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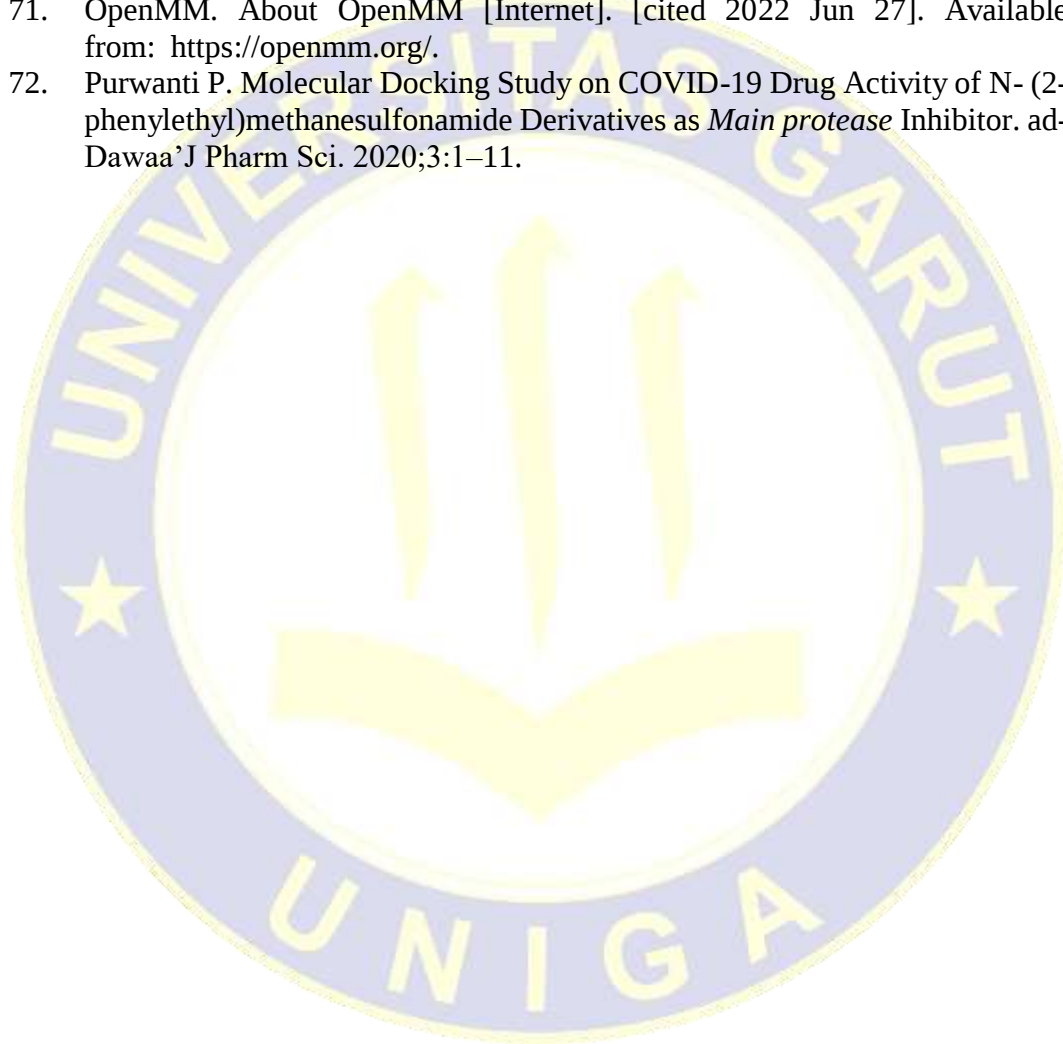
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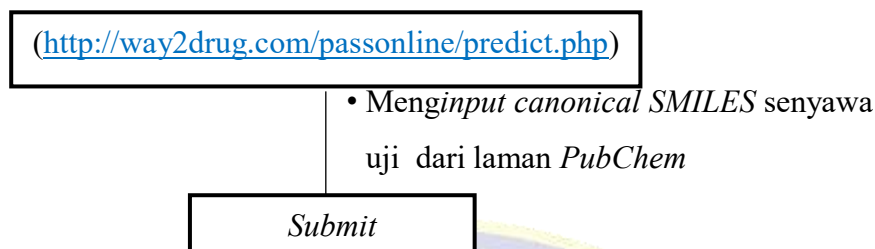
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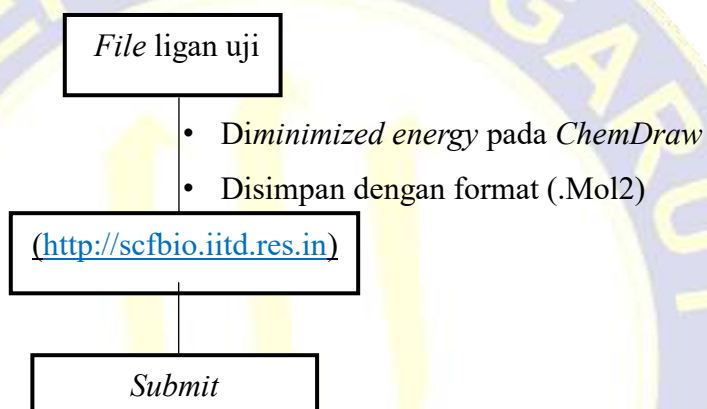


LAMPIRAN 1

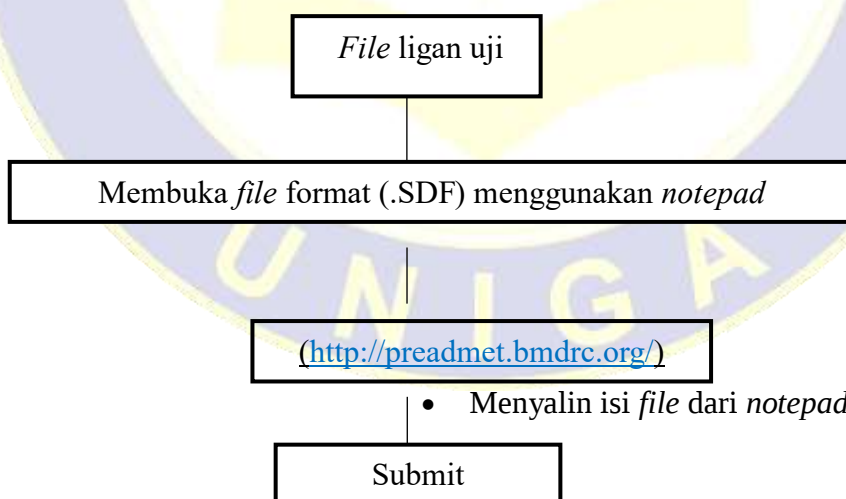
PREDIKSI AKTIVITAS ANTIVIRUS, *DRUGLIKENESS* DAN ADMET



Gambar VII. 1 Skema alur prediksi aktivitas antivirus



Gambar VII. 2 Skema alur prediksi *Druglikeness*



Gambar VII. 3 Skema alur prediksi ADMET

LAMPIRAN 2

PREDIKSI JALUR BIOSINTESIS

[\(https://chemairs.chemicalai.cn/#/\)](https://chemairs.chemicalai.cn/#/)

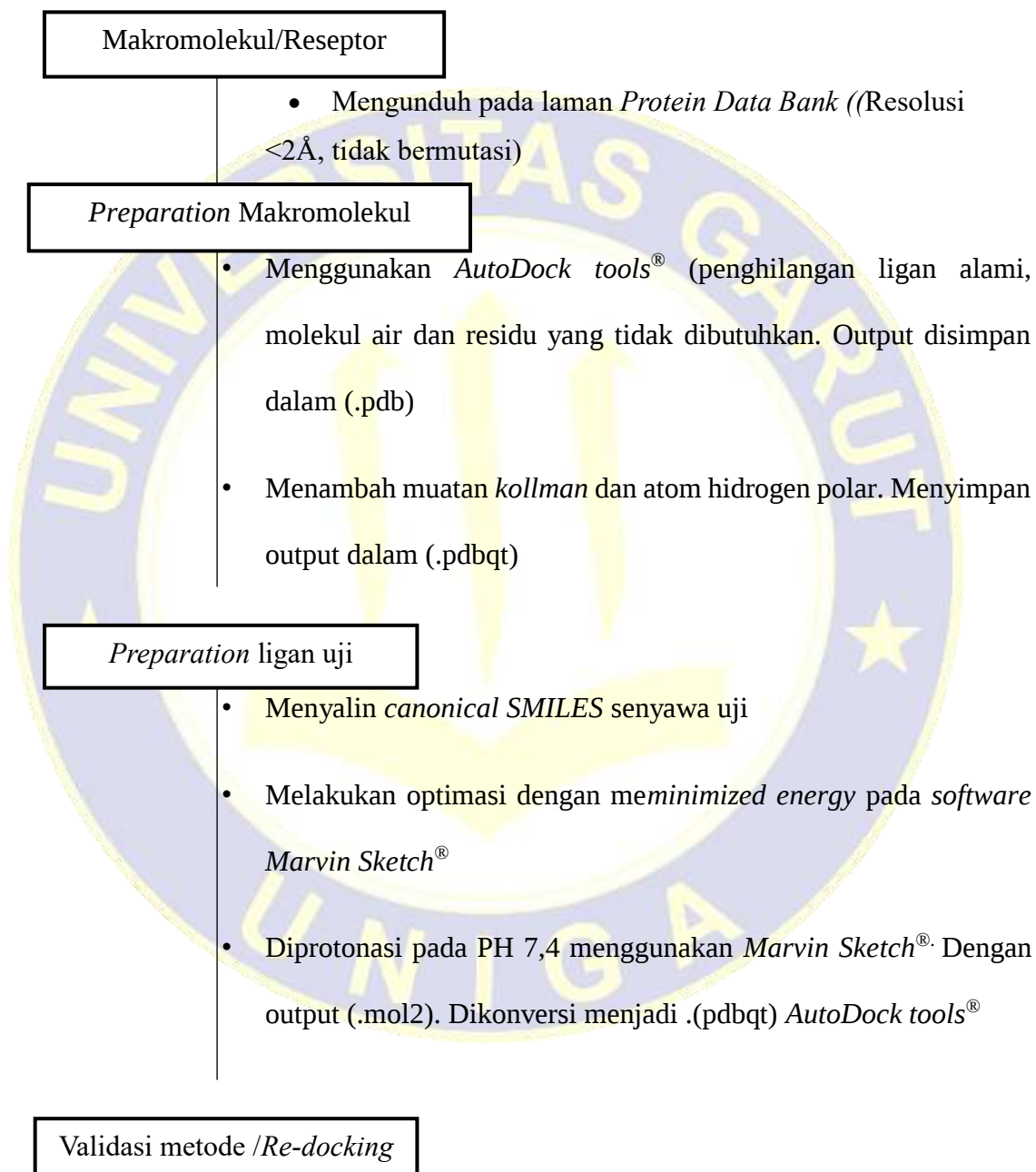
- Menginput *canonical SMILES* senyawa uji dari laman *PubChem*
- Pengaturan parameter pencarian (angka maksimum rute, waktu, kedalaman, level resiko dan estimasi harga material)
- Rute yang dipilih ialah rute yang paling mudah dengan biaya material paling rendah.

Submit

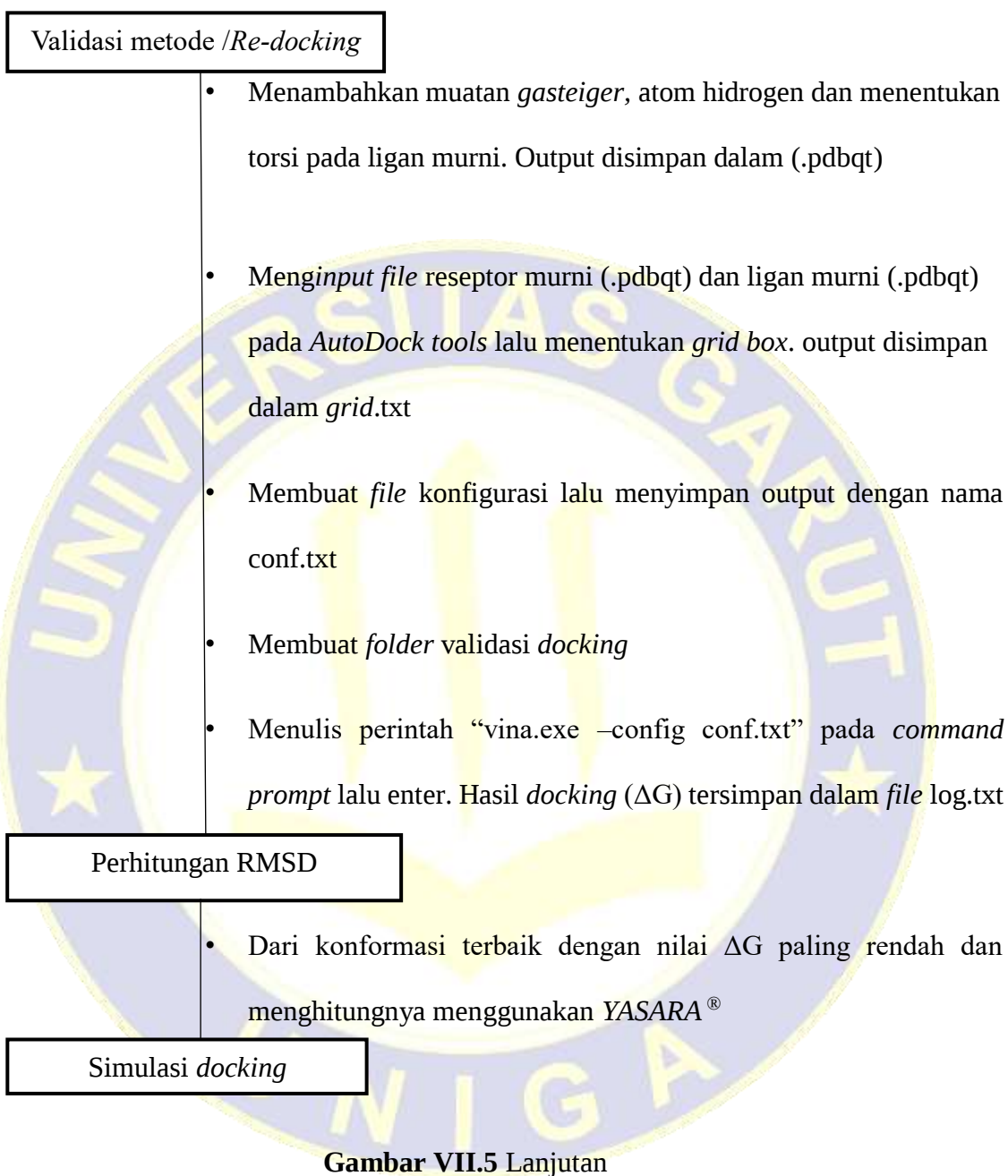
Gambar VII. 4 Skema alur prediksi biosintesis

LAMPIRAN 3

ALUR PENELITIAN SIMULASI MOLECULAR DOCKING

Gambar VII. 5 Skema alur molecular docking senyawa aktif *Gycyrrhiza glabra*

LAMPIRAN 3 (LANJUTAN)



LAMPIRAN 3 (LANJUTAN)

Simulasi *docking*

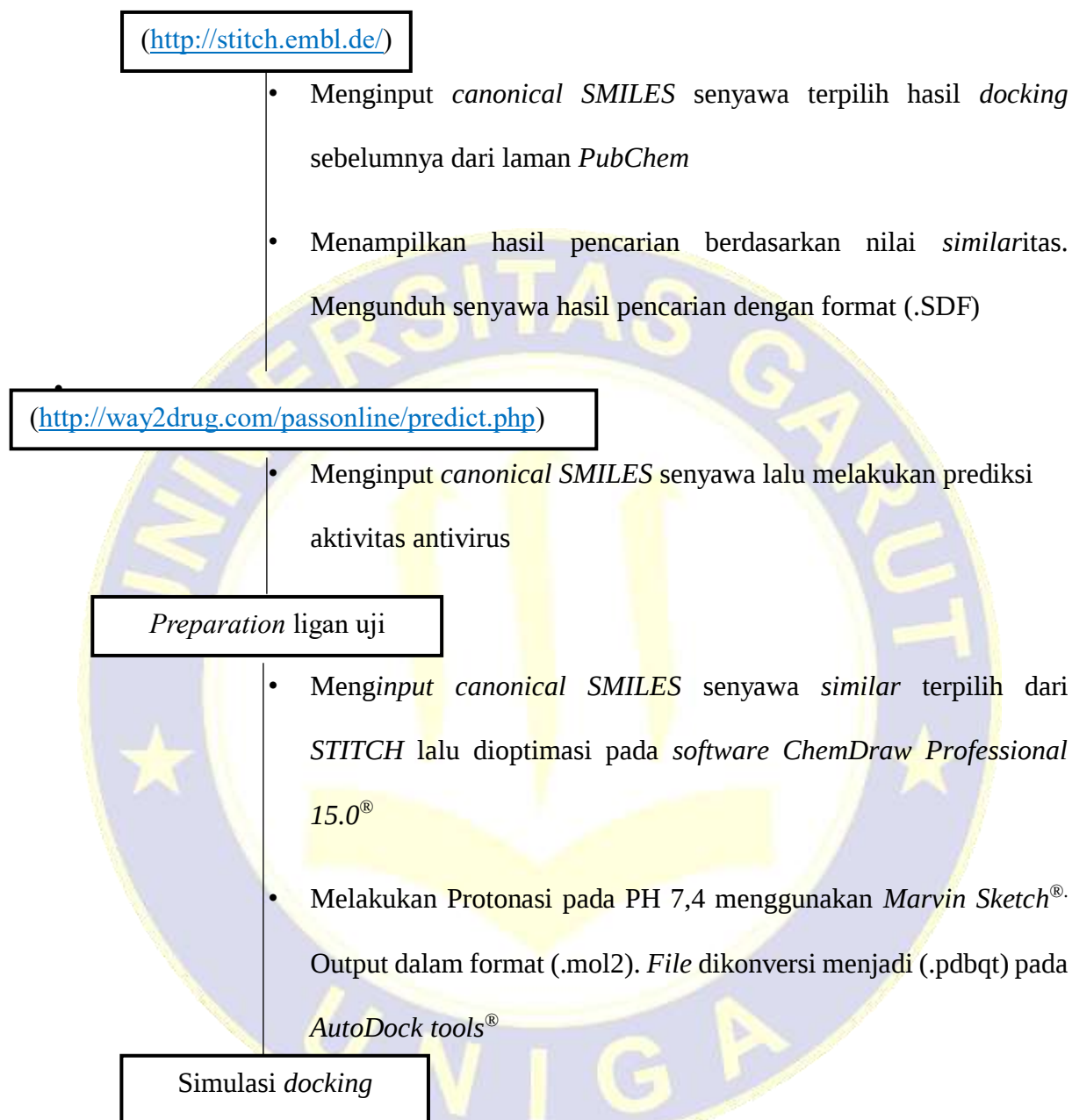
- Menggunakan *AutoDock Vina*®. Pertama membuat *folder* khusus untuk *docking* senyawa uji
- *me-running*

Analisa Hasil

- Hasil *docking* tersimpan pada *file* log.txt yang memuat nilai (ΔG) dianalisis interaksi molekul, dan residu asam amino menggunakan *Discovery Studio Visualizer*®

Gambar VII.5 Lanjutan

LAMPIRAN 4

ALUR PENELITIAN SIMULASI *MOLECULAR DOCKING* SENYAWA *SIMILAR*Gambar VII. 6 Skema alur *molecular docking* senyawa *similar*

LAMPIRAN 4 (LANJUTAN)

Simulasi *docking*

- Menggunakan *AutoDock Vina*®
- Membuat *folder* khusus untuk *docking* senyawa uji
- Menulis perintah “perl Vina_windows.pl” pada *command prompt* lalu enter kemudian “Ligan.txt” dan muncul tampilan sistem sudah mulai me-running

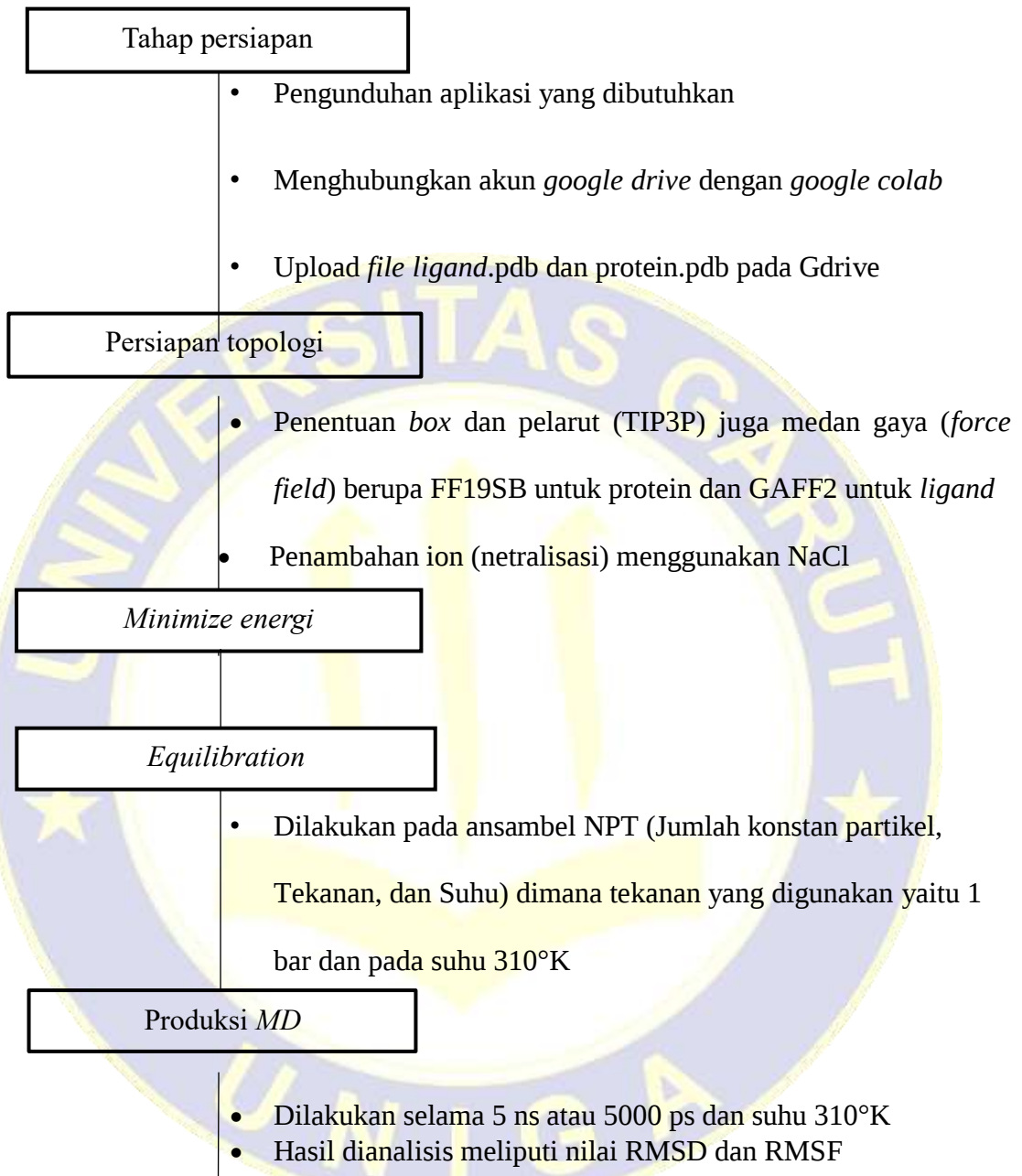
Analisa Hasil

- Hasil *docking* tersimpan otomatis pada *file log.txt* yang memuat nilai ΔG lalu dianalisis interaksi molekul, dan residu asam amino menggunakan *Discovery Studio Visualizer*®

Gambar VII.6 Lanjutan

LAMPIRAN 5

ALUR PENELITIAN SIMULASI DINAMIKA MOLEKULER (MD)



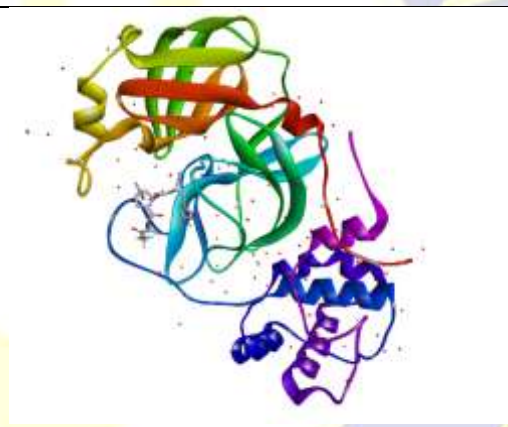
Gambar VII. 7 Skema alur dinamika molekuler (MD)

LAMPIRAN 6

STRUKTUR TIGA DIMENSI RESEPTOR

Tabel VII 1

Struktur 3D Komplek Reseptor *Ligand Main Protease*

PDB ID	Struktur Reseptor
7RN4	
7SI9	

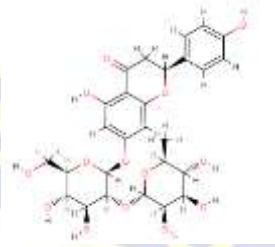
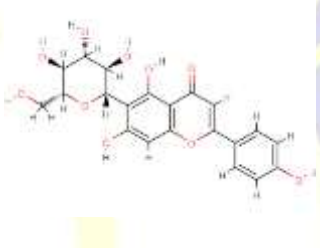
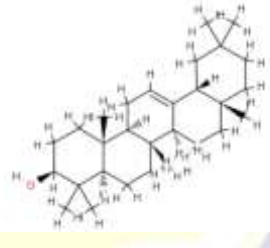
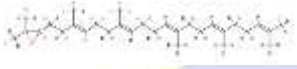
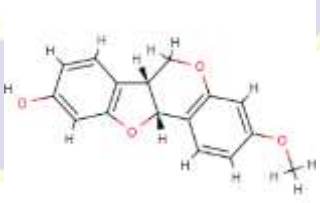
**LAMPIRAN 6
(LANJUTAN)****Tabel VII. 1**
Lanjutan

PDB ID	Struktur Reseptor
7DPU	
7NG6	

LAMPIRAN 7
STRUKTUR DUA DIMENSI SENYAWA UJI

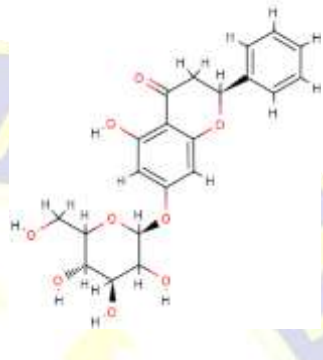
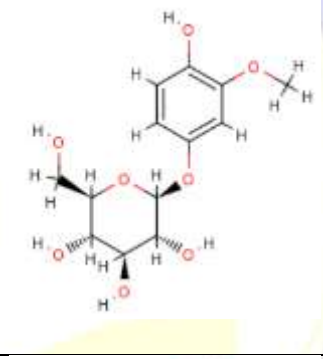
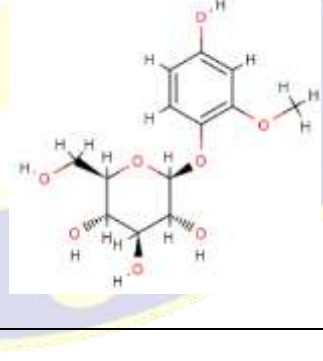
Tabel VII 2

Rumus Molekul dan Struktur 2D Senyawa Aktif Tanaman *Glycyrrhiza glabra*

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
1	Naringin	<u>C₂₇H₃₂O₁₄</u>	
2	Isovestin	<u>C₂₁H₂₀O₁₀</u>	
3	beta-Amyrin	<u>C₃₀H₅₀O</u>	
4	(S)-2,3-Epoxy-squalene	<u>C₃₀H₅₀O</u>	
5	Isomedicarpin	<u>C₁₆H₁₄O₄</u>	

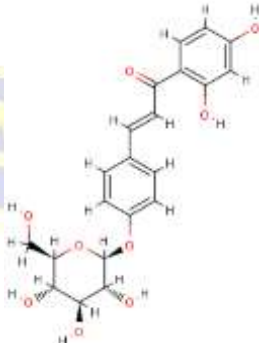
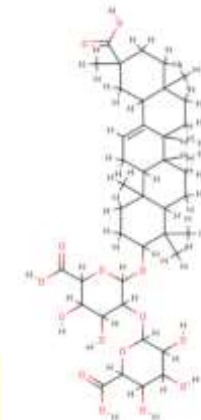
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
6	Pinocembroside	C₂₁H₂₂O₉	
7	Tachioside	C₁₃H₁₈O₈	
8	Isotachioside	C₁₃H₁₈O₈	

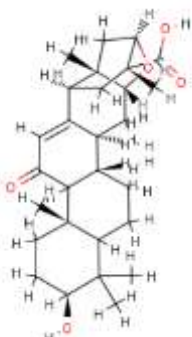
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
9	Isoliquiritin	$C_{21}H_{22}O_9$	
10	Licoricesaponin B2	$C_{42}H_{64}O_{15}$	
11	Licoricesaponin E2	$C_{42}H_{60}O_{16}$	

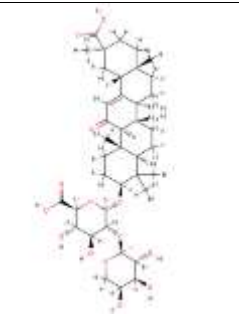
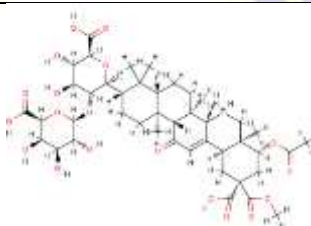
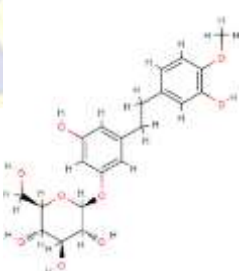
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
12	Licoricesaponin J2	C₄₂H₆₄O₁₆	
13	Liquiritic acid	C₃₀H₄₆O₄	
14	Liquoric acid	C₃₀H₄₄O₅	

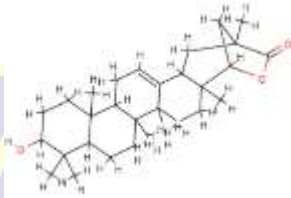
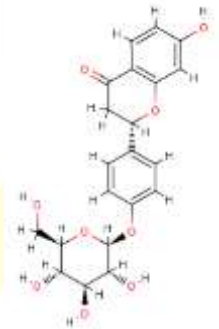
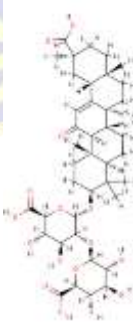
**LAMPIRAN 7
(LANJUTAN)**

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
15	Araboglycyrrhizin	<u>C₄₁H₆₂O₁₄</u>	
16	Uralsaponin M	<u>C₄₅H₆₄O₁₉</u>	
17	Anaphalisoleanenic acid	<u>C₃₀H₄₈O₃</u>	
18	alpha,beta-Dihydorhaponticin	<u>C₂₁H₂₆O₉</u>	

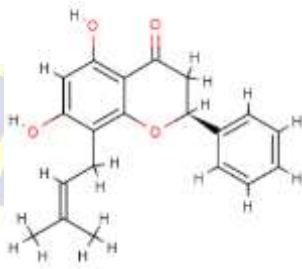
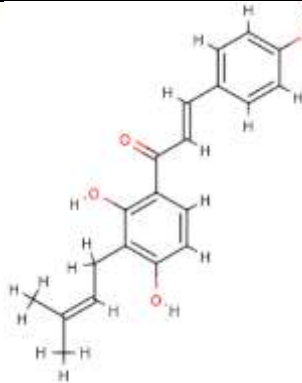
**LAMPIRAN 7
(LANJUTAN)**

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
19	Desoxoglabrolide	<u>C₃₀H₄₆O₃</u>	
20	Glycyrrhetic acid	<u>C₃₀H₄₆O₄</u>	
21	Liquiritin	<u>C₂₁H₂₂O₉</u>	
22	Glycyrrhizin	<u>C₄₂H₆₂O₁₆</u>	

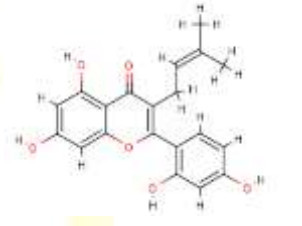
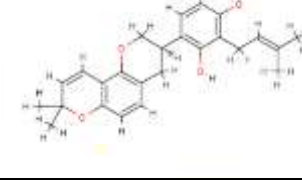
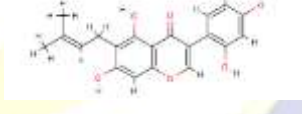
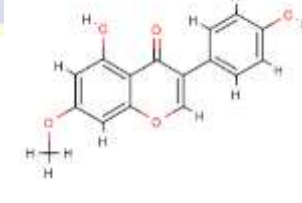
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
23	Glabranin	C₂₀H₂₀O₄	
24	Isobavachalcone	C₂₀H₂₀O₄	
25	Dihydrochrysin	C₁₅H₁₂O₄	
26	Genkwanin	C₁₆H₁₂O₅	

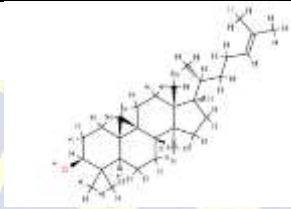
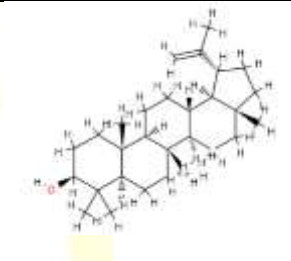
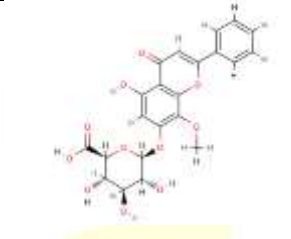
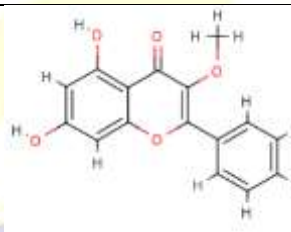
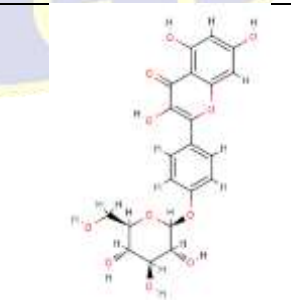
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
27	Kaempferol 3-O-methyl ether	C₁₆H₁₂O₆	
28	Albanin A	C₂₀H₁₈O₆	
29	Hispaglabridin A	C₂₅H₂₈O₄	
30	Luteone	C₂₀H₁₈O₆	
31	(-)-Phaseollinisoflavan	C₂₀H₂₀O₄	
32	Prunetin	C₁₆H₁₂O₅	

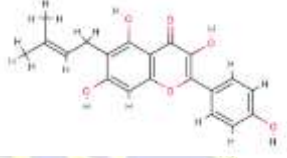
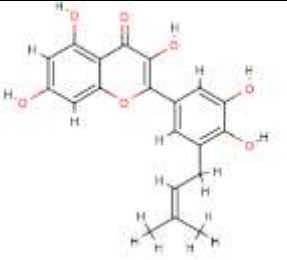
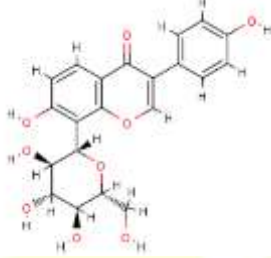
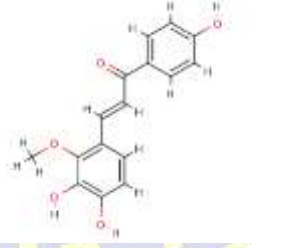
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
33	Cycloartenol	$C_{30}H_{50}O$	
34	Lupeol	$C_{30}H_{50}O$	
35	Wogonoside	$C_{22}H_{20}O_{11}$	
36	Galangin	$C_{16}H_{12}O_5$	
37	Kaempferol	$C_{21}H_{20}O_{11}$	

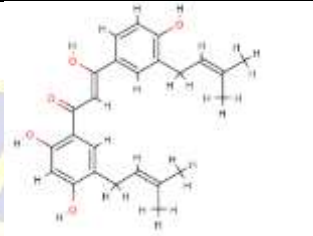
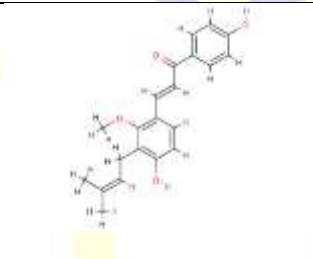
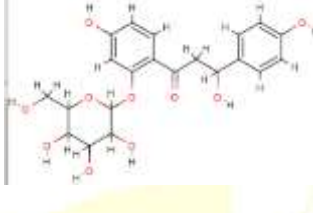
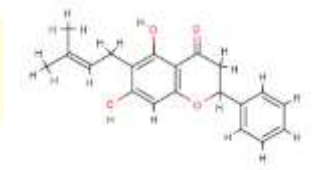
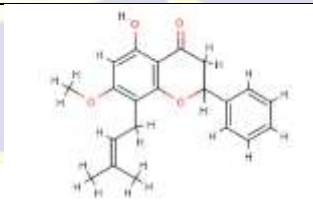
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
38	Licoflavonol	<u>C₂₀H₁₈O₆</u>	
39	Uralenol	<u>C₂₀H₁₈O₇</u>	
40	Puerarin	<u>C₂₁H₂₀O₉</u>	
41	Licochalcone B	<u>C₁₆H₁₄O₅</u>	
42	Glyinflanin B	<u>C₂₀H₁₈O₅</u>	

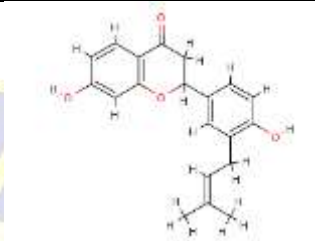
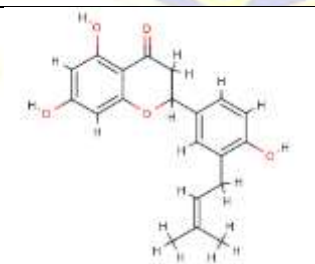
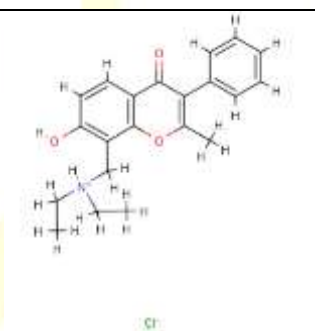
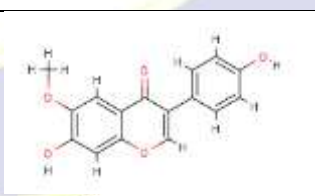
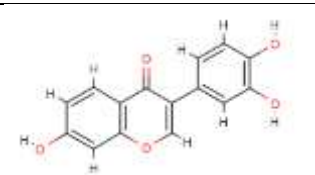
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
43	Glyinflanin A	C₂₅H₂₈O₅	
44	Licochalcone C	C₂₁H₂₂O₄	
45	Rocymosin B	C₂₁H₂₄O₁₀	
46	Isoglabranin	C₂₀H₂₀O₄	
47	Tephtrinone	C₂₁H₂₂O₄	

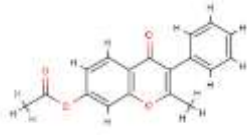
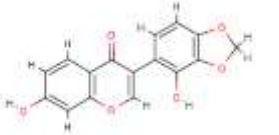
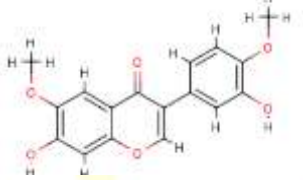
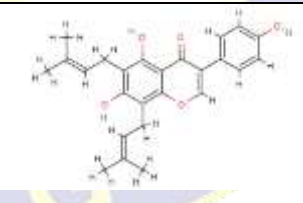
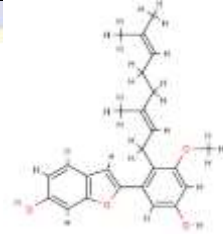
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
48	Abyssinone II	$C_{20}H_{20}O_4$	
49	Licoflavanone	$C_{20}H_{20}O_5$	
50	7-Hydroxy-2-methylisoflavone	$C_{16}H_{12}O_3$	
51	Glycitein	$C_{16}H_{12}O_5$	
52	3'-Hydroxydaidzein	$C_{15}H_{10}O_5$	

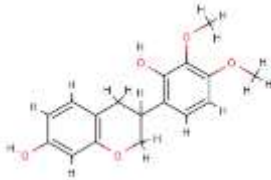
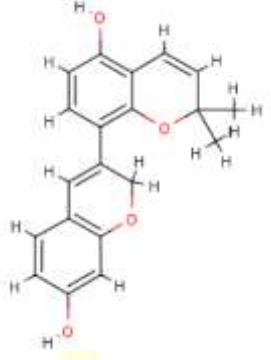
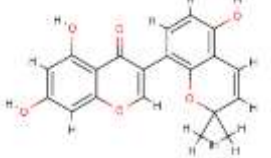
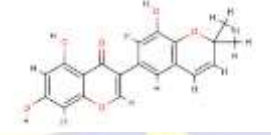
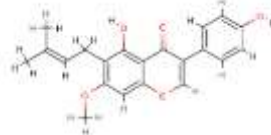
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
53	7-Acetoxy-2-methylisoflavone	$C_{18}H_{14}O_4$	
54	Glyzaglabrin	$C_{16}H_{10}O_6$	
55	Odoratin	$C_{17}H_{14}O_6$	
56	Parvisoflavone A	$C_{20}H_{16}O_6$	
57	6,8-Diprenylgenistein	$C_{25}H_{26}O_5$	
58	Mulberrofuran A	$C_{25}H_{28}O_4$	

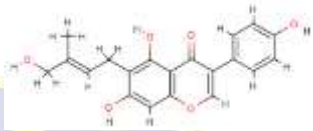
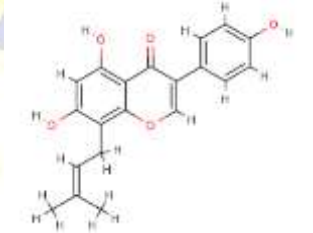
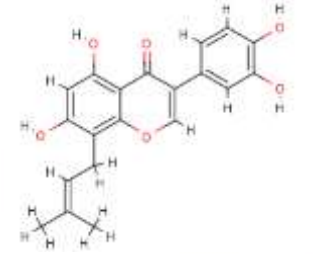
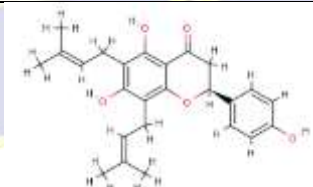
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
59	Isomucronulatoll	C₁₇H₁₈O₅	
60	Glabrene	C₂₀H₁₈O₄	
61	Sophoraisoflavone A	C₂₀H₁₆O₆	
62	Semilicoisoflavone B	C₂₀H₁₆O₆	
63	Gancaonin G	C₂₁H₂₀O₅	
64	6-C-prenylorobol	C₂₅H₂₆O₆	

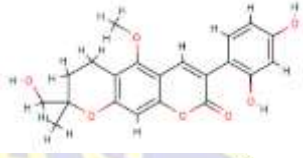
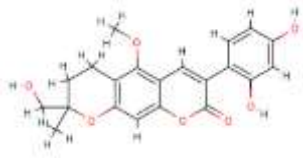
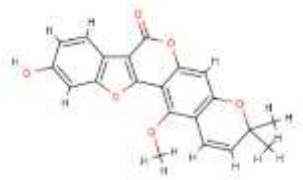
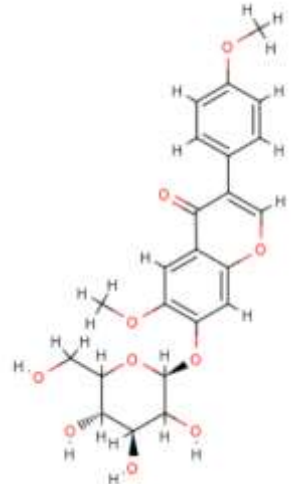
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
65	Hydroxywighteone	<u>C₂₀H₁₈O₆</u>	
66	Lupiwighteone	<u>C₂₀H₁₈O₅</u>	
67	Gancaonin L	<u>C₂₀H₁₈O₆</u>	
68	2'-Hydroxyisolupalbigenin	<u>C₂₅H₂₆O₆</u>	
69	Senegalensin	<u>C₂₅H₂₈O₅</u>	

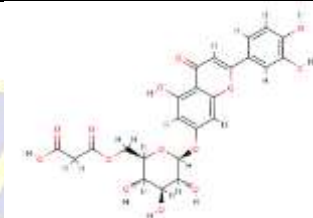
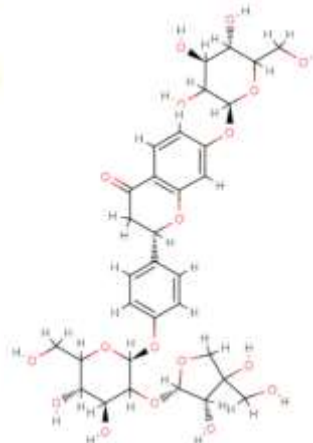
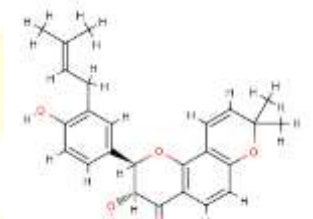
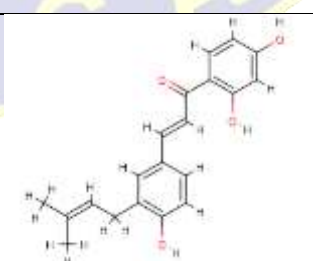
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
70	Licopyranocoumarin	<u>C₂₁H₂₀O₇</u>	
71	Licoarylcoumarin	<u>C₂₁H₂₀O₆</u>	
72	Gancaonin F	<u>C₂₁H₁₆O₆</u>	
73	Afrormosin 7-O-glucoside	<u>C₂₃H₂₄O₁₀</u>	

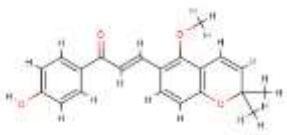
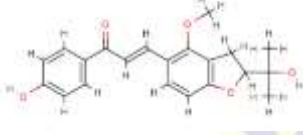
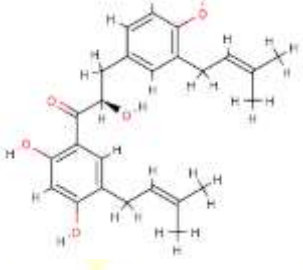
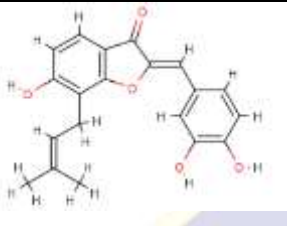
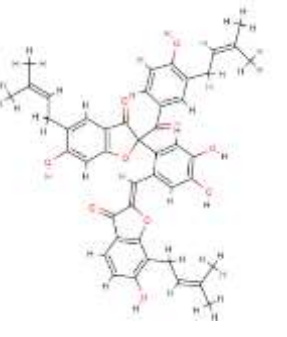
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
74	7-O-(6"-malonylglucoside)	C₂₄H₂₂O₁₄	
75	Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside	C₃₂H₄₀O₁₈	
76	Kanzonol Z	C₂₅H₂₆O₅	
77	Licoagrochalcone A	C₂₀H₂₀O₄	

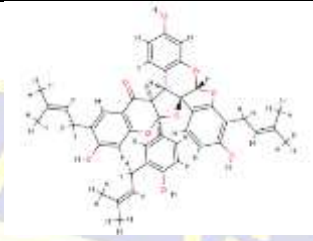
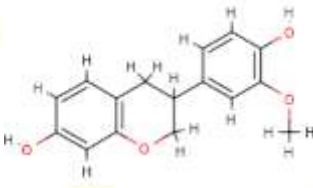
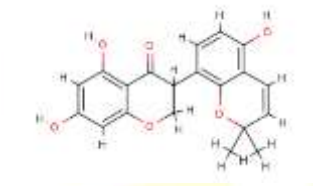
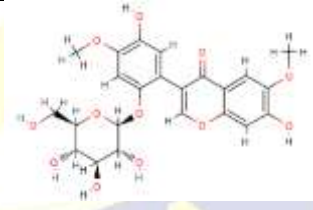
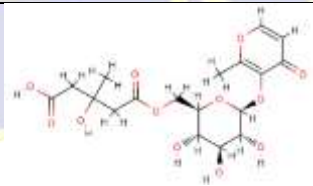
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
78	Licoagrochalcone B	<u>C₂₁H₂₀O₄</u>	
79	Licoagrochalcone D	<u>C₂₁H₂₂O₅</u>	
80	Kanzonol Y	<u>C₂₅H₃₀O₅</u>	
81	Licoagroaurone	<u>C₂₀H₁₈O₅</u>	
82	Licoagrone	<u>C₄₅H₄₂O₁₀</u>	

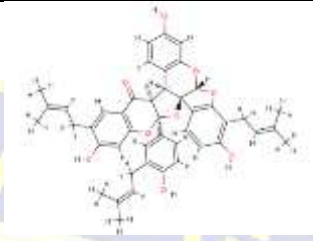
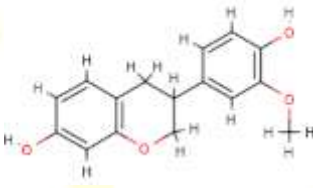
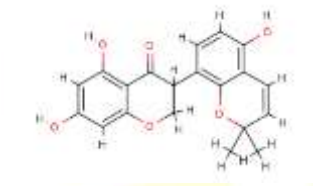
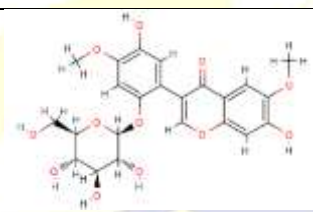
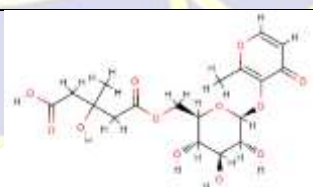
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
83	Licoagrodin	C₄₅H₄₄O₉	
84	7,4'-Dihydroxy-3'-methoxyisoflavan	C₁₆H₁₆O₄	
85	Glyasperin F	C₂₀H₁₈O₆	
86	Licoagroside A	C₂₃H₂₄O₁₂	
87	Tachiogroside B	C₁₈H₂₄O₁₂	

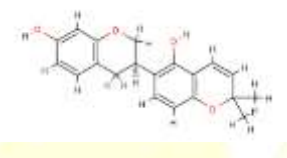
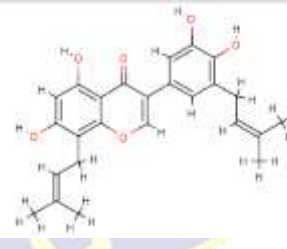
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
83	Licoagrodin	C₄₅H₄₄O₉	
84	7,4'-Dihydroxy-3'-methoxyisoflavan	C₁₆H₁₆O₄	
85	Glyasperin F	C₂₀H₁₈O₆	
86	Licoagroside A	C₂₃H₂₄O₁₂	
87	Tachiogroside B	C₁₈H₂₄O₁₂	

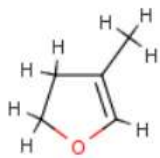
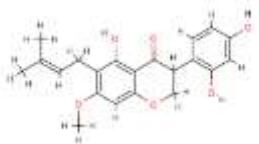
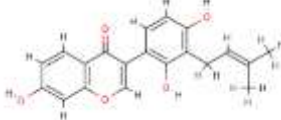
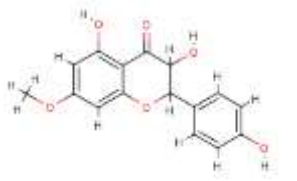
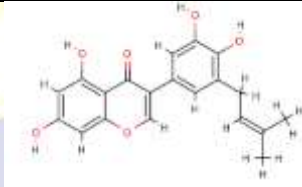
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
93	Glyasperin D	C₂₂H₂₆O₅	
94	Hirtellanine I	C₂₁H₁₆O₇	
95	phaseollinisoflavan	C₂₀H₂₀O₄	
96	Glyurallin B	C₂₅H₂₆O₆	

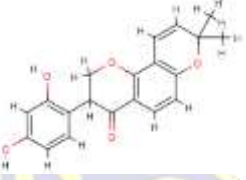
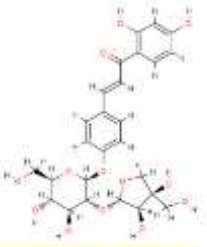
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
97	2,3-Dihydro-4-methylfuran	<u>C₅H₈O</u>	
98	Glyasperin B	<u>C₂₁H₂₂O₆</u>	
99	Eurycarpin A	<u>C₂₀H₁₈O₅</u>	
100	Folerogenin	<u>C₁₆H₁₄O₆</u>	
101	Glycyrrhisoflavone	<u>C₂₀H₁₈O₆</u>	
102	Glabrocoumarin	<u>C₂₀H₁₆O₅</u>	

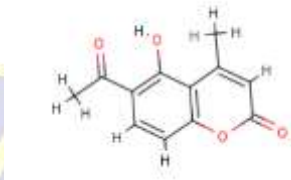
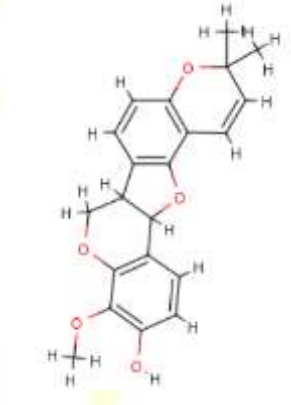
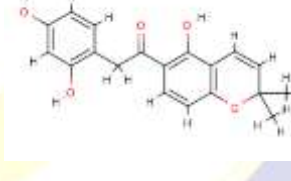
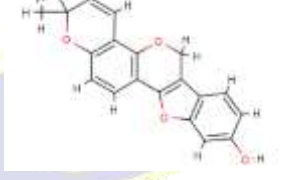
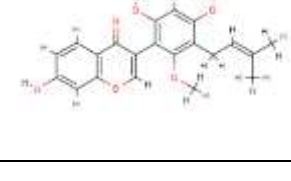
LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
103	Glabroisoflavano ne A	C₂₀H₁₈O₅	
104	Glicophenone	C₂₀H₂₂O₆	
105	Isoliquiritin apioside	C₂₆H₃₀O₁₃	
106	Docosyl-3,4- dihydroxy-trans- cinnamate	C₃₁H₅₂O₄	
107	Isoglabrolide	C₃₀H₄₄O₄	

LAMPIRAN 7 (LANJUTAN)

Tabel VII. 2
Lanjutan

No	Nama Senyawa	Rumus Molekul	Struktur Dua Dimensi
108	Liqcoumarin	C₁₂H₁₀O₄	
109	1-Methoxyphaseollin	C₂₁H₂₀O₅	
110	Erybacin B	C ₁₉ H ₁₈ O ₅	
111	Dehydroglyceollin I	C ₂₀ H ₁₆ O ₄	
112	Glicoricone	C₂₁H₂₀O₆	

LAMPIRAN 8

HASIL DOCKING 112 SENYAWA TERHADAP RESEPTOR 7NG6

Tabel VII 3
 Hasil Docking 7NG6

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
1	<i>Naringin</i>	-8.6	<	<	<
2	<i>alpha,beta-Dihydrorhaponticin</i>	-8.1	<	<	<
3	<i>Isomucronulatoll</i>	-7.1	<	<	<
4	<i>(-)-Phaseollinisoflavan</i>	-7,6	<	<	<
5	<i>(S)-2,3-Epoxy-squalene</i>	-5,3	>	>	>
6	<i>1-Methoxyphaseollin</i>	-1,7	>	>	>
7	<i>2,3-Dihydro-4-methylfuran</i>	-3,4	>	>	>
8	<i>2'-Hydroxyisolupalbigenin</i>	-7,6	<	<	<
9	<i>3'-Hydroxydaidzein</i>	-7.1	<	<	<
10	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	-6,7	<	<	<
11	<i>5,2',4'-Trihydroxy-7-methoxy-6-prenylisoflavone</i>	-7.6	<	<	<
12	<i>6,8-Diprenylgenistein</i>	-8,1	<	<	<
13	<i>6-C-prenylorobol</i>	-8,3	<	<	<
14	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	-7,8	<	<	<
15	<i>7-Acetoxy-2-methylisoflavone</i>	-7.4	<	<	<
16	<i>7-Hydroxy-2-methylisoflavone</i>	-7,7	<	<	<
17	<i>7-O-(6"-malonylglucoside)</i>	-7,4	<	<	<
18	<i>Abyssinone II</i>	-8.1	<	<	<
19	<i>Afrormosin 7-O-glucoside</i>	-7.5	<	<	<

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII. 3
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
20	<i>Albanin A</i>	-7.8	<	<	<
21	<i>Anaphalisoleanenoic acid</i>	-7.1	<	<	<
22	<i>AraboGlycyrrhizin</i>	-7.9	<	<	<
23	<i>beta-Amyrin</i>	-7.9	<	<	<
24	<i>Cycloartenol</i>	-6,9	<	<	<
25	<i>Dehydroglyceollin I</i>	-8,2	<	<	<
26	<i>Desoxoglabrolide</i>	-7.7	<	<	<
27	<i>Dihydrochrysin</i>	-6.7	<	<	<
28	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	-5.0	>	>	>
29	<i>Erybacin B</i>	-7.3	<	<	<
30	<i>Eurycarpin A</i>	-7.9	<	<	<
31	<i>Folerogenin</i>	-7.0	<	<	<
32	<i>Galangin</i>	-7.2	<	<	<
33	<i>Gancaonin F</i>	-8.3	<	<	<
34	<i>Gancaonin G</i>	-7,2	<	<	<
35	<i>Gancaonin L</i>	-7.8	<	<	<
36	<i>Genkwanin</i>	-7.2	<	<	<
37	<i>Glabranin</i>	-7.2	<	<	<
38	<i>Glabrene</i>	-8.3	<	<	<
39	<i>Glabrocoumarin</i>	-8.5	<	<	<
40	<i>Glabroisoflavanone A</i>	-7.7	<	<	<
41	<i>Glicophenone</i>	-6.8	<	<	<
42	<i>Glicoricone</i>	-7.5	<	<	<
43	<i>Glyasperin B</i>	-6.8	<	<	<
44	<i>Glyasperin D</i>	-6.6	<	<	<
45	<i>Glyasperin F</i>	-8.3	<	<	<
46	<i>Glycitein</i>	-6.7	<	<	<
47	<i>Glycyrrhetic acid</i>	-8.4	<	<	<
48	<i>Glycyrrhisoflavone</i>	-8.5	<	<	<

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII. 3
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
49	<i>Glycyrrhizin</i>	-9.1	<	<	<
50	<i>Glyinflanin A</i>	-7.5	<	<	<
51	<i>Glyinflanin B</i>	-7.1	<	<	<
52	<i>Glyurallin B</i>	-7.9	<	<	<
53	<i>Glyzaglabrin</i>	-8.2	<	<	<
54	<i>Hirtellanine I</i>	-8.6	<	<	<
55	<i>Hispaglabridin A</i>	-7.6	<	<	<
56	<i>Hydroxywighteone</i>	-7.7	<	<	<
57	<i>Isobavachalcone</i>	-7.3	<	<	<
58	<i>Isoglabranin</i>	-7.5	<	<	<
59	<i>Isoglabrolide</i>	-7.7	<	<	<
60	<i>Isoliquiritin</i>	-7.5	<	<	<
61	<i>Isoliquiritin apioside</i>	-9.0	<	<	<
62	<i>Isomedicarpin</i>	-7.0	<	<	<
63	<i>Isotachioside</i>	-6.4	<	>	>
64	<i>Isovestin</i>	-7.4	<	<	<
65	<i>Kaempferol</i>	-7.7	<	<	<
66	<i>Kaempferol 3-O-methyl ether</i>	-7.4	<	<	<
67	<i>Kanzonol R</i>	-6.9	<	<	<
68	<i>Kanzonol Y</i>	-6.7	<	<	<
69	<i>Kanzonol Z</i>	-7.5	<	<	<
70	<i>Licoagroaurone</i>	-8.1	<	<	<
71	<i>Licoagrochalcone A</i>	-7.3	<	<	<
72	<i>Licoagrochalcone B</i>	-7.0	<	<	<
73	<i>Licoagrochalcone D</i>	-6.7	<	<	<
74	<i>Licoagrodin</i>	-8.8	<	<	<
75	<i>Licoagrone</i>	-8.2	<	<	<
76	<i>Licoagroside A</i>	-7.4	<	<	<
77	<i>Licoarylcoumarin</i>	-7.3	<	<	<

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII. 3
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
78	<i>Licochalcone B</i>	-6.6	<	<	=
79	<i>Licochalcone C</i>	-6.9	<	<	<
80	<i>Licocoumarin A</i>	-7.5	<	<	<
81	<i>Licoflavanone</i>	-8.2	<	<	<
82	<i>Licoflavonol</i>	-7.0	<	<	<
83	<i>Licopyranocoumarin</i>	-7.3	<	<	<
84	<i>Licoricesaponin B2</i>	-8.9	<	<	<
85	<i>Licoricesaponin E2</i>	-8.9	<	<	<
86	<i>Licoricesaponin J2</i>	-8.3	<	<	<
87	<i>Liqcoumarin</i>	-6.3	<	>	>
88	<i>Liquiritic acid</i>	-8.3	<	<	<
89	<i>Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside</i>	-8.1	<	<	<
90	<i>Liquiritin</i>	-8.1	<	<	<
91	<i>Liquoric acid</i>	-7.1	<	<	<
92	<i>Lupeol</i>	-7.0	<	<	<
93	<i>Lupiwighteone</i>	-7.6	<	<	<
94	<i>Luteone</i>	-7.2	<	<	<
95	<i>Mulberrofuran A</i>	-7.3	<	<	<
96	<i>Odoratin</i>	-7.2	<	<	<
97	<i>Parvisoflavone A</i>	-7.7	<	<	<
98	<i>Phaseollinisoflavan</i>	-7.3	<	<	<
99	<i>Pinocembroside</i>	-7.4	<	<	<
100	<i>Prunetin</i>	-7.4	<	<	<
101	<i>Puerarin</i>	-7.7	<	<	<
102	<i>Rocymosin B</i>	-7.1	<	<	<
103	<i>Scanderone</i>	-8.8	<	<	<
104	<i>Semilicoisoflavone B</i>	-9.0			
105	<i>Senegalensin</i>	-7.7	<	<	<
106	<i>Sophoraisoflavone A</i>	-8.3	<	<	<

**LAMPIRAN 8
(LANJUTAN)**

Tabel VII. 3
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
107	<i>Tachiogroside B</i>	-6.3	<	>	>
108	<i>Tachioside</i>	-6.9	<	<	<
109	<i>Tephrinone</i>	-7.3	<	<	<
110	<i>Uralenol</i>	-8.1	<	<	<
111	<i>Uralsaponin M</i>	-6.5	<	=	>
112	<i>Wogonoside</i>	-7.6	<	<	<

Native Ligand	-6,2
Molnupiravir	-6,5
Paxlovid	-6,6

LAMPIRAN 9

HASIL DOCKING 112 SENYAWA TERHADAP RESEPTOR 7DPU

Tabel VII 4
Hasil Docking 7DPU

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
1	<i>Naringin</i>	-8,8	<	<	<
2	<i>alpha,beta-Dihydrorhaponticin</i>	-7.1	>	<	<
3	<i>Isomucronulatoll</i>	-6.2	>	>	>
4	<i>(-)-Phaseollinisoflavan</i>	-7.1	>	<	<
5	<i>(S)-2,3-Epoxysqualene</i>	-5.0	>	>	>
6	<i>1-Methoxyphaseollin</i>	-1.7	>	>	>
7	<i>2,3-Dihydro-4-methylfuran</i>	-3.8	>	>	>
8	<i>2'-Hydroxyisolupalbigenin</i>	-7.1	>	<	<
9	<i>3'-Hydroxydaidzein</i>	-6.7	>	>	>
10	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	-7.0	>	=	<
11	<i>5,2',4'-Trihydroxy-7-methoxy-6-prenylisoflavone</i>	-7.3	>	<	<
12	<i>6,8-Diprenylgenistein</i>	-7.7	>	<	<
13	<i>6-C-prenylorobol</i>	-8.0	<	<	<
14	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	-6.0	>	>	>
15	<i>7-Acetoxy-2-methylisoflavone</i>	-6.7	>	>	>
16	<i>7-Hydroxy-2-methylisoflavone</i>	-6.5	>	>	>
17	<i>7-O-(6"-malonylglucoside)</i>	-7.1	>	<	<
18	<i>Abyssinone II</i>	-7.6	<	<	<
19	<i>Afrormosin 7-O-glucoside</i>	-6.5	>	>	>
20	<i>Albanin A</i>	-7.1	>	<	<
21	<i>Anaphalisoleanenoic acid</i>	-6.7	>	>	>

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII. 4
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
22	<i>AraboGlycyrrhizin</i>	-7.4	=	<	<
23	<i>beta-Amyrin</i>	-6.9	>	>	<
24	<i>Cycloartenol</i>	-7.2	>	<	<
25	<i>Dehydroglyceollin I</i>	-8.0	>	<	<
26	<i>Desoxoglabrolide</i>	-7.0	>	=	<
27	<i>Dihydrochrysin</i>	-6.6	>	>	>
28	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	-4.7	>	>	>
29	<i>Erybacin B</i>	-7.0	>	=	<
30	<i>Eurycarpin A</i>	-7.3	>	<	<
31	<i>Folerogenin</i>	-6.8	>	>	<
32	<i>Galangin</i>	-6.9	>	>	<
33	<i>Gancaonin F</i>	-8.2	<	<	<
34	<i>Gancaonin G</i>	-7,1	>	<	<
35	<i>Gancaonin L</i>	-7.8	<	<	<
36	<i>Genkwanin</i>	-7.8	<	<	<
37	<i>Glabranin</i>	-7.5	<	<	<
38	<i>Glabrene</i>	-7.3	>	<	<
39	<i>Glabrocoumarin</i>	-7.5	<	<	<
40	<i>Glabroisoflavanone A</i>	-7.0	>	=	<
41	<i>Glicophenone</i>	-6.6	>	>	>
42	<i>Glicoricone</i>	-6.9	>	>	<
43	<i>Glyasperin B</i>	-7.0	>	=	<
44	<i>Glyasperin D</i>	-6.5	>	>	>
45	<i>Glyasperin F</i>	-8.0	<	<	<
46	<i>Glycitein</i>	-6.8	>	>	=
47	<i>Glycyrrhetic acid</i>	-6.9	>	>	<
48	<i>Glycyrrhisoflavone</i>	-7.9	<	<	<
49	<i>Glycyrrhizin</i>	-7.2	>	<	<
50	<i>Glyinflarin A</i>	-7.3	>	<	<
51	<i>Glyinflarin B</i>	-7.5	<	<	<
52	<i>Glyurallin B</i>	-7.9	<	<	<

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII. 4
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
53	<i>Glyzaglabrin</i>	-6.8	>	>	=
54	<i>Hirtellanine I</i>	-7.9	<	<	<
55	<i>Hispaglabridin A</i>	-7.6	<	<	<
56	<i>Hydroxywighteone</i>	-7.6	<	<	<
57	<i>Isobavachalcone</i>	-7.3	>	<	<
58	<i>Isoglabranin</i>	-7.3	>	<	<
59	<i>Isoglabrolide</i>	-6.7	>	>	>
60	<i>Isoliquiritin</i>	-7.6	<	<	<
61	<i>Isoliquiritin apioside</i>	-7.5	<	<	<
62	<i>Isomedicarpin</i>	-7.4	=	<	<
63	<i>Isotachioside</i>	-6.4	>	>	>
64	<i>Isovestin</i>	-7.4	=	<	<
65	<i>Kaempferol</i>	-7.2	>	<	<
66	<i>Kaempferol 3-O-methyl ether</i>	-7.1	>	<	<
67	<i>Kanzonol R</i>	-7.2	>	<	<
68	<i>Kanzonol Y</i>	-7.2	>	<	<
69	<i>Kanzonol Z</i>	-7.09	>	<	<
70	<i>Licoagroaurone</i>	-7.4	=	<	<
71	<i>Licoagrochalcone A</i>	-7.3	>	<	<
72	<i>Licoagrochalcone B</i>	-7.4	>	<	<
73	<i>Licoagrochalcone D</i>	-7.1	>	<	<
74	<i>Licoagrodin</i>	-8.9	<	<	<
75	<i>Licoagrone</i>	-8.5	>	<	<
76	<i>Licoagroside A</i>	-7.8	>	<	<
77	<i>Licoarylcoumarin</i>	-7.6	<	<	<
78	<i>Licochalcone B</i>	-6.7	>	>	>
79	<i>Licochalcone C</i>	-6.6	>	>	>
80	<i>Licocoumarin A</i>	-7.8	<	<	<
81	<i>Licoflavanone</i>	-8.2	>	<	<
82	<i>Licoflavonol</i>	-7,7	<	<	<
83	<i>Licopyranocoumarin</i>	-6.7	>	>	>

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII. 4
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
84	<i>Licoricesaponin B2</i>	-6.8	>	>	=
85	<i>Licoricesaponin E2</i>	-6.7	>	>	>
86	<i>Licoricesaponin J2</i>	-4.9	>	>	>
87	<i>Liqcoumarin</i>	-6.5	>	>	>
88	<i>Liquiritic acid</i>	-7.2	>	<	<
89	<i>Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside</i>	-7.4	=	<	<
90	<i>Liquiritin</i>	-6.9	>	>	<
91	<i>Liquoric acid</i>	-6.8	>	>	>
92	<i>Lupeol</i>	-5.9	>	>	>
93	<i>Lupiwighteone</i>	-7.4	=	<	<
94	<i>Luteone</i>	-7.8	<	<	<
95	<i>Mulberrofurin A</i>	-6.5	>	>	>
96	<i>Odoratin</i>	-6.8	>	>	=
97	<i>Parvisoflavone A</i>	-7.3	>	<	<
98	<i>Phaseollinisoflavan</i>	-7.5	<	<	<
99	<i>Pinocembroside</i>	-8.2	<	<	<
100	<i>Prunetin</i>	-6,6	>	>	>
101	<i>Puerarin</i>	-7.2	>	<	<
102	<i>Rocymosin B</i>	-7.2	>	<	<
103	<i>Scanderone</i>	-8.1	<	<	<
104	<i>Semilicoisoflavone B</i>	-7.4	=	<	<
105	<i>Senegalensin</i>	-7.6	<	<	<
106	<i>Sophoraisoflavone A</i>	-7.3	>	<	<
107	<i>Tachiogroside B</i>	-7.1	>	<	<
108	<i>Tachioside</i>	-6.3	>	<	>
109	<i>Tephtrinone</i>	-7.2	>	<	<
110	<i>Uralenol</i>	-8.0	<	<	<
111	<i>Uralsaponin M</i>	-5.3	>	>	>
112	<i>Wogonoside</i>	-7.9	<	<	<

**LAMPIRAN 9
(LANJUTAN)****Tabel VII. 4**
Lanjutan

<i>Native Ligand</i>	-7.4
<i>Molnupiravir</i>	-7.0
<i>Paxlovid</i>	-6.8



LAMPIRAN 10

HASIL DOCKING 112 SENYAWA TERHADAP RESEPTOR 7SI9

Tabel VII 5
 Hasil Docking 7SI9

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
1	<i>Naringin</i>	-9.0	<	<	<
2	<i>alpha,beta-Dihydrorhaponticin</i>	-8.3	=	<	<
3	<i>Isomucronulatoll</i>	-7.2	>	<	>
4	<i>(-)-Phaseollinisoflavan</i>	-7.5	>	<	>
5	<i>(S)-2,3-Epoxysqualene</i>	-6.1	>	>	>
6	<i>1-Methoxyphaseollin</i>	-1.8	>	>	>
7	<i>2,3-Dihydro-4-methylfuran</i>	-3.5	>	>	>
8	<i>2'-Hydroxyisolupalbigenin</i>	-7.6	>	<	>
9	<i>3'-Hydroxydaidzein</i>	-7.1	>	<	>
10	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	-8.0	>	<	>
11	<i>5,2',4'-Trihydroxy-7-methoxy-6-prenylisoflavone</i>	-7.6	>	<	>
12	<i>6,8-Diprenylgenistein</i>	-7.6	>	<	>
13	<i>6-C-prenylorobol</i>	-7.8	>	<	>
14	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	-7.1	>	<	>
15	<i>7-Acetoxy-2-methylisoflavone</i>	-7.4	>	<	>
16	<i>7-Hydroxy-2-methylisoflavone</i>	-6.8	>	<	>
17	<i>7-O-(6''-malonylglucoside)</i>	-8.1	>	<	>
18	<i>Abyssinone II</i>	-8.1	>	<	>
19	<i>Afrormosin 7-O-glucoside</i>	-8.1	>	<	>
20	<i>Albanin A</i>	-7.5	>	<	>

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 5
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
21	<i>Anaphalisoleanenoic acid</i>	-8.0	>	<	>
22	<i>AraboGlycyrrhizin</i>	-9.1	<	<	<
23	<i>beta-Amyrin</i>	-7.5	>	<	>
24	<i>Cycloartenol</i>	-7.7	>	<	>
25	<i>Dehydroglyceollin I</i>	-7.7	>	<	>
26	<i>Desoxoglabrolide</i>	-8.1	>	<	>
27	<i>Dihydrochrysin</i>	-6.8	>	<	>
28	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	-5.5	>	>	>
29	<i>Erybacin B</i>	-7.2	>	<	>
30	<i>Eurycarpin A</i>	-8.0	>	<	>
31	<i>Folerogenin</i>	-7.3	>	<	>
32	<i>Galangin</i>	-7.6	>	<	>
33	<i>Gancaonin F</i>	-8.0	>	<	>
34	<i>Gancaonin G</i>	-7,2	>	<	>
35	<i>Gancaonin L</i>	-8.2	>	<	=
36	<i>Genkwanin</i>	-7.2	>	<	>
37	<i>Glabranin</i>	-7.1	>	<	>
38	<i>Glabrene</i>	-8.1	>	<	>
39	<i>Glabrocoumarin</i>	-8.2	>	<	=
40	<i>Glabroisoflavanone A</i>	-7.9	>	<	>
41	<i>Glicophenone</i>	-7.1	>	<	>
42	<i>Glicoricone</i>	-7.3	>	<	>
43	<i>Glyasperin B</i>	-7.5	>	<	>
44	<i>Glyasperin D</i>	-6,8	>	<	>
45	<i>Glyasperin F</i>	-8.6	<	<	<
46	<i>Glycitein</i>	-6.8	>	<	>
47	<i>Glycyrrhetic acid</i>	-7.9	>	<	>
48	<i>Glycyrrhisoflavone</i>	-8.7	<	<	<
49	<i>Glycyrrhizin</i>	-10.0	<	<	<

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 5
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
50	<i>Glyinflanin A</i>	-8.3	=	<	<
51	<i>Glyinflanin B</i>	-7.9	>	<	>
52	<i>Glyurallin B</i>	-8.7	<	<	<
53	<i>Glyzaglabrin</i>	-8.2	>	<	=
54	<i>Hirtellanine I</i>	-8.1	>	<	>
55	<i>Hispaglabridin A</i>	-7.7	>	<	>
56	<i>Hydroxywighteone</i>	-7.8	>	<	>
57	<i>Isobavachalcone</i>	-7.8	>	<	>
58	<i>Isoglabranin</i>	-7.6	>	<	>
59	<i>Isoglabrolide</i>	-7.9	>	<	>
60	<i>Isoliquiritin</i>	-7.7	>	<	>
61	<i>Isoliquiritin apioside</i>	-9.0	<	<	<
62	<i>Isomedicarpin</i>	-6.8	>	<	>
63	<i>Isotachioside</i>	-7.3	>	<	>
64	<i>Isovestin</i>	-8.4	<	<	<
65	<i>Kaempferol</i>	-7.5	>	<	>
66	<i>Kaempferol 3-O-methyl ether</i>	-7.3	>	<	>
67	<i>Kanzonol R</i>	-7.2	>	<	>
68	<i>Kanzonol Y</i>	-7.2	>	<	>
69	<i>Kanzonol Z</i>	-8.4	<	<	<
70	<i>Licoagroaurone</i>	-8.0	>	<	>
71	<i>Licoagrochalcone A</i>	-7.4	>	<	>
72	<i>Licoagrochalcone B</i>	-7.0	>	<	>
73	<i>Licoagrochalcone D</i>	-7.0	>	<	>
74	<i>Licoagrodin</i>	-8.5	<	<	<
75	<i>Licoagrone</i>	-8.7	<	<	<
76	<i>Licoagroside A</i>	-8.4	<	<	<
77	<i>Licoarylcoumarin</i>	-8.0	>	<	>

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 5
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
78	<i>Licochalcone B</i>	-6.9	>	<	>
79	<i>Licochalcone C</i>	-7.2	>	<	>
80	<i>Licocoumarin A</i>	-8.3	=	<	<
81	<i>Licoflavanone</i>	-8.3	=	<	<
82	<i>Licoflavanol</i>	-7,5	>	<	>
83	<i>Licopyranocoumarin</i>	-8.0	>	<	>
84	<i>Licoricesaponin B2</i>	-8.9	<	<	<
85	<i>Licoricesaponin E2</i>	-10.5	<	<	<
86	<i>Licoricesaponin J2</i>	-9.5	<	<	<
87	<i>Liquocoumarin</i>	-6.1	>	>	>
88	<i>Liquiritic acid</i>	-7.5	>	<	>
89	<i>Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside</i>	-8.1	>	<	>
90	<i>Liquiritin</i>	-8.1	>	<	>
91	<i>Liquoric acid</i>	-8.3	=	<	<
92	<i>Lupeol</i>	-7.6	>	<	>
93	<i>Lupiwighteone</i>	-7.8	>	<	>
94	<i>Luteone</i>	-7.8	>	<	>
95	<i>Mulberrofuran A</i>	-7.8	>	<	>
96	<i>Odoratin</i>	-6.7	>	<	>
97	<i>Parvisoflavone A</i>	-8.5	<	<	<
98	<i>Phaseollinisoflavan</i>	-7.3	>	<	>
99	<i>Pinocembroside</i>	-7.8	>	<	>
100	<i>Prunetin</i>	-6,8	>	<	>
101	<i>Puerarin</i>	-8.5	<	<	<
102	<i>Rocymosin B</i>	-8.7	<	<	<
103	<i>Scanderone</i>	-8.1	>	<	>
104	<i>Semilicoisoflavone B</i>	-8.0	>	<	>
105	<i>Senegalensin</i>	-7.7	>	<	>

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 5
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
106	<i>Sophoraisoflavone A</i>	-8.5	<	<	<
107	<i>Tachiogroside B</i>	-7.6	>	<	>
108	<i>Tachioside</i>	-7.2	>	<	>
109	<i>Tephrinone</i>	-7.1	>	<	>
110	<i>Uralenol</i>	-8.5	<	<	<
111	<i>Uralsaponin M</i>	-7.2	>	<	>
112	<i>Wogonoside</i>	-9.0	<	<	<

<i>Native Ligand</i>	-8.3
<i>Molnupiravir</i>	-6,5
<i>Paxlovid</i>	-8,2

LAMPIRAN 11

HASIL DOCKING 112 SENYAWA TERHADAP RESEPTOR 7RN4

Tabel VII 6
 Hasil Docking 7RN4

NO	Senyawa	ΔG	Keterangan		
			Native Ligand	Molnupiravir	Paxlovid
1	Naringin	-8.8	>	<	<
2	alpha,beta-Dihydrorhaponticin	-9.0	>	<	<
3	Isomucronulatoll	-7.0	>	>	<
4	(-)-Phaseollinisoflavan	-8.5	>	<	<
5	(S)-2,3-Epoxy-squalene	-5.7	>	>	>
6	1-Methoxyphaseollin	-1.7	>	>	>
7	2,3-Dihydro-4-methylfuran	-3.7	>	>	>
8	2'-Hydroxyisolupalbigenin	-7.8	>	<	<
9	3'-Hydroxydaidzein	-7,8	>	<	<
10	3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside	-7.6	>	<	<
11	5,2',4'-Trihydroxy-7-methoxy-6-prenylisoflavone		>	>	<
12	6,8-Diprenylgenistein	-9.0	>	<	<
13	6-C-prenylorobol	-8.3	>	<	<
14	7,4'-Dihydroxy-3'-methoxyisoflavan	-7.5	>	<	<
15	7-Acetoxy-2-methylisoflavone	-6.9	>	>	<
16	7-Hydroxy-2-methylisoflavone	-7.6	>	<	<
17	7-O-(6"-malonylglucoside)	-7.7	>	<	<
18	Abyssinone II	-8.3	>	<	<
19	Afrormosin 7-O-glucoside	-7.4	>	=	<

**LAMPIRAN 11
(LANJUTAN)**

Tabel VII. 6
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	<i>Paxlovid</i>
20	<i>Albanin A</i>	-8.3	>	<	<
21	<i>Anaphalisoleanenoic acid</i>	-7.0	>	>	<
22	<i>AraboGlycyrrhizin</i>	-6,9	>	>	<
23	<i>beta-Amyrin</i>	-6.8	>	>	<
24	<i>Cycloartenol</i>	-6.9	>	>	<
25	<i>Dehydroglyceollin I</i>	-8.9	>	<	<
26	<i>Desoxoglabrolide</i>	-6.8	>	<	<
27	<i>Dihydrochrysin</i>	-7.3	>	<	<
28	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	-5.5	>	>	>
29	<i>Erybacin B</i>	-8.1	>	<	<
30	<i>Eurycarpin A</i>	-8.6	>	<	<
31	<i>Folerogenin</i>	-7.7	>	<	<
32	<i>Galangin</i>	-7.9	>	<	<
33	<i>Gancaonin F</i>	-9.1	>	<	<
34	<i>Gancaonin G</i>	-7,9	>	<	<
35	<i>Gancaonin L</i>	-8.8	>	<	<
36	<i>Genkwanin</i>	-8,4	>	<	<
37	<i>Glabranin</i>	-7.4	>	=	<
38	<i>Glabrene</i>	-9.2	<	<	<
39	<i>Glabrocoumarin</i>	-8,2	>	<	<
40	<i>Glabroisoflavanone A</i>	-7.8	>	<	<
41	<i>Glicophenone</i>	-8.1	>	<	<
42	<i>Glicoricone</i>	-8.1	>	<	<
43	<i>Glyasperin B</i>	-7.7	>	<	<
44	<i>Glyasperin D</i>	-7.1	>	>	<
45	<i>Glyasperin F</i>	-8,1	>	<	<
46	<i>Glycitein</i>	-7,7	>	<	<
47	<i>Glycyrrhetic acid</i>	-7.1	>	>	<
48	<i>Glycyrrhisoflavone</i>	-9.2	<	<	<
49	<i>Glycyrrhizin</i>	-9.0	>	<	<

LAMPIRAN 11
(LANJUTAN)

Tabel VII. 6
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	<i>Paxlovid</i>
50	<i>Glyinflanin A</i>	-7.9	>	<	<
51	<i>Glyinflanin B</i>	-8.1	>	<	<
52	<i>Glyurallin B</i>	-8.2	>	<	<
53	<i>Glyzaglabrin</i>	-8.2	>	<	<
54	<i>Hirtellanine I</i>	-9.0	>	<	<
55	<i>Hispaglabridin A</i>	-8.1	>	<	<
56	<i>Hydroxywighteone</i>	-8.5	>	<	<
57	<i>Isobavachalcone</i>	-7.4	>	=	<
58	<i>Isoglabranin</i>	-7,8	>	<	<
59	<i>Isoglabrolide</i>	-7.1	>	>	<
60	<i>Isoliquiritin</i>	-8.1	>	<	<
61	<i>Isoliquiritin apioside</i>	-8.8	>	>	<
62	<i>Isomedicarpin</i>	-7.3	>	>	<
63	<i>Isotachioside</i>	-7.0	>	>	<
64	<i>Isovestin</i>	-8,8	>	<	<
65	<i>Kaempferol</i>	-8.6	>	<	<
66	<i>Kaempferol 3-O-methyl ether</i>	-7,8	>	<	<
67	<i>Kanzonol R</i>	-7.3	>	>	<
68	<i>Kanzonol Y</i>	-7.5	>	<	<
69	<i>Kanzonol Z</i>	-8,5	>	<	<
70	<i>Licoagroaurone</i>	-8.5	>	<	<
71	<i>Licoagrochalcone A</i>	-8,1	>	<	<
72	<i>Licoagrochalcone B</i>	-7.5	>	<	<
73	<i>Licoagrochalcone D</i>	-7,5	>	<	<
74	<i>Licoagrodin</i>	-7.6	>	<	<
75	<i>Licoagrone</i>	-9,3	<	<	<
76	<i>Licoagroside A</i>	-8.6	>	<	<
77	<i>Licoarylcoumarin</i>	-7,7	>	<	<
78	<i>Licochalcone B</i>	-7.4	>	=	<
79	<i>Licochalcone C</i>	-7,3	>	>	<

LAMPIRAN 11
(LANJUTAN)

Tabel VII. 6
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	<i>Paxlovid</i>
80	<i>Licocoumarin A</i>	-8.1	>	<	<
81	<i>Licoflavanone</i>	-8.6	>	<	<
82	<i>Licoflavonol</i>	-7.4	>	=	<
83	<i>Licopyranocoumarin</i>	-7.4	>	=	<
84	<i>Licoricesaponin B2</i>	-9.0	>	<	<
85	<i>Licoricesaponin E2</i>	-8.1	>	<	<
86	<i>Licoricesaponin J2</i>	-6,7	>	>	=
87	<i>Liqcoumarin</i>	-7.1	>	>	<
88	<i>Liquiritic acid</i>	-7,5	>	<	<
89	<i>Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside</i>	-8.1	>	<	<
90	<i>Liquiritin</i>	-7.8	>	<	<
91	<i>Liquoric acid</i>	-7.1	>	>	<
92	<i>Lupeol</i>	-6.9	>	>	<
93	<i>Lupiwighteone</i>	-8.9	>	<	<
94	<i>Luteone</i>	-7,8	>	<	<
95	<i>Mulberrofurin A</i>	-8.4	>	<	<
96	<i>Odoratin</i>	-7.8	>	<	<
97	<i>Parvisoflavone A</i>	-9.2	>	<	<
98	<i>Phaseollinisoflavan</i>	-7.8	>	<	<
99	<i>Pinocembroside</i>	-9.0	>	<	<
100	<i>Prunetin</i>	-8.0	>	<	<
101	<i>Puerarin</i>	-9.2	>	<	<
102	<i>Rocymosin B</i>	-8.8	>	<	<
103	<i>Scanderone</i>	-8,9	>	<	<
104	<i>Semilicoisoflavone B</i>	-10	<	<	<
105	<i>Senegalensin</i>	-7,5	>	<	<
106	<i>Sophoraisoflavone A</i>	-9.5	<	<	<
107	<i>Tachiogroside B</i>	-7.5	>	<	<
108	<i>Tachioside</i>	-6.9	>	>	<

LAMPIRAN 11
(LANJUTAN)

Tabel VII. 6
Lanjutan

NO	Senyawa	ΔG	Keterangan		
			<i>Native Ligand</i>	<i>Molnupiravir</i>	Paxlovid
109	<i>Tephrinone</i>	-7.7	>	<	<
110	<i>Uralenol</i>	-9.4	<	<	<
111	<i>Uralsaponin M</i>	-8,4	>	<	<
112	<i>Wogonoside</i>	-8.5	>	<	<

<i>Native Ligand</i>	9,1
<i>Molnupiravir</i>	-7,4
<i>Paxlovid</i>	-6,7

LAMPIRAN 12
PREDIKSI DRUGLIKENESS

Tabel VII 7
Prediksi Druglikeness

NO	Senyawa	Massa	Hidrogen Donor	Hidrogen Akseptor	Log P	MR	Total Memenuhi
1	<i>Naringin</i>	556	0	14	-4,512	115,735	3
2	<i>alpha,beta-Dihydrorhaponticin</i>	-	-	-	-	-	0
3	<i>Isomucronulatoll</i>	-	-	-	-	-	0
4	<i>(-)-Phaseollinisoflavan</i>	306	0	4	0	0	4
5	<i>(S)-2,3-Epoxysqualene</i>	323	0	5	-1,392	77,55	5
6	<i>1-Methoxyphaseollin</i>	333	0	5	1,25	79,936	5
7	<i>2,3-Dihydro-4-methylfuran</i>	76	0	1	0,153	19,5	4
8	<i>2'-Hydroxyisolupalbigenin</i>	400	0	6	0	0	4
9	<i>3'-Hydroxydaidzein</i>	263	0	5	-1,912	61,301	5
10	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	358	0	10	-7,28	68,038	4
11	<i>5,2',4'-Trihydroxy-7-methoxy-6-prenylisoflavone</i>	395	0	5	0	0	4
12	<i>6,8-Diprenylgenistein</i>	383	0	5	-0,906	93,127	5
13	<i>6-C-prenylorobol</i>						4
14	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	258	0	4	-0,198	62,261	5
15	<i>7-Acetoxy-2-methylisoflavone</i>	280	0	4	0,593	68,902	5
16	<i>7-Hydroxy-2-methylisoflavone</i>	258	0	4	-0,198	62,261	5
17	<i>7-O-(6''-malonylglucoside)</i>	519	0	14	-3,535	104,575	3
18	<i>Abyssinone II</i>	306	0	4	-0,534	75,001	5

**LAMPIRAN 12
(LANJUTAN)**

Tabel VII. 7
Lanjutan

NO	Senyawa	Massa	Hidrogen Donor	Hidrogen Akseptor	Log P	MR	Total Memenuhi
19	<i>Afrormosin 7-O-glucoside</i>	306	0	4	-0,534	75,001	5
20	<i>Albanin A</i>	354	4	6	3,851	95,969	5
21	<i>Anaphalisoleanoic acid</i>	410	0	3	0,421	100,325	5
22	<i>AraboGlycyrrhizin</i>	778	7	14	2,792	192,881	1
23	<i>beta-Amyrin</i>	426	1	1	8,168	130,719	3
24	<i>Cycloartenol</i>	377	0	1	1,226	96,796	5
25	<i>Dehydroglyceollin I</i>	305	0	4	0,77	75,112	5
26	<i>Desoxoglabrolide</i>	409	0	3	0,717	99,022	5
27	<i>Dihydrochrysin</i>	246	0	4	-0,784	58,35	5
28	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	430	0	4	-0,644	109,097	5
29	<i>Erybacin B</i>	311	0	5	0	0	4
30	<i>Eurycarpin A</i>	323	0	5	-1,279	77,411	5
31	<i>Folerogenin</i>	28	0	1	-0,597	5,683	4
32	<i>Galangin</i>	263	0	5	0	0	4
33	<i>Gancaonin F</i>	364	1	6	4,35	98,566	5
34	<i>Gancaonin G</i>	352	2	5	4,231	98,836	5
35	<i>Gancaonin L</i>	340	0	6	-1,978	78,676	5
36	<i>Genkwanin</i>	274	0	5	-0,863	64,4	5
37	<i>Glabranin</i>	306	0	4	-0,241	75,383	5
38	<i>Glabrene</i>	306	0	4	0	0	4
39	<i>Glabrocoumarin</i>	322	0	5	-0,694	78,561	5
40	<i>Glabroisoflavanone A</i>	322	0	5	-0,696	78,561	5
41	<i>Glicophenone</i>	340	0	6	0	0	4
42	<i>Glicoricone</i>	351	0	6	1,048	85,382	5
43	<i>Glyasperin B</i>	351	0	6	1,789	83,603	5
44	<i>Glyasperin D</i>	346	0	5	0	0	4
45	<i>Glyasperin F</i>	339	0	6	-1,276	80,254	5
46	<i>Glycitein</i>	274	0	5	-0,71	64,025	5
47	<i>Glycyrrhetic acid</i>	426	0	4	-0,591	100,294	5

**LAMPIRAN 12
(LANJUTAN)**

Tabel VII. 7
Lanjutan

NO	Senyawa	Massa	Hidrogen Donor	Hidrogen Akseptor	Log P	MR	Total Memenuhi
48	<i>Glycyrrhisoflavone</i>	340	0	6	-1,546	79,897	5
49	<i>Glycyrrhizin</i>	768	0	16	-4,504	163,274	2
50	<i>Glyinflanin A</i>	384	0	5	0	0	4
51	<i>Glyinflanin B</i>	322	0	5	0	0	4
52	<i>Glyurallin B</i>	422	4	6	4,837	118,943	5
53	<i>Glyzaglabrin</i>	298	2	6	2,137	65,467	5
54	<i>Hirtellanine I</i>	380	3	7	4,373	99,785	5
55	<i>Hispaglabridin A</i>	366	0	4	-0,283	91,691	5
56	<i>Hydroxywighteone</i>	354	4	6	2,9	95,36	5
57	<i>Isobavachalcone</i>	307	0	4	-0,619	76,187	5
58	<i>Isoglabranin</i>	306	0	4	-0,216	72,421	5
59	<i>Isoglabrolide</i>	468	1	4	6	130,768	3
60	<i>Isoliquiritin</i>	402	0	9	0	0	4
61	<i>Isoliquiritin apioside</i>	482	0	11	0	0	3
62	<i>Isomedicarpin</i>	370	1	4	3,01	72,705	5
63	<i>Isotachioside</i>	289	0	8	0,488	63,683	5
64	<i>Isovestin</i>	419	0	10	-1,583	90,605	4
65	<i>Kaempferol</i>	280	0	6	0	0	4
66	<i>Kaempferol 3-O-methyl ether</i>	-	-	-	-	-	0
67	<i>Kanzonol R</i>	346	0	5	0,998	82,859	5
68	<i>Kanzonol Y</i>	384	0	5	-0,011	96,266	5
69	<i>Kanzonol Z</i>	328	0	5	-0,562	92,434	5
70	<i>Licoagroaurone</i>	338	3	5	3,924	93,548	5
71	<i>Licoagrochalcone A</i>	-	-	-	-	-	0
72	<i>Licoagrochalcone B</i>	-	-	-	-	-	0
73	<i>Licoagrochalcone D</i>	-	-	-	-	-	0
74	<i>Licoagrodin</i>	-	-	-	-	-	0
75	<i>Licoagrone</i>	-	-	-	-	-	0
76	<i>Licoagroside A</i>	474	0	12	0	0	3
77	<i>Licoarylcoumarin</i>	351	0	6	0	0	4
78	<i>Licochalcone B</i>	-	-	-	-	-	0

**LAMPIRAN 12
(LANJUTAN)**

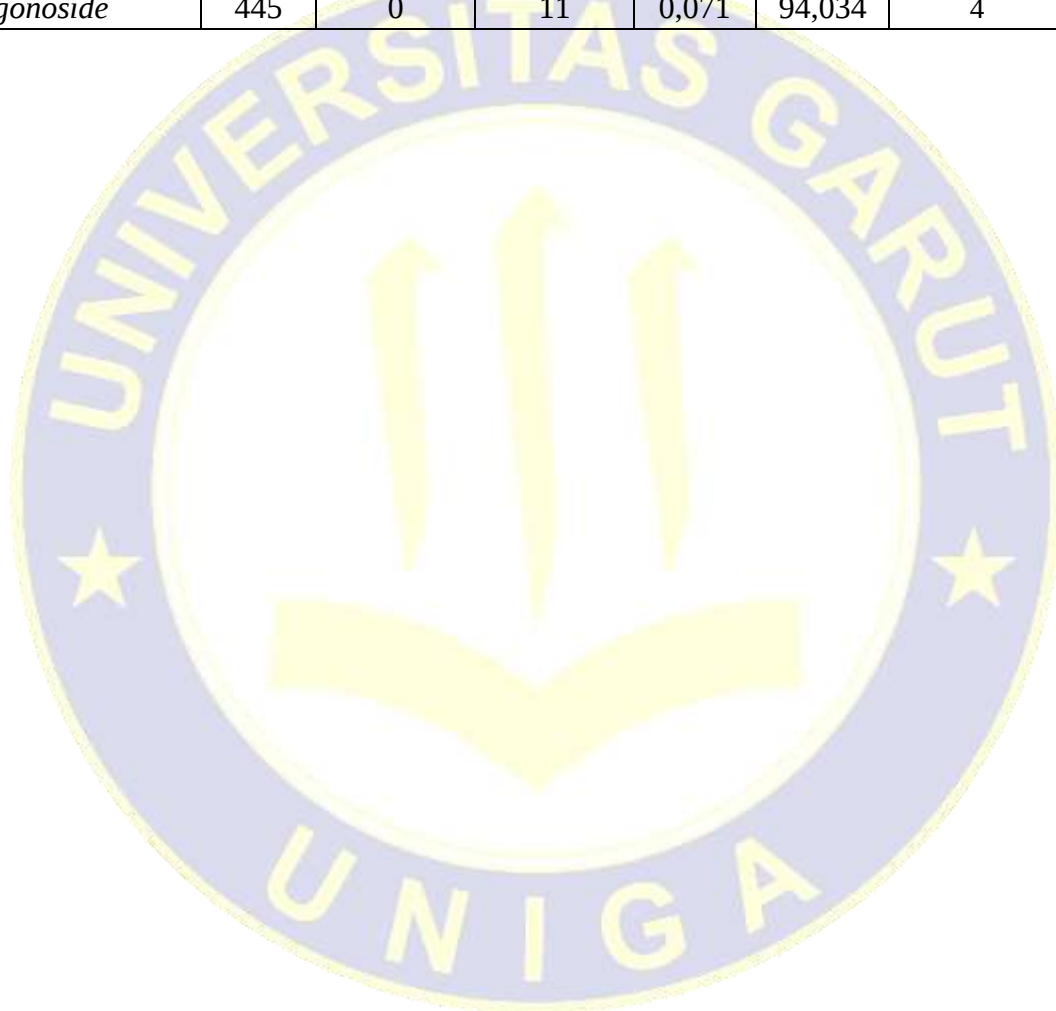
Tabel VII. 7
Lanjutan

NO	Senyawa	Massa	Hidrogen Donor	Hidrogen Akseptor	Log P	MR	Total Memenuhi
79	<i>Licochalcone C</i>	-	-	-	-	-	0
80	<i>Licocoumarin A</i>	-	-	-	-	-	0
81	<i>Licoflavanone</i>	323	0	5	0	0	4
82	<i>Licoflavanol</i>	340	0	6	-1,628	79,756	5
83	<i>Licopyranocoumarin</i>	367	0	7	0	0	4
84	<i>Licoricesaponin B2</i>	752	0	15	0	0	2
85	<i>Licoricesaponin E2</i>	769	0	16	-5,029	158,952	2
86	<i>Licoricesaponin J2</i>	769	0	16	-4,785	153,445	2
87	<i>Liquocoumarin</i>	218	1	4	1,917	57,597	5
88	<i>Liquiritic acid</i>	426	0	4	-0,591	100,294	5
89	<i>Liquiritigenin 7-glucoside-4'-apiosyl-(1->2)-glucoside</i>	-	-	-	-	-	0
90	<i>Liquiritin</i>	401	0	9	0,458	93,789	5
91	<i>Liquoric acid</i>	442	0	5	0	0	4
92	<i>Lupeol</i>	377	0	1	1,429	97,68	5
93	<i>Lupiwighteone</i>	323	0	5	-1,392	77,557	5
94	<i>Luteone</i>	339	0	6	0	0	4
95	<i>Mulberrofurin A</i>	366	0	4	0,341	89,594	5
96	<i>Odoratin</i>	302	0	6	0,21	67,118	5
97	<i>Parvisoflavone A</i>	339	0	6	0	0	4
98	<i>Phaseollinisoflavan</i>	306	0	4	0	0	4
99	<i>Pinocembroside</i>	401	0	9	-2,317	85,375	5
100	<i>Prunetin</i>	-	-	-	-	-	0
101	<i>Puerarin</i>	402	0	9	-0,878	89,375	5
102	<i>Rocymosin B</i>	419	0	10	-3,435	89,717	4
103	<i>Scanderone</i>	410	2	5	3,94	114,794	5
104	<i>Semilicoisoflavone B</i>	339	0	6	-1,281	80,354	5
105	<i>Senegalensin</i>	383	0	5	-0,906	93,137	5
106	<i>Sophoraisoflavone A</i>	339	0	6	-1,276	80,254	5
107	<i>Tachigroside B</i>	413	0	12	-2,393	80,189	4
108	<i>Tachioside</i>	289	0	8	-1,037	57,057	5

**LAMPIRAN 12
(LANJUTAN)**

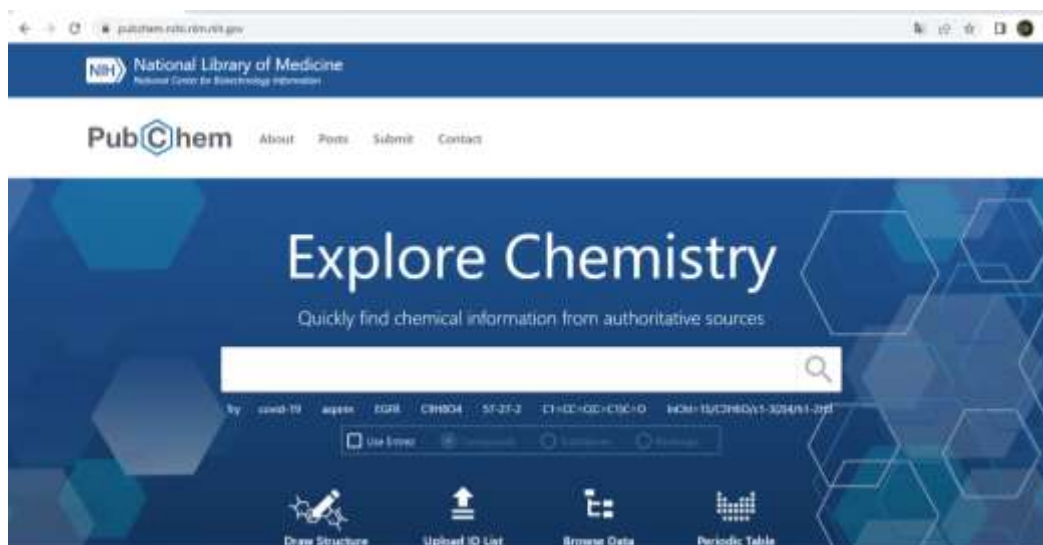
Tabel VII. 7
Lanjutan

NO	Senyawa	Massa	Hidrogen Donor	Hidrogen Akseptor	Log P	MR	Total Memenuhi
109	<i>Tephrinone</i>	317	0	4	0,913	76,705	5
110	<i>Uralenol</i>	375	0	7	0	0	4
111	<i>Uralsaponin M</i>	852	0	19	-2,225	179,827	2
112	<i>Wogonoside</i>	445	0	11	0,071	94,034	4



LAMPIRAN 13

SITUS DAN APLIKASI



Gambar VII. 5 Tampilan situs *pubChem*



Gambar VII. 6 Tampilan situs *PASS-online*

LAMPIRAN 13 (LANJUTAN)

scfbio-ibd.res.in/software/drugdesign/lipinski.jsp#anchortag

Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi

Lipinski Rule of Five

Lipinski rule of 5 helps in distinguishing between drug like and non drug like molecules. It predicts high probability of success or failure due to drug likeness for molecules complying with 2 or more of the following rules

- Molecular mass less than 500 Dalton
- High lipophilicity (expressed as LogP less than 5)
- Less than 5 hydrogen bond donors
- Less than 10 hydrogen bond acceptors
- Polar refractivity should be between 40-130

These filters help in early preclinical development and could help avoid costly late-stage preclinical and clinical failure. To draw a chemical structure [Click here](#) and follow the instructions given.

Step 1: Input Drug File.

Input PDB file No file chosen

Step 2: Input pH Value

pH Value [Value ranges from 0.0 to 14.0]

Step 3: Click on 'Submit' to submit your job

How to Use the Tool

OPTION 1:-

- The input File should be in the following format(*.pdb, *.mol, *.sdf, *.mol2, *.xyz, *.cif, *.mol)
- The input file name should not contain whitespace(s).

PreADMET

Tel: +91-32-212-9555 / Fax: +91-32-212-9672 | webmaster@brndrc.org

208, Vardas A Hall, Yonsei University 55 Songdo-dong, Yeosu-gu, Incheon 21953, Republic of Korea

Home | About | Drug-likeness | 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: Desktop, Endpoint, Standard and Professional.

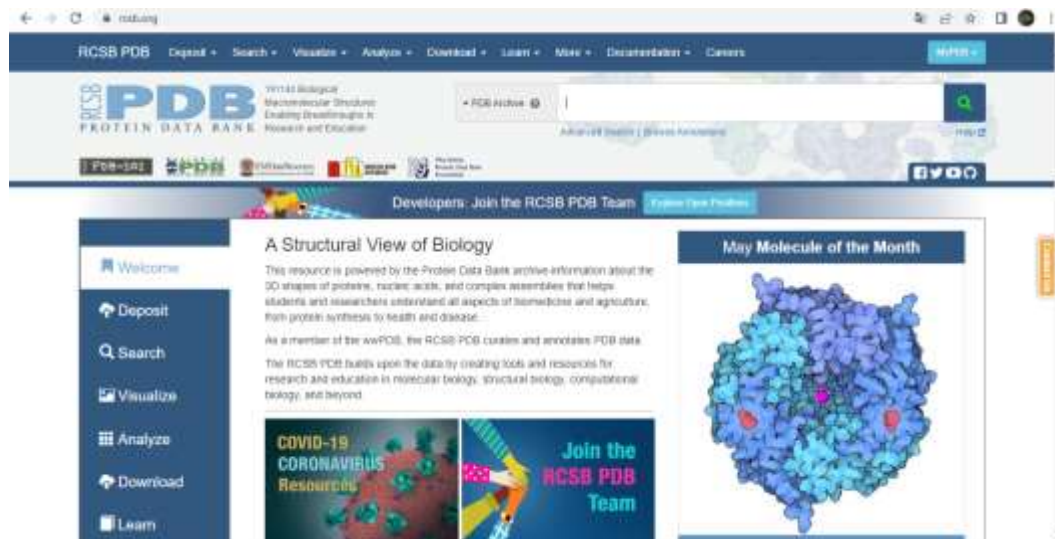
- Drug-Likeness Prediction**
Lipinski's rule, lead-like rule, Drug-DB like rule
- ADME Prediction**
Tox21, MDCK, BBB, HSA, plasma protein binding and skin permeability data
- Toxicity Prediction**
 Ames test and rodent carcinogenicity assay

Latest News

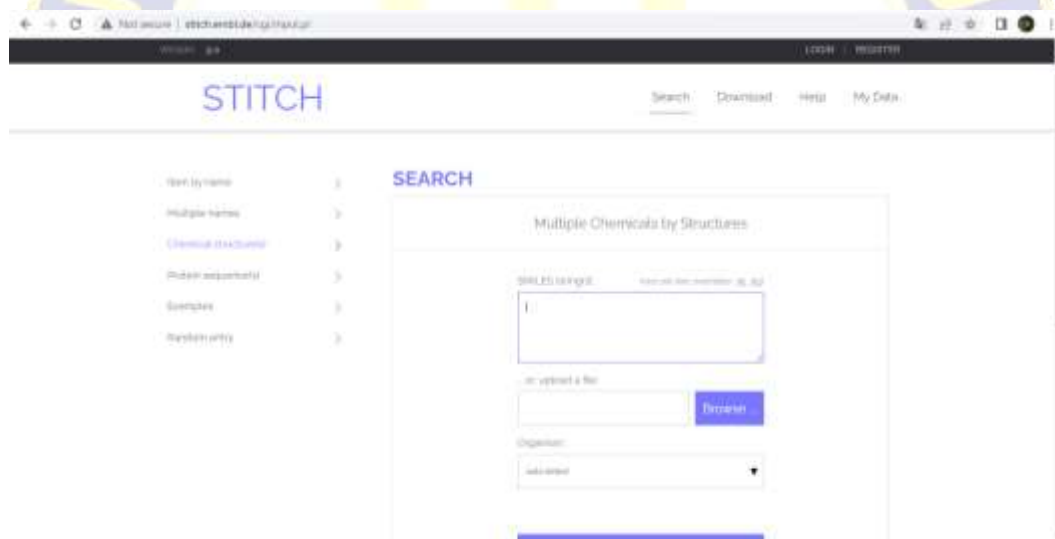
- G-SPED and Human hepatotoxicity models will be added in Aug 2017
January 24, 2017
- PreADMET Ver 2.1 is coming soon in 10th month
January 6, 2017
- [2008/11] PreADMET is one of the most popular sites by Cheminformatics.org
November 27, 2008
- [2008/10] New release of PreADMET v2.0 windows version
October 27, 2008
- [2008/09] New PreADMET web site

Gambar VII. 8 Tampilan situs pre-ADMET

LAMPIRAN 13 (LANJUTAN)



Gambar VII. 9 Tampilan situs *protein data bank*



Gambar VII. 10 Tampilan situs *STITCH*

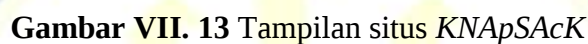
LAMPIRAN 13 (LANJUTAN)



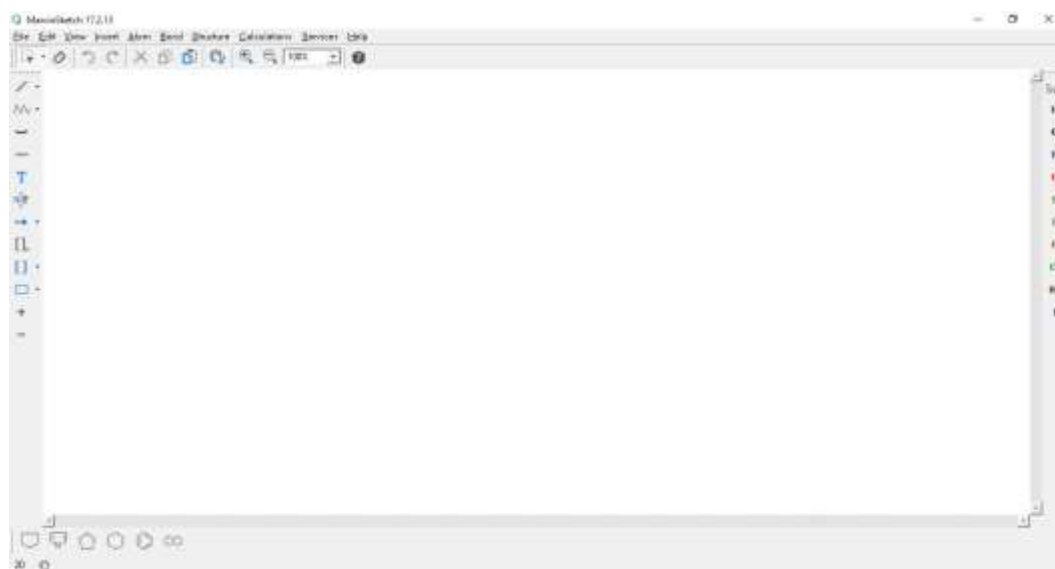
Gambar VII. 11 Tampilan situs CHARMM-GUI



Gambar VII. 12 Tampilan situs google colab



LAMPIRAN 13 (LANJUTAN)

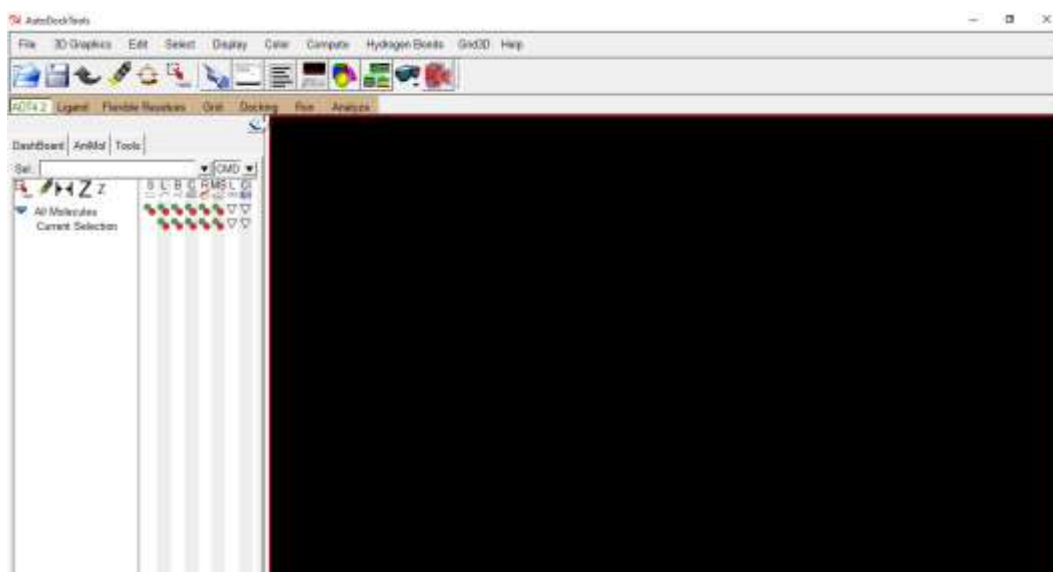


Gambar VII. 15 Tampilan software *Marvin Sketch*

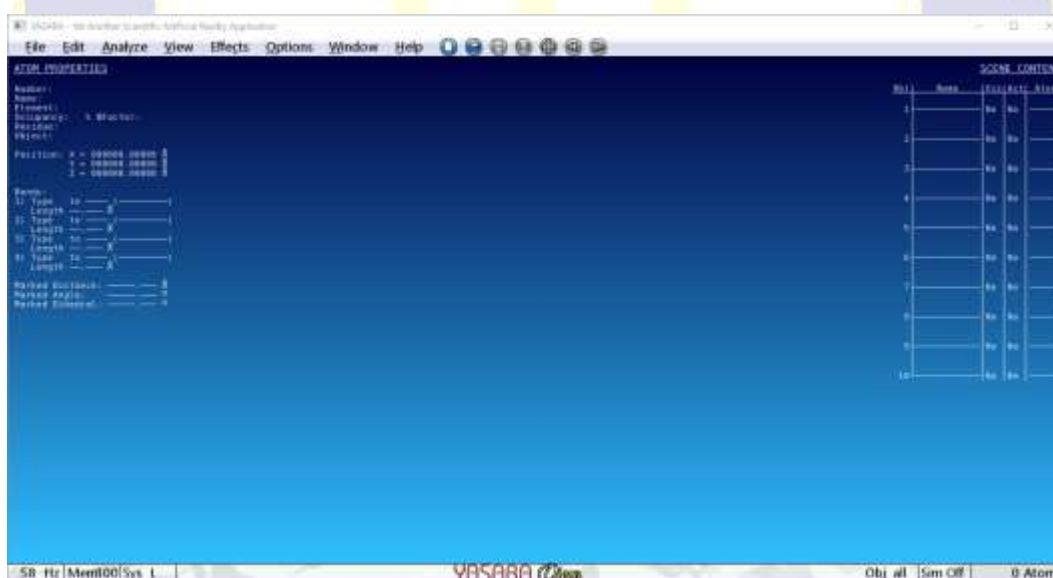


Gambar VII. 16 Tampilan software *Open Babel*

LAMPIRAN 13 (LANJUTAN)

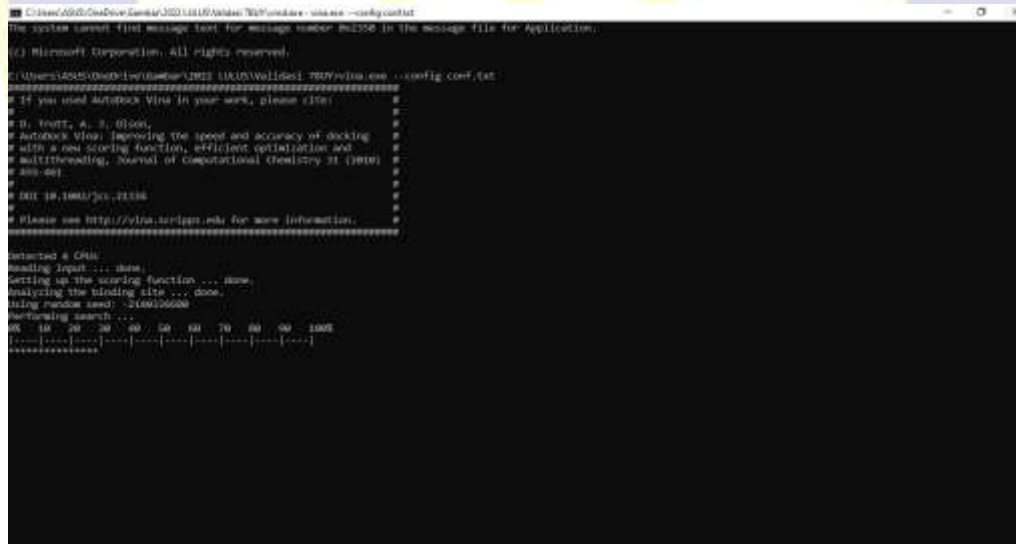


Gambar VII. 17 Tampilan software *AutoDock tools*



Gambar VII. 18 Tampilan software *YASARA*

Gambar VII. 19 Tampilan *software CHIMERA*



Gambar VII. 20 Tampilan *software* AutoDock Vina

LAMPIRAN 14
PREDIKSI ADME

Tabel VII 8
Prediksi Aktivitas Absorpsi, Distribusi dan Metabolisme

Senyawa	Absorpsi		Distribusi	Metabolisme
	CaCo-2 Cell (nm sec)	HIA (%)	Protein Plasma Binding	Substrat CYP2D6
<i>Licoricesaponin E2</i>	20,72 **	15,95 ***	78,50 **	non
<i>Glycyrrhizin</i>	20,79 **	9,45 ***	82,48 **	non
<i>Licoricesaponin J2</i>	20,70 **	7,07 ***	81,24 **	non
<i>Licoagrodin</i>	28,47 **	95,54 *	100 *	non
<i>Naringin</i>	7,89 **	11,74 ***	51,06 **	non
<i>Licoagrone</i>	14,39 **	93,69 *	100 *	non
<i>Semilicoisoflavone B</i>	10,2 **	90,6 *	90,96 *	non
<i>Sophoraisoflavone A</i>	7,8 **	90,60 *	97,19 *	non
<i>Uralenol</i>	10,1 **	75,82 *	100 *	non
<i>Isoliquiritin apiosid</i>	15,25 **	15,79 ***	62,37 **	non
<i>Similar</i>				
<i>Apioglycyrrhizin</i>	20,63 **	29,95 **	83,31 **	non
<i>Poncirin</i>	7,97 **	21,41 **	47,99 **	non
DHS-1	20,42 **	6,42 ***	56,08 **	non

PPB (%) :

* : >90 terikat kuat

** : <90 terikat lemah

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

LAMPIRAN 15
PREDIKSI TOKSISITAS

Tabel VII 9
Predeiksi Profil Toksisitas Senyawa Aktif

Senyawa	Karsinogenik		Mutagen (Amestest)
	Mencit	Tikus	
<i>Licoricesaponin E2</i>	+	+	Mutagen
<i>Glycyrrhizin</i>	+	+	Non Mutagen
<i>Licoricesaponin J2</i>	+	+	Non Mutagen
<i>Licoagrodin</i>	+	-	Non Mutagen
<i>Naringin</i>	-	-	Non Mutagen
<i>Licoagrone</i>	+	-	Non Mutagen
<i>Semilicoisoflavone B</i>	-	+	Non Mutagen
<i>Sophoraisoflavone A</i>	-	-	Non Mutagen
Uralenol	+	-	Mutagen
Isoliquiritin apiosid	-	-	Non Mutagen
<i>Similar</i>			
<i>Apioglycyrrhizin</i>	+	+	Non Mutagen
<i>Poncirin</i>	-	-	Non Mutagen
DHS-1	-	+	Non Mutagen

LAMPIRAN 16

VISUALISASI RESIDU ASAM AMINO 7SI9

Tabel VII 10

Visualisasi Residu Asam Amino 112 Senyawa Aktif Terhadap Reseptor 7SI9

NO	LIGAND	RESIDU ASAM AMINO
1	<i>1-(S)-2,3-Epoxy-squalene</i>	
2	<i>phaseollinisolavan</i>	PRO 168, GLN 192, THR 190, LEU 167, GLU 166, CYS 145, HIS 41, GLN 189, ARG 188
3	<i>2,3-Dihydro-4-methylfuran</i>	HIS 41
4	<i>2'-Hydroxyisolupalbigenin</i>	GLN 192
5	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	ASN 142, SER 144, GLY 143, CYS 145, LEU 141, HIS 163, PHE 140, GLU 166, HIS 41, MET 165, ASP 187
6	<i>3'-Hydroxydaidzein</i>	GLU 166, PHE 140, HIS 163, HIS 41, ASP 187
7	<i>6-C-diprenylorobol</i>	GLU 166, HIS 163, SER 144, GLY 143, LEU 141, CYS 145, ASN 142
8	<i>6-prenylisoflavone</i>	SER 144, GLY 143, LEU 141, CYS 145, HIS 163, GLU 166, PRO 168, MET 165, LEU 167
9	<i>6,8-Diprenylgenistein</i>	HIS 41, MET 165, GLU 166, LEU 141, GLY 143, ASN 142, THR 26, THR 24, THR 25
10	<i>7-Acetoxy-2-methylisoflavone</i>	HIS 41, GLY 143, CYS 145, LEU 141, SER 144, GLU 166, MET 165
11	<i>7-Hydroxy-2-methylisoflavone</i>	HIS 41, GLU 166, MET 49,
12	<i>7-O-(6''-malonylglucoside)</i>	ASN 142, HIS 164, THR 25, MET 49, HIS 41, GLY 143, CYS 145, GLU 166, SER 144
13	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	MET 165, SER 144, GLY 143, LEU 141, CYS 145, GLU 166
14	<i>Aalpha,beta-Dihydorhaponticin</i>	HIS 164, LEU 141, GLU 166, HIS 163, GLY 143, SER 144, THR 26, CYS 145, THR 25, HIS 41, ASN 142

LAMPIRAN 16
(LANJUTAN)

Tabel VII.10
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
15	<i>Afrormosin 7-O-glucoside</i>	GLN 189, MET 165, SER 144, CYS 145, ASN 142, GLY 143, LEU 141, HIS 163, GLU 166
16	<i>Anaphalisoleanenoic acid</i>	
17	<i>AraboGlycyrrhizin_out</i>	GLU 166, PHE 140, SER 144, CYS 145, GLY 143, LEU 141
18	<i>beta-Myrrin</i>	GLU 166, CYS 145, GLY 143
19	<i>Cycloartenol</i>	GLU 166, PRO 168
20	<i>Dehydroglyceollin I</i>	CYS 145, GLU 166, LEU 141
21	<i>Desoxoglabrolide</i>	GLU 166, HIS 41
22	<i>Dihydrochrysin</i>	MET 49, HIS 41, HIS 172, HIS 163, SER 144, CYS 145, GLY 143
23	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	GLN 192, PRO 168
24	<i>Erybacin B</i>	MET 165, ASN 142, SER 144, LEU 141, CYS 145
25	<i>Eurycarpin A</i>	GLN 189, ASN 142, CYS 145, LEU 141, GLY 143, SER 144, HIS 164, MET 165
26	<i>Folerogenin</i>	HIS 41, GLY 143, ASN 142, CYS 145, LEU 141, SER 144, PHE 140, GLU 166, HIS 164
27	<i>Galangin</i>	HIS 41, GLY 143, ASN 142, HIS 163, PHE 140, LEU 141, GLU 166
28	<i>Gancaonin F</i>	TYR 54, CYS 145, CYS 44, GLY 143, HIS 163, LEU 141, ASN 142
29	<i>Gancaonin I</i>	GLN 189, MET 165, GLU 166, HIS 163, SER 144, GLY 143, LEU 141, CYS 145
30	<i>Gancaonin G</i>	
31	<i>Genkwanin</i>	ARG 188, GLN 189, GLY 143, CYS 145, SER 144, LEU 141, HIS 163, GLU 166, PHE 140, MET 165
32	<i>Glabranin</i>	CYS 145, GLY 143, SER 144, PHE 140, MET 165, GLU 166, GLN 189
33	<i>Glabrene</i>	PHE 140, CYS 145, ARG 188, GLU 166

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Tabel VII.10
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NO	LIGAND	RESIDU ASAM AMINO
34	<i>Glabrocoumarin</i>	LEU 141, GLY 143, CYS 145, SER 144, ARG 188, GLN 189
35	<i>Glabroisoflavanone A</i>	TYR 54, MET 49, GLN 189, HIS 41
36	<i>Glicophenone</i>	GLY 143, ASN 142, HIS 163, CYS 145, HIS 41
37	<i>Glicoricone</i>	HIS 163, SER 144, GLY 143, CYS 145, HIS 41, ASN 142
38	<i>Glyasperin B</i>	HIS 41, GLN 189, ASN 142, LEU 141, HIS 163, SER 144
39	<i>Glyasperin D</i>	GLU 126, HIS 41, LEU 141, ASN 142, SER 144
40	<i>Glyasperin F</i>	MET 165, HIS 163, CYS 145, LEU 141, SER 144
41	<i>Glycitein</i>	LEU 141, SER 144, CYS 145, GLY 143, HIS 163, MET 165, GLN 189, THR 190, ARG 168
42	<i>Glycyrrhetic acid</i>	GLY 143, GLN 189, THR 190, CYS 145
43	<i>Glycyrrhisoflavone</i>	GLN 189, HIS 164, HIS 163, GLY 143, SER 144, LEU 141, CYS 145
44	<i>Glycirrhizin</i>	HIS 164, GLU 166, MET 165, HIS 41, MET 49, GLN 189, ARG 188, HIS 163, CYS 145, LEU 141, SER 144, GLY 143
45	<i>Glyinflarin B</i>	HIS 41, MET 49, GLN 189, ARG 188, MET 165, GLU 166, HIS 163, SER 144, CYS 145, LEU 141
46	<i>Glyinflarin A</i>	ARG 188, GLN 192, HIS 41, SER 144, GLY 143, CYS 145, HIS 163, LEU 141, GLU 166
47	<i>Glyurallin</i>	ARG 188, GLN 189, GLU 166, HIS 41, CYS 145, SER 144, LEU 141, GLY 143, HIS 163, HIS 164
48	<i>Glyzaglabrin</i>	ASP 187, GLN 189, GLU 166, HIS 163, LEU 141, ASN 142, CYS 145, HIS 164

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Tabel VII.10
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
49	<i>Hirtellanin I</i>	GLU 166, HIS 41, MET 165, ASP 187, HIS 164, LEU 141, ASN 142
50	<i>Hispaglabridin</i>	
51	<i>Hydroxywighteone</i>	GLN 192, GLU 166, CYS 145, GLY 143, SER 144, LEU 141, HIS 41, HIS 164, MET 165, ARG 188
52	<i>Isobavachalcone</i>	ASP 187, ARG 188, MET 49, HIS 41, GLU 166, GLN 192, THR 190, PRO 168, THR 190, ALA 191
53	<i>Isoglabrolide</i>	ASP 187, ARG 188, MET 49, HIS 41, GLU 166, GLN 192, THR 190, PRO 168, THR 190, ALA 191
54	<i>Isoliquiritin apioside</i>	HIS 41, THR 26, MET 49, GLY 143, ASN 142, CYS 145, PRO 168, ALA 191, THR 190, GLN 192, ARG 188, MET 165,
55	<i>Isoliquiritin</i>	
56	<i>Isomedicarpin</i>	HIS 163, ASN 142, PRO 168, THR 190, GLN 192, ARG 188
57	<i>Isomucronulatoll</i>	PHE 140, ASN 142, HIS 41, MET 165, CYS 145, HIS 163, LEU 141
58	<i>Isotachioside</i>	THR 25, HIS 41, MET 165, GLU 166, HIS 163, PHE 140, LEU 141, SER 144, CYS 145, GLY 143, ASN 142
59	<i>Isovitexin</i>	CYS 145, LEU 141, SER 144, GLY 143, HIS 41, ASN 142, MET 165, PRO 168, GLN 192, GLU 166
60	<i>Kaempferol 3-O-methyl ether</i>	ASN 142, THR 25, HIS 41, LEU 141, CYS 145, SER 144, HIS 163, MET 165, GLU 166
61	<i>Kanazolol Y</i>	GLU 166, MET 165, ARG 188, CYS 145, GLY 143, HIS 163, ASN 142, GLN 189
62	<i>Kanazolol Z</i>	GLN 189, ARG 188, HIS 41, PRO 168, MET 165, GLU 166, CYS 145, HIS 163, ASN 142, LEU 141

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Tabel VII.10
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NO	LIGAND	RESIDU ASAM AMINO
63	Kanazolol R	HIS 41, GLN 192
64	Licoagroaurone	HIS 163, CYS 149, GLY 143, SER 144, GLU 166, GLN 192, ARG 188, GLN 189, MET 165, HIS 41, MET 49,
65	Licoagrochalcone A	HIS 41, MET 165, GLN 189, ARG 188, GLU 166, HIS 163, SER 144, CYS 145, GLY 143, ASN 142
66	Licoagrochalcone B	ARG 188, MET 165, ASN 142, CYS 145, GLN 189
67	Licoagrochalcone D	HIS 41, ARG 188, MET 165, THR 190, GLN 189
68	<i>Licoagrodin</i>	CYS 145, HIS 41, GLN 189, ARG 188, GLN 192, THR 190
69	<i>Licoagrone</i>	CYS 145, HIS 41, MET 49, GLN 192, PRO 168, MET 165, GLU 166
70	Licoagroside A	MET 49, GLY 143, CYS 145, SER 144, HIS 163, GLU 166, MET 165, PRO 168, GLN 192
71	Licoarylcoumarin	ASN 142, CYS 145, LEU 141, GLY 143, SER 144, HIS 163, GLU 166, MET 165, GLN 192, GLN 189, PRO 188
72	Licochalcone B	ASN 142, SER 144, CYS 145, LEU 141, GLY 143, MET 165, HIS 41, GLN 189, MET 49, GLU 166
73	Licochalcone C	MET 49, HIS 41, GLN 189, LEU 141, SER 144, CYS 145, GLY 143
74	Licocoumarin A	GLN 189, GLU 166, MET 165, HIS 41, CYS 145, PRO 168, GLN 192
75	Licoflavanone	GLN 192, HIS 41, ASN 142, HIS 163 SER 144, GLU 166, MWT 165, CYS 145
76	Licoflavanol	ASN 142, HIS 41, PRO 168, GLN 192
77	Licopyranocoumarin	HIS 164, HIS 41, ASN 142, GLY 143

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Tabel VII.10
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
78	<i>Licoricesaponin B2</i>	GLN 189, ASN 142, GLY 143, SER 144, HIS 163, CYS 145, GLU 166, HIS 164, HIS 41
79	<i>Licoricesaponin E2</i>	GLN 192, THR 190, PRO 168, GLU 166, GLN 189, ASN 142, GLY 143, LEU 141, HIS 163, SER 144, MET 165, CYS 145, HIS 164, HIS 41
80	<i>Licoricesaponin J2</i>	GLU 166, PRO 168, GLN 192, THR 190, GLN 189, HIS 41, MET 165, ASN 142, SER 144, LEU 141, GLY 143, CYS 145, HIS 163
81	<i>Native ligan</i>	PRO 168, GLN 192, THR 190, GLU 166, PHE 140, HIS 163, HIS 172, MET 49, HIS 41, GLN 189, LEU 167, PRO 168
82	<i>Luqcoumarin</i>	GLU 166, ASN 142, GLN 189, HIS 41, MET 49, MET 165
83	<i>Liquiritic acid</i>	HIS 41, MET 49, MET 165, GLU 166, ASN 142
84	<i>Liquiritigenin 7-glucoside-4'-apiosyl</i>	THR 26, GLY 143, ASN 142, GLU 166, LEU 141, SER 144, HIS 41
85	<i>Liquiritin</i>	HIS 41, MET 49, CYS 145, SER 144, MET 165, GLU 166, HIS 163, LEU 141, GLY 143, ASN 142, THR 26, THR 25
86	<i>Liquoric acid</i>	ASN 142, MET 165, CYS 145, HIS 41, MET 49, GLY 143, THR 25, THR 26
87	<i>Lupeol</i>	ASN 142, THR 26, HIS 41
88	<i>Lupiwighteone</i>	ASN 142, HIS 41
89	<i>Luteone</i>	GLU 166, ASN 142, SER 144, GLY 143, CYS 145
90	<i>Molnupiravir</i>	GLU 166, HIS 41, CYS 145, GLY 143, SER 144, ASN 142, GLN 189, GLU 166
91	<i>Mulberoffuran A</i>	THR 190, PRO 168, GLN 192, GLN 189, MET 49, HIS 41, GLU 166

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Tabel VII.10
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NO	LIGAND	RESIDU ASAM AMINO
92	<i>Naringin</i>	GLU 166, CYS 145, PRO 168, THR 190, GLN 192, HIS 164, HIS 41, MET 49
93	<i>Odoratin</i>	HIS 41, GLN 192, THR 190, PRO 168, GLU 166, MET 49
94	<i>Parvisoflavone</i>	LEU 141, ASN 142, GLY 143, SER 144, CYS 145
95	<i>Paxlovid</i>	GLN 189, GLN 192, LEU 167, PRO 168, THR 190, MET 165, GLU 166, CYS 145, LEU 141, ASN 142, GLY 143, ASN 142, SER 144
96	<i>phaseollinisoflavan</i>	PRO 168, LEU 167, GLU 166, HIS 41, MET 165 GLN 189, GLN 192, THR 190
97	<i>Pinocembroside</i>	HIS 41, GLU 166, HIS 163, PHE 140, GLY 143
98	<i>Prunetin</i>	GLU 166, HIS 41, HIS 163, PHE 140
99	<i>Puerarin</i>	THR 190, PRO 168, GLN 192, GLN 189, GLU 166, LEU 141, CYS 145, SER 144, GLY 143, HIS 164
100	<i>Rocymosin B</i>	GLN 189, ASP 187, TYR 54, HIS 164, ASN 142, GLU 166, HIS 163, LEU 141, SER 144, GLY 143, CYS 145
101	<i>Scanderone</i>	GLU 166, ASN 142, SER 144, LEU 141, GLY 143, CYS 145, HIS 163
102	<i>Semilicoisoflavone B</i>	LEU 141, SER 144, PHE 140, HIS 41, ASN 142
103	<i>Senegalensin</i>	PHE 140, HIS 163, MET 165, HIS 41, PRO 168, GLN 189, ARG 188, LEU 141
104	<i>Sophoraisoflavone A</i>	SER 144, GLY 143, LEU 141, CYS 145, HIS 163, HIS 164, MET 165, GLN 189, ARG 188
105	<i>Tachiogroside B</i>	LEU 141, ASN 142, SER 144, GLY 143, HIS 164, CYS 145, HIS 41, ASP 187, TYR 54, GLN 189, HIS 163

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NO	LIGAND	RESIDU ASAM AMINO
106	<i>Tachioside</i>	ASN 142, GLY 143, HIS 164, MET 165, HIS 163, CYS 145, SER 144, LEU 141, HIS 41
107	<i>Tephtrinone</i>	ASN 142, GLY 143, CYS 145, HIS 41, MET 165
108	<i>Uralenol</i>	HIS 41, ASN 142, HIS 163, SER 144, MET 165, GLU 166
109	<i>Uralsaponin M</i>	GLU 166, PRO 168, ASN 142, THR 25, SER 144, HIS 41, CYS 145, MET 165
110	<i>Wogonoside</i>	PRO 168, GLU 166, ASN 142, THR 25, THR 26, GLY 143, CYS 145, SER 144, MET 165
111	<i>(S)-2,3-Epoxysqualene</i>	ARG 188, HIS 41, CYS 145, LEU 167, PRO 168, GLN 192
112	<i>Kaempferol</i>	ARG 188, GLN 189, GLY 143, ASN 142, CYS 145, SER 144, HIS 163, LEU 141, GLU 166, MET 165

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VISUALISASI RESIDU ASAM AMINO 7NG6

Tabel VII 11

Visualisasi Residu Asam Amino 112 Senyawa Aktif Terhadap Reseptor 7NG6

NO	LIGAND	RESIDU ASAM AMINO
1	<i>1-(S)-2,3-Epoxyqualene</i>	
2	<i>phaseollinisolavan</i>	ASP 187
3	<i>2,3-Dihydro-4-methylfuran</i>	
4	<i>2'-Hydroxyisolupalbigenin</i>	GLN 189, CYS 145
5	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	ASN 142, SER 144, LEU 141, PHE 140, CYS 145, HIS 163, GLU 166, GLN 189, ARG 188
6	<i>3'-Hydroxydaidzein</i>	
7	<i>6-C-diprenylorobol</i>	GLU 166, ALA 191, GLN 192, GLN 189
8	<i>6-prenylisoflavone</i>	GLN 189, HIS 41, MET 49, CYS 44, CYS 145, MET 165, PRO 168, ALA 191, GLN 192
9	<i>6,8-Diprenylgenistein</i>	GLN 192, GLU 166, HIS 163, LEU 141, ASN 142, SER 144, CYS 145, ARG 188, GLN 189, ALA 191, GLN 192
10	<i>7-Acetoxy-2-methylisoflavone</i>	CYS 145, HIS 41, LEU 141, ASN 142, GLU 166, GLN 189
11	<i>7-Hydroxy-2-methylisoflavone</i>	HIS 41, CYS 145, ASN 142, GLU 166
12	<i>7-O-(6''-malonylglucoside)</i>	TYR 54, CYS 145, HIS 41, GLN 189, ASN 142, MET 49
13	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	MET 49, GLN 189, GLU 166, HIS 163, LEU 141, SER 144, CYS 145, MET 165, HIS 41
14	<i>Aalpha,beta-Dihydrorhaponticin</i>	CYS 145, ASN 142, LEU 141, PHE 140, HIS 163, HIS 172, HIS 41, GLN 192, GLN 189, GLU 166
15	<i>Afrormosin 7-O-glucoside</i>	GLN 189, MET 165, SER 144, LEU 141, ASN 142, CYS 145, HIS 163, HIS 172, PHE 140, GLU 166
16	<i>Anaphalisoleanenoic acid</i>	PHE 140, HIS 163, CYS 145, MET 165
17	<i>Araboglycyrrhizin</i>	GLN 189, PHE 140, HIS 163, SER 144, GLU 166, GLN 192, ASN 142

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NO	LIGAND	RESIDU ASAM AMINO
18	<i>beta-Amyrin</i>	ASN 142, GLN 192, ALA 191, GLU 166, GLN 189, PHE 140
19	<i>Cycloartenol</i>	
20	<i>Dehydroglyceollin I</i>	MET 165, HIS 41, CYS 145
21	<i>Desoxoglabrolide</i>	MET 165
22	<i>Dihydrochrysin</i>	MET 165, HIS 41, CYS 145, HIS 163, PHE 140
23	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	HIS 41, HIS 163, PHE 140, ASN 142
24	<i>Erybacin B</i>	PHE 140, HIS 163, GLU 166, ASN 142
25	<i>Eurycarpin A</i>	GLN 189, GLU 166, HIS 163, LEU 141, PHE 140
26	<i>Folerogenin</i>	HIS 41, HIS 163, SER 144, LEU 141, GLN 189, GLU 166
27	<i>Galangin</i>	HIS 41, GLN 189, GLU 166
28	<i>Gancaonin F</i>	HIS 41, MET 165, GLU 166, GLN 189
29	<i>Gancaonin I</i>	HIS 41, CYS 145, HIS 163, MET 165, GLU 166, GLN 189, THR 190, GLN 192, ALA 191
30	<i>Gancaonin G</i>	
31	<i>Genkwanin</i>	ALA 191, GLN 192
32	<i>Glabranin</i>	MET 165, MET 49, HIS 41
33	<i>Glabrene</i>	ASP 187, CYS 145, GLU 166, PHE 140
34	<i>Glabrocoumarin</i>	ASP 187, CYS 145, MET 165, PHE 140, GLU 166
35	<i>Glabroisoflavanone A</i>	MET 165, GLN 189
36	<i>Glicophenone</i>	
37	<i>Glicoricone</i>	LEU 141, HIS 164, GLN 189
38	<i>Glyasperin B</i>	GLN 189, HIS 164
39	<i>Glyasperin D</i>	GLN 189, HIS 164, HIS 41, LEU 141
40	<i>Glyasperin F</i>	HIS 163, PHE 140, HIS 41, ARG 188, ASN 142
41	<i>Glycitein</i>	ASN 142, ARG 188

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NO	LIGAND	RESIDU ASAM AMINO
42	<i>Glycyrrhetic acid</i>	SER 144, ASN 142, CYS 145, GLU 166, ALA 191, GLN 192, LEU 141, PHE 140
43	<i>Glycyrrhisoflavone</i>	HIS 163, LEU 141, SER 144, PHE 140, GLU 166
44	<i>Glycirrhizin</i>	GLN 189, ASN 142, THR 190, ALA 191, HIS 41, CYS 145, HIS 164
45	<i>Glyinflanin B</i>	SER 144, CYS 145, GLU 166
46	<i>Glyinflanin A</i>	PHE 140, HIS 163, ARG 188, CYS 145, ASN 142, GLY 143
47	<i>Glyurallin</i>	ALA 191, GLN 192, ARG 188, CYS 145
48	<i>Glyzaglabrin</i>	GLU 166, CYS 145
49	<i>Hirtellanin I</i>	GLU 166, MET 165, VAL 186, ARG 188, HIS 41, LEU 141, PHE 140
50	<i>Hispaglabridin</i>	ARG 188, MET 165, PHE 140, LEU 141, GLU 166, CYS 145, ASN 142
51	<i>Hydroxywighteone</i>	GLN 192, GLU 166, ASN 142, PHE 140, SER 144, HIS 163, CYS 145, HIS 41, ARG 188, ALA 191
52	<i>Isobavachalcone</i>	ASN 142, LEU 141, PHE 140, HIS 163, SER 144, CYS 145, MET 49, MET 165, ARG 188, ASP 187, HIS 41, GLU 166
53	<i>Isoglabrolide</i>	GLU 166, HIS 163, LEU 141, MET 165
54	<i>Isoliquiritin apioside</i>	MET 49, GLN 189, ARG 188, GLY 143, GLU 166, SER 144, LEU 141, PHE 140, CYS 145, HIS 163, ASN 119, MET 165, ASN 142, THR 26, THR 25
55	<i>Isoliquiritin</i>	THR 190, GLN 192, MET 165, GLU 166, HIS 163, LEU 141, SER 144, ASN 142, HIS 164, CYS 145, GLY 143, GLN 189
56	<i>Isomedicarpin</i>	LEU 141, SER 144, HIS 163, GLN 189, THR 190
57	<i>Isomucronulatoll</i>	MET 165, HIS 164, HIS 163, LEU 141, ASN 142, CYS 145

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Tabel VII.11
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NO	LIGAND	RESIDU ASAM AMINO
58	<i>Isotachioside</i>	HIS 164, MET 165, PHE 140, GLU 166, LEU 141, CYS 145, GLY 143, ASN 142, GLN 189
59	<i>Isovitexin</i>	GLN 189, THR 190, ARG 188, MET 165, ASN 142, LEU 141, GLY 143, SER 144, CYS 145, PHE 140, GLU 166, GLN 192, PRO 168
60	<i>Kaempferol 3-O-methyl ether</i>	GLU 166, HIS 172, MET 165, ARG 188, GLN 189, MET 49, ASN 142, LEU 141, HIS 163, PHE 140
61	<i>Kanazolol Y</i>	
62	<i>Kanazolol Z</i>	GLU 166, MET 165, GLN 189, CYS 145, MET 49, HIS 41
63	<i>Kanazolol R</i>	
64	<i>Licoagroaurone</i>	PHE 140, GLU 166, ASN 142, LEU 141, CYS 145, HIS 41, VAL 186, MET 165
65	<i>Licoagrochalcone A</i>	PHE 140, HIS 163, HIS 41, ARG 188, VAL 186, GLY 143, CYS 145, LEU 141, ASN 142, GLU 166, MET 165
66	<i>Licoagrochalcone B</i>	CYS 145, LEU 141, ASN 142, PHE 140, GLU 166, ARG 188, HIS 41
67	<i>Licoagrochalcone D</i>	PHE 140, ASN 142, HIS 41, GLU 166, ARG 188
68	<i>Licoagrodin</i>	THR 190, ARG 188, GLN 192, HS 41, ASN 142, PHE 140
69	<i>Licoagrone</i>	HIS 163, CYS 145, HIS 41, ASN 142, MET 49, LEU 167, GLU 166, GLN 192, THR 190, PRO 168, LEU 141
70	<i>Licoagroside A</i>	PRO 168, LEU 167, ARG 188, MET 49, VAL 186, HIS 41, HIS 163, ASN 142, GLU 166, GLN 189
71	<i>Licoarylcoumarin</i>	ASN 142, CYS 145, HIS 145, ARG 188, MET 165, GLN 189, GLN 192, ALA 191, THR 190, GLU 166

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NO	LIGAND	RESIDU ASAM AMINO
72	<i>Licochalcone B</i>	HIS 41, MET 165, GLN 189, ALA 191, THR 190, GLN 192
73	<i>Licochalcone C</i>	ALA 191, MET 165, GLU 168, CYS 145, ASN 142, HIS 41, GLN 189
74	<i>Licocoumarin A</i>	HIS 41, GLU 166, HIS 163, ALA 191, GLN 192, MET 165
75	<i>Licoflavanone</i>	HIS 163, PHE 140, GLU 166, HIS 172, MET 165, GLN 192, VAL 186, MET 49, HIS 41, ASN 142
76	<i>Licoflavonol</i>	MET 49, TYR 54, ASP 187, CYS 145, HIS 41, ASN 142, LEU 141, PHE 140, GLU 166, MET 165
77	<i>Licopyranocoumarin</i>	HIS 164, THR 190, GLN 192, GLN 189, MET 49, ASN 142, GLY 143, CYS 145, LEU 141
78	<i>Licoricesaponin B2</i>	HIS 41, HIS 164, PHE 140, LEU 141, ASN 142, GLU 166, GLN 189, GLN 192, THR 190, VAL 189, ARG 188
79	<i>Licoricesaponin E2</i>	GLN 189, THR 190, ARG 188, GLU 166, PHE 140, ASN 142, SER 144, CYS 145, HIS 163, MET 165, LEU 141
80	<i>Licoricesaponin J2</i>	MET 49, HIS 164, HIS 41, ASP 187, GLN 189, VAL 186, CYS 145, GLU 166, HIS 163, ARG 188, MET 165, ASN 142, THR 190, ALA 191
81	<i>Native ligan</i>	PRO 168, ALA 191, GLN 192, THR 190, ARG 188, GLU 166, GLN 189, HIS 164, MET 49, HIS 41, MET 165, CYS 145, ASP 187, HIS 163, PHE 140, ASN 142
82	<i>Luqcoumarin</i>	MET 49, HIS 41, CYS 145, HIS 163, GLU 166, MET 165, GLN 189
83	<i>Liquiritic acid</i>	PHE 140, GLU 166, CYS 145, HIS 163, GLN 189, MET 165, PRO 168, ALA 191, GLN 192

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NO	LIGAND	RESIDU ASAM AMINO
84	<i>Liquiritigenin 7-glucoside-4'-apiosyl</i>	PRO 168, LEU 167, THR 169, HIS 164, HIS 41, GLN 189, GLU 166, MET 165, CYS 145, ASN 142, LEU 141, PHE 140
85	<i>Liquiritin</i>	GLN 189, MET 165, HIS 164, ASN 142, LEU 141, HIS 163, GLU 166, THR 190, GLN 192, ARG 188, PRO 168, LEU 167
86	<i>Liquoric acid</i>	GLN 192, GLN 189, PRO 168, THR 190, MET 165, GLU 166, PHE 140, ASN 142
87	<i>Lupeol</i>	GLN 189, HIS 41, ASN 142
88	<i>Lupiwighteone</i>	GLN 192, ARG 188, ALA 191, HIS 41, CYS 145, ASN 142, GLU 166, THR 190, ALA 191
89	<i>Luteone</i>	GLN 192, GLU 166, ASN 142, CYS 145, HIS 41, ARG 188, ALA 191
90	<i>Molnupiravir</i>	PHE 140, HIS 163, GLU 166, SER 144, HIS 172, LEU 141
91	<i>Mulberoffuran A</i>	GLN 189, THR 190, GLU 166, HIS 163, PHE 140, LEU 141, SER 144
92	<i>Naringin</i>	PHE 140, HIS 163, CYS 145, HIS 164, GLU 166, HIS 164, PRO 168, GLN 192, THR 190, GLN 189, HIS 41, MET 48
93	<i>Odoratin</i>	PHE 140, HIS 164, GLU 166, CYS 145, HIS 41, MET 49, VAL 186, ARG 188, GLN 189
94	<i>Parvisoflavone</i>	ASN 142, PHE 140, HIS 163, MET 165, GLU 166, HIS 164, MET 49, HIS 41, ARG 188, GLN 189
95	<i>Paxlovid</i>	HIS 41, ASN 142, SER 144, LEU 141, MET 165, HIS 163, CYS 145, PHE 140, HIS 172, GLU 166, GLN 189, THR 190, HIS 164, THR 190, ARG 188
96	<i>phaseollinisoflavan</i>	ASN 142, CYS 145, HIS 41, HIS 164, GLU 166, MET 165, ARG 188, THR 190

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Tabel VII.11
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
97	<i>Pinocembroside</i>	ASN 142, CYS 44, THR 25, SER 46, THR 24, MET 49, HIS 41, CYS 145, ARG 188, HIS 164, GLN 189, GLU 166
98	<i>Prunetin</i>	PHE 140, ASN 142, GLU 166, GLN 189, HIS 41, MET 49, HIS 164
99	<i>Puerarin</i>	GLN 192, ARG 188, HIS 41, CYS 154, ASN 142, PHE 140, GLU 166, GLN 189, ALA 191
100	<i>Rocymosin B</i>	LEU 141, PHE 140, HIS 163, ASN 142, GLU 166, MET 165, HIS 164, CYS 145, HIS 41, MET 49
101	<i>Scanderone</i>	LEU 141, PHE 140, HIS 163, GLU 166, CYS 145, METT 165, HIS 164, HIS 41, ASN 142, ARG 188, VAL 186
102	<i>Semilicoisoflavone B</i>	HIS 163, PHE 140, GLU 166, ARG 188, MET 49, HIS 164, CYS 145, ASN 142
103	<i>Senegalensin</i>	ARG 188, MET 165, HIS 41, CYS 44, MET 49, GLU 166, CYS 45, SER 144, PHE 140, HIS 163
104	<i>Sophoraisoflavone A</i>	PHE 140, HIS 163, GLU 166, MET 165, ARG 188, MET 49, HIS 41, CYS 145
105	<i>Tachiogroside B</i>	SER 144, PHE 140, LEU 141, ASN 142, MET 49, VAL 186, ARG 188, GLU 166, THR 190
106	<i>Tachioside</i>	SER 144, HIS 163, LEU 141, ASN 142, CYS 145, HIS 164, PHE 140, GLN 189, HIS 41, GLU 166, HIS 172, ARG 188
107	<i>Tephrinone</i>	GLN 189, HIS 41, HIS 164
108	<i>Uralenol</i>	HIS 41, ALA 191, GLN 192, GLU 166
109	<i>Uralsaponin M</i>	THR 169, HIS 164, GLN 189, GLU 166, CYS 145, SER 144, ASN 142, LEU 141, PHE 140

**LAMPIRAN 17
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Tabel VII.11
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
110	<i>Wogonoside</i>	ARG 188, GLN 189, THR 190, PHE 140, ASN 142, GLU 166, HIS 163, GLU 166, HIS 163, SER 144, LEU 141, GLY 143, CYS 145, HIS 164
111	<i>(S)-2,3-Epoxysqualene</i>	ASP 187, HIS 41
112	<i>Kaempferol</i>	MET 49, GLN 189, ASN 142, PHE 140, HIS 163, SER 144, LEU 141, CYS 145, GLU 166, MET 165

LAMPIRAN 18

VISUALISASI RESIDU ASAM AMINO 7DPU

Tabel VII 12

Visualisasi Residu Asam Amino 112 Senyawa Aktif Terhadap Reseptor 7SI9

NO	LIGAND	RESIDU ASAM AMINO
1	<i>1-(S)-2,3-Epoxyqualene</i>	MET49, HIS41, GLN189
2	<i>phaseollinisolavan</i>	HIS41, GLN189, ASN119
3	<i>2,3-Dihydro-4-methylfuran</i>	TYR54
4	<i>2'-Hydroxyisolupalbigenin</i>	HIS41, THR25, THR24, GLU166, GLN189, PRO168, ASN142, MET165
5	<i>3-Methyl-2-butenyl 6-O-alpha-L-arabinopyranosyl-beta-D-glucopyranoside</i>	GLU166, GLU166, CYS44, MET49, HIS41, THR25, GLN189,
6	<i>3'-Hydroxydaidzein</i>	MET165, ARG188, HIS41, MET49, THR25, THR26, GLU166, GLN189
7	<i>6-C-diprenylorobol</i>	MET165, ARG188, HIS41, MET49, GLY143, GLU166, GLN189, PRO168
8	<i>6-prenylisoflavone</i>	MET165, ARG188, HIS41, MET49, CYS145, GLU166, GLN189, THR24, THR26, GLY143
9	<i>6,8-Diprenylgenistein</i>	MET165, ARG188, HIS41, MET49, CYS145, GLU166, GLN189, GLY143, ASN142, LEU167
10	<i>7-Acetoxy-2-methylisoflavone</i>	GLY143, LEU27, THR26, MET49, HIS41, THR25, GLN189
11	<i>7-Hydroxy-2-methylisoflavone</i>	MET165, ARG188, HIS41, MET49, GLY143, GLU166, GLN189, PRO168, CYS145
12	<i>7-O-(6''-malonylglucoside)</i>	MET165, ARG188, HIS41, MET49, CYS145, GLU166, GLN189, GLY143, ASN142, LEU167, CYS44
13	<i>7,4'-Dihydroxy-3'-methoxyisoflavan</i>	GLU166, GLN189, GLY143, MET49, ASN142, MET165
14	<i>Aalpha,beta-Dihydrohaponticin</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, ARG188
15	<i>Afrormosin 7-O-glucoside</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, ARG188, THR26, THR25, CYS145, GLY143
16	<i>Anaphalisoleanoic acid</i>	GLU166, GLN189, MET165, THR25, HIS41, ARG188, THR25, CYS145, GLY143, LEU27, GLY143
17	<i>Araboglycyrrhizin</i>	GLU166, GLN189, MET165, THR26, HIS41, ARG188, THR24, CYS145, GLY143, LEU27, GLY143, ASN119

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
18	<i>beta-Amyrin</i>	GLN189, MET49, HIS41, MET165, GLU166, ASN142, GLY143
19	<i>Cycloartenol</i>	MET165, MET49, HIS41, GLN189, GLY143, ASN142, GLU166,
20	<i>Dehydroglyceollin I</i>	GLU166, GLN189, MET165, THR26, HIS41, ARG188, THR24, CYS145, GLY143, THR25, GLY143, ASN119
21	<i>Desoxoglabrolide</i>	GLU166, GLN189, MET165, THR25, HIS41, ARG188, THR24, CYS145, GLY143, LEU27, GLY143, ASN142
22	<i>Dihydrochrysin</i>	ARG188, CYS145, HIS41, GLN189, MET165, GLU166, THR25
23	<i>Docosyl-3,4-dihydroxy-trans-cinnamate</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, THR25, CYS145, GLY143, PRO52, SER46
24	<i>Erybacin B</i>	ARG188, CYS145, HIS41, GLN189, MET165, GLU166, THR25, MET49, GLY143, CYS145
25	<i>Eurycarpin A</i>	ARG188, CYS145, HIS41, GLN189, MET165, GLU166, THR25, THR26, MET49, GLY143, CYS145, HIS164
26	<i>Folerogenin</i>	ASP187, GLU166, GLN189, MET165, THR25, HIS41, ARG188, THR26, CYS145, GLY143, LEU27, GLY143, ASN142
27	<i>Galangin</i>	ASP187, GLU166, GLN189, MET165, THR25, HIS41, THR26, THR25, CYS145, LEU27
28	<i>Gancaonin F</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR26, HIS41, THR26, THR25, CYS145, GLY143, ASN142
29	<i>Gancaonin I</i>	ARG188, CYS145, HIS41, GLN189, MET165, GLU166, THR25, THR24, THR26
30	<i>Gancaonin G</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, THR26, HIS41, THR26, THR25, CYS145, MET49
31	<i>Genkwanin</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, GLY143, PRO52, CYS44
32	<i>Glabranin</i>	ASP187, GLU166, GLN189, MET165, THR25, THR26, HIS41, CYS145, MET49, LEU27

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
33	<i>Glabrene</i>	GLU166, GLN189, MET165, THR25, THR24, THR26, HIS41, THR26, CYS145, MET49, LEU27, SER46
34	<i>Glabrocoumarin</i>	THR45, GLU166, GLN189, MET165, THR25, THR24, THR26, HIS41, THR26, CYS145, MET49, CYS44
35	<i>Glabroisoflavanone A</i>	GLU166, GLY143, GLN189, MET165, HIS41, THR26, CYS145, MET49, LEU27, THR25,
36	<i>Glicophenone</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, GLY143, PRO52, CYS44
37	<i>Glicoricone</i>	ARG188, CYS145, HIS41, GLN189, MET165, GLU166, THR25, THR24, THR26, HIS164
38	<i>Glyasperin B</i>	ASP187, GLU166, GLN189, MET165, THR25, HIS41, THR26, GLY143, HIS164
39	<i>Glyasperin D</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, GLY143, ARG188
40	<i>Glyasperin F</i>	ASP187, GLU166, GLN189, MET165, HIS41, CYS145, MET49, LEU27, THR190, ASN142
41	<i>Glycitein</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, THR26, HIS41, THR26, CYS145, GLY143, PRO52
42	<i>Glycyrrhetic acid</i>	LEU167, PRO168, THR25, GLN189, CYS145, GLY143, MET49, MET165, ASN142, GLU166
43	<i>Glycyrrhisoflavone</i>	GLU166, GLN189, MET165, THR25, HIS41, THR26, THR24, GLY143, HIS164, ARG188, CYS145
44	<i>Glycirrhizin</i>	GLU166, GLN189, MET165, THR25, THR24, THR26, HIS41, THR26, CYS145, MET49, LEU27, SER46, ASN142, PRO168,ASN119,
45	<i>Glyinflarin B</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, GLY143, PRO52
46	<i>Glyinflarin A</i>	ASP187, TYR54, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, PRO52, SER46

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
47	<i>Glyurallin</i>	ASP187, TYR54, LEU167, PRO168, GLN189, CYS145, GLY143, MET49, MET165, ASN142, GLU166, GLU170
48	<i>Glyzaglabrin</i>	GLU166, GLN189, MET165, HIS41, CYS145, MET49, LEU27, ARG188, THR25, THR26
49	<i>Hirtellain I</i>	ASP187, GLU166, GLN189, MET165, THR25, HIS41, THR26, CYS145, GLY143, ASN142, CYS145, ARG188, MET49
50	<i>Hispaglabridin</i>	ASP187, TYR54, LEU27, GLN189, CYS145, GLY143, MET49, MET165, ASN142, GLU166, ARG188, HIS41
51	<i>Hydroxywighteone</i>	THR26, HIS41, ASP187, MET49, GLU166, TYR54, CYS44
52	<i>Isobavachalcone</i>	CYS145, HIS41, MET49, GLU166, GLN189, SER46, MET165
53	<i>Isoglabrolide</i>	CYS145, HIS41, MET49, GLU166, GLN189, MET165
54	<i>Isoliquiritin apioside</i>	ASP187, TYR54, LEU27, CYS145, GLY143, MET49, MET165, ASN142, GLU166, HIS41, SER46
55	<i>Isoliquiritin</i>	CYS145, HIS41, MET49, THR24, GLN189, THR26, ASN119, GLY143,
56	<i>Isomedicarpin</i>	GLN189, ASP187, MET49, HIS41
57	<i>Isomucronulatoll</i>	GLN189, GLU166, MET49, HIS41, MET165, CYS145
58	<i>Isotachioside</i>	ASP187, GLN189, GLU166, MET49, HIS41, MET165, CYS145, THR25, HIS164
59	<i>Isovitexin</i>	ASP187, GLN189, GLY143, MET49, HIS41, MET165, CYS145, THR26, ASN119
60	<i>Kaempferol 3-O-methyl ether</i>	GLN189, GLU166, HIS41, MET165, THR25
61	<i>Kanazolol Y</i>	GLN189, GLU166, HIS41, THR25, GLY143
62	<i>Kanazolol Z</i>	GLN189, GLU166, HIS41, MET165, THR25, CYS145
63	<i>Kanazolol R</i>	GLN189, GLU166, MET165, ARG188, ASP187, HIS41, CYS145
64	<i>Licoagroaurone</i>	GLN189, GLU166, MET165, ARG188, CYS145, HIS41

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
65	<i>Licoagrochalcone A</i>	GLN189, GLU166, MET165, ARG188, CYS145, HIS41, MET49
66	<i>Licoagrochalcone B</i>	ASP187, TYR54, GLN189, GLU166, MET165, CYS145, HIS41
67	<i>Licoagrochalcone D</i>	ASP187, TYR54, GLN189, GLU166, GLY143, THR26, HIS41
68	<i>Licoagrodin</i>	THR24, THR26, GLU166, CYS44
69	<i>Licoagrone</i>	LEU27, GLN189, GLU166, MET165, THR24, CYS145, HIS41, MET49, CYS145
70	<i>Licoagroside A</i>	LEU27, GLN189, GLY143, THR26, MET165, THR24, CYS145, HIS41, MET49, CYS145
71	<i>Licoarylcoumarin</i>	LEU27, GLN189, GLY143, THR26, MET165, THR24, CYS145, HIS41, MET49, CYS145, THR25, CYS44
72	<i>Licochalcone B</i>	ASP187, TYR54, GLN189, GLU166, GLY143, HIS41, CYS145, THR25,
73	<i>Licochalcone C</i>	ASP187, TYR54, GLN189, GLU166, GLY143, HIS41, CYS145,
74	<i>Licocoumarin A</i>	MET49, THR24, THR26, GLU166, CYS145, GLN189
75	<i>Licoflavanone</i>	ASP187, MET49, THR25, THR26, GLU166, CYS145, HIS41
76	<i>Licoflavanol</i>	HIS41, ASP187, GLU166, GLY143
77	<i>Licopyranocoumarin</i>	HIS41, HIS164, GLU166, GLY143, ASN142, PRO168
78	<i>Licoricesaponin B2</i>	THR24, SER46, GLN189, MET49, THR25, THR26, GLU166, CYS145, HIS41
79	<i>Licoricesaponin E2</i>	THR24, SER46, MET49, THR25, THR26, ASN142, HIS41
80	<i>Licoricesaponin J2</i>	THR24, LEU167, MET49, THR25, THR26, ASN142, HIS41, GLN189, GLU166
81	<i>Native ligan</i>	GLN189, CYS44, PRO52, MET49, THR25, THR26, GLU166, CYS145, HIS41, ASN142
82	<i>Luqcoumarin</i>	HIS41, GLU166, GLY143, PRO52, CYS44, GLN189, MET165
83	<i>Liquiritic acid</i>	HIS41, THR25

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
84	<i>Liquiritigenin 7-glucoside-4'-apiosyl</i>	CYS145, GLN189, GLU166, MET49, THR25, THR26, ASN142, HIS41
85	<i>Liquiritin</i>	HIS41, GLU166, GLY143, GLN189, CYS145
86	<i>Liquoric acid</i>	MET49, GLU166, GLY143, GLN189, CYS145, THR26
87	<i>Lupeol</i>	HIS41
88	<i>Lupiwighteone</i>	HIS41, THR24, THR26
89	<i>Luteone</i>	HIS41, THR24, THR26, GLU166, GLY143
90	<i>Molnupiravir</i>	ARG188, GLU166, GLY143, GLN189, CYS145, ASN142, HIS41
91	<i>Mulberoffuran A</i>	GLN189, GLY143, HIS41, MET165
92	<i>Naringin</i>	THR24, THR26, HIS164, CYS145, GLN189, GLU166, MET49, THR25, ARG188, MET165
93	<i>Odoratin</i>	ASP187, THR25, THR26, MET165, GLN189, HIS41
94	<i>Parvisoflavone</i>	PRO168, THR25, THR26, MET165, GLN189
95	<i>Paxlovid</i>	THR24, THR25, HIS41, GLN189
96	<i>phaseollinisoflavan</i>	ASP187, HIS41, GLN189, CYS145, GLY143
97	<i>Pinocembroside</i>	HIS164, HIS41, GLN189, CYS145, THR25
98	<i>Prunetin</i>	HIS41, CYS145, THR25, THR26, GLU166, GLN189
99	<i>Puerarin</i>	ASN142, HIS41, THR25, GLU166, GLN189
100	<i>Rocymosin B</i>	GLY143, ASN142, HIS41, THR25, GLU166, GLN189, CYS145
101	<i>Scanderone</i>	THR26, HIS41, THR25, GLU166, GLN189, CYS145
102	<i>Semilicoisoflavone B</i>	THR26, HIS41, GLU166
103	<i>Senegalensin</i>	LEU27, MET49, HIS41, THR25, GLU166, GLN189, CYS145, MET165
104	<i>Sophoraisoflavone A</i>	THR25, THR26, LEU27, HIS41, GLN189, CYS145, MET165
105	<i>Tachigroside B</i>	GLY143, HIS41, THR25, MET165, GLN189, CYS145, ASN142
106	<i>Tachioside</i>	ARG188, HIS41, THR25, MET165, GLN189
107	<i>Tephrinone</i>	THR26, HIS41, GLN189, ARG188

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Tabel VII.12
Lanjutan

NO	LIGAND	RESIDU ASAM AMINO
108	<i>Uralenol</i>	THR26, GLN289, ASP187, TYR54
109	<i>Uralsaponin M</i>	PRO168, THR26, GLN189
110	<i>Wogonoside</i>	THR25, THR26, SER46, HIS41, CYS44, GLY143, GLU166
111	<i>(S)-2,3-Epoxysqualene</i>	THR45, SER46, CYS44, HIS41, THR25, THR24, GLU166, GLN189, MET49, ASP187, LEU27, MET165, GLY143
112	<i>Kaempferol</i>	THR25, THR26, MET49, MET165, CYS145, HIS41, CYS44, GLY143, GLU166



Daftar Riwayat Hidup

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II. RIWAYAT PENDIDIKAN

Jenjang Pendidikan	Nama Sekolah/Perguruan Tinggi	Tahun Masuk	Tahun Lulus
SD/MI	SD Negeri 2 Wanasari	2006	2012
SMP/MTs	SMP Negeri 1 Sukawening	2012	2015
SMA/MA/SMK	SMA Negeri 6 Garut	2015	2018
Perguruan Tinggi	Universitas Garut	2018	2022

III. Kegiatan dan Organisasi

- Magang dan Studi Independen Bersertifikat (MSIB) *Batch 2* (2022)
- Beasiswa Talenta Inovasi (2021)
- Pertukaran Mahasiswa Merdeka Angkatan 1 (2021)
- Koordinator Program Kampus Mengajar Angkatan 1 Kab.Garut (2021)
- Paduan Suara Mahasiswa Gempita Swara Uniga (2018-2021)
- Kepala Divisi Media dan Publikasi Himpunan Mahasiswa Farmasi KEMA FMIPA UNIGA (2020-2021)
- Paduan Suara Dinas PPKBPPPA Kab.Garut (2019-2020)