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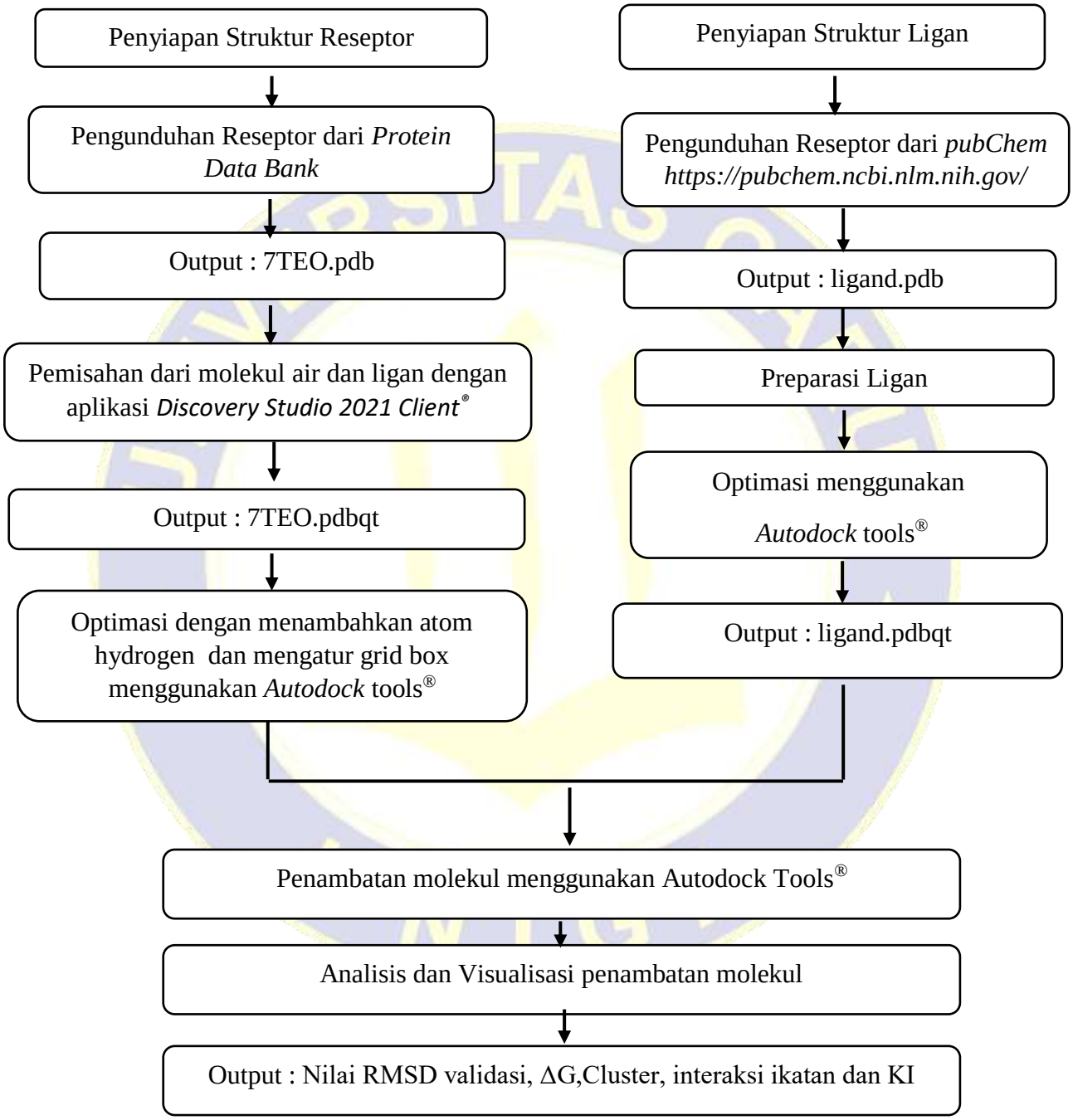
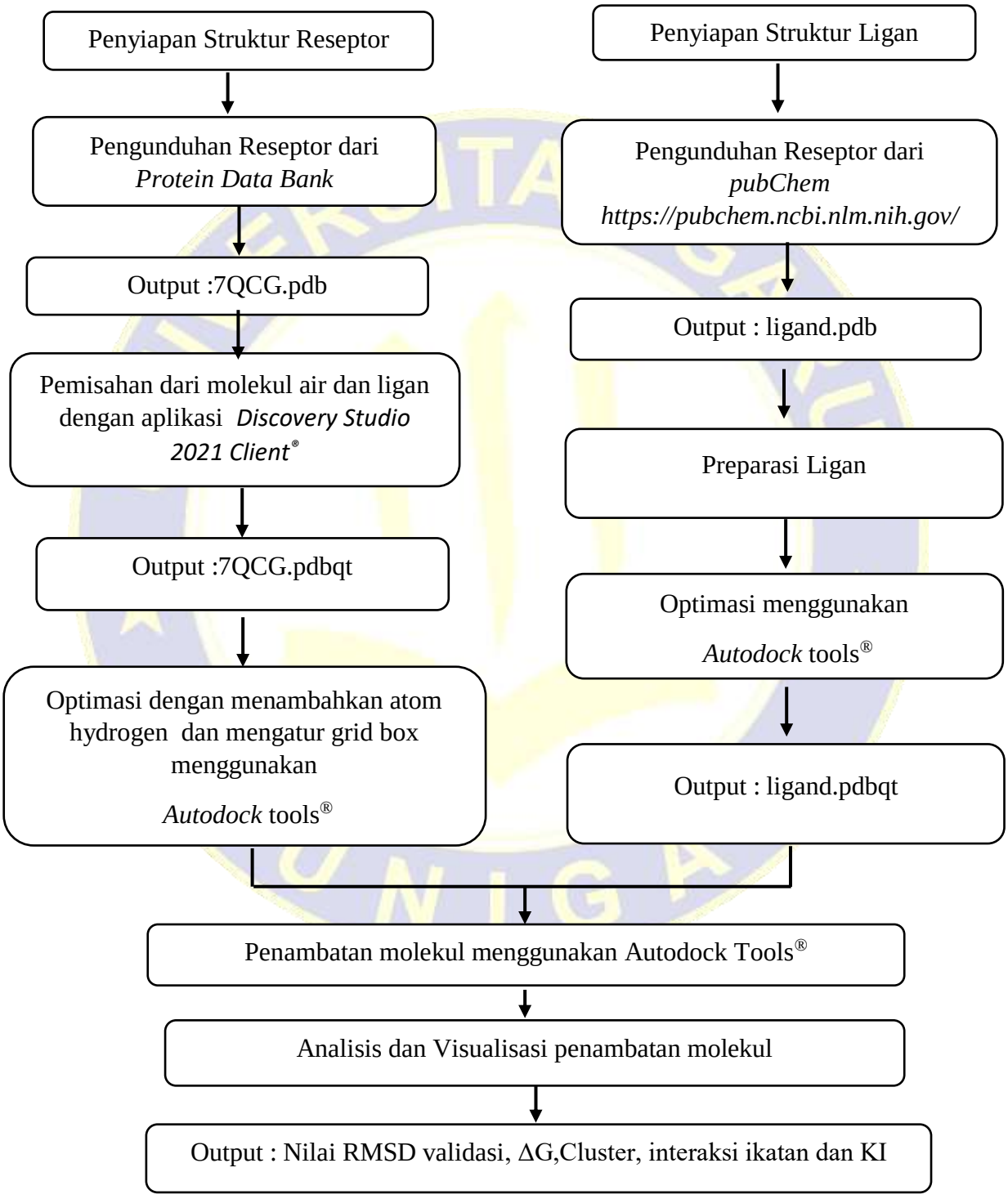
LAMPIRAN 1

ALUR PENELITIAN



Gambar IV.1 Alur penelitian penambatan molekul reseptor 7TEO

LAMPIRAN 1
(LANJUTAN)

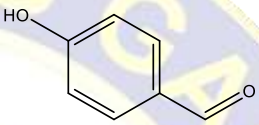
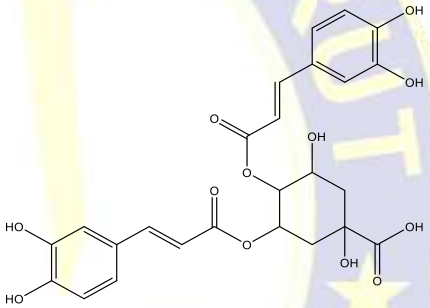
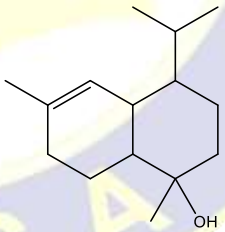
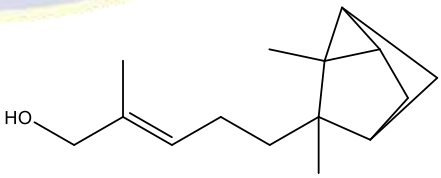


Gambar IV.1 Alur penelitian penambatan molekul reseptor 7QCG

LAMPIRAN 2

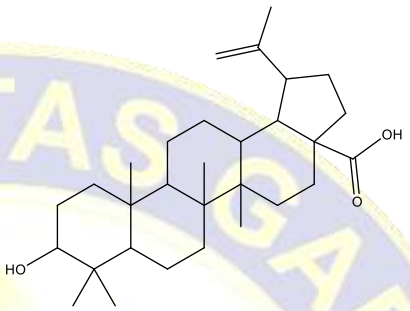
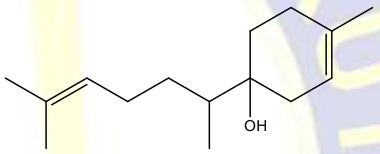
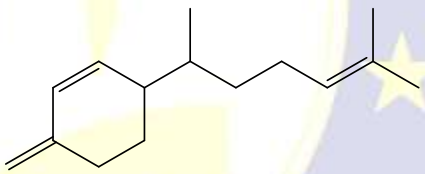
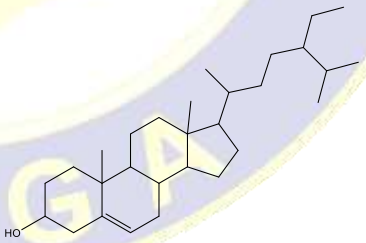
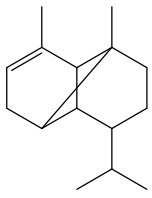
SENYAWA HERBA TAPAK LIMAN (*Elephantopus scaber* L)

Tabel V.1
SENYAWA HERBA TAPAK LIMAN (*Elephantopus scaber* L.)

No.	Nama Senyawa	Struktur 2D
1	4 Hydroxy-Benzaldehyde	
2	4,5Dicaffeoylquinic Acid	
3	Alpha Cadinol	
4	Alpha Santalol	

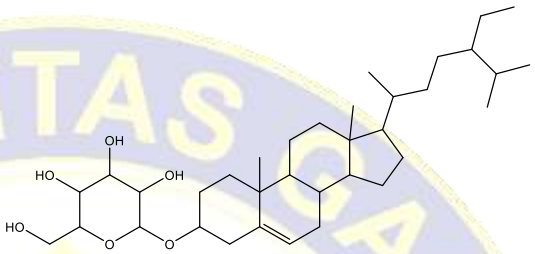
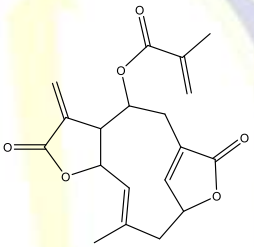
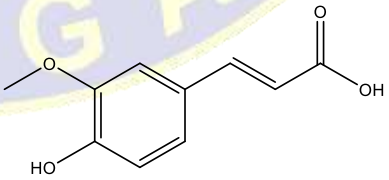
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
5	Betulinic Acid	
6	Beta Bisabolol	
7	Beta Sesquiphellandrene	
8	Beta Sitosterol	
9	Copaene	

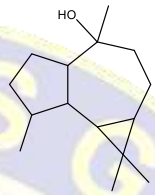
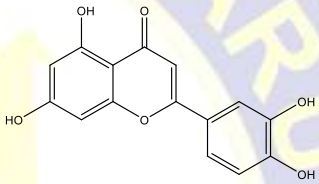
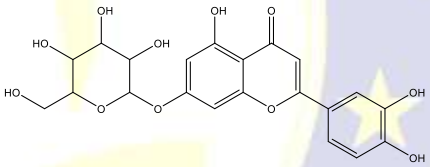
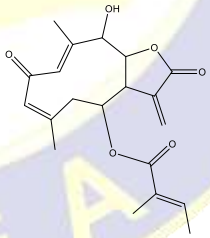
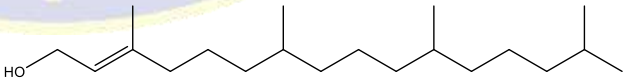
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
(Lanjutan)

NO	Nama Senyawa	Struktur 2D
10	Daucosterol	
11	Deoxyellephantopin	
12	Efipriedelanol	
13	Ferulic Acid	

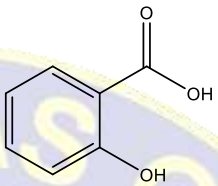
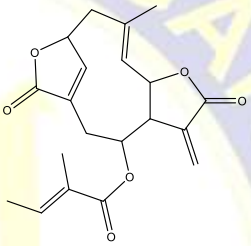
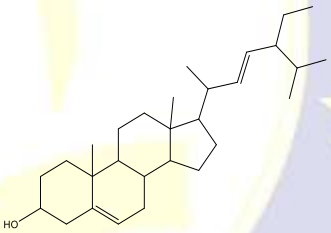
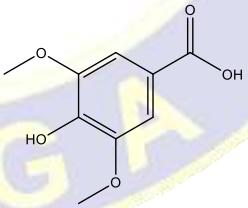
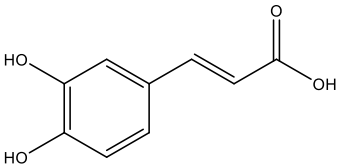
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Seyawa	Struktur 2D
14	Ledol	
15	Luteolin	
16	Luteolin-7-Glucoside	
17	Molephantinin	
18	Phytol	

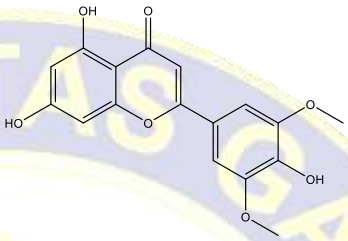
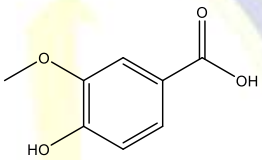
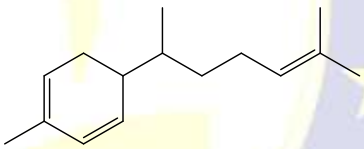
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
19	Salysilic acid	
20	Scabertopin	
21	Stigmasterol	
22	Syringic Acid	
23	Trans Caffeic Acid	

LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

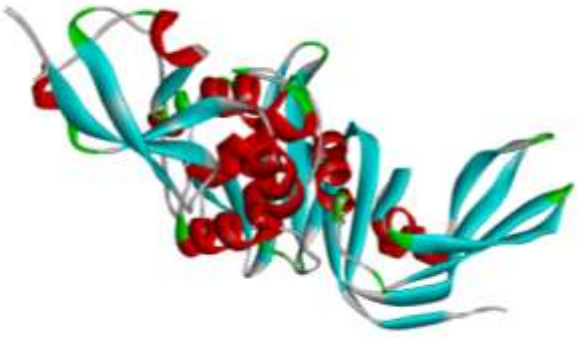
No	Nama Senyawa	Gambar 2D
24	Tricin	
25	Vanilic Acid	
26	Zingiberene	

LAMPIRAN 3

RESEPTOR

Reseptor *Main Protease* (Mpro) Kode 7TE0 dengan Resolusi 2Å

Gambar III.1 Struktur 3D reseptor Mpro

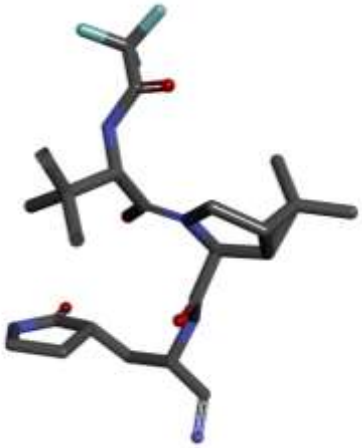


Reseptor *Papain like protease* (PLpro) Kode 7QCG dengan Resolusi 1.75Å

Gambar III.2 Struktur 3D Reseptor PLpro

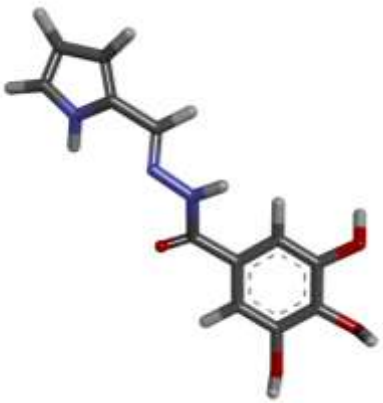
LAMPIRAN 4

LIGAN ALAMI



Ligan alami [*(1R,2S,5S)-N-{(1E,2S)-1-imino-3-[(3S)-2- oxopyrrolidin-3-yl] propan-2-yl}-6,6- dimethyl-3- [3-methyl-N- (trifluoroacetyl)-L-valyl]-3-azabicyclo[3.1.0] hexane-2-carboxamide*] dari reseptor *Main protease*.

Gambar IV.1 Ligan alami Mpro

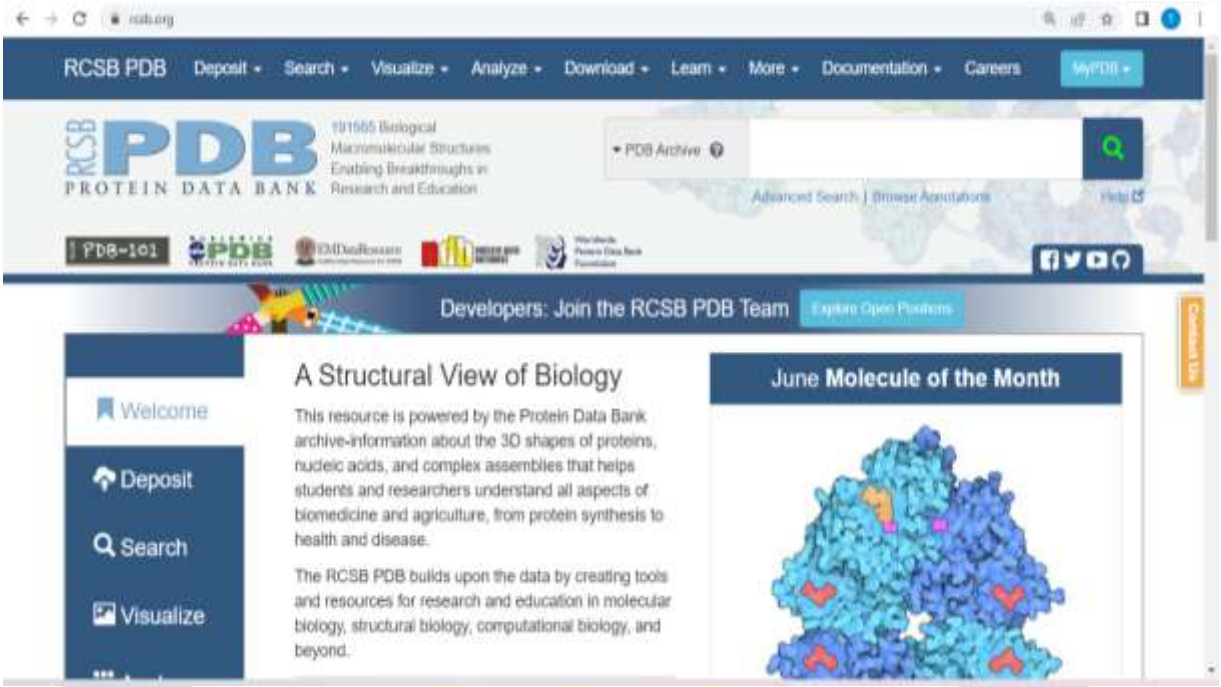


Ligan alami [*3,4,5-tris(oxidanyl)-N-[(E)-1H-pyrrol-2-ylmethylideneamino]benzamide*] dari reseptor *Papain like protease.*

Gambar IV.2 Ligan alami PLpro

LAMPIRAN 5

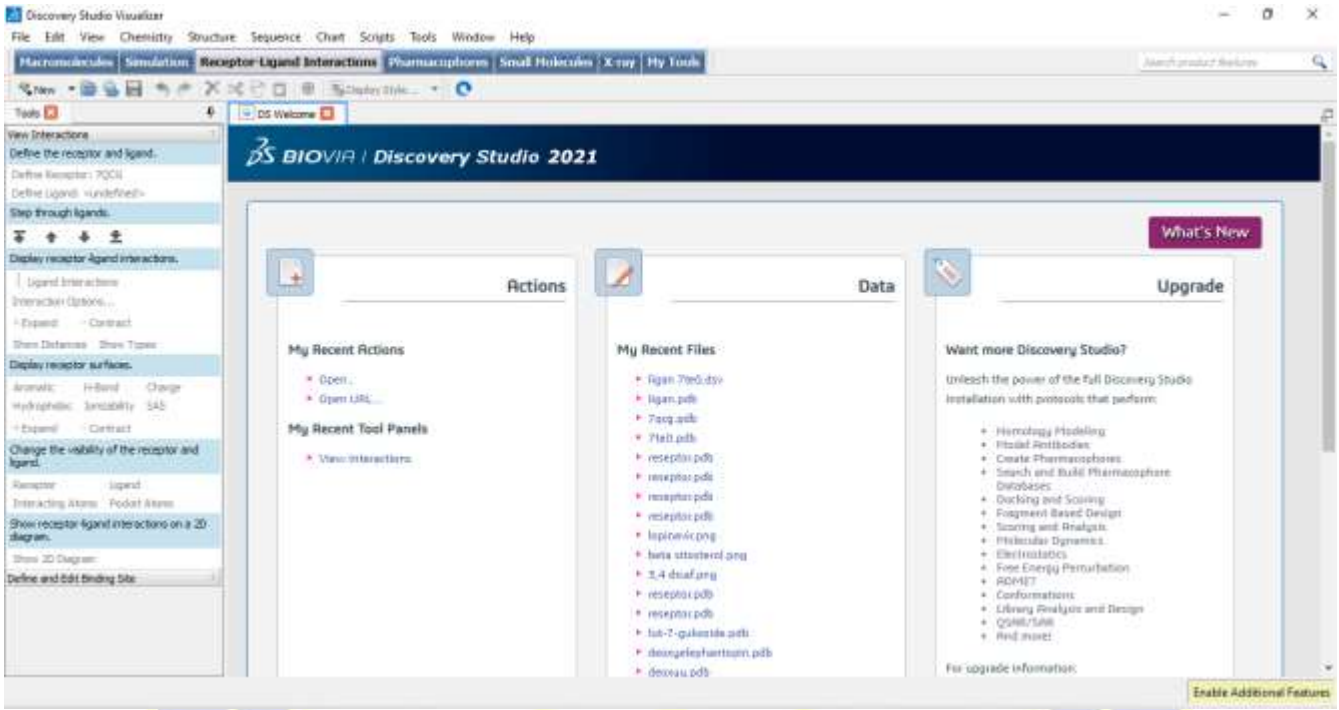
SITUS *Online* PDB (*PROTEIN DATA BANK*)



Gambar IV.3 Situs *online Protein Data Bank* (PDB)

LAMPIRAN 6

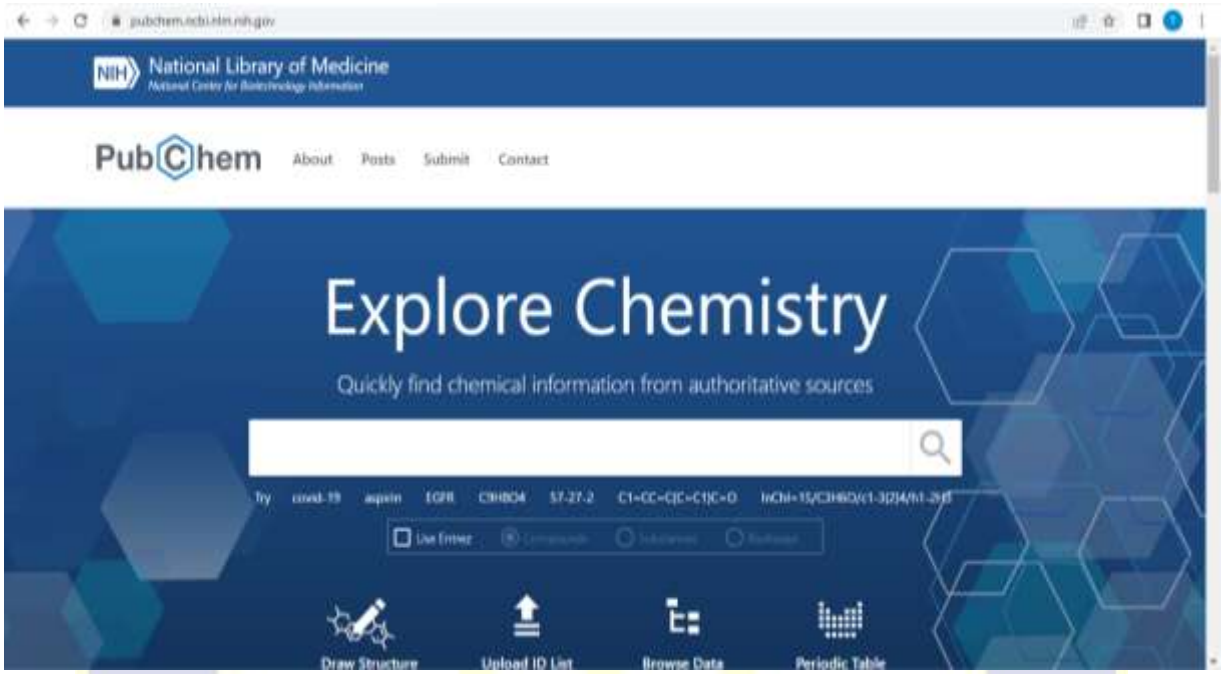
PROGRAM *DISCOVERY STUDIO VISULIZER*



Gambar IV.4 Program *Discovery Studio Visualizer*

LAMPIRAN 7

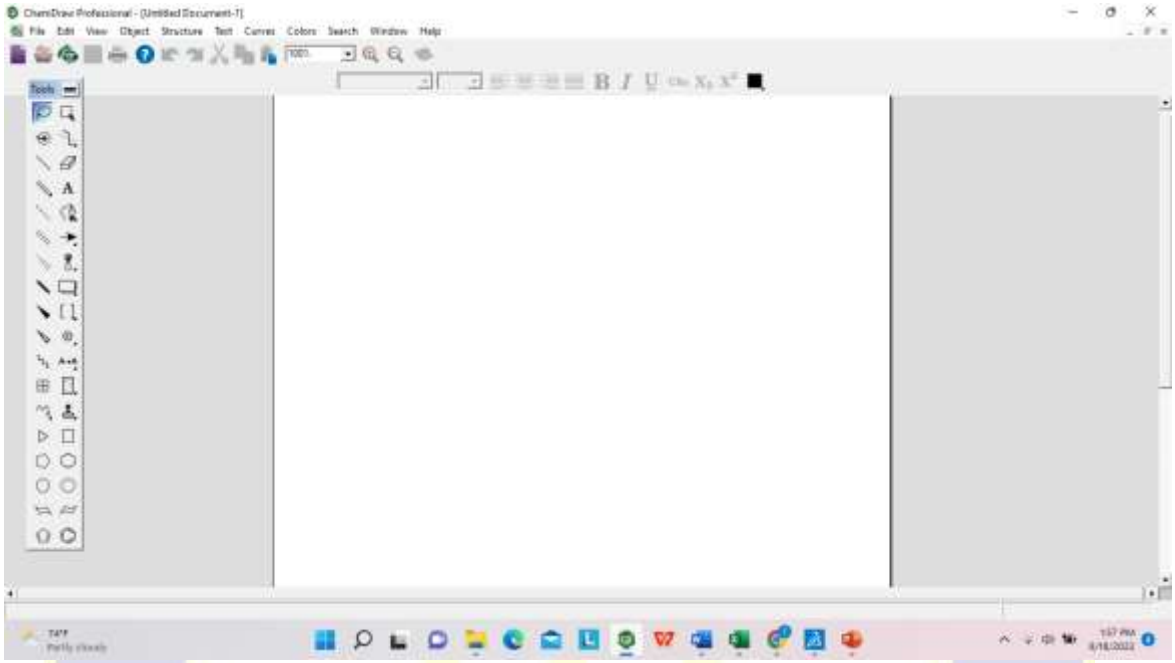
SITUS *ONLINE PUBCHEM*



Gambar IV.5 Situs *Online PubChem*

LAMPIRAN 8

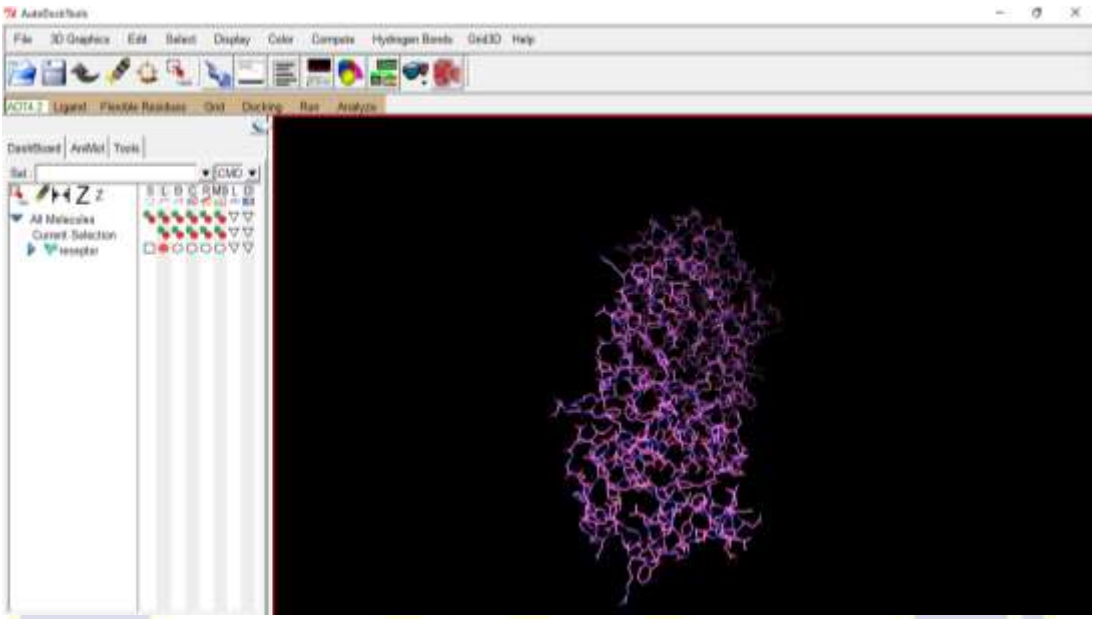
PROGRAM *CHEMDRAW ULTRA*



Gambar IV.6 Program *Chemdraw ultra*

LAMPIRAN 9

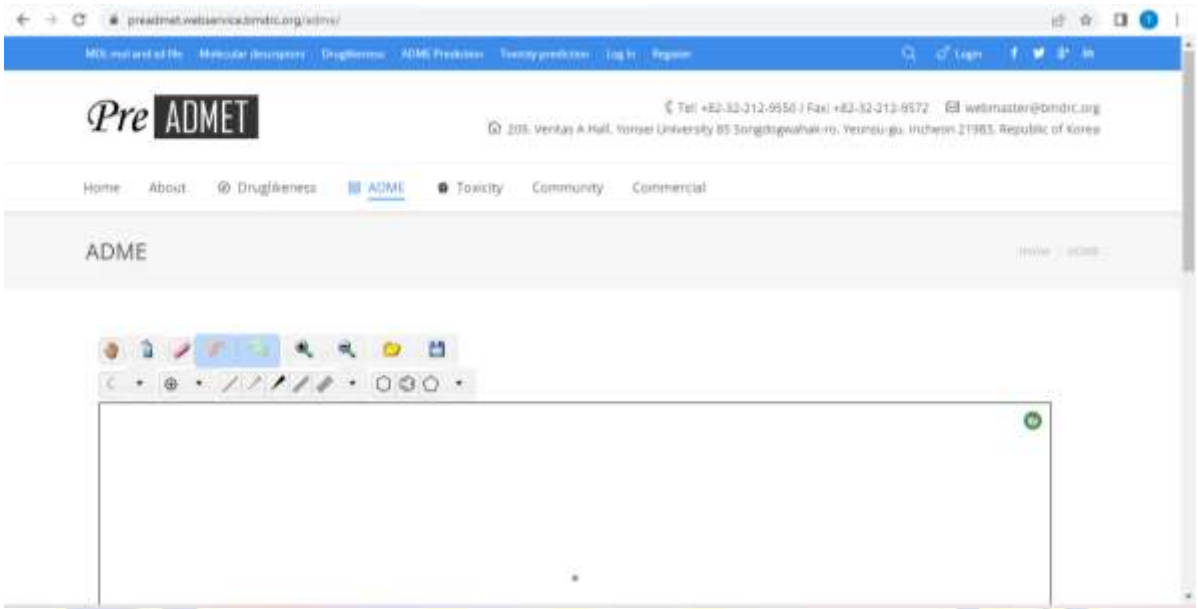
PROGRAM *AUTODOCK TOOLS*



Gambar IV.7 Program *Autodock Tools*

LAMPIRAN 10

SITUS *ONLINE PreADME*



Gambar IV.8 Situs *Online PreAdme*

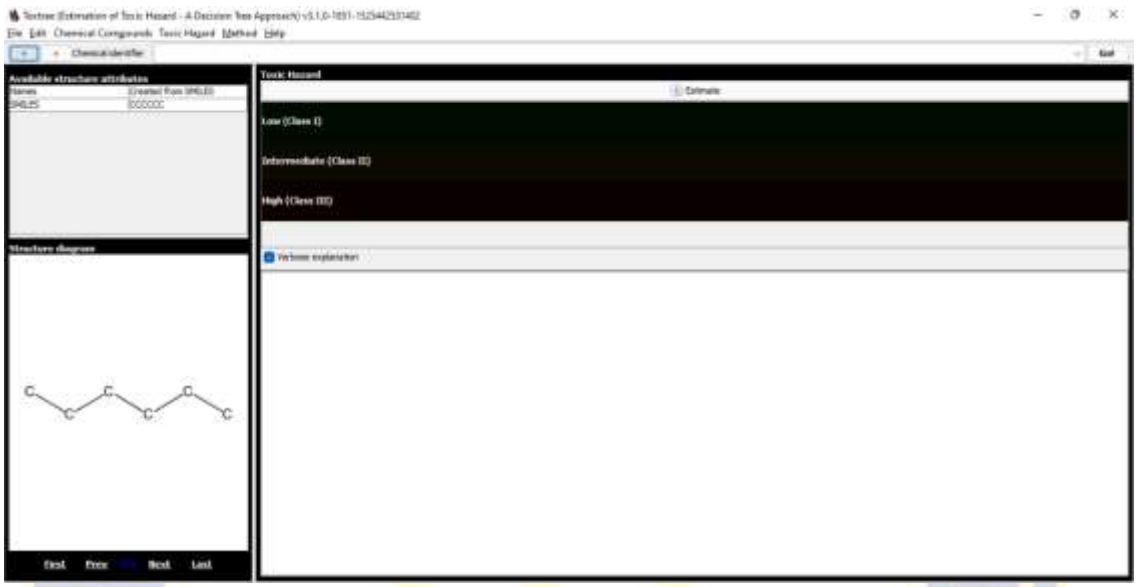
LAMPIRAN 11

SITUS *ONLINE LIPINSKI RULE'S OF FIVE*

Gambar IV.9 Situs *Online Lipinski Rule's of Five*

LAMPIRAN 12

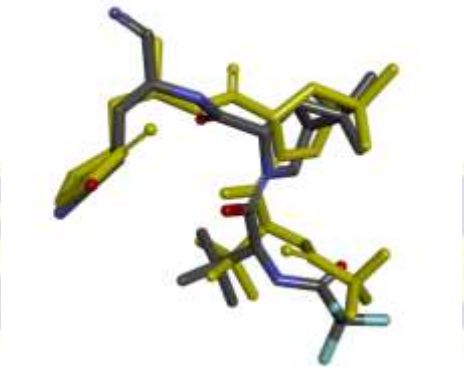
PROGRAM *TOXTREE*



Gambar IV.10 Program *Toxtree*

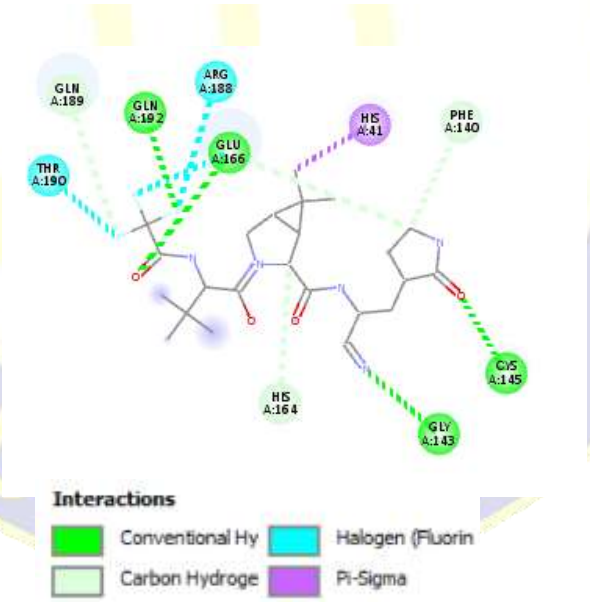
LAMPIRAN 13

HASIL VALIDASI



Visualisasi tumpang tindih ligan alami dengan ligan hasil redocking dari reseptor *Main protease* (Mpro) dengan Kode PDB 7TE0

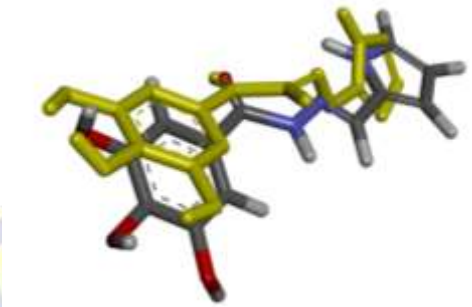
Gambar V.3 Hasil validasi tumpang tindih



Visualisasi interaksi asam amino ligan alami dengan reseptor *Main protease* (Mpro) dengan kode PDB 7TE0

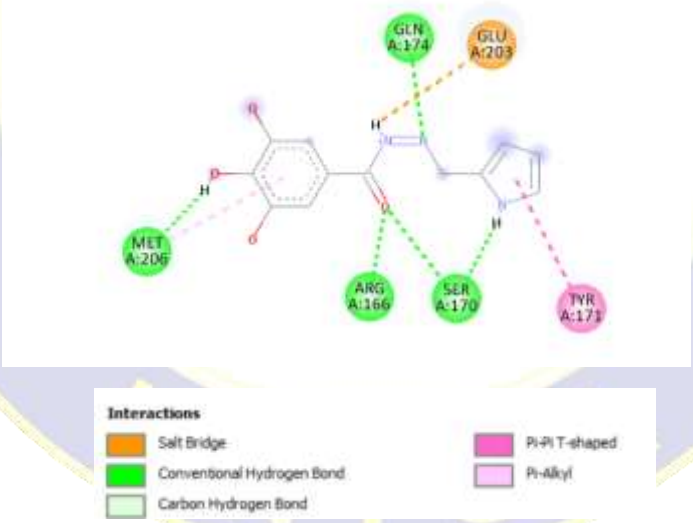
Gambar V.4 Interaksi asam amino ligan alami Mpro

LAMPIRAN 13
(LANJUTAN)



Visualisasi tumpang tindih ligan alami dengan ligan hasil redocking dari reseptor *Papain like protease* (PLpro) dengan kode PDB 7QCG

Gambar V.5 Hasil validasi



Visualisasi interaksi asam amino ligan alami dengan reseptor *Papain like protease* (PLpro) dengan kode PDB 7QCG

Gambar V.6 Interaksi asam amino ligan alami PLpro

LAMPIRAN 13
(LANJUTAN)

Tabel V.2
Hasil Validasi

No	Reseptor	Grid Box		RMSD (Å)	ΔG (Energi Bebas) kcal/mol	KI (Konstanta Inhibisi) μm
		Center	Size			
1	*Main protease* kode ID 7TE0	X : -10.360 Y : -15.079 Z : -17.201	X : 28 Y : 30 Z : 20	1.196	-11.93	0.0018
2	*Papain like protease* kode ID 7QCG	X : 70.154 Y : 29.471 Z : -29.331	X : 28 Y : 20 Z : 32	1.242	-4.03	1110

LAMPIRAN 14

HASIL PENAMBATAN MOLEKUL MPro

Hasil Penambatan Molekul terhadap reseptor *Main protease* (Mpro)

Tabel V.3
Hasil Penambatan Molekul

No	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan lain	Ikatan Hidrogen
1	(1R,2S,5S)-N-{(1E,2S)-1-imino-3-[(3S)-2- oxopyrrolidin-3-yl] propan-2-yl}-6,6- dimethyl-3-[3-methyl-N- (trifluoroacetyl)-L-valyl]-3azabicyclo[3.1.0] hexane-2-carboxamide*	-11.93	0.00179	HIS41 THR190 ARG188	GLN192 GLU166 CYS145 GLY143 GLN189 HIS164 PHE140
2	Lopinavir**	-7.88	0.00166	HIS41 MET49 MET165 LEU167 PRO168	CYS143 GLU166 ASN142
3	4-Hydroxybenzaldehyde	-4.89	262.16	CYS145	PHE140H IS172 ASN142 GLY143
4	4,5 Dicaffeoyl Quinic Acid	-6.36	21.77	GLN189 CYS145	GLN192 HIS164 GLN189 LEU141 SER144
5	Alpha Cadinol	-6.46	18.33	MET165 CYS145 HIS163	GLY143 ASN142

LAMPIRAN 14
(LANJUTAN)

Tabel V.3

No	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan lain	Ikatan Hidrogen
6	Alpha Santalol	-6.97	7780	HIS41 MET165 MET49	THR19 GLN192
7	Betulinic Acid	-8.94	0.28056	HIS41 CYS145	SER144 LEU141 THR190 GLN192
8	Beta Bisabolol	-6.41	20.11	HIS164 LEU167 PRO168 MET165 HIS41	GLU166
9	Beta Sesquiphellandrene	-4.48	17.77	HIS41 MET165 CYS145 HIS163	SER144 LEU141
10	Beta Sitosterol	-9.5	0.10943	HIS41 MET165 CYS145 HIS163	SER144 LEU141
11	Copaene	-6.91	8.56	HIS41 MET49 LEU167 MET165	-
12	Daucosterol	+3.66	-	MET165 THR190 ASN142	GLY143 CYS145 SER144
13	Deoxyellphantopin	-8.5	0.58776		GLN192 GLU166 MET165
14	Efipriedelanol	-6.42	19.18	GLY143	LEU141 SER144

LAMPIRAN 14
(LANJUTAN)

Tabel V.3

No	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan lain	Ikatan Hidrogen
15	Ferulic Acid	-4.37	626.32	MET165 HIS42 HIS164	GLN192 THR190
16	Ledol	-6.78	10.69	HIS163 CYS145	ASN142
17	Luteolin	-6.79	10.53	GLN192 GLU166 ASN142 SER144 LEU141	HIS163 CYS141 MET165 GLN189
18	Luteolin-7-Glucoside	-6.87	9.13	MET165 ASN142	CYS145 GLN192 LEU141 GLU166
19	Molephantinin	-8.54	0.54537	HIS163 CYS145 MET165	HIS41 GLU166
20	Phytol	-6.08	34.78	HIS163 HIS41 CYS145 MET165 MET49	GLU166
21	Salysilic Acid	-4.68	373.67	-	CYS145 SER144 ASN142
22	Scabertopin	-7.8	1.93	MET49 HIS41	ASN142 CYS145 GLY143 HIS172
23	Stigmasterol	-8.58	0.50951	HIS41 MET49 MET165 CYS145	THR190

LAMPIRAN 14
(LANJUTAN)

Tabel V.3

No	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan lain	**Ikatan Hidrogen**
24.	Syringic Acid	-5.14	168.75	HIS172 HIS163	PHE140 CYS145 GLU166 SER144 LEU141 GLY143 HIS164
25	Trans Caffeic Acid	-4.45	549.47	-	ASN142 GLU166 PHE140
26	Tricin	-7.88	1.68	MET165	GLN189 GLU166 SER144 LEU141 GLY143 CYS145 PHE140
27	Vanilic Acid	-4.71	350.64	-	CYS145 GLU166 ASN142
28	Zingiberene	-6.49	17.4	PRO168 LEU167 MET165 HIS41 MET49	-

* Ligan alami

** Ligan Pembanding

LAMPIRAN 15

HASIL PENAMBATAN MOLEKUL PLpro

Hasil Penambatan molekul Terhadap Reseptor *Papain Like Protease* (PLpro)

Tabel V.4
Hasil Penambatan molekul

No	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan Lain	Ikatan Hidrogen
1	*3,4,5-tris(oxidanyl)-N-[(E)-1H-pyrrol-2-ylmethylideneamino] benzamide**	-4.03	1110	GLU203 TYR171	GLN174 SER170 ARG161 MET206
2	Ribavirin**	-4.26	759.79	MET206	GLU203 GLN174 ARG166
3	4-Hydroxybenzaldehyde	-3.48	2830	-	SER170 ARG166 MET206
4	4,5 Dicaffeoyl Quinic Acid	-2.53	13980	MET206	MET208 GLU203 GLN174 SER170 VAL202 ARG166 TYR207
5	Alpha Cadinol	-4.88	264.96	MET206	ARG166
6	Alpha Santalol	-4.99	218.31	MET206	SER170

LAMPIRAN 15
(LANJUTAN)

Tabel V.4

NO	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan Lain	Ikatan Hidrogen
7	Betulinic Acid	-5.07	192.58	-	MET208 MET206 ARG166
8	Beta Bisabolol	4.7	357.06	MET206 MET208	ARG166
9	Beta Sesquiphellandrene	-4.36	636.31	MET206 TYR207	-
10	Beta Sitosterol	-5.19	157.17	TYR171	-
11	Copaene	-5.3	131.38	MET208 MET206	-
12	Daucosterol	-2.72	10150	TYR171	MET206
13	Deoxyellphantopin	-5.65	72.16	-	SER170 ARG166
14	Efipriedelanol	-5.35	120.15	TYR171	MET206
15	Ferulic Acid	-3.95	1280	VAL202	ARG166 SER170 MET206
16	Ledol	-4.77	320.03	MET206	-
17	Luteolin	+1.49	-	-	-
18	Luteolin-7-Glucoside	-3.05	5860	-	MET206 ARG166 GLN174 GLU203
19	Molephantinin	-5.64	73.95	-	SER170 ARG166
20	Phytol	-2.82	8.53	VAL202 MET206	ARG166
21	Salysilic Acid	-3.26	4090	MET206	MET208 ARG166

LAMPIRAN 15
(LANJUTAN)

Tabel V.4

NO	Ligan	ΔG (Kcal/mol)	KI (µm)	Residu asam amino yang berikatan	
				Ikatan Lain	Ikatan Hidrogen
22	Scabertopin	-5.13	174.59	TYR207	MET206 GLN174 ARG166
23	Stigmasterol	-5.72	64.49	MET208	TYR171 MET206
24	Syringic Acid	-3.83	1570	MET206 VAL202 TYR207	MET208 ARG166 GLU203
25	Trans Caffeic Acid	-3.96	1260	VAL202 MET208	GLN174 MET206 ARG166 GLU203
26	Tricin	-4.56	456.24	-	ARG166 SER170 GLU203 MET208 MET206
27	Vanilic Acid	-3.64	2150	MET208	SER170 ARG166 MET206 TYR207
28	Zingiberene	-4.51	497.62	TYR207 MET206 VAL202	-

* Ligan alami

** Ligan Pembanding

LAMPIRAN 16

HASIL PENGUJIAN *LIPINSKI RULE'S OF FIVE*

Tabel V.5
Hasil Pengujian *Lipinski Rule's of Five*

No	Senyawa	BM	Log P	Ikatan Hidrogen		Keterangan
				Donor	Akseptor	
1	4-Hydroxybenzaldehyde	122	0.7989	1	2	Memenuhi Syarat
2	4,5 Dicaffeoyl Quinic Acid	516	2.2182	7	12	Tidak Memenuhi Syarat
3	Alpha Cadinol	222	3.8970	1	1	Memenuhi Syarat
4	Alpha Santalol	220	3.6996	1	1	Memenuhi Syarat
5	Betulinic Acid	456	7.1833	2	3	Memenuhi Syarat
6	Beta Bisabolol	222	3.9918	1	1	Memenuhi Syarat
7	Beta Sesquiphellandrene	204	3.8705	0	0	Memenuhi Syarat
8	Beta Sitosterol	414	7.7456	1	1	Memenuhi Syarat
9	Copaene	286	0.8346	4	6	Memenuhi Syarat
10	Daucosterol	312	-0,053101	5	6	Memenuhi Syarat
11	Deoxyellphantopin	344	2.4146	0	6	Memenuhi Syarat
12	Efipriedelanol	428	8.0414	1	1	Memenuhi Syarat
13	Ferulic Acid	194	0.5561	2	4	Memenuhi Syarat
14	Ledol	222	3.8865	1	1	Memenuhi Syarat
15	Luteolin	386	0.8346	4	6	Memenuhi Syarat
16	Luteolin-7-Glucoside	448	1.5093	7	11	Tidak Memenuhi Syarat
17	Molephantinin	360	3.7351	0	6	Memenuhi Syarat
18	Phytol	296	5.7215	1	1	Memenuhi Syarat
19	Salysilic Acid	138	0.4867	2	3	Memenuhi Syarat
20	Scabertopin	358	2.8537	1	6	Memenuhi Syarat
21	Stigmasterol	412	7.5416	1	1	Memenuhi Syarat
22	Syringic Acid	198	0.8616	2	5	Memenuhi Syarat
23	Trans Caffeic Acid	180	0.0308	3	4	Memenuhi Syarat
24	Tricin	333	1.5854	3	7	Memenuhi Syarat
25	Vanilic Acid	168	0.6361	2	4	Memenuhi Syarat
26	Zingiberene	204	4.0033	0	0	Memenuhi Syarat

Keterangan: *BM (Berat molekul) <500 Dalton, Log P <5, Donor ikatan hidrogen <5, Adan Akseptor ikatan hidrogen <10.*

LAMPIRAN 17

HASIL PENGUJIAN *PreADME*

Tabel V.6
Hasil Pengujian *PreADME*

No	Senyawa	Absorpsi		Distribusi
		Caco2 (nm.sec-1)	HIA (%)	PPB (%)
1	4-Hydroxybenzaldehyde	20.52	94.09	6.00
2	4,5 Dicaffeoyl Quinic Acid	19.53	23.12	87.77
3	Alpha Cadinol	55.41	100	100
4	Alpha Santalol	18.57	100	91.62
5	Betulinic Acid	21.86	96.00	100
6	Beta Bisabolol	51.11	100	100
7	Beta Sesquiphellandrene	23.40	100	100
8	Beta Sitosterol	52.37	100	100
9	Copaene	23.63	100	100
10	Daucosterol	25.23	90.03	100.00
11	Deoxyellphantopin	23.80	97.94	92.35
12	Efipriedelanol	46.84	100	100.00
13	Ferulic Acid	21.12	90.60	50.41
14	Ledol	54.57	100	100
15	Luteolin	4.54	79.43	99.72
16	Luteolin-7-Glucoside	4.87	25.17	73.28
17	Molephantinin	21.34	95.81	88.23
18	Phytol	37.63	100	100
19	Salysilic Acid	20.31	88.14	8.77
20	Scabertopin	25.56	98.30	94.53
21	Stigmasterol	52.34	100	100
22	Syringic Acid	18.83	82.03	69.78
23	Trans Caffeic Acid	21.11	82.30	40.29
24	Tricin	3.00	87.82	87.08
25	Vanilic Acid	19.94	85.37	52.11
26	Zingiberene	23.40	100	100

LAMPIRAN 17
(LANJUTAN)

Keterangan:

- Permeabilitas sel CaCo-2 (nm. Sec^{-1}): >70 permeabilitas tinggi, 4-70 permeabilitas sedang, <4 permeabilitas rendah;
- % *human intestinal absorption* (HIA): 700-100% absorpsi baik,20-70% absorpsi cukup, 0-20% absorpsi buruk;
- %plasma protein binding (PBB) : >90% ikatan kuat, <90% ikatan lemah.

LAMPIRAN 18

HASIL PENGUJIAN TOKSISITAS

Tabel V.7
Hasil Pengujian Toksisitas

No	Senyawa	Crame Rules	Kroes TTC	Benigni/ Bosarulebase
1	4-Hydroxybenzaldehyde	1	2	1.9
2	4,5 Dicaffeoyl Quinic Acid	3	1	8.9
3	Alpha Cadinol	3	1	8.9
4	Alpha Santalol	1	1	8.9
5	Betulinic Acid	1	1	8.9
6	Beta Bisabolol	1	1	8.9
7	Beta Sesquiphellandrene	3	1	8.9
8	Beta Sitosterol	3	1	8.9
9	Copaene	1	1	8.9
10	Daucosterol	3	1	8.9
11	Deoxyellphantopin	3	1	8.9
12	Efipriedelanol	1	1	8.9
13	Ferulic Acid	1	1	8.9
14	Ledol	3	1	8.9
15	Luteolin	3	1	8.9
16	Luteolin-7-Glucoside	3	1	8.9
17	Molephantinin	3	2	1.9
18	Phytol	1	1	8.9
19	Salysilic Acid	1	1	8.9
20	Scabertopin	3	1	8.9
21	Stigmasterol	1	1	8.9
22	Syringic Acid	1	1	8.9
23	Trans Caffeic Acid	1	1	8.9
24	Tricin	3	1	8.9
25	Vanilic Acid	1	1	8.9
26	Zingiberene	1	1	8.9

LAMPIRAN 18
(LANJUTAN)

Keterangan:

- Cramer ruler kelas 1 : lemah, kelas 2 : sedang, kelas 3 : tinggi.
- Benigni/bosa rulebase 1 (peringatan struktural untuk karsinogenk genotoksik), 8 (negatif untuk karsinogenik genotoksik), 9 (negatif untuk karsinogenik non genotoksik).
- Kroes TTC decission tree 1 (Zat tidak mempunyai masalah keamanan), 2 (Resiko yang dapat diabaikan)

DAFTAR RIWAYAT HIDUP

DATA PRIBADI

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