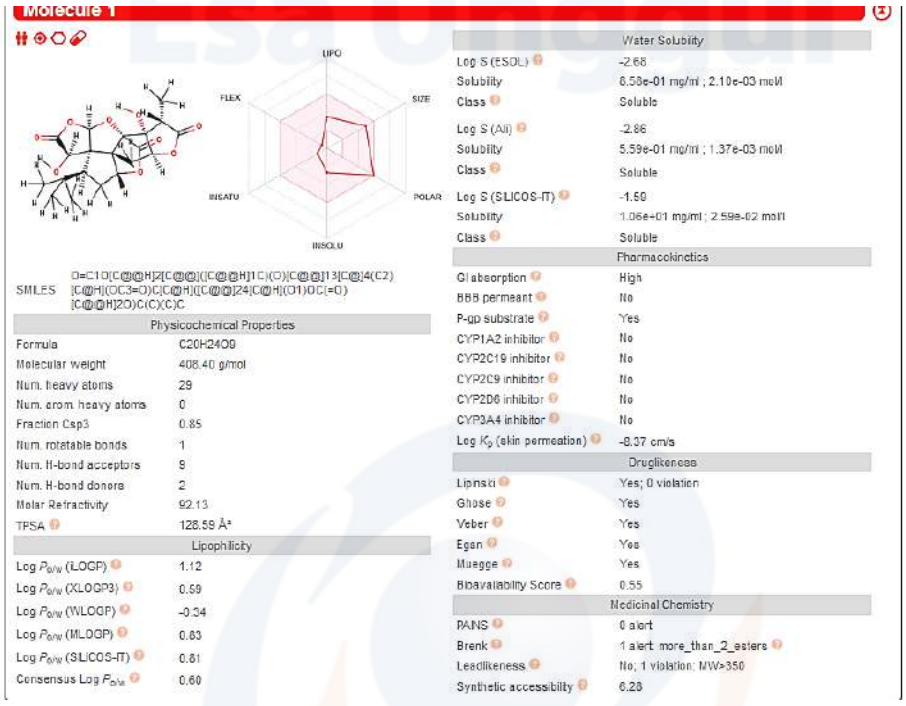
Pharmacokinetics	
GI absorption	High
BBB permeant	No
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-8.48 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: WLOGP<-0.4
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

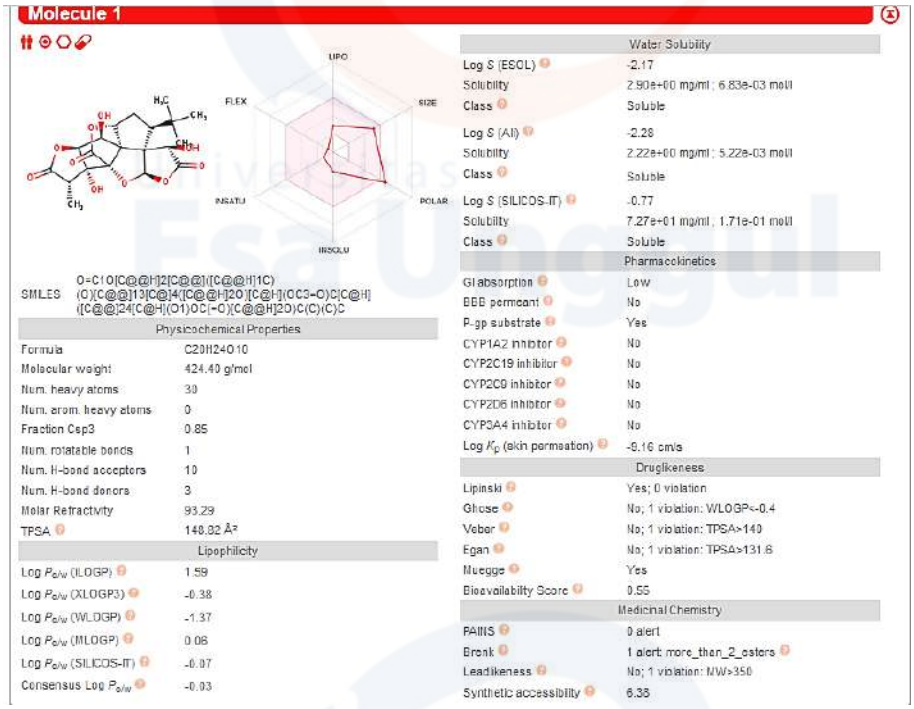
Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: more_than_2_esters
Leadlikeness	Yes
Synthetic accessibility	5.41

Bilobalida

(lanjutan)



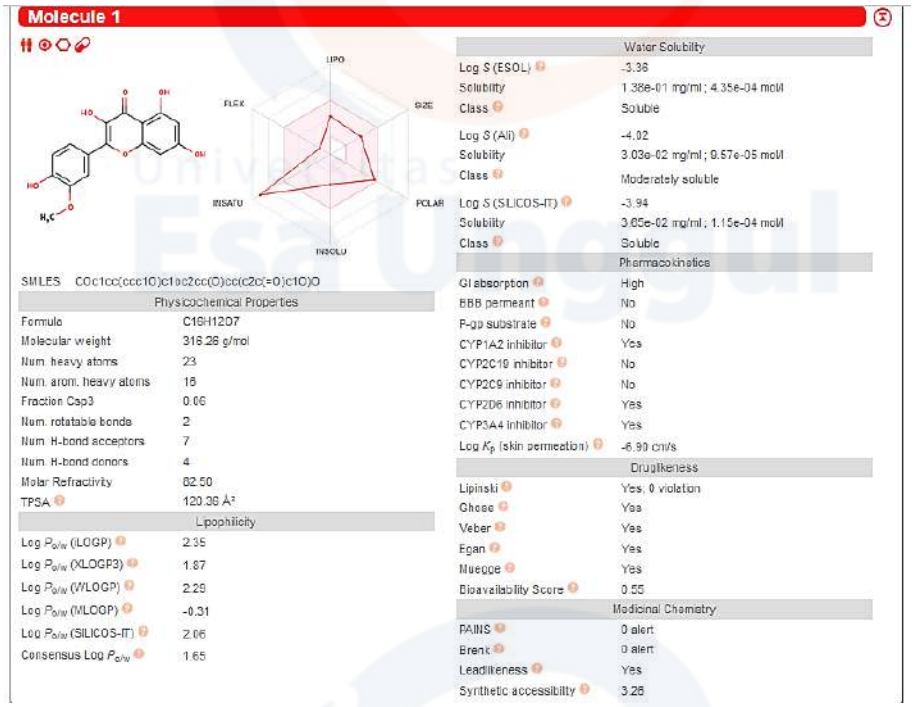
Ginkgolida A



Ginkgolida B

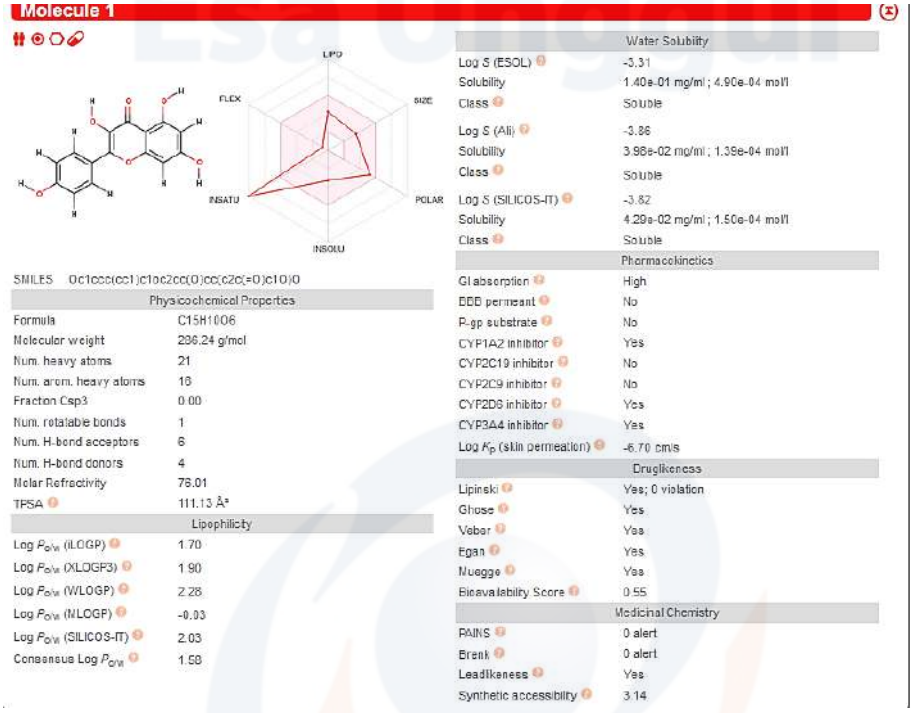
(lanjutan)

Ginkgolida C

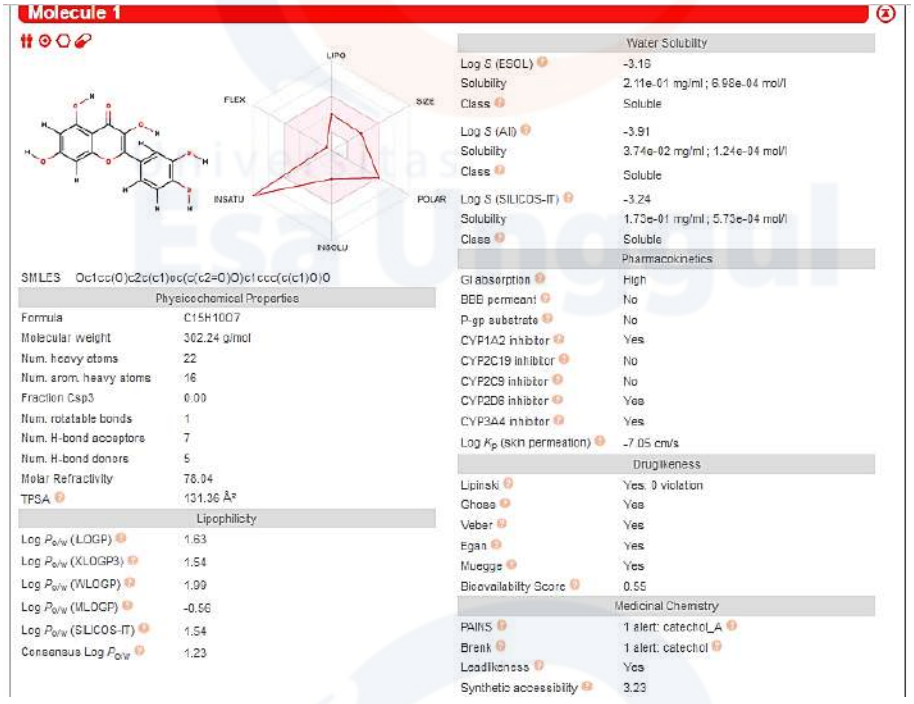


Isorhamnetin

(lanjutan)

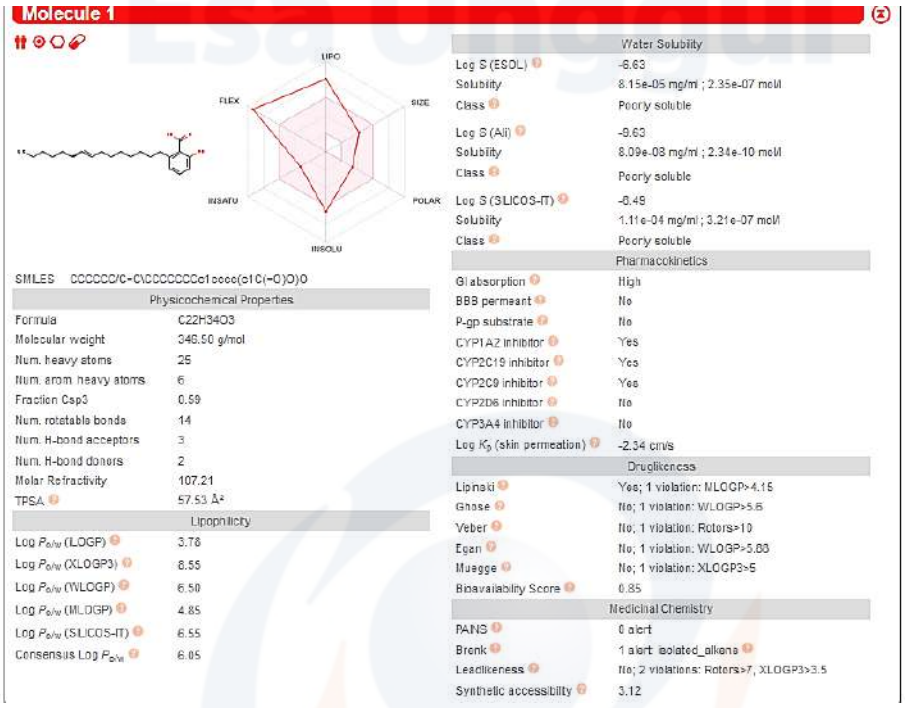


Kaempferol

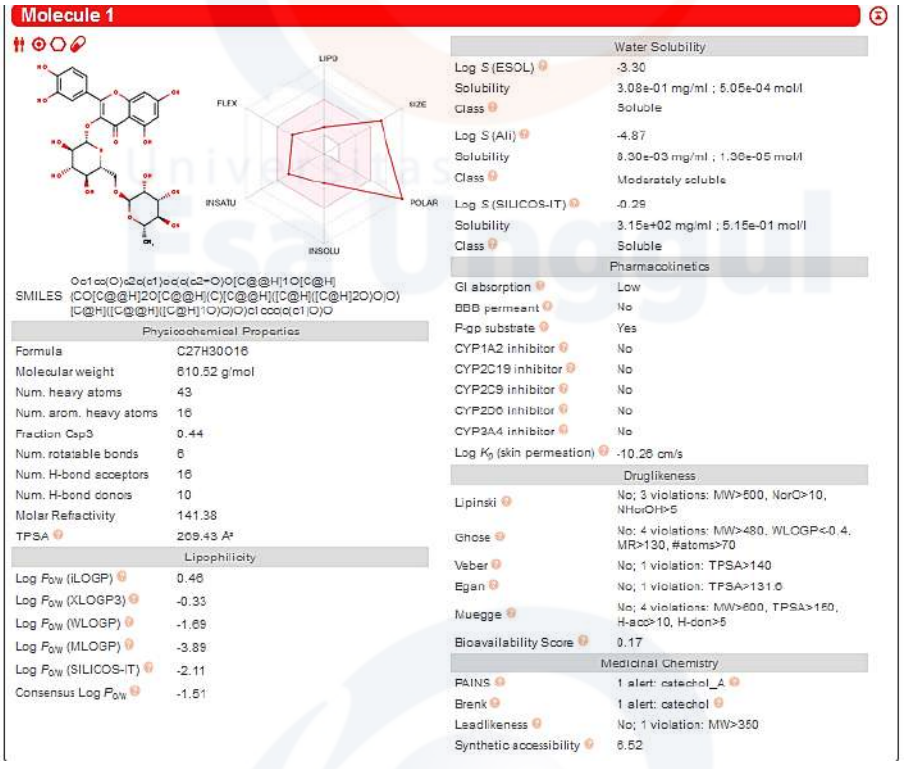


Kuersetin

(lanjutan)

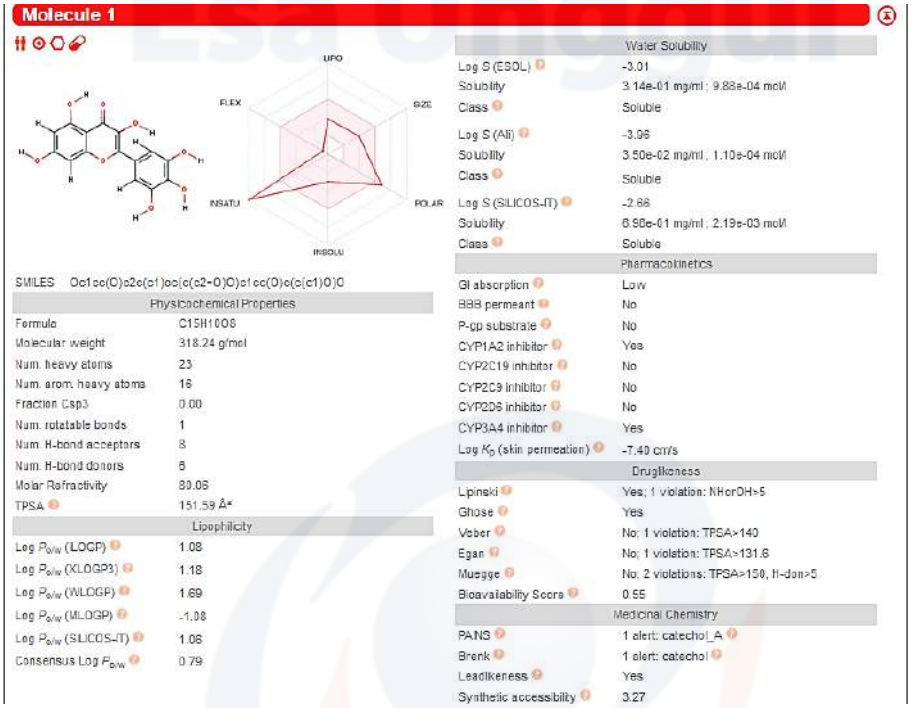


Asam ginkgolik



Rutin

(lanjutan)



Molecule 1

SMILES Oc1cc(O)c2c(c1)oc(c(c2=O)O)c1cc(O)c(O)c(O)c1

Physicochemical Properties	
Formula	C15H10O8
Molecular weight	318.24 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	16
Fraction Csp3	0.00
Num. rotatable bonds	1
Num. H-bond acceptors	8
Num. H-bond donors	6
Molar Refractivity	80.06
TPSA	151.59 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	1.08
Log $P_{o/w}$ (XLOGP3)	1.18
Log $P_{o/w}$ (WLOGP)	1.69
Log $P_{o/w}$ (MLOGP)	-1.08
Log $P_{o/w}$ (SILICOS-IT)	1.08
Consensus Log $P_{o/w}$	0.79

Water Solubility	
Log S (ESOL)	-3.01
Solubility	3.14e-01 mg/ml ; 9.88e-04 mol/l
Class	Soluble
Log S (Ali)	-3.06
Solubility	3.50e-02 mg/ml ; 1.10e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-2.88
Solubility	6.80e-01 mg/ml ; 2.13e-03 mol/l
Class	Soluble

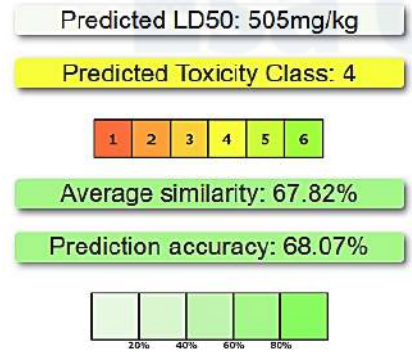
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	Yes
Log K_p (skin permeation)	-7.40 cm/s

Druglikeness	
Lipinski	Yes; 1 violation: NHorOH>5
Ghose	Yes
Veber	No; 1 violation: TPSA>140
Egan	No; 1 violation: TPSA>131.6
Muegge	No; 2 violations: TPSA>150, H-don>5
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	1 alert: catechol_A
Brenk	1 alert: catechol
Leadlikeness	Yes
Synthetic accessibility	3.27

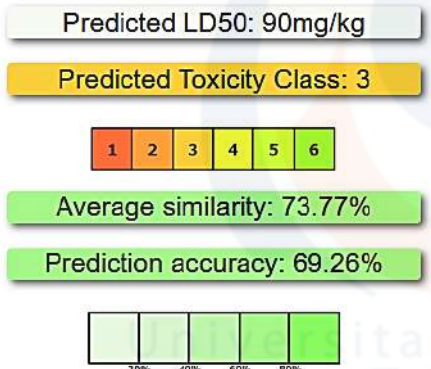
Mirisetin

Lampiran 8. Prediksi toksisitas pada ligan asli dan ligan uji



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.98
Toxicity end points	Carcinogenicity	carcino	Active	0.50
Toxicity end points	Immunotoxicity	immuno	Active	0.95
Toxicity end points	Mutagenicity	mutagen	Inactive	0.53
Toxicity end points	Cytotoxicity	cyto	Active	0.63

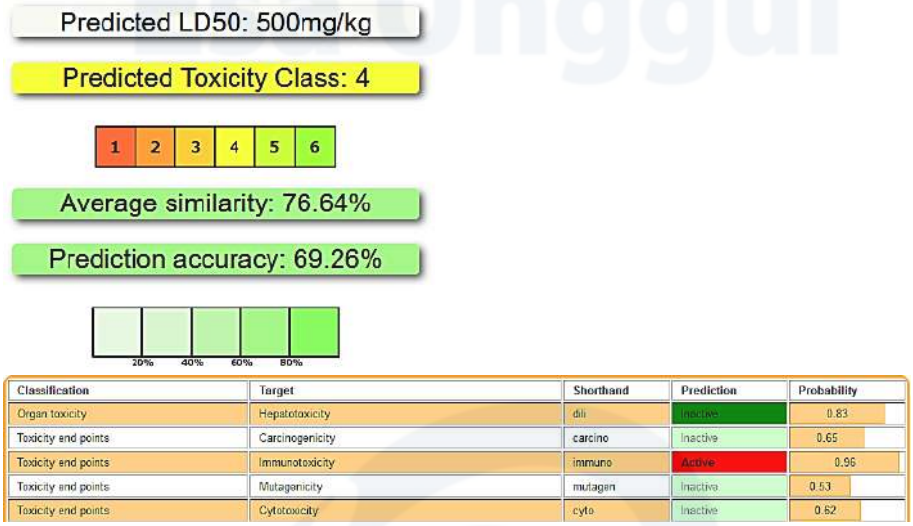
Donepezil



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.87
Toxicity end points	Carcinogenicity	carcino	Inactive	0.64
Toxicity end points	Immunotoxicity	immuno	Active	0.55
Toxicity end points	Mutagenicity	mutagen	Active	0.50
Toxicity end points	Cytotoxicity	cyto	Inactive	0.66

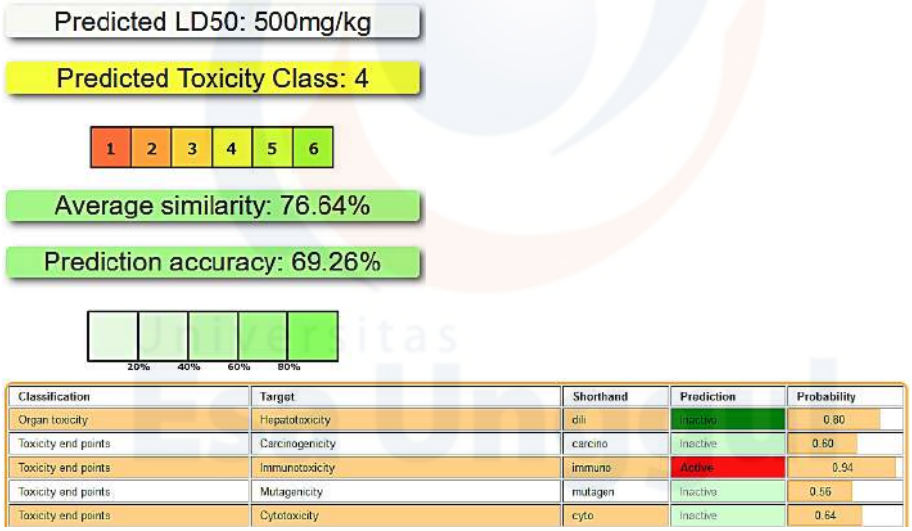
Bilobalida

(lanjutan)



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.83
Toxicity end points	Carcinogenicity	carcino	Inactive	0.65
Toxicity end points	Immunotoxicity	immuno	Active	0.96
Toxicity end points	Mutagenicity	mutagen	Inactive	0.53
Toxicity end points	Cytotoxicity	cyto	Inactive	0.62

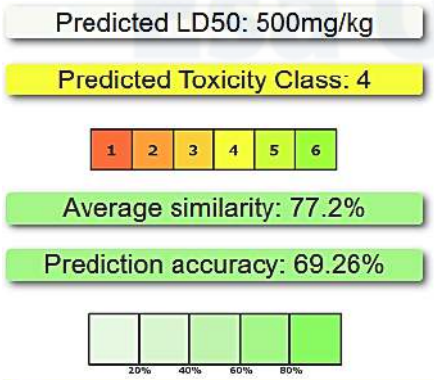
Ginkgolida A



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.80
Toxicity end points	Carcinogenicity	carcino	Inactive	0.60
Toxicity end points	Immunotoxicity	immuno	Active	0.94
Toxicity end points	Mutagenicity	mutagen	Inactive	0.56
Toxicity end points	Cytotoxicity	cyto	Inactive	0.64

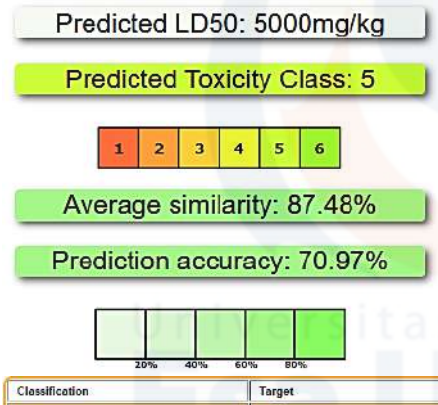
Ginkgolida B

(lanjutan)



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.82
Toxicity end points	Carcinogenicity	carcino	Inactive	0.55
Toxicity end points	Immunotoxicity	immuno	Active	0.77
Toxicity end points	Mutagenicity	mutagen	Inactive	0.63
Toxicity end points	Cytotoxicity	cyto	Inactive	0.65

Ginkgolida C



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.72
Toxicity end points	Carcinogenicity	carcino	Inactive	0.68
Toxicity end points	Immunotoxicity	immuno	Active	0.58
Toxicity end points	Mutagenicity	mutagen	Inactive	0.94
Toxicity end points	Cytotoxicity	cyto	Inactive	0.95

Isorhamnetin

(lanjutan)

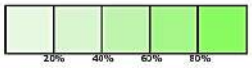
Predicted LD50: 3919mg/kg

Predicted Toxicity Class: 5

1 2 3 4 5 6

Average similarity: 82.46%

Prediction accuracy: 70.97%



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.68
Toxicity end points	Carcinogenicity	carcino	Inactive	0.72
Toxicity end points	Immunotoxicity	immuno	Inactive	0.96
Toxicity end points	Mutagenicity	mutagen	Inactive	0.52
Toxicity end points	Cytotoxicity	cyto	Inactive	0.98

Kaempferol

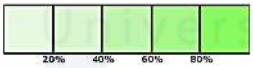
Predicted LD50: 159mg/kg

Predicted Toxicity Class: 3

1 2 3 4 5 6

Average similarity: 100%

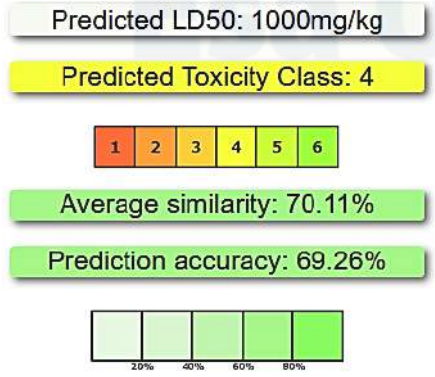
Prediction accuracy: 100%



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.69
Toxicity end points	Carcinogenicity	carcino	Active	0.68
Toxicity end points	Immunotoxicity	immuno	Inactive	0.87
Toxicity end points	Mutagenicity	mutagen	Active	0.51
Toxicity end points	Cytotoxicity	cyto	Inactive	0.99

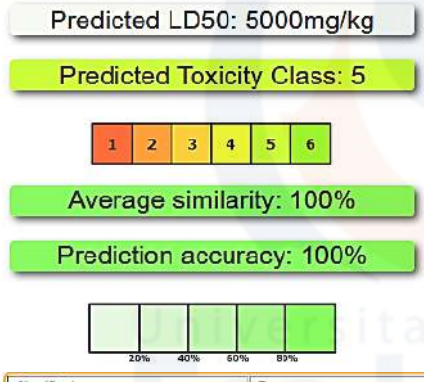
Kuersetin

(lanjutan)



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.77
Toxicity end points	Carcinogenicity	carcino	Inactive	0.72
Toxicity end points	Immunotoxicity	immuno	Active	0.60
Toxicity end points	Mutagenicity	mutagen	Inactive	0.89
Toxicity end points	Cytotoxicity	cyto	Inactive	0.75

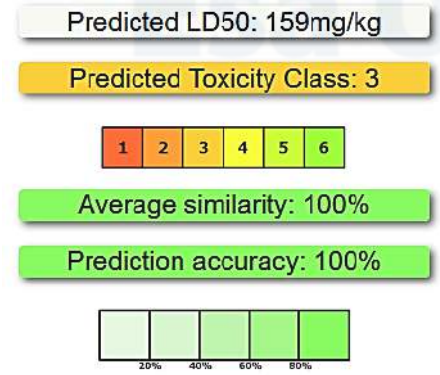
Asam ginkgolik



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.80
Toxicity end points	Carcinogenicity	carcino	Inactive	0.91
Toxicity end points	Immunotoxicity	immuno	Active	0.96
Toxicity end points	Mutagenicity	mutagen	Inactive	0.88
Toxicity end points	Cytotoxicity	cyto	Inactive	0.64

Rutin

(lanjutan)



Classification	Target	Shorthand	Prediction	Probability
Organ toxicity	Hepatotoxicity	dili	Inactive	0.69
Toxicity end points	Carcinogenicity	carcino	Active	0.68
Toxicity end points	Immunotoxicity	immuno	Inactive	0.86
Toxicity end points	Mutagenicity	mutagen	Active	0.51
Toxicity end points	Cytotoxicity	cyto	Inactive	0.99

Mirisetin