LAMPIRAN

Lampiran 1. Prediksi Aktivitas Biologis Senyawa Ikan Sidat dengan PASS Online

1. Senyawa dengan aktivitas biologis antiviral influenza dan influenza A dengan Pa>0,6

Nama Senyawa	CID	Pa	Pi	Aktivitas Biologis	SMILE
4-Hydroxybenzenesulfonic acid	4765	0.792	0.002	Antiviral (Influenza A)	C1=CC(=CC=C1O)S(=O)(=O)O
15(R)-Prostaglandin D2	132282632	0.749	0.004	Antiviral (Influenza)	CCCCCC(C=CC1C(C(CC1=O)O)CC=CCCCC(=O)O)O
1beta-Hydroxycholic acid	5283893	0.728	0.004	Antiviral (Influenza)	CC(CCC(=O)O)C1CCC2C1(C(CC3C2C(CC4C3(C(CC(C4)O)O)C)O)O)C
4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol	443212	0.72	0.004	Antiviral (Influenza)	CC(CCC=C(C)C)C1CC=C2C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C)C
Carboprost	5281075	0.709	0.005	Antiviral (Influenza)	CCCCCC(C)(C=CC1C(CC(C1CC=CCCCC(=O)O)O)O)O
4-Dodecylbenzenesulfonic acid	8485	0.672	0.008	Antiviral (Influenza)	CCCCCCCCCCCCC1=CC=C(C=C1)S(=O)(=O)O
10-HDA	5312738	0.642	0.01	Antiviral (Influenza)	C(CCCC=CC(=O)O)CCCO
10,16-Dihydroxyhexadecanoic acid	441449	0.621	0.011	Antiviral (Influenza)	C(CCCCC(=O)O)CCCC(CCCCCCO)O
9,10-Dihydroxystearic acid	89377	0.599	0.013	Antiviral (Influenza)	CCCCCCCCC(C(CCCCCCCC(=O)O)O)O
(R)-2-hydroxystearic acid	439885	0.619	0.012	Antiviral (Influenza)	CCCCCCCCCCCCCCCCC(C(=O)O)O
2-Hydroxymyristic acid	1563	0.619	0.012	Antiviral (Influenza)	CCCCCCCCCCCCC(C(=O)O)O
2-Hydroxytetracosanoic acid	102430	0.619	0.012	Antiviral (Influenza)	CCCCCCCCCCCCCCCCCCCCCCC(C(=O)O)O
3-Hydroxysebacic acid	3017884	0.605	0.013	Antiviral (Influenza)	C(CCCC(=O)O)CCC(CC(=O)O)O
4-(Heptyloxy)benzoic acid	85154	0.625	0.011	Antiviral (Influenza)	CCCCCCCOC1=CC=C(C=C1)C(=O)O

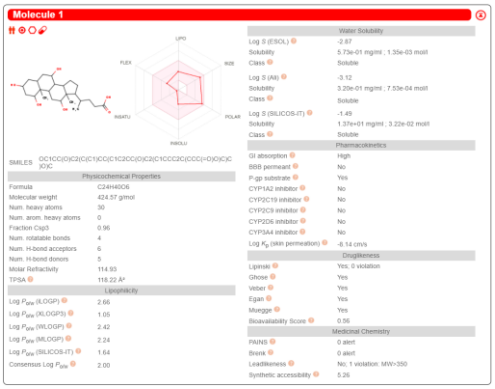
1,2,3-cyclopropanetricarboxylic acid	604010	0.609	0.012	Antiviral (Influenza)	CCOC(=O)C1C(C1C(=O)OCC)C(=O)OCC
(2R)-2,3-Dihydroxypropanoic acid	439194	0.6	0.013	Antiviral (Influenza)	C(C(C(=O)O)O)O
6-acetyloxy-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid	51694232	0.674	0.007	Antiviral (Influenza)	CC(=O)OC1CC2C(=CCC3C2(CCCC3(C)C(=O)O)C)CC1(C)C=C
(±)13-HODE	6443013	0.646	0.009	Antiviral (Influenza)	CCCCCC(C=CC=CCCCCCCCC(=O)O)O
(R)-3-Hydroxy myristic acid	5288266	0.635	0.01	Antiviral (Influenza)	CCCCCCCCCCCC(CC(=O)O)O
3-Hydroxypentadecanoic acid	182089	0.635	0.01	Antiviral (Influenza)	CCCCCCCCCCCCC(CC(=O)O)O
4-(hydroxymethyl)benzoic acid	76360	0.622	0.011	Antiviral (Influenza)	C1=CC(=CC=C1CO)C(=O)O
Androstanolone	10635	0.658	0.009	Antiviral (Influenza)	CC12CCC(=O)CC1CCC3C2CCC4(C3CCC4O)C
19(R)-hydroxy Prostaglandin A2	16061098	0.655	0.009	Antiviral (Influenza)	CC(CCCC(C=CC1C=CC(=O)C1CC=CCCCC(=O)O)O)O
4-[(2,4-Dihydroxyphenyl)diazenyl] benzenesulfonic acid	11035	0.653	0.009	Antiviral (Influenza)	C1=CC(=CC=C1N=NC2=C(C=C(C=C2)O)O)S(=O)(=O)O
14(Z)-Eicosenoic acid	5282770	0.652	0.009	Antiviral (Influenza)	CCCCCC=CCCCCCCCCCCCCC(=O)O
Androst-4-en-3-one	250294	0.646	0.009	Antiviral (Influenza)	CC12CCCC1C3CCC4=CC(=O)CCC4(C3CC2)C
13Z,16Z-docosadienoic acid	5312554	0.599	0.013	Antiviral (Influenza)	CCCCCC=CCC=CCCCCCCCCCCCC(=O)O
8Z,11Z,14Z-Eicosatrienoic acid	5280581	0.599	0.013	Antiviral (Influenza)	CCCCCC=CCC=CCC=CCCCCCCC(=O)O
Adrenic acid	5497181	0.599	0.013	Antiviral (Influenza)	CCCCCC=CCC=CCC=CCC=CCCCCCC(=O)O
Arachidonic acid	444899	0.599	0.013	Antiviral (Influenza)	CCCCCC=CCC=CCC=CCC=CCCCC(=O)O
(±)11(12)-EET	53480479	0.609	0.012	Antiviral (Influenza)	CCCCCC=CCC1C(O1)CC=CCC=CCCCC(=O)O
8-(4-Sulfophenyl) octanoic acid	53987276	0.668	0.008	Antiviral (Influenza)	C1=CC(=CC=C1CCCCCCCC(=O)O)S(=O)(=O)O

2. Senyawa dengan aktivitas biologis antiviral poxvirus, rhinovirus, dan picornavirus dengan Pa>0,7

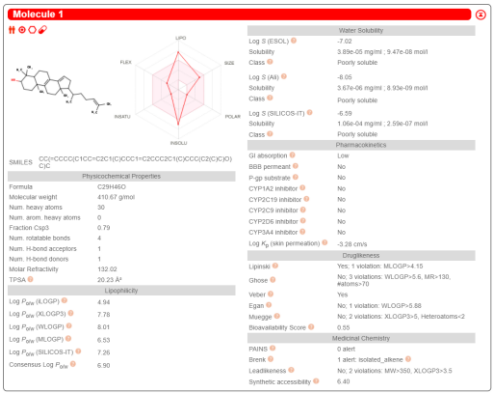
Nama Senyawa	CID	Pa	Pi	Aktivitas Biologis	SMILES
Adenosine-5'-diphosphate Di(monocyclohexylammonium)salt	197	0.956	0.001	Antiviral (Poxvirus)	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)COP(=O)(O)OP(=O)(O)O)O)O)N
(10S)-Juvenile hormone III diol	10859043	0.891	0	Antiviral (Rhinovirus)	CC(=CCCC(=CC(=O)OC)C)CCC(C(C)(C)O)O
9-(2,3-dihydroxypropoxy)-9-oxononanoic acid	45783154	0.762	0.002	Antiviral (Rhinovirus)	C(CCCC(=O)O)CCCC(=O)OCC(CO)O
2,3-dihydroxypropyl 12-methyltridecanoate	10828227	0.749	0.002	Antiviral (Rhinovirus)	CC(C)CCCCCCCCCCC(=O)OCC(CO)O
4-methyl-2-oxopentanoic acid	70	0.739	0.004	Antiviral	CC(C)CC(=O)C(=O)O
4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol	443212	0.719	0.002	Antiviral (Rhinovirus)	CC(CCC=C(C)C)C1CC=C2C1(CCC3=C2CCC4C3(CCC(C4(C)C)O)C)C
16-Heptadecyne-1,2,4-triol	3015189	0.717	0.002	Antiviral (Rhinovirus)	C#CCCCCCCCCCCCC(CC(CO)O)O
Chenodeoxycholic acid 3-sulfate	21252312	0.707	0.003	Antiviral (Rhinovirus)	CC(CCC(=O)O)C1CCC2C1(CCC3C2C(CC4C3(CCC(C4)OS(=O)(=O)O)C)O)C
Cannabigerol	5315659	0.703	0.003	Antiviral (Rhinovirus)	CCCCCC1=CC(=C(C(=C1)O)CC=C(C)CCC=C(C)C)O
2-Oxobutyric acid	58	0.7	0.004	Antiviral	CCC(=O)C(=O)O
Avocadyne Acetate	3952079	0.7	0.003	Antiviral (Rhinovirus)	CC(=O)OCC(CC(CCCCCCCCCCCC#C)O)O
C12-AE1S (TENTATIVE)	24761	0.701	0.003	Antiviral (Rhinovirus)	CCCCCCCCCCCCOCCOS(=O)(=O)O

Lampiran 2. Prediksi Molekul Obat SwissADME

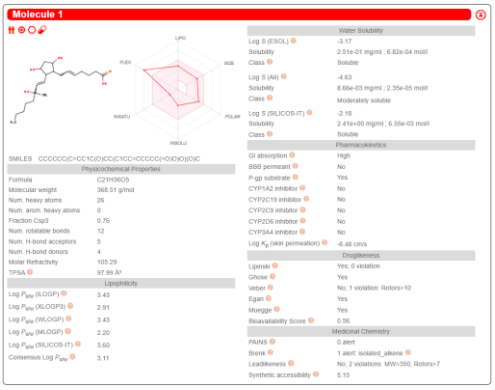
1. 1beta-Hydroxycholic acid



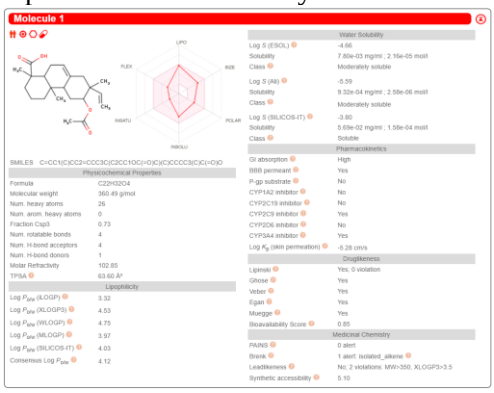
2. 4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol



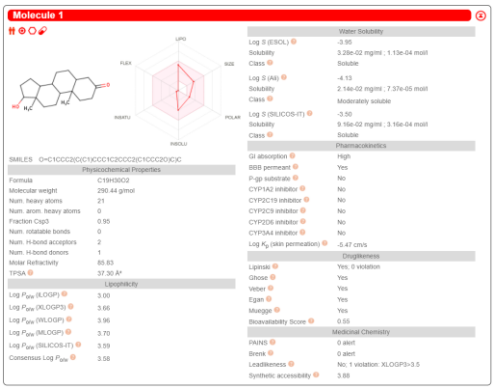
3. Carboprost



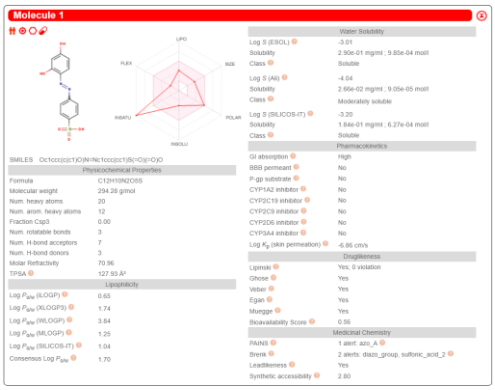
4. 6-acetyloxy-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid



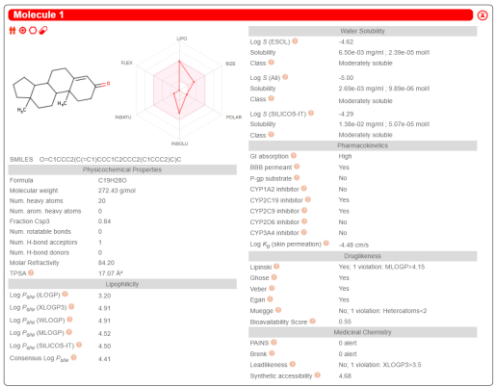
5. Androstanolone



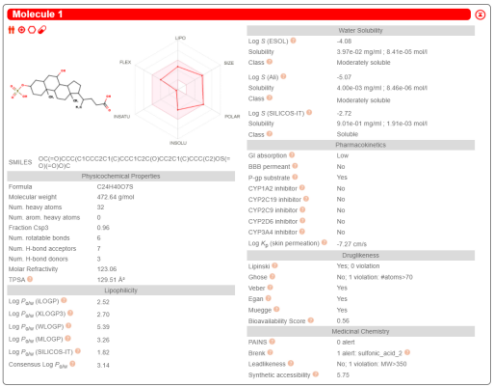
6. 4-[(2,4-Dihydroxyphenyl)diazenyl] benzenesulfonic acid



7. Androst-4-en-3-one



8. Chenodeoxycholic acid 3-sulfate



Lampiran 3. Konfigurasi Penambatan Molekuler Autodock Vina

1. Data input Main Protease (M^{pro}) Sars-CoV-2

*Conf6w63_Ligand - Notepad

File Edit Format View Help

```
receptor = 6w63_Mpro.pdbqt
ligand = Ligan_ID.pdbqt

out = out1.pdbqt

center_x = -19.340
center_y = 18.376
center_z = -27.228

size_x = 18
size_y = 18
size_z = 18

log = log.txt
num_modes = 9
exhaustiveness = 32
```

2. Data input Receptor Binding Domain (RBD) Sars-CoV-2

*Conf6m0jE_Ligand - Notepad

File Edit Format View Help

```
receptor = 6m0jE_RBD.pdbqt
ligand = Ligan_ID.pdbqt

out = out1.pdbqt

center_x = -36.588
center_y = 28.757
center_z = 3.603

size_x = 24
size_y = 40
size_z = 24

log = log.txt
num_modes = 9
exhaustiveness = 32
```

3. Data input Receptor Angiotensin-converting Enzyme (ACE2)

*Conf6m0jA_Ligand - Notepad

File Edit Format View Help

```
receptor = 6m0j_ACE2.pdbqt
ligand = Ligan_ID.pdbqt

out = out1.pdbqt

center_x = -34.607
center_y = 31.063
center_z = -3.383

size_x = 20
size_y = 40
size_z = 20

log = log.txt
num_modes = 9
exhaustiveness = 32
```

Lampiran 4. Log Penambatan M^{pro} Sars-CoV-2 Autodock Vina

1. Remdesivir

Log_6w63_Remdesivir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 234742180
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         -7.9      1.221      2.087
   3         -7.8      2.914      7.437
   4         -7.7      2.866      7.142
   5         -7.6      2.632      7.390
   6         -7.6      2.149      3.924
   7         -7.6      2.154      4.884
   8         -7.5      2.406      4.365
   9         -7.5      2.689      7.549
Writing output ... done.
```

2. Nelfinavir

Log6w63_Nelfinavir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 826519980
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      1.772      3.059
   3         -8.4      1.476      2.224
   4         -8.4      2.061      3.101
   5         -8.3      1.536      1.994
   6         -8.3      2.020      4.259
   7         -8.2      2.442      7.604
   8         -8.2      2.563      6.632
   9         -8.1      2.380      3.922
Writing output ... done.
```

3. Hydroxychloroquine

Log6w63_Hyedoxychloroquine - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -870692872
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.2      0.000      0.000
   2         -6.1      2.309      3.900
   3         -6.1      2.472      3.984
   4         -6.0      1.682      2.535
   5         -5.9      2.777      4.391
   6         -5.9      1.237      1.809
   7         -5.9      2.798      4.445
   8         -5.9      4.004      7.712
   9         -5.8      3.575      6.212
Writing output ... done.
```

4. Molnupiravir

log6w63_Molnupiravir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1646261760
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.8      0.000      0.000
   2         -6.6      3.726      5.667
   3         -6.4      2.918      5.839
   4         -6.4      2.142      5.070
   5         -6.4      3.030      6.572
   6         -6.4      3.692      6.050
   7         -6.4      2.234      5.149
   8         -6.4      3.272      5.558
   9         -6.3      3.359      6.916
Writing output ... done.
```

5. 1beta-Hydroxycholic acid

Log6w63_5283893 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1441435152
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -7.3      3.670      7.738
   3         -7.0      2.229      3.007
   4         -6.9      3.130      7.796
   5         -6.9      3.611      8.204
   6         -6.8      2.191      3.663
   7         -6.8      2.162      3.967
   8         -6.8      1.862      8.210
   9         -6.8      3.652      6.371
Writing output ... done.
```

6. 4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol

Log6w63_443212 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1875534124
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -7.3      2.605      5.072
   3         -7.2      3.549      9.335
   4         -7.0      1.539      3.543
   5         -6.9      2.113      3.614
   6         -6.9      2.282      3.941
   7         -6.8      3.158      8.240
   8         -6.8      2.232      4.945
   9         -6.8      1.560      3.189
Writing output ... done.
```

7. Carboprost

Log6w63_5281075 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2131044288
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.3      0.000      0.000
   2         -5.9      2.042      3.632
   3         -5.9      1.907      3.594
   4         -5.8      2.169      3.365
   5         -5.8      3.052      6.668
   6         -5.8      3.330      5.728
   7         -5.8      3.472      6.311
   8         -5.7      1.520      2.296
   9         -5.7      2.741      5.611
Writing output ... done.
```

8. 6-acetyloxy-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid

Log6w63_51694232 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1922542440
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.9      0.000      0.000
   2         -6.6      1.775      6.897
   3         -6.5      2.613      6.076
   4         -6.4      3.382      7.052
   5         -6.2      2.006      2.996
   6         -6.2      2.193      6.727
   7         -6.2      2.681      3.517
   8         -6.1      2.737      5.203
   9         -6.1      2.946      4.908
Writing output ... done.
```

9. Androstanolone

Log6w63_10635 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -195838696
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         -7.3      3.085      6.655
   3         -6.8      2.762      3.796
   4         -6.7      3.968      7.343
   5         -6.7      4.801      7.050
   6         -6.6      1.082      6.380
   7         -6.5      1.519      2.965
   8         -6.5      1.893      6.338
   9         -6.5      1.267      6.556
Writing output ... done.
```

10. 4-[(2,4-Dihydroxyphenyl)diazenyl] benzenesulfonic acid

Log6w63_11035 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2117621460
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.9      0.000      0.000
   2         -6.9      1.149      1.889
   3         -6.5      5.434      7.313
   4         -6.3      5.462      6.885
   5         -6.3      5.155      5.951
   6         -6.1      5.490      6.451
   7         -6.1      3.455      8.469
   8         -6.1      5.261      6.146
   9         -6.1      5.714      8.513
Writing output ... done.
```

11. Androst-4-en-3-one

Log6w63_250294 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1318792496
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.2      0.000      0.000
   2         -7.0      2.877      3.872
   3         -6.9      2.553      3.507
   4         -6.9      1.391      1.712
   5         -6.8      3.635      5.869
   6         -6.7      3.031      6.252
   7         -6.6      2.949      6.276
   8         -6.5      3.340      5.166
   9         -6.5      3.041      6.283
Writing output ... done.
```

12. Chenodeoxycholic acid 3-sulfate

Log6w63_21252312 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1217666832
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -8.1      0.000      0.000
   2         -7.8      2.069      3.236
   3         -7.4      2.852      4.230
   4         -7.3      3.478      9.110
   5         -7.2      1.866      2.506
   6         -7.2      3.712      9.028
   7         -7.1      3.422      8.824
   8         -7.1      4.047      8.517
   9         -7.0      3.426      8.918
Writing output ... done.
```

Lampiran 5. Log Penambatan RBD SARS-CoV-*2*- Autodock Vina

1. Remdesivir

Log6m0jE_Remdesivir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 736359356
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.7      0.000      0.000
   2         -6.5      1.554      1.955
   3         -6.4      4.106      9.074
   4         -6.4      1.748      2.281
   5         -6.4      4.729     10.111
   6         -6.3      1.741      2.265
   7         -6.2      3.078      9.011
   8         -6.2      3.360      8.983
   9         -6.2      1.972      2.848
Writing output ... done.
```

2. Nelfinavir

Log6m0jE_Nelfinavir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1757677536
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.0      0.000      0.000
   2         -6.9      2.251      3.773
   3         -6.8      5.017     11.608
   4         -6.7      7.919     11.519
   5         -6.7      3.581      6.305
   6         -6.6      5.126     11.180
   7         -6.6      2.674      5.485
   8         -6.6      1.698      4.829
   9         -6.6      1.141      1.444
Writing output ... done.
```

3. Hydroxychloroquine

Log6m0jE_Hyedoxychloroquine - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1592583664
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.2      0.000      0.000
   2         -5.1      2.156      3.160
   3         -5.0      3.615      5.726
   4         -5.0      3.818      6.098
   5         -4.9      2.921      4.347
   6         -4.9      2.846      4.604
   7         -4.9      4.284      6.702
   8         -4.9      2.683      4.188
   9         -4.9      3.536      5.076
Writing output ... done.
```

4. Molnupiravir

log6m0jE_Molnupiravir1 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1501864952
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.9      0.000      0.000
   2         -5.8      1.807      1.886
   3         -5.7      3.204      6.519
   4         -5.6      1.898      2.155
   5         -5.5      1.927      2.228
   6         -5.4      4.017      7.682
   7         -5.4      1.853      2.878
   8         -5.4      3.985      6.935
   9         -5.4      3.533      7.480
Writing output ... done.
```

5. 1beta-Hydroxycholic acid

*Log6m0jE_5283893 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1755523256
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.8      0.000      0.000
   2         -6.6      3.804      6.760
   3         -6.5      1.992      2.480
   4         -6.3      2.906      4.625
   5         -6.1      1.822      2.549
   6         -6.1      3.527      7.135
   7         -6.1      4.243      7.755
   8         -6.1      3.476      6.701
   9         -6.1      4.342      7.681
Writing output ... done.
```

6. 4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol

Log6m0jE_443212 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2080540416
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.9      0.000      0.000
   2         -6.4      2.772      8.344
   3         -6.3      1.697      3.335
   4         -6.2      1.800      3.363
   5         -6.1      8.450     13.683
   6         -6.0      4.060      5.820
   7         -5.9      2.320      3.571
   8         -5.9      4.351      6.039
   9         -5.9      2.424      4.587
Writing output ... done.
```

7. Carboprost

Log6m0jE_5281075 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1063172096
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.3      0.000      0.000
   2         -5.2      1.783      2.092
   3         -5.0      2.839      7.069
   4         -5.0      3.052      5.618
   5         -4.9      3.456      7.279
   6         -4.9      2.496      5.486
   7         -4.8      2.178      7.859
   8         -4.8      2.412      5.427
   9         -4.8      2.536      4.689
Writing output ... done.
```

8. 6-acetyloxy-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid

Log6m0jE_51694232 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -287040336
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.9      0.000      0.000
   2         -5.8      2.446      3.957
   3         -5.7      2.954      6.857
   4         -5.6      3.379      4.573
   5         -5.6      2.599      6.969
   6         -5.5      1.942      2.493
   7         -5.5      1.581      6.799
   8         -5.5      0.984      1.037
   9         -5.4      2.664      6.308
Writing output ... done.
```

9. Androstanolone

Log6m0jE_10635 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1391909756
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.9      0.000      0.000
   2         -5.7      3.321      5.047
   3         -5.7      2.075      6.691
   4         -5.6      2.140      2.867
   5         -5.5      2.057      6.652
   6         -5.5      4.051      6.272
   7         -5.5      1.695      2.487
   8         -5.4      1.160      6.691
   9         -5.4      2.702      4.431
Writing output ... done.
```

10. 4-[(2,4-Dihydroxyphenyl)diazenyl] benzenesulfonic acid

Log6m0jE_11035 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1667413348
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.2      0.000      0.000
   2         -6.1      0.270      1.368
   3         -5.8      1.056      1.846
   4         -5.8      6.324      8.753
   5         -5.7      1.443      1.890
   6         -5.7      1.287      1.875
   7         -5.7      7.046      9.496
   8         -5.5      5.897      9.278
   9         -5.5      6.325      8.885
Writing output ... done.
```

11. Androst-4-en-3-one

Log6m0jE_250294 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1059192832
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -5.7      0.000      0.000
   2         -5.7      2.620      6.000
   3         -5.7      5.319      7.767
   4         -5.7      2.211      4.006
   5         -5.6      5.691      7.985
   6         -5.5      3.035      4.961
   7         -5.5      3.194      5.999
   8         -5.4     14.310     16.473
   9         -5.4      5.186      7.835
Writing output ... done.
```

12. Chenodeoxycholic acid 3-sulfate

Log6m0jE_21252312 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 256506792
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.0      0.000      0.000
   2         -6.3      3.787      5.825
   3         -6.2      3.722      9.877
   4         -6.1      5.641     12.145
   5         -6.0      3.504      9.373
   6         -6.0      5.658      8.437
   7         -6.0      5.195      9.010
   8         -5.9      5.506      8.625
   9         -5.9      5.011      9.017
Writing output ... done.
```

Lampiran 6. Log Penambatan ACE2 Autodock Vina

1. Remdesivir

Log6m0jA_Remdesivir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 639636848
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.5      0.000      0.000
   2         -6.2      2.822     10.256
   3         -5.9      4.432      8.643
   4         -5.8      2.968      6.261
   5         -5.8      1.582      2.160
   6         -5.8      1.283      2.155
   7         -5.7      2.538      5.589
   8         -5.7      1.973      3.703
   9         -5.7     13.307     15.449
Writing output ... done.
```

2. Nelfinavir

Log6m0jA_Nelfinavir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 303451112
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.4      0.000      0.000
   2         -6.0     16.979     20.760
   3         -6.0      3.122      6.130
   4         -6.0     16.548     19.720
   5         -5.9     16.031     19.723
   6         -5.8     17.594     21.393
   7         -5.8      3.713      8.309
   8         -5.8      2.374      8.795
   9         -5.8      2.915      8.480
Writing output ... done.
```

3. Hydroxychloroquine

Log6m0jA_Hyedoxychloroquine - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1428733264
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.4      0.000      0.000
   2         -6.2      1.753      2.305
   3         -6.1      3.341      5.439
   4         -5.8      5.226      8.125
   5         -5.8      3.398      7.807
   6         -5.8      2.994      4.193
   7         -5.7      4.320      8.678
   8         -5.6      3.316      4.992
   9         -5.6      3.418      7.636
Writing output ... done.
```

4. Molnupiravir

log6m0jA_Molnupiravir - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1633839400
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.8      0.000      0.000
   2         -6.6      2.684      5.982
   3         -6.5      2.890      6.116
   4         -6.3      3.780      6.372
   5         -6.1      3.696      6.804
   6         -5.7      4.019      7.112
   7         -5.7     15.849     19.000
   8         -5.7     15.092     18.124
   9         -5.6     15.440     16.917
Writing output ... done.
```

5. 1beta-Hydroxycholic acid

Log6m0jA_5283893 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -458512792
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.2      0.000      0.000
   2         -6.2     14.698     19.419
   3         -6.0     15.395     19.248
   4         -5.9     12.473     15.326
   5         -5.9     15.655     18.900
   6         -5.8     15.010     17.626
   7         -5.7     14.587     17.946
   8         -5.6     15.075     19.078
   9         -5.5     14.306     17.841
Writing output ... done.
```

6. 4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol

Log6m0jA_443212 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 512043268
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.3      0.000      0.000
   2         -6.2      2.718      8.389
   3         -6.2     14.890     19.759
   4         -6.2      3.668      7.068
   5         -5.9     15.221     17.428
   6         -5.9     14.241     16.778
   7         -5.9     13.291     16.198
   8         -5.8     14.740     16.258
   9         -5.8     19.534     25.177
Writing output ... done.
```

7. Carboprost

Log6m0jA_5281075 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1214675844
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         -6.4      2.274      2.910
   3         -6.3      2.847      4.816
   4         -5.6      3.225      5.296
   5         -5.5      4.502      8.002
   6         -5.4     15.774     21.483
   7         -5.3     14.760     20.514
   8         -5.3     13.764     19.233
   9         -5.2      3.476      4.809
Writing output ... done.
```

8. 6-acetyloxy-7-ethenyl-1,4a,7-trimethyl-3,4,4b,5,6,8,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid

Log6m0jA_51694232 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 424532720
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.1      0.000      0.000
   2         -5.7      2.356      4.524
   3         -5.2     13.958     17.437
   4         -4.9      6.680     11.205
   5         -4.9      6.172      9.570
   6         -4.9     13.322     15.824
   7         -4.9      5.395      9.104
   8         -4.8     12.286     15.067
   9         -4.8     12.076     14.318
Writing output ... done.
```

9. Androstanolone

Log6m0jA_10635 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1468768272
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.9      0.000      0.000
   2         -6.6      6.409      8.877
   3         -6.5      0.908      6.647
   4         -6.4      6.844      9.990
   5         -6.1      3.867      8.317
   6         -5.9      2.957      7.602
   7         -5.7      6.269      9.002
   8         -5.6      2.181      6.951
   9         -5.6     13.776     15.233
Writing output ... done.
```

10. 4-[(2,4-Dihydroxyphenyl)diazenyl] benzenesulfonic acid

Log6m0jA_11035 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -298365312
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.0      0.000      0.000
   2         -5.7      3.478      8.120
   3         -5.7     14.229     15.175
   4         -5.5     14.139     15.390
   5         -5.5     14.327     16.840
   6         -5.4     16.854     18.423
   7         -5.4     14.493     17.813
   8         -5.4     14.203     15.157
   9         -5.3      1.820      2.182
Writing output ... done.
```

11. Androst-4-en-3-one

Log6m0jA_250294 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1233320584
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.9      0.000      0.000
   2         -6.7      8.026     10.270
   3         -6.4      4.039      7.416
   4         -6.3      2.885      6.044
   5         -6.2      6.932      9.367
   6         -6.2     13.343     15.368
   7         -6.2      2.738      5.110
   8         -5.9      4.487      7.627
   9         -5.9     18.010     20.528
Writing output ... done.
```

12. Chenodeoxycholic acid 3-sulfate

Log6m0jA_21252312 - Notepad

File Edit Format View Help

```
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1817535500
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -6.2      0.000      0.000
   2         -6.1      4.771     10.879
   3         -6.0      3.165      8.752
   4         -6.0     16.756     18.076
   5         -5.9      3.712      9.294
   6         -5.9      2.739      4.023
   7         -5.7      4.142      9.042
   8         -5.7      2.903      8.956
   9         -5.7      3.382      9.433
Writing output ... done.
```