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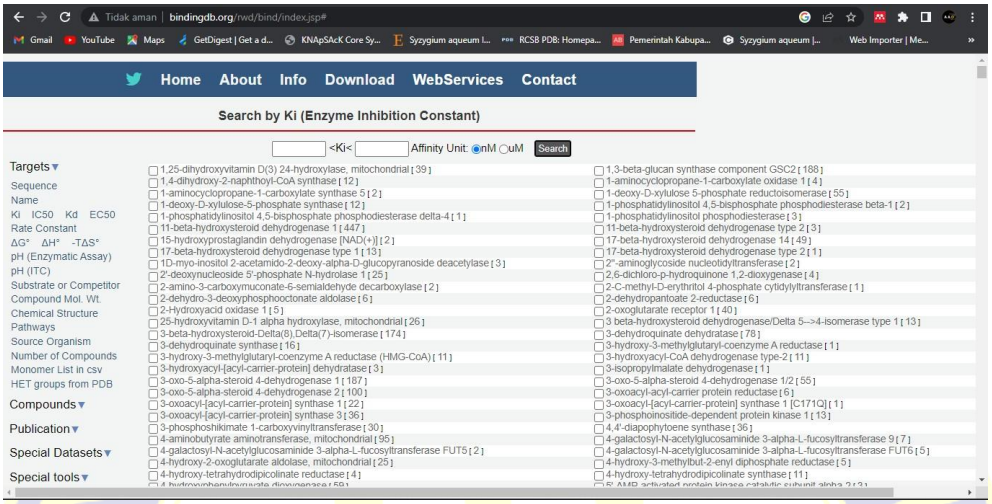
LAMPIRAN I

ALUR PENELITIAN *SKRINING* FARMAKOFOR DAN PENAMBATAN MOLEKUL

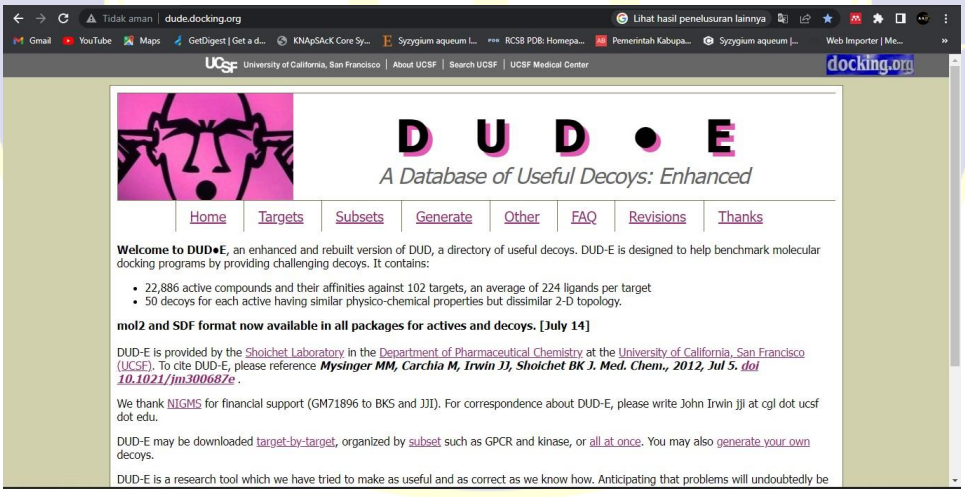
Gambar IV.1 Alur penelitian *screening phamracophore* dan penambatan molekul

LAMPIRAN 2

SITUS DAN PROGRAM

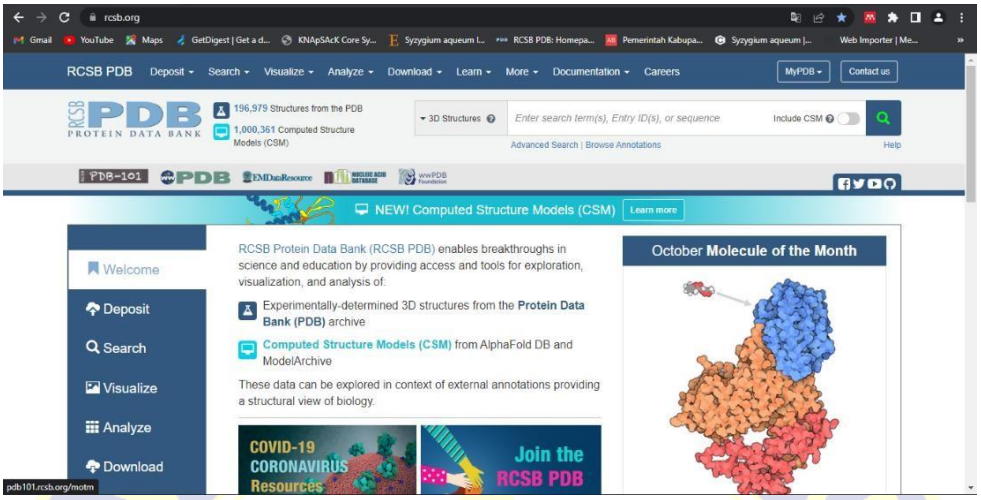


Gambar IV.1 Tampilan situs *binding database*

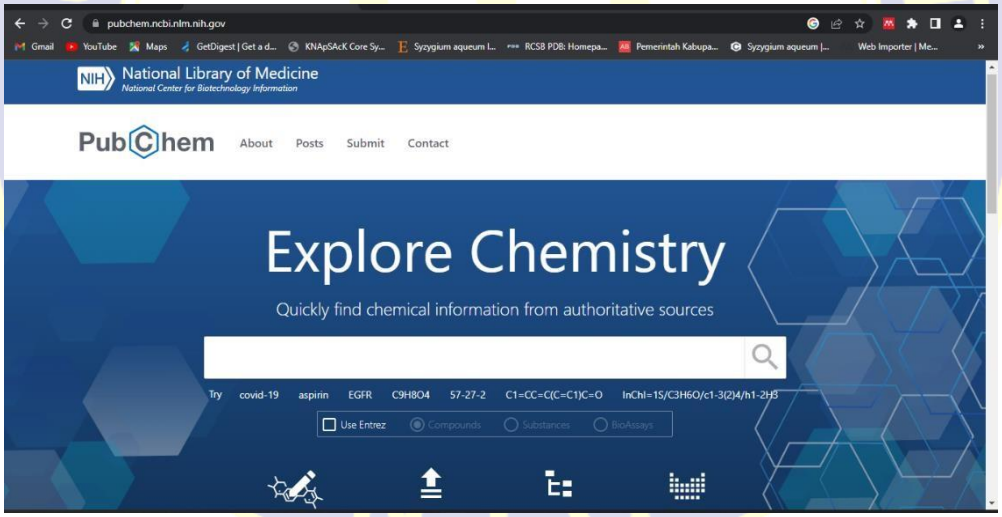


Gambar. IV.2 Tampilan situs DUD-E

LAMPIRAN 2
(LANJUTAN)

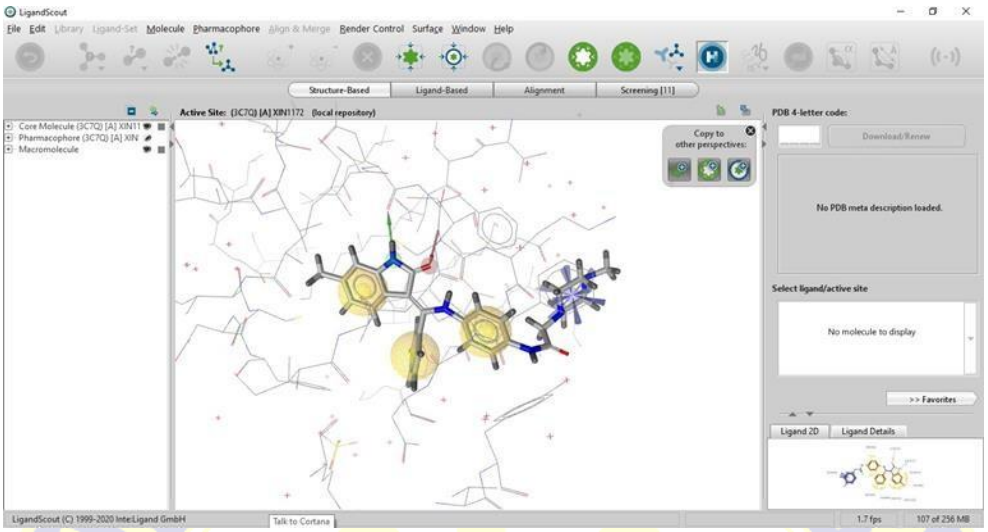


Gambar IV.3 Tampilan situs *protein data bank*

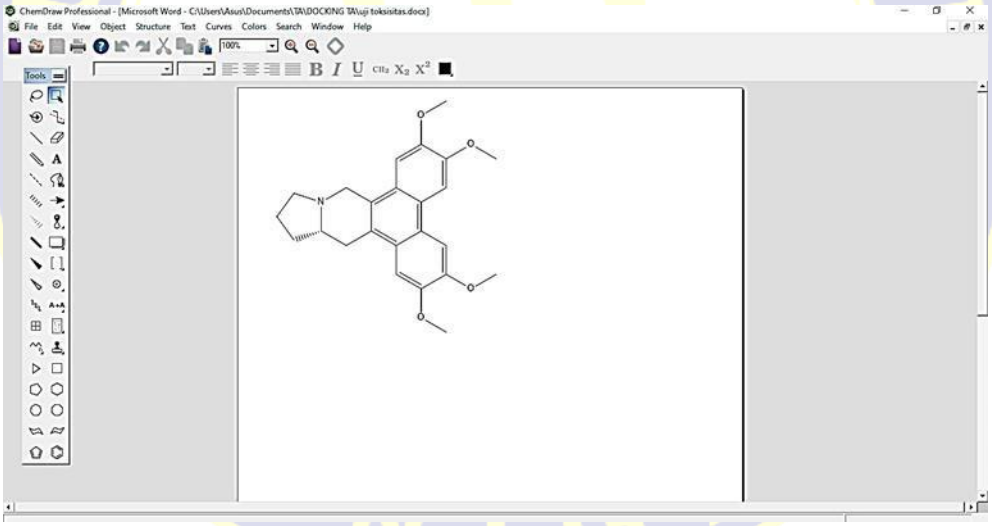


Gambar IV.4 Tampilan situs *pubchem*

LAMPIRAN 2
(LANJUTAN)

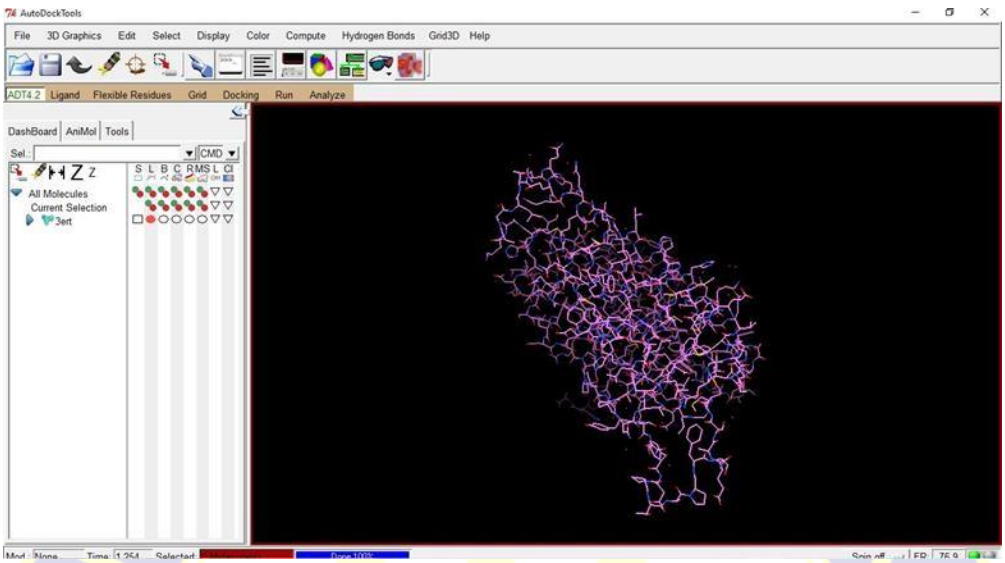


Gambar IV.5 Tampilan program *ligandscout*®

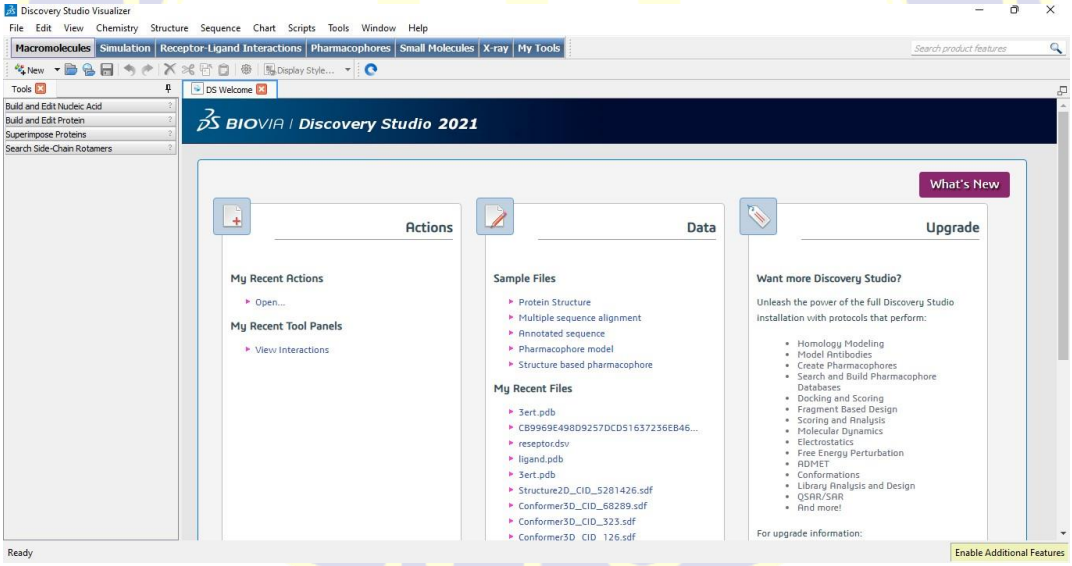


Gambar IV.6 Tampilan program *chemdraw*®

LAMPIRAN 2
(LANJUTAN)

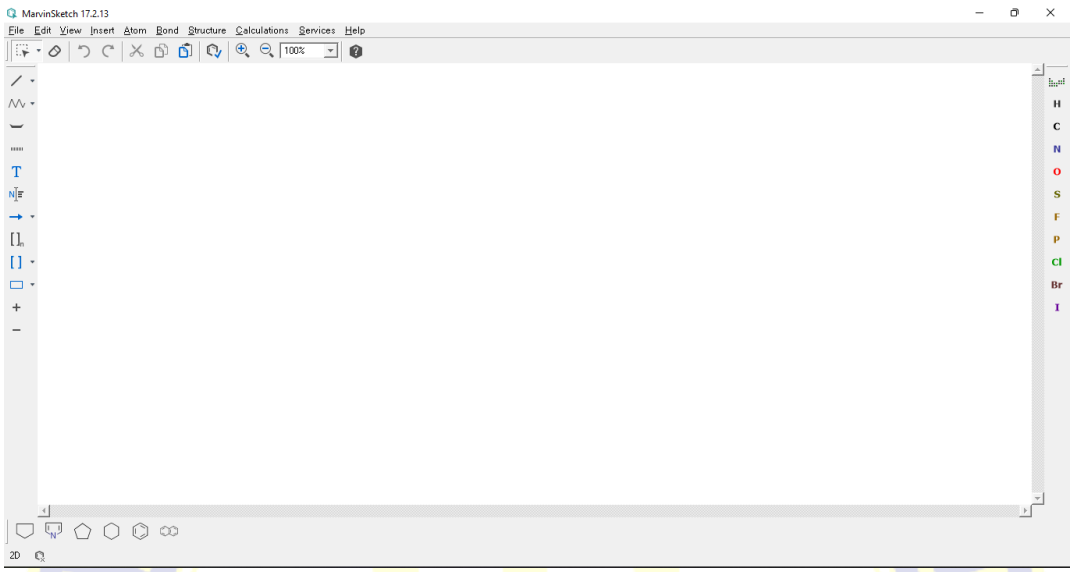


Gambar IV.7 Tampilan program *autodock tools*®

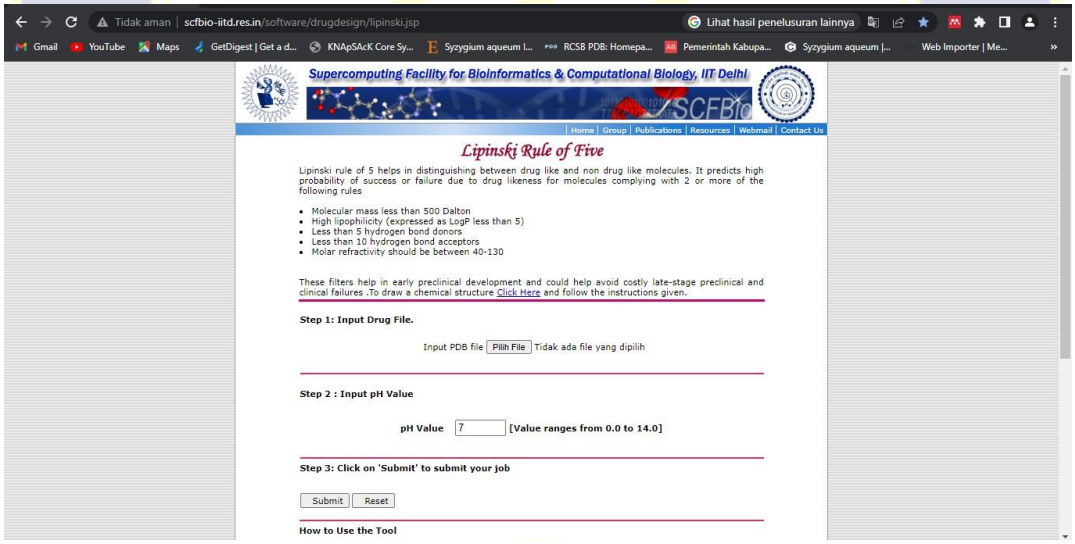


Gambar IV.8 Tampilan program *discovery studio visualizer*®

LAMPIRAN 2
(LANJUTAN)

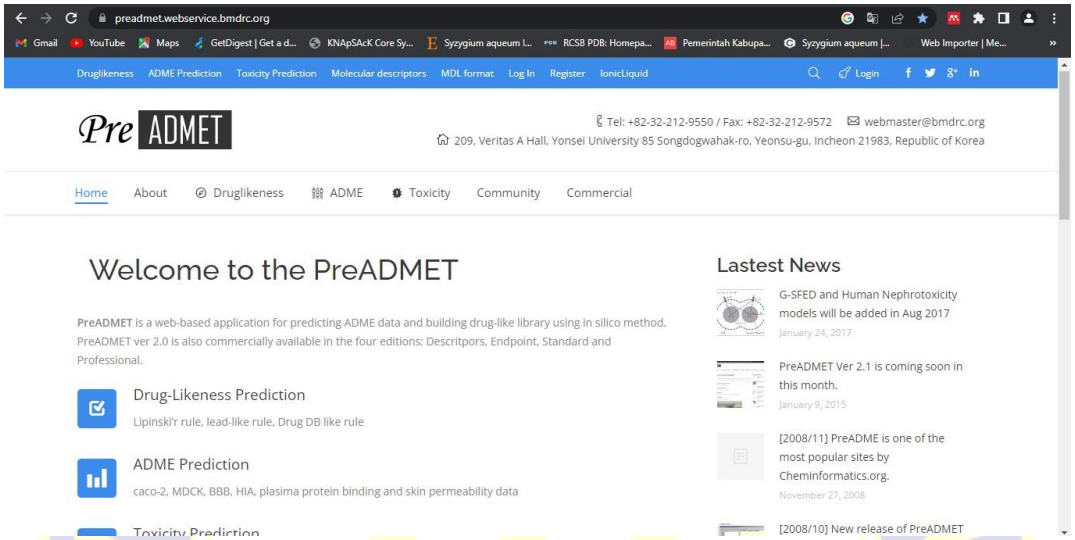


Gambar IV.9 Tampilan aplikasi *MarvinSketch 17.2.13*

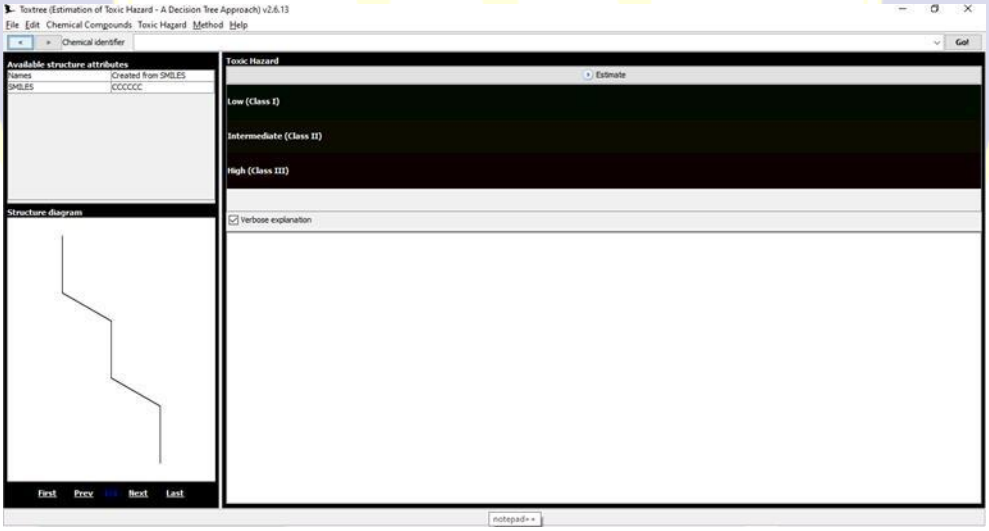


Gambar IV.10 Tampilan situs *online Lipins'ki Rule of Five*

LAMPIRAN 2
(LANJUTAN)



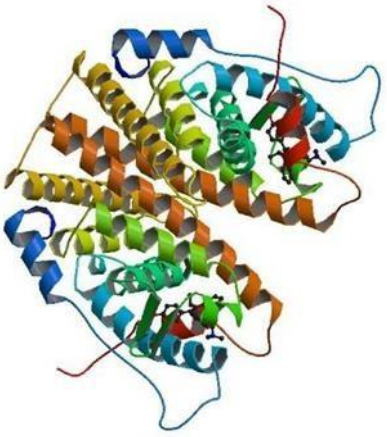
Gambar IV.11 Tampilan situs *online Pre* ADMET



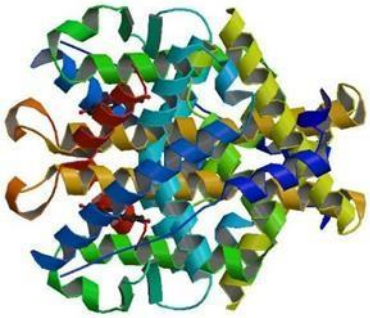
Gambar IV.12 Tampilan program *toxtree*®

LAMPIRAN 3

STRUKTUR 3D RESEPTOR



ER-*α* (Kode : 3ERT)



ER-Q (Kode : 1QKM)

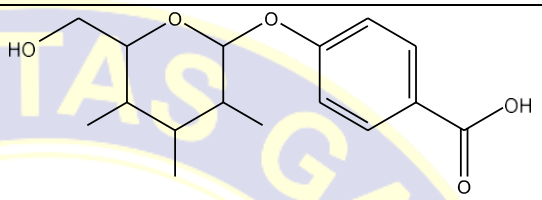
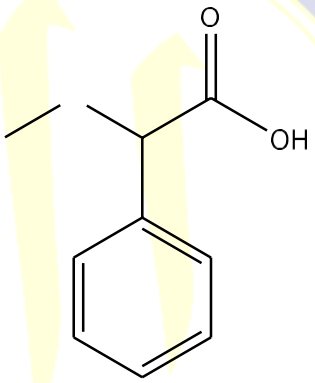
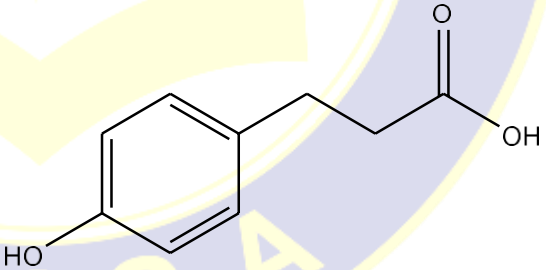
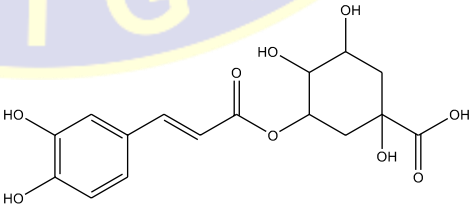
Gambar IV.15 Struktur 3D reseptor

LAMPIRAN 4

STRUKTUR SENYAWA DAUN JAMBU AIR (*Syzygium aqueum.*)

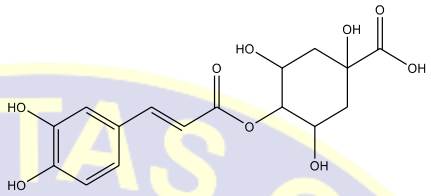
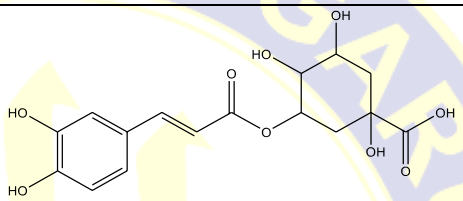
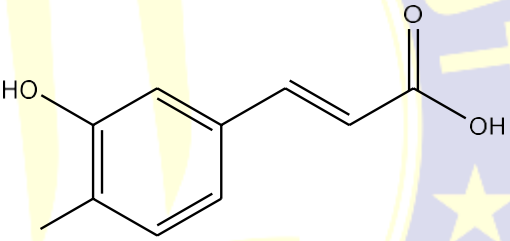
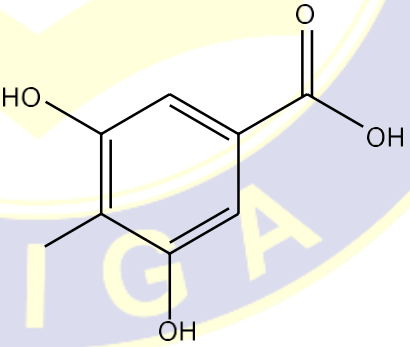
Tabel IV.1

Struktur 2D Senyawa Aktif Daun Jambu Air (*Syzygium aqueum.*)

No	Senyawa	Struktur 2D
1.	4-Hydroxybenzoic acid 4-O-glucoside	
2.	Methoxyphenylacetic acid	
3.	Dihydro-p-coumaric acid	
4.	5-Caffeoylquinic acid	

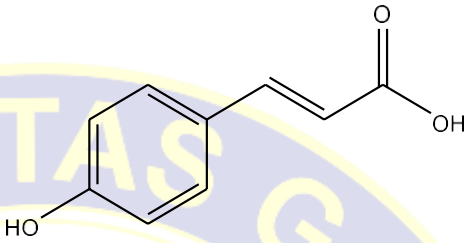
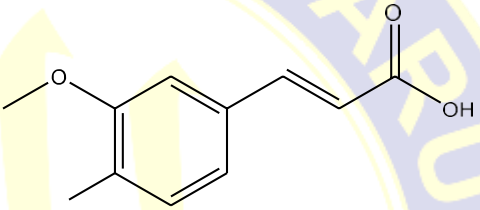
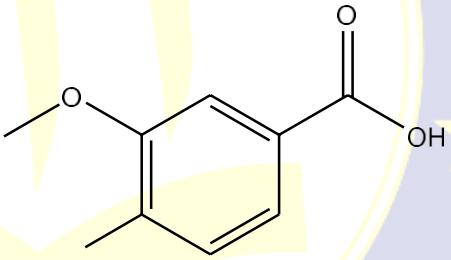
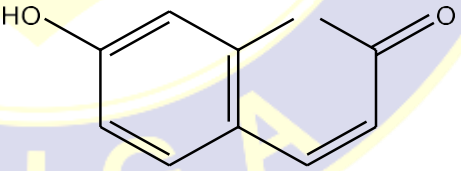
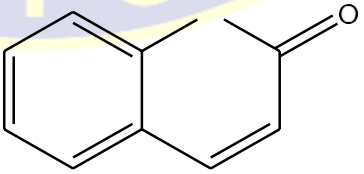
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
5.	4-Caffeoylquinic acid	
6.	Chlorogenic acid	
7.	Caffeic acid	
8.	Gallic acid	

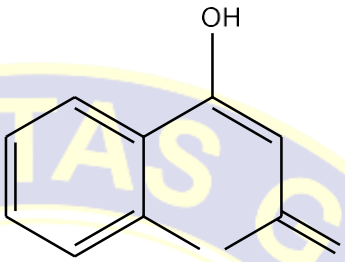
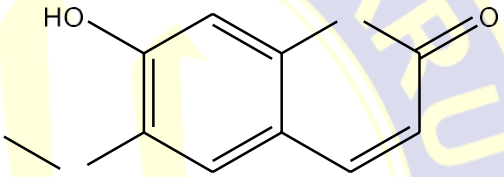
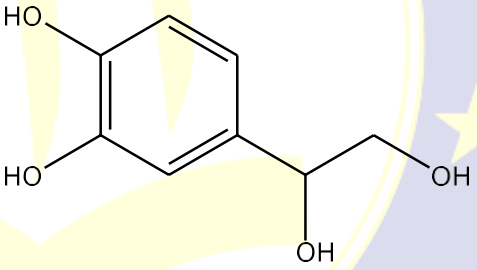
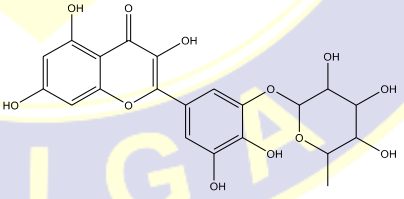
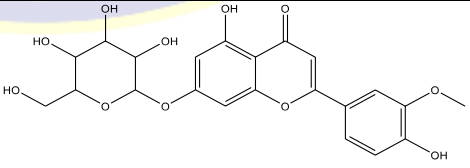
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
9.	p-Coumaric acid	
10.	Ferulic acid	
11.	Vanillic acid	
12.	Umbelliferone	
13.	Coumarin	

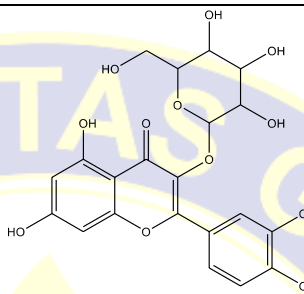
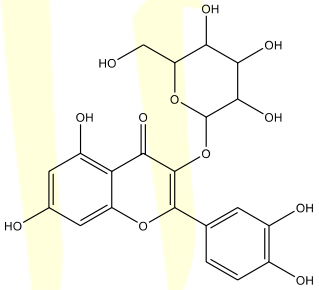
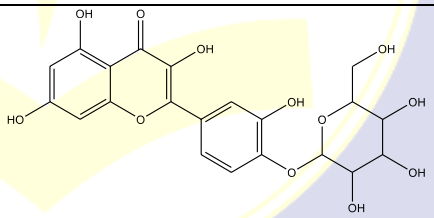
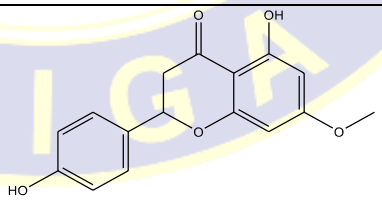
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
14.	4-Hydroxycoumarin	
15.	Scopoletin	
16.	3,4-Dihydroxyphenylglycol	
17.	Myricetin-3-O-rhamnoside	
18.	Chrysoeriol 7-O-glucoside	

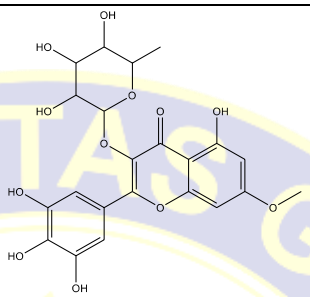
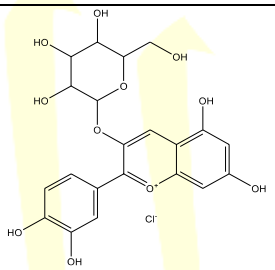
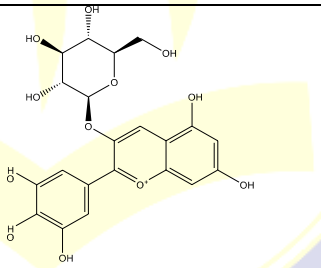
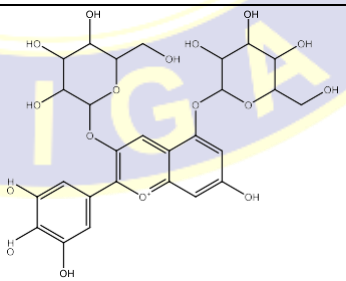
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
19.	Quercetin 3-O-galactoside	
20.	Quercetin 3-O-glucoside	
21.	Quercetin 4′-O-glucoside	
22.	Sakuranetin	

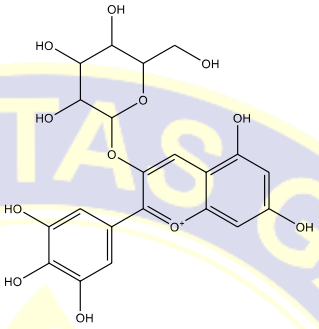
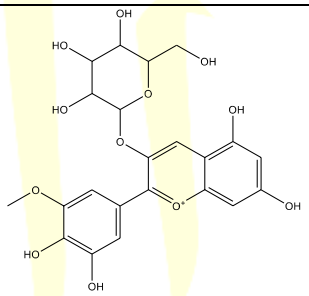
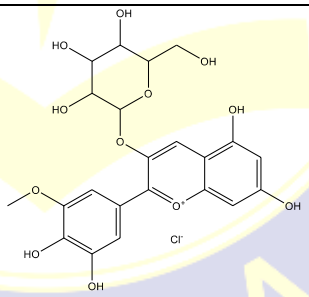
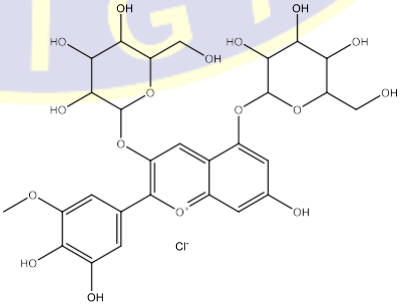
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
23.	Europetin 3-O-rhamnoside	
24.	Cyanidin 3-glucoside	
25.	Delphinidin 3-O-glucoside	
26.	Delphinidin 3,5-O-diglucoside	

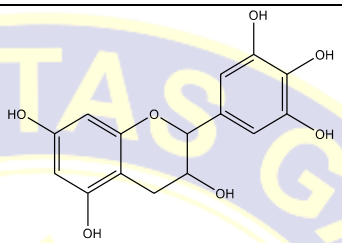
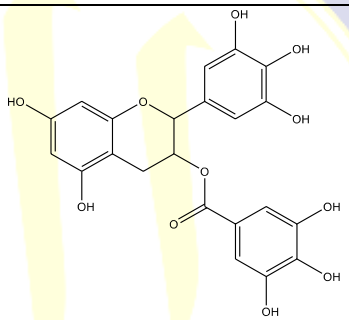
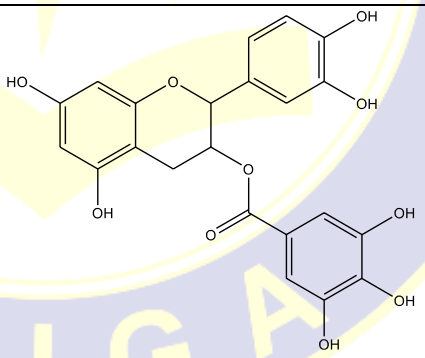
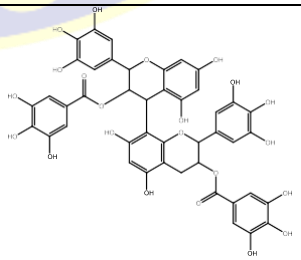
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
27.	Delphinidin 3-O-galactoside	
28.	Petunidin 3-O-glucoside	
29.	Petunidin 3-O-galactoside	
30.	Petunidin 3,5-O-diglucoside	

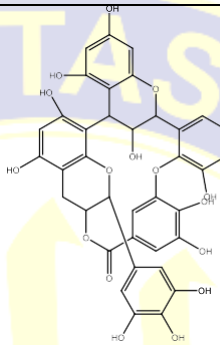
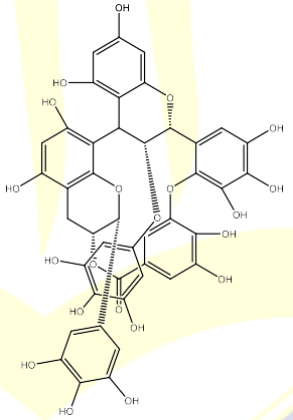
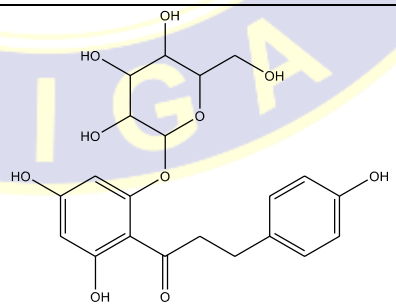
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
31.	(−)-Epigallocatechin	
32.	(−)-Epigallocatechin 3-gallate	
33.	Epicatechin 3-O-gallate	
34.	Prodelphinidin B-2,3,3″-di-O-gallate	

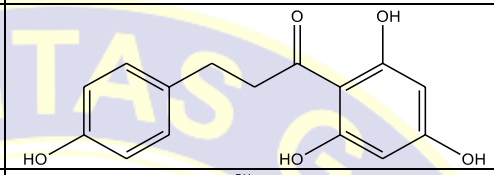
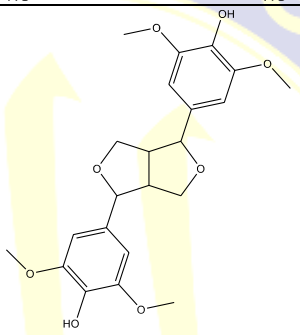
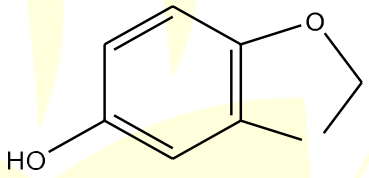
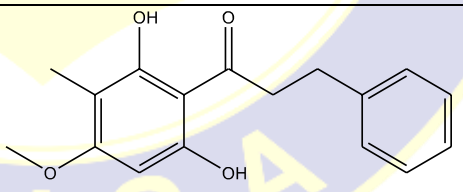
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
35.	Samarangenin A	
36.	Samarangenin B	
37.	Phlorizin	

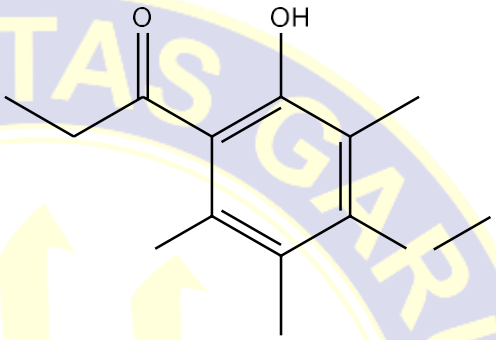
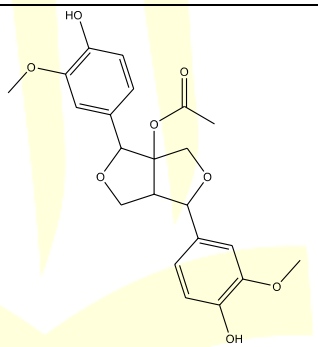
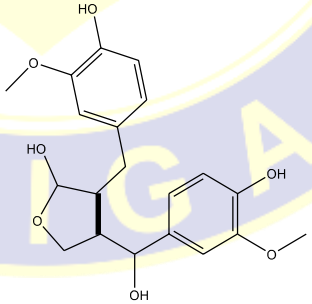
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
38.	Phloretin	
39.	Syringaresinol	
40.	Sesamol	
41.	Myrigalone G	

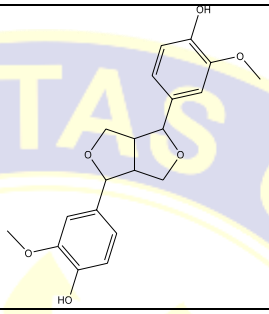
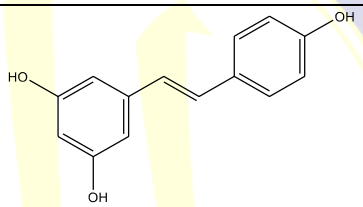
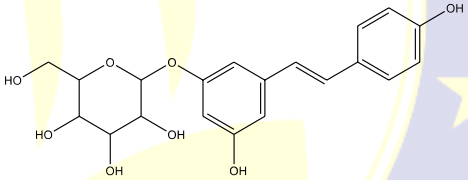
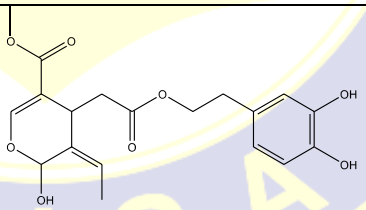
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
42.	Myrigalone B	
43.	1-Acetoxypinoresinol	
44.	Todolactol A	

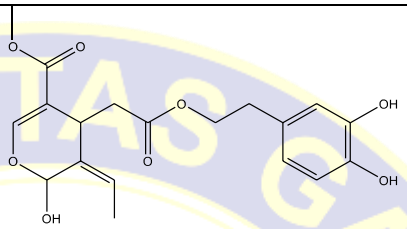
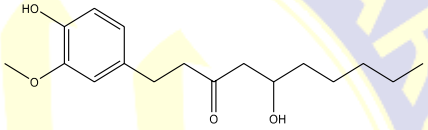
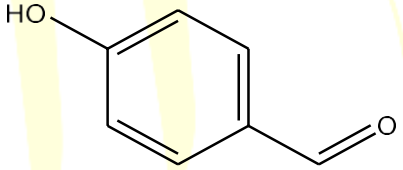
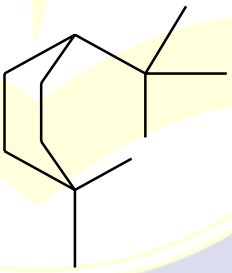
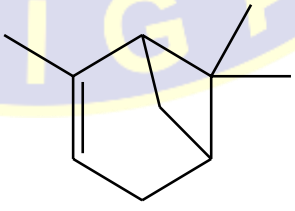
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
45.	Pinoresinol	
46.	Resveratrol	
47.	Resveratrol 5-O-glucoside	
48.	Oleuropein-aglycone	

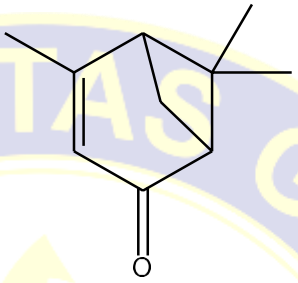
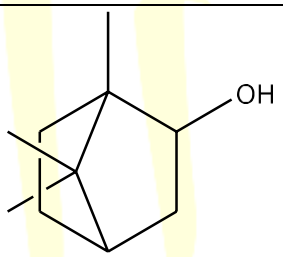
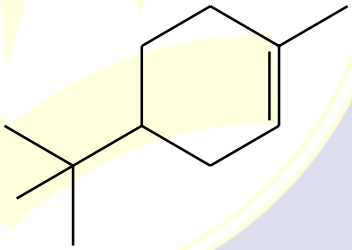
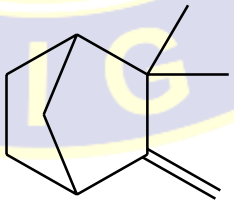
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
49.	3,4-DHPEA-Ea	
50.	6-Gingerol	
51.	4-Hydroxybenzaldehyde	
52.	Eucalyptol	
53.	α-Pinene	

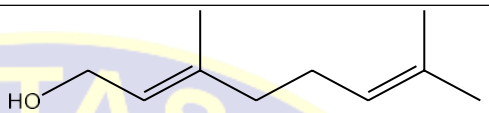
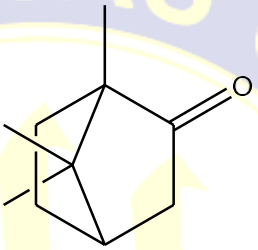
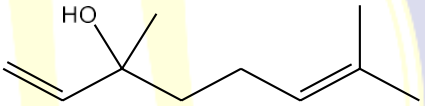
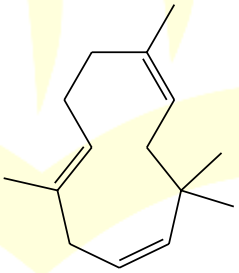
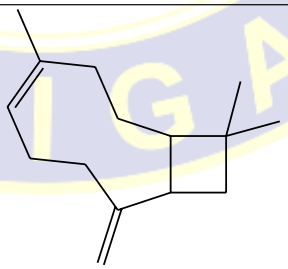
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
54.	L-Verbenone	
55.	Borneol	
56.	α-Terpineol	
57.	Camphene	

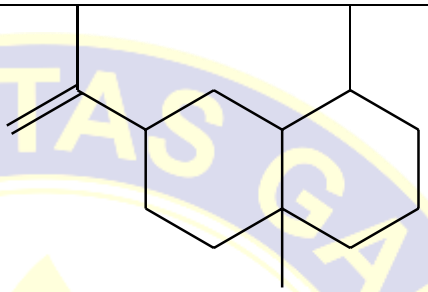
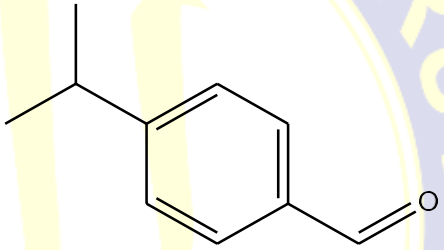
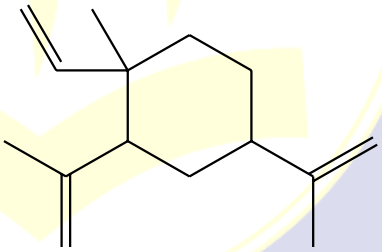
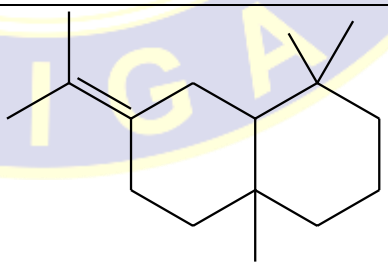
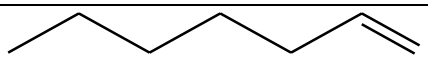
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
58.	Cis-Geraniol	
59.	Camphor	
60.	β-Linalool	
61.	α-Caryophyllene	
62.	β-Caryophyllene	

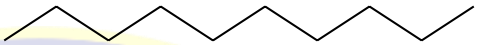
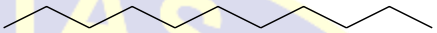
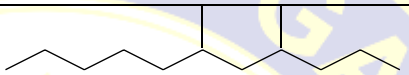
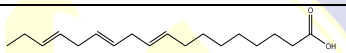
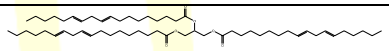
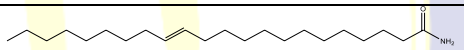
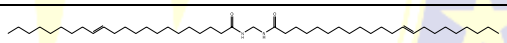
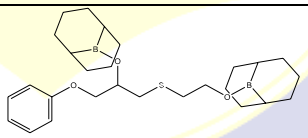
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
63.	β-Selinene	
64.	Cuminyl aldehyde	
65.	β-Elemene	
66.	Eudesm-7(11)-en-4-ola	
67.	Hexanal	

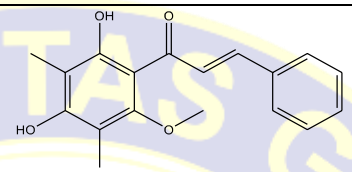
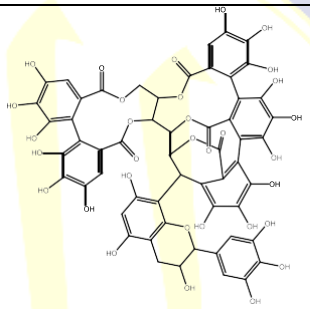
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

NO	SENYAWA	STUKTUR 2D
68.	Decane	
69.	Undecane	
70.	Undecane, 4,6-dimethyl-	
71.	9,12,15-Octadecatrienoic acid,	
72.	Trilinolein	
73.	13-Docosenamide, (Z)-	
74.	Bis(cis-13-docosenamido)methane	
75.	1,8-Dioxa-5-thiaoctane,8-(9-borabicyclo[3.3.1]non-9-yl)-3-(9-borabicyclo[3.3.1]non-9-yloxy)-1-phenyl-	

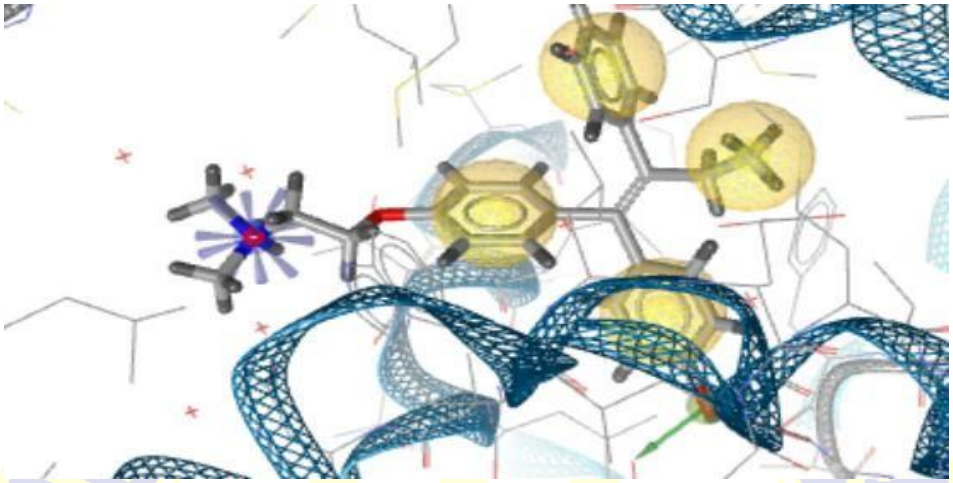
LAMPIRAN 4
(LANJUTAN)

Tabel IV.1
(lanjutan)

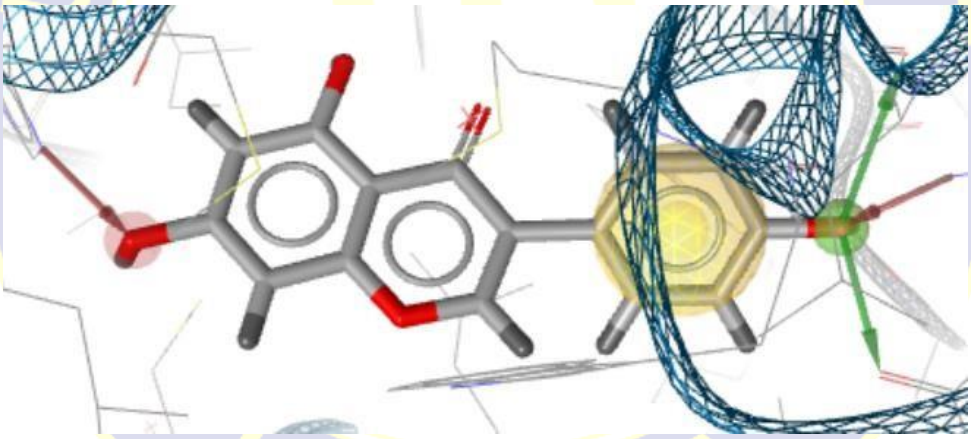
NO	SENYAWA	STUKTUR 2D
76.	2′,4′-Dihydroxy-6′-methoxy-3′,5′ dimethylchalcone	
77.	Eugenigrandin A	

LAMPIRAN 5

SKRINING FARMAKOFOR



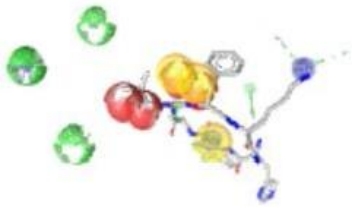
Gambar V.1 Hasil *screening pharmacophore* pada *estrogen receptor – alfa*



Gambar V.2 Hasil *screening pharmacophore* pada *estrogen receptor – beta*

LAMPIRAN 5
(LANJUTAN)

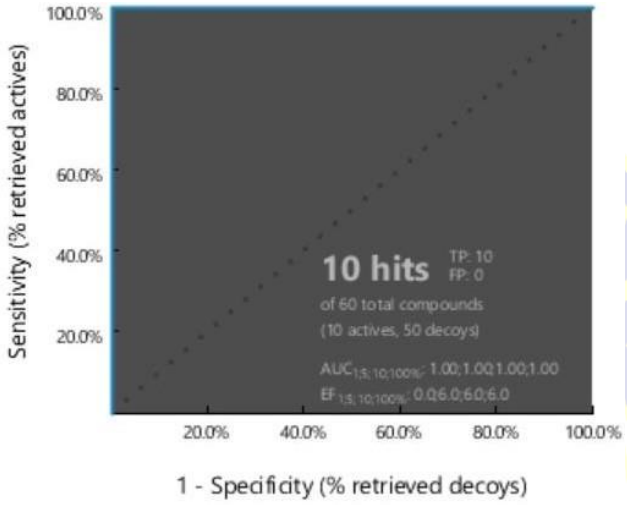
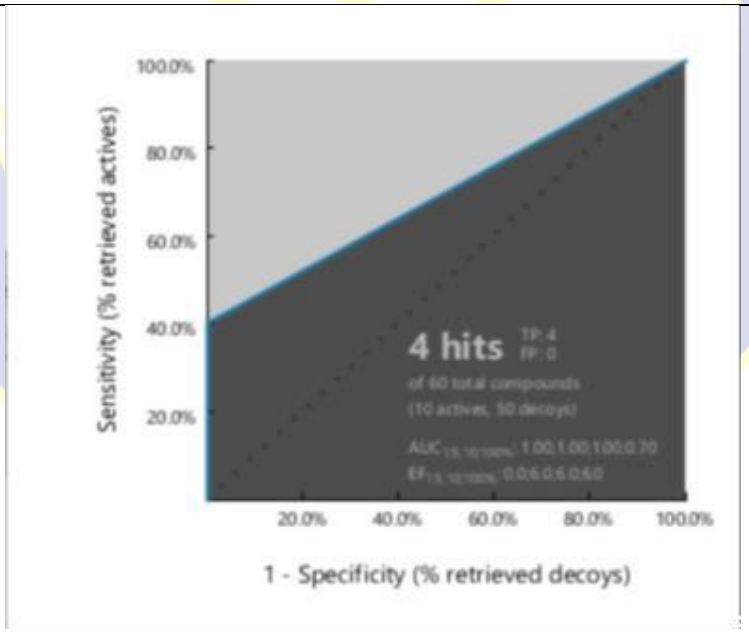
Gambar V.3 Model 1 *pharmacophore* ligan *estrogen receptor - alfa*



Gambar V.4 Model 1 *pharmacophore* ligan *estrogen receptor – beta*

LAMPIRAN 5
(LANJUTAN)

Tabel V.1
Hasil Validasi Model Farmakofor

Reseptor	**ROC *Curve***	**AUC**	**GH *Score***
ER-α		1.00	1.00
ER-β		0.70	0.85

LAMPIRAN 5
(LANJUTAN)

Tabel V.2
Hasil *Skrining* Farmakofor *Estrogen Receptor – Alfa*

No	Nama Senyawa	Matching Features	Fit Score
	TAMOXIFEN (LIGAN PEMBANDING)		
1	Pinoresinol		64.72
2	1-Acetoxypinoresinol		63.08
3	3,4-Dihydroxyphenylglycol		61.03
4	Oleuropein-aglycone		58.17
5	3,4-DHPEA-Ea		58.17
6	Todolactol A		57.1
7	4-Hydroxybenzaldehyde		56.76
8	Quercetin 3-O-glucoside		55.68
9	Dihydro-p-coumaric acid		55.18
10	Quercetin 3-O-galactoside		55.1
11	Epicatechin 3-O-gallate		54.73
12	p-Coumaric acid		54.42
13	Vanillic acid		54.34
14	Phloretin		53.88
15	Ferulic acid		48.54
16	Sakuranetin		47.98
17	Resveratrol 5-O-glucoside		47.78
18	Chrysoeriol 7-O-glucoside		47.72
19	4-Caffeoylquinic acid		47.46
20	Caffeic acid		47.06
21	Resveratrol		46.91
22	6-Gingerol		46.89
23	Chlorogenic acid		45.72
24	Phlorizin		45.5

LAMPIRAN 5
(LANJUTAN)

Tabel V.3

Hasil *Skrining* Farmakofor *Estrogen Receptor – Beta*

No	Nama Senyawa	Matching Features	Fit Score
#	GENISTEIN (LIGAN PEMBANDING)		
1	5-Caffeoylquinic acid		58.22
2	Chlorogenic acid		58.15
3	Resveratrol		57.61
4	Petunidin 3-O-galactoside		57.39
5	Phloretin		57.37
6	Petunidin 3-O-glucoside		57.37
7	Sakuranetin		57.15
8	Oleuropein-aglycone		56.95
9	3,4-DHPEA-Ea		56.95
10	4-Caffeoylquinic acid		56.32
11	Quercetin 3-O-glucoside		55.91
12	Delphinidin 3-O-glucoside		55.76
13	Cyanidin 3-glucoside		55.76

Keterangan :

Warna biru = Cincin aromatic

Warna kuning = Ikatan hidrofobik

Warna merah = Akseptor ikatan hidrogen

Warna hijau = Donor ikatan hidrogen

LAMPIRAN 6

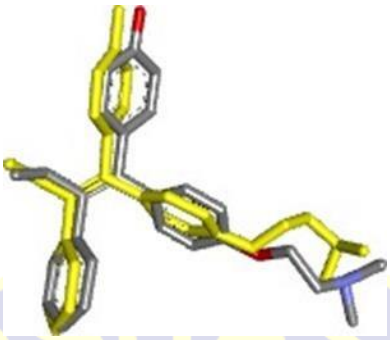
VALIDASI METODE PENAMBATAN MOLEKUL

Tabel V.4
Hasil Validasi Penambatan Molekul

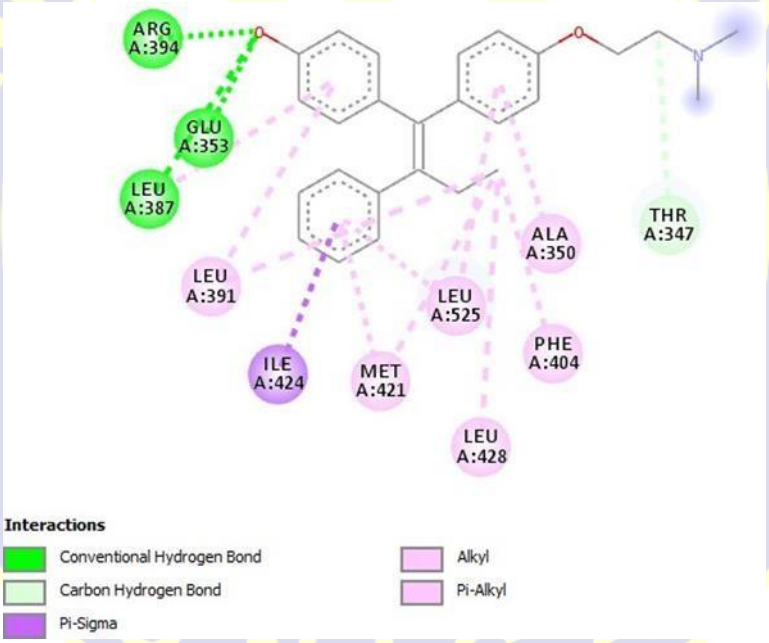
No	Kode PDB	Nilai RMSD	Grid Box
1	3ERT	1.158 Å	X : 30.282
			Y : -1.913
			Z : 24.207
2	1QKM	0.449 Å	X : 22.438
			Y : 8.003
			Z : 113.539

Keterangan : Nilai RMSD < 2Å

LAMPIRAN 6
(LANJUTAN)



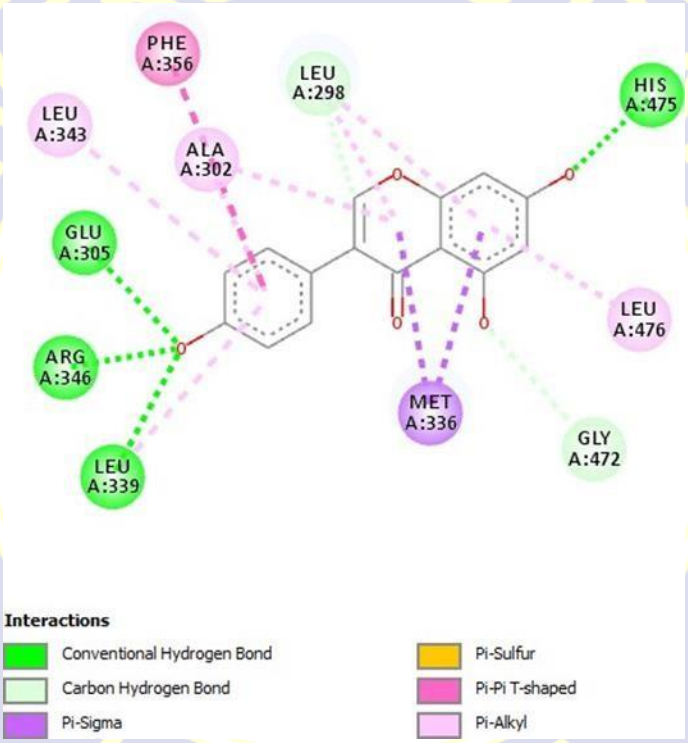
Gambar V.5 Visualisasi tumpang tindih ligan alami 3ERT (merah-abu-biru) dengan ligan hasil *redocking* (kuning)



Gambar V.6 Interaksi ligan alami dengan residu-residu asam amino pada *estrogen receptor – alfa*

LAMPIRAN 6
(LANJUTAN)

Gambar V.7 Visualisasi tumpang tindih ligan alami 1QKM (merah-abu) dengan ligan hasil *redocking* (kuning)



Gambar V.8 Interaksi ligan alami dengan residu-residu asam amino pada *estrogen receptor – beta*

LAMPIRAN 7

HASIL PENAMBATAN MOLEKUL

Tabel V.5
Hasil Penambatan Molekul pada *Estrogen Receptor-Alfa*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
	Tamoxifen (Ligan Pembanding)	-10.54	18.74	THR A:347	LEU A:387, LEU A:391, ALA A:350, MET A:421, LEU A:525, PHE A:404, LEU A:428, MET A:388
1	Pinoresinol	-8.02	1.33	ASP A:351, ARG A:394, LEU A:387	LEU A:525, LEU A:384, LEU A:391, ALA A:350
2	1-Acetoxypinoresinol	-8.01	1.35	ASP A:351, LEU A:387, GLY A:521	ALA A:350, LEU A:525, MET A:388
3	3,4-Dihydroxyphenylglycol	-4.38	616.15	GLU A:353, ARG A:394	LEU A:387, LEU A:391
4	Oleuropein-aglycone	-7.88	1.66	GLU A:353, LEU A:349, ARG A:394	LEU A:387, LEU A:391, ALA A:350
5	3,4-DHPEA-Ea	-6.79	10.62	ASP A:351, THR A:347, GLU A:353,	LEU A:525, ALA A:350, LEU A:346
6	Todolactol A	-7.08	6.43	ARG A:394, GLU A:353	MET A:388, ALA A:350, LEU A:346
7	4-Hydroxybenzaldehyde	-4.71	354.5	GLU A:353, ARG A:394	LEU A:391, LEU A:387
8	Quercetin 3-O-glucoside	-8.31	807.14	THR A:347, GLY A:521, HIS A:524, GLU A:419, PHE A:404	LEU A:525, LEU A:346, ALA A:350, LEU A:391

LAMPIRAN 7
(LANJUTAN)

Tabel V.5
Hasil Penambatan Molekul pada *Estrogen Receptor-Alfa*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
9	Dihydro-p-coumaric acid	-4.06	1.06	ARG A:394, GLU A:353	LEU A:391, LEU A:387
10	Quercetin 3-O-galactoside	-8.58	516.8	GLY A:521, ARG A:394, GLU A:353, LEU A:525, THR A:347	LEU A:387, LEU A:384, ALA A:350, LEU A:346, LEU A:391
11	Epicatechin 3-O-gallate	-9.43	123.34	GLU A:353, ASP A:351, GLU A:419, HIS A:524, PHE A:404THR A:347	LEU A:387, LEU A:349, ALA A:350, LEU A:525, MET A:343, MET A:421, LEU A:347
12	p-Coumaric acid	-4.06	1.06	ARG A:394, GLU A:353	LEU A:391, LEU A:387
13	Vanillic acid	-3.77	1.72	ARG A:394, GLU A:353, LEU A:346, HIS A:524, GLU A:419	LEU A:391, LEU A:387
14	Phloretin	-7.71	2.23	LEU A:346, GLU A:353, GLY A:521, HIS A:524,	LEU A:525, ILE A:424, LEU A:391, ALA A:350, LEU A:387
15	Ferulic acid	-4.15	905.98	ARG A:394, GLU A:353, LEU A:346, HIS A:524, GLU A:419	LEU A:391, LEU A:387

LAMPIRAN 7
(LANJUTAN)

Tabel V.5
Hasil Penambatan Molekul pada *Estrogen Receptor-Alfa*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
16	Sakuranetin	-7.08	6.51	LEU A:387, ARG A:394, THR A:347	LEU A:391, LEU A:346, MET A:343, LEU A:525
17	Resveratrol 5-O-glucoside	-7.48	3.3	ASP A:351, LEU A:346, GLU A:353, ARG A:394, LEU A:387, MET A:388	LEU A:384, ALA A:350
18	Chrysoeriol 7-O-glucoside	-7.1	6.21	ARG A:394, LEU A:387, MET A:343, THR A:347, ASP A:351	ALA A:350, LEU A:525, LEU A:346
19	4-Caffeoylquinic acid	-5.91	46.9	ARG A:394, GLU A:353, ASP A:351	ALA A:350, LEU A:525
20	Caffeic acid	-4.56	456.57	MET A:421, GLU A:353	LEU A:391, LEU A:387
21	Resveratrol	-7.41	3.73	GLY A:521, GLU A:353, ARG A:394, GLU A:419	ALA A:350, LEU A:387, LEU A:391, LEU A:525, MET A:421
22	6-Gingerol	-5.73	62.89	PHE A:404	LEU A:525, HIS A:524, MET A:343, LEU A:349, LEU A:346, ALA A:350, LEU A:391

LAMPIRAN 7
(LANJUTAN)

Tabel V.5
Hasil Penambatan Molekul pada *Estrogen Receptor-Alfa*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
23	Chlorogenic acid	-6.52	16.62	ARG A:394, GLU A:353, GLU A:419, HIS A:524, GJY A:420	LEU A:525
24	Phlorizin	-6.76	11.04	ASP A:351, THR A:347, GLY A:521, GLU A:419, GLU A:353	ALA A:350, LEU A:525, MET A:421

LAMPIRAN 7
(LANJUTAN)

Tabel V.6
Hasil Penambatan Molekul pada *Estrogen Receptor-Beta*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
	Genistein (Ligan Pembanding)	-9.49	110.71	ARG A:346, GLU A:305, HIS A:475, GLY A:472	MET A:336, ALA A:302, LEU A:339, LEU A:343, PHE A:356, LEU A:298
1	5-Caffeoylquinic acid	-8.29	841.05	ARG A:346, GLU A:305, GLY A:472, HIS A:475	LEU A:343, LEU A:339, PHE A:356, MET A:340
2	Chlorogenic acid	-8.33	788.88	GLY A:472, HIS A:475, ARG A:346, GLU A:305	PHE A:356, LEU A:339, MET A:340, LEU A:343
3	Resveratrol	-8.57	522.62	GLU A:305, GLY A:472, HIS A:475, LEU A:339	MET A:336, ALA A:302, PHE A:356, MET A:336, LEU A:298
4	Delphinidin 3-O-galactoside	-4.38	611.28	LEU A:339, GLU A:305	MET A:336, LEU A:343, PHE A:356, LEU A:298, ALA A:302
5	Phloretin	-8.81	350.54	LEU A:298, HIS A:475, MET A:336, GLU A:305	PHE A:356, LEU A:476, LEU A:301, ALA 302, LEU A:339
6	Petunidin 3-O-glucoside	-3.77	1.72	HIS A:475, ARG A:346, GLU A:305, GLY GLY A:472	LEU A:298, ALA A:302, PHE A:356, LEU A:339, LEU A:343, MET A:336
7	Sakuranetin	-8.86	318.63	GLU A:305, GLY A:472	MET A:336, LEU A:476, LEU A:298, ALA A:302, LEU A:339, PHE A:356

LAMPIRAN 7
(LANJUTAN)

Tabel V.6
Hasil Penambatan Molekul pada *Estrogen Receptor-Beta*

No	Nama Senyawa	Molekular Docking			
		ΔG (Kcal/mol)	**Ki (uM)**	**Residu Asam Amino (Ikatan Hidrogen)**	**Residu Asam Amino (Interaksi Hidrofobik)**
8	Oleuropein-aglycone	-8.32	791.24	GLY A:472, GLU A:305	LEU A:339, LEU A:343, LEU A:298, MEI A:295, LEU A:476
9	3,4-DHPEA-Ea	-8.34	765.32	GLY A:472, ARG A:346, LEU A:339	MET A:336, ALA A:302,
10	4-Caffeoylquinic acid	-6.78	10.74	GLY A:472, LEU A:339, ARG A:346, GLU A:305	PHE A:356, LEU A:343
11	Quercetin 3-O-glucoside	-3.43	3.05	ARG A:346, MET A:340	LEU A:343, LEU A:339, PHE A:356, LEU A:298, MET A:336, ALA A:302, LEU A:476, VAL A:487
12	Delphinidin 3-O-glucoside	-4.41	584.2	LEU A:339, PHE A:356	LEU A:301, MET A:336,LEU A:343, ALA A:302, LEU 298
13	Cyanidin 3-glucoside	-4.24	778.84	GLU A:305	PHE A:356, LEU A:339, LEU A:343, LEU A:298, MET A:336, ALA A:302, LEU A:476

LAMPIRAN 8

HASIL *SKRINING DRUG LIKENESS*

Tabel V.7
Hasil penelitian *skrining druglikeness* menggunakan situs *online lipin'ski rule of five.*

NO	SENYAWA	Prediksi Drugliknes				
		BM	Log P	Akseptor Ikatan Hidrogen	Donor ikatan Hidrogen	Keterangan
1	Pinoresinol	358	3.16	6	2	Memenuhi
2	1-Acetoxypinoresinol	416	3.31	8	2	Memenuhi
3	3,4-Dihydroxyphenylglycol	170	0.64	4	4	Memenuhi
4	Oleuropein-aglycone	378	2.48	8	3	Memenuhi
5	3,4-DHPEA-Ea	378	2.48	8	3	Memenuhi
6	Todolactol A	376	2.91	7	4	Memenuhi
7	4-Hydroxybenzaldehyde	122	0.79	2	1	Memenuhi
8	Quercetin 3-O-glucoside	464	1.03	12	8	Tidak memenuhi
9	Dihydro-p-coumaric acid	166	0.84	3	2	Memenuhi
10	Quercetin 3-O-galactoside	464	1.03	12	8	Tidak memenuhi
11	Epicatechin 3-O-gallate	442	1.31	10	7	Tidak memenuhi
12	p-Coumaric acid	164	0.15	3	2	Memenuhi
13	Vanillic acid	168	0.63	4	2	Memenuhi
14	Phloretin	274	1.22	5	4	Memenuhi
15	Ferulic acid	194	0.55	4	2	Memenuhi
16	Sakuranetin	286	1.87	5	2	Memenuhi
17	Resveratrol 5-O-glucoside	390	1.85	8	6	Tidak memenuhi
18	Chrysoeriol 7-O-glucoside	462	103.85	11	6	Tidak memenuhi
19	4-Caffeoylquinic acid	354	1.28	9	6	Tidak memenuhi
20	Caffeic acid	180	0.03	4	3	Memenuhi
21	Resveratrol	228	1.18	3	3	Memenuhi
22	6-Gingerol	294	3.58	4	2	Memenuhi
23	Chlorogenic acid	354	1.28	9	6	Tidak memenuhi
24	Phlorizin	274	1.22	5	4	Memenuhi
25	5-Caffeoylquinic acid	354	1.28	9	6	Tidak memenuhi
26	Petunidin 3-O-galactoside	514	2.16	12	8	Tidak memenuhi
27	Petunidin 3-O-glucoside	479	1.48	12	8	Tidak memenuhi
28	Oleuropein-aglycone	378	2.48	8	3	Memenuhi
29	Delphinidin 3-O-glucoside	465	0.96	12	9	Tidak memenuhi

LAMPIRAN 8
(LANJUTAN)

Keterangan : BM < 500 Dalton, Log P <5, Donor Ikatan Hidrogen <5, dan Akseptor Ikatan Hidrogen <10.

LAMPIRAN 9

HASIL PENELITIAN *SKRINING* FARMAKOKINETIKA

Tabel V.8
Hasil penelitian *skrining* farmakokinetika menggunakan *situs online Pre-ADMET*

NO	SENYAWA	Pre-ADMET		
		Absorbsi		Distribusi
		$CaCo_2$ Cell (nm sec-1)	Hia (%)	PPB (%)
1	Pinoresinol	35.13**	93.47***	81.60*
2	1-Acetoxypinoresinol	27.75**	93.96***	77.58*
3	3,4-Dihydroxyphenylglycol	17.20**	65.07**	0.72*
4	Oleuropein-aglycone	20.53**	81.36***	75.76*
5	3,4-DHPEA-Ea	20.53**	81.36***	75.76*
6	Todolactol A	20.98**	83.20***	78.41*
7	4-Hydroxybenzaldehyde	20.52**	94.08***	6.00*
8	Quercetin 3-O-glucoside	9.43**	11.77**	59.15*
9	Dihydro-p-coumaric acid	21.10**	90.67***	61.73*
10	Quercetin 3-O-galactoside	9.43**	11.77*	59.15*
11	Epicatechin 3-O-gallate	13.21**	40.58**	100**
12	p-Coumaric acid	21.10**	92.09***	63.05*
13	Vanillic acid	19.93**	85.36***	52.10*
14	Phloretin	18.10**	78.98***	100**
15	Ferulic acid	21.11**	90.60***	50.41*
16	Sakuranetin	12.82**	92.75***	95.21**
17	Resveratrol 5-O-glucoside	5.33**	59.21**	94.15**
18	Chrysoeriol 7-O-glucoside	5.02**	42.14**	62.67*
19	4-Caffeoylquinic acid	18.71**	20.42**	41.96*
20	Caffeic acid	21.10**	82.30***	40.29*
21	Resveratrol	5.19**	88.47***	100**
22	6-Gingerol	24.51**	91.96***	100**
23	Chlorogenic acid	18.71**	20.42**	41.96*
24	Phlorizin	9.51**	26.79**	75.47*
25	5-Caffeoylquinic acid	18.71**	20.42**	41.96*
26	Delphinidin 3-O-galactoside	4.85**	8.80**	80.17*
27	Petunidin 3-O-glucoside	6.14**	17.25**	70.59*
28	Oleuropein-aglycone	20.53**	81.36***	75.76*
29	Delphinidin 3-O-glucoside	4.85**	8.80**	80.17*

LAMPIRAN 9
(LANJUTAN)

HIA (%) :

*** : > 70 (terserap baik)

** : 20 - 70 (terserap cukup)

* : < 20 (kurang terserap)

CaCo-2 Cell (nm sec) :

*** : > 70 (permeabilitas tinggi)

** : 4-70 (permeabilitas sedang)

* : < 4 (permeabilitas rendah)

Protein Plasma Binding (%) :

** : > 90 (terikat kuat)

* : < 90 (terikat lemah)

LAMPIRAN 10

HASIL PENELITIAN *SKRINING* TOKSISITAS

Tabel V.9

Hasil penelitian *skrining* toksisitas menggunakan aplikasi *Toxree*®.

NO	SENYAWA	Toxtree		
		KROES TCC	CARCINOGENICITY	AMEST TEST
1	Pinoresinol	1	8,9	2
2	1-Acetoxypinoresinol	1	8,9	2
3	3,4-Dihydroxyphenylglycol	2	8,9	2
4	Oleuropein-aglycone	1	8,9	2
5	3,4-DHPEA-Ea	1	8,9	2
6	Todolactol A	1	8,9	2
7	4-Hydroxybenzaldehyde	1	8,9	1
8	Quercetin 3-O-glucoside	1	8,9	1
9	Dihydro-p-coumaric acid	1	8,9	2
10	Quercetin 3-O-galactoside	1	8,9	1
11	Epicatechin 3-O-gallate	1	8,9	2
12	p-Coumaric acid	1	8,9	2
13	Vanillic acid	1	8,9	2
14	Phloretin	1	8,9	2
15	Ferulic acid	1	8,9	2
16	Sakuranetin	1	8,9	1
17	Resveratrol 5-O-glucoside	1	8,9	2
18	Chrysoeriol 7-O-glucoside	1	8,9	1
19	4-Caffeoylquinic acid	1	8,9	2
20	Caffeic acid	1	8,9	2
21	Resveratrol	1	8,9	2
22	6-Gingerol	1	8,9	1
23	Chlorogenic acid	1	8,9	2
24	Phlorizin	1	8,9	2
25	5-Caffeoylquinic acid	1	8,9	2
26	Delphinidin 3-O-galactoside	1	8,9	2
27	Petunidin 3-O-glucoside	1	8,9	2
28	Oleuropein-aglycone	1	8,9	2
29	Delphinidin 3-O-glucoside	1	8,9	2

LAMPIRAN 10
(LANJUTAN)

Keterangan :

Cramer rules:

1 *Substances with sample chemical structures and fix which efficient modes of metabolism exist, suggesting a low order oforal toxicity*
2 *Substances which possess structures that are less innocuous than class I substances, but do not contain structural featuressuggestive 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 ir have reactive functional groups*

Benigni/bose rulebase:

8. *Negative for genotoxic carcinogenity*
9. *Negative for non-genotoxic carcinogencity*

Kroes TTC decision tree:

1. *Subtance would not be expected to be a safety concern*
2. *Negligible risk (loe probability of life-time cancer risk greater than 1 in 10)*