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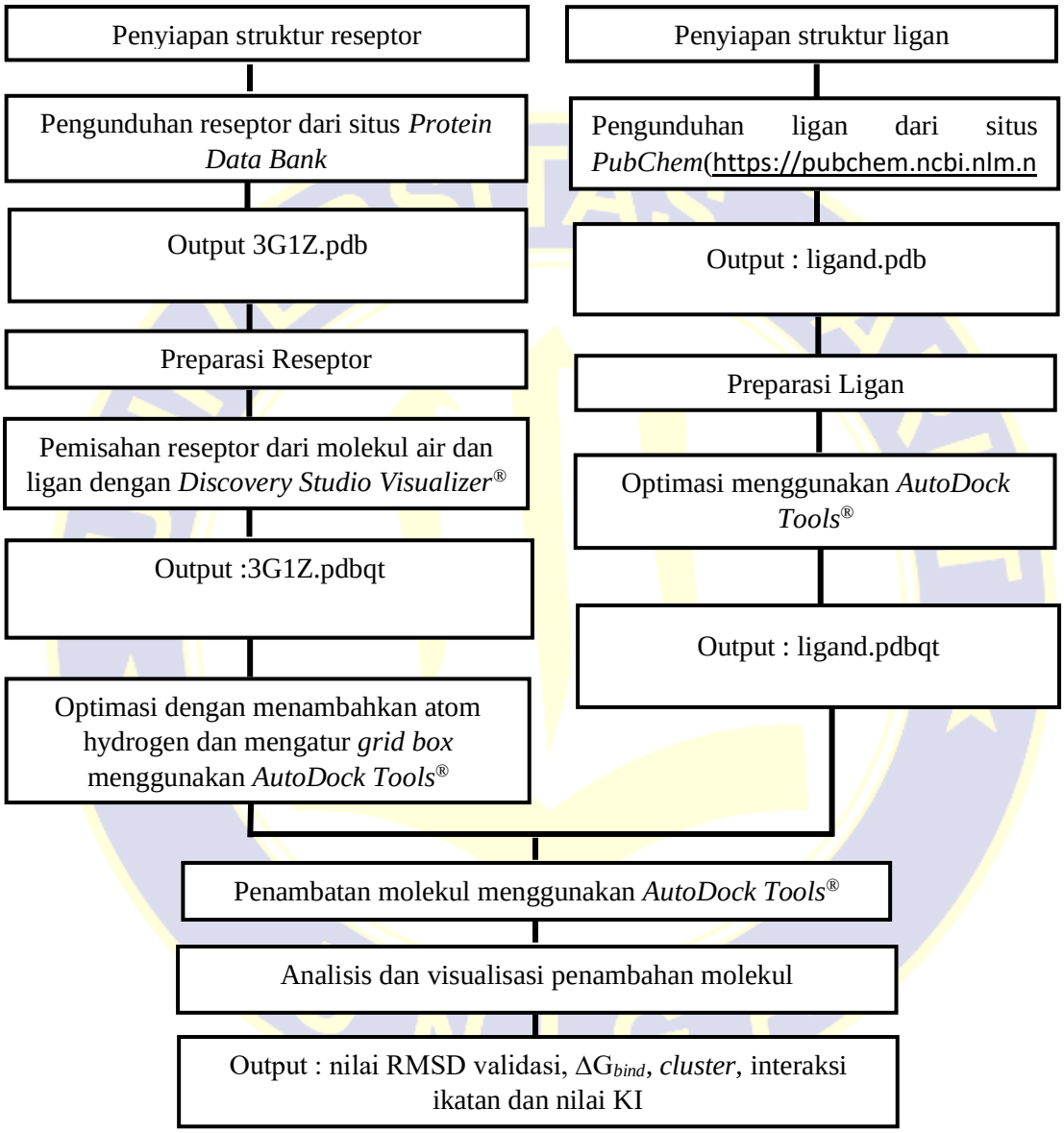
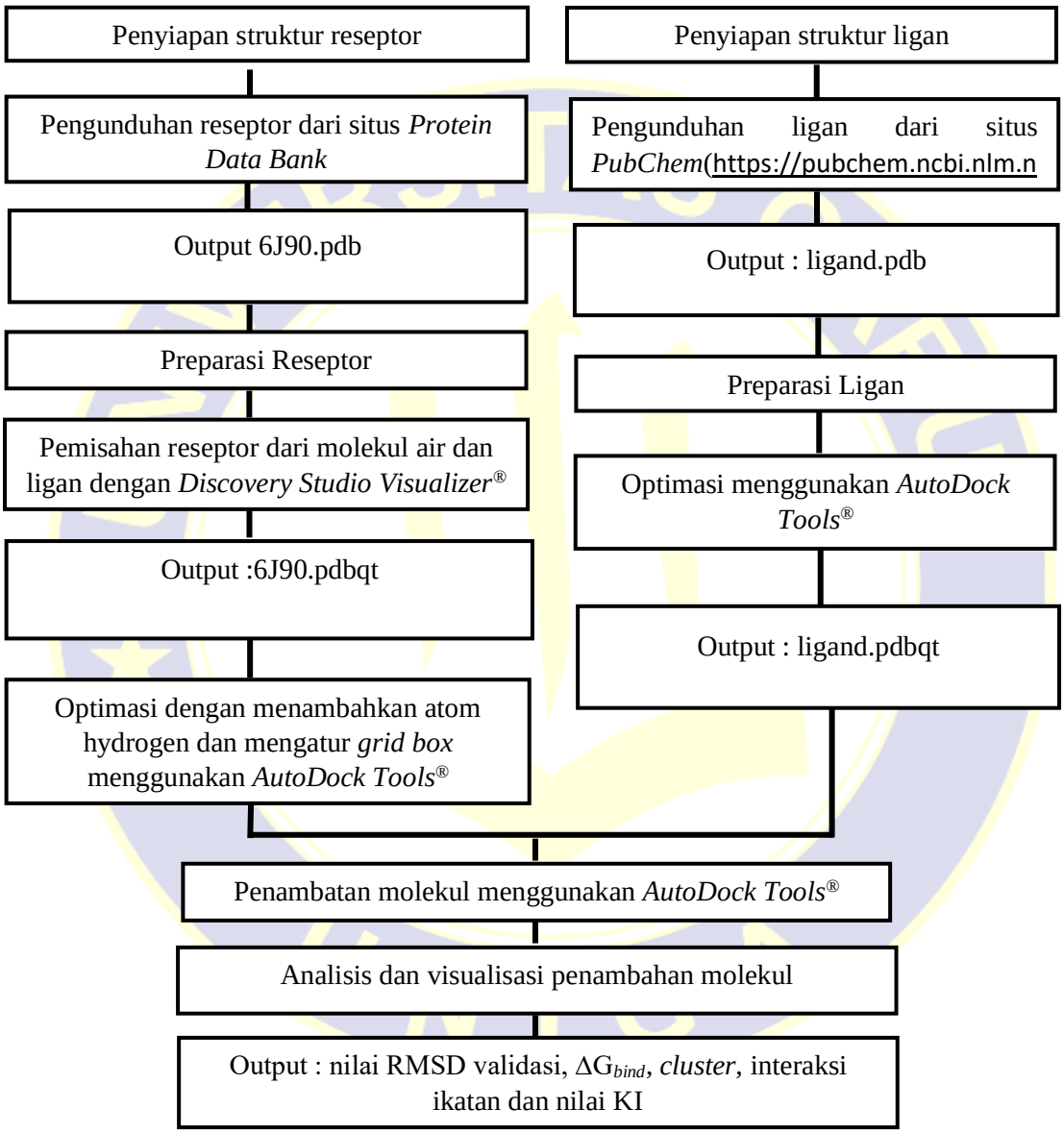


Gambar IV.1 Alur penelitian penambatan molekul reseptor 3G1Z

LAMPIRAN 1
(LANJUTAN)

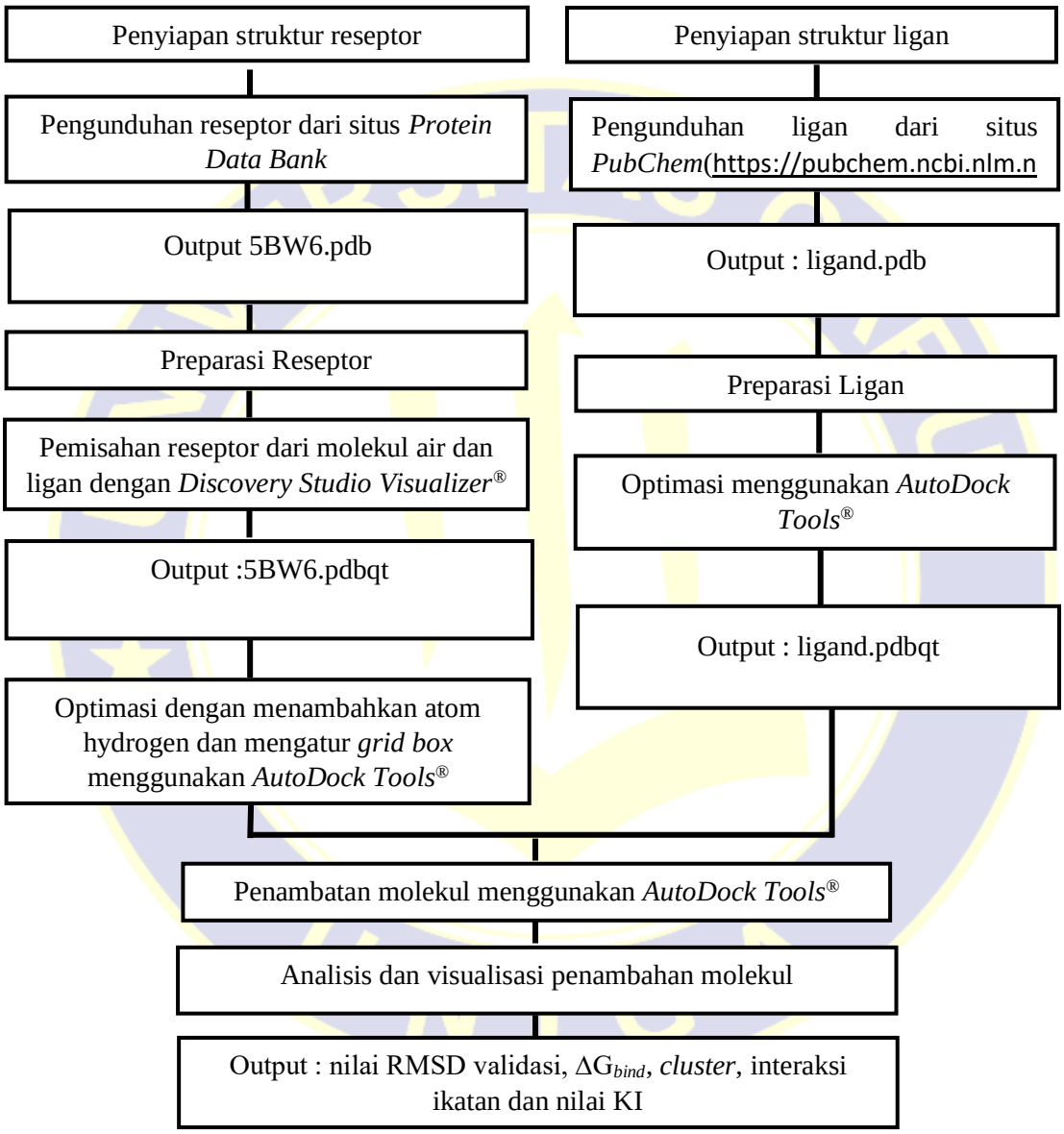
ALUR PENELITIAN



Gambar IV.2 Alur penelitian penambatan molekul reseptor 6J90

LAMPIRAN 1
(LANJUTAN)

ALUR PENELITIAN



Gambar IV.3 Alur penelitian penambatan molekul reseptor 5BW6

LAMPIRAN 2

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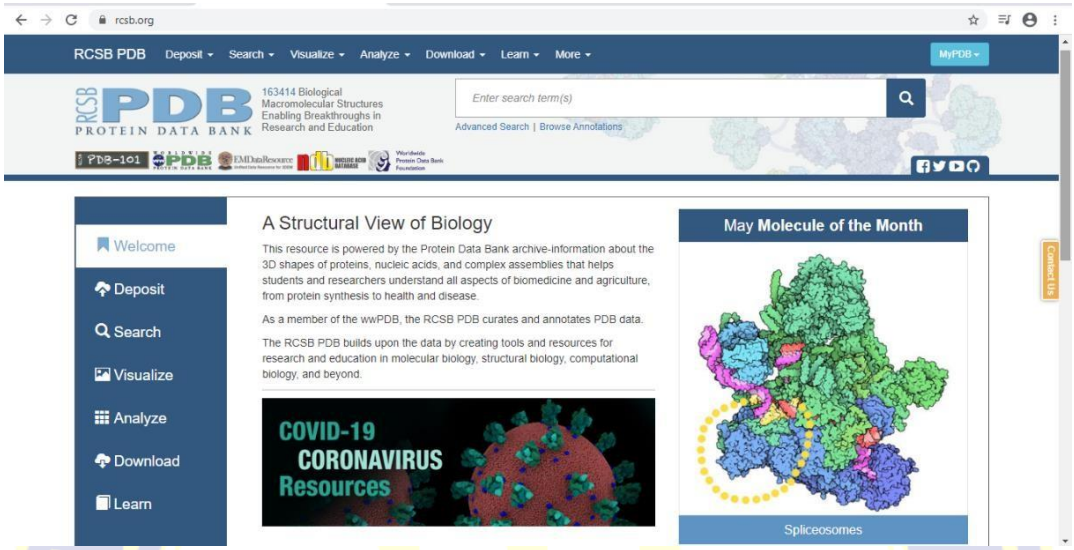
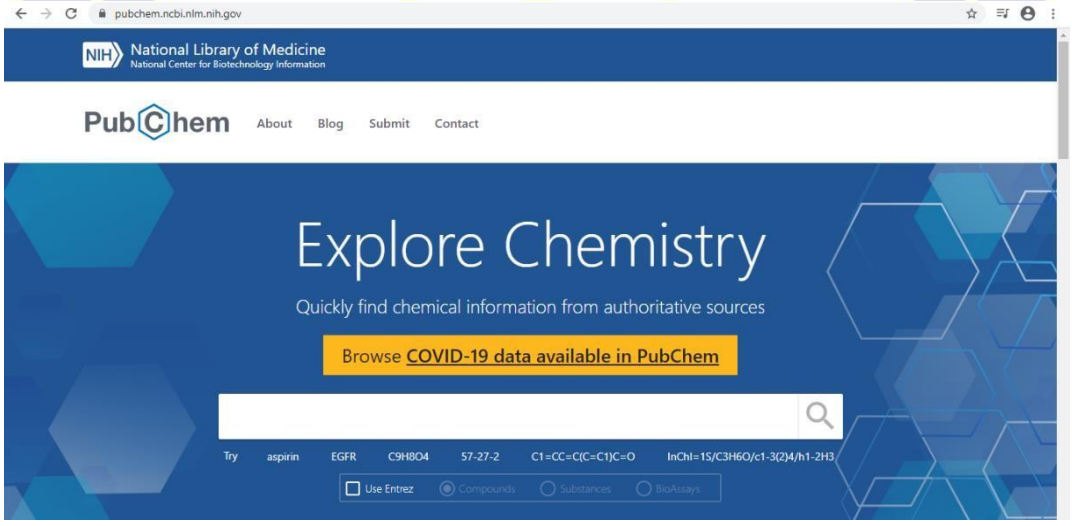


Gambar IV.4 Tampilan situs *Protein Data Bank*



Gambar IV.5 Tampilan situs *PubChem*

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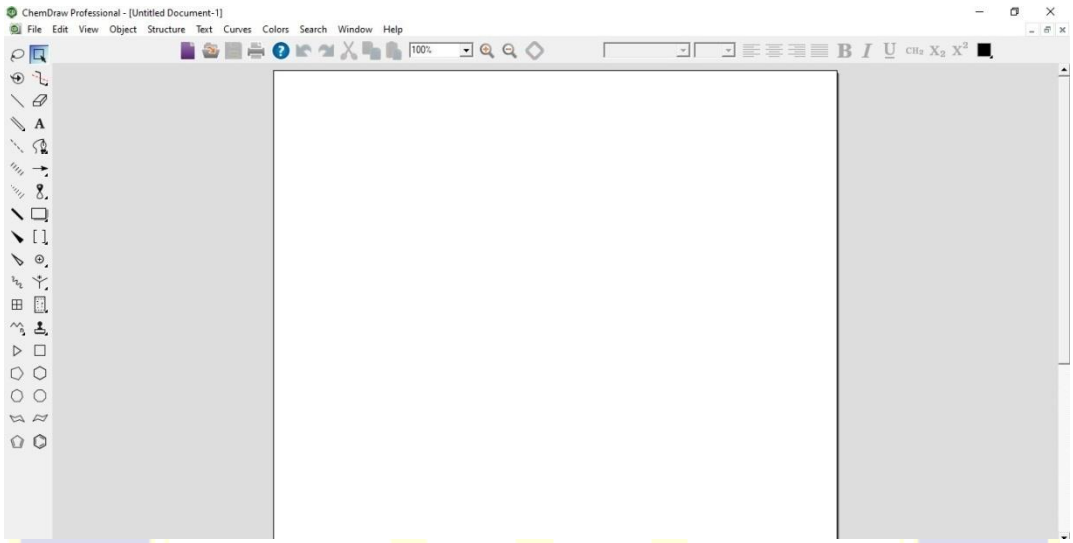
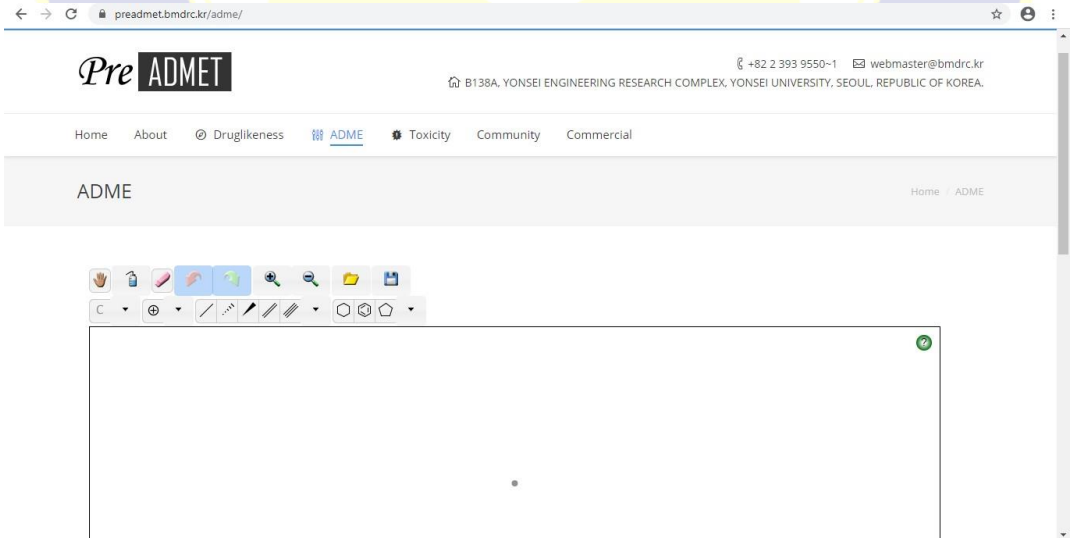


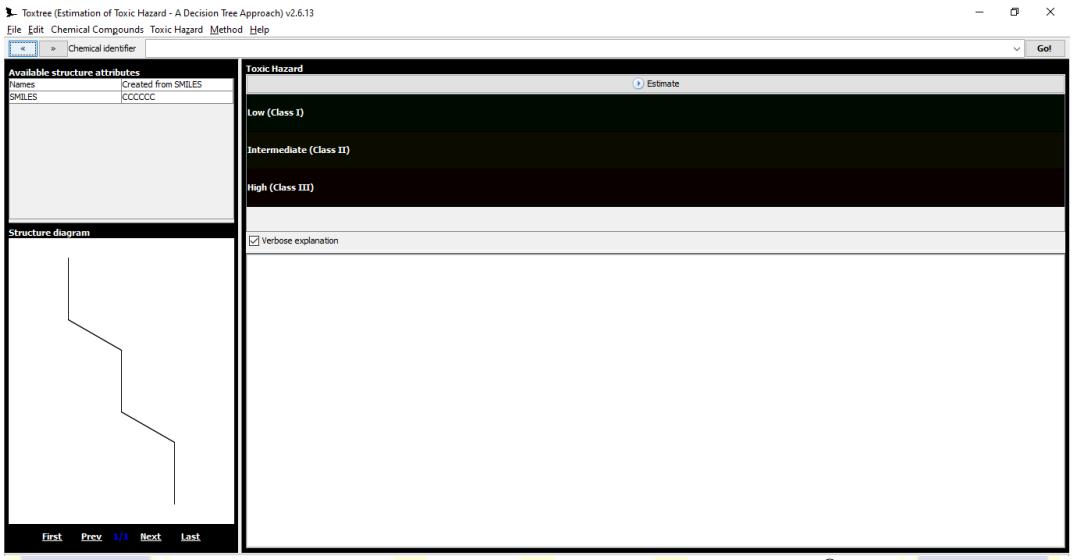
Gambar IV.6 Tampilan aplikasi *ChemDraw Professional 15.0*®



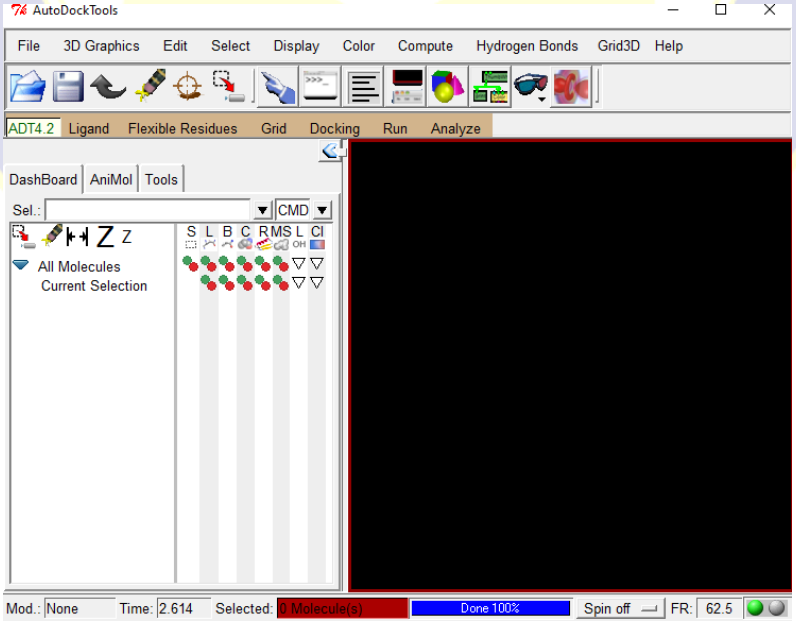
Gambar IV.7 Tampilan situs *Pre*-ADMET

LAMPIRAN 2
(LANJUTAN)

SITUS DAN APLIKASI



Gambar IV.8 Tampilan aplikasi *Toxtree*®



Gambar IV.9 Tampilan aplikasi *AutoDock Tools*®

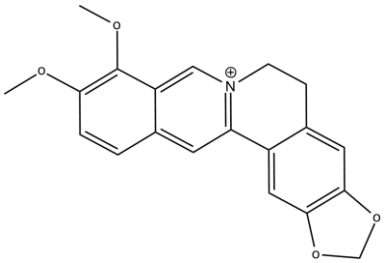
LAMPIRAN 3

TANAMAN KAYU KUNING

Gambar II.3 Tanaman kayu kuning

LAMPIRAN 4

STRUKTUR SENYAWA



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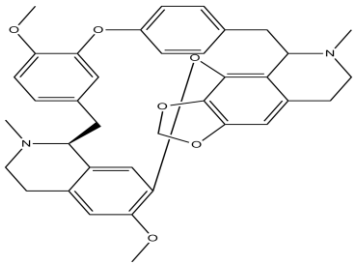

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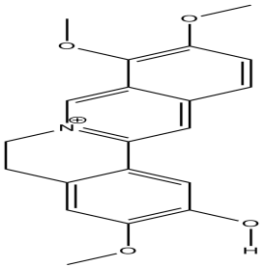

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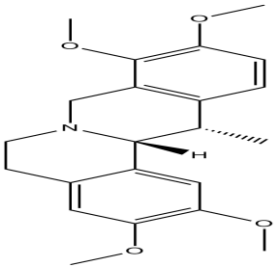

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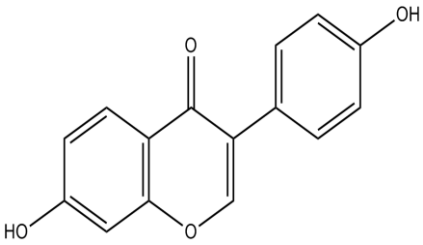

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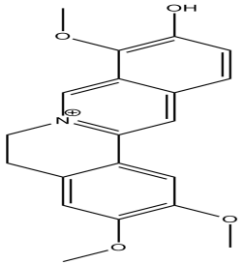

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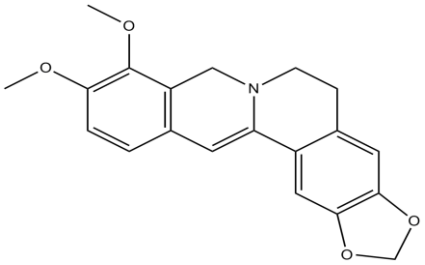

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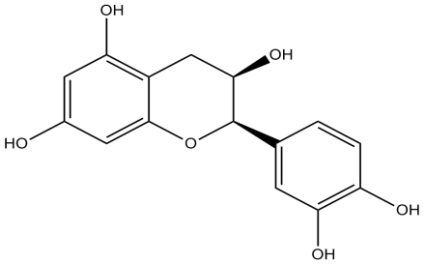

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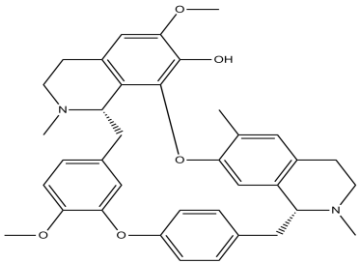
LAMPIRAN 4
(LANJUTAN)

STRUKTUR SENYAWA



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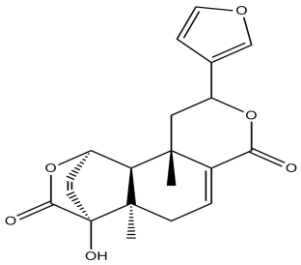

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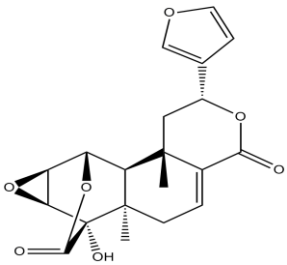

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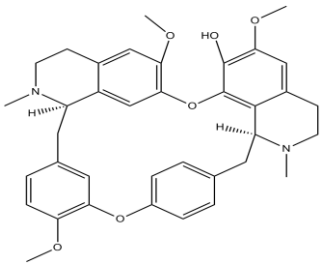

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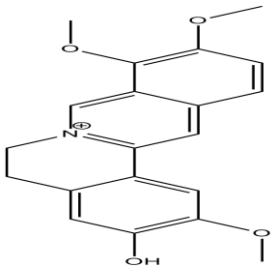

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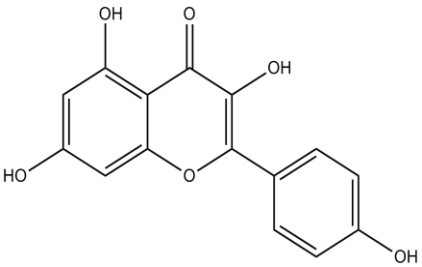

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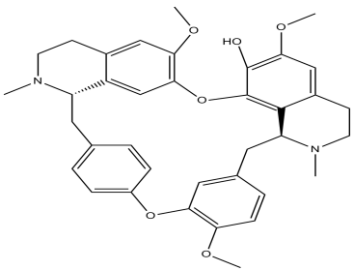

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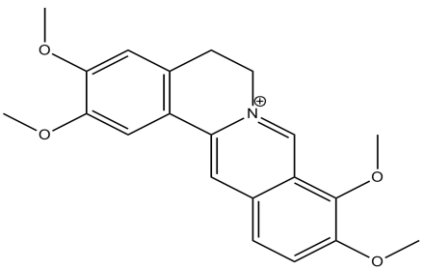

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LAMPIRAN 4
(LANJUTAN)

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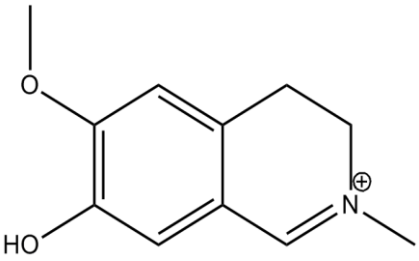

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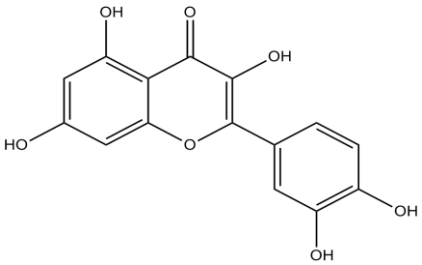

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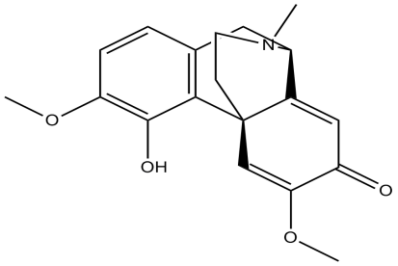

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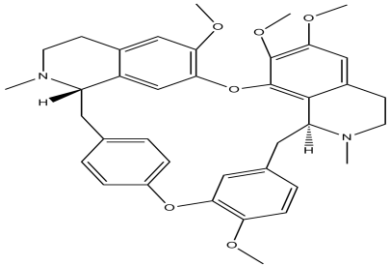

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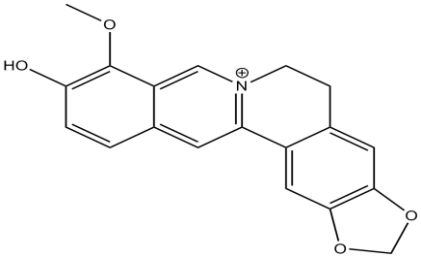

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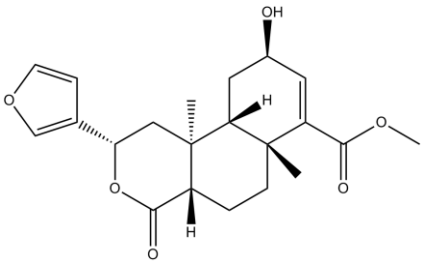

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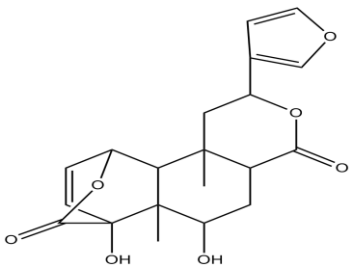
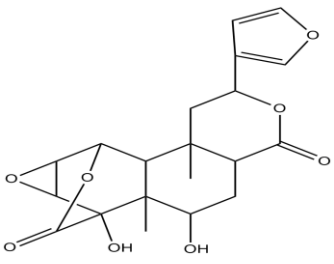


2-HYDROXYARCANGELISINOL



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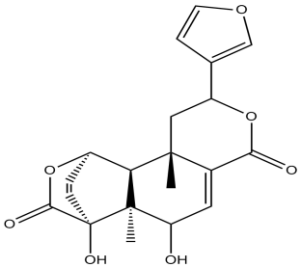
LAMPIRAN 4
(LANJUTAN)

STRUKTUR SENYAWA



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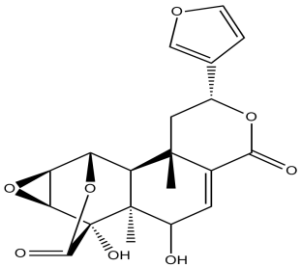

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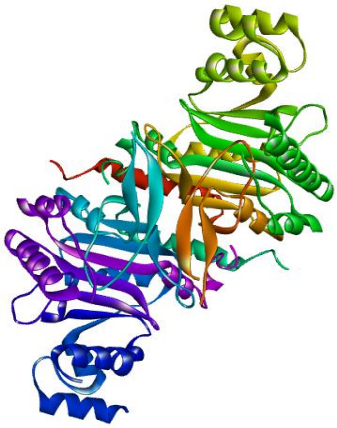
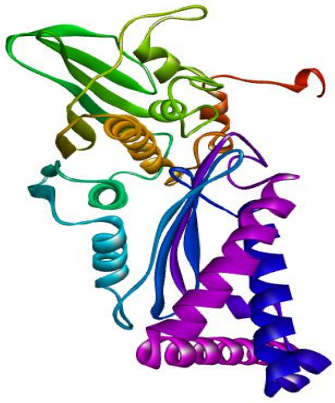
LAMPIRAN 5

RESEPTOR



Reseptor 3G1Z

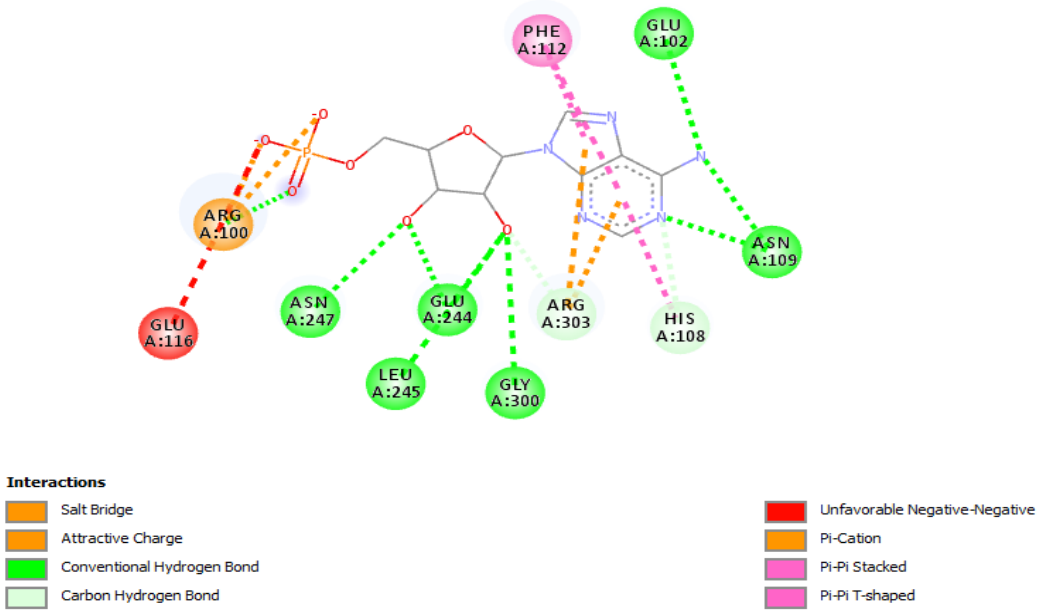


Reseptor 6J90

Reseptor 5BW6

LAMPIRAN 6

VALIDASI METODE

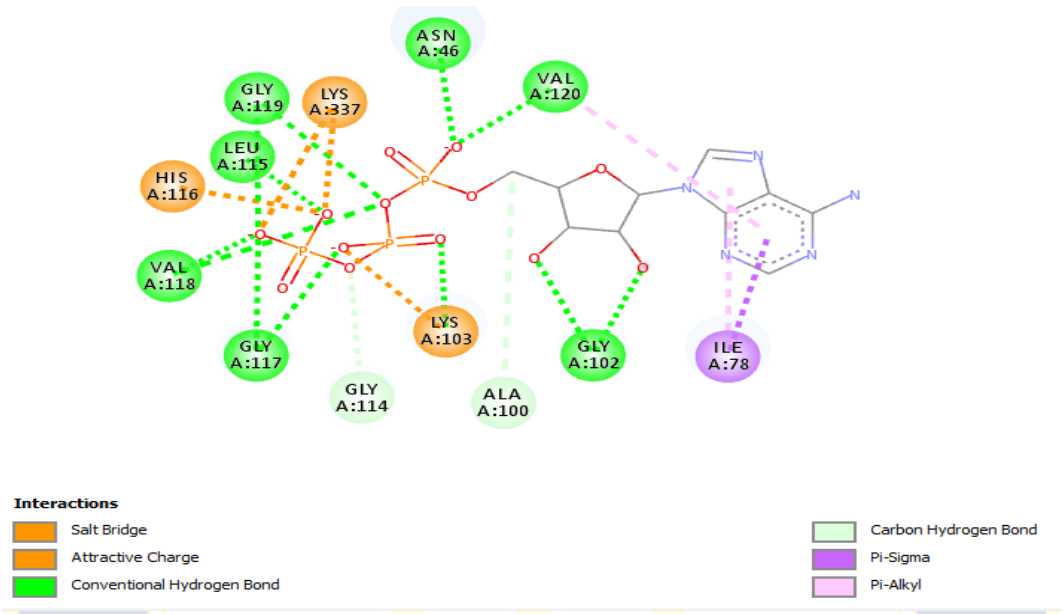


Gambar V.4 Interaksi Hasil Validasi Reseptor 3G1Z

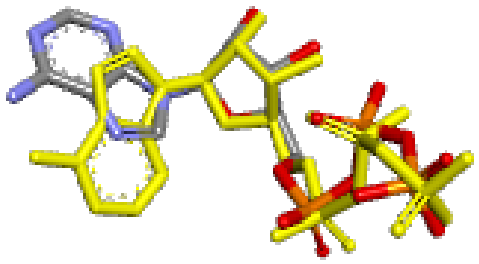
Gambar V.5 Tumpang tindih ligan alami 3G1Z (Merah-Abu) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 6
(LANJUTAN)

VALIDASI METODE



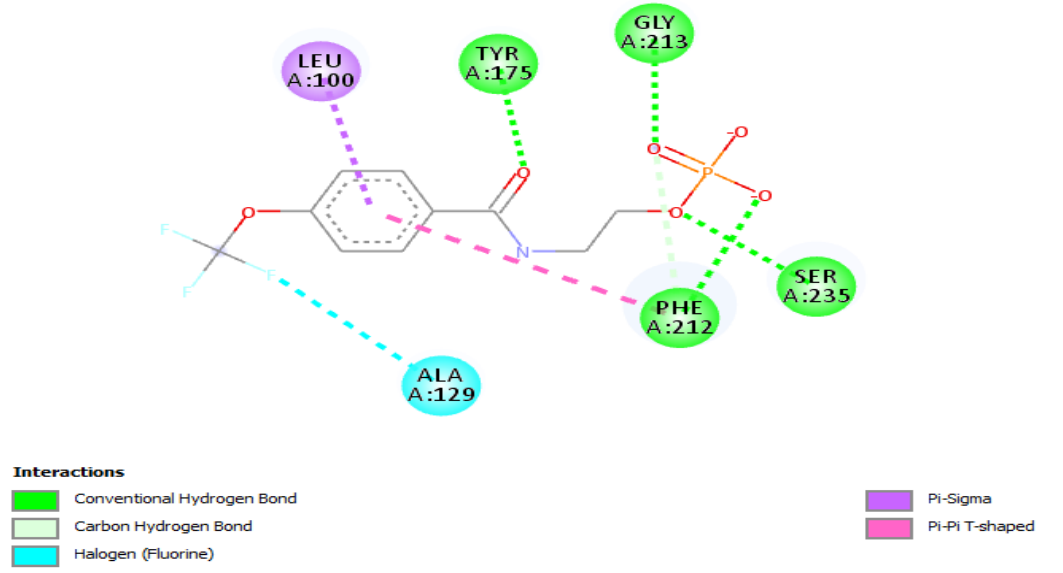
Gambar V.6 Interaksi Hasil Validasi Reseptor 6J90



Gambar V.7 Tumpang tindih ligan alami 6J90 (merah-abu-biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 6
(LANJUTAN)

VALIDASI METODE



Gambar V.8 Interaksi Hasil Validasi 5BW6

Gambar V.9 Tumpang tindih ligan alami 5BW6 (merah-abu-biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 7

HASIL PENAMBATAN MOLEKUL SENYAWA UJI

TABEL V.1

HASIL PENAMBATAN PADA RESEPTOR 3G1Z

No	SENYAWA	ΔG (kcal/Mol)	ki (µmolar)	ASAM AMINO
1	2-dehydroxyarcangelisinol	-7,76	2,06	GLU:116,GLY:300,ARG:303,PHE:112
2	6-hydroxyarcangelisin	-7,76	9,72	ARG:100
3	6-hydroxyfibleucin	-8,07	1,22	GLY:300,LEU:245,ASN:247,ARG:100,
4	6-hydroxyfibraurin	-7,67	2,37	ARG:100
5	Berberin	-9,73	0,0733	HIS:108,ASN:109,ARG:303:100,PHE:112,GLU:244
6	Cepharantine	-8,43	0,666	ARG:303,GLU:102:244PHE:112
7	Columbamine	-9,10	0,214	HIS:108,ARG:303:100,GLU:244,PHE:112
8	Corrydalin	-11,10	0,00727	HIS:108,ASN:109,PHE:112,ARG:303:100
9	Daidzein	-7,66	2,42	ASN:109:247,ARG:303,PHE:112,GLU:244
10	Dehydrocorydalmin	-9,28	0,158	ASN:109,ARG:303:100,GLU:244
11	Dihydroberberine	-9,33	0,146	HIS:108,ARG:303:100,ALA:298,PHE:112
12	Epicathecin	-8,42	0,677	ASN:109:247,PHE:112,ARG:303,GLU:244
13	Fangchinolin	-6,50	17,20	ASN:247,GLU:244,ARG:100,HIS:108
14	Fibleucin	-7,14	5,83	HIS:108,ASN:247,PHE:112

LAMPIRAN 7
(LANJUTAN)

TABEL V.1
LANJUTAN

No	SENYAWA	ΔG (kcal/Mol)	ki (μmolar)	ASAM AMINO
15	Fibraurin	-8,16	1,05	ASN:247,GLY:300,ARG:303:100,HIS:108,GLU:102,PHE:112
16	Homoaromoline	-7,94	1,52	GLU:244:102,ARG:100:303,PHE:112,HIS:108
17	Jathorrizine	-8,68	0,437	HIS:108,ASN:109,ARG:303:100,PHE:112,GLU:244
18	Kaempferol	-8,23	0,932	GLU:244:102,ARG:100:303,PHE:112,ASN:109
19	Limacine	-10,06	0,00422	HIS:108,ARG:100:303,PHE:112,GLU:102:244
20	Palmatine	-9,45	0,118	HIS:108,ASN:109,ARG:303:100,GLU:244
21	Pycnarrhine	-6,21	27,96	LEU:245,GLU:244,ARG:303,PHE:112,GLU:102,ASN:109
22	Quercetine	-8,73	0,3999	ASN:109:247,PHE:112,ARG:100:303,GLU:244
23	Sinoacutin	-7,24	4,96	LEU:245,ARG:100,GLU:102,PHE:112,HIS:108,ARG:303
24	Tetrandrin	-7,89	1,64	HIS:108,ARG:303:100,ASN:247,GLU:244
25	Thalifendin	-9,58	0,096	GLU:244,ARG:303:100,HIS:108,ASN:109,PHE:112
26	Thiamphenicol	-7,45	3,46	ARG:303,ASN:109
27	Tynophyllol	-7,58	2,79	ARG:303:100,MET:114,PHE:112,ALA:298,LEU:53
28	Adenosine Monophospate (Ligan Alami)	-7,34	4,14	GLU:116:244:102,ARG:100:303,HIS:108,ASN:247:109,PHE:112,LEU:245,GLY:300

LAMPIRAN 7
(LANJUTAN)

TABEL V.2

HASIL PENAMBATAN MOLEKUL RESEPTOR 6J90

No	SENYAWA	ΔG (kcal/Mol)	ki (µmolar)	ASAM AMINO
1	2-dehydroxyarcangelisinol	-8,64	0,466	VAL:120,LYS:103,GLY:102:101,ILE:78
2	6-hydroxyarcangelisin	-8,45	0,645	GLY:101,102,ILE,:78,LYS:103
3	6-hydroxyfibleucin	-8,79	0,363	ALA:100,LYS:103,VAL:120:118,GLY:119
4	6-hydroxyfibraurin	-8,87	0,317	GLY:102,LYS:103,ILE:78
5	Berberin	-9,02	0,243	GLY:119:102,VAL:118,ASN:46,LYS:103,ILE:78
6	Cepharantine	+30,65	-	LYS:103,GLY:102,VAL:120,ILE:78,ASN:46
7	Ciprofloxacin	-8,64	0,462	LYS:103:337,LEU:115,HIS:116,GLY:119,ASN:46
8	Columbamine	-8,83	0,339	LYS:337:103,GLY:119:102
9	Corrydalin	-9,32	0,146	GLU:50,PRO:79,TYR:109,ILE:94,VAL:118:120,LYS:103
10	Daidzein	-7,76	2,06	LYS:337:103,VAL:102:118,ASN:46
11	Dehydrocorydalmin	-8,55	0,541	ILE:78,ASN:46,GLY:119,LYS:337:103,HIS:116
12	Dihydroberberine	-8,69	0,425	ASN:46,ILE:78
13	Epicathecin	-7.18	5,45	ALA:100, LYS:103, ILE:78,ASN:46
14	Fangchinolin	+9,39	-	VAL:120,LYS:103,ILE:78
15	Fibleucin	-9,31	0,150	LYS:337:103,VAL:120:118,GLY:119

LAMPIRAN 7
(LANJUTAN)

TABEL V.2
LANJUTAN

No	SENYAWA	ΔG (kcal/Mol)	ki (µmolar)	ASAM AMINO
16	Fibraurin	-9,11	0,211	LYS:103,GLY:102,ILE:78
17	Homoaromoline	+33,44	-	ILE:78,GLY:102,LYS:103
18	Jathorrizine	-8,43	0,661	ILE:78,ASN:46
19	Kaempferol	-7,70	2,27	GLY:119,,LYS:103:337
20	Limacine	+15,20	-	GLY:117:102,ALA:100,LYS:103,ILE:78,VAL120,ASN:46
21	Palmatine	-9,22	0,175	ILE:78,ASN:46,GLY:119,LYS:337:103,HIS:116
22	Pycnarrhine	-6,42	19,71	GLY:119,LYS:103,LEU:115,HIS:116
23	Quercetine	-7,32	4,28	ALA:100,GLY:117:102:119,VAL:120:118,LYS:103,ASN:46
24	Sinoacutin	-7,71	2,25	ILE:78,VAL:120,ASN:46,GLY:119:117,LYS:103
25	Tetrandrin	+2,51	-	GLY:119:117:102,ALA:100,LYS:103,ILE:78,ASN:46
26	Thalifendin	-8,49	0,597	ALA:100,VAL:120:118,LYS:103,GLY:117:119:102:101,ILE:78,ASN:46
27	Tynophyllol	-8,53	0,558	GLY:102:119,VAL:120,LYS:103,ASN:46,ILE:78,ALA:100,
28	Adenosine-5'-Triposphate (Ligan Alami)	-12,44	0,000756	GLY: 119:102:117:114,LEU:115,HIS:116, LYS:337:103,ASN:46,VAL:120:118,ALA:100,ILE:78

LAMPIRAN 7
(LANJUTAN)

TABEL V.3

HASIL PENAMBATAN MOLEKUL RESEPTOR 5BW6

No	SENYAWA	ΔG (kcal/Mol)	ki (µmolar)	ASAM AMINO
1	2-dehydroxyarcangelisinol	-9,06	0,230	ALA:129,LEU:100,SER:235,PHE:212,TYR:175
2	6-hydroxyarcangelisin	-8,51	0,580	ALA:129,TYR:175,LEU:100,SER:235,PHE:212
3	6-hydroxyfibleucin	-6,52	16,69	PHE:212
4	6-hydroxyfibraurin	-8,31	0,809	ALA:129,SER:235,PHE:212,LEU:100
5	Berberin	-7,55	2,90	GLY:213,SER:235,PHE:212
6	Cepharantine	+15,25	-	LEU:100,ALA:129
7	Columbamine	-6,74	11,51	ALA:129,PHE:212,GLY:213,SER:235,LEU:100
8	Corrydalin	8,03	1,30	PHE:212,SER:235,LEU:100,ALA:129
9	Daidzein	-7,76	2,04	ALA:129,PHE:212
10	Dehydrocorydalmin	-7,10	6,21	PHE:212
11	Dihydroberberine	-7,49	3,25	SER:235GLY:213,PHE:212
12	Epicathecin	-8,49	0,597	ALA:129,PHE:212,LEU:100,TYR:175
13	Fangchinolin	-2,35	18880	LEU:100,PHE:212,GLY:234
14	Fibleucin	-6,98	7,70	ALA:129,PHE:212

LAMPIRAN 7
(LANJUTAN)

TABEL V.3
LANJUTAN

No	SENYAWA	ΔG (kcal/Mol)	ki (µmolar)	ASAM AMINO
15	Fibraurin	-8,55	0,541	SER:235,PHE:212,LEU:100
16	Homoaromoline	+43,36	-	ALA:129,TYR:175,LEU:100
17	Jathorrizine	-7,54	2,95	SER:235,PHE:212
18	Kaempferol	-8,43	0,663	ALA:129,LEU:100,PHE:212,TYR:175
19	Limacine	-1,70	56460	LEU:100,PHE:212
20	Palmatine	-7,20	5,28	SER:235,PHE:212
21	Pycnarrhine	-6,46	18,50	PHE:212
22	Quercetine	-9,65	0,0847	PHE:212,SER:235,TYR:175
23	Sinoacutin	-9,19	0,184	SER:235,PHE:212
24	Tetrandrin	-2,21	23980	PHE:212,LEU:100,TYR:175
25	Thalifendin	-7,14	5,82	SER:235,GLY:213,PHE212
26	Thiamphenicol	-8,25	0,899	PHE:212,SER:235
27	Tynophyllol	-9,94	0,0565	LEU:100,GLY:213,SER:215,PHE:212,TYR:175
28	2-{[4-(Trifluoromethoxy)Benzoyl]Amino}Ethyl Dihydrogen Phosphate	-7,47	3,34	LEU:100,TYR:175,GLY:213,SER:235,PHE:212,ALA:129

LAMPIRAN 8

TABEL V.4

HASIL PREDIKSI *DRUG LIKENESS* BERDASARKAN ATURAN *LIPINSKI RULE OF FIVE*

NO	SENYAWA	BM	Log P	Ikatan Hidrogen		Keterangan
				Donor	Akseptor	
1	2-dehydroxyarcangelisinol	374	1,5	2	7	Memenuhi Syarat
2	6-hydroxyarcangelisin	390	0,715	2	8	Memenuhi Syarat
3	6-hydroxyfibleucin	372	1,42	2	7	Memenuhi Syarat
4	6-hydroxyfibraurin	388	0,635	2	8	Memenuhi Syarat
5	Berberin	336	3,89	0	4	Memenuhi Syarat
6	Cepharantine	606	6,87	0	8	Tidak Memenuhi Syarat
7	Columbamine	338	3,88	1	4	Memenuhi Syarat
8	Corrydalin	369	3,53	0	5	Memenuhi Syarat
9	Daidzein	254	2,71	2	4	Memenuhi Syarat
10	Dehydrocorydalmin	338	3,07	1	4	Memenuhi Syarat
11	Dihydroberberine	337	3,07	0	5	Memenuhi Syarat
12	Epicathecin	290	1,55	5	6	Memenuhi Syarat
13	Fangchinolin	608	6,86	1	8	Tidak Memenuhi Syarat
14	Fibleucin	356	2,45	1	6	Memenuhi Syarat
15	Fibraurin	372	1,66	1	7	Memenuhi Syarat
16	Homoaromoline	541	5,85	2	9	Tidak Memenuhi Syarat
17	Jathorrizine	338	3,64	1	4	Memenuhi Syarat
18	Kaempferol	286	2,31	4	6	Memenuhi Syarat

LAMPIRAN 8
(LANJUTAN)

TABEL V.4
LANJUTAN

NO	SENYAWA	BM	Log P	Ikatan Hidrogen		Keterangan
				Donor	Akseptor	
19	Limacine	608	6,86	1	8	Tidak Memenuhi Syarat
20	Palmatine	352	4,18	0	4	Memenuhi Syarat
21	Pycnarrhine	192	1,02	1	2	Memenuhi Syarat
22	Quercetine	302	2,01	5	7	Memenuhi Syarat
23	Sinoacutin	327	1,71	1	5	Memenuhi Syarat
24	Tetrandrin	622	6,61	0	8	Tidak Memenuhi Syarat
25	Thalifendin	322	3,59	1	4	Memenuhi Syarat
26	Tynophyllol	374	3,17	1	6	Memenuhi Syarat

LAMPIRAN 9

TABEL V.5

HASIL PREDIKSI TOKSISITAS LIGAN PEMBANDING DAN SENYAWA AKTIF TANAMAN KAYU KUNING (*Arcangelisia flava* (L.) Merr.)

NO	SENYAWA	Crame Rules	Kross TTC	Benigni
1	2-dehydroxyarcangelisinol	3	2	1,9
2	6-hydroxyarcangelisin	3	2	1,9
3	6-hydroxyfibleucin	3	2	1,9
4	6-hydroxyfibraurin	3	2	1,9
5	Berberin	3	2	1,2
6	Cepharantine	3	1	2,8
7	Ciprofloxacin	3	1	8,9
8	Columbamine	3	2	1,9
9	Corrydalin	3	1	8,9
10	Daidzein	3	2	1,9
11	Dehydrocorydalmin	3	2	1,9
12	Dihydroberberine	3	1	2,8
13	Epicathecin	3	1	8,9
14	Fangchinolin	3	1	8,9
15	Fibleucin	3	1	8,9

LAMPIRAN 9
(LANJUTAN)

TABEL V.5
LANJUTAN

NO	SENYAWA	Crame Rules	Kross TTC	Benigni
16	Fibraurin	3	2	1,9
17	Homoaromoline	3	1	8,9
18	Jathorrizine	3	2	1,9
19	Kaempferol	3	1	8,9
20	Limacine	3	1	8,9
21	Palmatine	3	2	1,9
22	Pycnarrhine	3	1	8,9
23	Quercetine	3	1	2,8
24	Sinoacutin	3	2	1,9
25	Tetrandrin	3	1	8,9
26	Thalifendin	3	2	1,2
27	Tynophyllol	3	1	8,9
28	Thyamphenicol	3	2	1,9

LAMPIRAN 9
(LANJUTAN)

TABEL V.5
LANJUTAN (KETERANGAN TABEL)

Keterangan :

Cramer rules	=	(1)	*Substances with sample chemical structures and fix which efficient modes of meabolism exist, suggesting a low order of oral toxicity.*
		(2)	*Substances which possess structures that are less innocuous than class I Substances, but do not contain structural features suggestive of toxicity like those substances in class III.*
		(3)	*Substances with chemical structures that permit no strong unitial presumption of safety or may even suggest significant toxicity it have reactive functional groups.*
Benigni/Bossa rulebase	=	(1)	*Structural Alert for genotoxic carcinogenicity.*
		(2)	*Structural Alert for nongenotoxic carcinogenicity.*
		(3)	*Negative for genotoxic carcinogenicity.*
		(4)	*Negative for nongenotoxic carcinogenicity.*
Kroes TTC	=	(1)	*Substance would not be expected to be a safety concern.*
		(2)	*Negligible risk (low probability of life-time cancer risk greater than 1 in 10^6).*

LAMPIRAN 10

TABEL V.6
HASIL PREDIKSI PROFIL ABSORBSI DAN DISTRIBUSI LIGAN PEMBANDING DAN SENYAWA AKTIF TANAMAN KAYU KUNING (*Arcangelisia flava* (L.) Merr.)

NO	SENYAWA	HIA	Caco-2	Protein Plasma Binding
1	2-dehydroxyarcangelisinol	95.80	22.327	90.293
2	6-hydroxyarcangelisin	88.718	20.667	57.05
3	6-hydroxyfibleucin	98.65	27.76	97.119
4	6-hydroxyfibraurin	88.471	19.862	59.195
5	Berberin	97.884	55.578	58.542
6	Cepharantine	98.01	54.229	82.20
7	Ciprofloxacin	96.270	21.280	31.053
8	Columbamine	96.14	46.74	56.82
9	Corrydalin	97.762	56.776	82.937
10	Daidzein	92.646	7.72	88.704
11	Dehydrocorydalmin	96.143	46.74	57.061
12	Dihydroberberine	97.867	55.732	89.321
13	Epicathecin	66.707	0.656	100
14	Fangchinolin	97.523	52.287	81.99
15	Fibleucin	95.942	21.847	87.398

LAMPIRAN 10
(LANJUTAN)

TABEL V.6
LANJUTAN

NO	SENYAWA	HIA	Caco-2	Protein Plasma Binding
16	Fibraurin	92.457	21.154	72.768
17	Homoaromoline	97.523	50.052	81.99
18	Jathorrizine	96.143	46.741	55.352
19	Kaempferol	77.833	9.565	89.671
20	Limacine	97.523	52.287	81.99
21	Palmatine	97.923	55.956	58.381
22	Pycnarrhine	95.84	44.502	16.482
23	Quercetine	63.485	3.412	93.236
24	Sinoacutin	95.75	29.392	30.186
25	Tetrandrin	98.056	54.338	84.203
26	Thalifendin	95.923	36.814	34.293
27	Tynophyllol	95.789	21.885	93.58
28	Thyamphenicol	91.779	0.498	69.998

LAMPIRAN 10
(LANJUTAN)

TABEL V.6
LANJUTAN (KETERANGAN TABEL)

Keterangan :

% Human Intestinal Absorbsi (% HIA)	=	(1)	70-100% *well absorbed*
		(2)	20-70% *moderately absorbed*
		(3)	0-20% *poorly absorbed*
In Vitro Caco-2 cell permeability (nm sec-1)	=	(1)	>70 *higher permeability*
		(2)	4-70 *medium permeability*
		(3)	<4 *low permeability*
Plasma Protein Binding	=	(1)	>90 *strongly bound*
		(2)	<90 *weakly bound*