

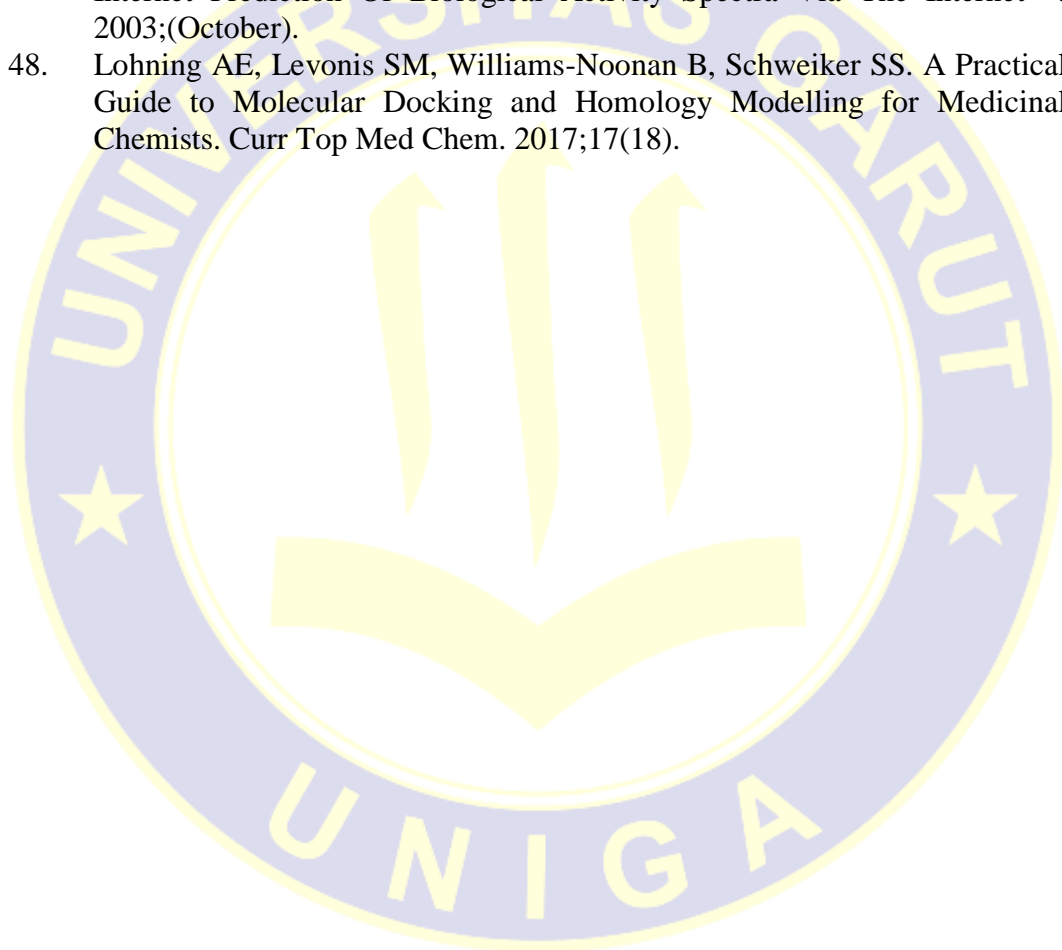
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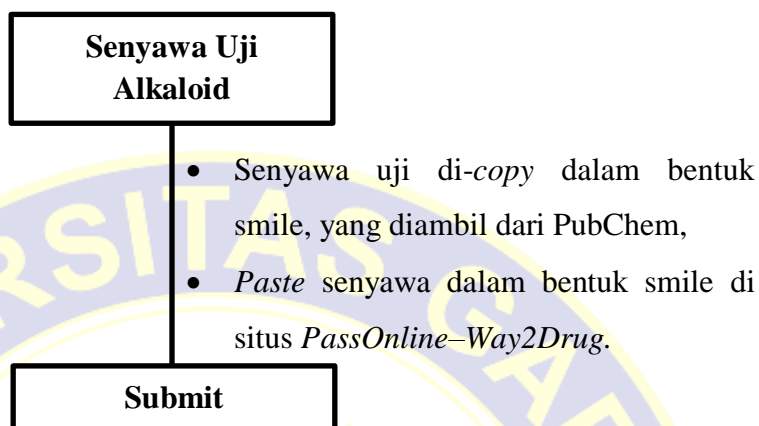
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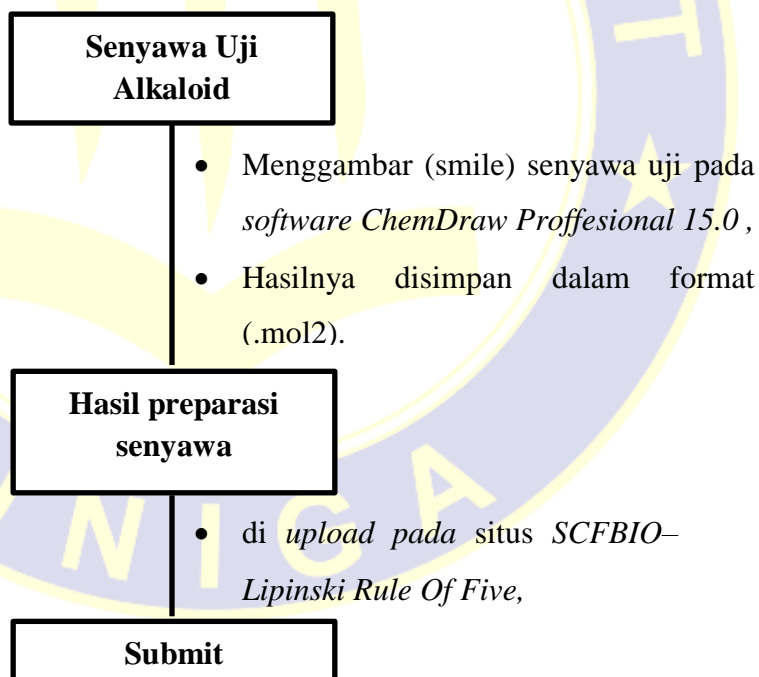


LAMPIRAN 1

ALUR *SCREENING* ANTIVIRUS, ANALISIS FISIKOKIMIA, ANALISIS FARMAKOKINETIK DAN ANALISIS TOKSISITAS

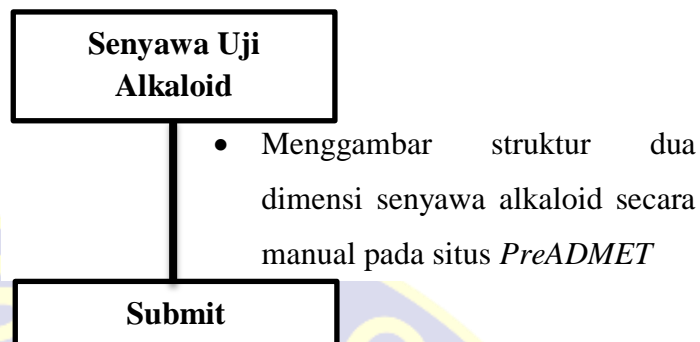


Gambar VII.1 Skema alur penelitian *Screening* Antivirus

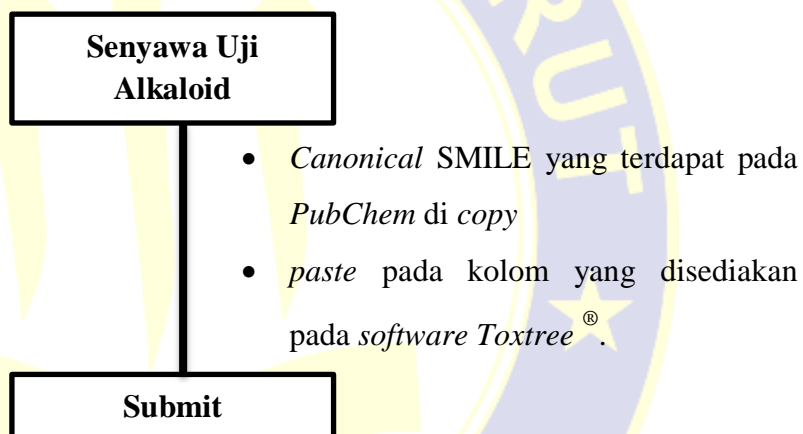


Gambar VII.2 Skema alur penelitian Analisis Fisikokimia

**LAMPIRAN 1
(LANJUTAN)**



Gambar VII.3 Skema alur penelitian Analisis Farmakokinetik

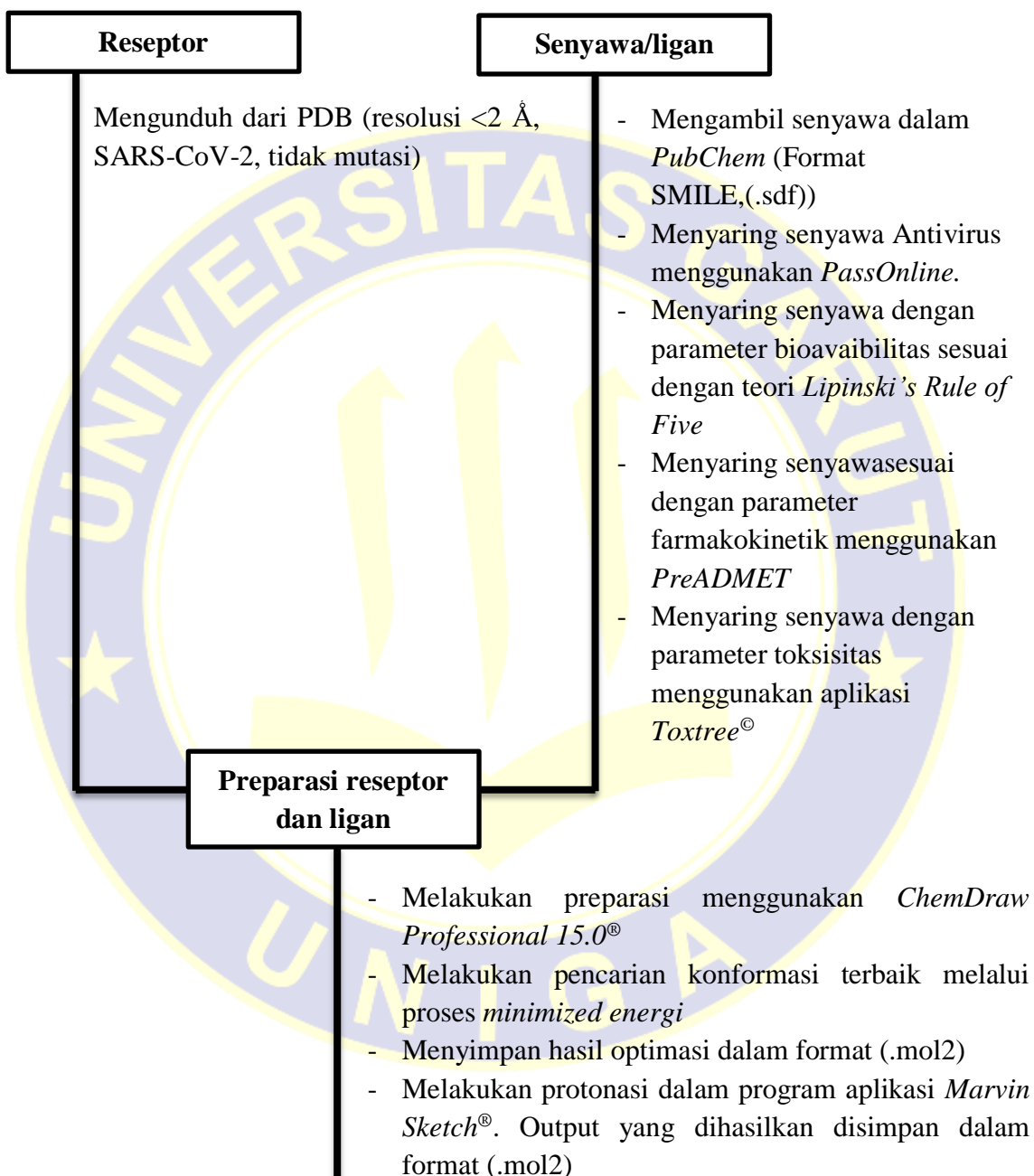


Pilih *method*, pilih “*select decision tree*”.
Lalu pilih parameter *cross TCC decision tree*, *carcinogenicity (genotox and nongenotox)* and *mutagenicity rulebase by ISS* serta *in vitro mutagenicity (Amest Test) alerts by ISS*

Gambar VII.4 Skema alur penelitian Analisis Toksisistas

LAMPIRAN 2

ALUR PENELITIAN SIMULASI MOLECULAR DOCKING



LAMPIRAN 2 (LANJUTAN)

Validasi

- Melakukan preparasi reseptor dan ligan uji menggunakan *AutodockTools*[®]
- Menambahkan muatan *gestaiger*, atom hydrogen dan mengoreksi titik rotasi ligan
- Menyimpan dalam format (.pdbqt)
Menyiapkan reseptor selanjutnya menambahkan muatan *Kollman charges* dan atom hydrogen, simpan dalam format (.pdbqt)
- Mengatur *grid-box*, simpan dalam format (.gpf)
- Mengatur parameter docking dengan metode *Lamarckian GA*, simpan dalam format (.dpf)

Simulasi *docking*

- Menyiapkan reseptor hasil validasi yang telah dipisahkan *native ligand-nya* dari reseptor tersebut dalam format (.pdb).
- Meng-*upload* pada situs *SwissDock*
- Menyiapkan ligan uji yang telah dipreparasi yang disimpan dalam format (.mol2) di-*upload* pada situs *SwissDock*.

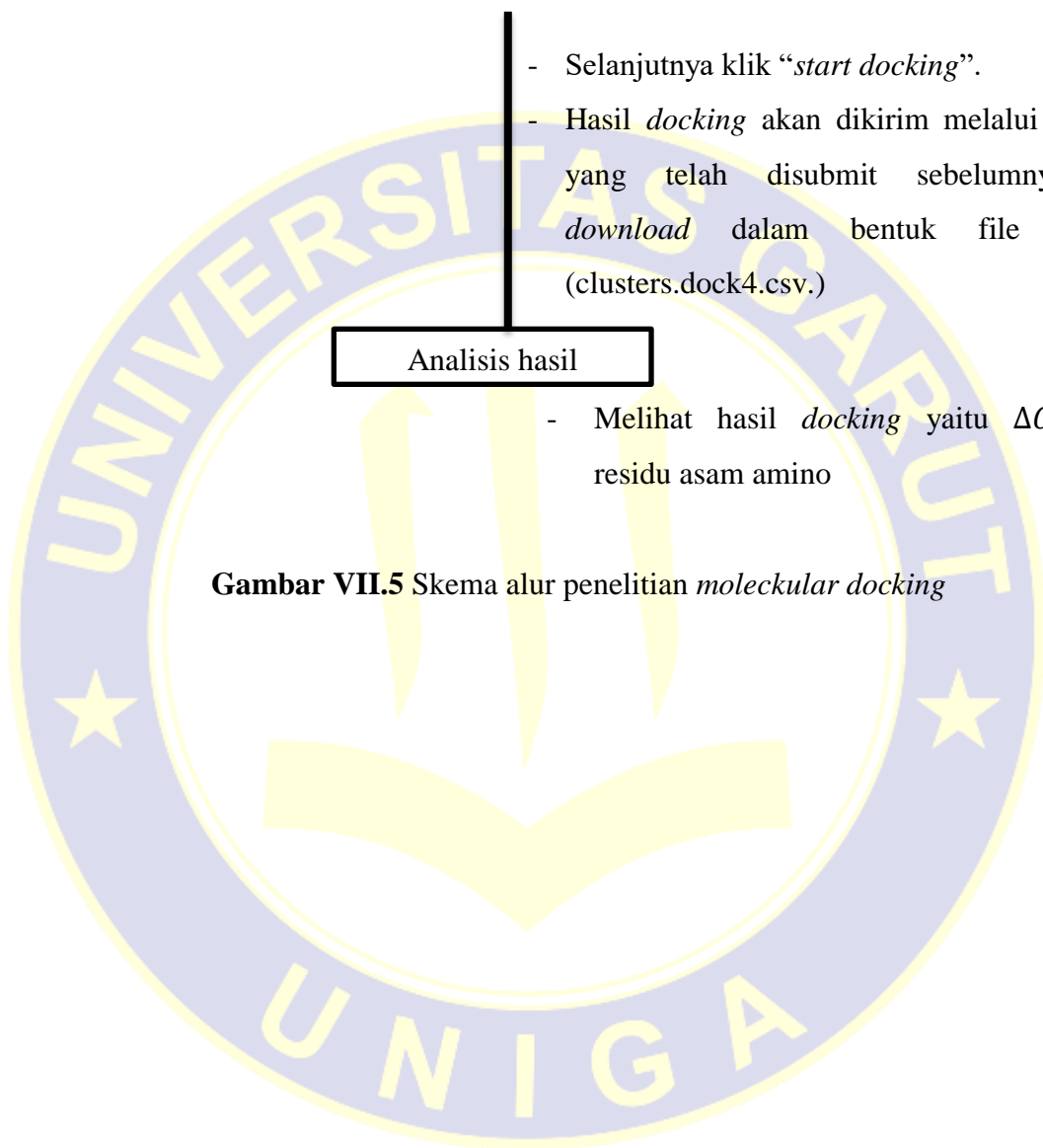
LAMPIRAN 2 (LANJUTAN)

- Selanjutnya klik “*start docking*”.
- Hasil *docking* akan dikirim melalui *email* yang telah disubmit sebelumnya. .
download dalam bentuk file CSV (clusters.dock4.csv.)

Analisis hasil

- Melihat hasil *docking* yaitu ΔG dan residu asam amino

Gambar VII.5 Skema alur penelitian *moleckular docking*

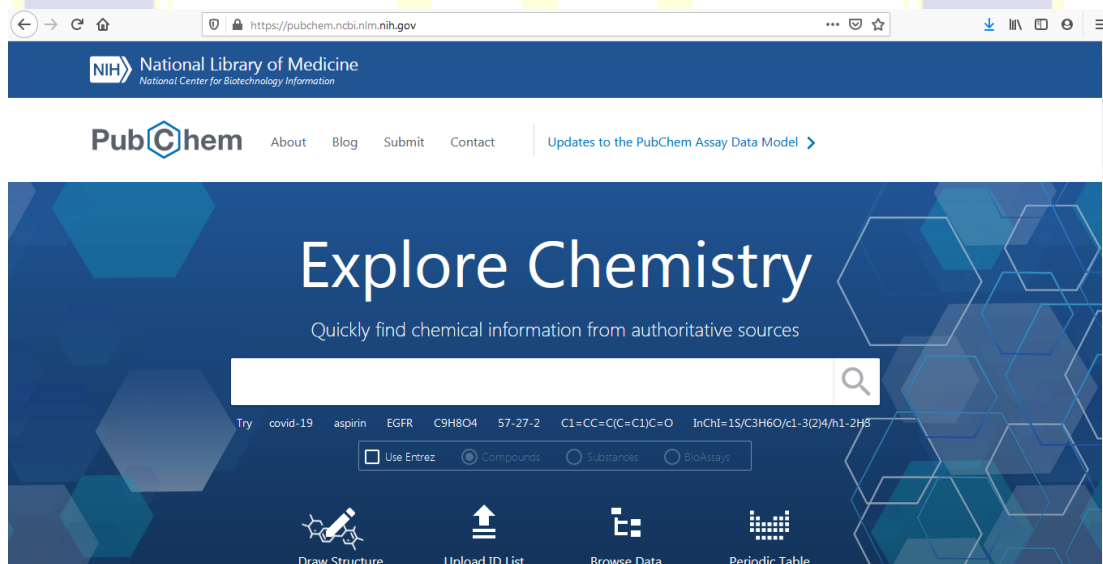


LAMPIRAN 3

SITUS DAN APLIKASI

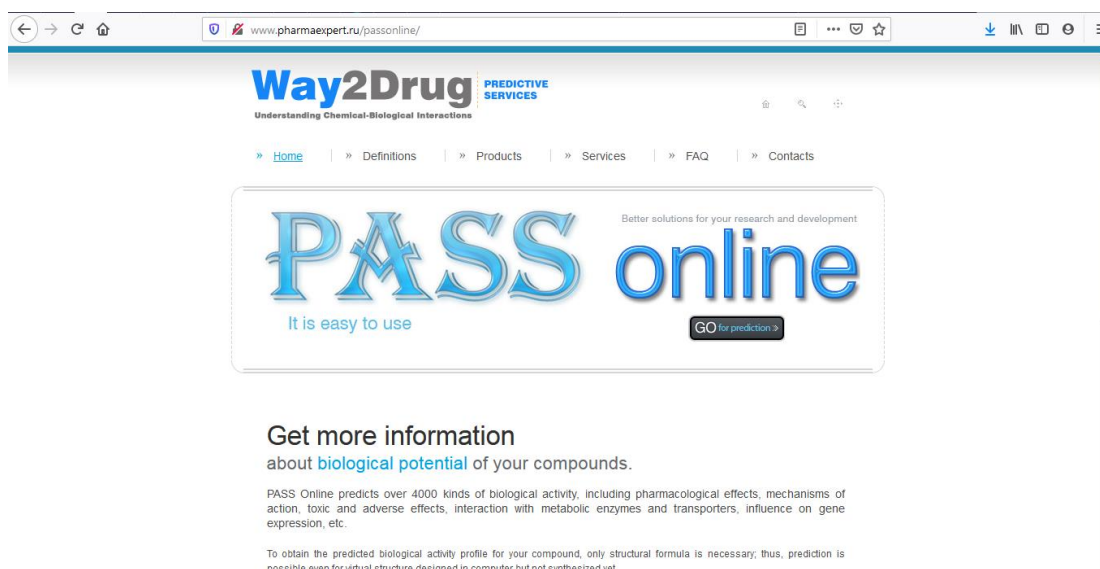


Gambar VII.6 Tampilan situs *Protein Data Bank (PDB)*

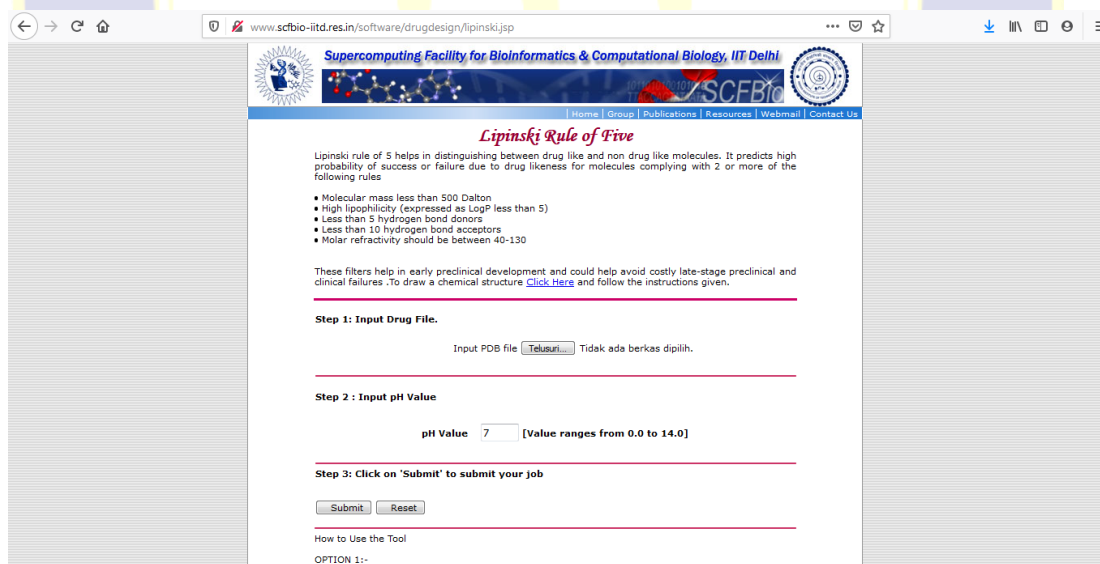


Gambar VII.7 Tampilan situs *PubChem*

LAMPIRAN 3 (LANJUTAN)



Gambar VII.8 Tampilan situs PASS-Online



Gambar VII.9 Tampilan situs *Lipinski Rule of Five*

LAMPIRAN 3 (LANJUTAN)

The screenshot shows the PreADMET website homepage. The browser address bar displays <https://preadmet.bmdrcr>. The navigation menu includes: MDL mol and sd file, Molecular descriptors, Druglikeness, ADME Prediction, Toxicity prediction, Log In, Register, Login, and social media icons. The main header features the PreADMET logo, contact information (Tel: +82-32-212-9550, Fax: +82-32-212-9572, webmaster@bmdrcr.kr), and the address (209, Veritas A Hall, Yonsei University 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, Republic of Korea). The navigation bar contains: Home, About, Druglikeness, ADME, Toxicity, Community, Commercial.

Welcome to the PreADMET

PreADMET is a web-based application for predicting ADME data and building drug-like library using in silico method. PreADMET ver 2.0 is also commercially available in the four editions: Descriptors, Endpoint, Standard and Professional.

- Drug-Likeness Prediction**
Lipinski's rule, lead-like rule, Drug DB like rule
- ADME Prediction**
caco-2, MDCK, BBB, HIA, plasma protein binding and skin permeability data
- Toxicity Prediction**
Ames test and rodent carcinogenicity assay

Lastest News

- G-SFED and Human Nephrotoxicity models will be added in Aug 2017
January 24, 2017
- PreADMET Ver 2.1 is coming soon in this month.
January 9, 2015
- [2008/11] PreADME is one of the most popular sites by Cheminformatics.org.
November 27, 2008
- [2008/10] New release of PreADMET v2.0 windows version

Gambar VII.10 Tampilan situs PreADMET

The screenshot shows the SwissDock website interface. The browser address bar displays www.swissdock.ch/docking. The navigation menu includes: Click2Drug, SwissDock, SwissParam, SwissSidechain, SwissBioisostere, SwissTargetPrediction, SwissADME, SwissSimilarity, About us.

SwissDock
Swiss Institute of Bioinformatics

Home | Target Database | Submit Docking | Command Line Access | Help Forum | Contact

You might be unable to find PDB native structures but only S3DB prepared structures, via a search by PDB ID or protein name. We are working to fix this issue. In the meantime, you can search protein structural files directly on the PDB web site, and upload the selected ones on SwissDock. We are sorry for the inconvenience.

Due to a technical problem, some outputs have been erased before the usual 7 days deadline. We are sorry for the inconvenience. Please, resubmit your job if it was lost.

Target selection
Search for targets:

ie. PDB code, protein name, sequence, or URL
or upload file (max 5MB)

Ligand selection
Search for ligands:

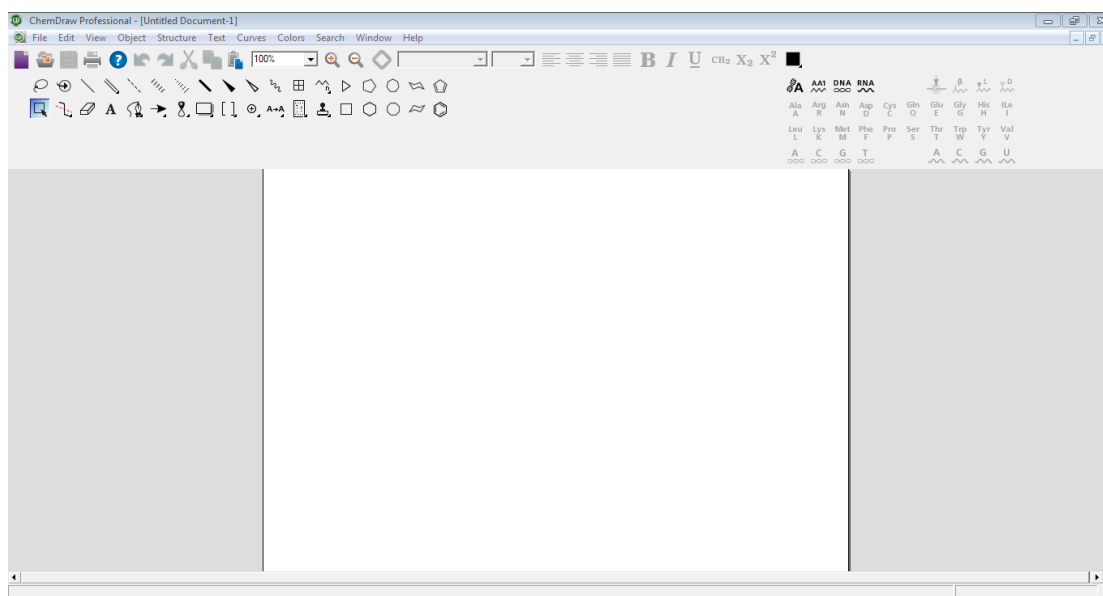
Help
Search for a target protein
You can search for targets using a PDB code, a name, an aminoacid sequence, or even load it from a URL.
PDB codes, names and aminoacid sequence will be looked for in the PDB database.
Names will also be searched for in our database of clean targets.

Load a target protein from a URL
You can also load a file from a URL, provided that it is either:

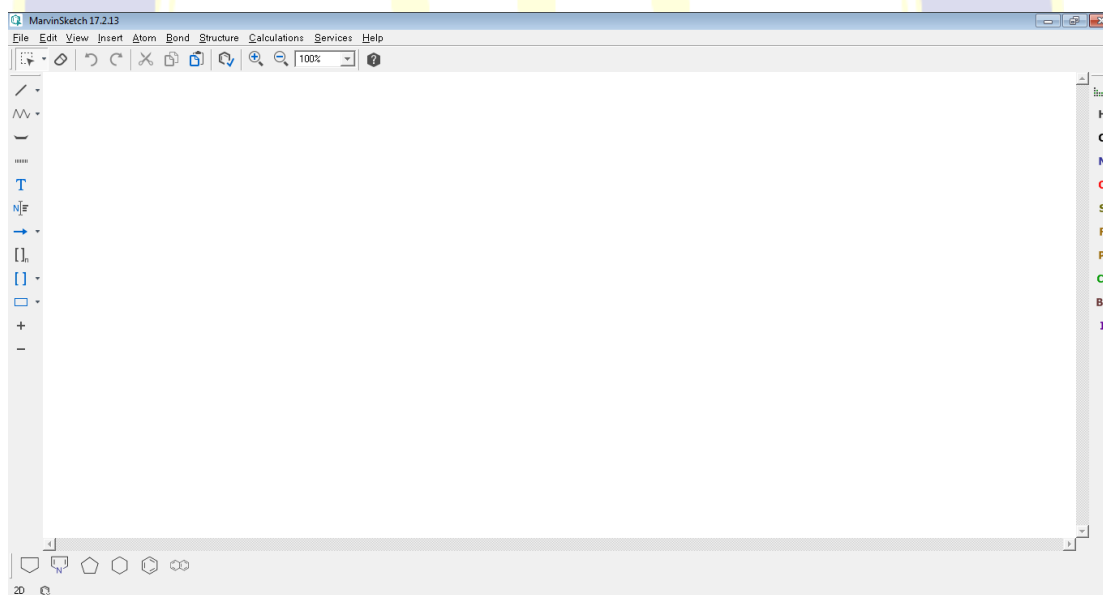
- a PDB file
- a ZIP file containing your target protein in the CHARMM format (PSF, CRD and, if needed, extra RTF,IPAR).

Gambar VII.11 Tampilan situs *SwissDock*

LAMPIRAN 3 (LANJUTAN)

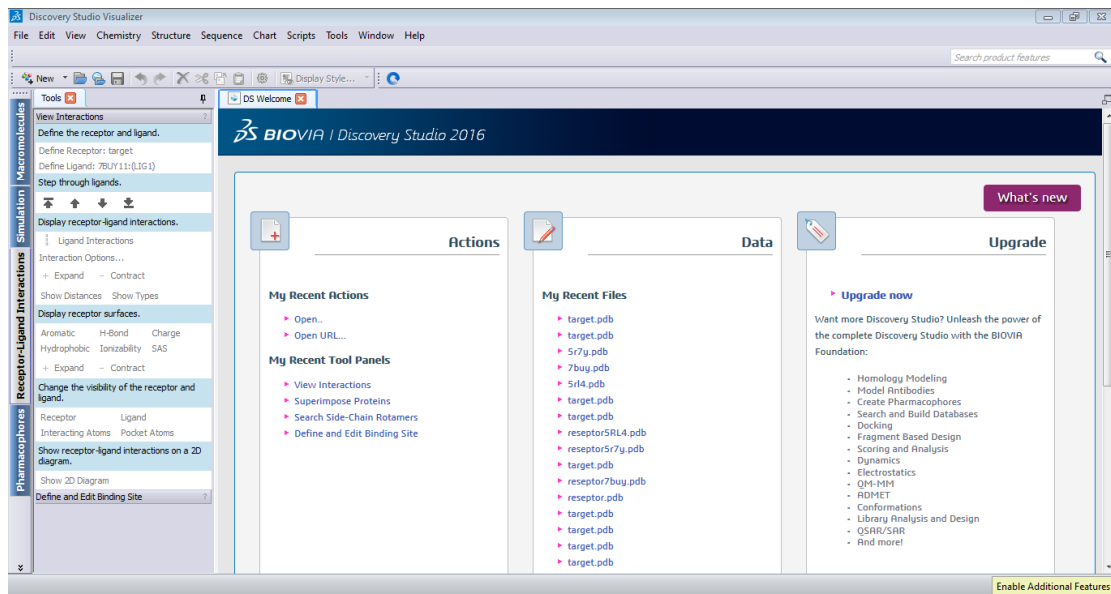


Gambar VII.12 Tampilan aplikasi *ChemDraw Professional 15.0*[®]

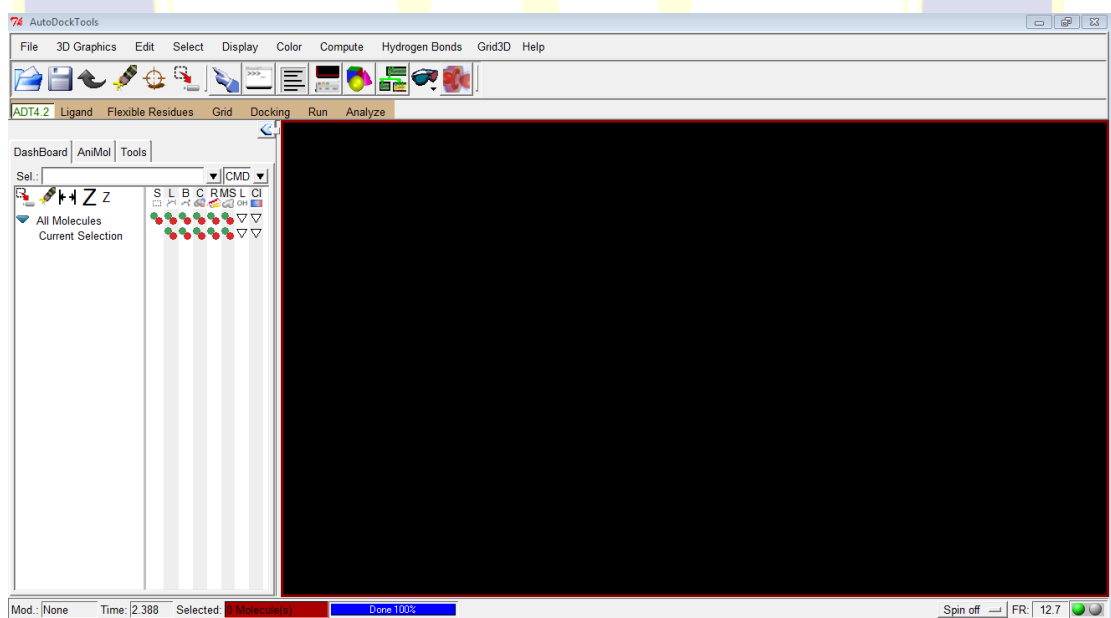


Gambar VII.13 Tampilan aplikasi *Marvisn Sketch*[®]

LAMPIRAN 3 (LANJUTAN)

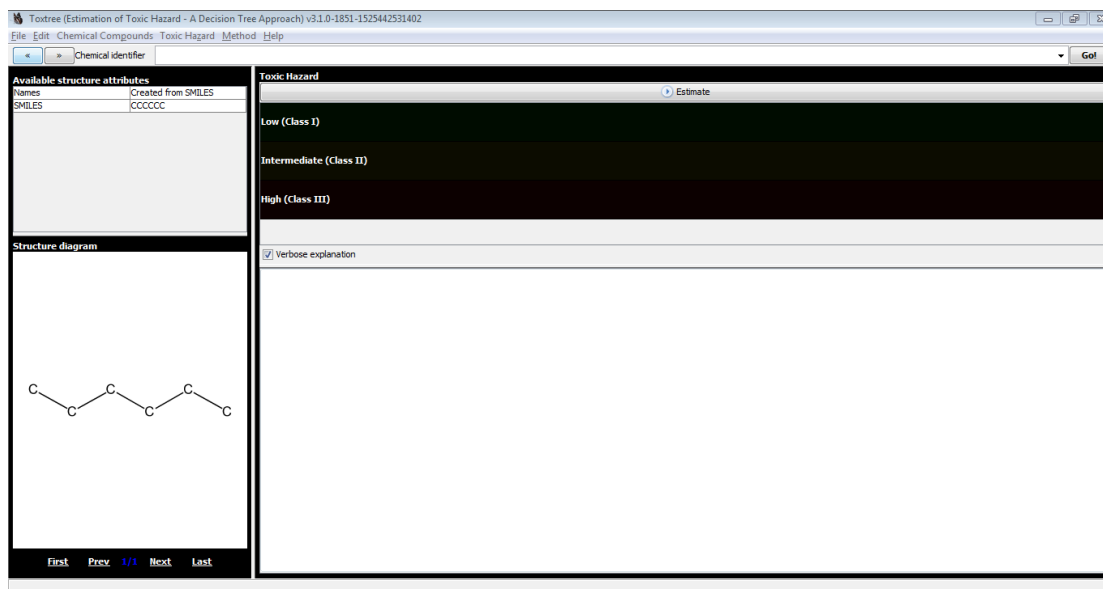


Gambar VII.14 Tampilan aplikasi *Discovery Studio Visualizer*[®]

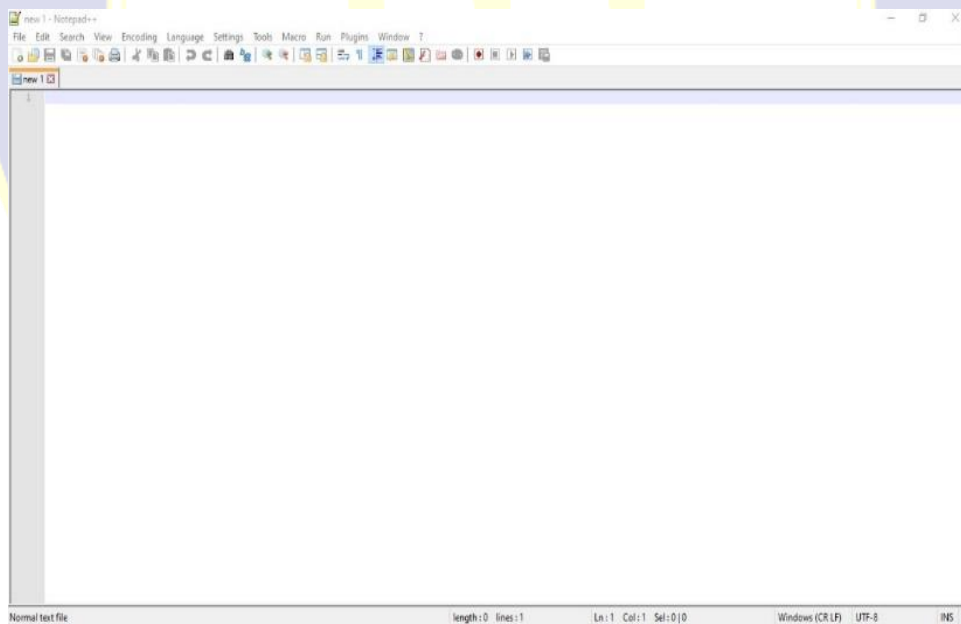


Gambar VII.15 Tampilan aplikasi *AutoDock Tools*[®]

LAMPIRAN 3 (LANJUTAN)



Gambar VII.16 Tampilan aplikasi *Toxtree*[®]



Gambar VII.17 Tampilan aplikasi *Notepad*^{++®}

LAMPIRAN 4

HASIL SCREENING ANTIVIRUS

Tabel VII.1

Screening Senyawa Alkaloid Berdasarkan Aturan PASS-Online

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
1	Cryptospirolepine	0,321	0,195	Picornavirus
		0,231	0,163	Adenovirus
2	Isocryptolepine	0,481	0,059	Picornavirus
		0,349	0,055	Adenovirus
		0,285	0,068	Poxvirus
		0,264	0,059	CMV
		0,206	0,134	Viral entry inhibitor
		0,222	0,154	Herpes
		0,112	0,112	HIV-2 reverse transcriptase inhibitor
3	Jozipeltine A	0,233	0,071	Antiviral
		0,214	0,074	Hepatitis B
		0,140	0,078	HIV
		0,089	0,053	HIV-1 integrase inhibitor
4	Normelicopicine	0,437	0,082	Picornavirus
		0,374	0,041	Adenovirus
		0,234	0,103	CMV
		0,254	0,126	Herpes
		0,214	0,106	Viral entry inhibitor
		0,209	0,152	3C-like protease (Human coronavirus) inhibitor
		0,202	0,156	Poxvirus
		0,130	0,086	HIV-2 reverse transcriptase inhibitor
		0,108	0,031	HIV-1 integrase inhibitor
0,086	0,061	Trachoma		

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
5	Isostrychnopentamine	0,179	0,019	Hepatitis
		0,137	0,023	Hepatitis C
6	Strychnopentamine	0,179	0,019	Hepatitis
		0,137	0,023	Hepatitis C
7	Liriodenine	0,393	0,032	Adenovirus
		0,307	0,032	Hepatitis B
		0,266	0,054	3C-like protease (Human coronavirus) inhibitor
		0,132	0,018	HIV-1 integrase inhibitor
		0,131	0,017	HIV-1 integrase (Strand Transfer) inhibitor
		0,103	0,024	HIV-1 integrase (3'- Processing) inhibitor
8	Dioncopeltine A	0,219	0,070	Hepatitis B
		0,225	0,076	Antiviral
		0,136	0,083	HIV
		0,193	0,185	Herpes
		0,092	0,048	HIV-1 integrase inhibitor
9	Dihydranitidine	0,363	0,074	Adenovirus
		0,192	0,189	Viral entry inhibitor
		0,221	0,127	3C-like protease (Human coronavirus) inhibitor
10	Cryptoheptine	0,485	0,057	Picornavirus
		0,394	0,147	Adenovirus
		0,248	0,079	CMV

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
10	Cryptoheptine	0,241	0,199	Simian immunodeficiency virus proteinase inhibitor
		0,225	0,120	3C-like protease (Human coronavirus) inhibitor
		0,222	0,166	Influenza
		0,197	0,163	Poxvirus
11	Annonidine F	0,483	0,058	Picornavirus
		0,221	0,130	CMV
		0,122	0,110	HIV
12	Ancistrotanzanine C	0,199	0,159	Viral entry inhibitor
		0,122	0,022	HIV-1 integrase inhibitor
		0,071	0,046	HIV-1 integrase (Strand Transfer) inhibitor
13	Alstonine	0,081	0,072	Trachoma
14	Chelidonine	0,410	0,025	Adenovirus
		0,195	0,094	Hepatitis B
		0,235	0,194	Influenza
		0,208	0,200	Influenza A
15	Berbamine	0,167	0,139	Hepatitis B
		0,064	0,051	HIV-1 integrase (Strand Transfer) inhibitor
		0,064	0,052	HIV-1 integrase (3'-Processing) inhibitor

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
16	Dicentrine	0,401	0,029	Adenovirus
		0,228	0,063	Hepatitis B
17	Cepharanthine	0,264	0,143	Adenovirus
18	Quinine	0,298	0,257	Rhinovirus
		0,435	0,036	influenza
		0,150	0,034	Hepatitis
		0,121	0,034	Hepatitis C
		0,170	0,134	Antiviral
19	Quinidine	0,435	0,036	Influenza
		0,150	0,034	Hepatitis
		0,121	0,034	hepatitis C
		0,298	0,257	Rhinovirus
		0,170	0,134	Antiviral
20	Cinchonine	0,471	0,028	Influenza
		0,163	0,026	Hepatitis
		0,203	0,093	Antiviral
		0,130	0,027	Hepatitis C
21	Cinchonidine	0,471	0,028	Influenza
		0,163	0,026	Hepatitis
		0,203	0,093	Antiviral
		0,130	0,027	Hepatitis C
22	Dictamine	0,438	0,083	Picornavirus
		0,354	0,058	Herpes
		0,271	0,116	Adenovirus
		0,142	0,041	Hepatitis
		0,112	0,043	Hepatitis C
		0,209	0,158	CMV

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
22	Dictamine	0,200	0,159	Poxvirus
		0,119	0,100	HIV-2 reverse transcriptase inhibitor
		0,081	0,066	HIV-1 integrase inhibitor
23	Ellipticine	0,193	0,185	Viral entry inhibitor
24	Evolitrine	0,333	0,070	Herpes
		0,365	0,142	Picornavirus
		0,150	0,035	Hepatitis
		0,120	0,035	Hepatitis C
		0,234	0,159	Adenovirus
		0,203	0,176	CMV
		0,077	0,073	HIV-1 integrase inhibitor
		0,275	0,044	3C-like protease (Human coronavirus) inhibitor
25	Fagarine	0,379	0,128	Picornavirus
		0,315	0,081	Herpes
		0,234	0,158	Adenovirus
		0,127	0,059	Hepatitis
		0,098	0,066	Hepatitis C
		0,201	0,181	CMV
		0,115	0,026	HIV-1 integrase inhibitor

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
25	Fagarine	0,067	0,048	HIV-1 integrase (Strand Transfer) inhibitor
		0,257	0,044	3C-like protease (Human coronavirus) inhibitor
		0,271	0,156	Simian immunodeficiency virus proteinase inhibitor
26	Skimmianine	0,312	0,083	Herpes
		0,343	0,167	Picornavirus
		0,124	0,064	Hepatitis
		0,222	0,176	Adenovirus
		0,097	0,068	Hepatitis C
		0,113	0,028	HIV-1 integrase inhibitor
		0,070	0,045	HIV-1 integrase (Strand Transfer) inhibitor
		0,259	0,063	3C-like protease (Human coronavirus) inhibitor
27	Cryptolepine	0,583	0,023	Picornavirus
		0,343	0,058	Adenovirus
		0,275	0,074	Poxvirus
		0,283	0,203	Herpes

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
27	Cryptolepine	0,225	0,078	Viral entry inhibitor
		0,238	0,096	CMV
		0,242	0,141	Influenza
		0,156	0,154	Antiviral
		0,010	0,010	Viral fusion inhibitor
		0,135	0,080	HIV-2 reverse transcriptase inhibitor
		0,267	0,161	Simian immunodeficiency virus proteinase inhibitor
		0,213	0,143	3C-like protease (Human coronavirus) inhibitor
28	Harmine	0,250	0,035	Viral entry inhibitor
		0,323	0,192	Picornavirus
		0,249	0,140	Adenovirus
		0,212	0,150	CMV
		0,245	0,098	HIV attachment inhibitor
		0,257	0,066	3C-like protease (Human coronavirus) inhibitor
		0,243	0,196	Simian immunodeficiency virus proteinase inhibitor
29	Harmaline	0,297	0,091	Influenza
		0,202	0,149	Viral entry inhibitor
		0,288	0,280	Rhinovirus

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
29	Harmaline	0,240	0,201	Simian immunodeficiency virus proteinase inhibitor
		0,196	0,182	3C-like protease (Human coronavirus) inhibitor
30	Yohimbine	0,302	0,088	Influenza
		0,352	0,155	Rhinovirus
		0,247	0,103	Influenza A
31	Scopolamine	0,429	0,063	Rhinovirus
		0,384	0,124	Picornavirus
		0,319	0,074	Adenovirus
		0,228	0,149	Herpes
		0,213	0,149	CMV
		0,173	0,128	Hepatitis B
		0,199	0,161	Poxvirus
		0,242	0,198	Simian immunodeficiency virus proteinase inhibitor
32	Atropine	0,421	0,070	Rhinovirus
		0,373	0,041	Adenovirus
		0,421	0,100	Picornavirus
		0,261	0,063	CMV
		0,210	0,137	Poxvirus
		0,222	0,165	Imfluenza
		0,168	0,137	Hepatitis B
		0,201	0,176	Herpes

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
33	Colchicine	0,367	0,058	Influenza
		0,272	0,067	Influenza A
		0,241	0,150	Adenovirus
34	Allantoin	0,465	0,067	Picornavirus
		0,359	0,037	Poxvirus
		0,324	0,076	Influenza
		0,262	0,120	Herpes
		0,237	0,122	Influenza A
		0,247	0,142	Adenovirus
		0,160	0,149	Antiviral
		0,400	0,052	Simian immunodeficiency virus proteinase inhibitor
0,084	0,080	HIV-1 integrase (overall integration) inhibitor		
35	Trigonelline	0,503	0,005	Adenovirus
		0,520	0,042	Picornavirus
		0,453	0,047	Rhinovirus
		0,338	0,014	CMV
		0,277	0,073	Poxvirus
		0,219	0,093	Viral entry inhibitor
		0,246	0,133	Herpes
		0,046	0,026	Parainfluenza
0,180	0,043	HIV-2 reverse transcriptase inhibitor		

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
35	Trigonelline	0,101	0,058	HIV-1 integrase (overall integration) inhibitor
		0,089	0,053	HIV-1 integrasi inhibitor
		0,064	0,084	HIV-1 integrase (Strand Transfer) inhibitor
		0,338	0,089	Simian immunodeficiency virus proteinase inhibitor
		0,245	0,083	3C-like protease (Human coronavirus) inhibitor
36	Octopamine	0,576	0,025	Picornavirus
		0,423	0,040	Influenza
		0,378	0,039	Adenovirus
		0,371	0,034	Poxvirus
		0,366	0,051	Herpes
		0,274	0,064	Influenza A
		0,242	0,089	CMV
		0,181	0,113	Hepatitis B
		0,194	0,181	Viral entry inhibitor
		0,042	0,032	Parainfluenza
		0,220	0,010	HIV-1 integrase (overall integration) inhibitor
		0,192	0,038	HIV-2 reverse transcriptase inhibitor

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
36	Octopamine	0,438	0,037	Simian immunodeficiency virus proteinase inhibitor
		0,235	0,100	3C-like protease (Human coronavirus) inhibitor
37	Synephrine	0,478	0,060	Picornavirus
		0,398	0,030	Poxvirus
		0,393	0,032	Adenovirus
		0,332	0,071	Influenza
		0,327	0,074	Herpes
		0,242	0,113	Influenza A
		0,201	0,151	Viral entry inhibitor
		0,377	0,064	Simian immunodeficiency virus proteinase inhibitor
		0,238	0,096	3C-like protease (Human coronavirus) inhibitor
		0,158	0,058	HIV-2 reverse transcriptase inhibitor
38	Capsaicin	0,103	0,056	HIV-1 integrase (overall integration) inhibitor
		0,415	0,076	Rhinovirus
		0,375	0,047	Herpes
		0,348	0,065	Influenza
		0,229	0,069	Viral entry inhibitor

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
38	Capsaicin	0,231	0,085	Antiviral
		0,164	0,052	HIV
		0,207	0,163	CMV
		0,214	0,181	Influenza A
		0,164	0,147	Hepatitis B
		0,313	0,109	Simian immunodeficiency virus proteinase inhibitor
		0,212	0,147	3C-like protease (Human coronavirus) inhibitor
		0,098	0,041	HIV-1 integrase inhibitor
		0,135	0,094	HIV-2 reverse transcriptase inhibitor
		0,066	0,050	HIV-1 integrase (3'-Processing) inhibitor
39	Quinolizidine	0,544	0,034	Picornavirus
		0,408	0,026	Adenovirus
		0,399	0,047	Influenza
		0,340	0,013	CMV
		0,376	0,121	Rhinovirus
		0,251	0,033	Viral entry inhibitor
		0,284	0,068	Poxvirus
		0,289	0,099	Herpes
		0,129	0,057	Hepatitis
		0,113	0,042	Hepatitis C

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
39	Quinolizidine	0,446	0,035	Simian immunodeficiency virus proteinase inhibitor
		0,245	0,084	3C-like protease (Human coronavirus) inhibitor
		0,020	0,011	Protease (Human cytomegalovirus) inhibitor
		0,372	0,018	HIV attachment inhibitor
		0,173	0,048	HIV-2 reverse transcriptase inhibitor
		0,064	0,001	Viral fusion inhibitor
40	Cytisine	0,465	0,005	Influenza A
		0,437	0,083	Picornavirus
		0,331	0,072	Influenza
		0,286	0,101	Adenovirus
		0,212	0,141	Poxvirus
		0,197	0,191	CMV
		0,311	0,112	Simian immunodeficiency virus proteinase inhibitor
41	Tomatidine	0,407	0,044	Influenza
		0,279	0,106	Herpes
		0,249	0,100	Influenza A
42	Theonelladin A	0,409	0,081	Rhinovirus
		0,389	0,119	Picornavirus

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
42	Theonelladin A	0,297	0,031	CMV
		0,296	0,094	Herpes
		0,281	0,103	Influenza
		0,280	0,107	Adenovirus
		0,220	0,130	Poxvirus
		0,214	0,180	Influenza A
		0,247	0,190	Simian immunodeficiency virus proteinase inhibitor
43	Theonelladin C	0,449	0,076	Picornavirus
		0,324	0,071	Adenovirus
		0,262	0,061	CMV
		0,271	0,078	Poxvirus
		0,239	0,119	Influenza A
		0,248	0,134	Influenza
		0,208	0,128	Viral entry inhibitor
		0,202	0,174	Herpes
		0,293	0,267	Rhinovirus
		0,302	0,120	Simian immunodeficiency virus proteinase inhibitor
		0,212	0,146	3C-like protease (Human coronavirus) inhibitor
		0,116	0,104	HIV-2 reverse transcriptase inhibitor

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
44	Makaluvamine	0,068	0,047	HIV-1 integrase (Strand Transfer) inhibitor
		0,080	0,069	HIV-1 integrase inhibitor
		0,063	0,054	HIV-1 integrase (3'-Processing) inhibitor
45	Neoamphimedine	0,223	0,175	Adenovirus
		0,290	0,244	Picornavirus
		0,138	0,017	HIV-1 integrase inhibitor
		0,073	0,041	HIV-1 integrase (Strand Transfer) inhibitor
46	Granulatimide	0,413	0,099	Picornavirus
		0,279	0,072	Poxvirus
		0,254	0,126	Herpes
47	Isogranulatimide	0,413	0,099	Picornavirus
		0,279	0,072	Poxvirus
		0,254	0,126	Herpes
48	Rigidin	0,250	0,095	Poxvirus
		0,328	0,186	Picornavirus
		0,222	0,084	Viral entry inhibitor
		0,243	0,135	Herpes
		0,164	0,146	Hepatitis B
		0,129	0,037	HiV-1 integrase (overall integration) inhibitor
		0,141	0,074	HIV-2 reverse transcriptase inhibitor

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
48	Rigidin	0,243	0,196	Simian immunodeficiency virus proteinase inhibitor
49	Coscinamide	0,248	0,036	Viral entry inhibitor
		0,219	0,131	3C-like protease (Human coronavirus) inhibitor
		0,473	0,005	HIV attachment inhibitor
		0,077	0,073	HIV-1 integrase inhibitor
50	Asterriquinone	0,290	0,099	Herpes
		0,276	0,111	Adenovirus
		0,244	0,086	CMV
		0,317	0,201	Picornavirus
		0,216	0,101	Viral entry inhibitor
		0,115	0,078	Hepatitis
		0,096	0,069	Hepatitis C
		0,102	0,037	HIV-1 integrase inhibitor
		0,091	0,030	HIV-1 integrase (Strand Transfer) inhibitor
		0,133	0,083	HIV-2 reverse transcriptase inhibitor
0,080	0,037	HIV-1 integrase (3'-Processing) inhibitor		

LAMPIRAN 4 (LANJUTAN)

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
51	Topsentin	0,236	0,099	3C-like protease (Human coronavirus) inhibitor
52	Nortopsentin	0,245	0,084	CMV
		0,237	0,109	Poxvirus
		0,204	0,141	Viral entry inhibitor
		0,271	0,067	HIV attachment inhibitor
		0,254	0,071	3C-like protease (Human coronavirus) inhibitor
53	Dispacamide	0,360	0,037	Poxvirus
		0,304	0,086	Adenovirus
		0,282	0,104	Herpes
		0,219	0,170	Influenza
		0,208	0,198	Influenza A
54	Polyandrocarpamine	0,470	0,010	Adenovirus
		0,455	0,073	Picornavirus
		0,392	0,039	Herpes
		0,311	0,033	Antiviral
		0,298	0,031	CMV
		0,273	0,041	Hepatitis B
		0,274	0,075	Poxvirus
		0,265	0,075	Influenza
		0,268	0,113	Influenza
		0,132	0,089	HIV
0,294	0,004	HIV-1 integrase (overall integration) inhibitor		

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
54	Polyandrocarpamine	0,126	0,020	HIV-1 integrase inhibitor
		0,114	0,021	HIV-1 integrase (3'-Processing) inhibitor
		0,101	0,205	HIV-2 reverse transcriptase inhibitor
		0,052	0,044	HIV-1 reverse transcriptase inhibitor
		0,304	0,118	Simian immunodeficiency virus proteinase inhibitor
		0,221	0,218	3C-like protease (Human coronavirus) inhibitor
55	Leucettamine	0,462	0,011	Adenovirus
		0,364	0,143	Picornavirus
		0,235	0,102	CMV
		0,200	0,096	Antiviral
		0,164	0,051	HIV
		0,223	0,123	3C-like protease (Human coronavirus) inhibitor
56	Camptothecin	0,449	0,019	Herpes
57	Vinblastine			Tidak Memiliki Aktivitas Antivirus
58	β -Carboline			Tidak Memiliki Aktivitas Antivirus
59	Dragmacidin			Tidak Memiliki Aktivitas Antivirus

**LAMPIRAN 4
(LANJUTAN)**

Tabel VII.1

Lanjutan

NO	ALKALOID	Pa	Pi	Aktivitas Antivirus
60	Emetine			Tidak Memiliki Aktivitas Antivirus
61	Jatrorrhizine			Tidak Memiliki Aktivitas Antivirus
62	Palmatine			Tidak Memiliki Aktivitas Antivirus
63	Tetrandrine			Tidak Memiliki Aktivitas Antivirus
64	Sanguinarine			Tidak Memiliki Aktivitas Antivirus
65	Chelerythrine			Tidak Memiliki Aktivitas Antivirus
66	Berberrubine			Tidak Memiliki Aktivitas Antivirus
67	Coptisine			Tidak Memiliki Aktivitas Antivirus
68	Berberine			Tidak Memiliki Aktivitas Antivirus
69	Fagaronine			Tidak Memiliki Aktivitas Antivirus
70	Hydroxycryptolepine			Tidak Memiliki Aktivitas Antivirus
71	Chrysopentamine			Tidak Memiliki Aktivitas Antivirus
72	10-Hydroxyusambarensine			Tidak Memiliki Aktivitas Antivirus

LAMPIRAN 5

HASIL ANALISIS SIFAT FISIKOKIMIA

Tabel VII.2

Sifat Fisikokimia *Native Ligand*, Ligan Perbandingan dan Senyawa Alkaloid Berdasarkan Aturan *Lipinski's Rule of Five*

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
1	Lovinapir	628	4,33	4	9	Tidak Memenuhi
2	Remdesivir	602	2,31	5	13	Tidak Memenuhi
3	HexylcarbamicAcid_7buy	145	1,83	2	3	Memenuhi
4	N-(2-phenylethyl) methanesulfonamide_5r7y	199	0,63	1	3	Memenuhi
5	N-(4-tert-butylphenyl)-N-[(1R)-2-(methylamino)-2-oxo-1-(pyridin-3-yl) ethyl]propanamide	326	-0,13	0	5	Memenuhi
6	10 – Hydroxyusambarensine	448	5,93	3	5	Tidak Memenuhi
7	Cryptospirolepine	504	5,38	1	3	Tidak Memenuhi
8	Chrysopentamine	595	6,26	4	4	Tidak Memenuhi
9	Isocryptolepine	232	2,2	0	0	Memenuhi
10	Jozipeltine A	312	-0,05	5	6	Memenuhi
11	Normelicopicine	315	2,42	0	5	Memenuhi
12	Isostrychnopentamine	549	6,46	3	4	Tidak Memenuhi
13	Strychnopentamine	549	6,46	3	4	Tidak Memenuhi
14	Liriodenine	275	1,65	0	4	Memenuhi
15	Dioncopeltine A	379	3,64	3	4	Memenuhi
16	Dihydranitidine	349	1,94	0	4	Memenuhi
17	Hydroxycryptolepine	248	3,48	1	2	Memenuhi
18	Cryptoheptine	262	2,31	1	1	Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

Tabel VII.2

Lanjutan

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
19	Annonidine A	368	7,26	2	0	Tidak Memenuhi
20	Ancistrotanzanine C	407	5,18	2	5	Tidak Memenuhi
21	Fagaronine	350	4,29	1	4	Memenuhi
22	Alstonine	348	3,37	0	4	Memenuhi
23	Sanguinarine	332	3,43	0	4	Memenuhi
24	Chelerythrine	348	3,72	0	4	Memenuhi
25	Chelidonine	353	2,33	1	6	Memenuhi
26	Berberine	336	2,91	0	4	Memenuhi
27	Berbamine	608	5,23	1	7	Tidak Memenuhi
28	Berberrubine	357	2,5	1	4	Memenuhi
29	Coptisine	320	2,57	0	4	Memenuhi
30	Dicentrine	339	3,18	0	5	Memenuhi
31	Jatrorrhizine	338	3,08	1	4	Memenuhi
32	Palmatine	352	3,38	0	4	Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

Tabel VII.2

Lanjutan

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
33	Tetrandrine	622	5,88	0	7	Tidak Memenuhi
34	Cepharanthine	606	5,87	0	8	Tidak Memenuhi
35	Quinine	324	3,17	1	4	Memenuhi
36	Quinidine	324	3,17	1	4	Memenuhi
37	Cinchonine	294	3,17	1	3	Memenuhi
38	Cinchonidine	294	3,16	1	3	Memenuhi
39	Emetine	480	3,71	1	6	Memenuhi
40	Dictamine	199	2,99	0	3	Memenuhi
41	Ellipticine	246	4,49	1	1	Memenuhi
42	Evolitrine	229	2,99	0	4	Memenuhi
43	Fagarine	229	2,99	0	4	Memenuhi
44	Skimmianine	259	3,01	0	5	Memenuhi
45	Cryptolepine	232	3,88	0	1	Memenuhi
46	Harmine	212	3,03	1	2	Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

Tabel VII.2

Lanjutan

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
47	Harmaline	214	2,31	1	2	Memenuhi
48	Yohimbine	354	2,65	2	4	Memenuhi
49	Scopolamine	303	0,92	1	5	Memenuhi
50	Atropine	289	1,93	1	3	Memenuhi
51	Colchicine	399	2,59	1	7	Memenuhi
52	Allantoin	158	-2,71	5	7	Memenuhi
53	Trigonelline	137	-1,12	0	2	Memenuhi
54	Octopamine	153	0,38	4	3	Memenuhi
55	Synephrine	167	0,65	3	3	Memenuhi
56	Capsaicin	305	3,79	2	4	Memenuhi
57	Quinolizidine	139	2,02	0	1	Memenuhi
58	Cytisine	190	0,5	1	3	Memenuhi
59	Tomatidine	415	5,37	2	3	Tidak Memenuhi
60	Theonelladin A	288	5,03	2	2	Tidak Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

Tabel VII.2

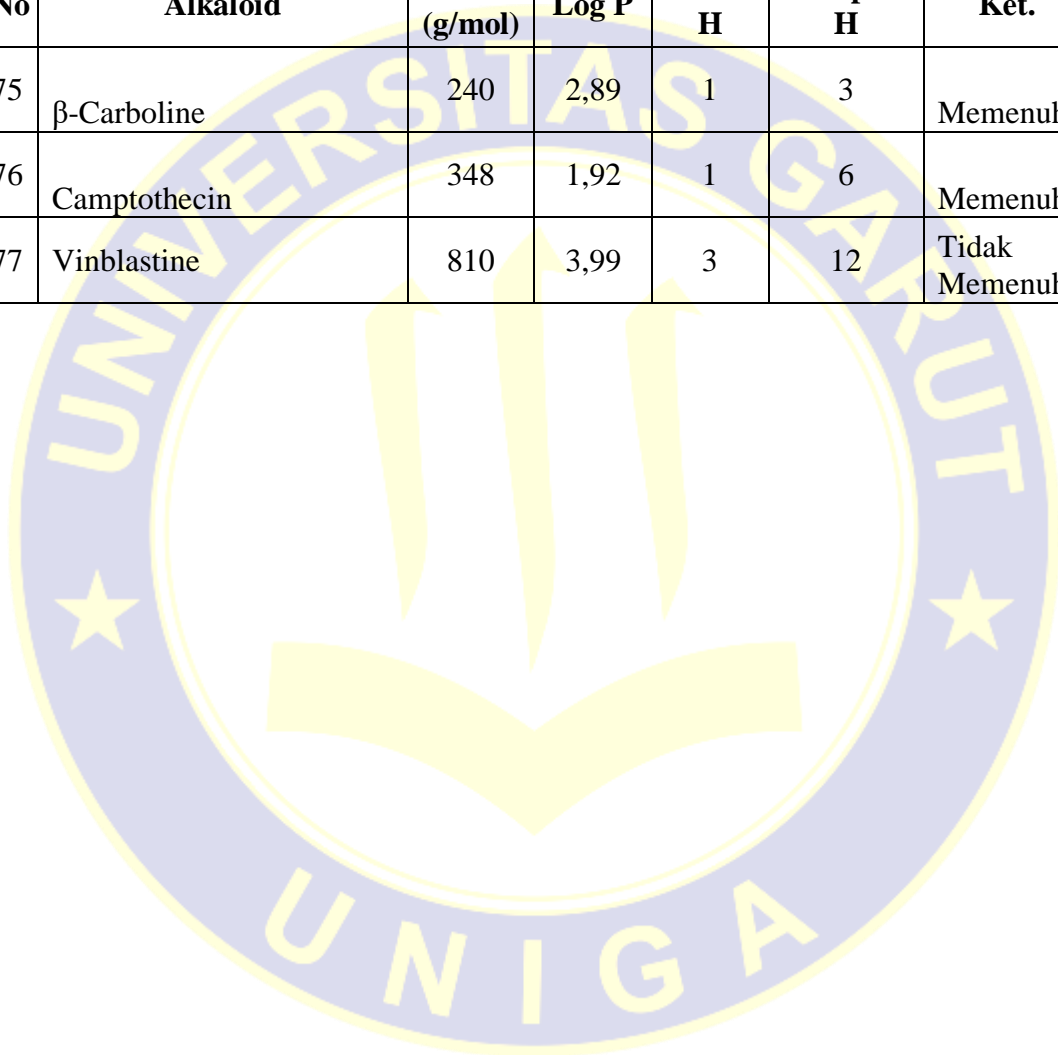
Lanjutan

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
61	Theonelladin C	276	4,87	2	2	Memenuhi
62	Makaluvamine	415	4,04	3	5	Memenuhi
63	Neoamphimedine	313	2,72	0	5	Memenuhi
64	Granulatimide	276	2,08	3	4	Memenuhi
65	Isogranulatimide	276	2,02	2	5	Memenuhi
66	Rigidin	363	3,59	5	7	Memenuhi
67	Coscinamide	407	4,38	3	3	Memenuhi
68	Asterriquinone	506	6,48	2	4	Tidak Memenuhi
69	Dragmacidin	580	5,96	4	3	Tidak Memenuhi
70	Topsentin	342	3,98	4	3	Memenuhi
71	Nortopsentin	454	6,04	3	1	Tidak Memenuhi
72	Dispacamide	403	0,98	5	6	Memenuhi
73	Polyandrocarpamine	219	-0,12	5	6	Memenuhi
74	Leucettamine	231	0,82	2	5	Memenuhi

**LAMPIRAN 5
(LANJUTAN)****Tabel VII.2**

Lanjutan

No	Alkaloid	BM (g/mol)	Log P	Donor H	Akseptor H	Ket.
75	β -Carboline	240	2,89	1	3	Memenuhi
76	Camptothecin	348	1,92	1	6	Memenuhi
77	Vinblastine	810	3,99	3	12	Tidak Memenuhi



LAMPIRAN 6

HASIL ANALISIS FARMAKOKINETIK

Tabel VII.3

Analisis Farmakokinetik *Native Ligand*, Ligan Pembanding dan Senyawa Alkaloid Berdasarkan PreADMET

No	Nama Senyawa	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
1	Lovinapir	93,80 ^a	24,06 ^b	89,71 ^b
2	Remdesivir	38,21 ^b	2,89 ^c	74,45 ^b
3	HexylcarbamicAcid_7buy	85,33 ^a	11,08 ^b	73,92 ^b
4	N-(2-phenylethyl) methanesulfonamide_5r7y	94,47 ^a	7,83 ^b	58,35 ^b
5	N-(4-tert-butylphenyl)-N-[(1R)-2-(methylamino)-2-oxo-1-(pyridin-3-yl)ethyl]propanamide	97,64 ^a	22,44 ^b	87,14 ^b
6	10 -Hydroxyusambarensine	93,72 ^a	30,6 ^b	90,09 ^a
7	Cryptospirolepine	95,11 ^a	52 ^b	97,35 ^a
8	Chrysopentamine	93,02 ^a	44,37 ^b	75,33 ^b
9	Isocryptolepine	100 ^a	53,26 ^b	86,54 ^b
10	Jozipeltine A	90,06 ^a	19,98 ^b	92,24 ^a
11	Normelicopicine	96,17 ^a	33,19 ^b	85,37 ^b
12	Isostrychnopentamine	94,03 ^a	37,29 ^b	62,63 ^b
13	Strychnopentamine	94,03 ^a	37,29 ^b	62,63 ^b
14	Liriodenine	97,45 ^a	27,54 ^b	87,25 ^b
15	Dioncopeltine A	87,69 ^a	20,99 ^b	75,67 ^b
16	Dihydronitidine	98,03 ^a	55,98 ^b	91,02 ^a
17	Hydroxycryptolepine	93,39 ^a	52,58 ^b	93,39 ^a
18	Cryptoheptine	97,09 ^a	52,81 ^b	90,89 ^a
19	Annonidine A	94,32 ^a	32,22 ^b	87,33 ^a
20	Ancistrotanzanine C	96,26 ^a	36,42 ^b	85,52 ^b
21	Fagaronine	96,84 ^a	47,71 ^b	61,8 ^b
22	Alstonine	97,46 ^a	43,06 ^b	53,81 ^b

LAMPIRAN 6 (LANJUTAN)

Tabel VII.3

Lanjutan

No	Nama Senyawa	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
23	Sanguinarine	98,2 ^a	54,32 ^b	69,46 ^b
24	Chelerythrine	98,25 ^a	55,73 ^b	64,98 ^b
25	Chelidonine	93,85 ^a	19,06 ^b	50,06 ^b
26	Berberine	97,88 ^a	55,57 ^b	58,54 ^b
27	Berbamine	97,52 ^a	52,69 ^b	82,06 ^b
28	Berberrubine	96,04 ^a	36,04 ^b	57,31 ^b
29	Coptisine	97,85 ^a	54,28 ^b	60,75 ^b
30	Dicentrine	97,76 ^a	56,52 ^b	64,84 ^b
31	Jatrorrhizine	96,14 ^a	46,74 ^b	55,35 ^b
32	Palmatine	97,92 ^a	55,96 ^b	58,38 ^b
33	Tetrandrine	98,06 ^a	54,34 ^b	84,2 ^b
34	Cepharanthine	98,01 ^a	54,23 ^b	82,2 ^b
35	Quinine	96,09 ^a	50,17 ^b	59,46 ^b
36	Quinidine	96,09 ^a	50,17 ^b	59,45 ^b
37	Cinchonine	96,48 ^a	52,98 ^b	66,28 ^b
38	Cinchonidine	96,48 ^a	52,98 ^b	66,28 ^b
39	Emetine	96,59 ^a	56,69 ^b	63,09 ^b
40	Dictamine	98,74 ^a	55,85 ^b	92,08 ^a
41	Ellipticine	95,03 ^a	27,78 ^b	86,79 ^b
42	Evolitrine	97,71 ^a	56,36 ^b	88,47 ^b
43	Fagarine	97,71 ^a	55,92 ^b	82,37 ^b
44	Skimmianine	97,89 ^a	56,68 ^b	84,15 ^b
45	Cryptolepine	100 ^a	37,55 ^b	83,88 ^b
46	Harmine	92,83 ^a	42,21 ^b	64,05 ^b
47	Harmaline	91,81 ^a	42,26 ^b	62,09 ^b

**LAMPIRAN 6
(LANJUTAN)**

Tabel VII.3

Lanjutan

No	Nama Senyawa	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
48	Yohimbine	90,73 ^a	15,67 ^b	66,43 ^b
49	Scopolamine	95,82 ^a	25,72 ^b	24,86 ^b
50	Atropine	95,4 ^a	26,28 ^b	35,26 ^b
51	Colchicine	96,9 ^a	37,44 ^b	65,42 ^b
52	Allantoin	35,76 ^b	15,73 ^b	12 ^b
53	Trigonelline	95,13 ^a	21,09 ^b	0 ^b
54	Octopamine	82,98 ^a	17,68 ^b	0 ^b
55	Synephrine	82,25 ^a	0,2 ^c	3,92 ^b
56	Capsaicin	92,48 ^a	37,37 ^b	92,86 ^a
57	Quinolizidine	100 ^a	25,44 ^b	100 ^a
58	Cytisine	95,29 ^a	24,25 ^b	3,53 ^b
59	Tomatidine	93,85 ^a	53,89 ^b	89,08 ^b
60	Theonelladin A	96,32 ^a	47,14 ^b	100 ^a
61	Theonelladin C	96,24 ^a	45,26 ^b	100 ^a
62	Makaluvamine	94,01 ^a	20,77 ^b	85,67 ^a
63	Neoamphimedine	97,45 ^a	19,25 ^b	91,98 ^a
64	Granulatimide	89,28 ^a	0,22 ^c	89,61 ^b
65	Isogranulatimide	94,33 ^a	0,22 ^c	90,21 ^a
66	Rigidin	72,62 ^a	19,77 ^b	88,47 ^b
67	Coscinamide	92,82 ^a	21,16 ^b	95,65 ^a
68	Asterriquinone	96,92 ^a	19,34 ^b	96,99 ^a
69	Dragmacidin	93,38 ^a	33,81 ^b	99,62 ^a
70	Topsentin	89,09 ^a	17,87 ^b	93,09 ^a
71	Nortopsentin	94,21 ^a	39,98 ^b	100 ^a
72	Dispacamide	83,77 ^a	13,33 ^b	35,29 ^b
73	Polyandrocarpamine	69,23 ^a	21,04 ^b	31,37 ^b

LAMPIRAN 6 (LANJUTAN)

Tabel VII.3

Lanjutan

No	Nama Senyawa	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
74	Leucettamine	95,74 ^a	21,32 ^b	45,81 ^b
75	β -Carboline	92,52 ^a	11,36 ^b	92,09 ^a
76	camptothecin	96,86 ^a	18,5 ^b	79,32 ^b
77	Vinblastine	94,16 ^a	34,11 ^b	46,94 ^b

Keterangan :

HIA (%) : 70-100 terserap baik^a

20-70 terserap cukup^b

<20 kurang terserap^c

CaCo-2 (nm sec) : >70 permeabilitas tinggi^a

4-70 permeabilitas sedang^b

<4 permeabilitas rendah^c

PPB (%) : >90 terikat kuat^a

<90 terikat lemah^b

LAMPIRAN 7

HASIL ANALISIS TOKSISITAS

Tabel VII.4

Analisis Toksisitas *Native Ligand*, Ligan Pembanding dan Senyawa Alkaloid Berdasarkan Aplikasi *Toxtree*[®]

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
1	Lovinapir	Tidak Berisiko	-	-	-
2	Remdesivir	Sangat berisiko	+	+	+
3	Hexylcarbamic Acid	Tidak Berisiko	-	-	-
4	N-(2-phenylethyl)methanesulfonamide	Tidak Berisiko	-	-	-
5	N-(4-tert-butylphenyl)-N-[(1R)-2-(methylamino)-2-oxo-1-(pyridin-3-yl)ethyl]propanamide	Tidak Berisiko	-	-	-
6	10 – Hydroxyusambarensin	Berisiko Rendah	+	-	+
7	Cryptospirolepine	Berisiko Rendah	+	-	+
8	Chrysopentamine	Berisiko Rendah	+	-	+
9	Isocryptolepine	Berisiko Rendah	+	-	+
10	Jozipeltine A	Tidak Berisiko	-	+	-
11	Normelicopicine	Berisiko Rendah	+	-	+
12	Isostrychnopentamine	Tidak Berisiko	+	-	-
13	Strychnopentamine	Tidak Berisiko	-	-	-

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Lanjutan

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
14	Liriodenine	Berisiko Rendah	+	+	+
15	Dioncopeltine A	Tidak Berisiko	-	+	-
16	Dihydranitidine	Berisiko Rendah	+	+	+
17	Hydroxycryptolepine	Berisiko Rendah	+	-	+
18	Cryptoheptine	Berisiko Rendah	+	-	+
19	Annonidine A	Berisiko Rendah	+	-	+
20	Ancistrotanzanine C	Tidak Berisiko	-	+	-
21	Fagaronine	Berisiko Rendah	+	-	+
22	Alstonine	Berisiko Rendah	-	-	+
23	Sanguinarine	Berisiko Rendah	+	+	+
24	Chelerythrine	Berisiko Rendah	+	+	+
25	Chelidonine	Tidak Berisiko	-	+	-
26	Berberine	Berisiko Rendah	+	+	+
27	Berbamine	Tidak Berisiko	-	-	-
28	Berberrubine	Berisiko Rendah	+	+	+

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Lanjutan

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
29	Coptisine	Berisiko Rendah	+	+	+
30	Dicentrine	Tidak Berisiko	-	+	+
31	Jatrorrhizine	Berisiko Rendah	+	-	+
32	Palmatine	Berisiko Rendah	+	-	+
33	Tetrandrine	Tidak Berisiko	-	-	+
34	Cepharanthine	Tidak Berisiko	-	+	-
35	Quinine	Tidak Berisiko	-	-	-
36	Quinidine	Tidak Berisiko	-	-	-
37	Cinchonine	Tidak Berisiko	-	-	-
38	Cinchonidine	Tidak Berisiko	-	-	-
39	Emetine	Tidak Berisiko	-	-	-
40	Dictamine	Berisiko Rendah	+	-	+
41	Ellipticine	Berisiko Rendah	+	-	+
42	Evolitrine	Berisiko Rendah	+	-	+
43	Fagarine	Berisiko Rendah	+	-	+

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Lanjutan

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
44	Skimmianine	Berisiko Rendah	+	-	+
45	Cryptolepine	Berisiko Rendah	+	-	+
46	Harmine	Berisiko Rendah	+	-	+
47	Harmaline	Tidak Berisiko	-	-	-
48	Yohimbine	Tidak Berisiko	-	-	-
49	Scopolamine	Berisiko Rendah	+	-	+
50	Atropine	Tidak Berisiko	-	-	-
51	Colchicine	Tidak Berisiko	-	-	-
52	Allantoin	Tidak Berisiko	-	-	-
53	Trigonelline	Tidak Berisiko	-	-	-
54	Octopamine	Tidak Berisiko	-	-	-
55	Synephrine	Tidak Berisiko	-	-	-
56	Capsaicin	Tidak Berisiko	-	-	-
57	Quinolizidine	Tidak Berisiko	-	-	-
58	Cytisine	Tidak Berisiko	-	-	-

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Lanjutan

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
59	Tomatidine	Tidak Berisiko	-	-	-
60	Theonelladin A	Tidak Berisiko	-	-	-
61	Theonelladin C	Tidak Berisiko	-	-	-
62	Makaluvamine	Tidak Berisiko	+	+	+
63	Neoamphimedine	Berisiko Rendah	+	-	+
64	Granulatimide	Berisiko Rendah	+	+	+
65	Isogranulatimide	Berisiko Rendah	+	-	+
66	Rigidin	Tidak Berisiko	-	-	-
67	Coscinamide	Tidak Berisiko	-	-	-
68	Asterriquinone	Berisiko Rendah	+	-	+
69	Dragmacidin	Tidak Berisiko	-	-	-
70	Topsentin	Tidak Berisiko	-	+	-
71	Nortopsentin	Tidak Berisiko	-	+	-
72	Dispacamide	Berisiko Rendah	+	-	+
73	Polyandrocarpamine	Tidak Berisiko	-	-	-

**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.4

Lanjutan

No	Nama Senyawa	<i>Kroes TCC</i>	Karsinogenik		Mutagen (<i>Amest Test</i>)
			Genotoksik	Non Genotoksik	
74	Leucettamine	Tidak Berisiko	-	-	-
75	β -Carboline	Berisiko Rendah	+	-	+
76	Camptothecin	Berisiko Rendah	-	-	+
77	Vinblastine	Tidak Berisiko	-	-	-

LAMPIRAN 8

ENERGI BEBAS DAN RESIDU ASAM AMINO RESEPTOR

5RL4

Tabel VII.5

Energi Bebas dan Residu asam amino simulasi *molecular docking* senyawa Alkaloid terhadap reseptor *Main Protease* ID 5RL4

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
1	N-(4-tert-butylphenyl)-N-[(1R)-2-(methylamino)-2-oxo-1-(pyridin-3-yl)ethyl]propanamide	-8.5	ASN 142, CYS 145, GLU 166, GLY 143, LEU 141, MET 49
2	Lovinapir	-10.56	ASN 142, CYS 44, GLU 166, GLY 143, LEU 27, MET 48, PRO 168
3	Remdesivir	-10.82	ASN 142, CYS 145, GLU 145, LEU 167, MET 165, PRO 168, THR 24, THR 25, THR 26
4	10 -Hydroxyusambarensine	-8.88	ASN 142, CYS 44, GLU 166, HSD 41, MET 49, PHE 140
5	Cryptospirolepine	-8.8	ASN 142, CYS 44, CYS 145, GLU 166, HSD 41, MET 49
6	Chrysopentamine	-9.21	CYS 44, CYS 145, MET 49, SER 46
7	Isocryptolepine	-7.32	ASN 142, CYS 145, GLU 166, MET 165
8	Jozipeltine A	-9.74	CYS 44, GLU 166, LEU 167, MET 49, PRO 168, THR 26, THR 190
9	Normelicopicine	-8.12	CYS 44, CYS 145, GLU 166, GLY 143, MET 49, MET 165, LEU
10	Isostrychnopentamine	-9.8	ARG 188, ASN 142, GLU166, LEU 167, MET 49, MET 165
11	Strychnopentamine	-10.11	ASN 142, GLU 166, MET 49, MET 165
12	Liriodenine	-7.54	ASN 142, CYS 145, MET 49, MET 165
13	Dioncopeltine A	-9.8	ASN 142, GLU 166, MET 165
14	Dihydranitidine	-8.33	GLU 166, MET 49, MET 165, THR 190

LAMPIRAN 8 (LANJUTAN)

Tabel VII.5

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
15	Hydroxycryptolepine	-7.15	CYS 44, MET 49, MET 165
16	Cryptoheptine	-7.72	ASN 142, GLU 166, MET 165
17	Annonidine A	-8.44	ASN 142, CYS 145, MET 49, MET 165
18	Ancistrotanzanine C	-9.73	CYS 44, GLU 166, HSD 41, MET 49, MET 165
19	Fagaronine	-8.42	ASN 142, GLU 166, PHE 140, PRO 168
20	Alstonine	-8.65	ASN 142, GLU 166
21	Sanguinarine	-8.28	GLU 166, MET 165, PRO 168
22	Chelerythrine	-8.87	ASN 142, GLU 166, LEU 141, PRO 168
23	Chelidonine	-8.58	CYS 44, GLN 189, MET 49, MET 165, THR 190
24	Berberine	-8.48	ASN 142, GLU 166, LEU 141, PHE 140, PRO 168
25	Berbamine	-8.91	CYS 44, CYS 145, GLU 166, MET 165, SER 46, THR 25, THR 45
26	Berberrubine	-8.1	GLU 166, LEU 141, PRO 168
27	Coptisine	-7.98	ASN 142, GLU 166, MET 165
28	Dicentrine	-8.75	ASN 142, CYS 44, CYS 145, LEU 141, MET 49
29	Jatrorrhizine	-8.43	GLU 166, LEU 141, PHE 140, PRO 168, THR 190
30	Palmatine	-8.61	GLU 166, LEU 141, PRO 168, THR 190
31	Tetrandrine	-9.11	CYS 145, GLU 166, MET 165, SER 46, THR 25, THR 45
32	Cepharanthine	-7.66	CYS 145, GLU 166, GLY 143
33	Quinine	-8.21	GLU 166, PHE 140, PRO 168
34	Quinidine	-8.35	GLU 166, PHE 140, PRO 168

LAMPIRAN 8 (LANJUTAN)

Tabel VII.5

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
35	Cinchonine	-8.1	ASN 142, GLU 166, PRO 168
36	Cinchonidine	-8.16	ASN 142, GLU 166, PRO 168
37	Emetine	-9.97	GLU 166, MET 166
38	Dictamine	-6.92	CYS 44, MET 49, HSE 164
39	Ellipticine	-7.35	ASN 142, CYS 44, CYS 145, GLY 143, MET 49
40	Evolitrine	-7.18	CYS 145, LEU 141, MET 49, MET 165
41	Fagarine	-7.29	ASN 142, CYS 145, GLY 143, LEU 141, MET 165, THR 26
42	Skimmianine	-7.62	GLU 166, HSE 164, MET 165, THR 190
43	Cryptolepine	-7.3	CYS 44, HSD 41, MET 49
44	Harmine	-7.06	ARG 188, GLU 166, LEU 141, MET 165
45	Harmaline	-7.96	GLU 166, MET 165
46	Yohimbine	-8.46	CYS 145, GLN 189, GLU 166, PRO 168
47	Scopolamine	-8.66	ARS 188, ASN 142, GLU 166, MET 49
48	Atropine	-8.01	ARG 188, GLU 166, LEU 167, MET 49, MET 165
49	Colchicine	-8.37	LEU 141, MET 49
50	Allantoin	-6.58	GLU 14, GLY 15, MET 17
51	Trigonelline	-7.13	ASN 142, GLY 143, MET 165, PHE 140
52	Octopamine	-8.02	ASN 142, GLU 166, HSE 164, LEU 141, PHE 140

LAMPIRAN 8 (LANJUTAN)

Tabel VII.5

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
53	Synephrine	-7.84	ASN 142, GLU 166, LEU 167
54	Capsaicin	-8.79	CYS 145, GLY 143, LEU 167, MET 165, PRO 168
55	Quinolizidine	-6.68	ASN 142, CYS 145, LEU 141, GLU 166
56	Cytisine	-7.3	GLU 166, LEU 167, PRO 168
57	Tomatidine	-8.29	CYS 145, LEU 27, MET 49, MET 165, THR 24
58	Theonelladin A	-9.32	GLN 189, GLU 166, LEU 141, MET 165, PHE 140, THR 190
59	Theonelladin C	-9.75	ASN 142, CYS 44, HSD 41, GLU 166, LEU 141, MET 49, PHE 140
60	Makaluvamine	-9.81	GLU 166, MET 49, PHE 140
61	Neoamphimedine	-8.21	ASN 142, CYS 44, CYS 145, GLY 143, LEU 141, MET 149, MET 165
62	Granulatimide	-7.35	ASN 142, GLU 166
63	Isogranulatimide	-7.74	ASN 142, CYS 145, GLY 143, MET 49
64	Rigidin	-8.28	CYS 145, GLN 189, GLY 143, GLU 166, MET 49, MET 165, PRO 168
65	Coscinamide	-8.23	ASN 142, GLU 166, PRO 168, MET 165
66	Asterriquinone	-9.24	ASN 142, GLY 143, MET 49, MET 165, THR 25
67	Dragmacidin	-8.57	ASN 142, CYS 145, GLN 189, GLY 143, MET 165, PRO 168, THR 26
68	Topsentin	-7.96	CYS 145, GLN 189, HSD 41, MET 49, MET 165
69	Nortopsentin	-8.16	CYS 44, GLU 166, MET 49, MET 165

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII.5

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
70	Dispacamide	-8.78	ARG 188, ASN 142, GLN 189, GLU 166, MET 165, PHE 140
71	Polyandrocarpamine	-7.36	ASN 142, GLU 166, MET 165
72	Leucettamine	-7.93	ARG 188, ASN 142, GLU 166, MET 165, PHE 140
73	β -Carboline	-7.43	CYS 44, CYS 145, GLU 166, LEU 141, MET 49
74	camptothecin	-7.88	ARG 188, GLU 166, GLN 189, MET 49, MET 165
75	vinblastine	-9.74	ASN 142, CYS 44, CYS 166, GLU 166, GLY 143, HSD 41, LEU 27, MET 49, THR 45

LAMPIRAN 9

ENERGI BEBAS DAN RESIDU ASAM AMINO RESEPTOR

7BUY

Tabel VII.6

Residu asam amino simulasi *molecular docking* senyawa Alkaloid terhadap reseptor *Main Protease* ID 7BUY

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
1	HexylcarbamicAcid	-6.6	GLU 166, MET 49, MET 165
2	Remdesivir	-10.01	ASN 142, CYS 145, GLN 189, GLU 166, MET 165, THR 190
3	Lovinapir	-10.16	ASN 142, GLU 166, GLY 143, MET 49, MET 165
4	10 -Hydroxyusambarensine	-8.44	ASN 166, CYS 145, GLU 166, MET 49, MET 165
5	Cryptospirolepine	-7.75	GLU 166, MET 49, MET 165, PRO 168
6	Chrysopentamine	-9.28	GLU 166, 49, MET 165, PRO 168
7	Isocryptolepine	-7.21	MET 49, MET 165, PRO 168
8	Jozipeltine A	-9.53	ASN 142, CYS 44, GLU 166, GLY 143, MET 165, THR 24, THR 25
9	Normelicopicine	-7.7	ARG 188, GLU 166, MET 165, PRO 1668
10	Isostrychnopentamine	-8.78	CYS 145, GLU 166, GLY 143, LEU 141, MET 49, PRO 168
11	Strychnopentamine	-8.86	CYS 44, CYS 145, GLU 166, MET 49, MET 165
12	Liriodenine	-7.14	GLU 166, MET 49, MET 165
13	Dioncopeltine A	-9.1	GLU 166, MET 165
14	Dihydranitidine	-8.27	CYS 145, GLY 143, MET 165, THR 190
15	Hydroxycryptolepine	-6.78	CYS 145, HSE 41, MET 49, MET 165
16	Cryptoheptine	-7.31	NET 49, MET 165, PRO 168, THR 190
17	Annonidine A	-8.11	ASN 142, CYS 145, GLU 166, LEU 167, MET 49, MET 165

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.6

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
18	Ancistrotanzanine C	-9.12	CYS 145, GLU 166, MET 49, MET 165
19	Fagaronine	-8.39	CYS 145, GLU 166, GLY 143, HSE 41, MET 165, THR 190
20	Alstonine	-7.99	CYS 145, GLY 143, MET 49, MET 165
21	Sanguinarine	-8.43	GLU 166, MET 165, THR 190
22	Chelerythrine	-8.36	CYS 145, GLU 166, MET 165, THR 190
23	Chelidonine	-7.72	CYS 145, GLY 143, MET 165
24	Berberine	-8.04	GLN 192, GLU 166, PRO 168, THR 190
25	Berbamine	-8.35	GLU 166, PRO 168, SER 46
26	Berberrubine	-7.74	GLU 166, MET 165, PRO 168
27	Coptisine	-8.28	GLN 192, GLU 166, LEU 141, MET 165, THR 190
28	Dicentrine	-8.09	CYS 145, GLY 143, GLU 166, MET 49, MET 165
29	Jatrorrhizine	-8.14	GLU 166, LEU 141, LEU 167, MET 165, PHE 140, PRO 168
30	Palmatine	-8.07	GLU 166, LEU 141, MET 165, PRO168
31	Tetrandrine	-8.87	ASN 142, GLU 165, MET 49, MET 165,
32	Cepharanthine	-9.26	CYS 145, GLN 189, GLU 166, LEU 141, MET 49, MET 165
33	Quinine	-7.9	GLU 166, MET 165
34	Quinidine	-7.98	ARG 188, CYS 145, GLN 189, GLU 166, MET 49, MET 165
34	Quinidine	-8.35	GLU 166, PHE 140, PRO 168

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.6

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
35	Cinchonine	-8.32	ASN 142, GLU 166
36	Cinchonidine	-7.85	ASN 142, GLU 166, PRO 168
37	Emetine	-9.56	GLU 166, LEU 141, PRO 168
38	Dictamine	-6.74	MET 49, MET 165
39	Ellipticine	-7.05	ARG 188, MET 49, MET 165
40	Evolitrine	-7.11	GLU 166, MET 165, PRO 168
41	Fagarine	-7.08	CYS 145, GLY 143, LEU 165, MET 141
42	Skimmianine	-7.36	CYS 145, GLY 143
43	Cryptolepine	-7.25	GLU 166, LEU 167, MET 49, MET 165, PRO 168
44	Harmine	-6.79	GLU 166, MET 49, MET 165
45	Harmaline	-7.94	GLU 166, MET 165, PHE 140
46	Yohimbine	-8.04	CYS 145, MET 165, PRO 168
47	Scopolamine	-7.65	CYS 145, GLU 166, GLY 143, LEU 141, MET 165, SER 144, THR 26
48	Atropine	-8.2	GLU 166, MET 49, MET 165
49	Colchicine	-8.54	GLY 143, HSE 41, MET 49
50	Allantoin	-6.63	ASN 142
51	Trigonelline	-7	ASN 42, CYS 145, GLY 143, SER 144

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.6

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
52	Octopamine	-8.13	ASN 142, GLU 166, PRO 141
53	Synephrine	-7.82	ASN 142, GLU 166
54	Capsaicin	-8.33	CYS 145, GLY 143, LEU 165, MET 165, SER 144
55	Quinolizidine	-6.98	ASN 142, GLU 166, LEU 141
56	Cytisine	-6.92	GLU 166, LEU 167, MET 165
57	Tomatidine	-8.14	CYS 145, MET 49, MET 165
58	Theonelladin A	-9.29	ASN 142, GLU 166, LEU 141, MET 49, MET 165, PHE 140
59	Theonelladin C	-9.02	ARG 188, ASN 142, GLU 166, THR 190
60	Makaluvamine	-9.62	GLU 166, MET 49, PHE 140
61	Neoamphimedine	-7.62	CYS 145, GLY 143, MET 49, MET 165, SER 144
62	Granulatimide	-7.28	ARG 188, GLU 166, LEU 167, MET 165, PRO 168, THR 190
63	Isogranulatimide	-6.87	ARG 188, MET 49, MET 165, PRO 168, THR 190
64	Rigidin	-7.89	ARG 188, CYS 145, GLU 166, GLY 143, MET 49, MET 165, THR 190
65	Coscinamide	-8.5	GLY 143, HSE 41, MET 49, MET 165
66	Asterriquinone	-8.2	ASN 142, GLY 143, MET 49, MET 165, THR 26
67	Dragmacidin	-7.81	ALA 191, CYS 145, GLU 166, HSE 41, LEU 167, MET 165, PRO 168, THR 190
68	Topsentin	-7.52	CYS 145, MET 49, MET 165, THR 190

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.6

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
69	Nortopsentin	-7.8	ARG 188, CYS 145, HSE 41, MET 49, MET 165, PRO 168
70	Dispacamide	-8.57	ASN 142, CYS 145, GLY 143, HSE 41, LEU 141, MET 49, MET 165, SER 144
71	Polyandrocarpamine	-7.3	CYS 145, GLU 166, GLY 143, LEU 141, MET 165, PHE 140
72	Leucettamine	-7.61	GLU 166, MET 165, PHE 140
73	β -Carboline	-7.08	GLU 166, MET 49, MET 165
74	camptothecin	-7.55	GLY 143, HSE 41, MET 165, PRO 168
75	vinblastine	-9.29	GLN 189, GLU 166

LAMPIRAN 10

ENERGI BEBAS DAN RESIDU ASAM AMINO

Tabel VII.7

Residu asam amino simulasi *molecular docking* senyawa Alkaloid terhadap reseptor *Main Protease* ID 5R7Y

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
1	N-(2-phenylethyl) methanesulfonamide	-6.91	GLN 189, GLU 166, LEU 167, MET 165, THR 190
2	Lovinapir	-9.76	CYS 44, GLU 166, HSE 41, LEU 167, MET 49, MET 165, PRO 168
3	Remdesivir	-9.61	CYS 44, GLU 166, MET 49, PRO 168, SER 46, THR 46
4	10 -Hydroxyusambarensine	-7.84	CYS 44, GLU 166, MET 49, THR 25
5	Cryptospirolepine	-7.87	MET 49, MET 165
6	Chrysopentamine	-9.2	CYS 145, GLU 166, MET 49, SER 46
7	Isocryptolepine	-6.9	ASN 142, GLU 166, MET 165
8	Jozipeltine A	-8.97	ARG 188, ASN 142, CLA 6, CYS 44, GLN 189, GLU 166, PRO 168, THR 26, THR 190
9	Normelicopicine	-7.58	GLU 166, THR 190
10	Isostrychnopentamine	-8.55	CLA 6, CYS 145, GLU 166, LEU 141, MET 49, MET 165, THR 25
11	Strychnopentamine	-8.54	GLU 166, MET 49, MET 165, THR 25, THR 26
12	Liriodenine	-7.13	GLU 166, LEU 167, MET 165, PRO 168, THR 190
13	Dioncopeltine A	-9.05	ASN 142, CYS 44, GLU 166, HSE 41, MET 49
14	Dihydronitidine	-7.62	ARG 188, GLU 166, MET 165, PRO 168
15	Hydroxycryptolepine	-6.99	GLU 166, ME 165
16	Cryptoheptine	-7.34	ASN 142, GLU 166, MET 49, MET 165
17	Annonidine A	-8.03	CYS 145, MET 49, MET 165

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.7

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
18	Ancistrotanzanine C	-8.95	CLA 6, GLN 189, GLU 166, MET 49, MET 165, THR 25
19	Fagaronine	-8.6	GLU 166, MET 165, PRO 168
20	Alstonine	-7.82	GLN 189, MET 49, MET 165
21	Sanguinarine	-8.5	GLU 166, MET 165, PRO 168
22	Chelerythrine	-8.78	CLA 6, GLU 166, MET 49, SER 46
23	Chelidone	-7.77	GLU 166, PRO 168
24	Berberine	-8.67	ARG 188, CYS 145, MET 49
25	Berbamine	-9.95	CLA 6, GLU 166, MET 165, PRO 169, SER 46
26	Berberrubine	-8.4	CYS 44, CYS 145, SER 46
27	Coptisine	-8.3	CYS 145, GLU 166, MET 165, PHE 140
28	Dicentrine	-7.64	GLU 166
29	Jatrorrhizine	-8.57	GLU 166, LEU 141, PHE 140, PRO 168, THR 190
30	Palmatine	-8.74	ARG 188, CYS 145, GLU 166, MET 49
31	Tetrandrine	-10.09	ARG 188, CYS 44, CYS 145, CLA 6, GLU 166, SER 46
32	Cepharanthine	-9.5	CLA 6, GLU 166, MET 49, SER 46
33	Quinine	-9.14	ARG 188, CLA 6, GLU 166, HSE 41, MET 165

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.7

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
34	Quinidine	-8.98	CLA 6, HSE 44, LEU 141
35	Cinchonine	-8.88	CLA 6, CYS 145, HSE 41, GLU 166, MET 165
36	Cinchonidine	-8.78	CLA 6, GLU 166, HSE 164, MET 165
37	Emetine	-10.49	ASN 142, CLA 6, GLU 166, MET 165, SER 46, THR 24
38	Dictamine	-6.75	CYS 145, HSE 41, GLU 166, MET 165
39	Ellipticine	-6.79	ASN 142, CYS 145, GLU 166, MET 165
40	Evolitrine	-7.28	ARG 188, CYS 145, GLU 166, LEU 141, MET 49, MET 165
41	Fagarine	-7.24	CYS 145, GLU 166, MET 49, MET 165
42	Skimmianine	-7.27	ARG 188, CYS 145, GLU 166, LEU 141, MET 165
43	Cryptolepine	-7.23	ASN 142, GLU 165, MET 49, MET 165
44	Harmine	-6.86	GLU 166, LEU 141, MET 49, MET 165
45	Harmaline	-8.56	ASN 142, GLU 166, LEU 141, MET 165, PHE 140
46	Yohimbine	-8.8	CLA 6, GLU 166, MET 49, SER 46, THR 25
47	Scopolamine	-7.73	HSE 164, SER 46, MET 49
48	Atropine	-8.67	CLA 6, GLU 166, HSE 164, MET 165, PRO 168, THR 190
49	Colchicine	-8.37	CYS 44, GLU 166, HSE 41, MET 49

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.7

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
50	Allantoin	-6.8	ASN 142, PHE 140
51	Trigonelline	-7.03	ASN 142, LEU 141, PHE 140
52	Octopamine	-8.11	ASN 142, GLU 166, LEU 141, PHE 140
53	Synephrine	-7.85	ASN 142, CLA 6, MET 165
54	Capsaicin	-8.17	CYS 145, HSE 41, GLN 189, GLU 166, THR 190
55	Quinolizidine	-7.68	ASN 142, GLU 166, LEU 141, PHE 140
56	Cytisine	-7.87	ASN 142, CLA 6, MET 49
57	Tomatidine	-7.98	ARG 188, CYS 145, MET 49, THR 24
58	Theonelladin A	-9.83	ASN 142, GLU 166, LEU 141, PHE 140, PRO 168
59	Theonelladin C	-9.6	GLN 189, GLI 166, LEU 167, PRO 168, THR 190
60	Makaluvamine	-10.75	GLU 166, PHE 140, PRO 168
61	Neoamphimedine	-7.85	ARG 188, GLN 189, GLU 166, PRO 168, THR 190
62	Granulatimide	-7.13	ARG 188, GLN 189, GLU 166, MET 165, PRO
63	Isogranulatimide	-6.76	GLN189, GLU 166, MET 49, MET 165, PRO 168, THR 190
64	Rigidin	-7.42	ARG 188, CYS 145, GLU 166, MET 165
65	Coscinamide	-8.11	GLU 166, HSE 41, LEU 167, MET 49, PRO 168, THR 190

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.7

Lanjutan

NO	Nama Senyawa	(ΔG)	Residu Asam Amino
66	Asterriquinone	-8.14	CYS 145, GLU 166, MET 49, MET 165, PRO 168
67	Dragmacidin	-8.8	CLA 6, CYS 44, MET 165, PRO 168, SER 46, THR 45
68	Topsentin	-7.62	CYS 145, GLU 166, MET 165, PRO 168, THR 190
69	Nortopsentin	-7.69	ARG 188, CYS 145, GLU 166, LEU 167, MET 165, PRO 168
70	Dispacamide	-8.23	ARG 188, ASN 142, GLN 189, GLU 142, MET 165, PHE 140, PRO 168
71	Polyandrocarpamine	-7.22	ASN 142, GLU 166, MET 165, PHE 140
72	Leucettamine	-7.68	ARG 188, CYS 145, GLU 166, MET 165, PHE, 140
73	β -Carboline	-7.07	CYS 145, GLU 166, MET 49
74	camptothecin	-7.45	GLA 6, GLU 166, MET 49
75	vinblastine	-9.23	GLU 166

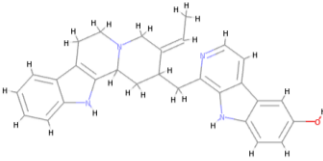
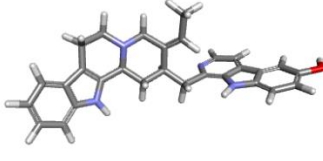
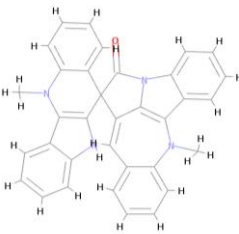
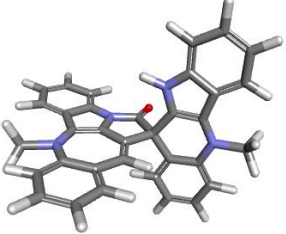
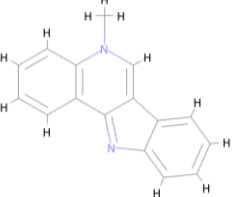
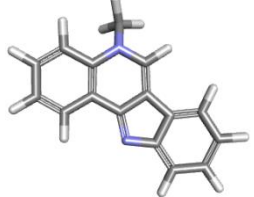
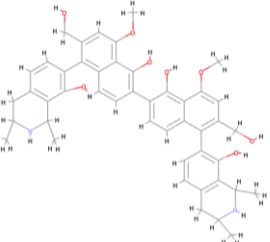
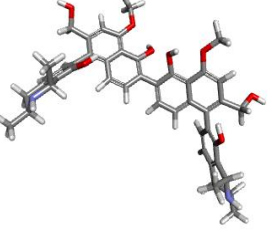
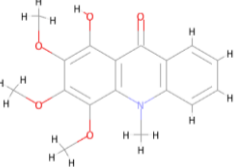

LAMPIRAN 11

STRUKTUR 2 DIMENSI DAN 3 DIMENSI

SENYAWA ALKALOID

Tabel VII.8

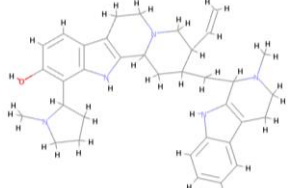
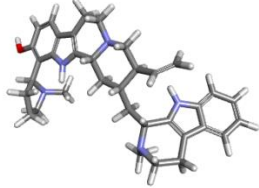
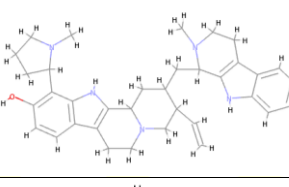
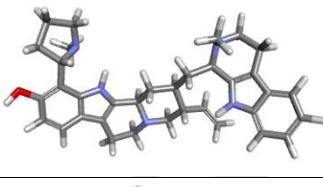
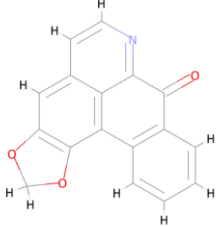
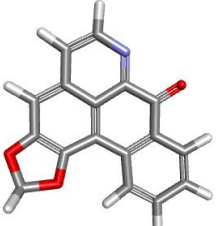
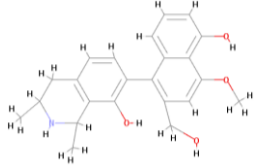
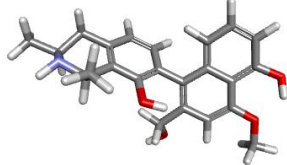
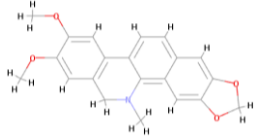
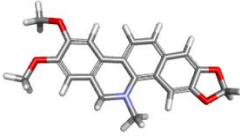
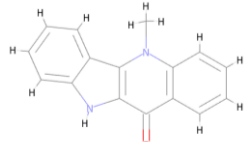
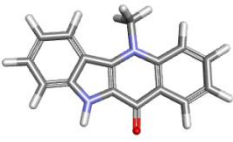
Struktur 2 Dimensi dan 3 Dimensi Alkaloid

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
10-Hydroxyusambarensine		
Cryptospirolepine		
Isocryptolepine		
Jozipeltine A		
Normelicopicine		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

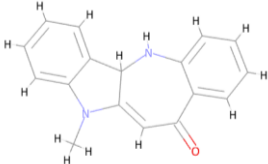

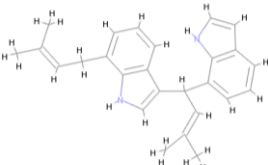
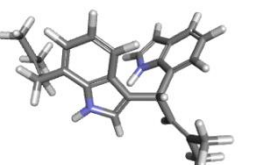
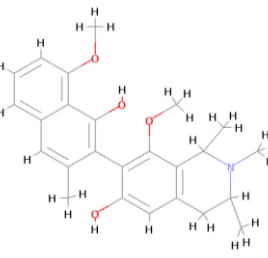
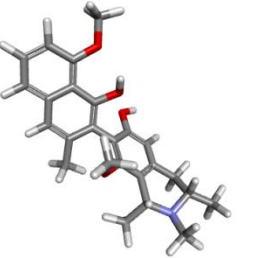
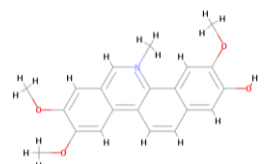
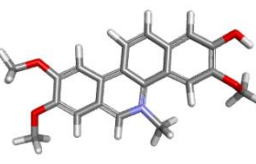
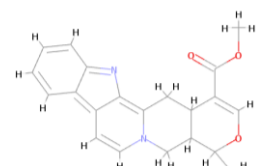
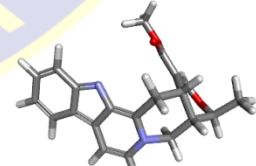
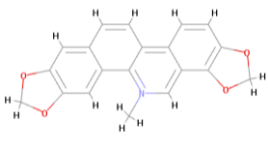
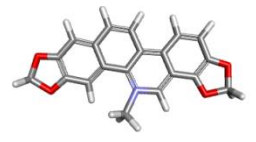
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Isostrychnopentamine		
Strychnopentamine		
Liriodenine		
Dioncopeltine A		
Dihydroneitidine		
Hydroxycryptolepine		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

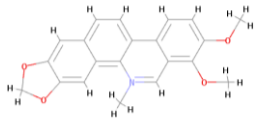
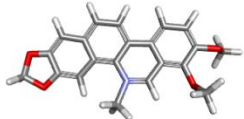
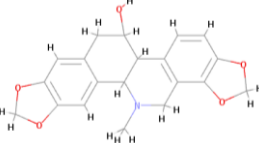

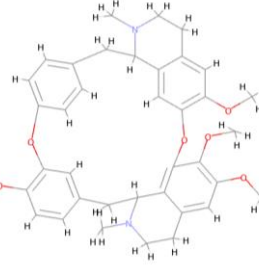
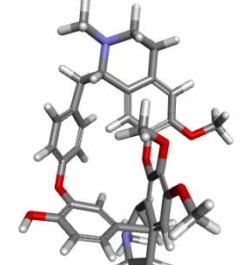
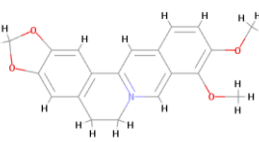
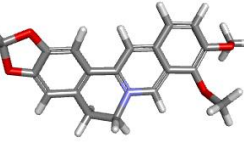
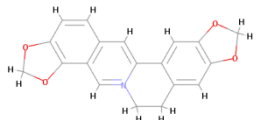
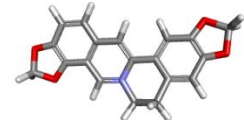
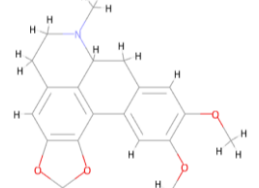

Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Cryptoheptine		
Annonidine A		
Ancistrotanzanine C		
Fagaronine		
Alstonine		
Sanguinarine		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

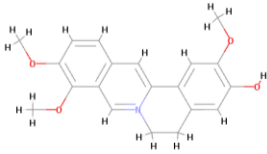

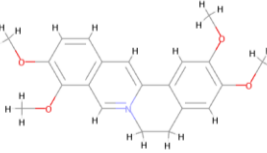
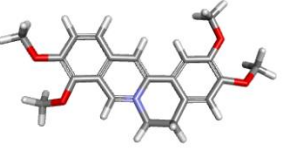
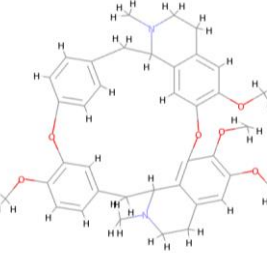
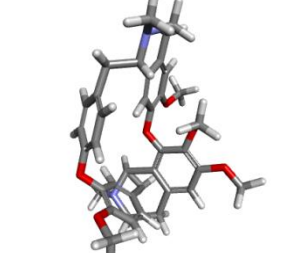
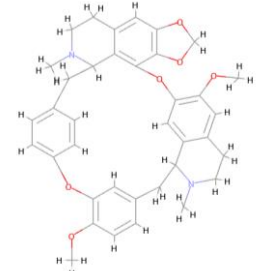
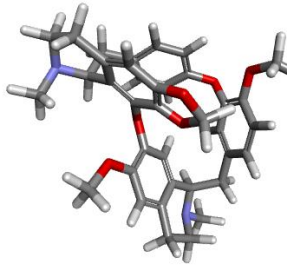
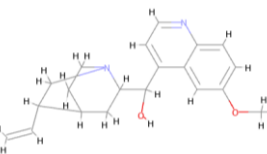
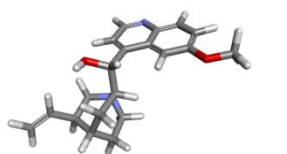
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Chelerythrine		
Chelidoniumine		
Berbamine		
Berberrubine		
Coptisine		
Dicentrine		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

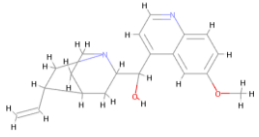
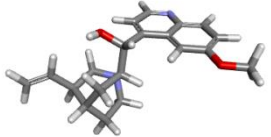
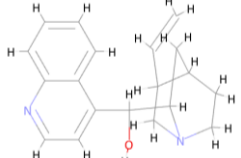
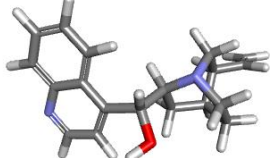
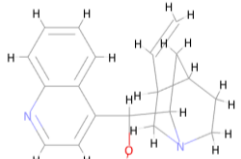
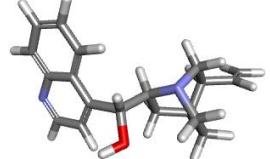
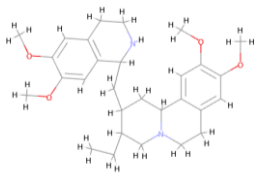
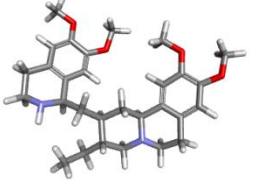
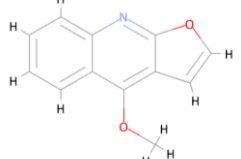
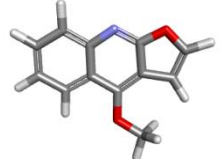
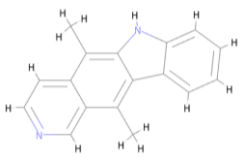
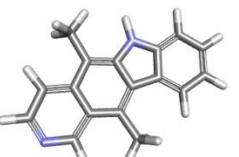
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Jatrorrhizine		
Palmatine		
Tetrandrine		
Cepharanthine		
Quinine		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

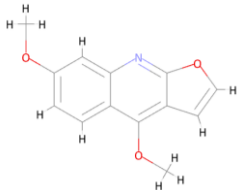
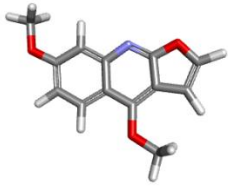
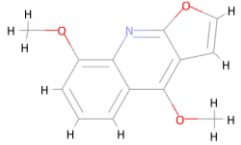
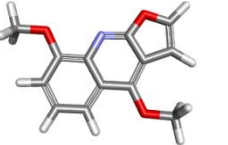
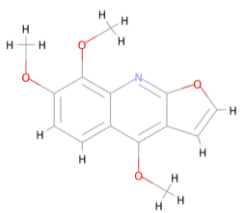
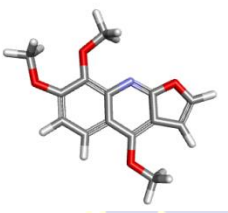
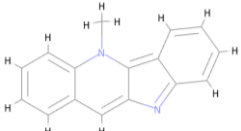
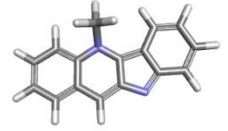
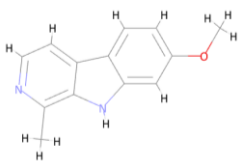
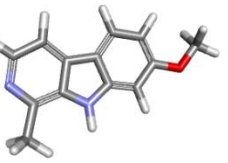
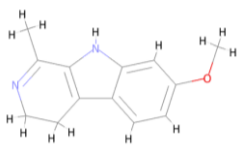
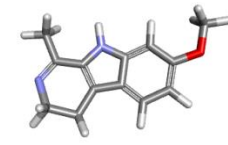
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Quinidine		
Cinchonine		
Cinchonidine		
Emetine		
Dictamine		
Ellipticine		

LAMPIRAN 11 (LANJUTAN)

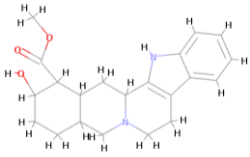
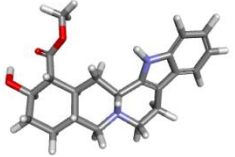
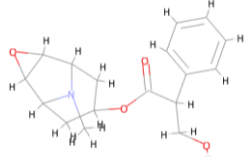
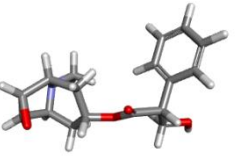
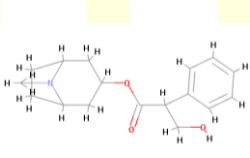
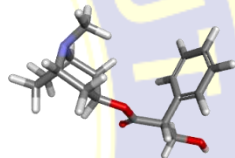
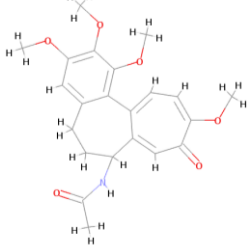
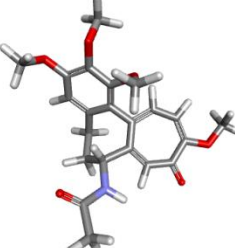
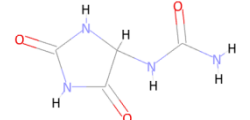
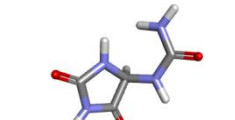
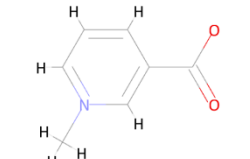
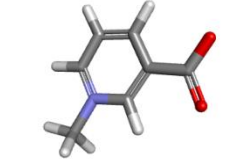
Tabel VII.8

Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Evolitrine		
Fagarine		
Skimmianine		
Cryptolepine		
Harmine		
Harmaline		

**LAMPIRAN 11
(LANJUTAN)****Tabel VII.8**

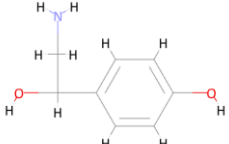
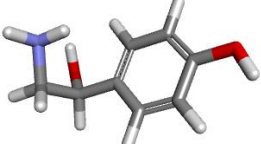
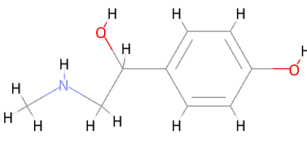
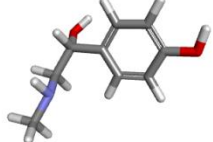
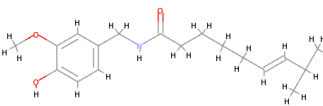
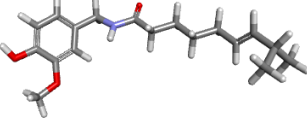
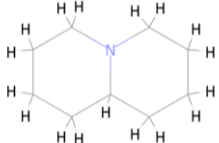
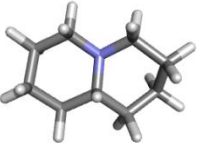
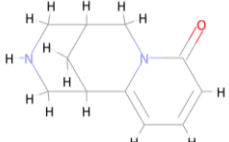

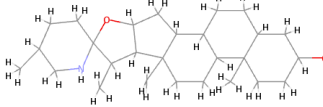

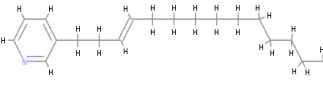
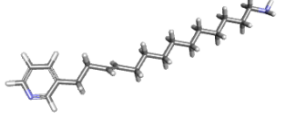
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Yohimbine	 The 2D structure of Yohimbine shows a complex polycyclic system. It features a hexahydroindole ring system fused to a pyridine ring, which is further fused to a benzene ring. A quaternary nitrogen atom is present in the hexahydroindole part, and a hydroxyl group is attached to the benzene ring.	 The 3D ball-and-stick model of Yohimbine illustrates the spatial arrangement of atoms. Carbon atoms are shown in grey, hydrogen in white, nitrogen in blue, and oxygen in red. The model highlights the three-dimensional conformation of the fused ring system.
Scopolamine	 The 2D structure of Scopolamine consists of a tropane bicyclic core (8-azabicyclo[3.2.1]octane) with an ester linkage to a tropane ring. The tropane ring has a methyl group and a hydroxyl group attached.	 The 3D ball-and-stick model of Scopolamine shows the tropane bicyclic core and the tropane ring in a perspective view, with atoms colored by element (C: grey, H: white, N: blue, O: red).
Atropine	 The 2D structure of Atropine is similar to scopolamine, featuring a tropane bicyclic core with an ester linkage to a tropane ring. The tropane ring has a methyl group and a hydroxyl group attached.	 The 3D ball-and-stick model of Atropine shows the tropane bicyclic core and the tropane ring in a perspective view, with atoms colored by element (C: grey, H: white, N: blue, O: red).
Colchicine	 The 2D structure of Colchicine is a complex polycyclic alkaloid. It features a tropane bicyclic core with a tropane ring, which is further fused to a benzene ring. The tropane ring has a methyl group and a hydroxyl group attached.	 The 3D ball-and-stick model of Colchicine shows the tropane bicyclic core and the tropane ring in a perspective view, with atoms colored by element (C: grey, H: white, N: blue, O: red).
Allantoin	 The 2D structure of Allantoin is a simple five-membered ring containing two nitrogen atoms and two carbonyl groups. It is a cyclic urea derivative.	 The 3D ball-and-stick model of Allantoin shows the five-membered ring structure in a perspective view, with atoms colored by element (C: grey, H: white, N: blue, O: red).
Trigonelline	 The 2D structure of Trigonelline is a pyridine ring with a methyl group and a carboxylate group attached to the nitrogen atom.	 The 3D ball-and-stick model of Trigonelline shows the pyridine ring and the methyl and carboxylate groups in a perspective view, with atoms colored by element (C: grey, H: white, N: blue, O: red).

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

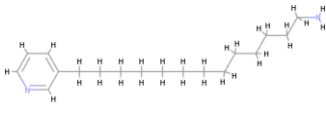
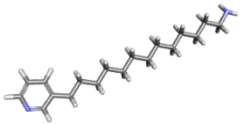
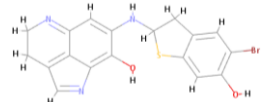
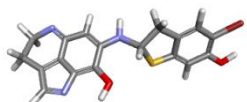
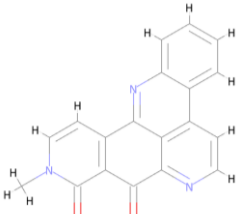

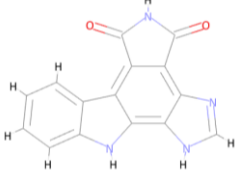
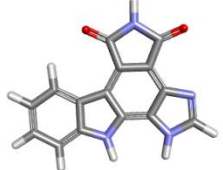
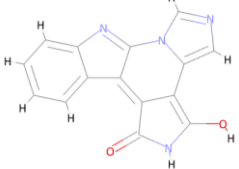
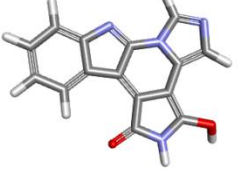
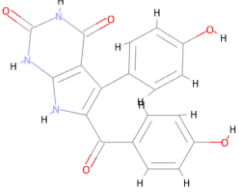

Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Octopamine		
Synephrine		
Capsaicin		
Quinolizidine		
Cytisine		
Tomatidine		
Theonelladin A		

LAMPIRAN 11 (LANJUTAN)

Tabel VII.8

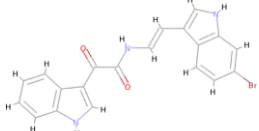
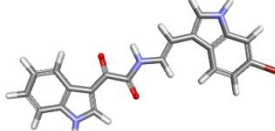
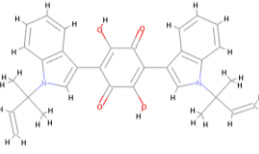
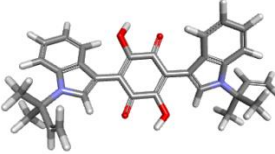
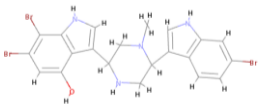
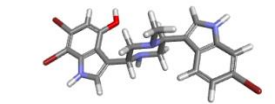
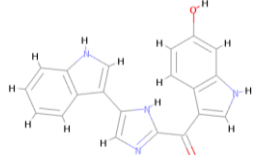

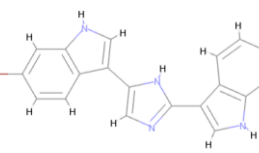
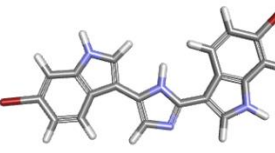
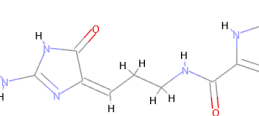

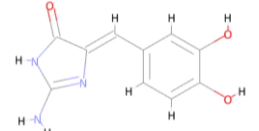
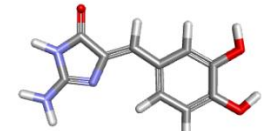
Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Theonelladin C		
Makaluvamine		
Neoamphimedine		
Granulatimide		
Isogranulatimide		
Rigidin		

LAMPIRAN 11 (LANJUTAN)

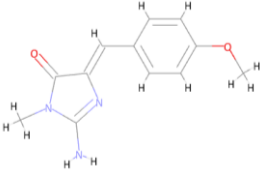
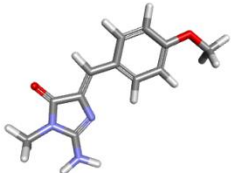
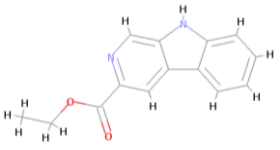
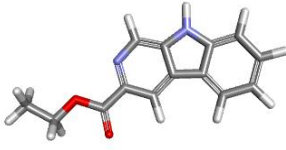
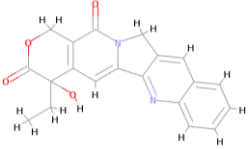
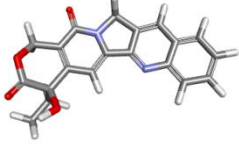
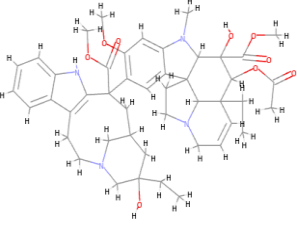
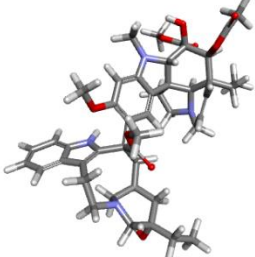
Tabel VII.8

Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Coscinamide		
Asterriquinone		
Dragmacidin		
Topsentin		
Nortopsentin		
Dispacamide		
Polyandrocarpamine		

**LAMPIRAN 11
(LANJUTAN)****Tabel VII.8**

Lanjutan

SENYAWA	STRUKTUR 2D	STRUKTUR 3D
Leucettamine	 <chem>Cc1ccc(cc1)C(=O)Nc2c[nH]c2</chem>	
β-Carboline	 <chem>Cc1ccc2c(c1)c[nH]2C(=O)O</chem>	
camptothecin	 <chem>Cc1c2c(c3c1O)c[nH]3C(=O)O2</chem>	
vinblastine	 <chem>Cc1c2c3c4c1c[nH]4C(=O)O3C(=O)O2</chem>	

DAFTAR RIWAYAT HIDUP

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 - LDK ASY - SYIFA FMIPQ UNIGA 2018 – 2019
- **Prestasi**
 - ON MIPA BIOLOGI 2019 Tingkat Provinsi
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 - PKL PT. Berkah Alam Nusantara, Garut
 - PKL Apotek Assyifa, Garut
 - Pelatihan Kimia *Atomic Absorption Spectrophotometer* (AAS) dan *Fourier Transform Infra Red* (FTIR) -2019

- Pertemuan Ilmiah PDPOTJI "*Integration of Traditional Medicine Into Evidence-Based Clinical Practice*" – 2020
- Pelatihan Series 3# HMF ITB "Pelatihan Kimia Komputasi (*Moleckular Docking*)" – 2021
- Virtual Workshop "Design of Experiments: How to Deal With 2-Level Factorial Design" – 2021

SMAN 22 Garut (2014-2017)

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 - OSIS SMAN 22 GARUT
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