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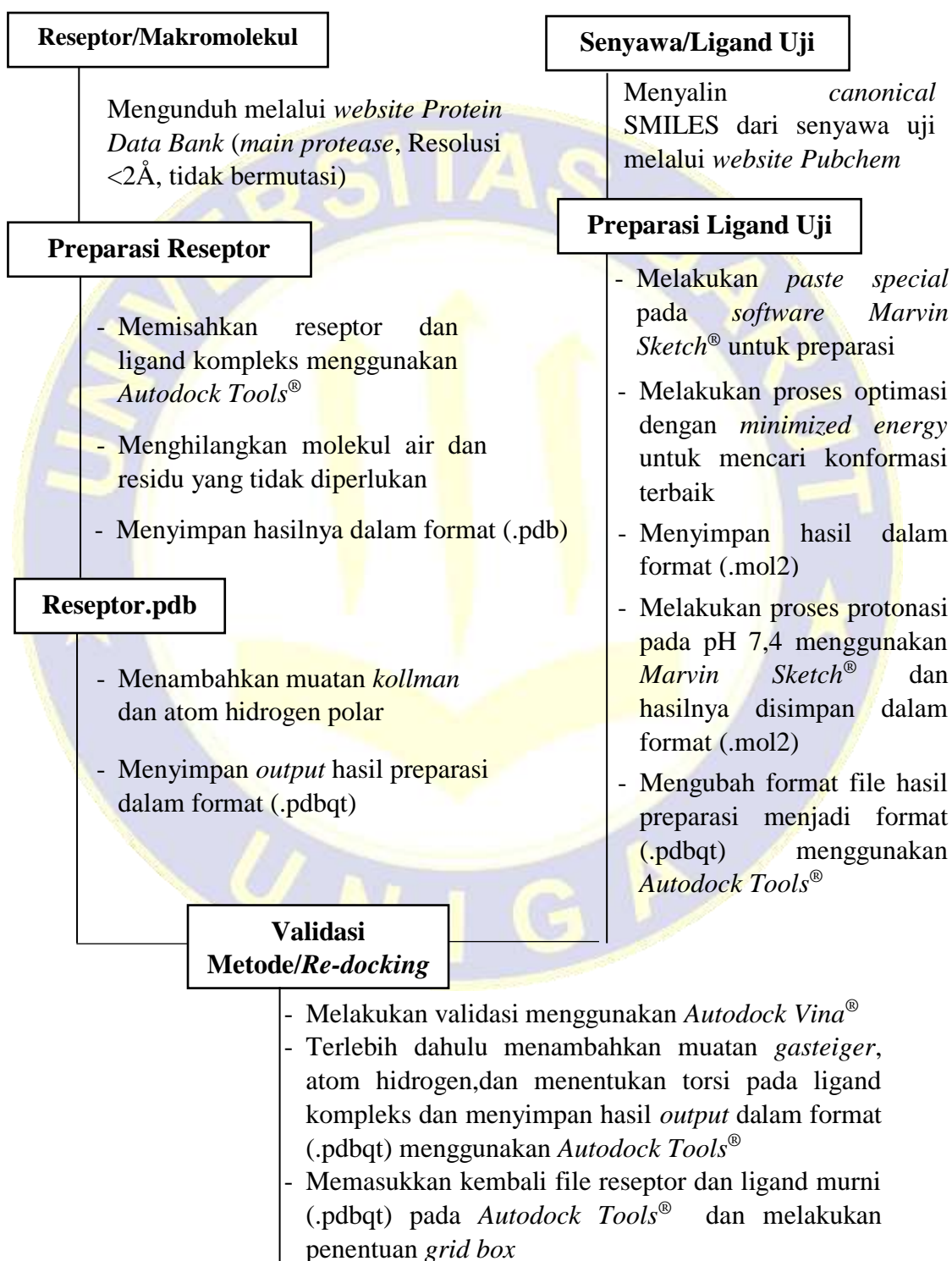
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LAMPIRAN 1

ALUR PENELITIAN SIMULASI *MOLECULAR DOCKING* SENYAWA

AKTIF TANAMAN SAMBILOTO (*Andrographis paniculata*)



LAMPIRAN 1 (LANJUTAN)

- Menyimpan hasil *output* grid dalam file *grid.txt*
- Membuat file konfigurasi pada *notepad* berisi file nama ligand, reseptor, ukuran *grid box*, *exhaustiveness*, *number of modes*, *output docking* dalam format *.pdbqt* dan *.txt* dan menyimpan hasilnya dengan nama file *conf.txt*
- Membuat folder khusus untuk validasi *docking* yang berisi file reseptor dan ligand dalam format *.pdbqt*, *grid.txt*, *conf.txt* dan file *software* vina meliputi *vina_lisence*, *vina_split* dan *vina.exe*, serta *command prompt* (*cmd*)
- Membuka file *command prompt* dan menuliskan perintah “*vina.exe --config conf.txt*” lalu *enter* dan proses *docking* akan berjalan. Hasil *docking* (ΔG) tersimpan dalam file *log.txt*

Perhitungan RMSD

- Menggunakan *software YASARA*[®] berdasarkan hasil *docking* dengan konformasi terbaik dan nilai (ΔG) paling rendah

Simulasi *docking*

- Menggunakan *Autodock Vina*[®]
- Membuat folder khusus untuk *docking* senyawa uji yang berisi file reseptor dan folder lig berisi ligand uji dalam format *.pdbqt*, *config.txt*, *vina_run.bat*, dan *vina.exe*, serta *command prompt* (*cmd*)
- Mengklik folder lig, diikuti klik reseptor dan buka file *command prompt* sehingga akan muncul tampilan proses *docking* sudah berjalan (*running*).

Analisis Hasil

- Hasil *docking* akan tersimpan dalam folder lig yang memuat nilai ΔG , ditandai dengan akhiran file (*_out*)
- Analisis hasil meliputi interaksi molekuler dan residu asam amino serta visualisasi menggunakan *Discovery Studio Visualizer*[®]

Gambar VII. 1 Alur penelitian *molecular docking* senyawa aktif tanaman (*Andrographis paniculata*)

LAMPIRAN 2

ALUR PENELITIAN PENCARIAN DAN PENAMBATAN MOLEKULER

SENYAWA SIMILAR

Senyawa Terpilih Hasil *Docking*

- Menginput *canonical SMILES* yang terdapat pada *website PubChem* ke *website STITCH* (<http://stitch.embl.de/>)
- Menampilkan hasil pencarian berdasarkan nilai similaritas
- Menyimpan senyawa similaritas terpilih hasil pencarian dengan format file (.SDF)

Senyawa Terpilih Hasil *STITCH*

- Menginput *canonical SMILES* yang terdapat pada *website PubChem* ke *website PASS Online* (<http://way2drug.com/passonline/predict.php>) dan submit
- Melakukan prediksi aktivitas antivirus

Preparasi Senyawa Terpilih Hasil *STITCH*

- Menyalin *canonical SMILES* dari senyawa uji melalui *website Pubchem*
- Melakukan *paste special* pada *software Marvin Skech*[®] untuk preparasi
- Melakukan proses optimasi dengan *minimized energy* untuk mencari konformasi terbaik dan Menyimpan hasil dalam format (.mol2)
- Melakukan proses protonasi pada pH 7,4 menggunakan *Marvin Sketch*[®] dan hasilnya disimpan dalam format (.mol2)
- Mengubah format file hasil preparasi menjadi format (.pdbqt) menggunakan *Autodock Tools*[®]

Simulasi *docking*

LAMPIRAN 2 (LANJUTAN)

Simulasi *docking*

- Menggunakan *Autodock Vina*[®]
- Membuat folder khusus untuk *docking* senyawa uji yang berisi file reseptor dan folder lig berisi ligand uji dalam format .pdbqt, config.txt, vina_run.bat, dan vina.exe, serta *command prompt* (cmd)
- Mengklik folder lig, diikuti klik reseptor dan buka file *command prompt* sehingga akan muncul tampilan proses *docking* sudah berjalan (*running*).

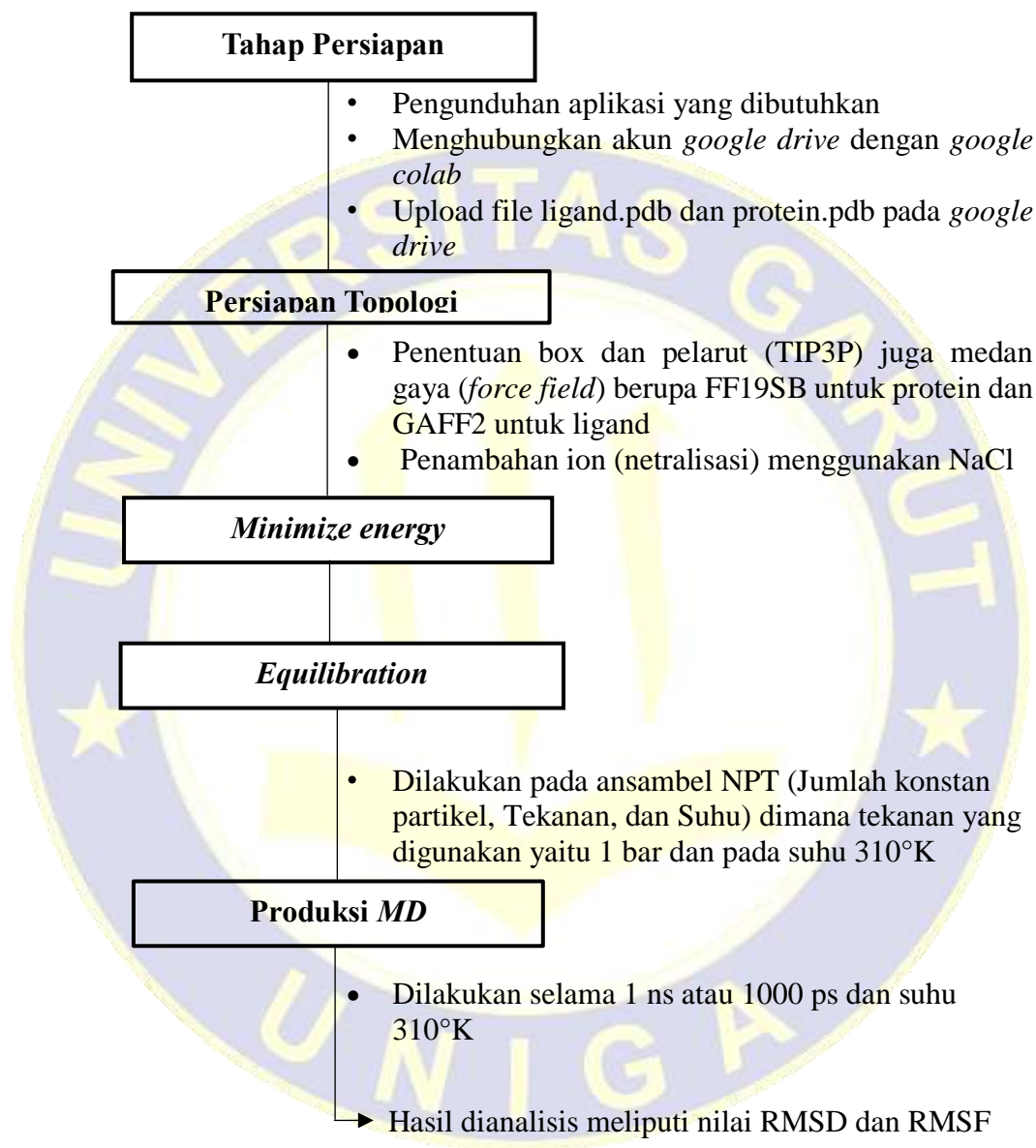
Analisis Hasil

- Hasil *docking* akan tersimpan dalam folder lig yang memuat nilai ΔG , ditandai dengan akhiran nama file (_out)
- Analisis hasil meliputi interaksi molekul dan residu asam amino serta visualisasi menggunakan *Discovery Studio Visualizer*[®]

Gambar VII. 2 Alur penelitian pencarian dan penambatan molekuler senyawa similar

LAMPIRAN 3

ALUR PENELITIAN SIMULASI DINAMIKA MOLEKULER (MD)



Gambar VII. 3 Alur penelitian simulasi dinamika molekuler

LAMPIRAN 4

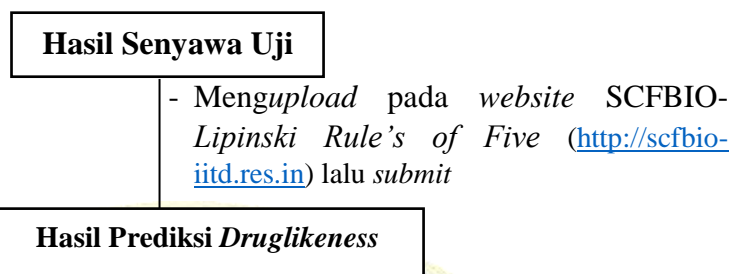
**ALUR PENCARIAN SENYAWA AKTIF, PREDIKSI AKTIVITAS
ANTIVIRUS, PREDIKSI DRUGLIKENESS, PREDIKSI ADMET, DAN
PREDIKSI JALUR SINTESIS**



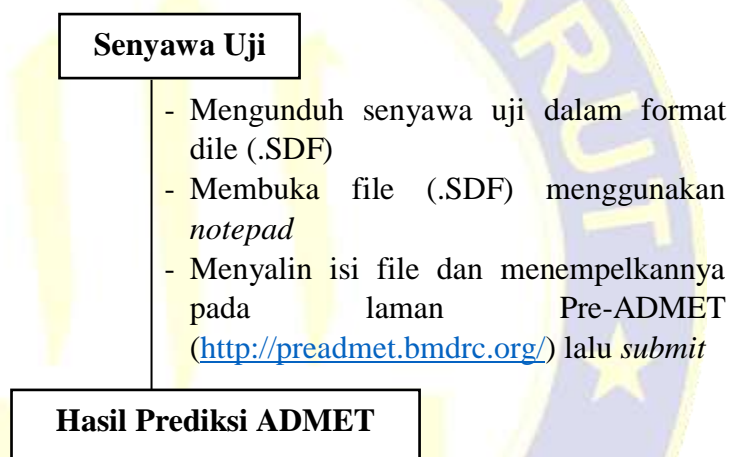
Senyawa Uji

- Menyalin *canonical SMILES* dari senyawa uji melalui *website Pubchem*
- Melakukan *paste special* pada *software Marvin Sketch*[®] untuk proses optimasi
- Menyimpan hasilnya dalam format file (.mol2)

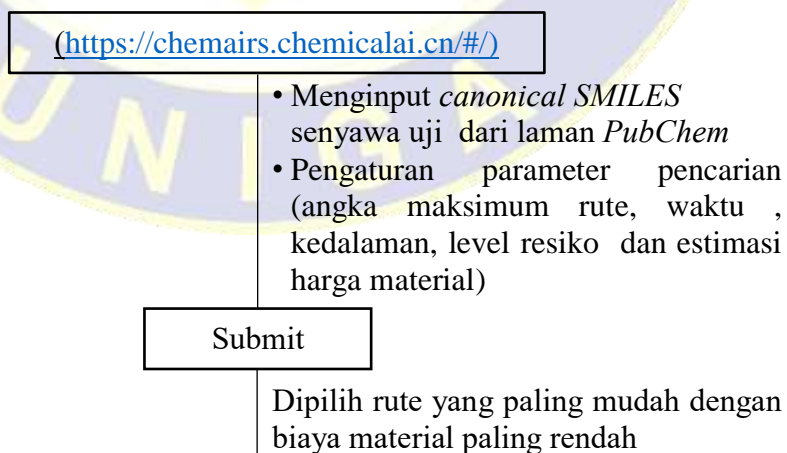
**LAMPIRAN 4
(LANJUTAN)**



Gambar VII. 6 Alur penelitian prediksi *druglikeness*



Gambar VII. 7 Alur penelitian prediksi ADMET

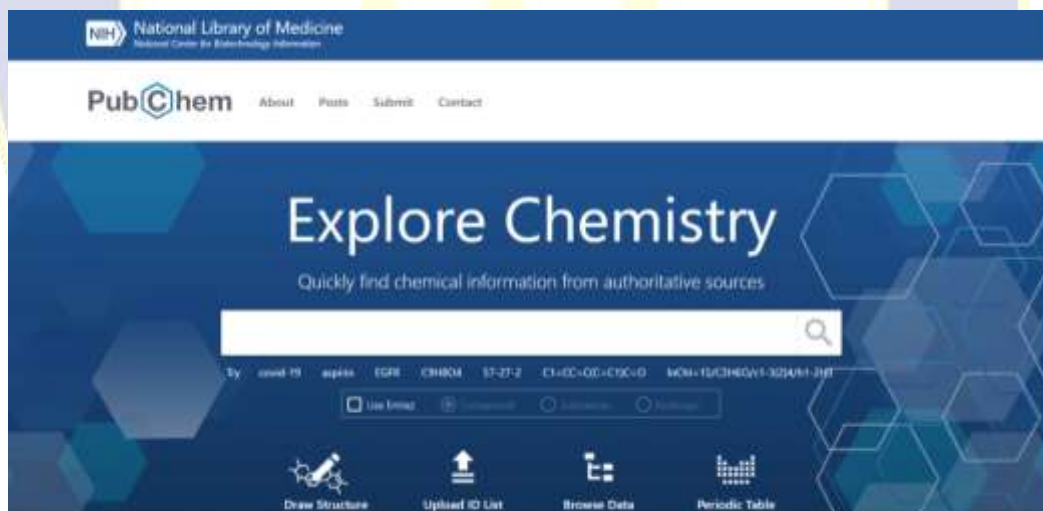


Gambar VII. 8 Alur penelitian prediksi sintesis senyawa

LAMPIRAN 5
SITUS DAN APLIKASI



Gambar VII. 9 Tampilan situs *PASS-Online*



Gambar VII. 10 Tampilan situs *Pubchem*

LAMPIRAN 5 (LANJUTAN)

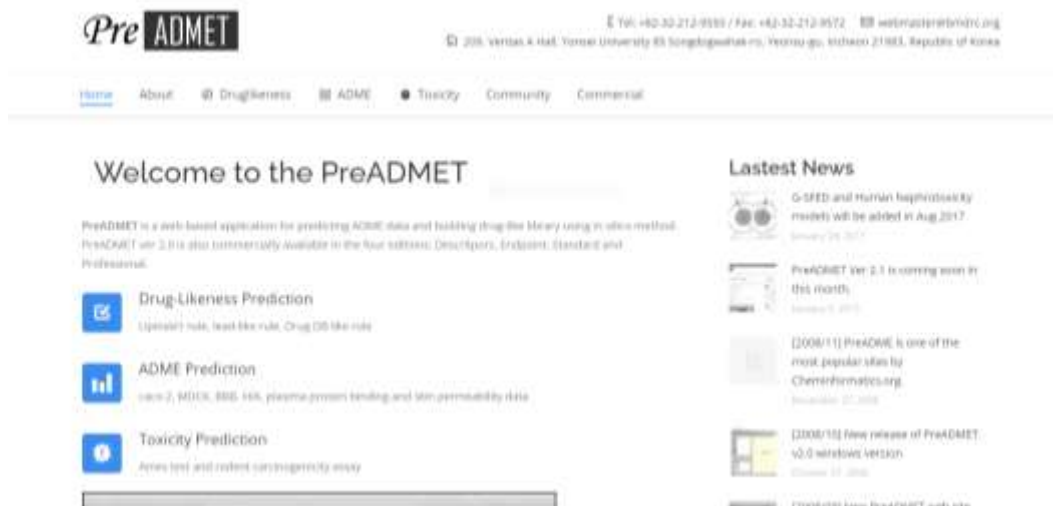


Gambar VII. 11 Tampilan situs *Protein Data Bank*

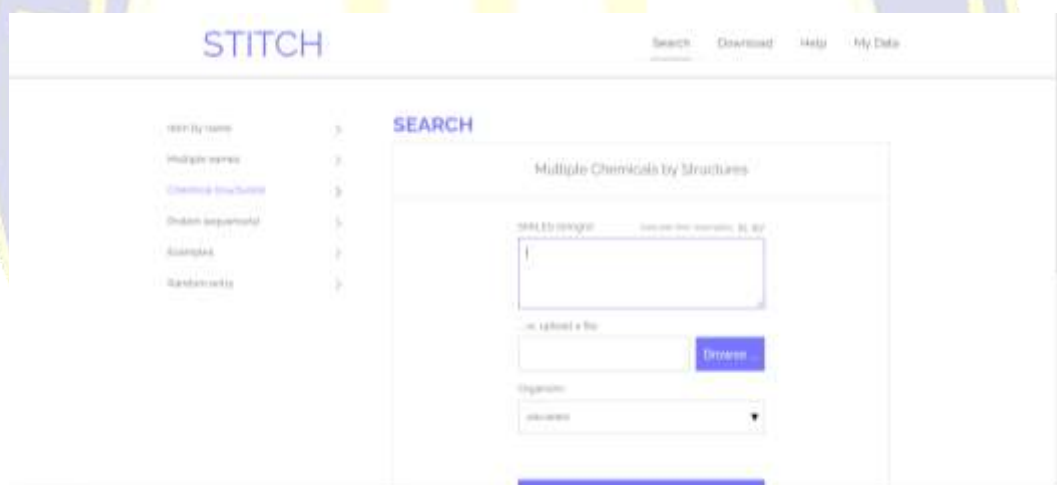


Gambar VII. 12 Tampilan situs *Lipinski's Rule of Five*

LAMPIRAN 5 (LANJUTAN)

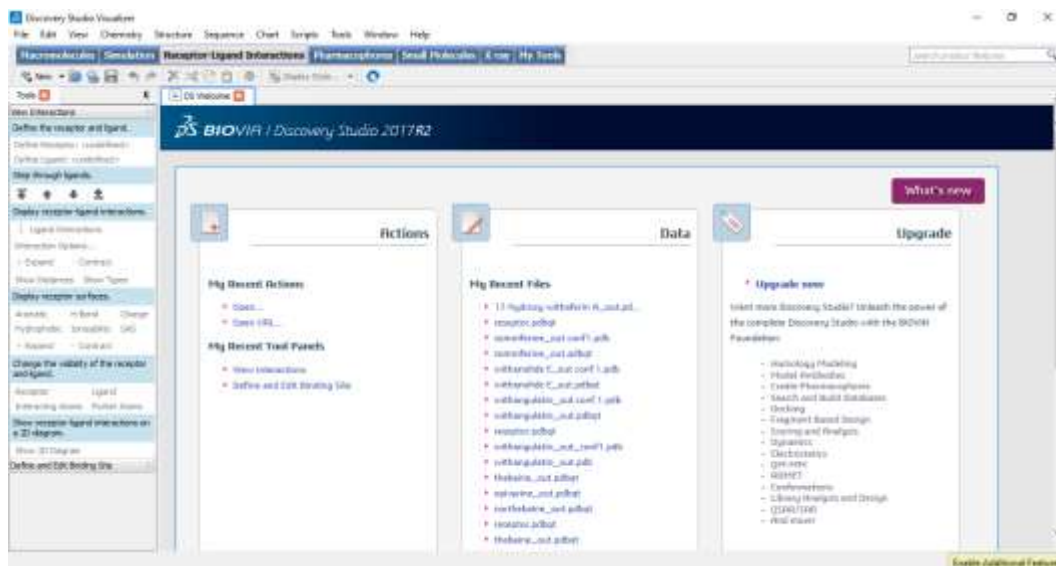


Gambar VII. 13 Tampilan situs *PreADMET*



Gambar VII. 14 Tampilan situs *STITCH*

LAMPIRAN 5 (LANJUTAN)

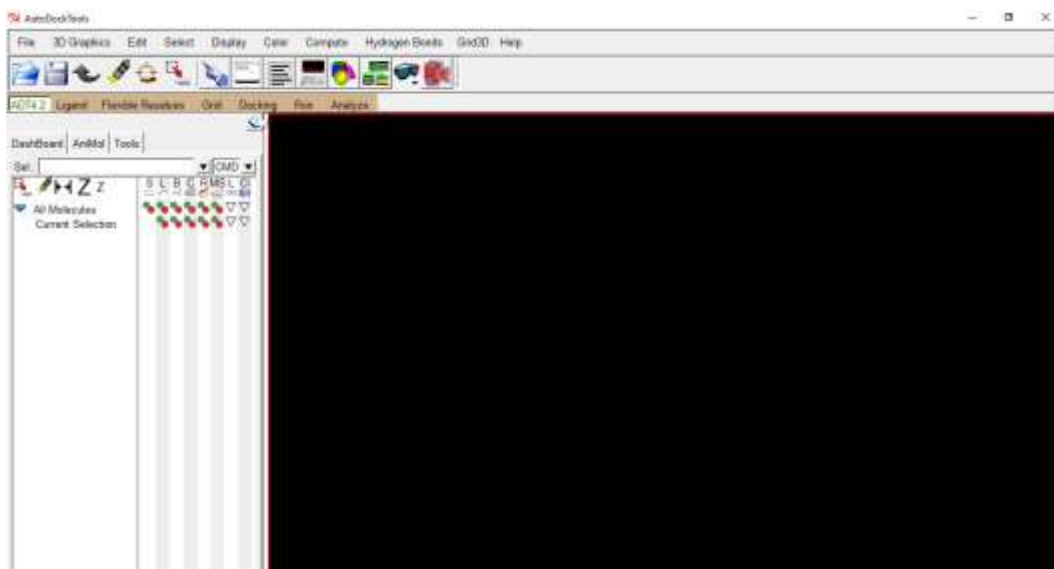


Gambar VII. 17 Tampilan software *Discovery Studio Visualizer*

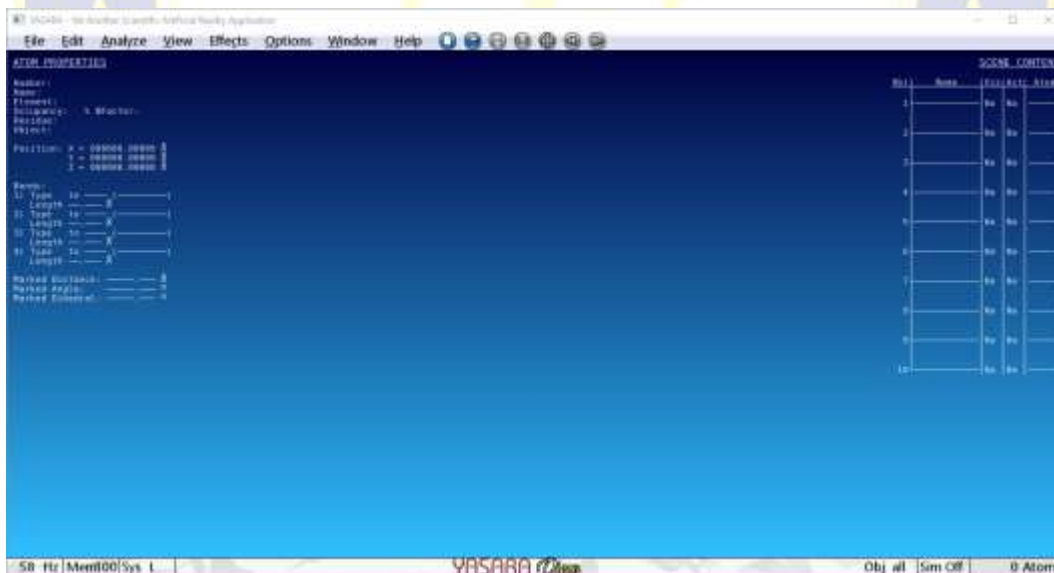


Gambar VII. 18 Tampilan software *Openbabel GUI*

LAMPIRAN 5 (LANJUTAN)

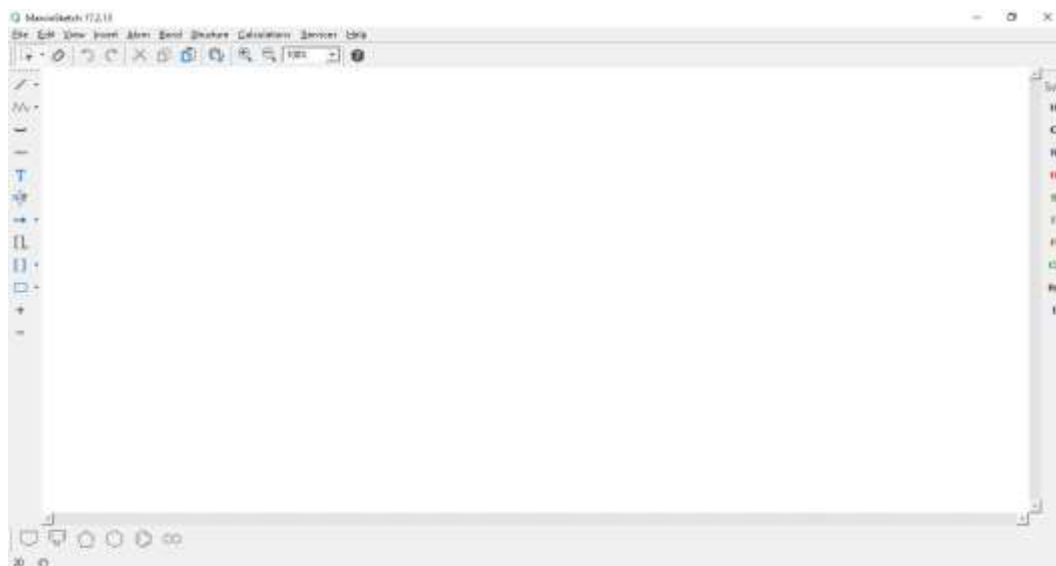


Gambar VII. 19 Tampilan *software Autodock Tools*



Gambar VII. 20 Tampilan *software YASARA*

LAMPIRAN 5 (LANJUTAN)



Gambar VII. 21 Tampilan *software MarvinSketch*

```
D:\LUTFI\KULIAH\SEMESTER B\TA II\Validasi\7519>vina.exe --config conf.txt
The system cannot find message text for message number 0x2350 in the message file for Application.

(c) Microsoft Corporation. All rights reserved.

D:\LUTFI\KULIAH\SEMESTER B\TA II\Validasi\7519>vina.exe --config conf.txt
*****
# 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.
*****
Detected 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1249274792
Performing search ...
0% 10 20 30 40 50 60 70 80 90 100%
|----|----|----|----|----|----|----|----|----|----|
```

Gambar VII. 22 Tampilan *Autodock vina*

LAMPIRAN 6

HASIL SCREENING AKTIVITAS ANTIVIRUS

Tabel VII.1

Hasil *Screening* Aktivitas Antivirus Menggunakan *PASS-Online*Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*)

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
1	<i>Andrographolide</i>	0.424	0.012	Antiviral
		0.203	0.029	Antiviral (HIV)
		0.217	0.071	Antiviral (Hepatitis B)
		0.421	0.027	Antiviral (Herpes)
		0.218	0.169	Antiviral (Influenza A)
		0.401	0.046	Antiviral (Influenza)
		0.367	0.133	Antiviral (Rhinovirus)
2	<i>Neoandrographolide</i>	0.26	0.054	Antiviral
		0.337	0.025	Antiviral (Hepatitis B)
		0.372	0.048	Antiviral (Herpes)
		0.701	0.005	Antiviral (Influenza)
		0.288	0.279	Antiviral (Rhinovirus)
3	<i>Ninandrographolide</i>	0.284	0.043	Antiviral
		0.132	0.09	Antiviral (HIV)
		0.333	0.026	Antiviral (Hepatitis B)
		0.396	0.037	Antiviral (Herpes)
		0.238	0.121	Antiviral (Influenza A)
		0.712	0.005	Antiviral (Influenza)
		0.288	0.279	Antiviral (Rhinovirus)
4	<i>Dihydroskullcap flavone I</i>	0.475	0.006	Antiviral (Hepatitis B)
		0.453	0.018	Antiviral (Herpes)
		0.48	0.026	Antiviral (Influenza)
		0.507	0.022	Antiviral (Rhinovirus)
5	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	0.247	0.142	Antiviral (Adenovirus)
		0.233	0.104	Antiviral (CMV)
		0.385	0.017	Antiviral (Hepatitis B)
		0.447	0.019	Antiviral (Herpes)
		0.432	0.037	Antiviral (Influenza)
		0.319	0.197	Antiviral (Picornavirus)
		0.355	0.151	Antiviral (Rhinovirus)
		0.088	0.059	Antiviral (Trachoma)

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**Tabel VII.1
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No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
6	<i>Paniculide C</i>	0.265	0.059	Antiviral (CMV)
		0.12	0.115	Antiviral (HIV)
		0.192	0.098	Antiviral (Hepatitis B)
		0.341	0.065	Antiviral (Herpes)
		0.203	0.192	Antiviral (Influenza)
		0.36	0.148	Antiviral (Picornavirus)
		0.587	0.007	Antiviral (Rhinovirus)
7	<i>Paniculide B</i>	0.238	0.067	Antiviral
		0.228	0.115	Antiviral (CMV)
		0.152	0.063	Antiviral (HIV)
		0.222	0.067	Antiviral (Hepatitis B)
		0.391	0.039	Antiviral (Herpes)
		0.259	0.123	Antiviral (Influenza)
		0.428	0.089	Antiviral (Picornavirus)
		0.19	0.175	Antiviral (Poxvirus)
		0.6	0.006	Antiviral (Rhinovirus)
8	<i>Paniculide A</i>	0.235	0.069	Antiviral
		0.198	0.188	Antiviral (CMV)
		0.132	0.09	Antiviral (HIV)
		0.176	0.121	Antiviral (Hepatitis B)
		0.376	0.047	Antiviral (Herpes)
		0.263	0.118	Antiviral (Influenza)
		0.43	0.088	Antiviral (Picornavirus)
		0.613	0.005	Antiviral (Rhinovirus)
9	<i>Andrographidin A</i>	0.282	0.043	Antiviral
		0.5	0.004	Antiviral (Hepatitis B)
		0.099	0.063	Antiviral (Hepatitis C)
		0.146	0.037	Antiviral (Hepatitis)
		0.533	0.007	Antiviral (Herpes)
		0.753	0.004	Antiviral (Influenza)
		0.463	0.041	Antiviral (Rhinovirus)
		0.078	0.077	Antiviral (Trachoma)

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
10	<i>Andrographiside</i>	0.525	0.006	Antiviral
		0.327	0.006	Antiviral (HIV)
		0.336	0.025	Antiviral (Hepatitis B)
		0.428	0.024	Antiviral (Herpes)
		0.21	0.193	Antiviral (Influenza A)
		0.496	0.023	Antiviral (Influenza)
11	<i>Andropanolide</i>	0.424	0.012	Antiviral
		0.203	0.029	Antiviral (HIV)
		0.217	0.071	Antiviral (Hepatitis B)
		0.421	0.027	Antiviral (Herpes)
		0.218	0.169	Antiviral (Influenza A)
		0.401	0.046	Antiviral (Influenza)
12	<i>Isoandrographolide</i>	0.367	0.133	Antiviral (Rhinovirus)
		0.424	0.012	Antiviral
		0.203	0.029	Antiviral (HIV)
		0.217	0.071	Antiviral (Hepatitis B)
		0.421	0.027	Antiviral (Herpes)
		0.218	0.169	Antiviral (Influenza A)
13	<i>Bisandrographolide C</i>	0.401	0.046	Antiviral (Influenza)
		0.367	0.133	Antiviral (Rhinovirus)
		0.293	0.039	Antiviral
		0.162	0.053	Antiviral (HIV)
		0.18	0.116	Antiviral (Hepatitis B)
		0.329	0.072	Antiviral (Herpes)
14	<i>Bisandrographolide B</i>	0.225	0.15	Antiviral (Influenza A)
		0.295	0.092	Antiviral (Influenza)
		0.343	0.171	Antiviral (Rhinovirus)
		0.333	0.027	Antiviral
		0.168	0.049	Antiviral (HIV)
		0.192	0.097	Antiviral (Hepatitis B)
		0.315	0.081	Antiviral (Herpes)
0.215	0.179	Antiviral (Influenza A)		
	0.24	0.143	Antiviral (Influenza)	
	0.311	0.23	Antiviral (Rhinovirus)	

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
15	<i>14-Acetylandrographolide</i>	0.473	0.008	Antiviral
		0.265	0.013	Antiviral (HIV)
		0.204	0.083	Antiviral (Hepatitis B)
		0.416	0.029	Antiviral (Herpes)
		0.335	0.07	Antiviral (Influenza)
		0.417	0.074	Antiviral (Rhinovirus)
16	<i>5,7,2',3'-Tetramethoxyflavanone</i>	0.357	0.021	Antiviral (Hepatitis B)
		0.435	0.022	Antiviral (Herpes)
		0.418	0.041	Antiviral (Influenza)
		0.551	0.012	Antiviral (Rhinovirus)
17	<i>14-Deoxy-17-hydroxyandrographolide</i>	0.369	0.019	Antiviral
		0.182	0.039	Antiviral (HIV)
		0.218	0.07	Antiviral (Hepatitis B)
		0.424	0.026	Antiviral (Herpes)
		0.262	0.08	Antiviral (Influenza A)
		0.702	0.005	Antiviral (Influenza)
18	<i>7S-Hydroxy-14-deoxyandrographolide (4-[2-[(1S,3S,4aS,5R,6R,8aR)-3,6-dihydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]ethyl]-2H-furan-5-one)</i>	0.368	0.132	Antiviral (Rhinovirus)
		0.351	0.023	Antiviral
		0.193	0.033	Antiviral (HIV)
		0.189	0.1	Antiviral (Hepatitis B)
		0.385	0.042	Antiviral (Herpes)
		0.237	0.124	Antiviral (Influenza A)
		0.604	0.013	Antiviral (Influenza)
19	<i>7R-Hydroxy-14-deoxyandrographolide (4-[2-[(1S,3R,4aS,5R,6R,8aR)-3,6-dihydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]ethyl]-2H-furan-5-one)</i>	0.355	0.15	Antiviral (Rhinovirus)
		0.351	0.023	Antiviral
		0.193	0.033	Antiviral (HIV)
		0.189	0.1	Antiviral (Hepatitis B)
		0.385	0.042	Antiviral (Herpes)
		0.237	0.124	Antiviral (Influenza A)
		0.604	0.013	Antiviral (Influenza)

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
20	<i>12R,13R-Hydroxyandrographolide ((3R,4S)-3-[(1R)-2-[(1R,4aS,5S,6R,8aR)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-1-hydroxyethyl]-4-hydroxyoxolan-2-one)</i>	0.302	0.036	Antiviral
		0.119	0.117	Antiviral (HIV)
		0.197	0.092	Antiviral (Hepatitis B)
		0.465	0.015	Antiviral (Herpes)
		0.216	0.176	Antiviral (Influenza A)
		0.517	0.02	Antiviral (Influenza)
21	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	0.168	0.137	Antiviral
		0.209	0.196	Antiviral (Adenovirus)
		0.197	0.193	Antiviral (CMV)
		0.404	0.014	Antiviral (Hepatitis B)
		0.433	0.023	Antiviral (Herpes)
		0.316	0.08	Antiviral (Influenza)
22	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	0.079	0.075	Antiviral (Trachoma)
		0.179	0.122	Antiviral
		0.492	0.005	Antiviral (Hepatitis B)
		0.113	0.081	Antiviral (Hepatitis)
		0.473	0.013	Antiviral (Herpes)
		0.585	0.014	Antiviral (Influenza)
23	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	0.557	0.011	Antiviral (Rhinovirus)
		0.17	0.134	Antiviral
		0.457	0.008	Antiviral (Hepatitis B)
		0.42	0.027	Antiviral (Herpes)
24	<i>Wogonin 5-glucoside</i>	0.261	0.12	Antiviral (Influenza)
		0.325	0.029	Antiviral
		0.131	0.092	Antiviral (HIV)
		0.502	0.004	Antiviral (Hepatitis B)
		0.097	0.067	Antiviral (Hepatitis C)
		0.144	0.039	Antiviral (Hepatitis)
		0.508	0.009	Antiviral (Herpes)
0.665	0.008	Antiviral (Influenza)		
0.086	0.061	Antiviral (Trachoma)		

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
25	<i>Caffeic acid</i>	0.252	0.058	Antiviral
		0.369	0.043	Antiviral (Adenovirus)
		0.294	0.033	Antiviral (CMV)
		0.202	0.029	Antiviral (HIV)
		0.294	0.035	Antiviral (Hepatitis B)
		0.112	0.082	Antiviral (Hepatitis)
		0.419	0.027	Antiviral (Herpes)
		0.013	0.005	Antiviral (Herpesvirus 3, Human)
		0.258	0.086	Antiviral (Influenza A)
		0.549	0.017	Antiviral (Influenza)
		0.508	0.047	Antiviral (Picornavirus)
		0.271	0.077	Antiviral (Poxvirus)
		0.389	0.103	Antiviral (Rhinovirus)
26	<i>Apigenin 7,4'-dimethyl ether</i>	0.164	0.143	Antiviral
		0.26	0.128	Antiviral (Adenovirus)
		0.224	0.122	Antiviral (CMV)
		0.419	0.013	Antiviral (Hepatitis B)
		0.45	0.018	Antiviral (Herpes)
		0.433	0.037	Antiviral (Influenza)
		0.316	0.203	Antiviral (Picornavirus)
		0.361	0.141	Antiviral (Rhinovirus)
0.085	0.063	Antiviral (Trachoma)		
27	<i>3-O-Caffeoylquinic acid</i>	0.303	0.035	Antiviral
		0.258	0.129	Antiviral (Adenovirus)
		0.234	0.019	Antiviral (HIV)
		0.528	0.004	Antiviral (Hepatitis B)
		0.136	0.048	Antiviral (Hepatitis)
		0.411	0.031	Antiviral (Herpes)
		0.231	0.137	Antiviral (Influenza A)
		0.537	0.018	Antiviral (Influenza)
		0.433	0.085	Antiviral (Picornavirus)
		0.472	0.036	Antiviral (Rhinovirus)
0.088	0.059	Antiviral (Trachoma)		

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
28	<i>beta-Sitosterol</i>	0.159	0.15	Antiviral
		0.136	0.084	Antiviral (HIV)
		0.205	0.171	Antiviral (Herpes)
		0.225	0.151	Antiviral (Influenza A)
		0.686	0.006	Antiviral (Influenza)
		0.547	0.013	Antiviral (Rhinovirus)
29	<i>7-O-Methylwogonin</i>	0.181	0.118	Antiviral
		0.487	0.005	Antiviral (Hepatitis B)
		0.437	0.022	Antiviral (Herpes)
		0.331	0.072	Antiviral (Influenza)
		0.286	0.283	Antiviral (Rhinovirus)
30	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	0.299	0.037	Antiviral
		0.496	0.005	Antiviral (Hepatitis B)
		0.092	0.079	Antiviral (Hepatitis C)
		0.137	0.046	Antiviral (Hepatitis)
		0.496	0.01	Antiviral (Herpes)
		0.645	0.01	Antiviral (Influenza)
		0.083	0.067	Antiviral (Trachoma)
31	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	0.282	0.043	Antiviral
		0.476	0.006	Antiviral (Hepatitis B)
		0.126	0.06	Antiviral (Hepatitis)
		0.495	0.01	Antiviral (Herpes)
		0.575	0.015	Antiviral (Influenza)
		0.08	0.072	Antiviral (Trachoma)
32	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	0.287	0.041	Antiviral
		0.132	0.09	Antiviral (HIV)
		0.489	0.005	Antiviral (Hepatitis B)
		0.517	0.008	Antiviral (Herpes)
		0.582	0.014	Antiviral (Influenza)
		0.091	0.053	Antiviral (Trachoma)

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**Tabel VII.1
Lanjutan**

No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
33	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	0.283	0.043	Antiviral
		0.476	0.006	Antiviral (Hepatitis B)
		0.128	0.058	Antiviral (Hepatitis)
		0.484	0.012	Antiviral (Herpes)
		0.575	0.015	Antiviral (Influenza)
		0.08	0.072	Antiviral (Trachoma)
34	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	0.288	0.041	Antiviral
		0.477	0.006	Antiviral (Hepatitis B)
		0.125	0.062	Antiviral (Hepatitis)
		0.482	0.012	Antiviral (Herpes)
		0.533	0.019	Antiviral (Influenza)
35	<i>Skullcapflavone 1 2'-O-glucoside</i>	0.297	0.038	Antiviral
		0.484	0.005	Antiviral (Hepatitis B)
		0.131	0.054	Antiviral (Hepatitis)
		0.508	0.009	Antiviral (Herpes)
		0.642	0.01	Antiviral (Influenza)
		0.095	0.049	Antiviral (Trachoma)
36	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	0.352	0.023	Antiviral
		0.165	0.051	Antiviral (HIV)
		0.28	0.106	Antiviral (Herpes)
		0.433	0.061	Antiviral (Rhinovirus)
37	<i>14-Deoxy-11,14-didehydroandrographolide</i>	0.245	0.063	Antiviral
		0.211	0.076	Antiviral (Hepatitis B)
		0.404	0.034	Antiviral (Herpes)
		0.251	0.097	Antiviral (Influenza A)
		0.441	0.034	Antiviral (Influenza)
		0.355	0.151	Antiviral (Rhinovirus)
38	<i>14-Deoxy-11-oxoandrographolide</i>	0.255	0.057	Antiviral
		0.127	0.1	Antiviral (HIV)
		0.205	0.082	Antiviral (Hepatitis B)
		0.387	0.041	Antiviral (Herpes)
		0.251	0.096	Antiviral (Influenza A)
		0.487	0.025	Antiviral (Influenza)
		0.392	0.099	Antiviral (Rhinovirus)

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Tabel VII.1
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No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
39	<i>Andrographic acid</i>	0.244	0.063	Antiviral
		0.2	0.087	Antiviral (Hepatitis B)
		0.452	0.018	Antiviral (Herpes)
		0.252	0.095	Antiviral (Influenza A)
		0.397	0.047	Antiviral (Influenza)
		0.384	0.109	Antiviral (Rhinovirus)
40	<i>Cinnamic acid</i>	0.213	0.085	Antiviral
		0.421	0.022	Antiviral (Adenovirus)
		0.34	0.013	Antiviral (CMV)
		0.165	0.051	Antiviral (HIV)
		0.262	0.046	Antiviral (Hepatitis B)
		0.11	0.087	Antiviral (Hepatitis)
		0.404	0.034	Antiviral (Herpes)
		0.02	0.003	Antiviral (Herpesvirus 3, Human)
		0.281	0.057	Antiviral (Influenza A)
		0.512	0.021	Antiviral (Influenza)
		0.05	0.021	Antiviral (Parainfluenza)
		0.629	0.014	Antiviral (Picornavirus)
		0.345	0.041	Antiviral (Poxvirus)
0.413	0.078	Antiviral (Rhinovirus)		
41	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	0.577	0.005	Antiviral
		0.344	0.005	Antiviral (HIV)
		0.286	0.037	Antiviral (Hepatitis B)
		0.439	0.021	Antiviral (Herpes)
		0.459	0.03	Antiviral (Influenza)
42	<i>14-Deoxyandrographolide</i>	0.321	0.03	Antiviral
		0.166	0.05	Antiviral (HIV)
		0.207	0.08	Antiviral (Hepatitis B)
		0.366	0.051	Antiviral (Herpes)
		0.246	0.106	Antiviral (Influenza A)
		0.617	0.012	Antiviral (Influenza)
		0.368	0.132	Antiviral (Rhinovirus)

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**Tabel VII.1
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No	Senyawa Aktif	Pa	Pi	Aktivitas Antivirus
43	<i>Andrograpanin</i>	0.264	0.052	Antiviral
		0.188	0.102	Antiviral (Hepatitis B)
		0.273	0.111	Antiviral (Herpes)
		0.488	0.024	Antiviral (Influenza)
		0.34	0.176	Antiviral (Rhinovirus)
44	<i>12S,13S-Hydroxyandrographolide ((3S,4S)-3-[(1R)-2-[(1R,4aS,5S,6R,8aR)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]-1-hydroxyethyl]-4-hydroxyoxolan-2-one)</i>	0.302	0.036	Antiviral
		0.119	0.117	Antiviral (HIV)
		0.197	0.092	Antiviral (Hepatitis B)
		0.465	0.015	Antiviral (Herpes)
		0.216	0.176	Antiviral (Influenza A)
		0.517	0.02	Antiviral (Influenza)
		0.346	0.166	Antiviral (Rhinovirus)
45	<i>12S-Hydroxyandrographolide</i>	0.302	0.036	Antiviral
		0.119	0.117	Antiviral (HIV)
		0.197	0.092	Antiviral (Hepatitis B)
		0.465	0.015	Antiviral (Herpes)
		0.216	0.176	Antiviral (Influenza A)
		0.517	0.02	Antiviral (Influenza)
		0.346	0.166	Antiviral (Rhinovirus)
46	<i>Ferulic acid</i>	0.188	0.109	Antiviral
		0.288	0.099	Antiviral (Adenovirus)
		0.261	0.063	Antiviral (CMV)
		0.154	0.06	Antiviral (HIV)
		0.261	0.046	Antiviral (Hepatitis B)
		0.401	0.035	Antiviral (Herpes)
		0.219	0.166	Antiviral (Influenza A)
		0.501	0.022	Antiviral (Influenza)
		0.412	0.1	Antiviral (Picornavirus)
		0.216	0.135	Antiviral (Poxvirus)
0.38	0.116	Antiviral (Rhinovirus)		
Senyawa Similar				
No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
1	<i>Deoxyelephantopin</i>	0.282	0.039	Antiviral (Hepatitis B)
		0.503	0.023	Antiviral (Rhinovirus)

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**Tabel VII.1
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No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
2	<i>3,19- Isopropylideneandrographolide</i>	0.488	0.008	Antiviral
		0.311	0.007	Antiviral (HIV)
		0.312	0.083	Antiviral (Herpes)
		0.393	0.099	Antiviral (Rhinovirus)
3	<i>Acetyl-3,19- Isopropylideneandrographolide</i>	0.352	0.023	Antiviral
		0.165	0.051	Antiviral (HIV)
		0.28	0.106	Antiviral (Herpes)
		0.433	0.061	Antiviral (Rhinovirus)
4	<i>Andrographidine C</i>	0.299	0.037	Antiviral
		0.496	0.005	Antiviral (Hepatitis B)
		0.092	0.079	Antiviral (Hepatitis C)
		0.137	0.046	Antiviral (Hepatitis)
		0.496	0.01	Antiviral (Herpes)
		0.645	0.01	Antiviral (Influenza)
		0.083	0.067	Antiviral (Trachoma)
5	<i>Andropanoside</i>	0.284	0.043	Antiviral
		0.132	0.09	Antiviral (HIV)
		0.333	0.026	Antiviral (Hepatitis B)
		0.396	0.037	Antiviral (Herpes)
		0.238	0.121	Antiviral (Influenza A)
		0.712	0.005	Antiviral (Influenza)
		0.288	0.279	Antiviral (Rhinovirus)
6	<i>Apigenin Glucopyranoside Arabinopyranoside</i>	0.392	0.015	Antiviral
		0.133	0.089	Antiviral (HIV)
		0.443	0.01	Antiviral (Hepatitis B)
		0.136	0.047	Antiviral (Hepatitis)
		0.842	0.002	Antiviral (Herpes)
		0.54	0.018	Antiviral (Influenza)
		0.349	0.159	Antiviral (Picornavirus)
		0.237	0.109	Antiviral (Poxvirus)
7	<i>Bemadienolide</i>	0.25	0.051	Antiviral (Hepatitis B)
		0.368	0.051	Antiviral (Herpes)
		0.379	0.053	Antiviral (Influenza)
		0.375	0.122	Antiviral (Rhinovirus)

**LAMPIRAN 6
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
8	<i>Apigenin Glucoside</i>	0.309	0.033	Antiviral
		0.146	0.071	Antiviral (HIV)
		0.49	0.005	Antiviral (Hepatitis B)
		0.111	0.085	Antiviral (Hepatitis)
		0.552	0.006	Antiviral (Herpes)
		0.73	0.004	Antiviral (Influenza)
		0.301	0.226	Antiviral (Picornavirus)
		0.097	0.046	Antiviral (Trachoma)
9	<i>Asperolide A</i>	0.19	0.106	Antiviral
		0.197	0.091	Antiviral (Hepatitis B)
		0.327	0.073	Antiviral (Herpes)
		0.265	0.117	Antiviral (Influenza)
		0.449	0.049	Antiviral (Rhinovirus)
10	<i>Baicalein-7-O-Diglucoside</i>	0.341	0.025	Antiviral
		0.174	0.044	Antiviral (HIV)
		0.502	0.004	Antiviral (Hepatitis B)
		0.11	0.086	Antiviral (Hepatitis)
		0.522	0.007	Antiviral (Herpes)
		0.745	0.004	Antiviral (Influenza)
11	<i>CHEMBL314507</i>	0.169	0.136	Antiviral
		0.282	0.102	Antiviral (Influenza)
		0.303	0.246	Antiviral (Rhinovirus)
12	<i>Cirsimarín</i>	0.266	0.051	Antiviral
		0.128	0.098	Antiviral (HIV)
		0.461	0.008	Antiviral (Hepatitis B)
		0.5	0.01	Antiviral (Herpes)
		0.657	0.009	Antiviral (Influenza)
		0.09	0.055	Antiviral (Trachoma)
13	<i>Helioscopinolide E</i>	0.319	0.029	Antiviral (Hepatitis B)
		0.377	0.046	Antiviral (Herpes)
		0.638	0.01	Antiviral (Influenza)
		0.505	0.023	Antiviral (Rhinovirus)

**LAMPIRAN 6
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
14	<i>Chrysin Glucoside</i>	0.37	0.019	Antiviral
		0.139	0.079	Antiviral (HIV)
		0.48	0.005	Antiviral (Hepatitis B)
		0.088	0.088	Antiviral (Hepatitis C)
		0.144	0.039	Antiviral (Hepatitis)
		0.744	0.002	Antiviral (Herpes)
		0.011	0.009	Antiviral (Herpesvirus 3, Human)
		0.231	0.136	Antiviral (Influenza A)
		0.744	0.004	Antiviral (Influenza)
		0.517	0.044	Antiviral (Picornavirus)
		0.344	0.041	Antiviral (Poxvirus)
15	<i>Chrysin-7-O-Glucoronide</i>	0.298	0.256	Antiviral (Rhinovirus)
		0.241	0.065	Antiviral
		0.122	0.109	Antiviral (HIV)
		0.426	0.012	Antiviral (Hepatitis B)
		0.453	0.017	Antiviral (Herpes)
		0.755	0.004	Antiviral (Influenza)
16	<i>Viscumneoside I</i>	0.299	0.254	Antiviral (Rhinovirus)
		0.124	0.027	Antiviral (Trachoma)
		0.19	0.106	Antiviral
		0.429	0.011	Antiviral (Hepatitis B)
		0.517	0.008	Antiviral (Herpes)
		0.666	0.008	Antiviral (Influenza)
17	<i>Deoxyandrographolide</i>	0.424	0.068	Antiviral (Rhinovirus)
		0.082	0.069	Antiviral (Trachoma)
		0.301	0.036	Antiviral
		0.163	0.053	Antiviral (HIV)
		0.191	0.098	Antiviral (Hepatitis B)
		0.411	0.03	Antiviral (Herpes)
		0.263	0.078	Antiviral (Influenza A)
0.671	0.008	Antiviral (Influenza)		
		0.375	0.122	Antiviral (Rhinovirus)

**LAMPIRAN 6
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
18	<i>Echioidin</i>	0.296	0.038	Antiviral
		0.126	0.103	Antiviral (HIV)
		0.449	0.009	Antiviral (Hepatitis B)
		0.128	0.058	Antiviral (Hepatitis)
		0.523	0.007	Antiviral (Herpes)
		0.703	0.005	Antiviral (Influenza)
		0.102	0.041	Antiviral (Trachoma)
19	<i>Echioidinin 5-O-Glucoside</i>	0.296	0.038	Antiviral
		0.126	0.103	Antiviral (HIV)
		0.449	0.009	Antiviral (Hepatitis B)
		0.128	0.058	Antiviral (Hepatitis)
		0.523	0.007	Antiviral (Herpes)
		0.703	0.005	Antiviral (Influenza)
		0.102	0.041	Antiviral (Trachoma)
20	<i>Homoplantaginin</i>	0.274	0.047	Antiviral
		0.133	0.088	Antiviral (HIV)
		0.464	0.007	Antiviral (Hepatitis B)
		0.508	0.009	Antiviral (Herpes)
		0.639	0.01	Antiviral (Influenza)
		0.09	0.055	Antiviral (Trachoma)
21	<i>Ikonnikoside I</i>	0.283	0.043	Antiviral
		0.162	0.053	Antiviral (HIV)
		0.417	0.013	Antiviral (Hepatitis B)
		0.46	0.016	Antiviral (Herpes)
		0.725	0.004	Antiviral (Influenza)
		0.292	0.27	Antiviral (Rhinovirus)
		0.118	0.03	Antiviral (Trachoma)
22	<i>Longipedlactone A</i>	0.363	0.138	Antiviral (Rhinovirus)
23	NSC624482 (<i>Saponaceolide A</i>)	0.464	0.009	Antiviral
		0.324	0.006	Antiviral (HIV)
24	NSC-677576 (<i>Saponaceolide B</i>)	0.19	0.106	Antiviral
25	<i>Pinusolide</i>	0.183	0.116	Antiviral
		0.571	0.015	Antiviral (Influenza)
		0.329	0.197	Antiviral (Rhinovirus)

**LAMPIRAN 6
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
26	<i>Luteolin 5-O-Glucoside</i>	0.334	0.026	Antiviral
		0.146	0.07	Antiviral (HIV)
		0.488	0.005	Antiviral (Hepatitis B)
		0.095	0.072	Antiviral (Hepatitis C)
		0.141	0.042	Antiviral (Hepatitis)
		0.542	0.006	Antiviral (Herpes)
		0.717	0.005	Antiviral (Influenza)
		0.081	0.072	Antiviral (Trachoma)
27	<i>Persicoside</i>	0.273	0.047	Antiviral
		0.471	0.006	Antiviral (Hepatitis B)
		0.094	0.074	Antiviral (Hepatitis C)
		0.137	0.046	Antiviral (Hepatitis)
		0.568	0.005	Antiviral (Herpes)
		0.791	0.003	Antiviral (Influenza)
		0.479	0.033	Antiviral (Rhinovirus)
28	<i>Pinusolidic Acid</i>	0.219	0.081	Antiviral
		0.163	0.15	Antiviral (Hepatitis B)
		0.618	0.012	Antiviral (Influenza)
		0.377	0.119	Antiviral (Rhinovirus)
29	<i>Rac-Tokinolide B</i>	0.195	0.094	Antiviral (Hepatitis B)
		0.311	0.084	Antiviral (Herpes)
		0.51	0.021	Antiviral (Rhinovirus)
30	<i>Riligustilide</i>	0.192	0.098	Antiviral (Hepatitis B)
		0.262	0.119	Antiviral (Herpes)
		0.504	0.023	Antiviral (Rhinovirus)
31	<i>Subvellerolactones D</i>	0.2	0.088	Antiviral (Hepatitis B)
		0.296	0.094	Antiviral (Herpes)
		0.338	0.179	Antiviral (Rhinovirus)
32	<i>Wogonin 7-O-Glucuronide (Wogonoside)</i>	0.226	0.076	Antiviral
		0.454	0.008	Antiviral (Hepatitis B)
		0.428	0.024	Antiviral (Herpes)
		0.691	0.006	Antiviral (Influenza)
		0.117	0.03	Antiviral (Trachoma)

**LAMPIRAN 6
(LANJUTAN)**

Tabel VII.1
Lanjutan

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
33	<i>Senkyunolide A</i>	0.256	0.132	Antiviral (Adenovirus)
		0.244	0.086	Antiviral (CMV)
		0.308	0.031	Antiviral (Hepatitis B)
		0.108	0.049	Antiviral (Hepatitis C)
		0.136	0.047	Antiviral (Hepatitis)
		0.429	0.024	Antiviral (Herpes)
		0.012	0.008	Antiviral (Herpesvirus 3, Human)
		0.315	0.08	Antiviral (Influenza)
		0.041	0.034	Antiviral (Parainfluenza)
		0.362	0.145	Antiviral (Picornavirus)
		0.237	0.108	Antiviral (Poxvirus)
	0.5	0.024	Antiviral (Rhinovirus)	
34	<i>Senkyunolide G</i>	0.34	0.025	Antiviral
		0.268	0.119	Antiviral (Adenovirus)
		0.244	0.086	Antiviral (CMV)
		0.275	0.041	Antiviral (Hepatitis B)
		0.122	0.033	Antiviral (Hepatitis C)
		0.146	0.037	Antiviral (Hepatitis)
		0.423	0.026	Antiviral (Herpes)
		0.286	0.099	Antiviral (Influenza)
		0.294	0.238	Antiviral (Picornavirus)
		0.225	0.123	Antiviral (Poxvirus)
	0.57	0.009	Antiviral (Rhinovirus)	
35	<i>Wightionolide</i>	0.318	0.03	Antiviral
		0.142	0.075	Antiviral (HIV)
		0.208	0.079	Antiviral (Hepatitis B)
		0.335	0.069	Antiviral (Herpes)
		0.206	0.206	Antiviral (Influenza A)
		0.664	0.008	Antiviral (Influenza)
	0.336	0.183	Antiviral (Rhinovirus)	

**LAMPIRAN 6
(LANJUTAN)**

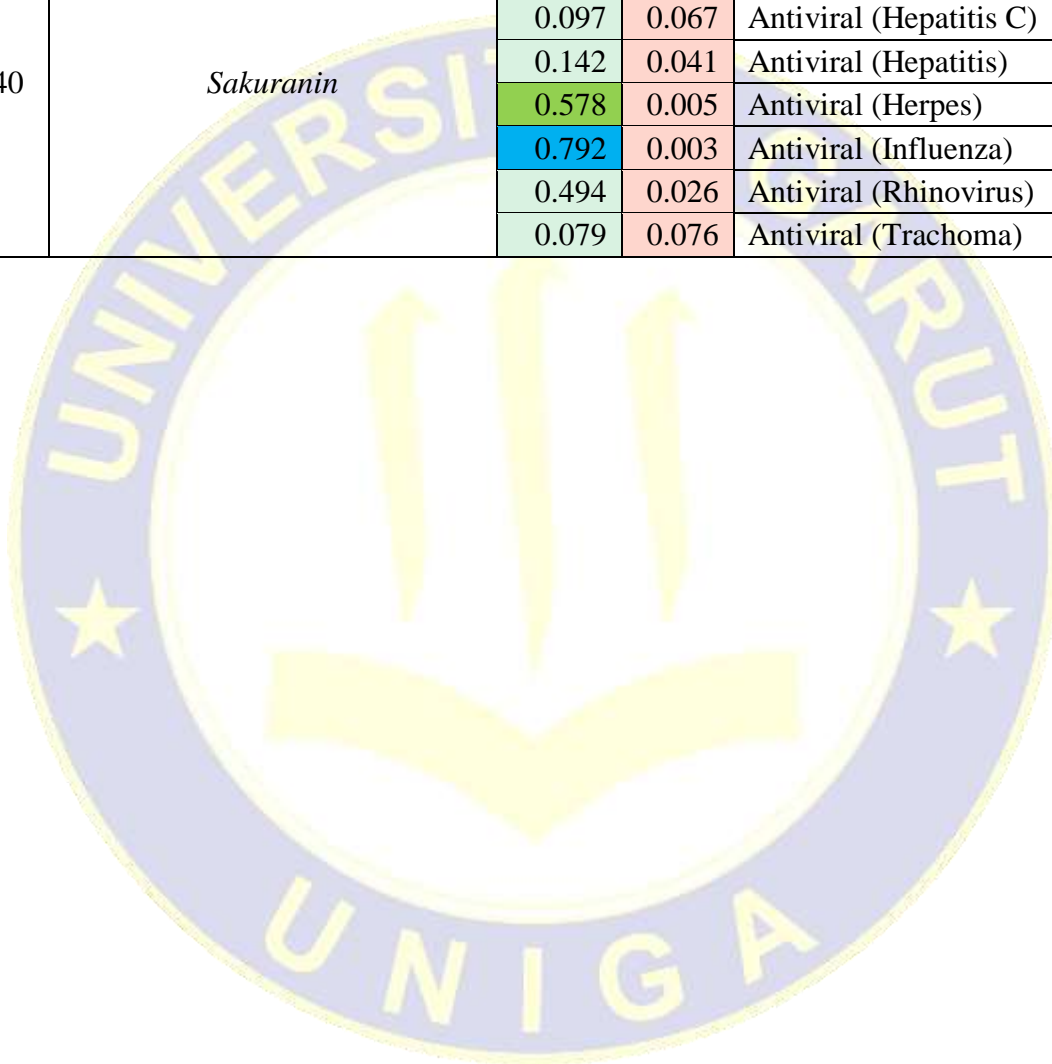
**Tabel VII.1
Lanjutan**

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
36	<i>Toringin</i>	0.336	0.026	Antiviral
		0.141	0.076	Antiviral (HIV)
		0.486	0.005	Antiviral (Hepatitis B)
		0.095	0.071	Antiviral (Hepatitis C)
		0.142	0.041	Antiviral (Hepatitis)
		0.539	0.006	Antiviral (Herpes)
		0.716	0.005	Antiviral (Influenza)
		0.304	0.221	Antiviral (Picornavirus)
		0.198	0.162	Antiviral (Poxvirus)
		0.087	0.059	Antiviral (Trachoma)
37	<i>Flavanomarein</i>	0.313	0.032	Antiviral
		0.139	0.079	Antiviral (HIV)
		0.5	0.005	Antiviral (Hepatitis B)
		0.119	0.071	Antiviral (Hepatitis)
		0.579	0.005	Antiviral (Herpes)
		0.739	0.004	Antiviral (Influenza)
38	<i>Naringenin 5-O-Beta-D-Glucopyranoside</i>	0.311	0.033	Antiviral
		0.494	0.005	Antiviral (Hepatitis B)
		0.102	0.059	Antiviral (Hepatitis C)
		0.15	0.034	Antiviral (Hepatitis)
		0.616	0.004	Antiviral (Herpes)
		0.809	0.003	Antiviral (Influenza)
		0.501	0.024	Antiviral (Rhinovirus)
39	<i>Pervianoside I</i>	0.3	0.037	Antiviral
		0.485	0.005	Antiviral (Hepatitis B)
		0.1	0.062	Antiviral (Hepatitis C)
		0.144	0.039	Antiviral (Hepatitis)
		0.606	0.004	Antiviral (Herpes)
		0.808	0.003	Antiviral (Influenza)
		0.471	0.037	Antiviral (Rhinovirus)

**LAMPIRAN 6
(LANJUTAN)**

Tabel VII.1
Lanjutan

No	Senyawa Similar	Pa	Pi	Aktivitas Antivirus
40	<i>Sakuranin</i>	0.274	0.047	Antiviral
		0.472	0.006	Antiviral (Hepatitis B)
		0.097	0.067	Antiviral (Hepatitis C)
		0.142	0.041	Antiviral (Hepatitis)
		0.578	0.005	Antiviral (Herpes)
		0.792	0.003	Antiviral (Influenza)
		0.494	0.026	Antiviral (Rhinovirus)
		0.079	0.076	Antiviral (Trachoma)



LAMPIRAN 7

HASIL PENAMBATAN SIMULASI *MOLECULAR DOCKING*

Tabel VII.2

Hasil Penambatan Molekuler Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*) Terhadap Reseptor ID PDB 7SI9

ID PDB 7SI9			
No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
1	<i>Bisandrographolide C</i>	-10.3	MET 165, GLN 192, PRO 168, SER 144, CYS 145, HIS 41
2	<i>Bisandrographolide B</i>	-9.5	THR 26, PHE 140, GLY 143, LEU 141, SER 144, ASN 142, CYS 145, MET 165, PRO 168
3	<i>Andrographiside</i>	-9.1	HIS 163, LEU 141, SER 144, HIS 172, PHE 140, ASN 142, GLN 192, MET 49, HIS 41
4	<i>Ninandrographolide</i>	-8.5	HIS 163, LEU 141, GLU 166, PRO 168, MET 49, HIS 41
5	<i>Wogonin 5-glucoside</i>	-8.4	HIS 41, SER 144, MET 165, PRO 168
6	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	-8.3	PRO168, GLN 192, MET 165, ASN 142, SER 144, GLY 143, LEU 141
7	<i>Neoandrographolide</i>	-8.2	GLN 192, MET 49, HIS 41, SER 144, LEU 141, GLU 166
8	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	-7.9	SER 144, CYS 145, GLY 143, ASN 142, GLU 166, THR 190, GLN 192,
9	<i>14-Deoxy-11-oxoandrographolide</i>	-7.9	MET 165, GLN 192, THR 190, CYS 145, SER 144, GLY 143
10	<i>Skullcapflavone I 2'-O-glucoside</i>	-7.8	GLY 143, CYS 145, SER 144, ASN 142, THR 190, GLN 192, GLU 166
11	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	-7.8	HIS 41, CYS 145
12	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	-7.7	CYS 145, HIS 41, MET 49, MET 165, GLU 166
13	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	-7.7	PRO 168, ARG 188, GLN 192, LEU 141, ASN 142
14	<i>Andrographidin A</i>	-7.6	PRO 168, LEU 141, SER 144, CYS 145, HIS 164, HIS 41, MET 164

**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
15	<i>3-O-Caffeoylquinic acid</i>	-7.6	GLY 143, CYS 145, HIS 163, SER 144
16	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	-7.6	MET 165, PRO 168, HIS 163, LEU 141, SER 144, CYS 145, HIS 164, HIS 41, GLN 189
17	<i>14-Acetylandrographolide</i>	-7.5	HIS 163, ASN 142, GLY 143, GLN 189
18	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	-7.5	GLU 166, PHE 140, LEU 141, CYS 145, SER 144, HIS 41, ARG 188, MET 49, MET 165, THR 190, PRO 168, ALA 191, GLN 192
19	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	-7.4	HIS 41, MET 49, LEU 141, SER 144, HIS 163, CYS 145, GLY 143, ASN 142
20	<i>5,7,2',3'-Tetramethoxyflavanone</i>	-7.4	MET 49, HIS 41, MET 165, GLN 189, ASN 142, GLU 166, PHE 140
21	<i>Dihydroskullcap flavone I</i>	-7.3	MET 49, GLU 166, CYS 145, LEU 27, THR 26, HIS 41
22	<i>12S-Hydroxyandrographolide</i>	-7.3	HIS 41, MET 49, GLN 189, HIS 163, CYS 145, PHE 140, MET 165, GLU 166
23	<i>12R,13R-Hydroxyandrographolide</i>	-7.3	HIS 41, MET 49, GLN 189, MET 165, HIS 163, CYS 145, GLU 166, PHE 140, ASN 142
24	<i>12S,13S-Hydroxyandrographolide</i>	-7.3	HIS 41, GLN 189, HIS 163, CYS 145, PHE 140, MET 165, GLU 166, ASN 142
25	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	-7.2	SER 144, CYS 145, GLU 166, GLN 189, THR 190, MET 165, ASN 142
26	<i>Beta-Sitosterol</i>	-7.2	HIS 41, MET 49, MET 165, CYS 145, THR 26
27	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	-7.1	GLU 166, MET 49, HIS 41, CYS 145, HIS 163, PHE 140, LEU 141
28	<i>Apigenin 7,4'-dimethyl ether</i>	-7.1	HIS 41, MET 49, MET 165, PRO 168, GLN 192

**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
29	<i>7-O-Methylwogonin</i>	-7.1	HIS 41, MET 49, GLU 166, LEU 141, PHE 140, ASN 142, HIS 163, CYS 145
30	<i>Molnupiravir</i>	-7.1	HIS 41, LEU 141, PHE 140, GLU 166, ASN 142
31	<i>Isoandrographolide</i>	-7	SER 144, CYS 145, HIS 163
32	<i>Andrograpanin</i>	-7	GLU 166, MET 165
33	<i>Andrographolide</i>	-6.9	ASN 142, PHE 140, GLU 166, MET 49, HIS 164
34	<i>Andropanolide</i>	-6.9	SER 144, CYS 145, HIS 163
35	<i>Andrographic acid</i>	-6.9	HIS 163, ASP 187, TYR 54, MET 165, ARG 188
36	<i>14-Deoxyandrographolide</i>	-6.9	MET 49, GLN 189, HIS 163, LEU 141
37	<i>14-Deoxy-11,14-didehydroandrographolide</i>	-6.8	CYS 145, MET 165, HIS 163, PHE 140
38	<i>7S-Hydroxy-14-deoxyandrographolide</i>	-6.8	CYS 145, HIS 41, GLN 189, MET 49, ARG 188, HIS 163, GLU 166
39	<i>7R-Hydroxy-14-deoxyandrographolide</i>	-6.8	HIS 163, GLU 166, HIS 41, CYS 145, MET 49, GLN 189
40	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	-6.6	MET 165, HIS 41, MET 49, ASP 187
41	<i>Paniculide C</i>	-6.4	GLU 166, ARG 188, MET 49, HIS 41, GLY 143, CYS 145, SER 144
42	<i>14-Deoxy-17-hydroxyandrographolide</i>	-6.4	HIS 41, MET 49, GLN 189, GLU 166
43	<i>Paniculide B</i>	-6.3	MET 165, HIS 41, ASN 142, CYS 145, SER 144, GLY 143, GLU 166
44	<i>Paniculide A</i>	-6.2	MET 49, CYS 145
45	<i>Caffeic acid</i>	-5.6	CYS 145, HIS 163, LEU 141
46	<i>Ferulic acid</i>	-5.4	CYS 145, GLU 166, PHE 140, LEU 141, HIS 163, SER 144, HIS 172
47	<i>Cinnamic acid</i>	-4.9	MET 49, MET 165

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.3

Hasil Penambatan Molekuler Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*) Terhadap Reseptor ID PDB 7RN4

ID PDB 7RN4			
No	Senyawa Aktif	ΔG (kcal/mol)	Residu Asam Amino
1	<i>Bisandrographolide C</i>	-10.8	MET 49, HIS 41, CYS 44, ASP 187, ARG 188, GLN 189
2	<i>Bisandrographolide B</i>	-9.8	HIS 41, MET 49, CYS 44, MET 165, CYS 145, HIS 172, GLU 166
3	<i>14-Deoxy-11-oxoandrographolide</i>	-9.3	HIS 41, MET 49, CYS 44, ASP 187, CYS 145, HIS 163, ASN 142
4	<i>Wogonin 5-glucoside</i>	-9	HIS 41, CYS 44, MET 49, ASN 142, CYS 145, GLU 166, LEU 141
5	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	-8.9	CYS 145, HIS 41, MET 49, CYS 44, GLN 189, MET 165, PHE 140, ASN 142
6	<i>5-Hydroxy-7,8-dimethoxyflavanone 5-glucoside</i>	-8.9	MET 49, CYS 145, CYS 44, HIS 41, LEU 141, GLU 166, ASN 142
7	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	-8.5	CYS 145, MET 165, LEU 141, CYS 44, HIS 41, MET 49, THR 25, THR 24
8	<i>beta-Sitosterol</i>	-8.3	HIS 163, CYS 145, HIS 41, MET 49, CYS 44, TYR 54
9	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	-8.1	CYS 145, HIS 41, MET 49, ASP 187, PRO 52, CYS 44, GLN 189, HIS 164, GLU 166
10	<i>Andrographidin A</i>	-7.9	CYS 145, ASN 142, LEU 141, GLU 166, HIS 41, MET 49, CYS 44
11	<i>3-O-Caffeoylquinic acid</i>	-7.8	CYS 145, THR 25, HIS 41, GLY 143, GLN 189, GLU 166
12	<i>5,7,2',3'-Tetramethoxyflavanone</i>	-7.8	HIS 41, GLY 143, CYS 145, GLU 166, MET 49, PRO 52, CYS 44, MET 165, ASP 187
13	<i>Neoandrographolide</i>	-7.8	MET 49, CYS 41, ASN 142, GLU 166, CYS 145, LEU 141, HIS 163
14	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	-7.7	HIS 41, CYS 145, ASN 142

**LAMPIRAN 7
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**Tabel VII.3
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
15	<i>Andrographiside</i>	-7.7	HIS 41, GLU 166, GLY 143, SER 144
16	<i>Apigenin 7,4'-dimethyl ether</i>	-7.7	HIS 41, GLY 143, CYS 145, MET 165, CYS 44, MET 49, PRO 52
17	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	-7.6	MET 49, HIS 41, CYS 145, LEU 141, HIS 172, GLU 166, ASN 142, GLN 189
18	<i>5-Hidroxy-7,8-dimethoxyflavanone</i>	-7.6	HIS 41, MET 165, HIS 164, GLY 143, CYS 145, LEU 141, GLU 166
19	<i>Skullcapflavone I 2'-O-glucoside</i>	-7.6	HIS 41, GLY 143, PHE 140, SER 144, MET 49, THR 25, THR 24
20	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	-7.5	HIS 41, THR 25, ASN 142, GLU 166, PHE 140, HIS 172, HIS 163, CYS 145, GLN 189
21	<i>5-Hidroxy-7,2',6'-trimethoxyflavone</i>	-7.5	HIS 41, MET 165, ASP 187, MET 49, PRO 52, THR 25, CYS 44
22	<i>7-O-Methylwogonin</i>	-7.5	CYS 44, MET 49, HIS 41, THR 24, THR 25
23	<i>Andropanolide</i>	-7.5	THR 26
24	<i>Isoandrographolide</i>	-7.5	MET 49, THR 26, GLY 143
25	<i>14-Acetylandrographolide</i>	-7.4	HIS 41, ASN 142, GLU 166
26	<i>Dihydroskullcap flavone I</i>	-7.4	HIS 41, MET 49, GLY 143, HIS 163, CYS 145, GLU 166
27	<i>12S-Hidroxyandrographolide</i>	-7.2	HIS 41, GLN 189, THR 26, GLY 143
28	<i>5-Hidroxy-3,7,8,2'-tetramethoxyflavone</i>	-7.2	CYS 145, GLN 189, MET 165, CYS 44, MET 49, PRO 52, ARG 188, HIS 41
29	<i>Molnupiravir</i>	-7.2	MET 49, CYS 44, ASP 187, HIS 41, HIS 163, HIS 164
30	<i>Ninandrographolide</i>	-7.2	ASN 142, GLN 189, TYR 54
31	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	-7.1	HIS 41, THR 24, THR 25, MET 49, LEU 141, GLY 143

**LAMPIRAN 7
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Tabel VII.3
Lanjutan

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
32	<i>12R,13R-Hydroxyandrographolide</i>	-7.1	HIS 41, GLN 189, THR 26
33	<i>12S,13S-Hydroxyandrographolide</i>	-7.1	HIS 41, GLN 189, THR 26, GLY 143
34	<i>Andrographic acid</i>	-7	HIS 41, MET 165, CYS 44, TYR 54, GLN 189, MET 49, ASN 142
35	<i>Andrographolide</i>	-7	HIS 41, THR 26
36	<i>14-Deoxy-11,14-didehydroandrographolide</i>	-6.9	HIS 41, CYS 145, ASN 142, ARG 188
37	<i>7R-Hydroxy-14-deoxyandrographolide</i>	-6.8	GLU 166, PHE 140, GLN 189
38	<i>7S-Hydroxy-14-deoxyandrographolide</i>	-6.8	GLU 166, PHE 140, ASN 142, GLN 189
39	<i>14-Deoxyandrographolide</i>	-6.7	ASN 142, THR 26
40	<i>Andrograpanin</i>	-6.7	HIS 41, CYS 145, ASN 142, ARG 188
41	<i>Paniculide C</i>	-6.7	MET 49, HIS 41, ASN 142, GLY 143, GLU 166, PHE 140
42	<i>14-Deoxy-17-hydroxyandrographolide</i>	-6.5	ASP 187
43	<i>Paniculide B</i>	-6.5	MET 49, MET 165, HIS 41, CYS 145, LEU 141, ASN 142
44	<i>Paniculide A</i>	-6.3	MET 49, HIS 41, CYS 145, MET 165
45	<i>Nirmatlervir</i>	-6.1	HIS 41, THR 26, THR 24, THR 25, ASN 142, SER 144, LEU 141, GLY 143
46	<i>Ferulic acid</i>	-6	HIS 41, MET 49, CYS 44, HIS 164, GLN 189
47	<i>Caffeic acid</i>	-5.8	HIS 41, MET 49, CYS 44, ARG 188, TYR 54
48	<i>Cinnamic acid</i>	-5.3	MET 49, HIS 41, THR 25, CYS 44

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Hasil Penambatan Molekuler Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*) Terhadap Reseptor ID PDB 7NG6

ID PDB 7NG6			
No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
1	<i>Bisandrographolide C</i>	-10	MET 49, CYS 145, CYS 44
2	<i>Bisandrographolide B</i>	-9.2	HIS 41, MET 165, SER 144, LEU 141, PHE 140, ASN 142, GLU 166
3	<i>14-Deoxy-11-oxoandrographolide</i>	-8.3	MET 49, HIS 41, CYS 145, GLU 166, PHE 140, HIS 164
4	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	-7.6	GLN 192, THR 190, GLU 166, GLN 189, HIS 41, CYS 145, LEU 27, LEU 141
5	<i>Wogonin 5-glucoside</i>	-7.6	MET 49, CYS 44, ARG 188, THR 190, GLN 192, GLU 166, CYS 145, HIS 41, MET 165
6	<i>3-O-Caffeoylquinic acid</i>	-7.5	ASN 142, GLY 166, GLN 189, THR 190, CYS 145, HIS 164, HIS 163, LEU 141
7	<i>beta-Sitosterol</i>	-7.3	MET 165, HIS 41, CYS 44, MET 49, PRO 168
8	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	-7.1	HIS 163, MET 165, ASN 142
9	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	-7.1	CYS 145, LEU 141, SER 144, PRO 168, ALA 191, GLN 192
10	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	-7.1	MET 165, THE 190, LEU 167, GLN 189, LEU 141, CYS 145, PRO 168
11	<i>5,7,2',3'-Tetramethoxyflavanone</i>	-7	MET 49, CYS 44, HIS 41, CYS 145, GLU 166, GLN 166, ALA 191, GLN 189, MET 165
12	<i>5-Hydroxy-7,8-dimethoxyflavanone 5-glucoside</i>	-7	CYS 145, MET 165, HIS 163, GLN 189, GLN 192, THR 190, GLU 166
13	<i>7-O-Methylwogonin</i>	-7	MET 49, MET 165, CYS 145, HIS 41, ASN 142, PHE 140, GLU 166
14	<i>Andrographidin A</i>	-7	SER 144, CYS 145, ASN 142

**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
15	<i>Skullcapflavone I 2'-O-glucoside</i>	-7	SER 144, GLY 143, GLN 189, PRO 168, ALA 191, GLN 192
16	<i>14-Acetylandrographolide</i>	-6.9	CYS 145, HIS 41, THR 190, ARG 188
17	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	-6.9	GLU 166, HIS 163, GLN 189, MET 165
18	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	-6.9	GLN 192, MET 165, HIS 163, CYS 145, GLU 166, ASN 142, LEU 141, GLN 189
19	<i>Apigenin 7,4'-dimethyl ether</i>	-6.9	MET 49, HIS 41, MET 165, CYS 145
20	<i>Neoandrographolide</i>	-6.9	HIS 163, ARG 188, THR 190, GLN 192
21	<i>Nirmatlervir</i>	-6.9	GLN 189, HIS 41, CYS 145, GLU 166
22	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	-6.8	HIS 41, PHE 140, MET 165
23	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	-6.8	MET 165, MET 49, GLU 166, CYS 145, SER 144, LEU 141, HIS 41, HIS 164
24	<i>Andrographiside</i>	-6.8	HIS 163, GLU 166, THR 190, GLN 192
25	<i>Ninandrographolide</i>	-6.8	HIS 163, GLN 189, GLN 192, THR 190, GLU 166
26	<i>14-Deoxyandrographolide</i>	-6.7	ARG 188
27	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	-6.7	GLU 166, PHE 140, ALA 191, GLN 192, THR 190, ARG 188, GLN 189
28	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	-6.7	HIS 41, MET 165, GLU 166
29	<i>Dihydroskullcap flavone I</i>	-6.7	HIS 41, CYS 145, MET 165, HIS 163, HIS 164, PHE 140, GLU 166
30	<i>Paniculide C</i>	-6.7	MET 49, HIS 41, PHE 140, GLU 166
31	<i>Molnupiravir</i>	-6.6	HIS 41, ARG 188, CYS 145, PHE 140
32	<i>7R-Hydroxy-14-deoxyandrographolide</i>	-6.6	ARG 188, ASN 142

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**Tabel VII.4
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
33	<i>7S-Hydroxy-14-deoxyandrographolide</i>	-6.6	ARG 188
34	<i>12S-Hydroxyandrographolide</i>	-6.5	ARG 188
35	<i>Paniculide B</i>	-6.5	MET 49, HIS 41, ASN 142, HIS 163
36	<i>12R,13R-Hydroxyandrographolide</i>	-6.5	PHE 140
37	<i>12S,13S-Hydroxyandrographolide</i>	-6.5	ARG 188
38	<i>Andrograpanin</i>	-6.3	ASN 142
39	<i>Andrographolide</i>	-6.2	GLU 166, ASN 142
40	<i>Andropanolide</i>	-6.2	ASN 142
41	<i>Isoandrographolide</i>	-6.2	ASN 142
42	<i>Paniculide A</i>	-6.2	MET 49, HIS 41, MET 165, SER 144, CYS 145, LEU 141, HIS 163, HIS 172
43	<i>14-Deoxy-11,14-didehydroandrographolide</i>	-6.2	HIS 164
44	<i>Andrographic acid</i>	-6	HIS 163, CYS 145, GLN 192, THR 190
45	<i>14-Deoxy-17-hydroxyandrographolide</i>	-5.8	ASN 142, PHE 140
46	<i>Caffeic acid</i>	-5.5	HIS 41, HIS 163, PHE 140, GLU 166, LEU 141, CYS 145, ASN 142
47	<i>Ferulic acid</i>	-5.4	ASN 142, CYS 145, HIS 41, ARG 188
48	<i>Cinnamic acid</i>	-4.7	MET 165, HIS 163, SER 144, PHE 140, GLU 166

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Tabel VII.5

Hasil Penambatan Molekuler Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*) Terhadap Reseptor ID PDB 7DPU

ID PDB 7DPU			
No	Nama Senyawa Aktif	ΔG	Residu Asam Amino
1	<i>Bisandrographolide C</i>	-8.4	HIS 41, TYR 54, MET 165, GLU 166, GLN 189, ASN 119
2	<i>Skullcapflavone 1 2'-O-glucoside</i>	-8.2	HIS 41, MET 49, MET 165, ARG 188, GLN 189, CYS 145, GLU 166, GLY 143, ASN 119, ASN 142, THR 25
3	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	-8.1	HIS 41, MET 49, MET 165, GLN 189, ARG 188, CYS 145, GLU 166, GLY 143, THR 26, ASN 119, ASN 142, THR 25, THR 24
4	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	-8	HIS 41, MET 49, GLN 189, MET 165, CYS 145, GLU 166, THR 26, GLY 143, THR 25, CYS 44
5	<i>Bisandrographolide B</i>	-7.8	LEU 27, CYS 145
6	<i>Wogonin 5-glucoside</i>	-7.8	MET 49, HIS 41, MET 165, CYS 145, GLY 143, THR 26, ASN 119, ASN 142, THR 25, CYS 44
7	<i>3-O-Caffeoylquinic acid</i>	-7.7	HIS 41, THR 25, MET 49, GLN 189, GLU 166
8	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	-7.7	MET 49, HIS 41, MET 165, CYS 145, GLY 143, ASN 142, CYS 44, THR 25
9	<i>Neoandrographolide</i>	-7.4	HIS 41, CYS 145, THR 26, ASN 119
10	<i>Andrographiside</i>	-7.4	GLN 189, ARG 188
11	<i>Apigenin 7,4'-dimethyl ether</i>	-7.4	HIS 41, MET 49, TYR 54, GLN 189, CYS 145, GLY 143
12	<i>Andrographidin A</i>	-7.2	CYS 145, MET 165, HIS 41, THR 25, THR 24, THR 26,
13	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	-7.1	MET 165, GLN 189, GLU 166, CYS 145, HIS 41, GLY 143, LEU 141, TYR 118, THR 26

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**Tabel VII.5
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
14	<i>Molnupiravir</i>	-7.1	MET 49, CYS 44, HIS 41, CYS 45, GLN 189
15	<i>Ninandrographolide</i>	-7	THR 26, ASN 119, ASN 142
16	<i>Dihydroskullcap flavone I</i>	-7	MET 49, MET 165, GLN 189, GLU 166, ASN 142, GLY 143, CYS 145
17	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	-7	CYS 145, GLY 143, HIS 41, CYS 44, MET 49, GLN 189, GLU 166
18	<i>14-Deoxy-11-oxoandrographolide</i>	-7	MET 165, HIS 41, THR 26, GLN 189
19	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	-7	HIS 41, GLU 166, GLN 189
20	<i>14-Acetylandrographolide</i>	-6.8	THR 25, CYS 44, GLU 166
21	<i>5,7,2',3'-Tetramethoxyflavanone</i>	-6.8	CYS 44, MET 49, PRO 52, HIS 41, CYS 145, GLN 189, GLU 166, MET 165
22	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	-6.8	THR 26
23	<i>Andrograpanin</i>	-6.8	CYS 145, HIS 41, THR 26
24	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	-6.7	MET 49, MET 165, CYS 145, ASN 142, GLU 166, GLN 189
25	<i>12S-Hydroxyandrographolide</i>	-6.7	THR 26, HIS 164
26	<i>12R,13R-Hydroxyandrographolide</i>	-6.7	CYS 145
27	<i>12S,13S-Hydroxyandrographolide</i>	-6.7	CYS 145, GLN 189, THR 26
28	<i>Paniculide C</i>	-6.6	MET 49, HIS 41, CYS 145, GLU 166
29	<i>7-O-Methylwogonin</i>	-6.6	GLU 166, GLN 189, MET 165, MET 49, HIS 41, CYS 145, ASN 142
30	<i>7S-Hydroxy-14-deoxyandrographolide</i>	-6.6	GLU 166, THR 26, GLN 189
31	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	-6.5	HIS 41, MET 49, GLU 166, CYS 145, LEU 27, GLY 143, THR 26, THR 25

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**Tabel VII.5
Lanjutan**

No	Senyawa Aktif	ΔG (kkal/mol)	Residu Asam Amino
32	<i>Andrographic acid</i>	-6.5	GLU 166, GLN 189, HIS 41
33	<i>7R-Hydroxy-14-deoxyandrographolide</i>	-6.5	GLU 166, GLY 143, GLN 189
34	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	-6.3	GLU 166, GLN 189, MET 49, HIS 41, CYS 145
35	<i>14-Deoxyandrographolide</i>	-6.3	GLN 189
36	<i>Andrographolide</i>	-6.2	GLN 189, GLU 166, ASN 119
37	<i>Andropanolide</i>	-6.2	GLN 189, ASN 119, THR 26, GLU 166
38	<i>Isoandrographolide</i>	-6.2	ASN 119, THR 26, GLU 166, GLN 189
39	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	-6.2	THR 26, CYS 145, GLU 166
40	<i>Nirmatlervir</i>	-6.2	HIS 164, CYS 145, GLN 189, GLU 166
41	<i>14-Deoxy-11,14-didehydroandrographolide</i>	-6.1	GLN 189
42	<i>Paniculide B</i>	-6	MET 165, HIS 41, THR 26, GLN 189
43	<i>14-Deoxy-17-hydroxyandrographolide</i>	-6	GLN 189, HIS 41
44	<i>Paniculide A</i>	-5.9	MET 49, GLU 166, GLN 189
45	<i>Caffeic acid</i>	-5.9	MET 49, ARG 188, GLU 166, MET 165
46	<i>beta-Sitosterol</i>	-5.9	MET 165, ARG 188, MET 49, HIS 41
47	<i>Ferulic acid</i>	-5.8	MET 165, CYS 44, ASP 187, MET 49, GLN 189, PRO 168, GLN 192
48	<i>Cinnamic acid</i>	-5.1	ARG 188, GLN 192, PRO 168, MET 165

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Tabel VII.6

Hasil Penambatan Molekuler Senyawa Similar Terhadap Reseptor ID PDB 7SI9

ID PDB 7SI9			
<i>Bisandrographolide C</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Deoxyelephantopin</i>	0.629	-7.5	GLU 166
<i>Riligustilide</i>	0.706	-7.2	HIS 41, MET 49, MET 165, PRO 168
<i>Rac-tokinolide B</i>	0.653	-6.4	CYS 145, MET 49
<i>Bemadienolide</i>	0.648	-6.2	CYS 145, MET 165
<i>Asperolide A</i>	0.635	-7.1	ASN 142, GLU 166
<i>Bisandrographolide B</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Senkyunolide A</i>	0.7	-5.4	GLY 143, SER 144, CYS 145, HIS 163
<i>Longipedlactone A</i>	0.622	-7.8	CYS 145
<i>Senkyunolide G</i>	0.663	-5.8	CYS 145, GLY 143, SER 144, HIS 163
<i>Subvellerolactones D</i>	0.643	-6.7	GLU 166, ASN 142, GLY 143
<i>Helioscopinolide E</i>	0.631	-7	HIS 41
<i>Andrographiside</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Nsc624482 (Saponaceolide A)</i>	0.832	-8.8	MET 165, HIS 41, PHE 140, THR 190, PRO 168
<i>3,19-Isopropylideneandrographolide</i>	0.824	-8.2	THR 190, ARG 188
<i>Nsc-677576 (Saponaceolide B)</i>	0.79	-8.8	MET 165, HIS 41, PHE 140, GLU 166
<i>Andropanoside</i>	0.711	-8.5	HIS 41, MET 49, PRO 168, ASN 142, GLU 166, PHE 140, LEU 141
<i>Acetyl-3,19-Isopropylideneandrographolide</i>	0.731	-7.8	HIS 41, CYS 145

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.7

Hasil Penambatan Molekuler Senyawa Similar Terhadap Reseptor ID PDB 7RN4

ID PDB 7RN4			
<i>Bisandrographolide C</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Deoxyelephantopin</i>	0.629	-6.6	HIS 41, CYS 145, SER 144, GLY 143, GLU 166, GLN 189
<i>Riligustilide</i>	0.706	-7.5	CYS 145, MET 49, HIS 41, PRO 52, CYS 44
<i>Rac-Tokinolide B</i>	0.653	-6.6	HIS 41, MET 49, CYS 145, LEU 27
<i>Bemadienolide</i>	0.648	-5.9	HIS 41
<i>Asperolide A</i>	0.635	-7.2	-
<i>Bisandrographolide B</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Senkyunolide A</i>	0.7	-5.7	HIS 41, MET 49, CYS 44
<i>Longipedlactone A</i>	0.622	-8.2	
<i>Senkyunolide G</i>	0.663	-5.6	CYS 44, MET 49, HIS 41
<i>Subvellerolactones D</i>	0.643	-7	HIS 41, ARG 188
<i>Helioscopinolide E</i>	0.631	-7.8	ARG 188, GLN 189
<i>14-Deoxy-11-oxoandrographolide</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Deoxyandrographolide</i>	0.875	-7.1	CYS 145, ARG 188
<i>Pinusolide</i>	0.852	-6.7	CYS 145, HIS 41, HIS 163
<i>Pinusolidic Acid</i>	0.852	-6.7	ASN 142, ARG 188
<i>Wightionolide</i>	0.789	-7.2	MET 49, HIS 163, SER 144, LEU 141, CYS 145, GLY 143
<i>CHEMBL314507</i>	0.852	-6.4	GLN 189

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Tabel VII.8

Hasil Penambatan Molekuler Senyawa Similar Terhadap Reseptor ID PDB 7NG6

ID PDB 7NG6			
<i>Bisandrographolide C</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Deoxyelephantopin</i>	0.629	-6.7	HIS 163, SER 144, GLU 166
<i>Riligustilide</i>	0.706	-7.5	HIS 41, MET 165, LEU 167
<i>Rac-Tokinolide B</i>	0.653	-5.9	MET 165, CYS 145
<i>Bemadienolide</i>	0.648	-5.8	CYS 145, GLU 166, PHE 140
<i>Asperolide A</i>	0.635	-6.7	HIS 41, GLN 189, LEU 141
<i>Bisandrographolide B</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Senkyunolide A</i>	0.7	-5.6	MET 49, CYS 44, PRO 52, HIS 41, MET 165, CYS 145, GLU 166
<i>Longipedlactone A</i>	0.622	-7.7	HIS 164, ARG 188, GLY 170, THR 169
<i>Senkyunolide G</i>	0.663	-5.4	CYS 145, HIS 163, LEU 141, ASN 142
<i>Subvellerolactones D</i>	0.643	-6.8	-
<i>Helioscopinolide E</i>	0.631	-6.6	GLU 166
<i>14-Deoxy-11-oxoandrographolide</i>			
Nama Senyawa	Tanimoto Score	ΔG (kcal/mol)	Residu Asam Amino
<i>Deoxyandrographolide</i>	0.875	-6.8	ARG 188, GLU 166
<i>Pinusolide</i>	0.852	-6.8	ARG 188, PHE 140
<i>Pinusolidic Acid</i>	0.852	-6.8	ARG 188
<i>Wightionolide</i>	0.789	-6.2	ARG 188, PHE 140, GLU 166
<i>CHEMBL314507</i>	0.852	-6.1	HIS 41, PHE 140

**LAMPIRAN 7
(LANJUTAN)**

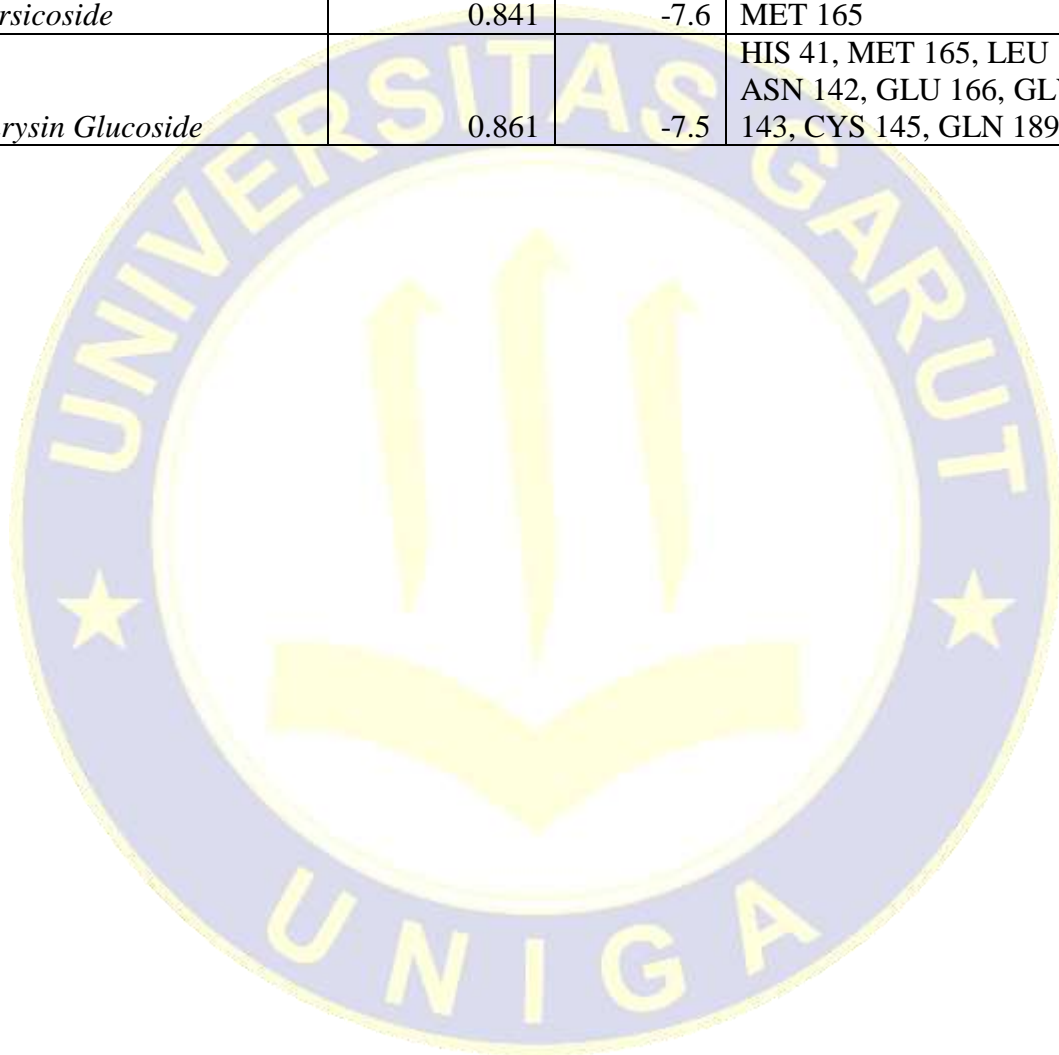
Tabel VII.9

Hasil Penambatan Molekuler Senyawa Similar Terhadap Reseptor ID PDB 7DPU

ID PDB 7DPU			
<i>Bisandrographolide C</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Deoxyelephantopin</i>	0.629	-6.1	HIS 41, GLN 189
<i>Riligustilide</i>	0.706	-6.8	HIS 41, MET 49, MET 165
<i>Rac-Tokinolide B</i>	0.653	-6.1	HIS 41, CYS 145, LEU 27
<i>Bemadienolide</i>	0.648	-5.7	GLU 166
<i>Asperolide A</i>	0.635	-6.7	HIS 41, TYR 54
<i>Skullcapflavone I 2'-O-glucoside</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Echioidin</i>	0.908	-8.4	MET 49, HIS 41, CYS 145, CYS 44, THR 25, THR 24, ARG 188, MET 165, PRO 52
<i>Ikonnikoside I</i>	0.757	-8.8	CYS 145, HIS 41, THR 26, THR 25, MET 165, GLN 189
<i>Homoplantagin</i>	0.749	-6.9	GLY 143, ASN 119, CYS 145, HIS 41, MET 165
<i>Cirsimar</i>	0.775	-7.6	CYS 44, MET 49, HIS 41, THR 25, THR 26, THR 24, ASN 119, GLY 143, CYS 145, GLN 189, ARG 188
<i>Wogonin 7-O-Glucuronide (Wogonoside)</i>	0.768	-7.9	MET 49, GLY 143, CYS 145, HIS 41, GLU 166, GLN 189, THR 25
<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>			
Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Echioidinin 5-O-Glucoside</i>	0.823	-7.7	MET 49, MET 165, HIS 41, THR 24, THR 26, CYS 145
<i>Chrysin-7-O-Glucoronide</i>	0.836	-8.3	GLU 166, GLN 189, MET 165, MET 49, HIS 41, CYS 145
<i>Andrographidine C</i>	0.872	-7.7	MET 49, HIS 41, MET 165, CYS 145, GLY 143, THR 25, CYS 44

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.9**
Lanjutan

Nama Senyawa	Tanimoto Score	ΔG (kkal/mol)	Residu Asam Amino
<i>Persicoside</i>	0.841	-7.6	HIS 41, CYS 44, THR 25, MET 165
<i>Chrysin Glucoside</i>	0.861	-7.5	HIS 41, MET 165, LEU 167, ASN 142, GLU 166, GLY 143, CYS 145, GLN 189



LAMPIRAN 8

HASIL PREDIKSI DRUGLIKENESS

Tabel VII.10

Hasil Prediksi Druglikeness Native Ligand, Ligand Pembanding, dan Senyawa Aktif Tanaman Sambiloto (*Andrographis Paniculata*) Berdasarkan Aturan Lipinski's Rule of Five

No	Senyawa Aktif	BM (g/mol)	Log P	Donor H	Akseptor H	Keterangan
1	<i>N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-1-hydroxy-4-methylpentan-2-yl]-L-leucinamide</i>	312	-0.05	5	6	Tidak memenuhi
2	<i>6-[4-(3,4-dichlorophenyl)piperidine-1-carbonyl]pyrimidine-2,4(1H,3H)-dione</i>	352	-1.3	0	8	Memenuhi
3	<i>(1R,2S,5S)-N-[(1E,2S)-1-imino-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]-6,6-dimethyl-3-[3-methyl-N-(trifluoroacetyl)-L-valyl]-3-azabicyclo[3.1.0]hexane-2-carboxamide</i>	477	5.06	4	5	Memenuhi
4	<i>7-methoxy-3,5-bis(oxidanyl)-2-[3,4,5-tris(oxidanyl)phenyl]chromen-4-one</i>	368	2.44	2	3	Memenuhi
5	<i>Andrographolide</i>	350	1.96	3	5	Memenuhi
6	<i>Neoandrographolide</i>	480	1.85	4	8	Memenuhi
7	<i>Ninandrographolide</i>	496	0.82	5	9	Tidak Memenuhi
8	<i>Dihydroskullcap flavone I</i>	316	2.82	2	6	Memenuhi
9	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	328	3.03	1	6	Memenuhi
10	<i>Paniculide C</i>	278	1.06	1	5	Memenuhi
11	<i>Paniculide B</i>	280	0.85	2	5	Memenuhi
12	<i>Paniculide A</i>	264	1.88	1	4	Memenuhi
13	<i>Nirmatrelvir</i>	499	1.09	3	9	Memenuhi

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII.10
Lanjutan

No	Senyawa Aktif	BM (g/mol)	Log P	Donor H	Akseptor H	Keterangan
14	<i>Andrographidin A</i>	462	0.59	4	10	Tidak Memenuhi
15	<i>Andrographiside</i>	512	-0.21	6	10	Tidak Memenuhi
16	<i>Andropanolide</i>	350	1.96	3	5	Memenuhi
17	<i>Isoandrographolide</i>	350	1.96	3	5	Memenuhi
18	<i>Bisandrographolide C</i>	664	5.37	4	8	Tidak Memenuhi
19	<i>Bisandrographolide B</i>	664	5.51	4	8	Tidak Memenuhi
20	<i>14-Acetylandrographolide</i>	392	2.53	2	6	Memenuhi
21	<i>5,7,2',3'-Tetramethoxyflavanone</i>	334	3.43	0	6	Memenuhi
22	<i>14-Deoxy-17-hydroxyandrographolide</i>	352	2.04	3	5	Memenuhi
23	<i>7S-Hydroxy-14-deoxyandrographolide</i>	350	1.96	3	5	Memenuhi
24	<i>7R-Hydroxy-14-deoxyandrographolide</i>	350	1.96	3	5	Memenuhi
25	<i>12R,13R-Hydroxyandrographolide</i>	368	1.01	4	6	Memenuhi
26	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	358	3.01	1	7	Memenuhi
27	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	300	3.12	1	5	Memenuhi
28	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	374	2.75	2	8	Memenuhi
29	<i>Caffeic acid</i>	180	1.19	3	4	Memenuhi
30	<i>Apigenin 7,4'-dimethyl ether</i>	298	3.026	1	5	Memenuhi
31	<i>3-O-Caffeoylquinic acid</i>	354	-0.65	6	9	Tidak Memenuhi
32	<i>Ferulic acid</i>	194	1.5	2	4	Memenuhi
33	<i>beta-Sitosterol</i>	414	8.02	1	1	Tidak Memenuhi

**LAMPIRAN 8
(LANJUTAN)**

**Tabel VII.10
Lanjutan**

No	Senyawa Aktif	BM (g/mol)	Log P	Donor H	Akseptor H	Keterangan
34	<i>7-O-Methylwogonin</i>	298	3.03	1	5	Memenuhi
35	<i>Wogonin 5-glucoside</i>	446	0.2	5	10	Tidak Memenuhi
36	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	460	0.5	4	10	Tidak Memenuhi
37	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	490	0.51	4	11	Tidak Memenuhi
38	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	492	-0.09	6	12	Tidak Memenuhi
39	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	520	0.52	4	12	Tidak Memenuhi
40	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	536	0.23	5	13	Tidak Memenuhi
41	<i>Skullcapflavone I 2'-O-glucoside</i>	536	0.23	5	13	Tidak Memenuhi
42	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	432	4.33	0	6	Memenuhi
43	<i>14-Deoxy-11,12-didehydroandrographolide</i>	332	2.77	2	4	Memenuhi
44	<i>14-Deoxy-11-oxoandrographolide</i>	312	-0.05	5	6	Tidak Memenuhi
45	<i>Andrographic acid</i>	364	2.38	4	6	Memenuhi
46	<i>Cinnamic acid</i>	148	1.78	1	2	Memenuhi
47	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	512	-0.21	6	10	Tidak Memenuhi
48	<i>14-Deoxyandrographolide</i>	334	2.99	2	4	Memenuhi
49	<i>Andrograpanin</i>	318	4.02	1	3	Memenuhi
50	<i>12S,13S-Hydroxyandrographolide</i>	368	1.01	4	6	Memenuhi
51	<i>12S-Hydroxyandrographolide</i>	368	1.01	4	6	Memenuhi
52	<i>Molnupiravir</i>	329	-1.14	4	10	Tidak Memenuhi

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII.11

Hasil Prediksi *Druglikeness* Senyawa Similar Berdasarkan Aturan *Lipinski's Rule of Five*

No	Senyawa Aktif	BM (g/mol)	Log P	Donor H	Akseptor H	Keterangan
1	3,19- <i>Isopropylideneandrographolide</i>	390	3.76	1	5	Memenuhi
2	Acetyl-3,19- <i>Isopropylideneandrographolide</i>	432	4.33	0	6	Memenuhi
3	<i>Andrographidine C</i>	460	0.49	4	10	Tidak Memenuhi
4	<i>Andropanoside</i>	496	0.82	5	9	Tidak Memenuhi
5	<i>Apigenin Glucopyranoside</i> <i>Arabinopyranoside</i>	564	-1.91	10	14	Tidak Memenuhi
6	<i>Apigenin Glucoside</i>	564	-1.91	10	14	Tidak Memenuhi
7	<i>Asperolide A</i>	288	0.89	1	5	Memenuhi
8	<i>Baicalein-7-O-Diglucoside</i>	594	-2.28	9	15	Tidak Memenuhi
9	<i>Bemadienolide</i>	232	3.24	0	2	Memenuhi
10	<i>Chembl314507</i>	364	3.25	1	5	Memenuhi
11	<i>Chrysin Glucoside</i>	416	0.23	6	9	Tidak Memenuhi
12	<i>Chrysin Glucuronide</i>	430	0.27	5	10	Tidak Memenuhi
13	<i>Cirsimarín</i>	476	0.2	5	11	Tidak Memenuhi
14	<i>Deoxyandrographolide</i>	334	3.14	2	4	Memenuhi
15	<i>Deoxyelephantopin</i>	344	2.16	0	6	Memenuhi
16	<i>Echioidin</i>	446	0.19	5	10	Tidak Memenuhi
17	<i>Echioidinin 5-O-Glucoside</i>	446	0.19	5	10	Tidak Memenuhi
18	<i>Helioscopinolide E</i>	314	3.98	0	3	Memenuhi
19	<i>Homoplantaginín</i>	462	-0.09	6	11	Tidak Memenuhi
20	<i>Ikonnikoside I</i>	462	-0.31	7	12	Tidak Memenuhi
21	<i>Longipedlactone A</i>	478	5.37	1	5	Memenuhi

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII.11
Lanjutan

No	Senyawa Aktif	BM (g/mol)	Log P	Donor H	Akseptor H	Keterangan
22	<i>Luteolin 5-O-Glucoside</i>	448	-0.4	7	11	Tidak Memenuhi
23	<i>NSC624482 (Saponaceolide A)</i>	518	4.8	2	7	Tidak Memenuhi
24	<i>NSC-677576 (Saponaceolide B)</i>	502	5.83	1	6	Tidak Memenuhi
25	<i>Persicoside</i>	478	0.3	5	11	Tidak Memenuhi
26	<i>Pinusolide</i>	346	4.2	0	4	Memenuhi
27	<i>Pinusolidic Acid</i>	332	4.11	1	4	Memenuhi
28	<i>Rac-Tokinolide B</i>	380	4.92	0	4	Memenuhi
29	<i>Riligustilide</i>	380	4.92	0	4	Memenuhi
30	<i>Senkyunolide A</i>	192	2.75	0	2	Memenuhi
31	<i>Senkyunolide G</i>	208	2.07	1	3	Memenuhi
32	<i>Subvellerolactones D</i>	280	0.5	3	5	Memenuhi
33	<i>Toringin</i>	416	0.19	5	9	Tidak Memenuhi
34	<i>Wightionolide</i>	352	2.05	3	5	Memenuhi
35	<i>Wogonin 7-O-Glucuronide (Wogonoside)</i>	460	0.29	5	11	Tidak Memenuhi
36	<i>Flavanomarein</i>	450	-0.31	7	11	Tidak Memenuhi
37	<i>Naringenin 5-O-Beta-D-Glucopyranoside</i>	434	-0.02	6	10	Tidak Memenuhi
38	<i>Pervianoside I</i>	494	0.0001	6	12	Tidak Memenuhi
39	<i>Sakuranin</i>	448	0.29	5	10	Tidak Memenuhi
40	<i>Viscumneoside I</i>	596	-1.9	8	15	Tidak Memenuhi

LAMPIRAN 9

HASIL PREDIKSI ADMET

Tabel VII.12

Hasil Prediksi Profil Farmakokinetika dan Toksisitas *Native Ligand*, Ligand Pemanding, dan Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*) Berdasarkan Pre-ADMET

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksisitas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
1	<i>Andrographolide</i>	87,69*	19,13**	94,87*	Non	+	+
2	<i>Neoandrographolide</i>	81,33*	18,12**	93,37*	Non	+	-
3	<i>Ninandrographolide</i>	64,13**	18,06**	80,97**	Non	+	-
4	<i>Dihydroskullcap flavone I</i>	92,98*	18,69**	89,2**	Non	-	-
5	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	96,49*	46,25**	87,28**	Non	+	-
6	<i>Paniculide C</i>	92,4*	16,53**	74,19**	Non	+	+
7	<i>Paniculide B</i>	88,83*	16,43**	65,18**	Non	+	+
8	<i>Paniculide A</i>	94,84*	21,77**	81,2**	Non	+	+
9	<i>Andrographidin A</i>	77,28*	5,82**	62,81**	Non	-	-
10	<i>Andrographiside</i>	40,19**	16,88**	63,91**	Non	+	-
11	<i>Andropanolide</i>	87,69*	19,13**	94,87*	Non	+	+
12	<i>Isoandrographolide</i>	87,69*	19,13**	94,87*	Non	+	+
13	<i>Bisandrographolide C</i>	91,83*	20,88**	93,94*	Non	+	+
14	<i>Bisandrographolide B</i>	91,83*	20,87**	94,74*	Non	+	+
15	<i>14-Acetylandrographolide</i>	92,69*	19,99**	86,8**	Non	+	+
16	<i>5,7,2',3'-Tetramethoxyflavanone</i>	98,54*	56,13**	87,25**	Non	+	-
17	<i>14-Deoxy-17-hydroxyandrographolide</i>	86,6*	21,13**	94,16*	Non	-	+
18	<i>7S-Hydroxy-14-deoxyandrographolide</i>	87,69*	21,03**	91*	Non	+	-
19	<i>7R-Hydroxy-14-deoxyandrographolide</i>	87,69*	21,03**	91*	Non	+	-
20	<i>12R,13R-Hydroxyandrographolide</i>	74,62*	20,66**	77,08**	Non	+	-
21	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	96,81*	41,33**	80,54**	Non	+	-

**LAMPIRAN 9
(LANJUTAN)**

**Tabel VII.12
Lanjutan**

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksisitas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
22	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	95,99*	22,48**	91,78*	Non	+	-
23	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	93,08*	20,81**	83,37*	Non	+	-
24	<i>Caffeic acid</i>	82,3*	21,11**	40,29**	Non	+	-
25	<i>Apigenin 7,4'-dimethyl ether</i>	95,99*	34,58**	88,96**	Non	+	+
26	<i>3-O-Caffeoylquinic acid</i>	20,43**	18,72**	41,96**	Non	+	-
27	<i>Ferulic acid</i>	90,6*	21,12**	50,41**	Non	+	-
28	<i>beta-Sitosterol</i>	100*	52,37**	100*	Non	-	+
29	<i>7-O-Methylwogonin</i>	95,99*	22,05**	88,64**	Non	+	-
30	<i>Wogonin 5-glucoside</i>	65,9**	4,7**	63,9**	Non	+	-
31	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	80,18*	5,82**	64,61**	Non	+	-
32	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	77,08*	7,49**	59,28**	Non	-	+
33	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	37**	10,3**	54,41**	Non	-	+
34	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	73,29*	7,33**	54,38**	Non	-	+
35	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	50,65**	5,85**	50,39**	Non	-	+
36	<i>Skullcapflavone I 2'-O-glucoside</i>	61,33**	6,39**	59,64**	Non	+	+
37	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	98,84*	47,67**	88,16**	Non	+	+

**LAMPIRAN 9
(LANJUTAN)**

**Tabel VII.12
Lanjutan**

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksisitas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
38	<i>14-Deoxy-11,14-didehydroandrographolide</i>	92,96*	20,6**	98,43*	Non	+	-
39	<i>14-Deoxy-11-oxoandrographolide</i>	92,51*	20,02**	91,1*	Non	+	+
40	<i>Andrographic acid</i>	79,27*	18,49**	97,56*	Non	+	+
41	<i>Cinnamic acid</i>	97,85*	21,03**	60,85**	Non	+	-
42	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	40,19**	15,68**	62,22**	Non	+	-
43	<i>14-Deoxyandrographolide</i>	92,67*	20,61**	100*	Non	+	+
44	<i>Andrograpanin</i>	95,37*	22,41**	100*	Non	+	+
45	<i>12S,13S-Hydroxyandrographolide</i>	74,62*	20,66**	77,08**	Non	+	-
46	<i>12S-Hydroxyandrographolide</i>	74,62*	20,66**	77,08**	Non	+	-
47	<i>Molnupiravir</i>	29,29**	4,51**	26,6**	Non	+	+
48	<i>Nirmatrelvir</i>	79,32*	20,59**	65,03**	Non	-	-
49	<i>7-methoxy-3,5-bis(oxidanyl)-2-[3,4,5-tris(oxidanyl)phenyl]chromen-4-one</i>	95.53*	20.78 *	89.21 **	Non	+	-
50	<i>N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-1-hydroxy-4-methylpentan-2-yl]-L-leucinamide</i>	65.00**	19.93 *	37.43**	Non	-	-
51	<i>6-[4-(3,4-dichlorophenyl)piperidine-1-carbonyl]pyrimidine-2,4(1H,3H)-dione</i>	46.31**	20.16 *	73.45**	Non	+	-

**LAMPIRAN 9
(LANJUTAN)**

**Tabel VII.12
Lanjutan**

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksistas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
52	<i>(1R,2S,5S)-N-((1E,2S)-1-imino-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl)-6,6-dimethyl-3-[3-methyl-N-(trifluoroacetyl)-L-valyl]-3-azabicyclo[3.1.0]hexane-2-carboxamide</i>	85.99*	21.47**	87.39**	Non	-	-

Keterangan :

HIA (%) :

70-100 terserap baik (*)
20-70 terserap cukup (**)
<20 kurang terserap (***)

CaCo-2 (nm sec) :

>70 permeabilitas tinggi (*)
4-70 permeabilitas sedang (**)
<4 permeabilitas rendah (***)

PPB (%) :

>90 terikat kuat (*)
<90 terikat lemah (**)

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.13
Hasil Prediksi Profil Farmakokinetika dan Toksisitas Senyawa Similar
Berdasarkan Pre-ADMET

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksisitas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
1	<i>3,19-Isopropylideneandrographolide</i>	96,14*	37,76**	92,4*	Non	+	+
2	<i>Acetyl-3,19-Isopropylideneandrographolide</i>	98,84*	47,67**	88,16**	Non	+	+
3	<i>Andrographidine C</i>	80,18*	5,82**	64,61**	Non	+	-
4	<i>Andropanoside</i>	64,13**	18,06**	80,97**	Non	+	-
5	<i>Apigenin Glucopyranoside</i> <i>Arabinopyranoside</i>	4,21***	6,61**	39,63**	Non	-	-
6	<i>Apigenin Glucoside</i>	4,21***	6,71**	40,1**	Non	-	-
7	<i>Asperolide A</i>	94,94*	21,17**	61,5**	Non	+	-
8	<i>Baicalein-7-O-Diglucoside</i>	6,33***	9,43**	47,03**	Non	-	-
9	<i>Bemadienolide</i>	100*	27,03**	100*	Non	+	-
10	<i>CHEMBL314507</i>	98,74*	33,15**	100*	Non	+	+
11	<i>Chrysin Glucoside</i>	54,39**	5,13**	61,27**	Non	+	-
12	<i>Chrysin-7-O-Glucoronide</i>	56,45**	7,79**	79,41**	Non	+	-
13	<i>Cirsimarín</i>	61,33**	4,56**	63,35**	Non	-	+
14	<i>Deoxyandrographolide</i>	92,67*	20,6**	90,18*	Non	-	+
15	<i>Deoxyelephantopin</i>	97,94*	23,8**	92,35*	Non	+	+
16	<i>Echioidin</i>	65,9**	8,8**	66,25**	Non	+	+
17	<i>Echioidinin 5-O-Glucoside</i>	65,9**	8,7**	65,62**	Non	+	-
18	<i>Helioscopinolide E</i>	98*	26,85**	98,68*	Non	-	+
19	<i>Homoplantaginín</i>	42,15**	9,25**	62,36**	Non	+	-
20	<i>Ikonnikoside I</i>	15,78** *	12,53**	73,84**	Non	-	+
21	<i>Longipedlactone A</i>	96,38*	36,95**	94,69*	Non	+	+
22	<i>Luteolin 5-O-Glucoside</i>	25,17**	3,12***	68,05**	Non	+	-
23	<i>NSC624482</i> <i>(Saponaceolide A)</i>	94,84*	37,4**	93,66*	Non	+	+

**LAMPIRAN 9
(LANJUTAN)**

**Tabel VII.13
Lanjutan**

No	Senyawa Aktif	Absorpsi		Distribusi	Metabolisme	Toksistas dan Mutagenitas	
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)	(Substrat CYP2D6)	Ames Test	Carsinogenity
24	<i>NSC-677576 (Saponaceolide B)</i>	96,43*	49,11**	95,07*	Non	+	+
25	<i>Persicoside</i>	56,48**	4,65**	59,44**	Non	-	-
26	<i>Pinusolide</i>	98,16*	23,26**	100*	Non	+	+
27	<i>Pinusolidic Acid</i>	98,15*	20,95**	100*	Non	+	+
28	<i>Rac-Tokinolide B</i>	97,58*	40,28**	100*	Non	-	+
29	<i>Riligustilide</i>	97,8*	40,23**	100*	Non	-	+
30	<i>Senkyunolide A</i>	100*	47,54**	100*	Non	+	+
31	<i>Senkyunolide G</i>	94,38*	22,3**	100*	Non	+	+
32	<i>Subvellerolactones D</i>	82,39**	2,4***	61,57**	Non	+	-
33	<i>Toringin</i>	69,58**	4,66**	70,75**	Non	+	-
34	<i>Wightionolide</i>	86,61*	21,12**	92,45*	Non	-	+
35	<i>Wogonin 7-O-Glucuronide (Wogonoside)</i>	50,57**	13,26**	70,56**	Non	+	-
36	<i>Flavanomarein</i>	21,74**	11,69**	67,49**	Non	-	-
37	<i>Naringenin 5-O-Beta-D-Glucoopyranoside</i>	42,27**	4,93**	66,79**	Non	+	-
38	<i>Pervianoside I</i>	32,36**	2,45***	53,97**	Non	-	-
39	<i>Sakuranin</i>	61,52**	5,83**	64,12**	Non	-	-
40	<i>Viscumneoside I</i>	8,82***	5,89**	35,97**	Non	+	-

Keterangan :

HIA (%) :

70-100 terserap baik (*)
20-70 terserap cukup (**)
<20 kurang terserap (***)

CaCo-2 (nm sec) :

>70 permeabilitas tinggi (*)
4-70 permeabilitas sedang (**)
<4 permeabilitas rendah (***)

PPB (%) :

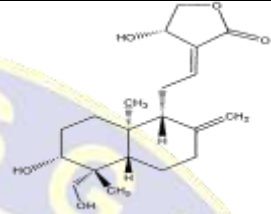
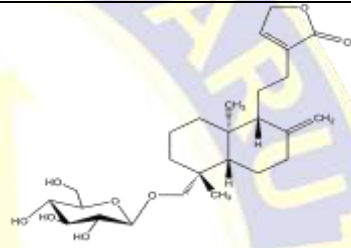
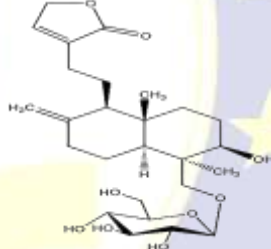
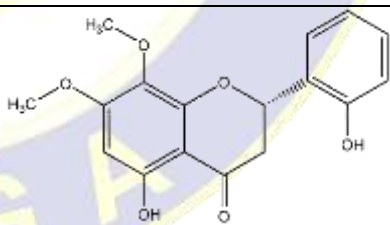
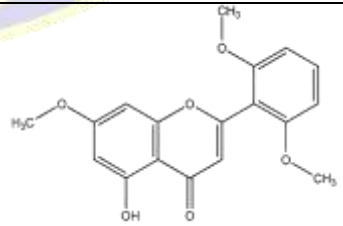
>90 terikat kuat (*)
<90 terikat lemah (**)

LAMPIRAN 10

STRUKTUR 2D SENYAWA UJI

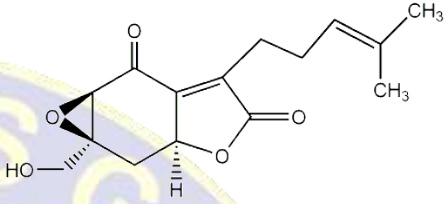
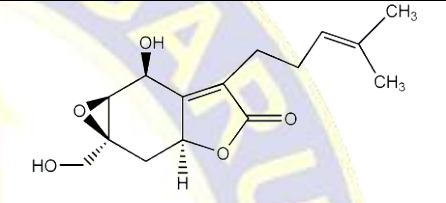
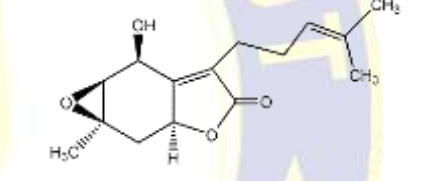
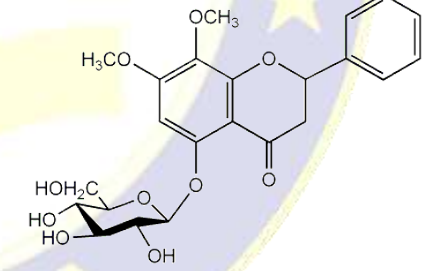
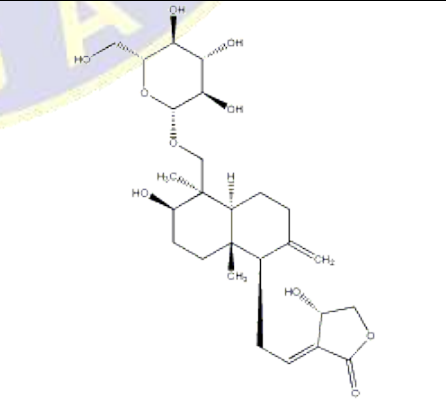
Tabel VII.14

Struktur 2D Senyawa Aktif Tanaman Sambiloto (*Andrographis paniculata*)

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
1	<i>Andrographolide</i>	$C_{20}H_{30}O_5$	
2	<i>Neoandrographolide</i>	$C_{26}H_{40}O_8$	
3	<i>Ninandrographolide</i>	$C_{26}H_{40}O_9$	
4	<i>Dihydroskullcap flavone I</i>	$C_{17}H_{16}O_6$	
5	<i>5-Hydroxy-7,2',6'-trimethoxyflavone</i>	$C_{18}H_{16}O_6$	

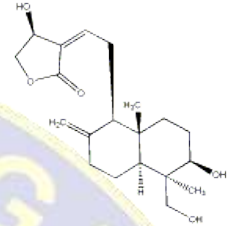
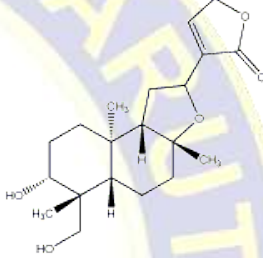
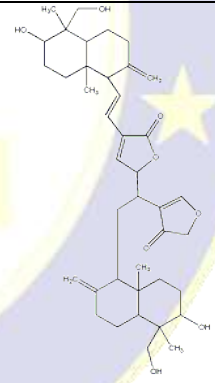
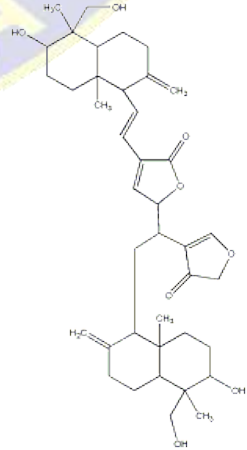
LAMPIRAN 10
(LANJUTAN)

Tabel VII.14
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
6	<i>Paniculide C</i>	$C_{15}H_{18}O_5$	
7	<i>Paniculide B</i>	$C_{15}H_{20}O_5$	
8	<i>Paniculide A</i>	$C_{15}H_{20}O_4$	
9	<i>Andrographidin A</i>	$C_{23}H_{26}O_{10}$	
10	<i>Andrographiside</i>	$C_{26}H_{40}O_{10}$	

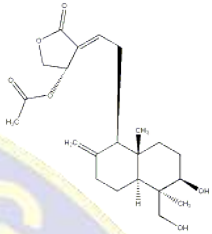
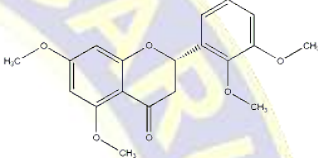
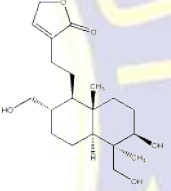
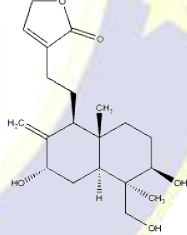
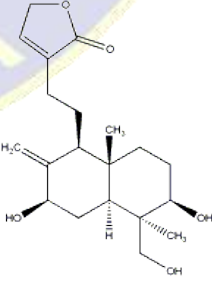
LAMPIRAN 10
(LANJUTAN)

Tabel VII.14
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
11	<i>Andropanolide</i>	$C_{20}H_{30}O_5$	
12	<i>Isoandrographolide</i>	$C_{20}H_{30}O_5$	
13	<i>Bisandrographolide C</i>	$C_{40}H_{56}O_8$	
14	<i>Bisandrographolide B</i>	$C_{40}H_{56}O_8$	

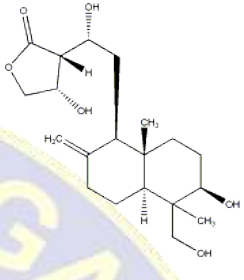
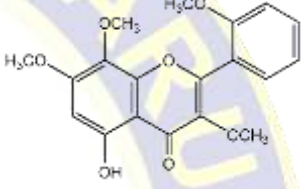
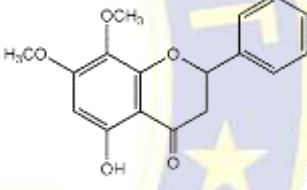
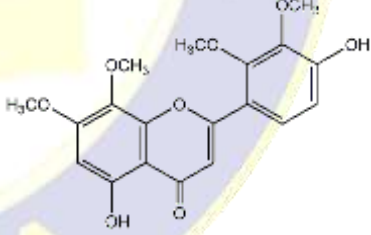
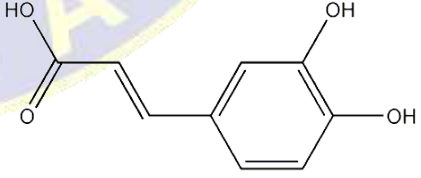
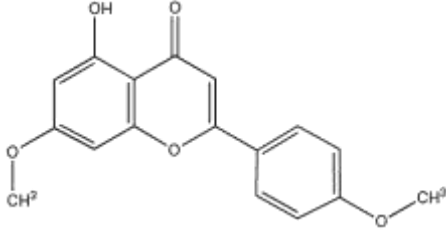
**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.14
Lanjutan**

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
15	<i>14-Acetylandrographolide</i>	$C_{22}H_{32}O_6$	
16	<i>5,7,2',3'-Tetramethoxyflavanone</i>	$C_{19}H_{20}O_6$	
17	<i>14-Deoxy-17-hydroxyandrographolide</i>	$C_{20}H_{32}O_5$	
18	<i>7S-Hydroxy-14-deoxyandrographolide</i>	$C_{20}H_{30}O_5$	
19	<i>7R-Hydroxy-14-deoxyandrographolide</i>	$C_{20}H_{30}O_5$	

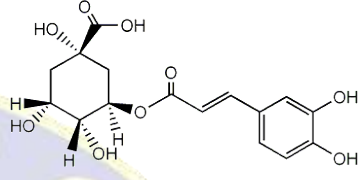
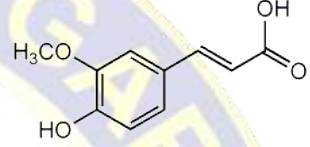
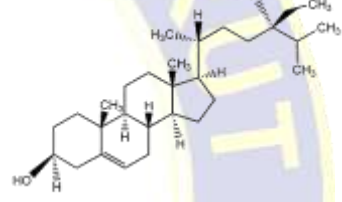
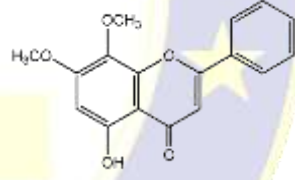
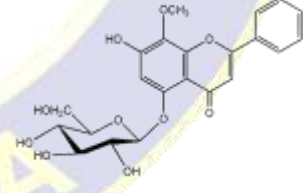
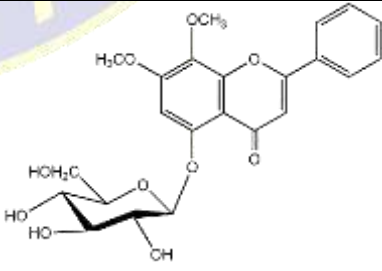
**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.14
Lanjutan**

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
20	<i>12R,13R-Hydroxyandrographolide</i>	$C_{20}H_{32}O_6$	
21	<i>5-Hydroxy-3,7,8,2'-tetramethoxyflavone</i>	$C_{19}H_{18}O_7$	
22	<i>5-Hydroxy-7,8-dimethoxyflavanone</i>	$C_{17}H_{16}O_5$	
23	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxyflavone</i>	$C_{19}H_{18}O_8$	
24	<i>Caffeic acid</i>	$C_9H_8O_4$	
25	<i>Apigenin 7,4'-dimethyl ether</i>	$C_{17}H_{14}O_5$	

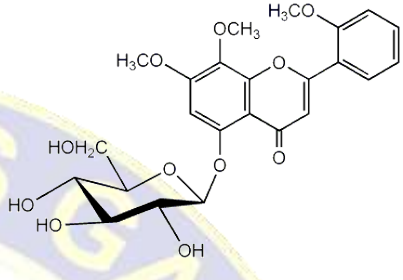
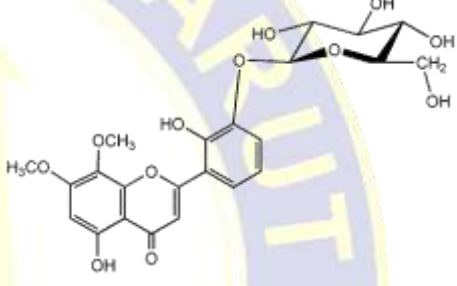
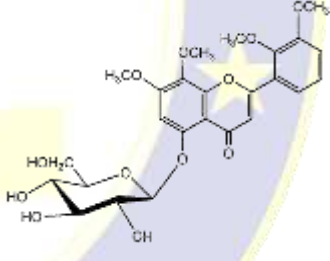
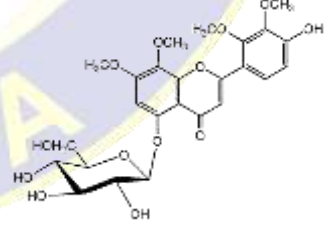
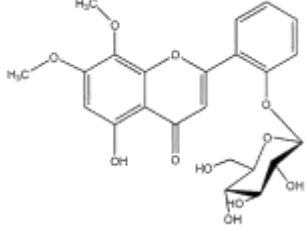
LAMPIRAN 10
(LANJUTAN)

Tabel VII.14
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
26	<i>3-O-Caffeoylquinic acid</i>	$C_{16}H_{18}O_9$	
27	<i>Ferulic acid</i>	$C_{10}H_{10}O_4$	
28	<i>beta-Sitosterol</i>	$C_{29}H_{50}O$	
29	<i>7-O-Methylwogonin</i>	$C_{17}H_{14}O_5$	
30	<i>Wogonin 5-glucoside</i>	$C_{22}H_{22}O_{10}$	
31	<i>5-Hydroxy-7,8-dimethoxyflavone 5-glucoside</i>	$C_{23}H_{24}O_{10}$	

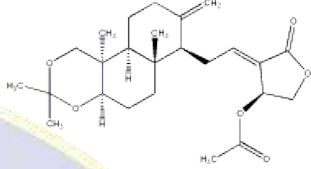

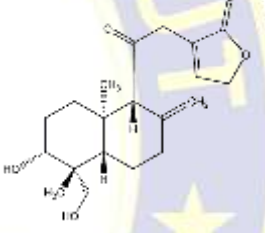
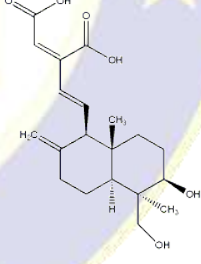
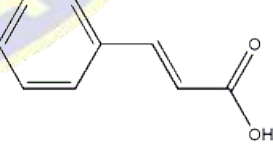
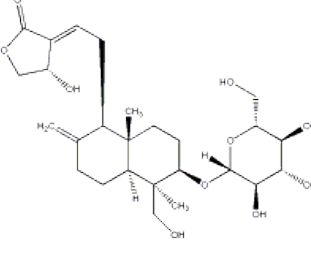
LAMPIRAN 10
(LANJUTAN)

Tabel VII.14
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
32	<i>5-Hydroxy-7,8,2'-trimethoxyflavone 5-glucoside</i>	$C_{24}H_{26}O_{11}$	
33	<i>5,2',3'-Trihydroxy-7,8-dimethoxyflavone 3'-glucoside</i>	$C_{23}H_{24}O_{12}$	
34	<i>5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside</i>	$C_{25}H_{28}O_{12}$	
35	<i>5,4'-Dihidroxy-7,8,2',3'-tetramethoxy flavone 5-glucoside</i>	$C_{25}H_{28}O_{13}$	
36	<i>Skullcapflavone 1 2'-O-glucoside</i>	$C_{23}H_{24}O_{11}$	

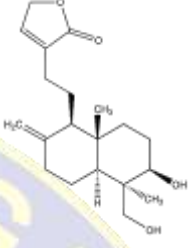

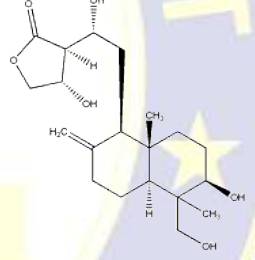
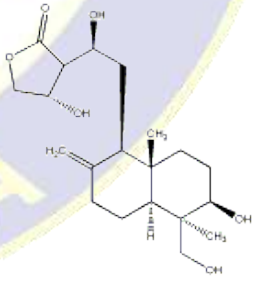
**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.14
Lanjutan**

No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
37	<i>14-Acetyl-3,19-isopropylideneandrographolide</i>	$C_{25}H_{36}O_6$	
38	<i>14-Deoxy-11,14-didehydroandrographolide</i>	$C_{20}H_{28}O_4$	
39	<i>14-Deoxy-11-oxoandrographolide</i>	$C_{20}H_{28}O_5$	
40	<i>Andrographic acid</i>	$C_{20}H_{28}O_6$	
41	<i>Cinnamic acid</i>	$C_9H_8O_2$	
42	<i>3-O-beta-D-Glucopyranosylandrographolide</i>	$C_{26}H_{40}O_{10}$	

**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.14
Lanjutan**



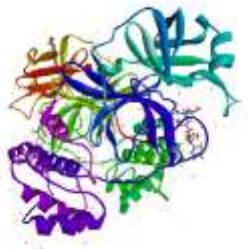
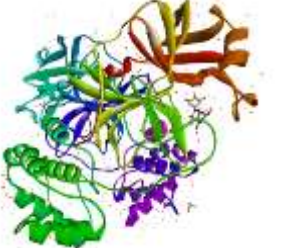
No	Nama Senyawa	Rumus Molekul	Struktur Senyawa
43	<i>14-Deoxyandrographolide</i>	$C_{20}H_{30}O_4$	
44	<i>Andrograpanin</i>	$C_{20}H_{30}O_3$	
45	<i>12S,13S-Hydroxyandrographolide</i>	$C_{20}H_{32}O_6$	
46	<i>12S-Hydroxyandrographolide</i>	$C_{20}H_{32}O_6$	

LAMPIRAN 11

STRUKTUR 3D RESEPTOR

Tabel VII.15

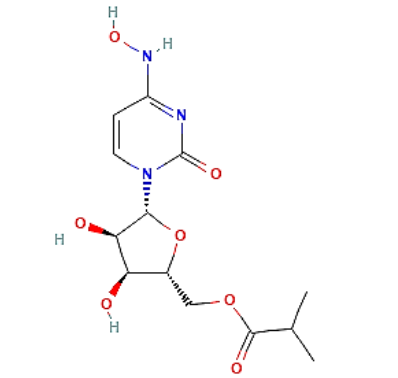
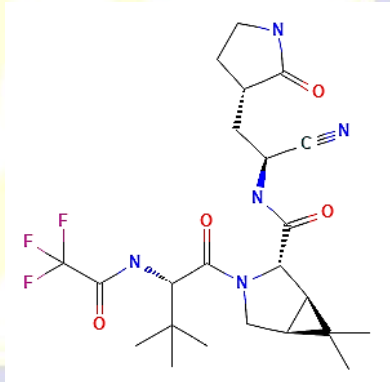
Struktur 3D Reseptor *Main Protease* SARS-CoV-2

ID PDB	STRUKTUR KOMPLEKS
7SI9	
7RN4	
7NG6	
7DPU	

LAMPIRAN 12

STRUKTUR 2D LIGAND PEMBANDING

Tabel VII.16
Struktur 2D Ligand Pembanding

LIGAND PEMBANDING	STRUKTUR SENYAWA
Molnupiravir	 <p>The chemical structure of Molnupiravir is shown. It features a central pyrimidine ring with a hydroxyl group at the 2-position and a methyl group at the 4-position. The 5-position of the pyrimidine ring is linked to a ribose sugar ring. The ribose sugar has hydroxyl groups at the 2' and 3' positions. The 4' position of the ribose is linked to a propanoic acid chain, which is further substituted with an isopropyl group.</p>
Nirmatrelvir (PF-07321332) + Ritonavir (Paxlovid™)	 <p>The chemical structure of Nirmatrelvir (PF-07321332) and Ritonavir (Paxlovid™) is shown. Nirmatrelvir is a complex molecule with a central nitrogen atom bonded to a propanoic acid chain, a nitrile group, and a proline ring. Ritonavir is a complex molecule with a central nitrogen atom bonded to a propanoic acid chain, a nitrile group, and a proline ring. The structure is a combination of the two molecules.</p>

DAFTAR RIWAYAT HIDUP

I. IDENTITAS DIRI

Nama : Lutfi Aulia Aliansyah
 Tempat, Tanggal Lahir : Garut, 23 April 2000
 Jenis Kelamin : Laki – Laki
 Agama : Islam
 Kewarganegaraan : Indonesia
 Status : Mahasiswa
 Alamat : Kp. Kaum RT 001 RW 005 Ds. Sudalarang
 Kec. Sukawening Kab. Garut, Jawa Barat 44184
 Telepon : 082317868676
 Email : lutfi.aulia.la@gmail.com



II. RIWAYAT PENDIDIKAN

Jenjang Pendidikan	Nama Sekolah/Perguruan Tinggi	Tahun Masuk	Tahun Lulus
SD/MI	SDN 3 Sudalarang	2006	2012
SMP/MTs	SMPN 1 Sukawening	2012	2015
SMA/MA/SMK	SMAN 14 Garut	2015	2018
Perguruan Tinggi	Universitas Garut	2018	2022

III. PENGALAMAN ORGANISASI

1. Sekretaris Departemen HUMAS BEM KEMA FMIPA UNIGA (2019 – 2020)
2. Wakil Sekretaris Umum BEM KEMA FMIPA UNIGA (2020 – 2021)
3. Relawan Creavil Garut dan Berdaya Foundation Garut (2020 – sekarang)
4. Relawan Pelita Intan Muda Garut (2021 – sekarang)