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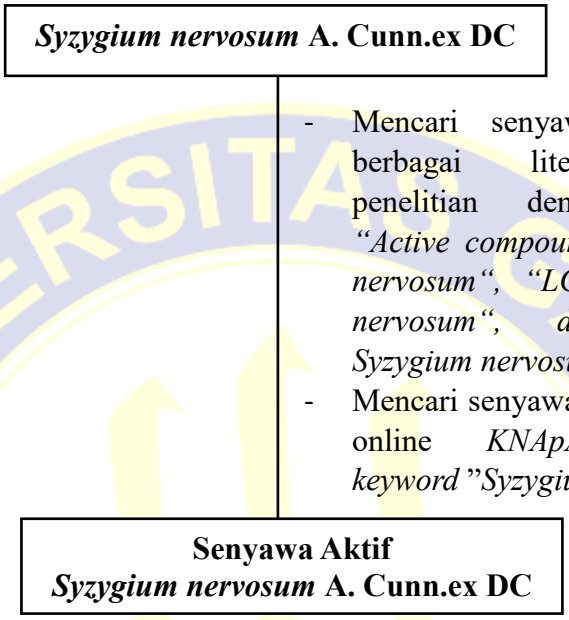
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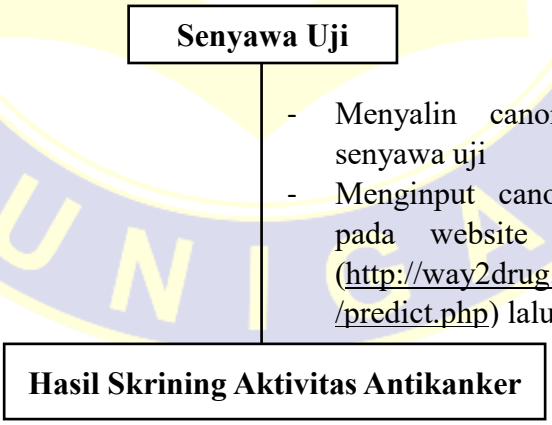
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LAMPIRAN 1

ALUR PENCARIAN SENYAWA AKTIF, SKRINING AKTIVITAS ANTIKANKER PAYUDARA, DAN STUDI FARMAKOFOR

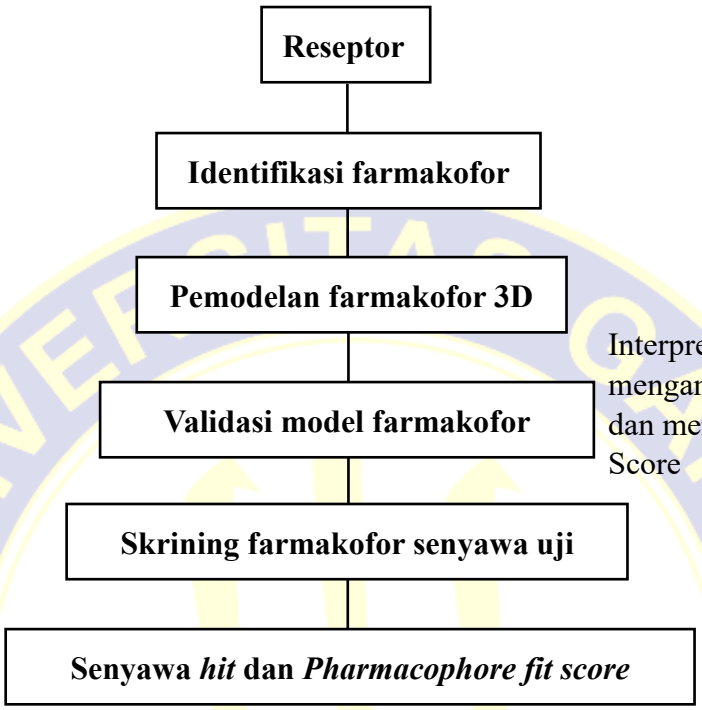


Gambar VII. 1 Alur penelitian pencarian senyawa aktif



Gambar VII. 2 Alur penelitian skrining aktivitas antikanker

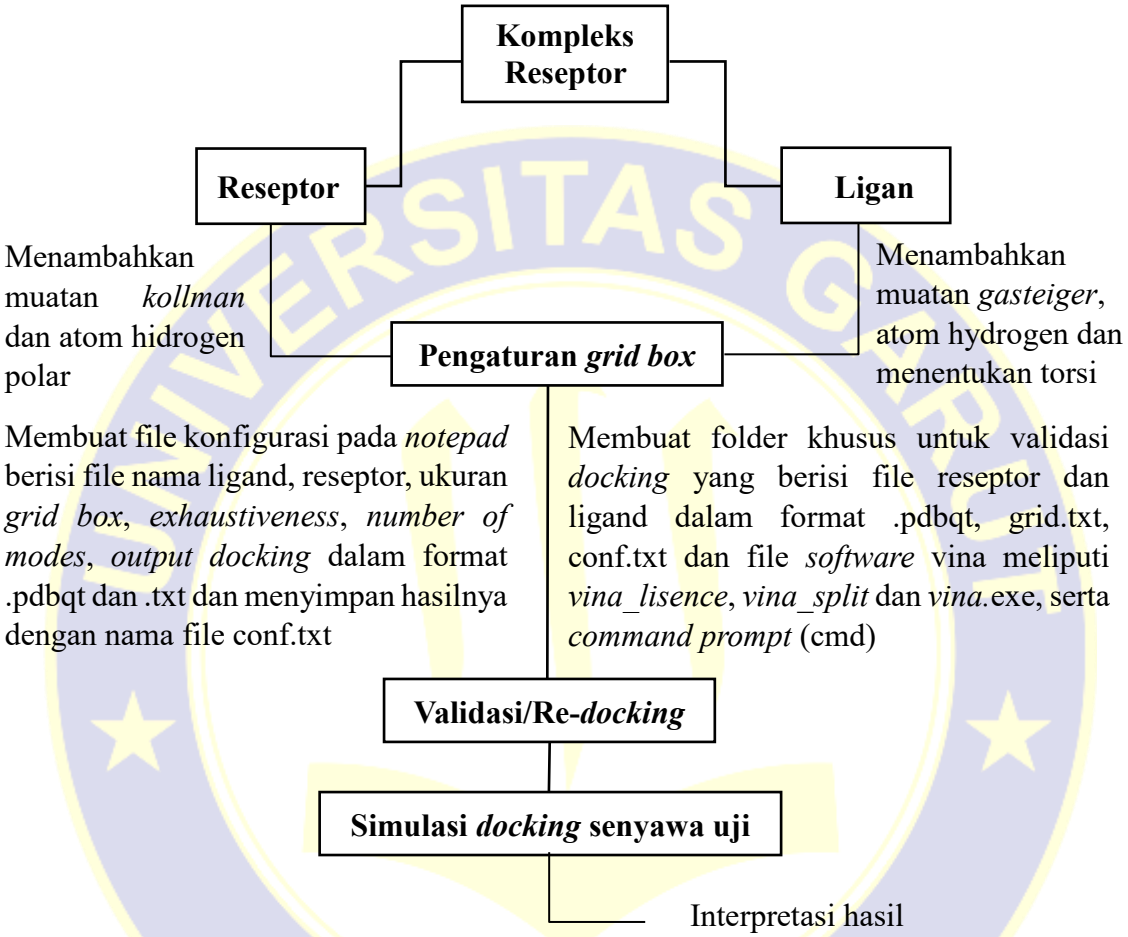
LAMPIRAN 1
(LANJUTAN)



Gambar VII. 3 Alur penelitian studi farmakofor

LAMPIRAN 2

ALUR SIMULASI *MOLECULAR DOCKING* DAN *SIMULASI MOLECULAR DYNAMIC*



Gambar VII. 4 Alur penelitian simulasi molecular docking

LAMPIRAN 2
(LANJUTAN)

Penggabungan kompleks ligan-reseptor

- Melakukan penggabungan reseptor-*native ligand*, reseptor-ligan pembanding, dan reseptor-senyawa uji terbaik hasil *docking* (format .pdbqt) di *Discovery Studio Visualizer*
- Memisahkan ligand dan ditambahkan hidrogen (save .pdb) di *Discovery Studio Visualizer*
- Memisahkan reseptor dan dihapus hidrogen (save .pdb) di *Autodock Tools*

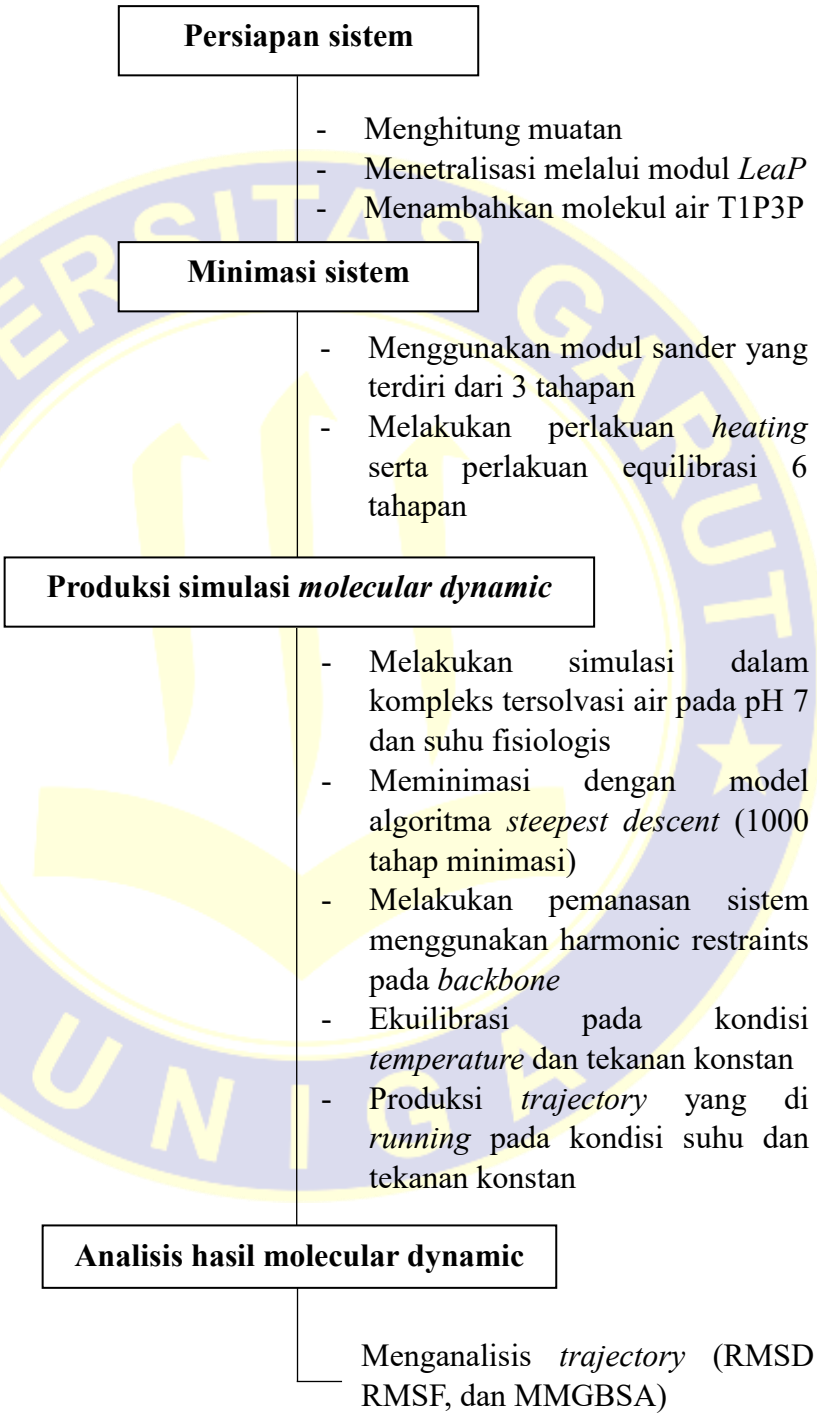
Persiapan reseptor

- Menghilangkan atom H dan optimasi di Sofware Autodock Tools
- Running pada program *Leap sd* dengan mode *force fields* ff14SB
- Menetralisasi dengan ion Na^+ atau Cl^-
- Mensolvasi dengan molekul air

Parameterisasi ligan

- Melakukan penambahan atom H melalui software Discovery Studio Visualizer
- Melakukan parameterisasi menggunakan modul *antechamber*
- Meminimasi sturktur dengan melalui modul *parmchk* ditambahkan medan gaya ff1SB

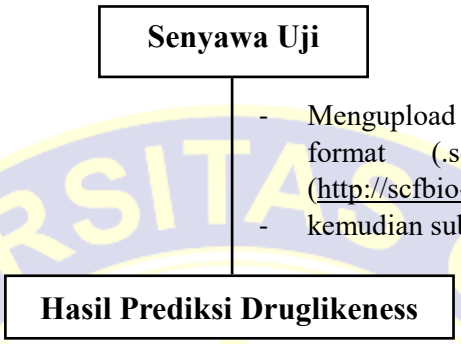
LAMPIRAN 2
(LANJUTAN)



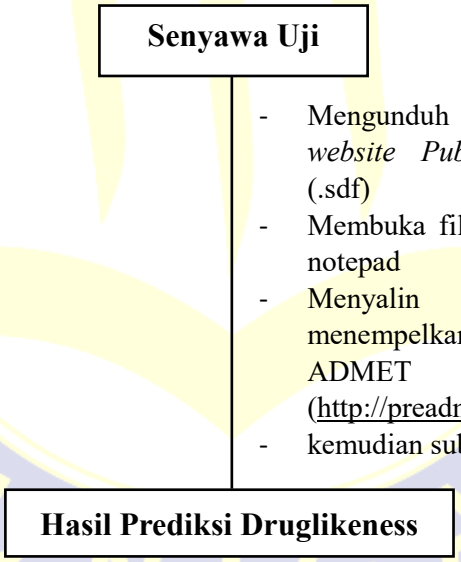
Gambar VII. 5 Alur penelitian simulasi molecular dynamic

LAMPIRAN 3

ALUR PREDIKSI *LIPINSKI'S RULE OF FIVE* (*DRUGLIKENESS*), PREDIKSI FARMAKOKINETIK DAN TOKSISITAS



Gambar VII. 6 Alur penelitian prediksi *Lipinski's Rule Of Five* (*Druglikeness*)



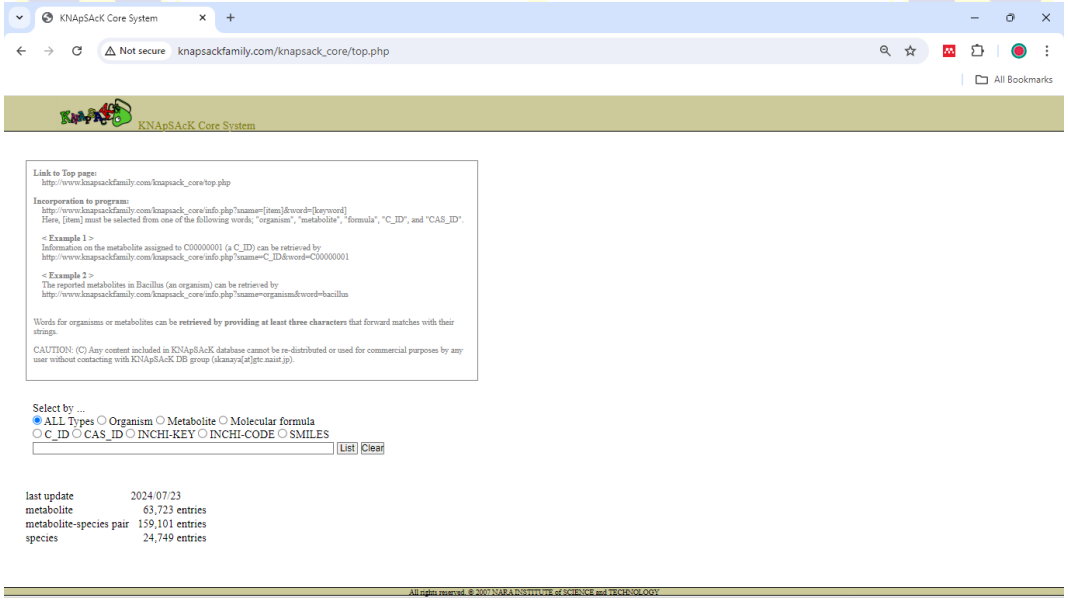
Gambar VII. 7 Alur penelitian prediksi farmakokinetik dan toksisitas

LAMPIRAN 4

SITUS DAN APLIKASI

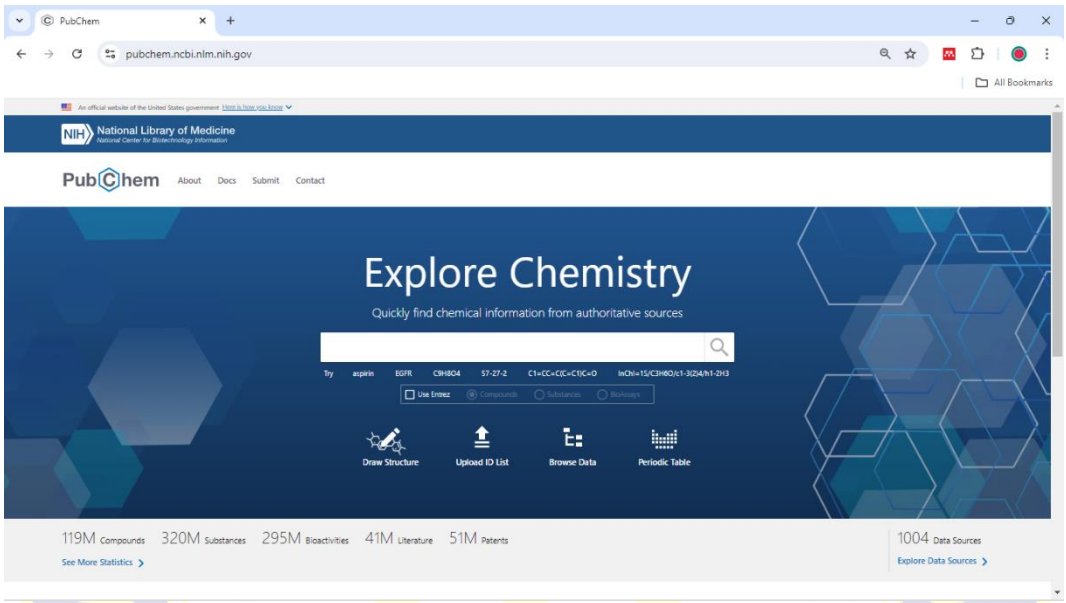


Gambar VII. 8 Tampilan situs *PASS Online*

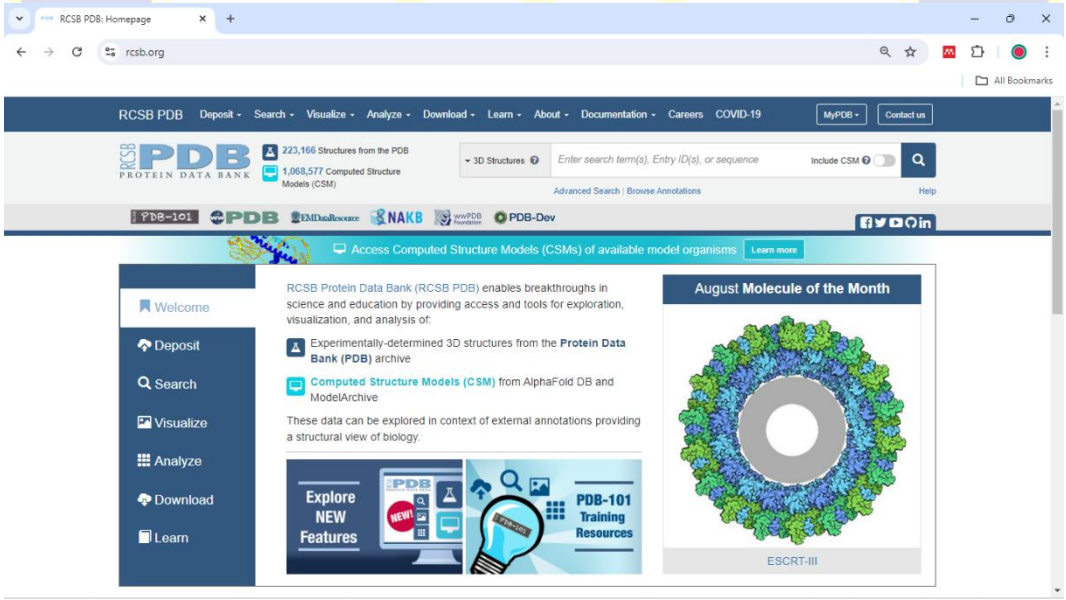


Gambar VII. 9 Tampilan situs *KNApSacK*

LAMPIRAN 4
(LANJUTAN)

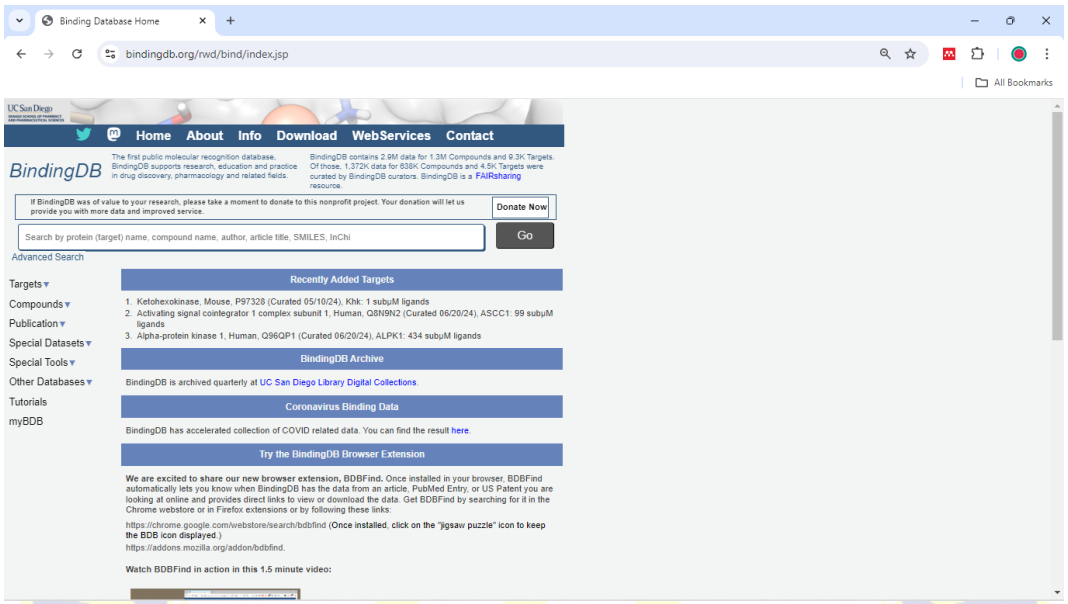


Gambar VII. 10 Tampilan situs *Pubchem*

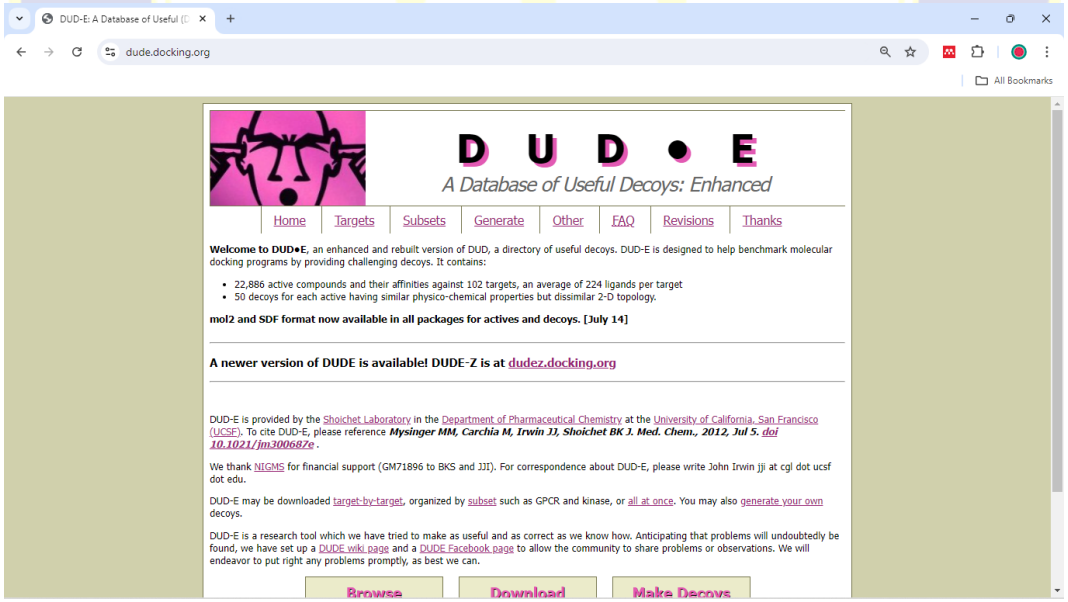


Gambar VII. 11 Tampilan situs Protein Data Bank

LAMPIRAN 4
(LANJUTAN)

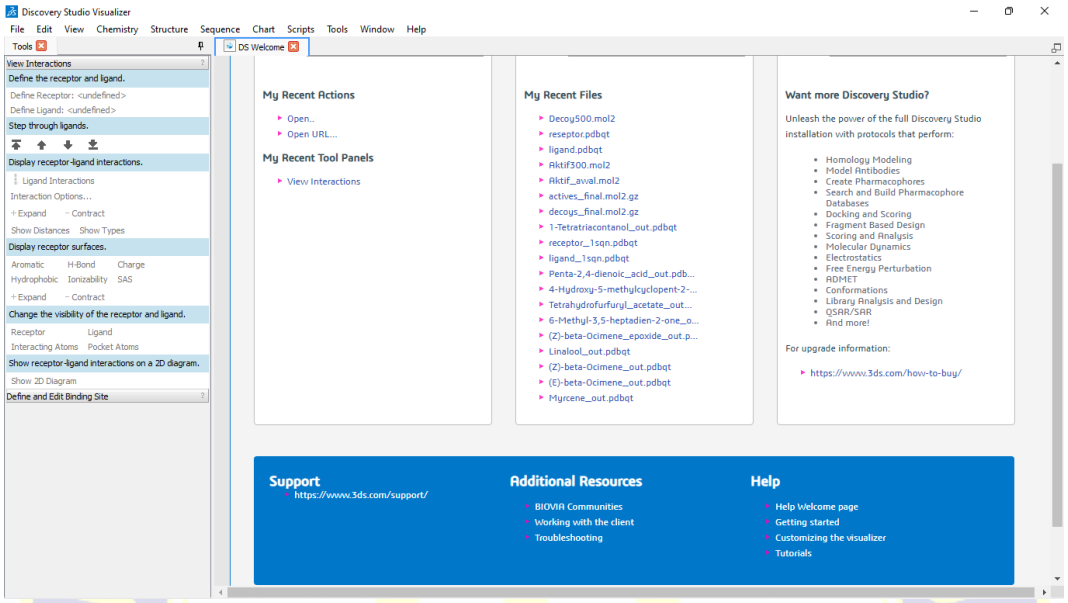


Gambar VII. 12 Tampilan situs *Binding Data Base*

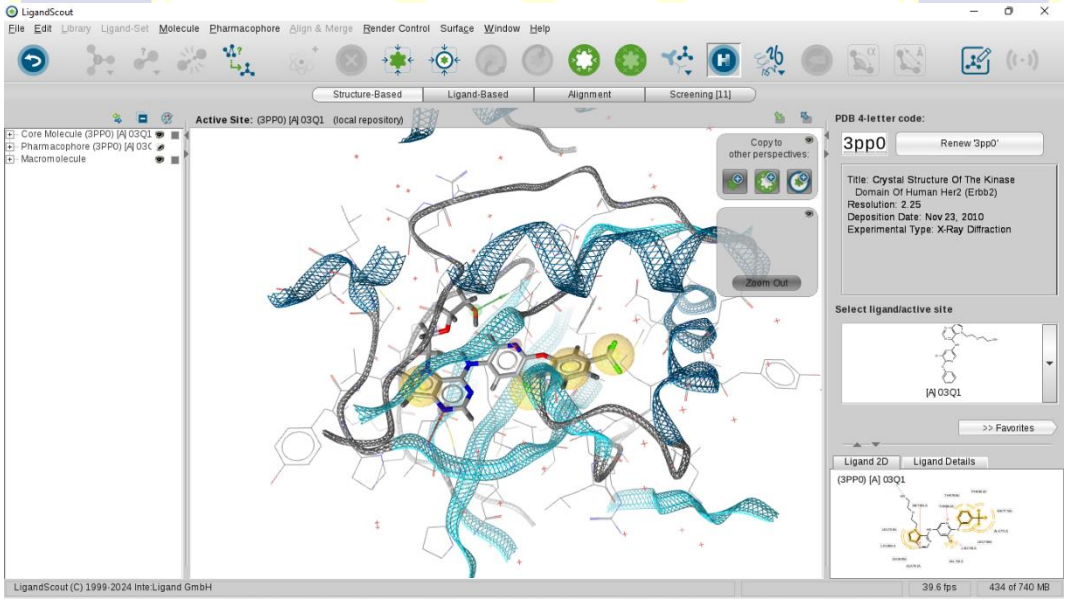


Gambar VII. 13 Tampilan situs DUD-E

LAMPIRAN 4
(LANJUTAN)

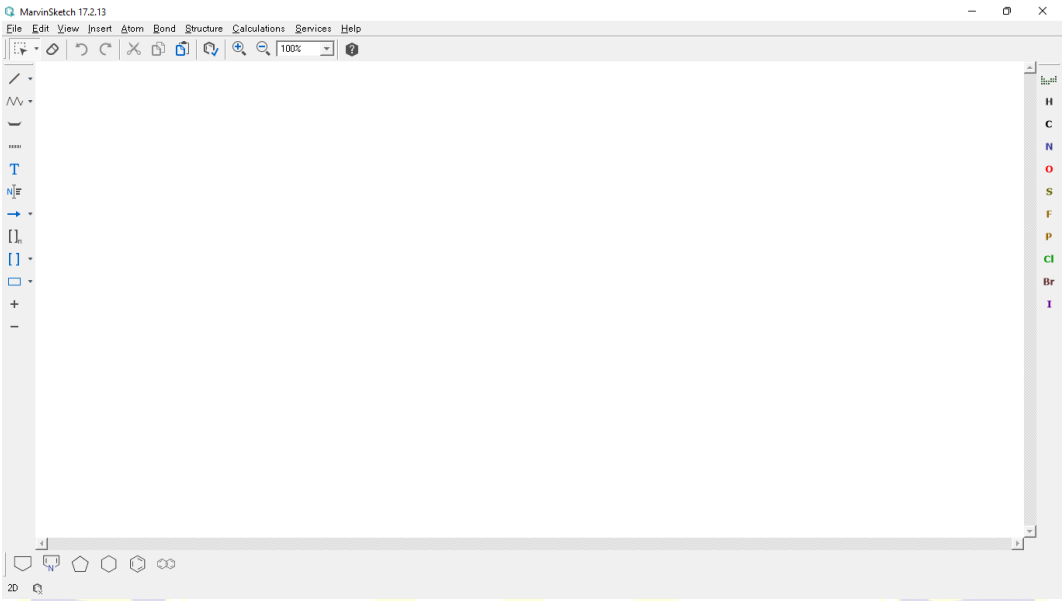


Gambar VII. 14 Tampilan *software Discovery Studio Visualizer*

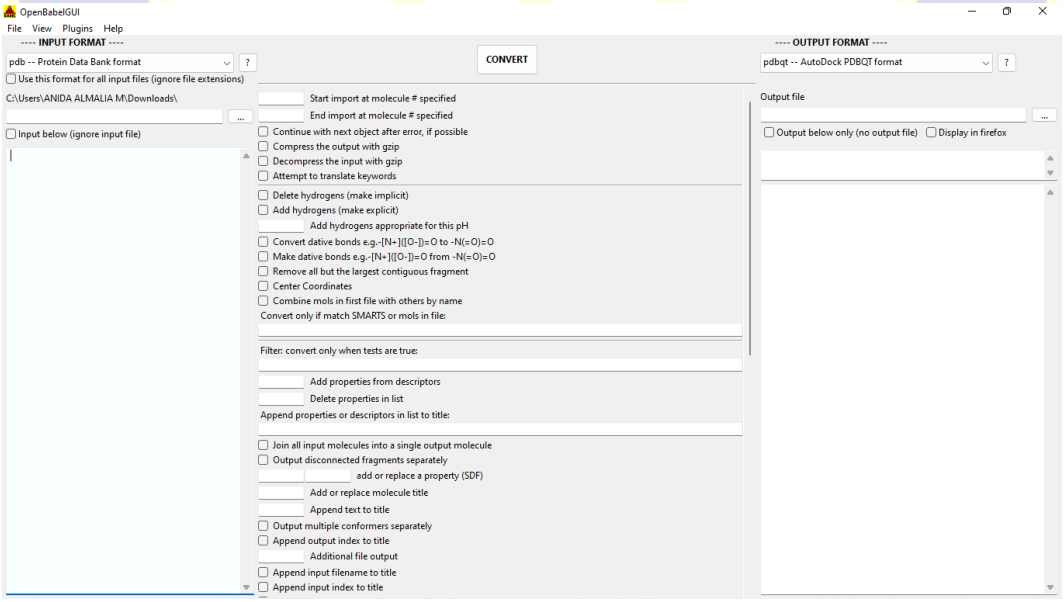


Gambar VII. 15 Tampilan software *Ligandscout*

LAMPIRAN 4
(LANJUTAN)



Gambar VII. 16 Tampilan software *Marvin Sketch*

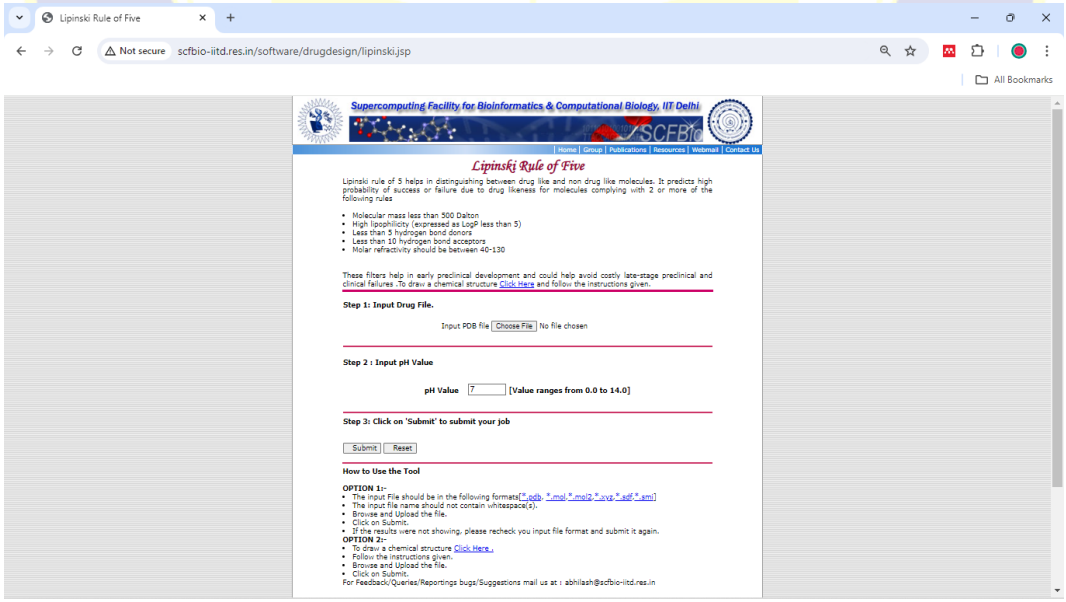


Gambar VII. 17 Tampilan software *Open Babel*

LAMPIRAN 4
(LANJUTAN)

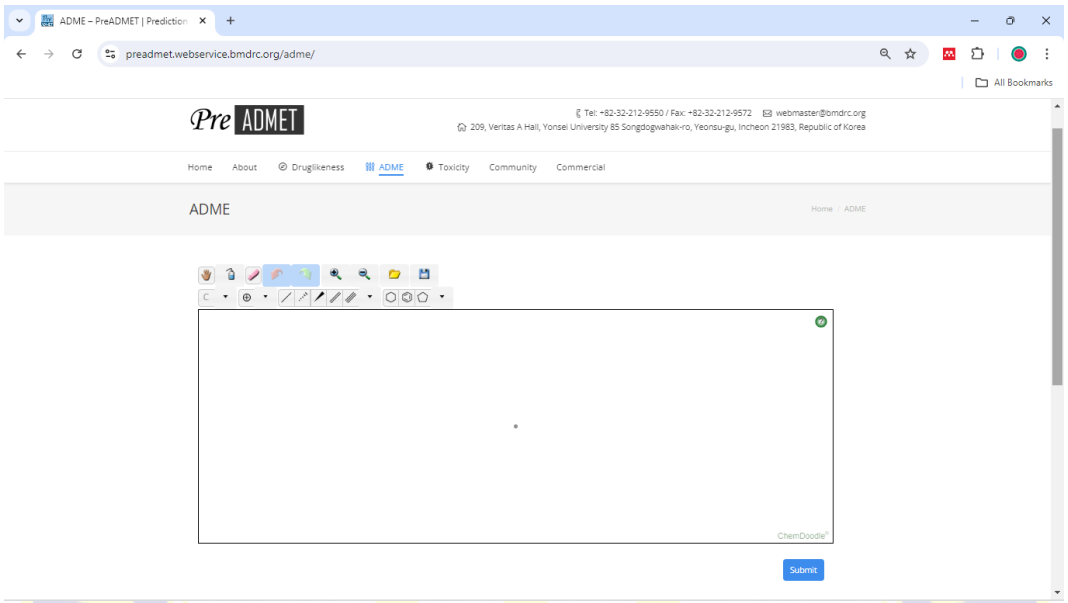


Gambar VII. 18 Tampilan software *AutodockTools*

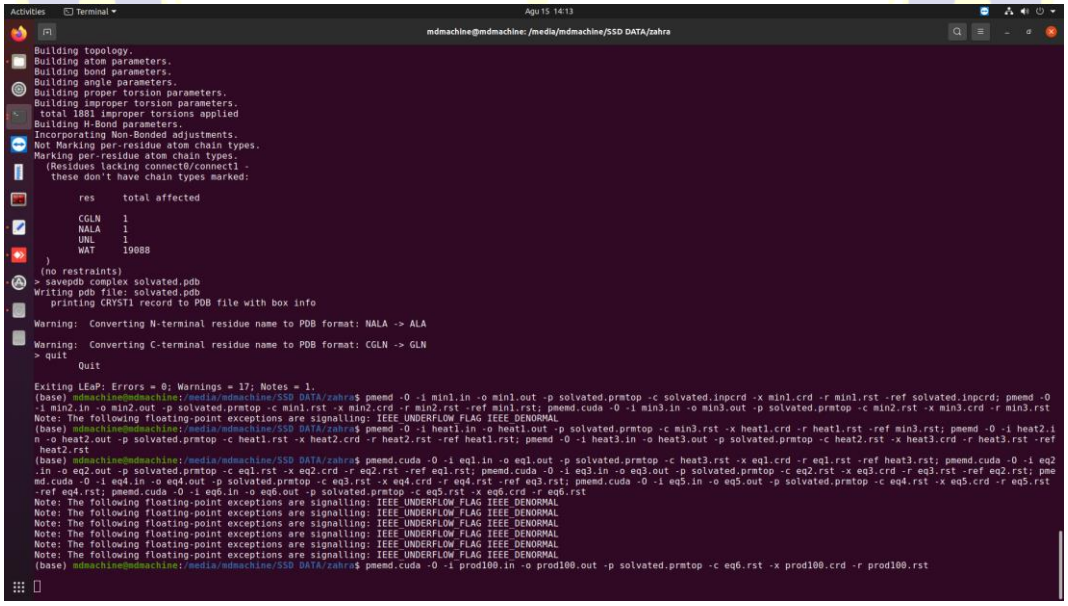


Gambar VII. 19 Tampilan situs *Lipinski Rule of Five*

LAMPIRAN 4
(LANJUTAN)

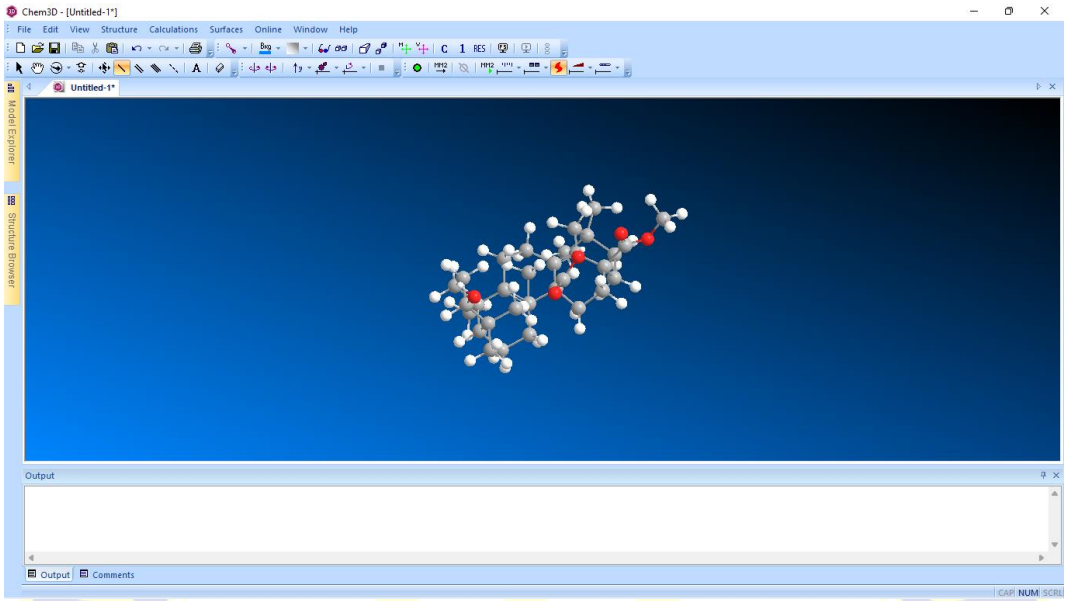


Gambar VII. 20 Tampilan situs PreADMET

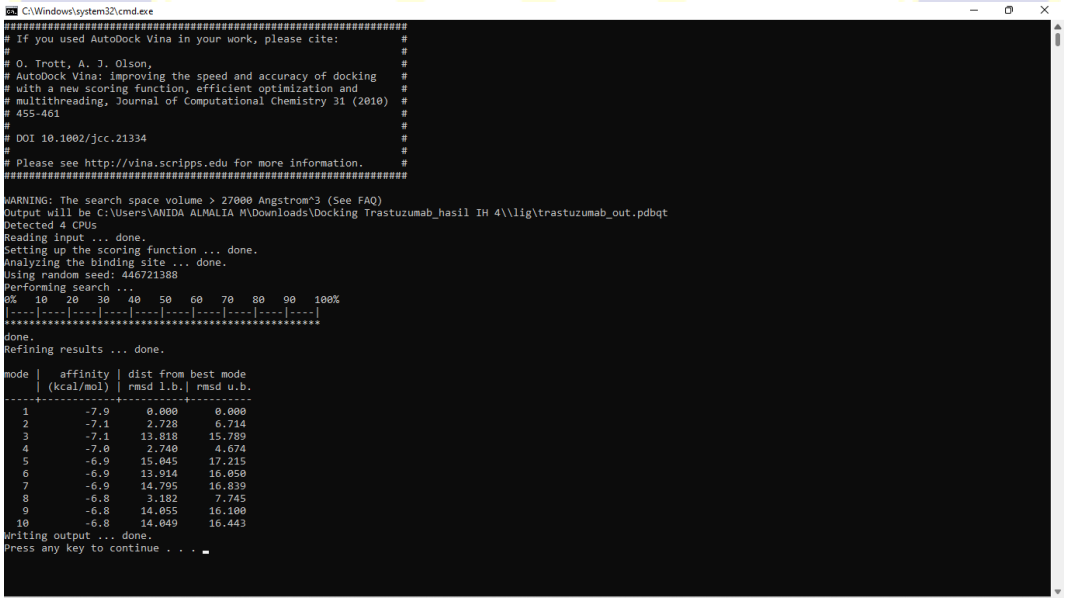


Gambar VII. 21 Tampilan situs Amber

LAMPIRAN 4
(LANJUTAN)



Gambar VII. 22 Tampilan situs *Chemdraw*

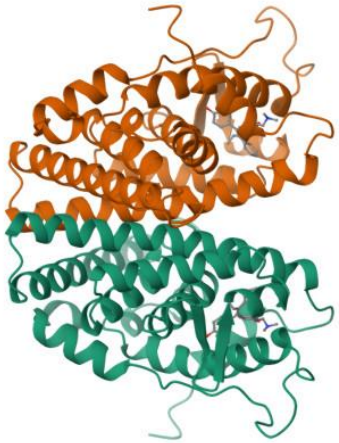
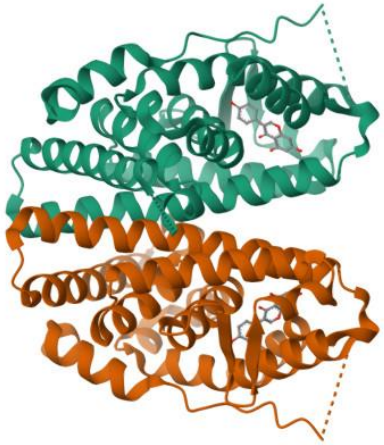


Gambar VII. 23 Tampilan situs Autodock Vina

LAMPIRAN 5

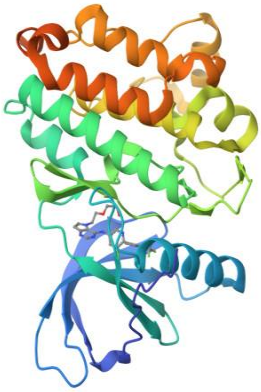
STRUKTUR 3D RESEPTOR

Tabel VII. 1
Struktur 3D Reseptor Kanker Payudara

ID PDB	STRUKTUR KOMPLEKS
3ERT	
1QKM	

LAMPIRAN 5
(LANJUTAN)

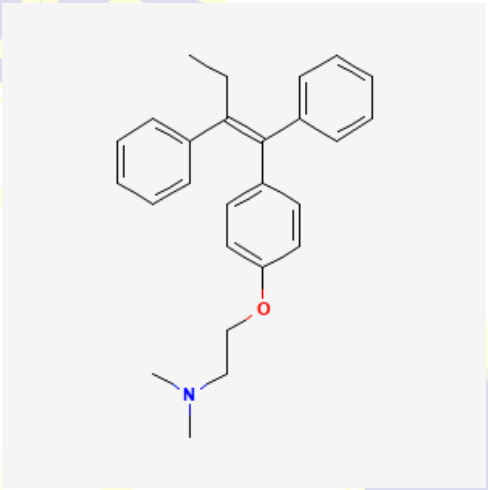
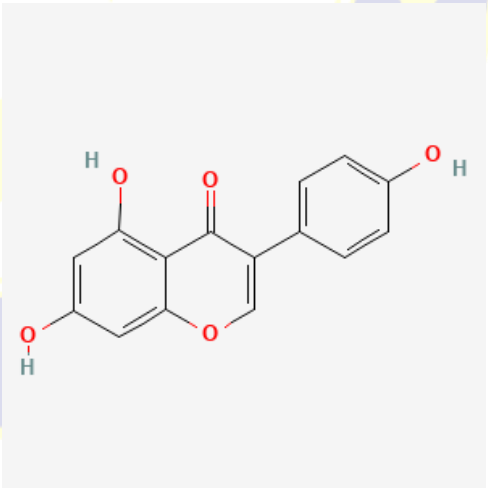
Tabel VII. 1
Lanjutan

ID PDB	STRUKTUR KOMPLEKS
3PPO	
1SQN	

LAMPIRAN 6

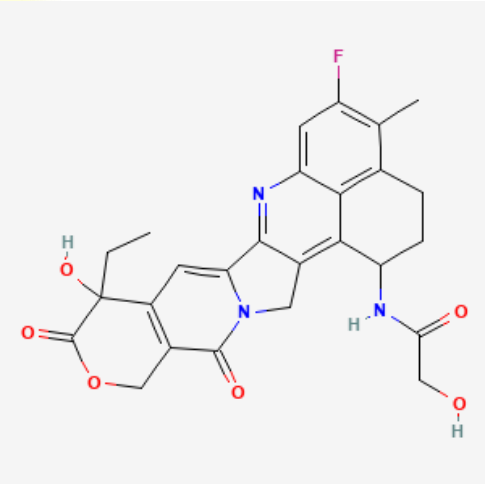
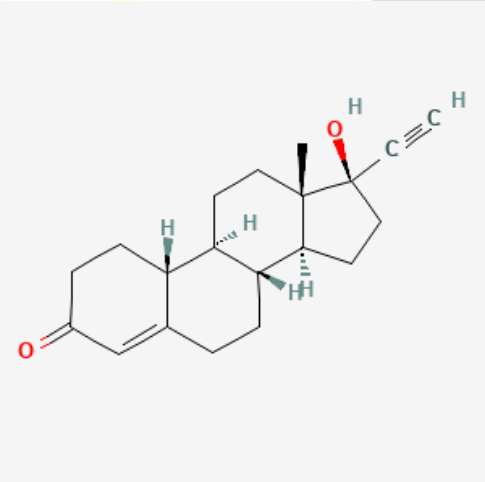
STRUKTUR 2D LIGAN PEMBANDING

Tabel VII. 2
Struktur 2D Ligan Pembanding

NAMA LIGAN PEMBANDING	STRUKTUR SENYAWA
Tamoxifen	
Genistein	

LAMPIRAN 6
(LANJUTAN)

Tabel VII. 2
Lanjutan

NAMA LIGAN PEMBANDING	STRUKTUR SENYAWA
Trastuzumab	
Norethindrone	

LAMPIRAN 7

HASIL PENCARIAN SENYAWA

Tabel VII. 3
Daftar Senyawa Aktif

No	Bagian Tanaman	Senyawa	Referensi
1	Daun	*Cleistocalyxic acid A*	[5]
2	Daun	*Cleistocalyxic acid B*	[5]
3	Daun	*Cleistocalyxic acid C*	[5]
4	Daun	*Cleistocalyxic acid D*	[5]
5	Daun	*Cleistocalyxolide B*	[5]
6	Daun	*Cleistocalyxic acid H*	[5]
7	Daun	*Actinidic acid*	[5]
8	Daun	*Cleistocalyxic acid I*	[5]
9	Daun	*Cleistocalyxic acid J*	[5]
10	Daun	*Cleistocalyxic acid K*	[5]
11	Daun, tunas	*Ursolic acid*	[5]
12	Daun	*Corosolic acid*	[5]
13	Daun	*Asiatic acid*	[5]
14	Daun	*2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid*	[5]
15	Daun	*2α,3β-Dihydroxy-24-nor-urs-4(23),12-dien-28-oic acid*	[5]
16	Daun, tunas	*β-Sitosterol*	[5]
17	Daun	*Betulinic acid*	[5]
18	Daun	*Alphitolic acid*	[5]
19	Daun, tunas	*Oleanolic acid*	[5]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
20	Daun, tunas	*Maslinic acid*	5
21	Tunas	*3-O-trans-p-Coumaroyl maslinic acid*	5
22	Tunas	*3-O-cis-p-Coumaroyl maslinic acid*	5
23	Daun	*Arjunolic acid*	5
24	Daun	*Cleistocalyxic acid E*	5
25	Daun	*Cleistocalyxic acid F*	5
26	Daun	*Cleistocalyxic acid G*	5
27	Daun, tunas, biji	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	5
28	Tunas	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	5
29	Tunas	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	5
30	Tunas	*3'-Formyl-6',4-dihydroxy-2'-methoxy-5'-methylchalcone 4'-O-β-D-glucopyranoside*	5
31	Tunas	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	5
32	Tunas	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	5
33	Daun, tunas	*Kaempferol*	5
34	Daun, tunas	*Quercetin*	5
35	Tunas	*Tamarixetin*	5

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
36	Daun, tunas	*Myricetin-3'-methylether 3-O-β-D-galactopyranoside*	5
37	Tunas	*Myricetin-3'-methylether*	5
38	Tunas	*Gossypetin-8,3'-dimethylether-3-O-β-D-galactoside*	5
39	Tunas	*Luteolin*	5
40	Tunas	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	5
41	Tunas	*(2S)-8-Formyl-6-methylnaringenin*	5
42	Tunas	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	5
43	Tunas	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	5
44	Tunas	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	5
45	Daun	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	5
46	Tunas	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	5
47	Tunas	*(2S)-8-methylpinocembrin*	5
48	Tunas	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	5
49	Tunas	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	5
50	Tunas	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	5
51	Tunas	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	5
52	Daun, tunas	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	5

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
53	Daun	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	[5]
54	Tunas	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	[5]
55	Tunas	*(trans)-4-Hydroxy-5-(2-hydroxypropan-2-yl)-2-methylcyclopent-2-en-1-one*	[5]
56	Tunas	*4-Hydroxy-2,2,5-trimethylcyclopent-4-ene-1,3-dione*	[5]
57	Tunas	*4'-Dihydrophaseic acid*	[5]
58	Tunas	*Pentadienoic acid*	[5]
59	Tunas	*4-Hydroxybenzoic acid*	[5]
60	Tunas	*Methyl 3,4,5-trihydroxybenzoate*	[5]
61	Tunas	*4-Hydroxy-3,5-dimethoxybenzoic acid*	[5]
62	Tunas	*Cinnamic acid*	[5]
63	Daun	*Cleistoperlone A*	[5]
64	Daun	*Operculatol A*	[5]
65	Daun	*1-Tetratriacontanol*	[5]
66	Tunas	*3-Hydroxy-3-phenylpropanoic acid*	[5]
67	Minyak	*Tetrahydrofurfuryl acetate*	[12]
68	Minyak	*β-Pinene*	[12]
69	Minyak	*Myrcene*	[12]
70	Minyak	*Limonene*	[12]
71	Minyak	*(Z)-β-Ocimene*	[12]
72	Minyak	*(E)-β-Ocimene*	[12]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
73	Minyak	*Rosefuran*	[12]
74	Minyak	*Linalool*	[12]
75	Minyak	*6-Methyl-3,5-heptadien-2-one*	[12]
76	Minyak	*allo-Ocimene*	[12]
77	Minyak	*(Z)-Epoxy ocimene (=(Z)-MyrOxide)*	[12]
78	Minyak	*(E)-Epoxy ocimene (= (E)-Myroxide)*	[12]
79	Minyak	*Naphthalene*	[12]
80	Minyak	*(3Z)-Octenyl acetate*	[12]
81	Minyak	*(3E)-Octenyl acetate*	[12]
82	Minyak	*Cyclosativene*	[12]
83	Minyak	*α-Copaene*	[12]
84	Minyak	*Geranyl acetate*	[12]
85	Minyak	*(E)-Caryophyllene*	[12]
86	Minyak	*β-Copaene*	[12]
87	Minyak	*Aromadendrene*	[12]
88	Minyak	*α-Humulene*	[12]
89	Minyak	*γ-Muurolene*	[12]
90	Minyak	*β-Selinene*	[12]
91	Minyak	*α-Selinene*	[12]
92	Minyak	*γ-Cadinene*	[12]
93	Minyak	*(E)-Nerolidol*	[12]
94	Minyak	*Spathulenol*	[12]
95	Minyak	*Caryophyllene oxide*	[12]
96	Minyak	*Humulene epoxide I*	[12]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
97	Minyak	*Humulene epoxide II*	[12]
98	Minyak	*Selina-6-en-4β-ol*	[12]
99	Minyak	*Caryophylla-4(12),8(13)-dien-5β-ol*	[12]
100	Minyak	*Selina-3,11-dien-6α-ol*	[12]
101	Minyak	*Selin-11-en-4α-ol*	[12]
102	Minyak	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	[12]
103	Minyak	*γ-Gurjunene*	[12]
104	Minyak	*δ-Cadinene*	[12]
105	Minyak	*cis-Cadin-4-en-7-ol*	[12]
106	Minyak	*p-Cymene*	[12]
107	Minyak	*Rosefuran epoxide*	[12]
108	Minyak	*α-Terpineol*	[12]
109	Minyak	*α-Terpinyl acetate*	[12]
110	Minyak	*cis-4-Caranone*	[12]
111	Minyak	*β-Oplopenone*	[12]
112	Minyak	*α-Amorphene*	[12]
113	Minyak	*α-Muurolene*	[12]
114	Minyak	*α-Cadinene*	[12]
115	Minyak	*τ-Cadinol*	[12]
116	Minyak	*τ-Muurolol*	[12]
117	Minyak	*α-Muurolol (= δ-Cadinol)*	[12]
118	Minyak	*α-Cadinol*	[12]
119	Minyak	*1-epi-Cubenol*	[12]
120	Minyak	*β-Calacorene*	[12]

LAMPIRAN 7
(LANJUTAN)

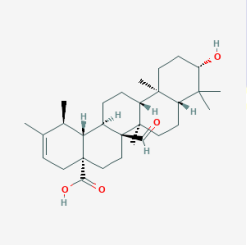
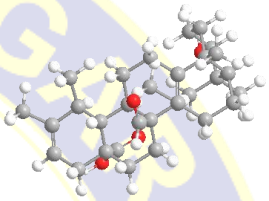
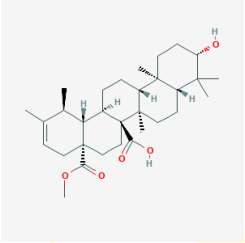
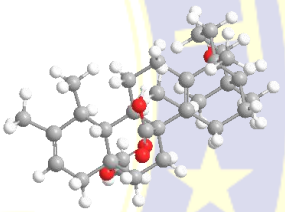
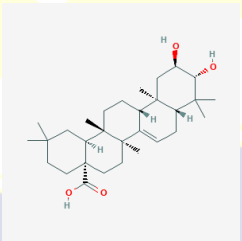
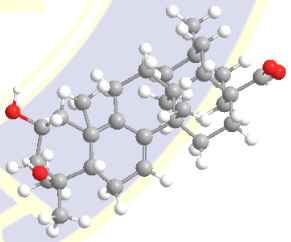
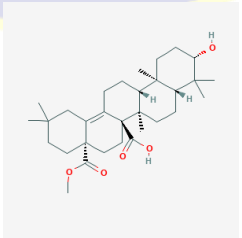
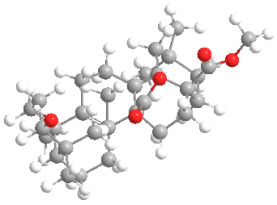
Tabel VII. 3
Lanjutan

No	Bagian Tanaman	Senyawa	Referensi
121	Minyak	*p-Mentha-1,5-dien-8-ol*	12
122	Minyak	*α-Pinene oxide*	12
123	Minyak	*Globulol*	12
124	Minyak	*Viridiflorol*	12
125	Minyak	*α-Pinene*	12
126	Minyak	*Guaiol*	12
127	Minyak	*α-Calcorene*	12

LAMPIRAN 8

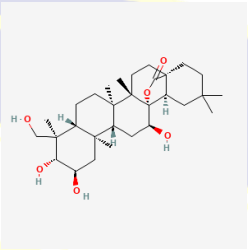
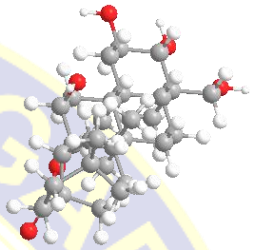
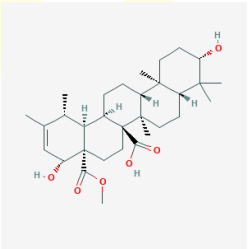
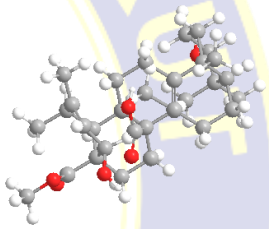
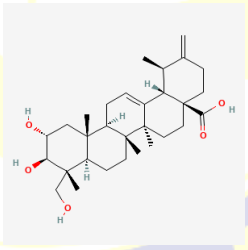
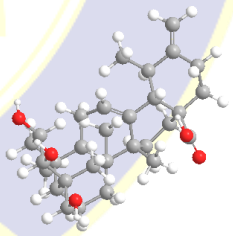
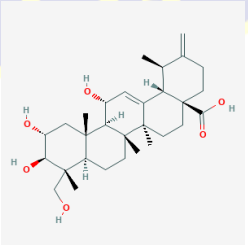
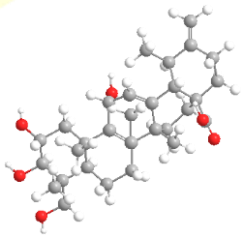
RUMUS MOLEKUL, STRUKTUR 2D DAN 3D SENYAWA UJI

Tabel VII. 4
Rumus Molekul, Struktur 2D dan 3D Senyawa Uji

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
1	*Cleistocalyxic acid A*	$C_{30}H_{46}O_4$		
2	*Cleistocalyxic acid B*	$C_{31}H_{48}O_5$		
3	*Cleistocalyxic acid C*	$C_{30}H_{48}O_4$		
4	*Cleistocalyxic acid D*	$C_{31}H_{48}O_5$		

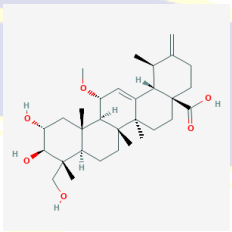
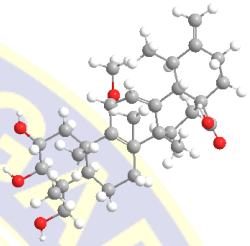
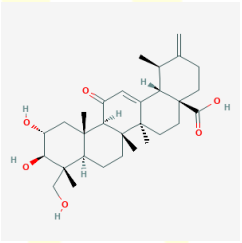
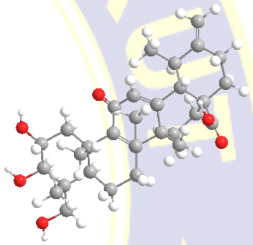
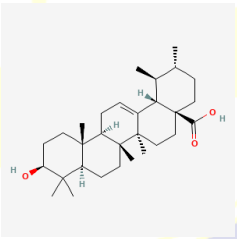
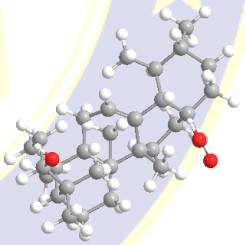
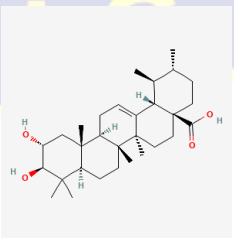
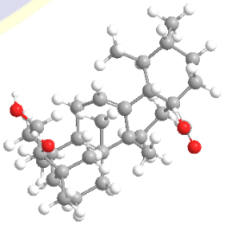
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
5	*Cleistocalyxolide B*	$C_{30}H_{48}O_6$		
6	*Cleistocalyxic acid H*	$C_{31}H_{48}O_6$		
7	*Actinidic acid*	$C_{30}H_{46}O_5$		
8	*Cleistocalyxic acid I*	$C_{30}H_{46}O_6$		

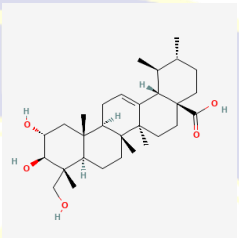
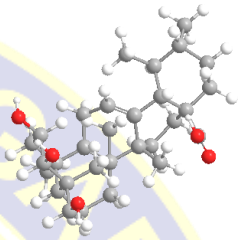
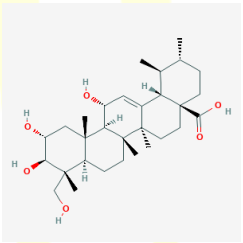
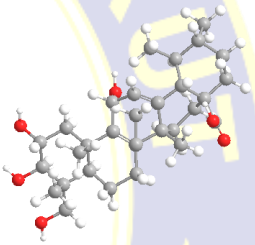
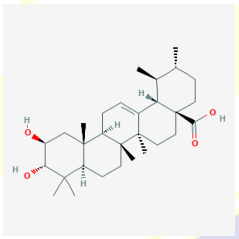
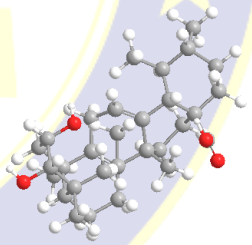
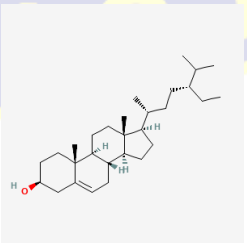
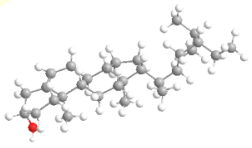
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
9	*Cleistocalyxic acid J*	$C_{31}H_{48}O_6$		
10	*Cleistocalyxic acid K*	$C_{30}H_{44}O_6$		
11	*Ursolic acid*	$C_{30}H_{48}O_3$		
12	*Corosolic acid*	$C_{30}H_{48}O_4$		

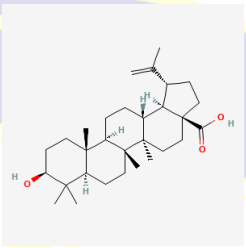
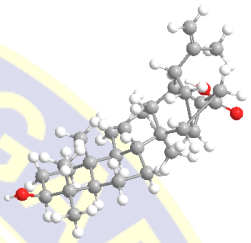
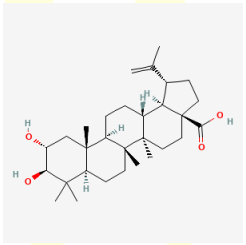
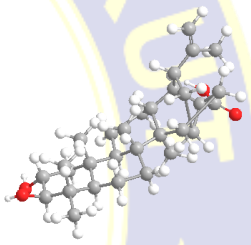
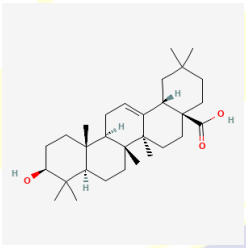
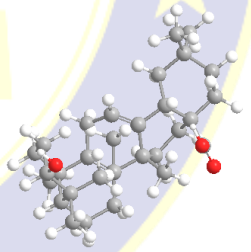
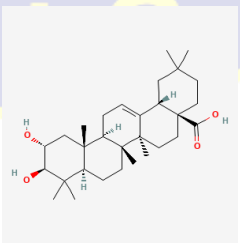
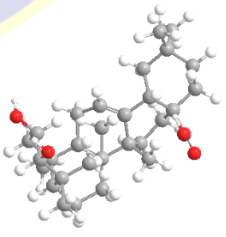
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
13	*Asiatic acid*	$C_{30}H_{48}O_5$		
14	*2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid*	$C_{30}H_{48}O_6$		
15	*2α,3β-Dihydroxy-24-nor-urs-4(23),12-dien-28-oic acid*	$C_{30}H_{48}O_4$		
16	*β-Sitosterol*	$C_{29}H_{50}O$		

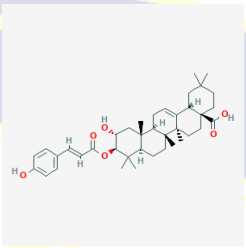
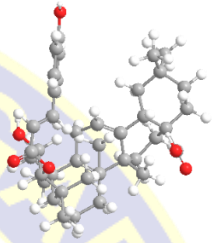
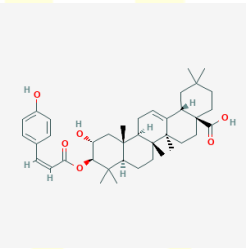
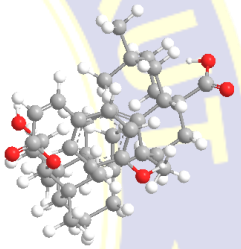
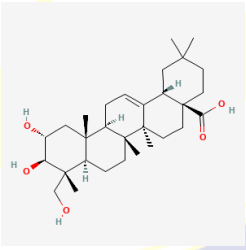
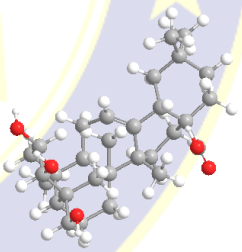
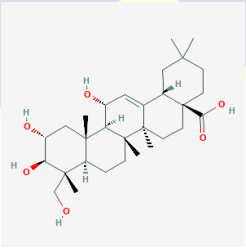
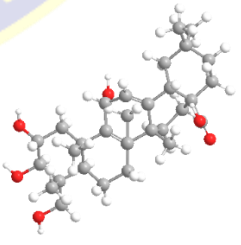
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
17	*Betulinic acid*	$C_{30}H_{48}O_3$		
18	*Alphitolic acid*	$C_{30}H_{48}O_4$		
19	*Oleanolic acid*	$C_{30}H_{48}O_3$		
20	*Maslinic acid*	$C_{30}H_{48}O_4$		

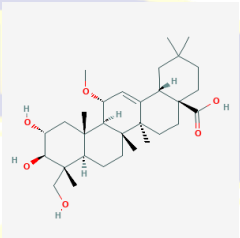
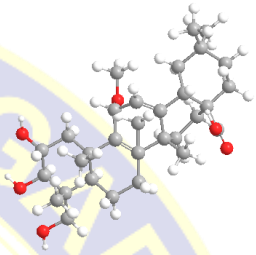
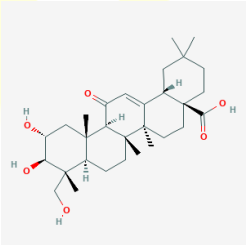
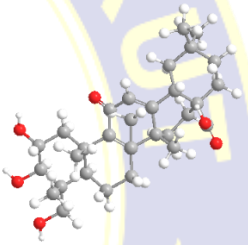
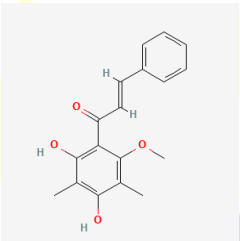
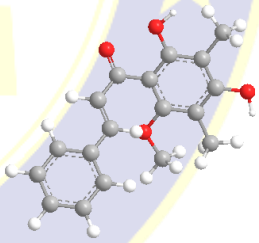
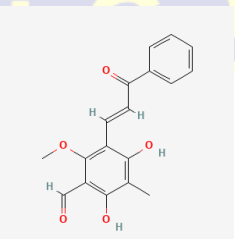
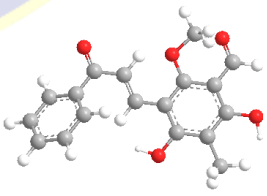
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
21	*3-O-trans-p-Coumaroyl maslinic acid*	$C_{39}H_{54}O_6$		
22	*3-O-cis-p-Coumaroyl maslinic acid*	$C_{39}H_{54}O_6$		
23	*Arjunolic acid*	$C_{30}H_{48}O_5$		
24	*Cleistocalyxic acid E*	$C_{30}H_{48}O_6$		

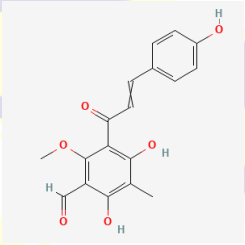
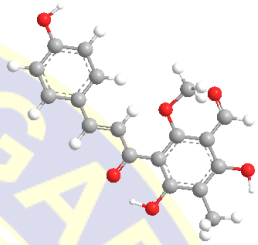
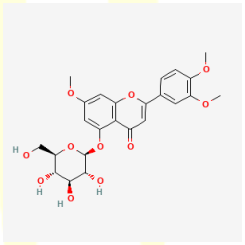
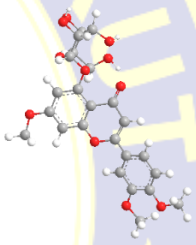
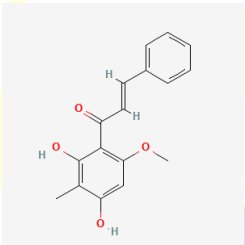
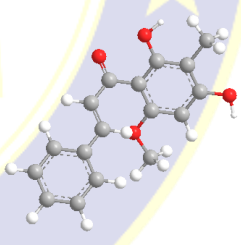
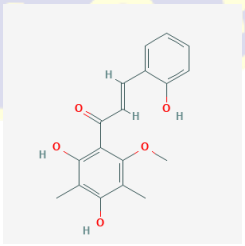
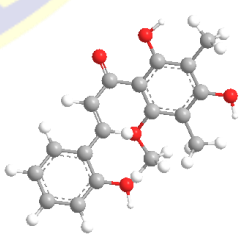
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
25	*Cleistocalyxic acid F*	$C_{31}H_{50}O_6$		
26	*Cleistocalyxic acid G*	$C_{30}H_{46}O_6$		
27	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	$C_{18}H_{18}O_4$		
28	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	$C_{18}H_{16}O_5$		

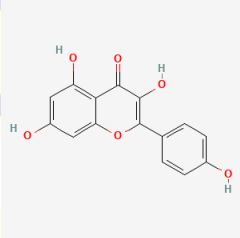
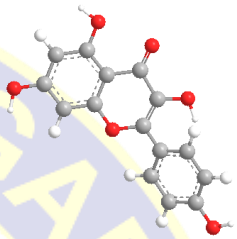
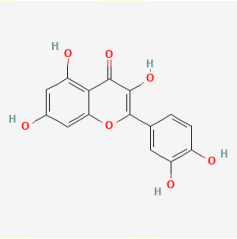
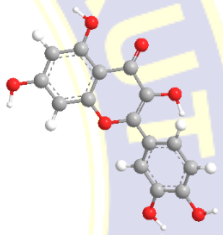
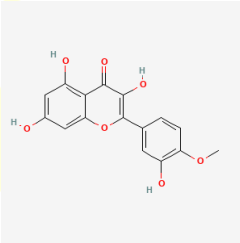
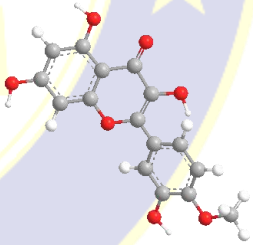
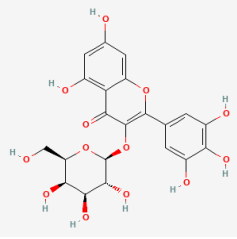
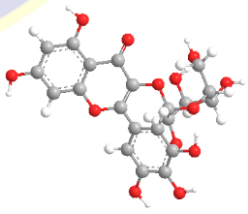
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
29	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	$C_{18}H_{16}O_6$		
30	*3'-Formyl-6',4-dihydroxy-2'-methoxy-5'-methylchalcone 4'-O-β-D-glucopyranoside*	$C_{24}H_{26}O_{11}$		
31	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	$C_{17}H_{16}O_4$		
32	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	$C_{18}H_{18}O_5$		

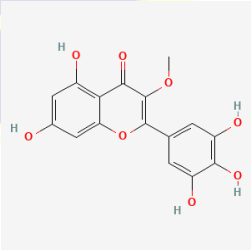
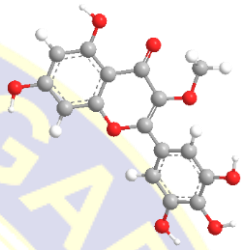
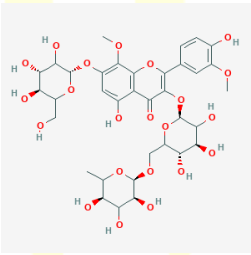
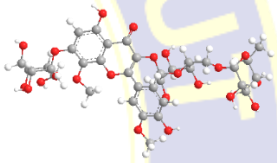
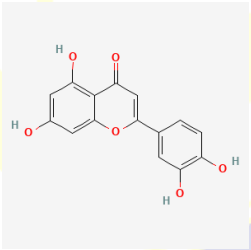
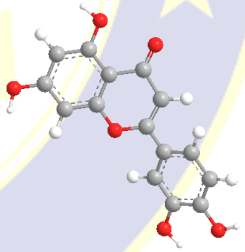
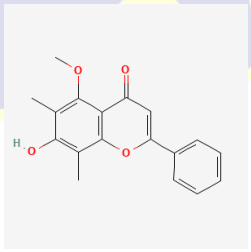
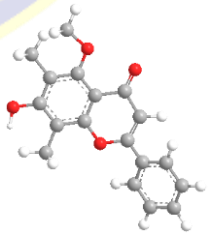
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
33	*Kaempferol*	$C_{15}H_{10}O_6$		
34	*Quercetin*	$C_{15}H_{10}O_7$		
35	*Tamarixetin*	$C_{16}H_{12}O_7$		
36	*Myricetin-3'-methylether 3-O-β-D-galactopyranoside*	$C_{21}H_{20}O_{13}$		

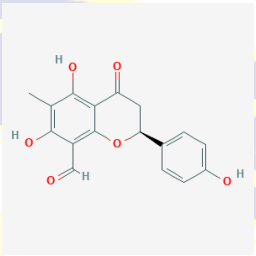
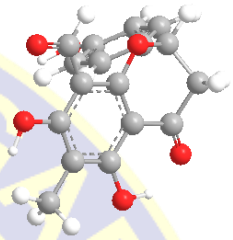
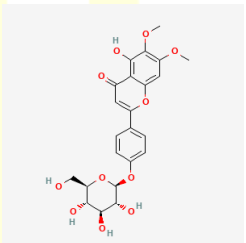
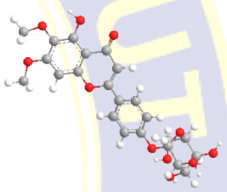
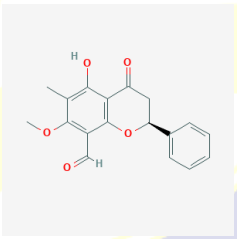
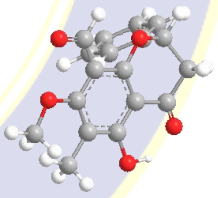
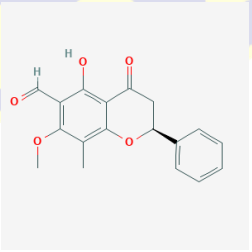
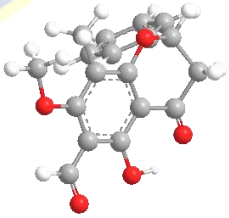
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
37	*Myricetin-3'-methylether*	$C_{16}H_{12}O_8$		
38	*Gossypetin-8,3'-dimethylether-3-O-β-D-galactoside*	$C_{35}H_{44}O_{22}$		
39	*Luteolin*	$C_{15}H_{10}O_6$		
40	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	$C_{18}H_{16}O_4$		

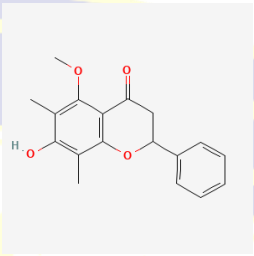
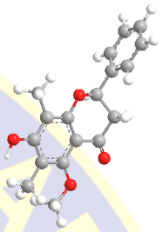
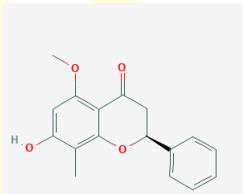
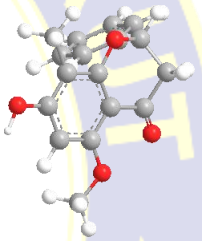
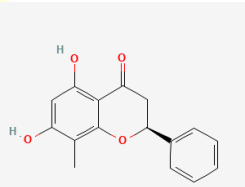
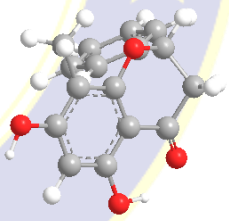
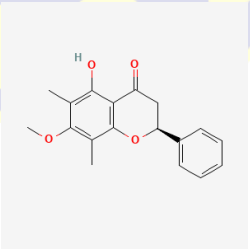
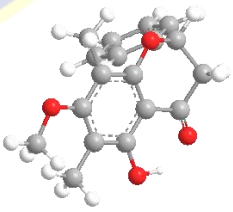
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
41	*(2S)-8-Formyl-6-methylnaringenin*	$C_{17}H_{14}O_6$		
42	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	$C_{23}H_{24}O_{11}$		
43	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	$C_{18}H_{16}O_5$		
44	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	$C_{18}H_{16}O_5$		

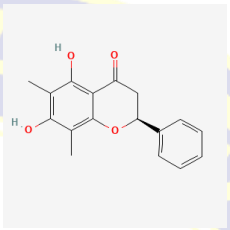
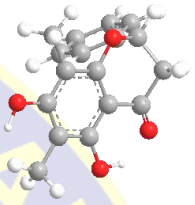
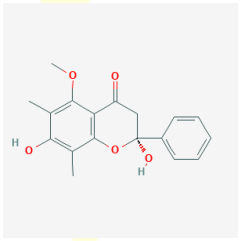
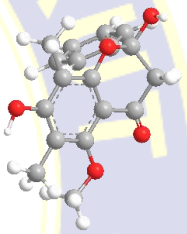
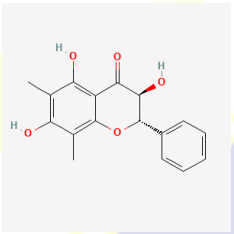
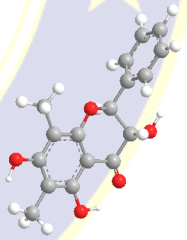
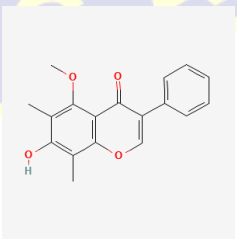
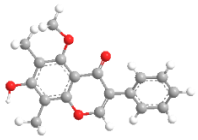
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
45	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	$C_{18}H_{18}O_4$		
46	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	$C_{17}H_{16}O_4$		
47	*(2S)-8-methylpinocembrin*	$C_{16}H_{14}O_4$		
48	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	$C_{18}H_{18}O_4$		

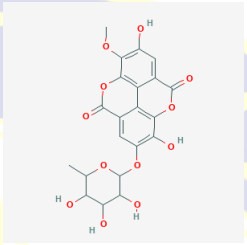
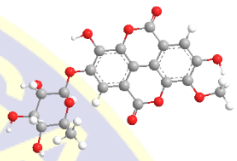
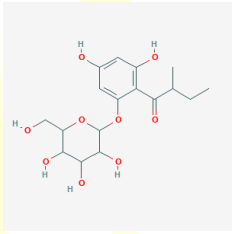
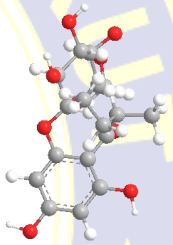
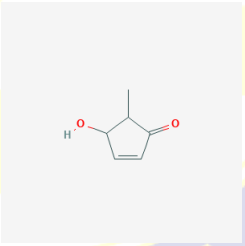
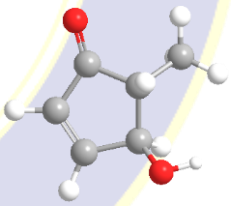
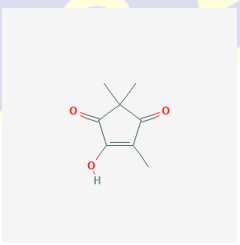
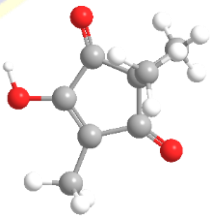
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
49	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	$C_{17}H_{16}O_4$		
50	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	$C_{18}H_{18}O_5$		
51	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	$C_{17}H_{16}O_5$		
52	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	$C_{18}H_{16}O_4$		

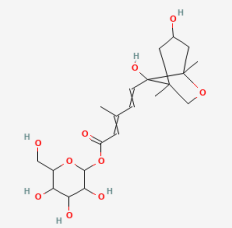
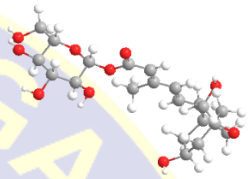
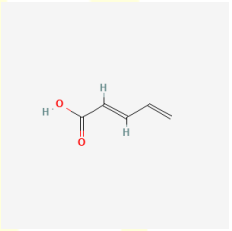
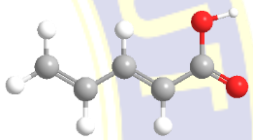
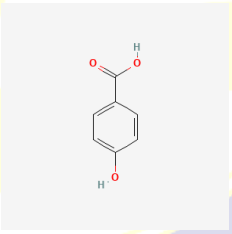
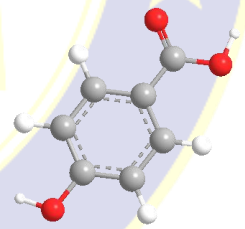
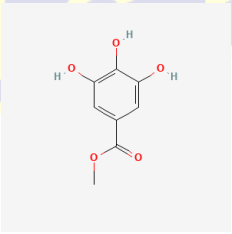
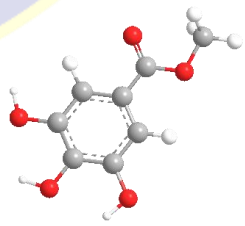
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
53	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	$C_{21}H_{18}O_{12}$		
54	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	$C_{17}H_{24}O_9$		
55	*(trans)-4-Hydroxy-5-(2-hydroxypropan-2-yl)-2-methylcyclopent-2-en-1-one*	$C_6H_8O_2$		
56	*4-Hydroxy-2,2,5-trimethylcyclopent-4-ene-1,3-dione*	$C_8H_{10}O_3$		

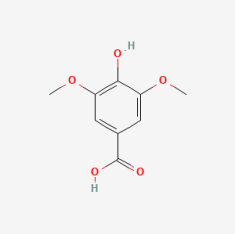
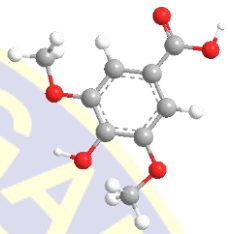
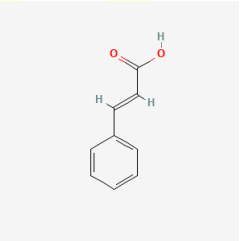
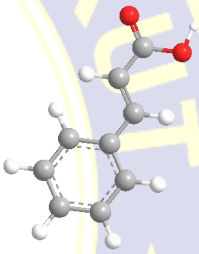
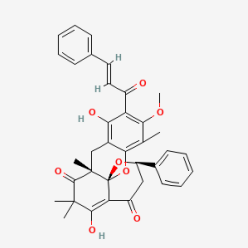
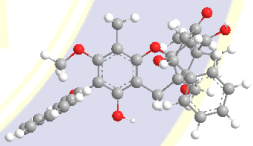
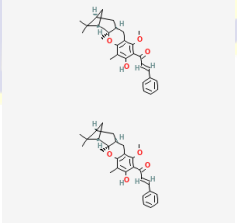
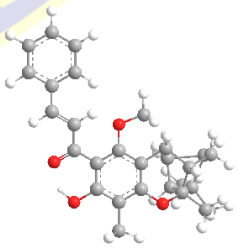
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
57	*4'-Dihydrophaseic acid*	$C_{21}H_{32}O_{10}$		
58	*Pentadienoic acid*	$C_5H_6O_2$		
59	*4-Hydroxybenzoic acid*	$C_7H_6O_3$		
60	*Methyl 3,4,5-trihydroxybenzoate*	$C_8H_8O_5$		

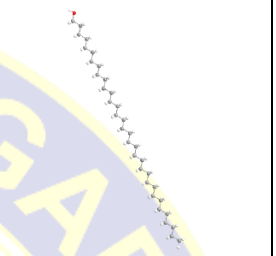
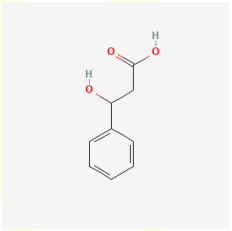
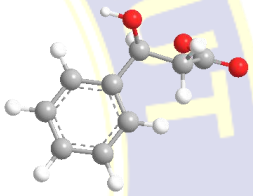
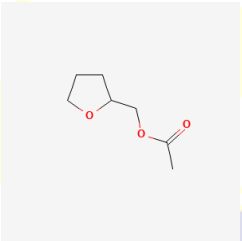
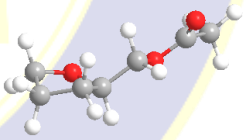
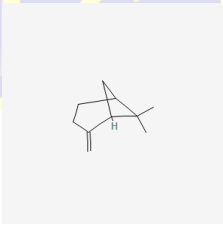
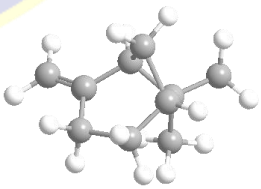
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
61	*4-Hydroxy-3,5-dimethoxybenzoic acid*	$C_9H_{10}O_5$		
62	*Cinnamic acid*	$C_9H_8O_2$		
63	*Cleistoperlone A*	$C_{36}H_{34}O_8$		
64	*Operculatol A*	$C_{56}H_{64}O_8$		

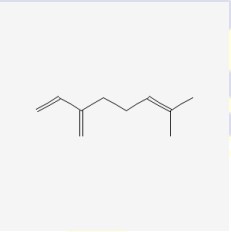
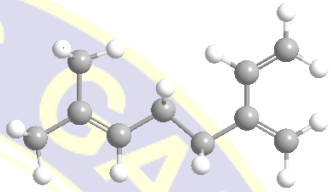
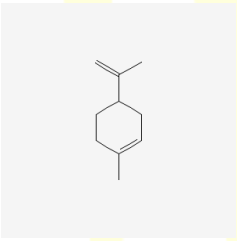
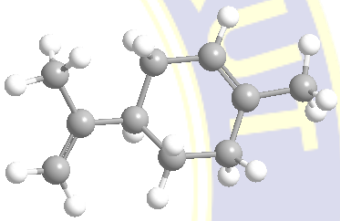
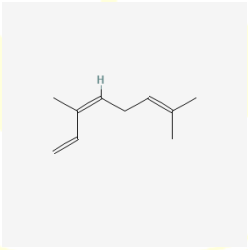
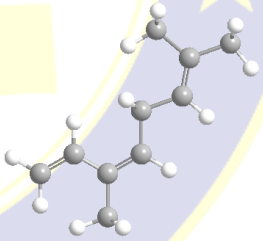
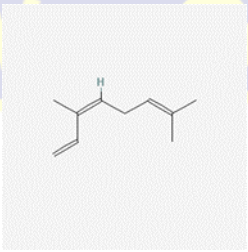
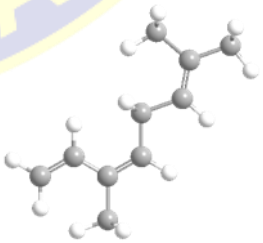
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
65	*1-Tetratriacontanol*	$C_{34}H_{70}O$		
66	*3-Hydroxy-3-phenylpropanoic acid*	$C_9H_{10}O_3$		
67	*Tetrahydrofurfuryl acetate*	$C_7H_{12}O_3$		
68	*β-Pinene*	$C_{10}H_{16}$		

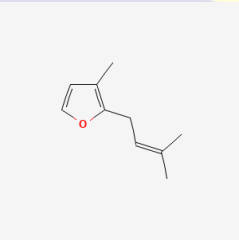
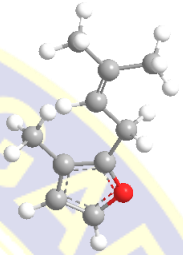
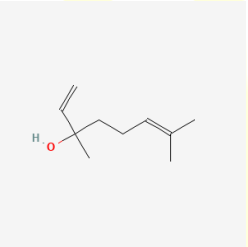
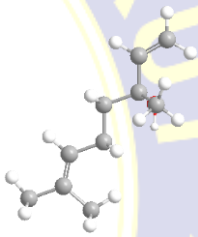
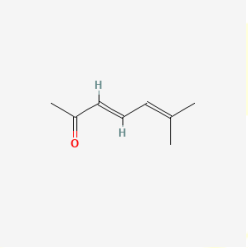
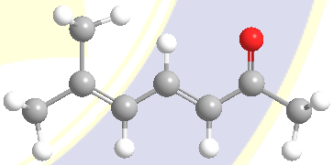
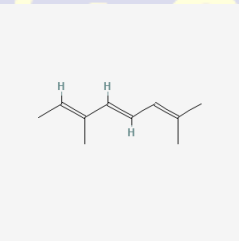
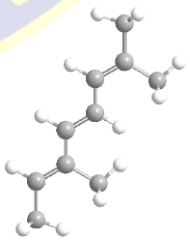
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
69	*Myrcene*	$C_{10}H_{16}$		
70	*Limonene*	$C_{10}H_{16}$		
71	*(Z)-β-Ocimene*	$C_{10}H_{16}$		
72	*(E)-β-Ocimene*	$C_{10}H_{16}$		

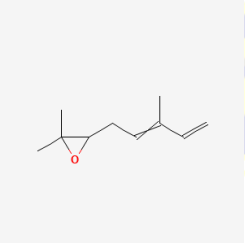
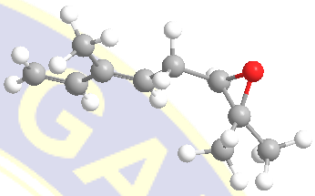
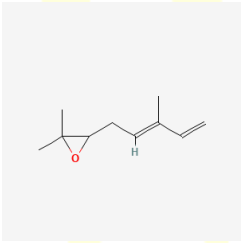
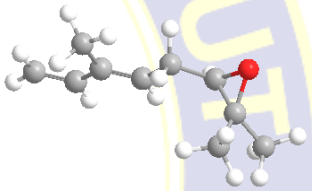
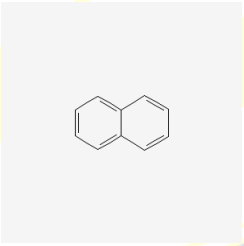
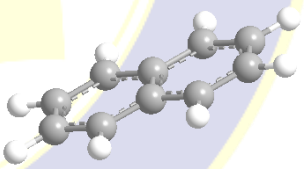
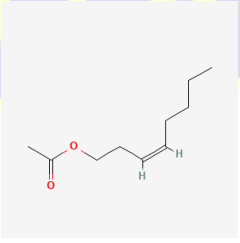
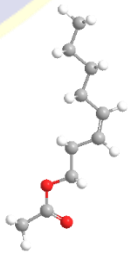
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
73	*Rosefuran*	$C_{10}H_{14}O$		
74	*Linalool*	$C_{10}H_{18}O$		
75	*6-Methyl-3,5-heptadien-2-one*	$C_8H_{12}O$		
76	*allo-Ocimene*	$C_{10}H_{16}$		

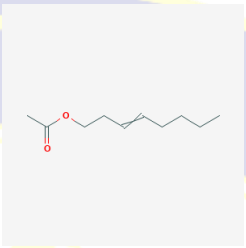
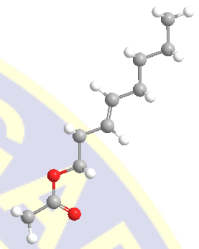
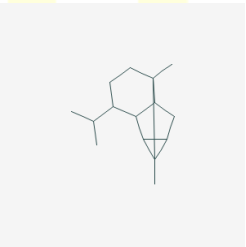
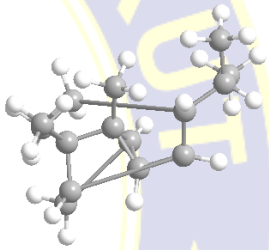
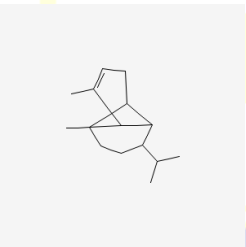
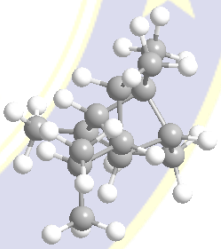
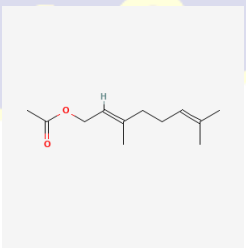
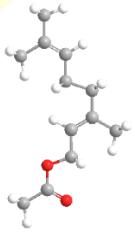
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
77	*(Z)-Epoxy ocimene (=(Z)-MyrOxide)*	$C_{10}H_{16}O$		
78	*(E)-Epoxy ocimene (=(E)-Myroxide)*	$C_8H_{12}O$		
79	*Naphthalene*	$C_{10}H_8$		
80	*(3Z)-Octenyl acetate*	$C_{10}H_{18}O_2$		

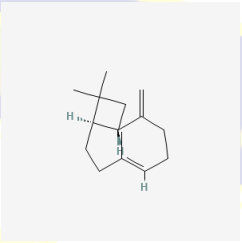
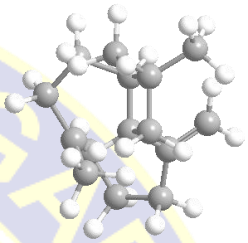
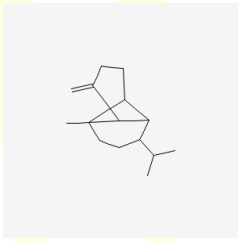
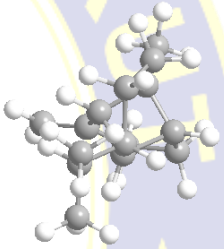
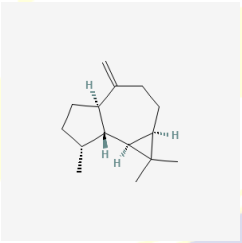
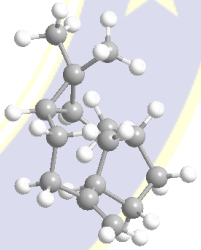
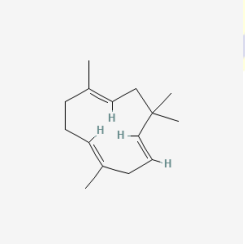
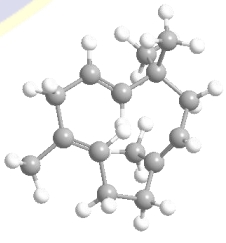
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
81	*(3E)-Octenyl acetate*	$C_{10}H_{18}O_2$		
82	*Cyclosativene*	$C_{15}H_{24}$		
83	*α-Copaene*	$C_{15}H_{24}$		
84	*Geranyl acetate*	$C_{12}H_{20}O_2$		

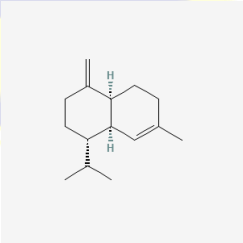
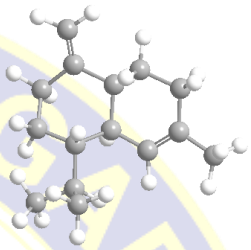
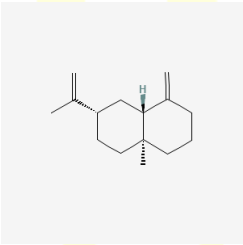
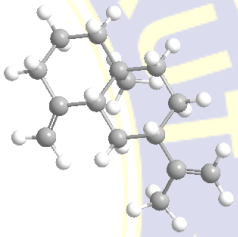
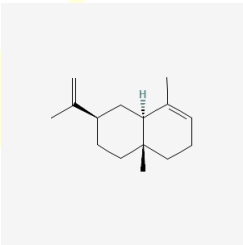
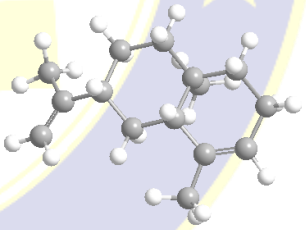
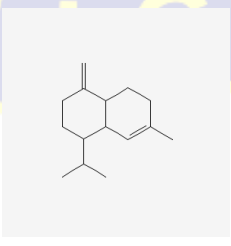
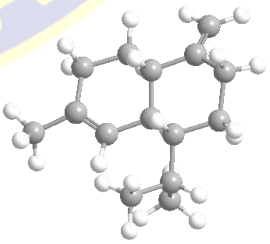
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
85	*(E)-Caryophyllene*	$C_{15}H_{24}$		
86	*β-Copaene*	$C_{15}H_{24}$		
87	*Aromadendrene*	$C_{15}H_{24}$		
88	*α-Humulene*	$C_{15}H_{24}$		

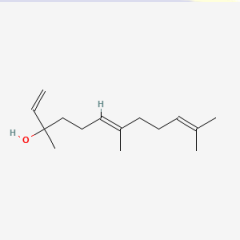
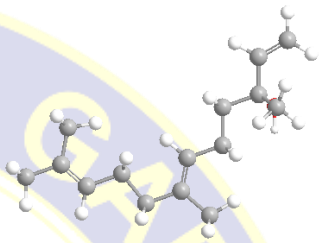
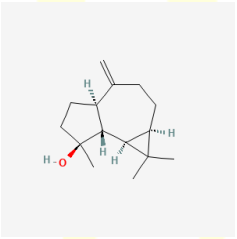
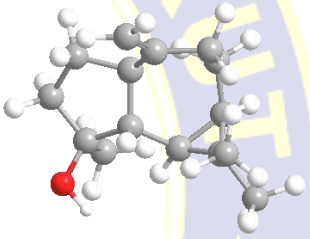
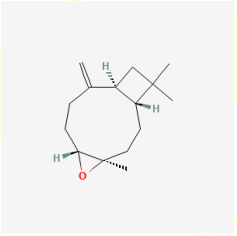
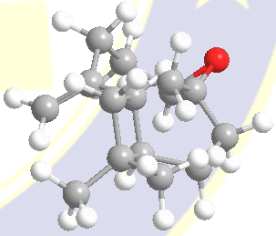
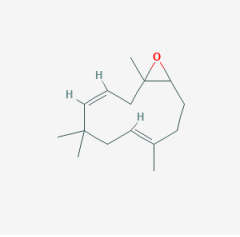
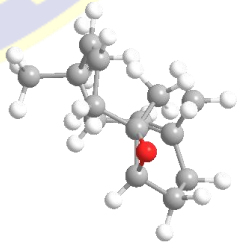
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
89	*γ-Muurolene*	$C_{15}H_{24}$		
90	*β-Selinene*	$C_{15}H_{24}$		
91	*α-Selinene*	$C_{15}H_{24}$		
92	*γ-Cadinene*	$C_{15}H_{24}$		

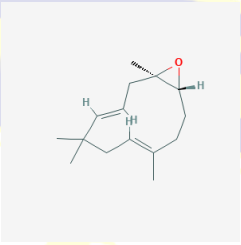
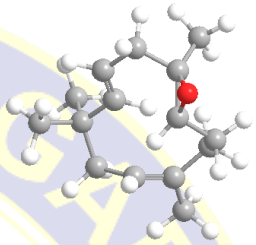
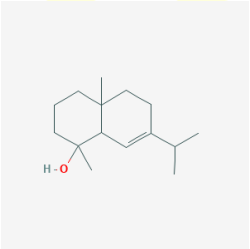
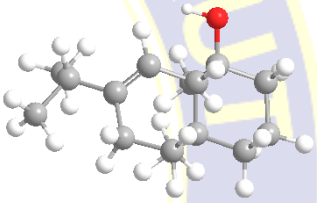
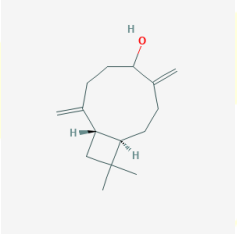
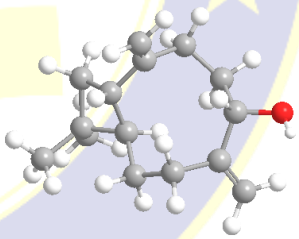
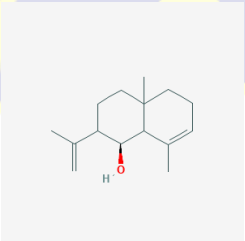
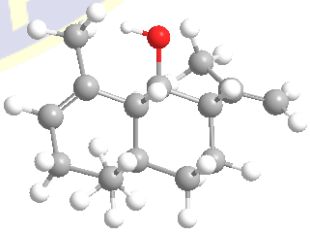
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
93	*(E)-Nerolidol*	$C_{15}H_{26}O$		
94	*Spathulenol*	$C_{15}H_{24}O$		
95	*Caryophyllene oxide*	$C_{15}H_{24}O$		
96	*Humulene epoxide I*	$C_{15}H_{24}O$		

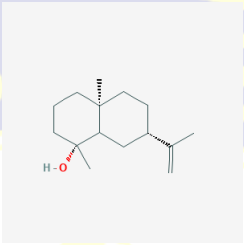
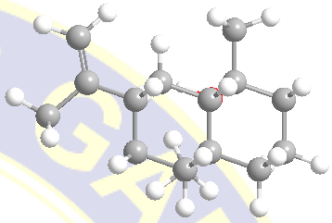
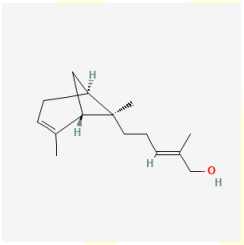
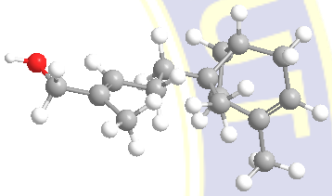
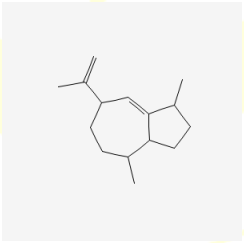
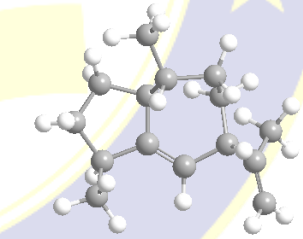
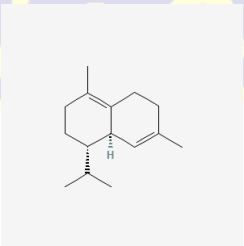
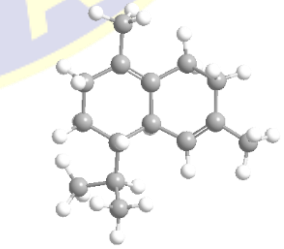
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
97	*Humulene epoxide II*	$C_{15}H_{24}O$		
98	*Selina-6-en-4β-ol*	$C_{15}H_{26}O$		
99	*Caryophylla-4(12),8(13)-dien-5β-ol*	$C_{15}H_{24}O$		
100	*Selina-3,11-dien-6α-ol*	$C_{15}H_{24}O$		

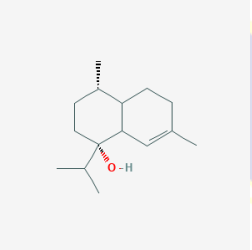
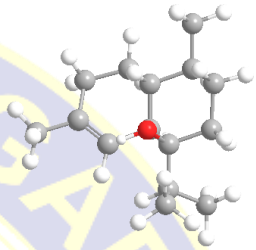
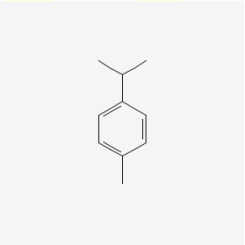
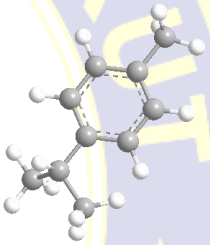
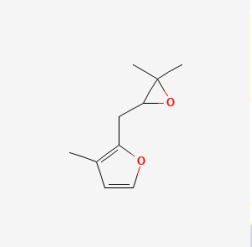
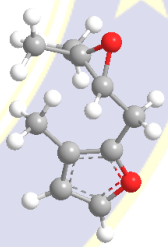
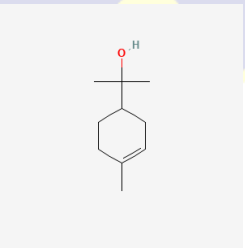
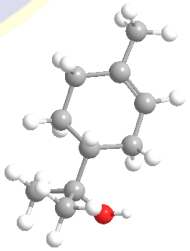
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
101	*Selin-11-en-4α-ol*	$C_{15}H_{26}O$		
102	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	$C_{15}H_{24}O$		
103	*γ-Gurjunene*	$C_{15}H_{24}$		
104	*δ-Cadinene*	$C_{15}H_{24}$		

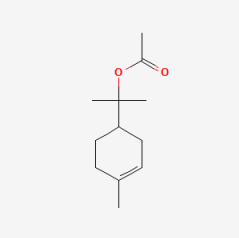
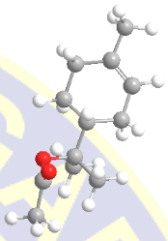
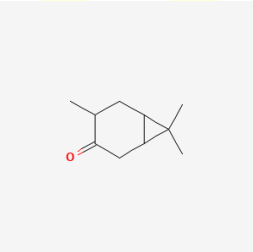
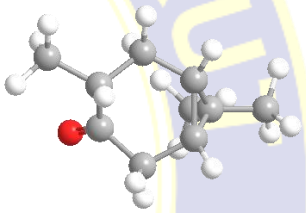
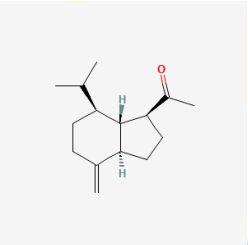
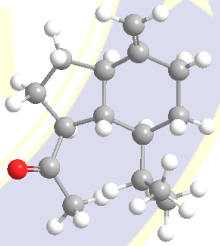
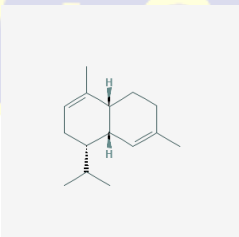
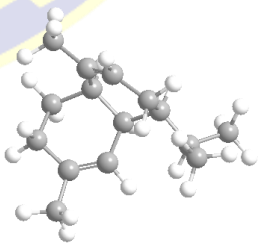
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
105	*cis-Cadin-4-en-7-ol*	$C_{15}H_{26}O$		
106	*p-Cymene*	$C_{10}H_{14}$		
107	*Rosefuran epoxide*	$C_{10}H_{14}O_2$		
108	*α-Terpineol*	$C_{10}H_{18}O$		

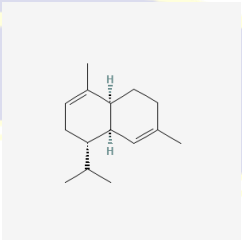
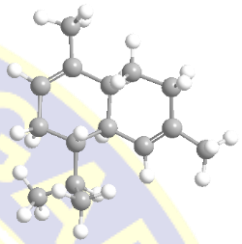
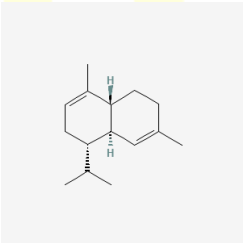
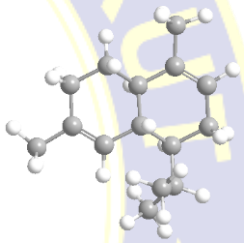
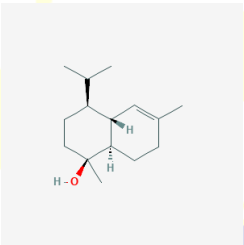
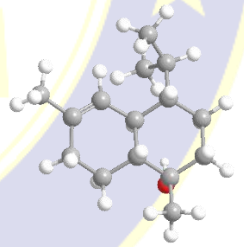
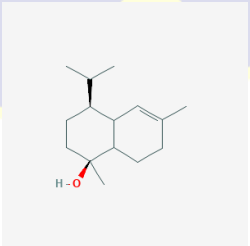
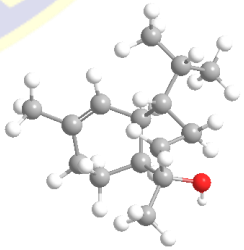
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
109	*α-Terpinyl acetate*	$C_{12}H_{20}O_2$		
110	*cis-4-Caranone*	$C_{10}H_{16}O$		
111	*β-Oplopenone*	$C_{15}H_{24}O$		
112	*α-Amorphene*	$C_{15}H_{24}$		

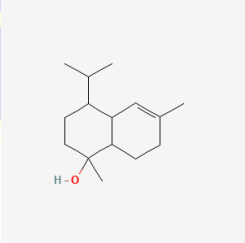
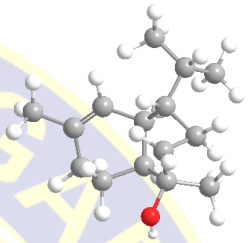
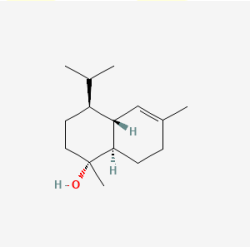
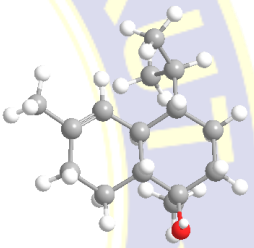
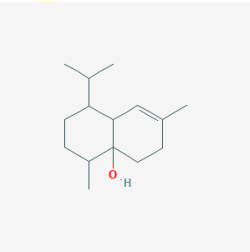
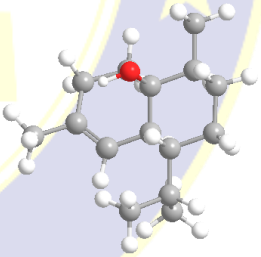
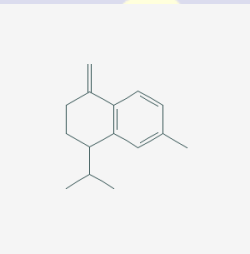
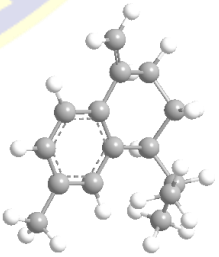
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
113	*α-Muurolene*	$C_{15}H_{24}$		
114	*α-Cadinene*	$C_{15}H_{24}$		
115	*τ-Cadinol*	$C_{15}H_{26}O$		
116	*τ-Muurolol*	$C_{15}H_{26}O$		

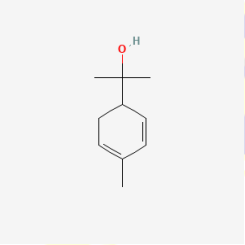
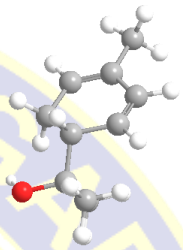
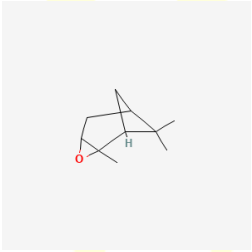
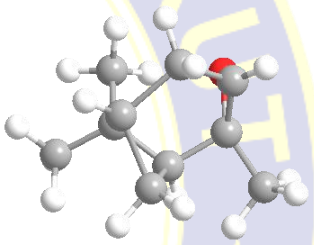
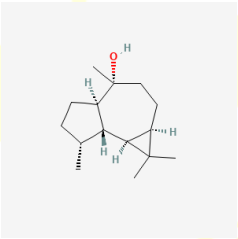
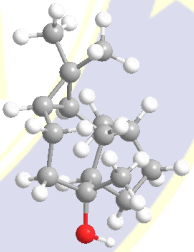
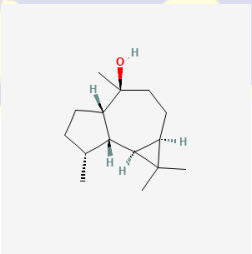
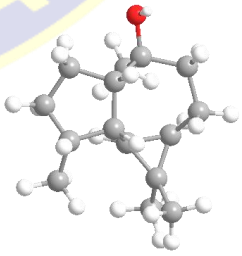
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
117	*α-Muurolol (= δ-Cadinol)*	$C_{15}H_{26}O$		
118	*α-Cadinol*	$C_{15}H_{26}O$		
119	*1-epi-Cubenol*	$C_{15}H_{26}O$		
120	*β-Calacorene*	$C_{15}H_{20}$		

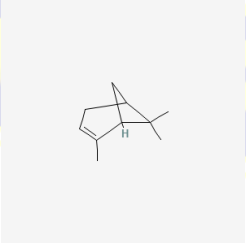
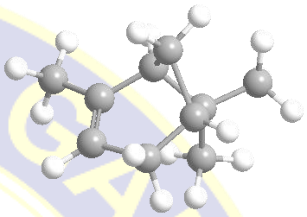
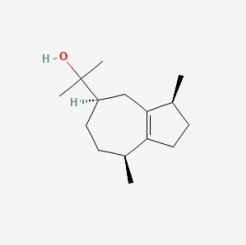
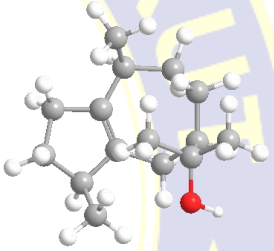
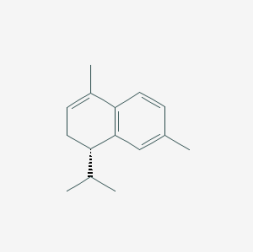
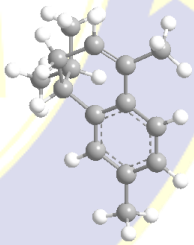
LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
121	*p-Mentha-1,5-dien-8-ol*	$C_{10}H_{16}O$		
122	*α-Pinene oxide*	$C_{10}H_{16}O$		
123	*Globulol*	$C_{15}H_{26}O$		
124	*Viridiflorol*	$C_{15}H_{26}O$		

LAMPIRAN 8
(LANJUTAN)

Tabel VII. 4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
125	*α-Pinene*	$C_{10}H_{16}$		
126	*Guaiol*	$C_{15}H_{26}O$		
127	*α-Calacorene*	$C_{15}H_{20}$		

LAMPIRAN 9

HASIL SKRINING AKTIVITAS ANTIKANKER PAYUDARA

Tabel VII. 5
Hasil Skrining Aktivitas Antikanker Payudara

No	Nama Senyawa	Pa	Pi	Aktivitas
1	*Myrcene*	0,892	0,004	*Antineoplastic (breast cancer)*
2	*(Z)-β-Ocimene*	0,755	0,005	*Antineoplastic (breast cancer)*
3	*(E)-β-Ocimene*	0,755	0,005	*Antineoplastic (breast cancer)*
4	*Betulinic acid*	0,724	0,005	*Antineoplastic (breast cancer)*
5	*Alphitolic acid*	0,686	0,006	*Antineoplastic (breast cancer)*
6	*Luteolin*	0,672	0,007	*Antineoplastic (breast cancer)*
7	*allo-Ocimene*	0,67	0,007	*Antineoplastic (breast cancer)*
8	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	0,638	0,008	*Antineoplastic (breast cancer)*
9	*Oleanolic acid*	0,627	0,009	*Antineoplastic (breast cancer)*
10	*Cleistocalyxic acid E*	0,627	0,009	*Antineoplastic (breast cancer)*
11	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	0,617	0,009	*Antineoplastic (breast cancer)*
12	*Cleistocalyxic acid G*	0,613	0,009	*Antineoplastic (breast cancer)*
13	*Cleistoperlone A*	0,613	0,009	*Antineoplastic (breast cancer)*
14	*Cleistocalyxic acid A*	0,612	0,01	*Antineoplastic (breast cancer)*
15	*Myricetin-3'-methylether*	0,612	0,009	*Antineoplastic (breast cancer)*
16	*(Z)-Epoxy ocimene (=(Z)-MyrOxide)*	0,612	0,01	*Antineoplastic (breast cancer)*
17	*(E)-Epoxy ocimene (= (E)-Myroxide)*	0,612	0,01	*Antineoplastic (breast cancer)*
18	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	0,61	0,01	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
19	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	0,606	0,01	*Antineoplastic (breast cancer)*
20	*(2S)-8-Formyl-6-methylnaringenin*	0,605	0,01	*Antineoplastic (breast cancer)*
21	*β-Selinene*	0,603	0,01	*Antineoplastic (breast cancer)*
22	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	0,601	0,01	*Antineoplastic (breast cancer)*
23	*3-O-trans-p-Coumaroyl maslinic acid*	0,6	0,01	*Antineoplastic (breast cancer)*
24	*3-O-cis-p-Coumaroyl maslinic acid*	0,6	0,01	*Antineoplastic (breast cancer)*
25	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	0,6	0,01	*Antineoplastic (breast cancer)*
26	*Tamarixetin*	0,6	0,01	*Antineoplastic (breast cancer)*
27	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	0,599	0,01	*Antineoplastic (breast cancer)*
28	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	0,594	0,011	*Antineoplastic (breast cancer)*
29	*Cleistocalyxic acid I*	0,593	0,011	*Antineoplastic (breast cancer)*
30	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	0,593	0,011	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
31	*Arjunolic acid*	0,591	0,011	*Antineoplastic (breast cancer)*
32	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	0,583	0,012	*Antineoplastic (breast cancer)*
33	*Cleistocalyxic acid C*	0,582	0,012	*Antineoplastic (breast cancer)*
34	*Maslinic acid*	0,582	0,012	*Antineoplastic (breast cancer)*
35	*Cleistocalyxic acid K*	0,58	0,012	*Antineoplastic (breast cancer)*
36	*(2S)-8-methylpinocembrin*	0,579	0,012	*Antineoplastic (breast cancer)*
37	*Quercetin*	0,577	0,012	*Antineoplastic (breast cancer)*
38	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	0,574	0,013	*Antineoplastic (breast cancer)*
39	*Cleistocalyxic acid F*	0,572	0,013	*Antineoplastic (breast cancer)*
40	*Kaempferol*	0,566	0,013	*Antineoplastic (breast cancer)*
41	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	0,566	0,013	*Antineoplastic (breast cancer)*
42	*Pentadienoic acid*	0,565	0,013	*Antineoplastic (breast cancer)*
43	*6-Methyl-3,5-heptadien-2-one*	0,562	0,014	*Antineoplastic (breast cancer)*
44	*Geranyl acetate*	0,562	0,014	*Antineoplastic (breast cancer)*
45	*4-Hydroxy-2,2,5-trimethylcyclopent-4-ene-1,3-dione*	0,557	0,014	*Antineoplastic (breast cancer)*
46	*Actinidic acid*	0,556	0,014	*Antineoplastic (breast cancer)*
47	*Cleistocalyxic acid B*	0,551	0,014	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
48	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	0,542	0,015	*Antineoplastic (breast cancer)*
49	*Cleistocalyxic acid J*	0,538	0,015	*Antineoplastic (breast cancer)*
50	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	0,537	0,015	*Antineoplastic (breast cancer)*
51	*(E)-Caryophyllene*	0,527	0,016	*Antineoplastic (breast cancer)*
52	*α-Selinene*	0,521	0,017	*Antineoplastic (breast cancer)*
53	*Limonene*	0,515	0,018	*Antineoplastic (breast cancer)*
54	*3'-Formyl-6',4-dihydroxy-2'-methoxy-5'-methylchalcone 4'-O-β-D-glucopyranoside*	0,506	0,018	*Antineoplastic (breast cancer)*
55	*Myricetin-3'-methylether 3-O-β-D-galactopyranoside*	0,501	0,019	*Antineoplastic (breast cancer)*
56	*Gossypetin-8,3'-dimethylether-3-O-β-D-galactoside*	0,468	0,023	*Antineoplastic (breast cancer)*
57	*2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid*	0,441	0,026	*Antineoplastic (breast cancer)*
58	*2α,3β-Dihydroxy-24-nor-urs-4(23),12-dien-28-oic acid*	0,441	0,026	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
59	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	0,423	0,028	*Antineoplastic (breast cancer)*
60	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	0,421	0,028	*Antineoplastic (breast cancer)*
61	*Ursolic acid*	0,416	0,029	*Antineoplastic (breast cancer)*
62	*Caryophylla-4(12),8(13)-dien-5β-ol*	0,409	0,03	*Antineoplastic (breast cancer)*
63	*Cleistocalyxic acid H*	0,39	0,033	*Antineoplastic (breast cancer)*
64	*Cleistocalyxolide B*	0,389	0,033	*Antineoplastic (breast cancer)*
65	*Selin-11-en-4α-ol*	0,389	0,033	*Antineoplastic (breast cancer)*
66	*Asiatic acid*	0,388	0,034	*Antineoplastic (breast cancer)*
67	*(E)-Nerolidol*	0,359	0,04	*Antineoplastic (breast cancer)*
68	*Corosolic acid*	0,357	0,04	*Antineoplastic (breast cancer)*
69	*Selina-3,11-dien-6α-ol*	0,338	0,045	*Antineoplastic (breast cancer)*
70	*Cleistocalyxic acid D*	0,33	0,047	*Antineoplastic (breast cancer)*
71	*Cinnamic acid*	0,3	0,055	*Antineoplastic (breast cancer)*
72	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	0,297	0,056	*Antineoplastic (breast cancer)*
73	*β-Copaene*	0,287	0,059	*Antineoplastic (breast cancer)*
74	*4-Hydroxy-3,5-dimethoxybenzoic acid*	0,278	0,062	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
75	*(trans)-4-Hydroxy-5-(2-hydroxypropan-2-yl)-2-methylcyclopent-2-en-1-one*	0,273	0,063	*Antineoplastic (breast cancer)*
76	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	0,271	0,064	*Antineoplastic (breast cancer)*
77	*Methyl 3,4,5-trihydroxybenzoate*	0,27	0,064	*Antineoplastic (breast cancer)*
78	*Caryophyllene oxide*	0,264	0,066	*Antineoplastic (breast cancer)*
79	*Linalool*	0,259	0,068	*Antineoplastic (breast cancer)*
80	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	0,259	0,068	*Antineoplastic (breast cancer)*
81	*4'-Dihydrophaseic acid*	0,256	0,069	*Antineoplastic (breast cancer)*
82	*α-Humulene*	0,254	0,07	*Antineoplastic (breast cancer)*
83	*Operculatol A*	0,25	0,071	*Antineoplastic (breast cancer)*
84	*Humulene epoxide I*	0,246	0,073	*Antineoplastic (breast cancer)*
85	*Humulene epoxide II*	0,246	0,073	*Antineoplastic (breast cancer)*
86	*(3Z)-Octenyl acetate*	0,236	0,078	*Antineoplastic (breast cancer)*
87	*(3E)-Octenyl acetate*	0,236	0,078	*Antineoplastic (breast cancer)*
88	*Cyclosativene*	0,235	0,078	*Antineoplastic (breast cancer)*
89	*Rosefuran*	0,229	0,081	*Antineoplastic (breast cancer)*
90	*α-Copaene*	0,186	0,103	*Antineoplastic (breast cancer)*
91	*Aromadendrene*	0,184	0,105	*Antineoplastic (breast cancer)*
92	*4-Hydroxybenzoic acid*	0,168	0,118	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 5
Lanjutan

No	Nama Senyawa	Pa	Pi	Aktivitas
93	*γ-Muurolene*	0,167	0,119	*Antineoplastic (breast cancer)*
94	*γ-Cadinene*	0,167	0,119	*Antineoplastic (breast cancer)*
95	*β-Pinene*	0,163	0,124	*Antineoplastic (breast cancer)*
96	*Selina-6-en-4β-ol*	0,159	0,129	*Antineoplastic (breast cancer)*
97	*β-Sitosterol*	0,153	0,134	*Antineoplastic (breast cancer)*
98	*Tetrahydrofurfuryl acetate*	0,148	0,139	*Antineoplastic (breast cancer)*
99	*Spathulenol*	0,144	0,144	*Antineoplastic (breast cancer)*
100	*Naphthalene*	0,118	0,011	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

Tabel VII. 6
Hasil Skrining Aktivitas Antikanker

No	Nama Senyawa	Pa	Pi	Aktivitas
1	*β-Oplopenone*	0,827	0,009	*Antineoplastic*
2	*α-Amorphene*	0,821	0,009	*Antineoplastic*
3	*α-Muurolene*	0,821	0,009	*Antineoplastic*
4	*α-Cadinene*	0,821	0,009	*Antineoplastic*
5	*τ-Cadinol*	0,739	0,02	*Antineoplastic*
6	*τ-Muurolol*	0,739	0,02	*Antineoplastic*
7	*α-Muurolol (= δ-Cadinol)*	0,739	0,02	*Antineoplastic*
8	*α-Cadinol*	0,739	0,02	*Antineoplastic*
9	*1-epi-Cubenol*	0,713	0,024	*Antineoplastic*
10	*β-Calacorene*	0,668	0,032	*Antineoplastic*
11	*p-Mentha-1,5-dien-8-ol*	0,623	0,04	*Antineoplastic*
12	*α-Pinene oxide*	0,575	0,051	*Antineoplastic*
13	*Globulol*	0,527	0,063	*Antineoplastic*
14	*Viridiflorol*	0,527	0,063	*Antineoplastic*
15	*α-Pinene*	0,22	0,149	*Antineoplastic*
16	*Guaiol*	0,162	0,093	*Antineoplastic*
17	*α-Calcorene*	0,161	0,087	*Antineoplastic*

LAMPIRAN 9
(LANJUTAN)

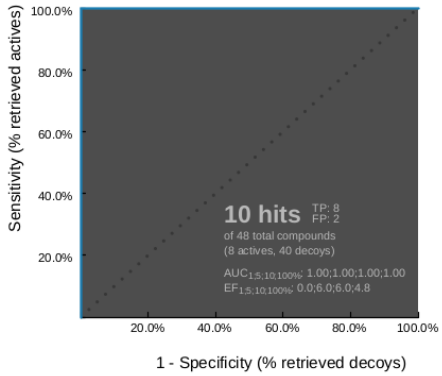
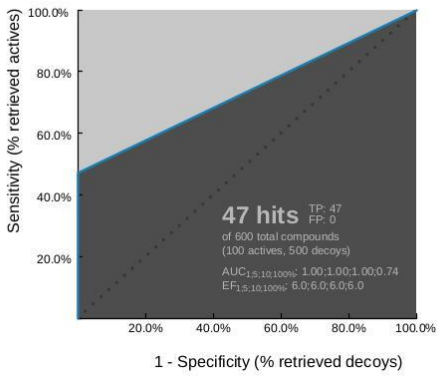
Tabel VII. 7
Hasil Skrining Aktivitas Antioksidan

No	Nama Senyawa	Pa	Pi	Aktivitas
1	1-Tetratriacontanol	0,229	0,043	*Antioxidant*
2	γ-Gurjunene	0,168	0,081	*Antioxidant*
3	3-Hydroxy-3-phenylpropanoic acid	0,164	0,086	*Antioxidant*
4	δ-Cadinene	0,147	0,107	*Antioxidant*
5	cis-Cadin-4-en-7-ol	0,145	0,108	*Antioxidant*
6	p-Cymene	0,144	0,11	*Antioxidant*
7	Rosefuran epoxide	0,14	0,114	*Antioxidant*
8	α-Terpineol	0,137	0,118	*Antioxidant*
9	α-Terpinyl acetate	0,132	0,125	*Antioxidant*
10	cis-4-Caranone	0,13	0,128	*Antioxidant*

LAMPIRAN 10

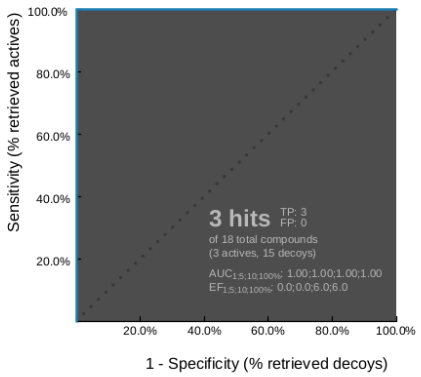
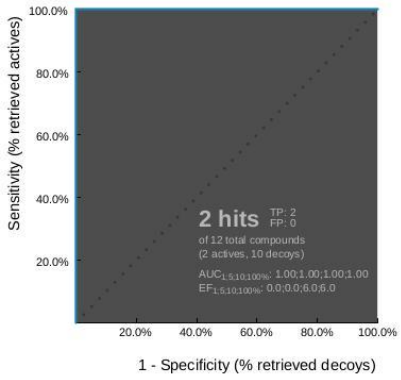
HASIL STUDI FARMAKOFOR

Tabel VII. 8
Hasil Validasi Farmakofor

Reseptor	ROC Curve	AUC	GH Score
ER-α		1	0,81
ER-β		0,74	0,87

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 8
Lanjutan

Reseptor	ROC Curve	AUC	GH Score
Progesteron		1	1,00
HER-2		1	1,00

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 9
Hasil Skrining Farmakofor Ligan Uji Terhadap Reseptor ER-α

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	52.71
2	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	52.68
3	*Cleistocalyxic acid H*	52.38
4	*Limocitrin 3-rutinoside-7-glucoside*	51.96
5	*Kaempferol*	51.59
6	*Luteolin*	51.43
7	*Quercetin*	51.42
8	*Tamarixetin*	51.25
9	*Myricetin 3-galactoside*	51.24
10	*4'-Dihydrophaseic acid*	51.05
11	*(2S)-8-Formyl-6-methylnaringenin*	50.81
12	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	50.62
13	*Cleistocalyxic acid D*	45.51
14	*Cleistocalyxic acid A*	45.46
15	*Maslinic acid*	44.99
16	*Lethedoside A*	44.58
17	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	44.34
18	*Cleistocalyxic acid K*	43.85
19	*Asiatic acid*	43.76
20	*Oleanolic acid*	43.73

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 9
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
21	*3-O-cis-p-Coumaroyl_maslinic_acid*	43.73
22	*Cleistocalyxic acid G*	43.72
23	*Arjunolic acid*	43.70
24	*Corosolic acid*	43.67
25	*Ursolic acid*	43.62
26	*(S)-2,3-Dihydro-5,7-dihydroxy-8-methyl-2-phenyl-4-benzopyrone*	43.60
27	*Stercurensin*	43.59
28	*Actinidic acid*	43.47
29	*Cleistocalyxolide B*	43.45
30	*Cirsimarin*	43.40
31	*Cleistocalyxic acid F*	43.37
32	*Cleistocalyxic acid E*	43.37
33	*(2beta,3alpha)-2,3-Dihydroxy-urs-12-en-28-oic acid*	43.34
34	*Alphitolic acid*	43.28
35	*11alpha-Hydroxyasiatic acid*	43.28
36	*Betulinic acid*	43.26
37	*Cleistocalyxic acid J*	43.12
38	*Annulatin*	43.06
39	*Cleistocalyxic acid I*	43.01
40	*Cleistocalyxic acid C*	42.99
41	*Operculatol A*	42.73
42	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	42.66

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 9
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
43	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	42.00
44	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	41.90
45	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	41.87
46	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	41.58
47	*(E)-Nerolidol*	41.26
48	*3-beta-O-(trans-p-Coumaroyl)maslinic_acid*	41.20
49	*p-Mentha-1,5-dien-8-ol*	37.96
50	*Linalool*	37.79
51	*4-Hydroxybenzoic acid*	37.70
52	*α-Terpineol*	36.88
53	*Cleistoperlone A*	36.55
54	*3-Hydroxy-3-phenylpropanoic acid*	36.50
55	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	35.59
56	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	35.58
57	*Demethoxymatteucinol*	35.56
58	*(2S,3S)-3,5,7-trihydroxy-6,8-dimethylflavanone*	35.56
59	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	35.56

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 9
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
60	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	35.55
61	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	35.47
62	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	35.47
63	*Cleistocalyxic acid B*	35.15
64	*Guaiol*	34.41
65	*Viridiflorol*	34.36
66	*Caryophylla-4(12),8(13)-dien-5β-ol*	34.36
67	*Globulol*	33.83

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 10
Hasil Skrining Farmakofor Ligan Uji Terhadap Reseptor ER-β

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*Luteolin*	75.13
2	*Kaempferol*	67.27
3	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	67.16
4	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	66.75
5	*(2S)-8-Formyl-6-methylnaringenin*	66.52
6	*Quercetin*	66.35
7	*3-O-cis-p-Coumaroyl_maslinic_acid*	56.77
8	*3-beta-O-(trans-p-Coumaroyl)maslinic_acid*	56.77
9	*Tamarixetin*	56.63

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 11
Hasil Skrining Farmakofor Ligan Uji Terhadap Reseptor Progesteron

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	52.34
2	*4'-Dihydrophaseic acid*	52.17
3	*Quercetin*	43.47
4	*Tamarixetin*	43.37
5	*Luteolin*	43.32
6	*Corosolic acid*	43.27
7	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	43.17
8	*Cleistocalyxic acid E*	43.16
9	*Cleistocalyxic acid A*	43.16
10	*Cleistocalyxic acid H*	43.14
11	*Kaempferol*	43.03
12	*Maslinic acid*	42.81
13	*Cleistocalyxic acid B*	42.60
14	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	42.53
15	*(2S)-8-Formyl-6-methylnaringenin*	42.50
16	*Cleistocalyxic acid G*	41.88
17	*Lethedoside A*	35.23
18	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	34.91
19	*(2beta,3alpha)-2,3-Dihydroxy-urs-12-en-28-oic acid*	34.84

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
20	*Annulatin*	34.63
21	*Cleistocalyxic acid F*	34.43
22	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	34.20
23	*Actinidic acid*	33.97
24	*Alphitolic_acid*	33.94
25	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	33.88
26	*Cleistocalyxic acid K*	33.85
27	*11alpha-Hydroxyasiatic acid*	33.85
28	*Myricetin 3-galactoside*	33.69
29	*Operculatol A*	33.65
30	*Ursolic acid*	33.57
31	*Cleistocalyxolide B*	33.57
32	*Cleistocalyxic acid C*	33.40
33	*Oleanolic acid*	33.32
34	*Arjunolic acid*	33.32
35	*Cleistocalyxic acid D*	33.22
36	*Cleistocalyxic acid J*	33.11
37	*Cleistocalyxic acid I*	33.11
38	*Betulinic acid*	33.07
39	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	33.05
40	*Asiatic acid*	32.99
41	*Cirsimarin*	32.92

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
42	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	32.86
43	*Viridiflorol*	32.69
44	*Guaiol*	32.32
45	*Globulol*	32.30
46	*(E)-Nerolidol*	32.06
47	*(3Z)-Octenyl acetate*	31.80
48	*(3E)-Octenyl acetate*	31.80
49	*Caryophylla-4(12),8(13)-dien-5β-ol*	31.65
50	*Geranyl acetate*	23.34

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 12
Hasil Skrining Farmakofor Ligan Uji Terhadap Reseptor HER2

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*Luteolin*	55.21
2	*4-Hydroxybenzoic acid*	54.00
3	*(2S)-8-Formyl-6-methylnaringenin*	50.88
4	*Cleistocalyxic acid C*	49.97
5	*Cleistocalyxic acid E*	49.49
6	*Cleistocalyxic acid G*	49.24
7	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	46.55
8	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	46.47
9	*(2S)-8-methylpinocembrin*	45.77
10	*Tamarixetin*	45.70
11	*Cinnamic acid*	45.45
12	*Asiatic acid*	44.79
13	*Pentadienoic acid*	44.65
14	*2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid*	44.51
15	*Arjunolic acid*	44.43
16	*Cleistocalyxic acid A*	44.29
17	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	43.56
18	*Selina-6-en-4β-ol*	42.90
19	*β-Sitosterol*	42.75
20	*Cleistocalyxic acid H*	42.71

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 12
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
21	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	42.66
22	*Maslinic acid*	42.49
23	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	42.33
24	*Cleistocalyxic acid K*	42.00
25	*Actinidic acid*	42.00
26	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	40.95
27	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	36.74
28	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	36.44
29	*Kaempferol*	36.20
30	*Quercetin*	36.09
31	*Ursolic acid*	35.86
32	*Oleanolic acid*	35.81
33	*4'-Dihydrophaseic acid*	35.78
34	*Methyl 3,4,5-trihydroxybenzoate*	35.52
35	*4-Hydroxy-3,5-dimethoxybenzoic acid*	35.50
36	*Myricetin-3'-methylether*	35.47
37	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	35.31
38	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	35.28

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 12
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
39	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	35.28
40	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	34.44
41	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	34.43
42	*Cleistocalyxolide B*	34.40
43	*3-Hydroxy-3-phenylpropanoic acid*	34.40
44	*τ-Cadinol*	34.27
45	*Spathulenol*	34.27
46	*α-Cadinol*	34.27
47	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	34.27
48	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	34.26
49	*τ-Muurolol*	34.25
50	*Viridiflorol*	34.23
51	*α-Muurolol (= δ-Cadinol)*	34.23
52	*Rosefuran epoxide*	34.21
53	*cis-Cadin-4-en-7-ol*	34.20
54	*Caryophylla-4(12),8(13)-dien-5β-ol*	34.18
55	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	34.16
56	*Guaiol*	34.14
57	*Globulol*	34.12

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 12
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
58	*α-Terpineol*	34.08
59	*p-Mentha-1,5-dien-8-ol*	34.06
60	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	34.05
61	*Selina-3,11-dien-6α-ol*	34.04
62	*Selin-11-en-4α-ol*	34.04
63	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	34.04
64	*Linalool*	34.03
65	*(E)-Nerolidol*	34.01
66	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	33.92
67	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	33.63
68	*Cleistocalyxic acid I*	33.38
58	*α-Terpineol*	34.08
59	*p-Mentha-1,5-dien-8-ol*	34.06
60	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	34.05
61	*Selina-3,11-dien-6α-ol*	34.04
62	*Selin-11-en-4α-ol*	34.04
63	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	34.04
64	*Linalool*	34.03
65	*(E)-Nerolidol*	34.01

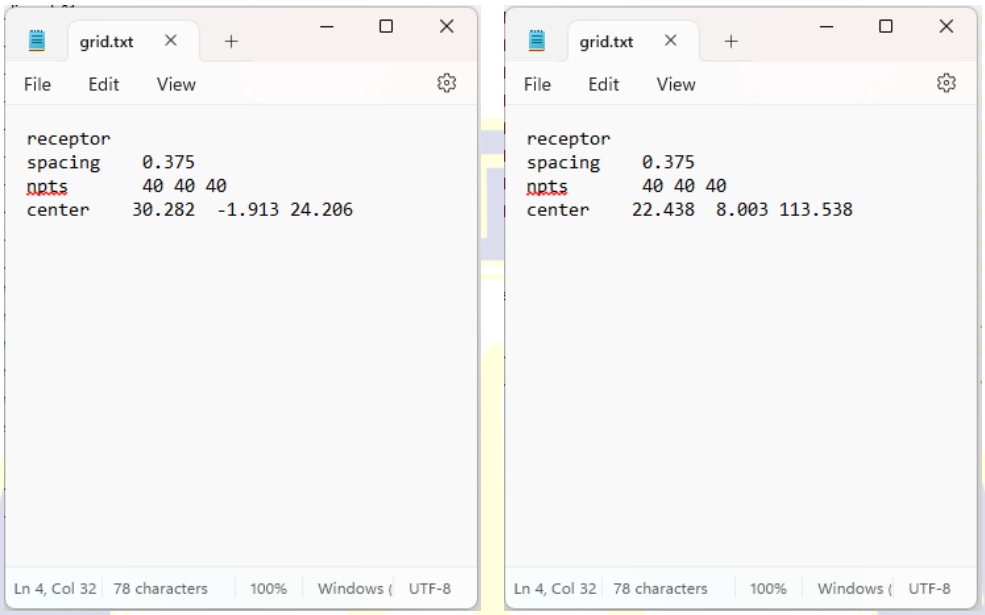
LAMPIRAN 10
(LANJUTAN)

Tabel VII. 12
Lanjutan

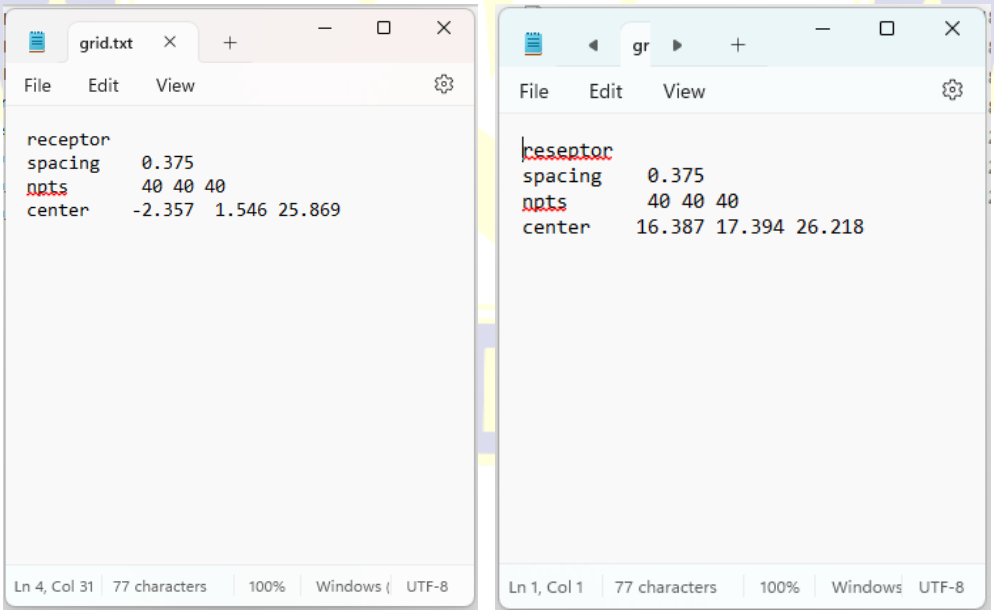
No.	Ligan Uji	*Pharmacophore-Fit Score*
66	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	33.92
67	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	33.63
68	*Cleistocalyxic acid I*	33.38

LAMPIRAN 11

GRID-BOX VALIDASI *DOCKING*



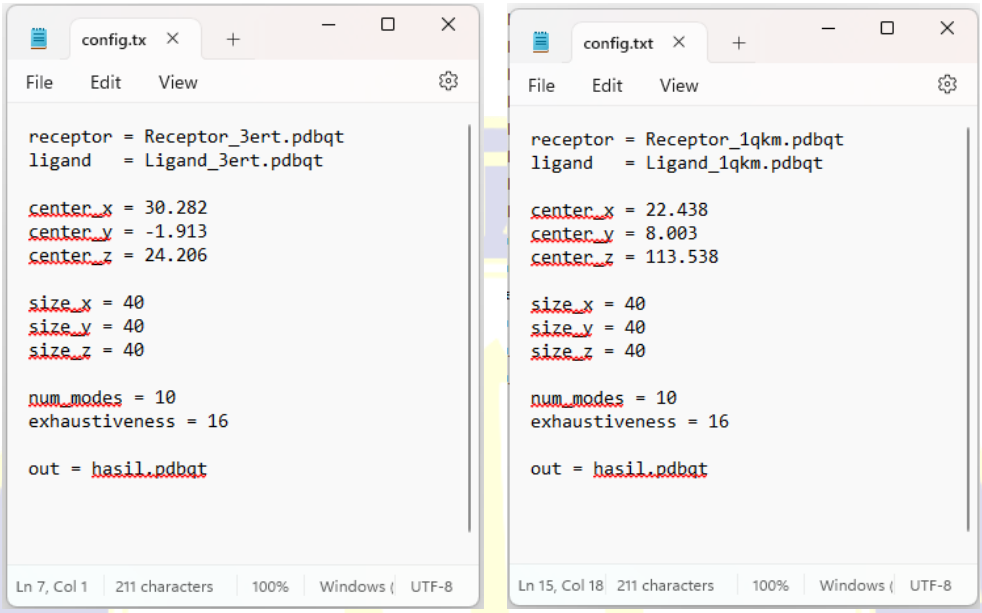
Gambar VII. 24 *Grid-box* validasi ER-α dan ER-β



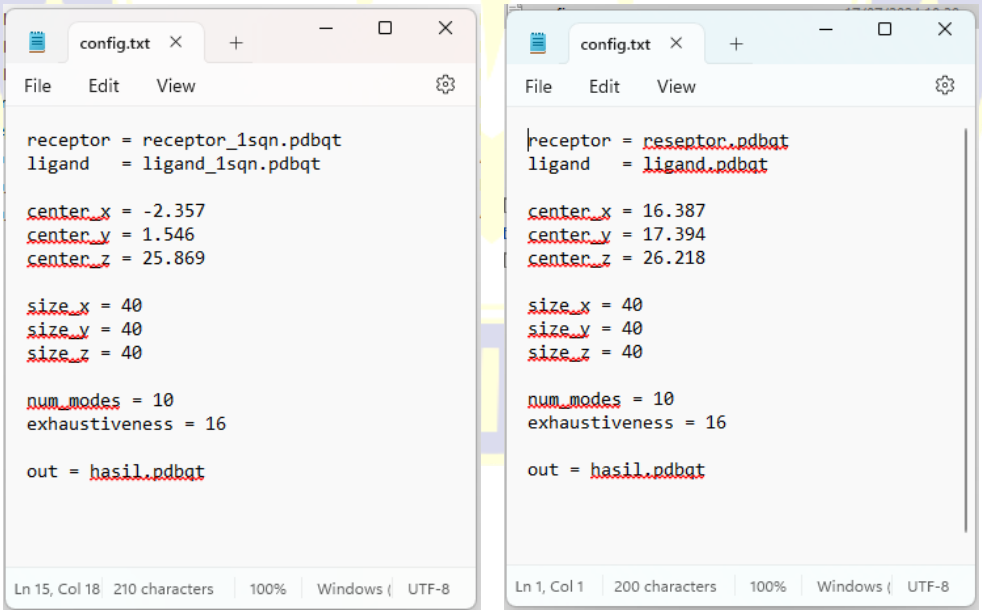
Gambar VII. 25 *Grid-box* validasi Progesteron dan HER2

LAMPIRAN 12

CONFIG DOCKING



Gambar VII. 26 *Config* validasi ER-α dan ER-β



Gambar VII. 27 *Config* validasi Progesteron dan HER2

LAMPIRAN 13

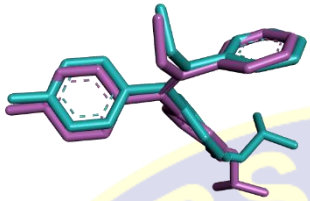
HASIL VALIDASI *DOCKING*

Tabel VII. 13
Hasil Validasi *Docking*

PDB ID	Grid Center			Grid Box			RMSD	Keterangan
	X	Y	Z	X	Y	Z		
3ERT	30.282	-1.913	24.206	40	40	40	1.1066 Å	Valid
1QKM	22.438	8.003	113.538	40	40	40	0.2887 Å	
1SQN	-2.357	1.546	25.869	40	40	40	0.3845 Å	
3PP0	16.387	17.394	26.218	40	40	40	0.5775 Å	

LAMPIRAN 14

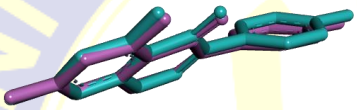
VISUALISASI TUMPANG TINDIH HASIL VALIDASI *DOCKING*



Redocking : pink (#ffaaff)

Hasil validasi : Hijau tosca (#55ffff

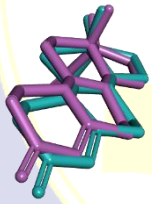
Gambar VII. 28 Visualisasi tumpang tindih validasi *docking* ER-α



Redocking : pink (#ffaaff)

Hasil validasi : Hijau tosca (#55ffff

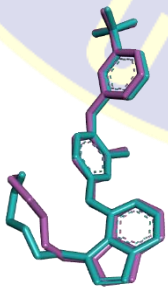
Gambar VII. 29 Visualisasi tumpang tindih validasi *docking* ER-β



Redocking : pink (#ffaaff)

Hasil validasi : Hijau tosca (#55ffff

Gambar VII. 30 Visualisasi tumpang tindih validasi *docking* Progesteron



Redocking : pink (#ffaaff)

Hasil validasi : Hijau tosca (#55ffff

Gambar VII. 31 Visualisasi tumpang tindih validasi *docking* HER2

LAMPIRAN 15

HASIL SIMULASI *MOLECULAR DOCKING*

Tabel VII. 14
Hasil *Molecular Docking* ER-α dan Analisis Residu Asam Amino

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
1	*3-O-cis-p-Coumaroyl_maslinic_acid*	-10,7	-	ALA 350, LEU 525	
2	*3-beta-O-(trans-p-Coumaroyl)maslinic_acid*	-10,7	LEU 536	LEU 525, LEU 346, ALA 350	
3	*Cleistocalyxolide B*	-10,4	-	-	TRP 383 (Pi-Sigma)
4	*(2beta,3alpha)-2,3-Dihydroxy-urs-12-en-28-oic acid*	-10,4	-	-	
5	*Corosolic acid*	-10,3	VAL 533	-	
6	*Cleistocalyxic acid I*	-10,2	VAL 534	-	
7	*Ursolic acid*	-10,1	-	-	
8	*Maslinic acid*	-10	-	-	TRP 383 (Pi-Sigma)
9	*Cleistocalyxic acid K*	-10	LEU 536	-	
10	*11alpha-Hydroxyasiatic acid*	-10	VAL 533, VAL 534	-	
11	*Operculatol A*	-10	-	LEU 525	THR 347 (Carbon Hidrogen Bond), TRP 383 (Pi-Donor Hidrogen Bond), TRP 383 (Pi-Pi Stacked)
12	*Cleistoperlone A*	-10	MET 522, LEU 536	TYR 526, LYS 529	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
13	*Cleistocalyxic acid C*	-9,9	-	-	TYR 526 (van der Waals)
14	*Ligan Alami 4 OHT (Pembanding)*	-9,8	ARG 394, GLU 353	LEU 387, LEU 391, LEU 346, MET 421, ALA 350, LEU 525, MET 388	
15	*Oleanolic acid*	-9,8	-	-	TRP 383 (Pi-Sigma)
16	*Asiatic acid*	-9,7	VAL 533	-	TRP 383 (Pi-Sigma)
17	*Cleistocalyxic acid J*	-9,7	-	-	
18	*Alphitolic acid*	-9,6	CYS 530	LEU 536	
19	*Cleistocalyxic acid G*	-9,5	-	-	
20	*Arjunolic acid*	-9,4	ASP 351	-	
21	*Actinidic acid*	-9,4	ASP 351	-	ASP 351 (Carbon Hidrogen Bond)
22	*Cleistocalyxic acid E*	-9,4	LEU 536, VAL 534	-	TRP 383 (Pi-Sigma)
23	*Betulinic acid*	-9,3	CYS 530	LEU 536	
24	*Cleistocalyxic acid A*	-9,2	TRP 383	TYR 526	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
25	*Cleistocalyxic acid D*	-9,1	-	-	TRP 383 (Pi-Sigma), LYS 529 (Carbon Hidrogen Bond)
26	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	-9,1	-	LEU 536, LEU 539, LEU 525, ALA 350	TRP 383 (Pi-Pi Stacked), ASP 351 (Pi-Anion), THR 347 (Carbon Hidrogen Bond)
27	*Cleistocalyxic acid B*	-9	-	-	TYR 526 (Carbon Hidrogen Bond), GLU 380 (Carbon Hidrogen Bond)
28	*Cleistocalyxic acid H*	-8,9	TRP 383	-	
29	*Quercetin*	-8,9	ARG 394, GLU 353, LEU 387	LEU 391, MET 388, LEU 384, ALA 350	MET 343 (Pi-Sulfur), LEU 525 (Pi-Sigma), THR 347 (van der Waals), LEU 346 (Amide-Pi Stacked)
30	*Kaempferol*	-8,8	ARG 394, GLU 353, LEU 387	LEU 391, MET 388, ALA 350, LEU 387, LEU 525, LEU 384	LEU 384 (Pi-Sigma), LEU 525 (Pi-Sigma), THR 347 (van der Waals), LEU 346 (Amide-Pi Stacked), MET 343 (Pi-Sulfur)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
31	*Cleistocalyxic acid F*	-8,8	-	-	GLU 380 (Carbon Hidrogen Bond)
32	*Tamarixetin*	-8,7	ARG 394, GLU 353, LEU 387	LEU 391, LEU 387, LEU 384, LEU 525, ALA 350	LEU 525 (Pi-Sigma), THR 347 (van der Waals), LEU 346 (Amide-Pi Stacked), MET 343 (Pi-Sulfur)
33	*Viridiflorol*	-8,7	-	ALA 350, LEU 525, TRP 383, LEU 384, LEU 346	
34	*Luteolin*	-8,6	LEU 387, GLU 353, ARG 394	ALA 350, LEU 384, LEU 391, LEU 387	LEU 346 (Amide-Pi Stacked), LEU 525 (Pi-Sigma), THR 347 (van der Waals), MET 343 (Pi-Sulfur)
35	*Myricetin 3-galactoside*	-8,6	MET 522, THR 347, ASP 351	MET 522, LEU 525	LEU 525 (Pi-Sigma)
36	*4'-Dihydrophaseic acid*	-8,6	-	-	
37	*(2S,3S)-3,5,7-trihydroxy-6,8-dimethylflavanone*	-8,6	-	ALA 350, LEU 346	LEU 346 (Amide-Pi Stacked), LEU 525 (Pi-Sigma), THR 347 (van der Waals), MET 343 (Pi-Sulfur)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
38	*Annulatin*	-8,5	ARG 394, GLU 353, MET 343, THR 347	LEU 387, LEU 391, ALA 350	LEU 384 (Pi-Sigma), LEU 525 (Pi-Sigma), MET 343 (Pi-Sulfur)
39	*Caryophylla-4(12),8(13)-dien-5β-ol*	-8,4	-	LEU 347	
40	*Globulol*	-8,3	-	LEU 384, ALA 350, PHE 404, LEU 346	
41	*Limocitrin 3-rutinoside-7-glucoside*	-8,2	CYS 530, LEU 525	MET 522, LEU 354, LEU 536	TRP 383 (Pi-Sigma), LEU 536 (Pi-Sigma)
42	*(S)-2,3-Dihydro-5,7-dihydroxy-8-methyl-2-phenyl-4-benzopyrone*	-8,2	ARG 394	ALA 350, LEU 391	LEU 525 (Pi-Sigma), THR 347 (van der Waals), LEU 346 (Amide-Pi Stacked), MET 343 (Pi-Sulfur)
43	*Lethedoside A*	-8,1	CYS 530, MET 528	LEU 354, LEU 536, ALA 350, LEU 387, LEU 525, LEU 346, MET 421	TRP 383 (Pi-Sigma), ASP 351 (Pi-Anion), THR 347 (van der Waals), MET 343 (Pi-Sulfur), LEU 346 (Amide-Pi Stacked)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
44	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	-8,1	-	VAL 533, LEU 536, ALA 350, LEU 354	TRP 383 (Pi-Pi Stacked)
45	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	-8	-	ALA 350, LEU 525, LEU 346	MET 343 (Pi-Sulfur)
46	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	-8	-	LEU 525, ALA 350, MET 421, ILE 424, LEU 428, MET 388, LEU 346	MET 343 (Pi-Sulfur)
47	*Guaiol*	-8	GLU 353	LEU 346, LEU 525, MET 343	
48	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-7,9	LEU 346	ALA 350, LEU 346	ASP 351 (Pi-Anion), TRP 383 (Pi-Pi Stacked), LEU 384 (Pi-Sigma)
49	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-7,9	LEU 346	LEU 525, ALA 350, LEU 346, LEU 384	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
50	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	-7,9	-	VAL 533, ALA 350, LEU 536, LEU 354	TRP 383 (Pi-Pi Stacked)
51	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	-7,9	-	ALA 350, LEU 536, LEU 354, VAL 533	TRP 383 (Pi-Pi Stacked)
52	*Demethoxymatteucinol*	-7,9	VAL 534	VAL 533, LEU 536, ALA 350, LEU 354	TRP 383 (Pi-Pi Stacked), PRO 535 (Carbon Hidrogen Bond)
53	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	-7,9	-	LEU 354, ALA 351	ASP 351 (Pi-Anion), TRP 383 (Pi-Pi Stacked)
54	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	-7,8	ARG 394	MET 388, LEU 387, ALA 350	LEU 346 (Carbon Hidrogen Bond), MET 388 (Carbon Hidrogen Bond), LEU 387 (Carbon Hidrogen Bond), MET 343 (Pi-Sulfur), LEU 525 (Pi-Sigma)
55	*(2S)-8-Formyl-6-methylnaringenin*	-7,8	LEU 525, TRP 383, ALA 350	LEU 536, LEU 354, ALA 350	TRP 383 (Pi-Pi Stacked)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
56	*Cirsimarin*	-7,8	LEU 525, TRP 383, ALA 350	LEU 536, LEU 354, ALA 350	TRP 383 (Pi-Pi Stacked)
57	*(E)-Nerolidol*	-7,8	-	LEU 391, PHE 404, LEU 349, LEU 346, ALA 350	
58	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	-7,8	ARG 394	MET 388, LEU 387, ALA 350	LEU 346 (Carbon Hidrogen Bond), MET 388 (Carbon Hidrogen Bond), LEU 387 (Carbon Hidrogen Bond), MET 343 (Pi-Sulfur), LEU 525 (Pi-Sigma)
59	*Stercurensin*	-7,7	-	ALA 350, LEU 525, LEU 384	
60	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	-7,7	-	MET 388, LEU 387, ALA 350, LEU 346, LEU 391	
61	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	-7,7	-	LEU 354, ALA 350, LEU 536	TRP 383 (Pi-Pi Stacked)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 14
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
62	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	-6,8	VAL 534, CYS 530, MET 522	-	
63	*p-Mentha-1,5-dien-8-ol*	-6,3	GLU 323, LYS 449	PRO 324, MET 357, LEU 387	
64	*3-Hydroxy-3-phenylpropanoic acid*	-6,3	ARG 394, GLU 353, LYS 449	MET 357, PRO 324	GLY 390 (Carbon Hidrogen Bond), TRP 393 (Carbon Hidrogen Bond)
65	*α-Terpineol*	-6,1	ARG 395	LEU 346, ALA 350, LEU 384, LEU 525	
66	*4-Hydroxybenzoic acid*	-5,7	GLU 353, ARG 394, LYS 449	PRO 324	GLU 353 (Pi-Anion)
67	*Linalool*	-5,5	LEU 387, GLU 353, ARG 394	LEU 387, LEU 384, ILE 424, LEU 391, MET 388, MET 421	
68	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-	-	-	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 15
Hasil *Molecular Docking* ER-β dan Analisis Residu Asam Amino

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
1	*Ligan Alami Genistein (Pembanding)*	-10,4	ARG 346, GLU 305, LEU 339, HIS 475	LEU 476, LEU 298, LEU 343, ALA 302, LEU 339	PHE 356 (Pi-Pi T-shaped), MET 336 (Pi-Sigma), PHE 356 (Pi-Sulfur)
2	*Luteolin*	-9,2	ARG 346, GLU 305, LEU 339,	LEU 343, LEU 339, ALA 302, LEU 298, LEU 476	PHE 356 (Pi-Pi T-shaped), MET 336 (Pi-Sigma), MET 336 (Pi-Sulfur), GLY 472 (Carbon Hidrogen Bond), HIS 475 (Pi-Donor Hidrogen Bond)
3	*3-beta-O-(trans-p-Coumaroyl)maslinic_acid*	-9,2	GLU 305, HIS 279	-	PRO 277 (Pi-Sigma), ARG 346 (Pi-Cation), GLU 305 (Pi-Donor Hidrogen Bond)
4	*(2S)-8-Formyl-6-methylnaringenin*	-9,1	ARG 346	LEU 339, LEU 343, ALA 302, LEU 298, LEU 476	PHE 356 (Pi-Pi T-shaped), MET 336 (Pi-Sigma), THR 299 (Carbon Hidrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
5	*Quercetin*	-9,1	TRP 345, VAL 280, GLU 305	ARG 346, PRO 277,	ARG 346 (Pi-Cation), GLU 305 (Pi-Anion), HIS 279 (Pi-Sigma), HIS 279 (Pi-Pi T-shaped), HIS 279 (Carbon Hidrogen Bond)
6	*3-O-cis-p-Coumaroyl_maslinic_acid*	-9	HIS 279, LYS 401, TYR 397	-	ARG 346 (Pi-Cation), PRO 277 (Pi-Sigma), GLY 342 (Carbon Hidrogen Bond)
7	*Kaempferol*	-8,9	ARG 346, GLU 305, LEU 339, LEU 298	LEU 298, LEU 339, ALA 302, LEU 343	MET 336 (Pi-Sigma), PHE 356 (Pi-Pi T-shaped), PHE 356 (Pi-Sulfur)
8	*Tamarixetin*	-7,9	GLU 305, VAL 280, HIS 279, TRP 345	LEU 273, PRO 277	ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped), HIS 279 (Carbon Hidrogen Bond), HIS 279 (Pi-Donor Hidrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
9	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	-7,5	ARG 346, GLU 305, LYS 401, HIS 279	PRO 277	ARG 346 (Pi-Sigma), ARG 346 (Pi-Cation), HIS 279 (Pi-Pi T-shaped), GLY 342 (Pi-Donor Hidrogen Bond), GLY 342 (Carbon Hidrogen Bond)
10	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-	-	-	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Hasil *Molecular Docking* Progesteron dan Analisis Residu Asam Amino

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
1	*Ligan Alami Norethindrone (Pembanding)*	-12	ARG 766	MET 759, LEU 718, LEU 715, PHE 794, LEU 797, TYR 890	
2	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	-11,1	GLN 815, TRP 765, GLU 695, ILE 699, ARG 766, LYS 822	VAL 698, ARG 766	GLY 762 (Carbon Hydrogen Bond), VAL 698 (Carbon Hydrogen Bond)
3	*Quercetin*	-9,9	ASN 719, MET 756, GLN 725, ARG 766	CYS 891, LEU 718, LEU 763, MET 759	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-shaped)
4	*Luteolin*	-9,8	ASN 719, MET 756, GLN 725, ARG 766	CYS 891, LEU 718, LEU 763, MET 759	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-shaped)
5	*Kaempferol*	-9,3	MET 756, MET 759, GLN 725, ARG 766	LEU 718, LEU 763, MET 759	PHE 778 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
6	*Lethedoside A*	-9,3	ARG 766, MET 759, GLN 725, LEU 758, LYS 822, VAL 729, ILE 699, GLN 815	PRO 780, VAL 698, ALA 779, ILE 699, PRO 696, MET 692	LEU 758 PHE 778 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), TRP 765 (Pi-Pi T-shaped), ARG 766 (Pi-Sigma)
7	*4'-Dihydrophaseic acid*	-9,2	HIS 770, TRP 765, GLN 815, LYS 822, GLN 725, MET 759, ARG 766	PRO 696, ILE 699	TRP 765, LYS 769 (Carbon Hydrogen Bond)
8	*(2S)-8-Formyl-6-methylnaringenin*	-9,2	MET 759, ARG 766, GLN 725	LEU 763, LEU 718	MET 801 CYS 891 (Pi-Sulfur), PHE 778 (Pi-Pi T-shaped), MET 759 (Pi-Sigma)
9	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	-9,2	-	LEU 763, MET 759, LEU 718	ASN 719 (Carbon Hydrogen Bond), PHE 778 (Pi-Pi T-shaped)
10	*Cirsimarin*	-9,2	LYS 822, GLN 725, ARG 766, LEU 758, TRP 765	PRO 696, ARG 766, HIS 770, VAL 698	LEU 758 GLY 762 LYS 769 (Carbon Hydrogen Bond), ARG 766 HIS 770 (Pi-Cation), TRP 765 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
11	*Ursolic acid*	-8,8	TYR 700	-	ARG 724 (Carbon Hydrogen Bond)
12	*Actinidic acid*	-8,7	SER 728, LYS 731, TYR 700, ARG 724	-	
13	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-8,6	-	LEU 763, MET 759, LEU 721	CYS 891 MET 756 (Pi-Sulfur), PHE 778 (Pi-Pi T-shaped)
14	*Annulatin*	-8,6	LYS 822, LEU 758	PRO 696, ARG 766	ARG 766, PRO 696 (Pi-Cation)
15	*Corosolic acid*	-8,5	SER 728, ARG 724, TYR 700	-	
16	*Maslinic acid*	-8,5	SER 728	-	ARG 724 (Carbon Hydrogen Bond)
17	*11alpha-Hydroxyasiatic acid*	-8,5	SER 728, LYS 731, ARG 724	-	ARG 724 (Carbon Hydrogen Bond)
18	*Myricetin 3-galactoside*	-8,5	ILE 699, HIS 770, TRP 765, GLN 815, MET 692	ILE 699, ARG 766, PRO 696	ARG 766 (Carbon Hydrogen Bond), ARG 766 (PI-Cation), GLU 695 (Pi-Anion)
19	*Operculatol A*	-8,5	GLU 695, ARG 766	PRO 696, ARG 766	TRP 765 (Carbon Hydrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
20	*Oleanolic acid*	-8,5	ARG 724	-	
21	*Cleistocalyxic acid I*	-8,5	SER 728, LYS 731, ARG 724	-	
22	*Tamarixetin*	-8,4	LYS 822, LEU 758, TRP 765	PRO 696, ARG 766, MET 692	ARG 766 (PI-Cation), GLU 695 (Pi-Anion)
23	*Cleistocalyxic acid E*	-8,3	LYS 731, ARG 724	-	SER 728 (Carbon Hydrogen Bond)
24	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	-8,2	MET 801	MET 759, CYS 891, LEU 715	LEU 718 (Carbon Hydrogen Bond), PHE 778 TYR 890 (PI-Pi T-shaped)
25	*Cleistocalyxolide B*	-8,2	ASP 704, ASN 705, GLN 720	-	
26	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	-8,1	HIS 770, GLN 815, TRP 765, GLU 695, PRO 696	PRO 696	ARG 766 (Pi-Cation)
27	*Asiatic acid*	-8,1	SER 728, LYS 731, TYR 700	ARG 724	ILE 699 (Carbon Hydrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
28	*(2beta,3alpha)-2,3-Dihydroxy-urs-12-en-28-oic acid*	-8	LYS 822, LEU 758, GLN 725, ARG 766, GLN 815, MET 692	-	HIS 770 (Pi-Sigma)
29	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	-8	ARG 766, GLN 725	LEU 718, PHE 778, LEU 797, LEU 887, TYR 890, CYS 891	MET 759 (Carbon Hydrogen Bond)
30	*Cleistocalyxic acid H*	-7,9	LYS 731, ARG 724	-	
31	*Cleistocalyxic acid K*	-7,9	ASP 704, ASN 705, ASP 709	-	
32	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	-7,9	ILE 699, TRP 765, HIS 770	PRO 696, ILE 699	ARG 766 (Pi-Cation), HIS 770 (Pi-Sigma)
33	*Viridiflorol*	-7,9	-	LEU 718, MET 759, PHE 778, LEU 721	
34	*Guaiol*	-7,8	-	LEU 718, MET 759, LEU 721	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
35	*(E)-Nerolidol*	-7,8	ASN 719, LEU 718	MET 801, PHE 778, PHE 794, LEU 797, LEU 718, CYS 891	
36	*Caryophylla-4(12),8(13)-dien-5β-ol*	-7,8	-	LEU 718	
37	*Globulol*	-7,7	ARG 766	PRO 696	
38	*Cleistocalyxic acid G*	-7,5	LYS 790, ASN 705	-	ASP 709, HIS 703 (Carbon Hydrogen Bond)
39	*Cleistocalyxic acid C*	-7,5	-	-	GLY 762 (Carbon Hydrogen Bond)
40	*Cleistocalyxic acid J*	-7,4	LYS 790, ASN 705	-	ILE 783, LYS 790, GLN 787 (Carbon Hydrogen Bond)
41	*Betulinic acid*	-7,4	GLN 725, TRP 765, HIS 770	VAL 698	ARG 766 (Unfavorable Bump)
42	*Cleistocalyxic acid A*	-7,3	PRO 708	-	SER 717 (Unfavorable Acceptor-Acceptor)
43	*Cleistocalyxic acid B*	-7,3	PRO 708, SER 713, SER 717	-	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 16
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
44	*Arjunolic acid*	-7,3	ARG 899, SER 910	-	
45	*Cleistocalyxic acid D*	-7,3	ASN 705, ASN 785	-	ASN 705, LYS 790 (Carbon Hydrogen Bond)
46	*Cleistocalyxic acid F*	-7,2	GLN 720	-	
47	*Alphitolic_acid*	-7	THR 800, ASN 893	-	LEU 797 (Carbon Hydrogen Bond), TYR 890 (Pi-Sigma)
48	*(3E)-Octenyl acetate*	-5,7	GLN 725, ARG 766	LEU 718, LEU 715, PHE 778	
49	*(3Z)-Octenyl acetate*	-5,5	ARG 766, GLN 725	LEU 718, PHE 794, LEU 797, MET 801, PHE 778	
50	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-	-	-	-
51	*Geranyl acetate*	-6,3	ARG 766	MET 759, LEU 721, LEU 718, MET 756, LEU 797, MET 801, LEU 887	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Hasil *Molecular Docking* HER2 dan Analisis Residu Asam Amino

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
1	Ligan Alami	-11,4	ASP 863, MET 801, ASN 850	LYS 753, ALA 751, LEU 785, LEU 796, VAL 734, MET 774, PHE 864	GLN 799 SER 728 (Carbon Hidrogen Bond), LEU 852 LEU 726 (Pi-Sigma), PHE 864 (Pi-Pi T-shaped), GLU 770 Halogen (Fluorine)
2	3-O-Methylellagic acid-4′-O-α-L-rhamnopyranoside	-10,4	ASP 863, CYS 805, SER 728	LEU 726, LEU 852, ALA 751, VAL 734, LYS 753	GLY 729 (Carbon Hidrogen Bond), VAL 734 LEU 852 (Pi-Sigma)
3	7-Hydroxy-5-methoxy-6,8-dimethylisoflavone	-10,3	-	LYS 753, LEU 796, VAL 734	VAL 734 LEU 852 (Pi-Sigma)
4	Luteolin	-10,1	-	VAL 734, ALA 751, LEU 852, LYS 753, LEU 796	VAL 734 LEU 852 (Pi-Sigma), GLY 729 (Carbon Hydrogen Bond)
5	(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside	-10,1	ASP 863, LEU 796, SER 728, SER 783	LEU 852, VAL 734, ALA 751, LEU 726, LYS 753	THR 862 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
6	Tamarixetin	-10,1	ASP 863, MET 801, ALA 751, LYS 753, LEU 796	LEU 852, VAL 734, LEU 726, ALA 751, LEU 785, LEU 796	GLY 804 GLY 729 (Carbon Hydrogen Bond), LEU 852 VAL 734 (Pi-Sigma)
7	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-10,1	ASP 863, THR 862	LEU 796, LYS 753, LEU 726	ARG 849 (Carbon Hydrogen Bond), THR 798 VAL 734 LEU 852 (Pi-Sigma)
8	*(2S)-8-Formyl-6-methylnaringenin*	-9,9	LEU 726	ALA 751, LYS 753, VAL 734	GLY 804 (Carbon Hydrogen Bond), LEU 726 (Pi-Sigma)
9	*Quercetin*	-9,9	ASP 863, MET 801	VAL 734, ALA 751, LEU 726, LYS 753, LEU 852	GLY 804 (Carbon Hydrogen Bond), LEU 852 VAL 734 THR 798 (Pi-Sigma)
10	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	-9,7	LEU 726, MET 801	ALA 751, LYS 753, CYS 805, LEU 852, LEU 726	GLY 804 (Carbon Hydrogen Bond), VAL 734 (Pi-Sigma)
11	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	-9,7	CYS 805	LYS 753, VAL 734, ALA 751	GLY 804 (Carbon Hydrogen Bond), LEU 726 LEU 852 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
12	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	-9,6	-	ALA 751, LYS 753, VAL 734, LEU 852	GLY 804 ASP 808 (Carbon Hydrogen Bond)
13	*(2S)-8-methylpinocembrin*	-9,5	MET 801, LEU 726	LYS 753, LEU 852, ALA 751	VAL 734 LEU 726 (Pi-Sigma)
14	*Ursolic acid*	-9,5	PHE 731, LYS 887, ILE 886	-	
15	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	-9,5	CYS 805	ALA 751, LYS 753, LEU 852, LEU 726, VAL 734	GLY 804 GLY 727 (Carbon Hydrogen Bond)
16	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-9,5	-	LYS 753, LEU 726, LEU 796	ARG 849 (Carbon Hydrogen Bond), LEU 852 VAL 734 (Pi-Sigma)
17	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	-9,4	-	LYS 753, VAL 734, LEU 852, LEU 726	GLY 729 SER 728 (Carbon Hydrogen Bond), VAL 734 LEU 852 (Pi-Sigma)
18	*Kaempferol*	-9,4	ASP 863	VAL 734, ALA 751, LEU 726, LYS 753	GLY 804 (Carbon Hydrogen Bond), LEU 852 VAL 734 THR 798 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
19	*Myricetin-3'-methylether*	-9,4	ASP 863, MET 801, ALA 751, LYS 753, LEU 796	ALA 751, LYS 753	ASP 863 (Carbon Hydrogen Bond), LEU 852 LEU 726 VAL 734 THR 798 (Pi-Sigma)
20	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	-9,4	-	LYS 753, ALA 751, VAL 734, LEU 726	ASP 808 GLY 804 (Carbon Hydrogen Bond)
21	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	-9,2	-	LYS 753, VAL 734, ALA 751, CYS 805	GLY 729 (Carbon Hydrogen Bond), LEU 852 (Pi-Sigma)
22	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	-9,2	ASP 863	LEU 796, LEU 726, VAL 734, ALA 751, LYS 753	ARG 849 (Carbon Hydrogen Bond), LEU 852 (Pi-Sigma)
23	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	-9,1	-	LYS 753, VAL 734, LEU 726	SER 728 GLY 729 (Carbon Hydrogen Bond), LEU 852 (Pi-Sigma)
24	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	-9	THR 862	ALA 751, LYS 753	ARG 849, GLY 729 (Carbon Hydrogen Bond), VAL 734 LEU 852 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
25	*Oleanolic acid*	-9	PHE 731, LYS 887, ILE 886	-	
26	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	-8,9	ASP 863	LEU 796, ALA 751, LEU 852, VAL 734, LEU 726	LEU 785 (Pi-Sigma)
27	*Cleistocalyxic acid K*	-8,9	ARG 756, LYS 883, GLY 729, PHE 731, ARG 849, ILE 886, LYS 887	-	ALA 730 (Carbon Hydrogen Bond)
28	*Cleistocalyxic acid G*	-8,8	PHE 731, GLY 729, ARG 849, LYS 887, ILE 886	-	ALA 730 (Carbon Hydrogen Bond)
29	*Maslinic acid*	-8,8	PHE 731, GLY 729, LYS 887	-	
30	*Actinidic acid*	-8,8	PHE 731, LYS 887, ILE 886	-	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
31	*Cleistocalyxic acid E*	-8,7	PHE 731, GLY 729, LYS 887, ILE 886	-	
32	*2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid*	-8,6	ARG 756, PHE 731, GLY 729, ARG 849, LYS 887, ILE 886	-	ALA 730 (Carbon Hydrogen Bond)
33	*Cleistocalyxolide B*	-8,6	PHE 731, GLY 729, LYS 887	-	ALA 730, ARG 849, TRP 888, ALA 928, LYS 921, PRO 922, ILE 886, PRO 885, VAL 884, LYS 883 (van der Waals)
34	*Guaiol*	-8,6	THR 862	VAL 734, LEU 726, LEU 852	
35	*Cleistocalyxic acid C*	-8,5	ARG 811, VAL 884	-	PHE 731 (Pi-Sigma)
36	*α-Cadinol*	-8,5	-	LEU 852, ALA 751, LEU 726, VAL 734, CYS 805	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
37	*Cleistocalyxic acid I*	-8,5	LYS 883, ARG 756, GLY 729, PHE 731, ARG 849, ILE 886, LYS 887	-	ALA 730 (Carbon Hydrogen Bond)
38	*Asiatic acid*	-8,4	ARG 868, GLY 865	-	
39	*Cleistocalyxic acid H*	-8,4	PHE 731, LYS 887	-	
40	*Arjunolic acid*	-8,3	ARG 868, GLY 865	-	
41	*Cleistocalyxic acid A*	-8,2	LYS 887	LYS 883, PHE 731	
42	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	-8	ASP 863	PHE 864, MET 774, LEU 785, LEU 796	
43	*Trastuzumab*	-7,9	ASP 863, ALA 751, LYS 753, THR 862, LEU 796	ALA 751, VAL 734	LYS 753 (Unfavorable Donor-donor), LEU 852 VAL 734 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
44	*τ-Muurolol*	-7,9	-	VAL 734, LEU 852, ALA 751, LEU 800, LYS 753, LEU 726	
45	*α-Muurolol (= δ-Cadinol)*	-7,9	SER 728	LEU 726, VAL 734, LEU 852, LYS 753	
46	*τ-Cadinol*	-7,8	ASN 758	ALA 763, ARG 756, ILE 767, LEU 755, PHE 731	THR 759 (Carbon Hydrogen Bond), PHE 731 (Pi-Sigma)
47	*Globulol*	-7,7	-	ARG 756, ALA 763, PHE 731	
48	*Spathulenol*	-7,6	ARG 868, GLU 766	LEU 755, ALA 763, ARG 756	PHE 731 (Pi-Sigma)
49	*Caryophylla-4(12),8(13)-dien-5β-ol*	-7,5	PHE 731, ARG 756	ALA 763, ARG 756, PHE 731	PHE 731 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
50	*Selin-11-en-4α-ol*	-7,5	-	ARG 756, LEU 755, PHE 731	PHE 731 (Carbon Hydrogen Bond), ALA 763 LEU 866 ARG 868 GLU 766 GLY 865 GLU 770 ILE 767 THR 759 (van der Waals)
51	*Methyl 3,4,5-trihydroxybenzoate*	-7,4	SER 783, THR 862	LEU 785, LEU 796	ILE 767 (Carbon Hydrogen Bond), PHE 864 (Pi-Pi T-shaped)
52	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	-7,2	GLY 865	LYS 762, ALA 763, ARG 756	PHE 731 (Pi-Sigma), PHE 731 (Pi-Pi Stacked)
53	*4'-Dihydrophaseic acid*	-7,2	ARG 756, PHE 731	LEU 866, PHE 731	
54	*Selina-6-en-4β-ol*	-7,1	-	ALA 763, ARG 756, PHE 731	PHE 731 (Pi-Sigma)
55	*Viridiflorol*	-7,1	-	ARG 756, ALA 763, PHE 731	
56	*(E)-Nerolidol*	-7,1	GLU 766, ARG 868	PHE 731, ILE 767, ARG 756, ALA 763	

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
57	*β-Sitosterol*	-7	-	ALA 730, TRP 888, LYS 921, LYS 887	PHE 731 (Pi-Sigma)
58	*Rosefuran epoxide*	-7	ASP 863	LYS 753, VAL 734, PHE 864, LEU 796	ASP 863 (Carbon Hydrogen Bond), LEU 785 (Pi-Sigma)
59	*p-Mentha-1,5-dien-8-ol*	-7	THR 862	LEU 852, VAL 734, LYS 753, ALA 751	
60	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	-6,9	ARG 844, ARG 868, GLY 865, ALA 763, SER 760	ALA 763	LYS 762 (Carbon Hydrogen Bond)
61	*α-Terpineol*	-6,7	THR 862	PHE 864, MET 774, LEU 785, LEU 796, LYS 753	
62	*4-Hydroxybenzoic acid*	-6,6	SER 783, GLU 770	MET 774, LEU 785	PHE 864 (Pi-Pi T-shaped)
63	*Cinnamic acid*	-6,6	MET 801	LYS 753, ALA 751	VAL 734 (Pi-Sigma)

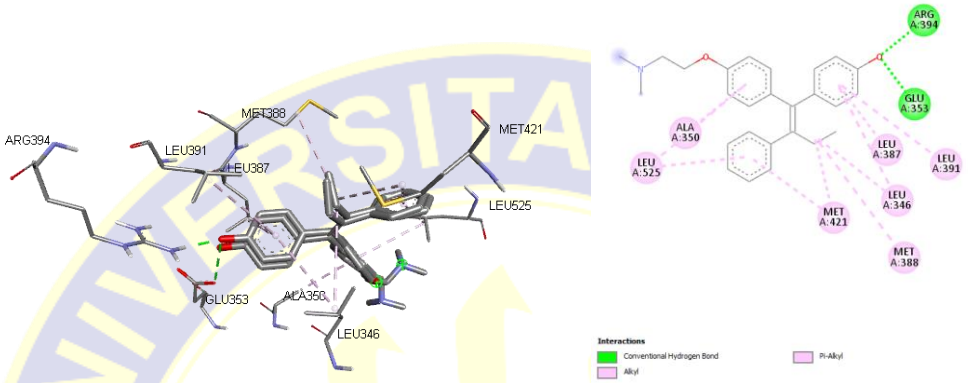
LAMPIRAN 15
(LANJUTAN)

Tabel VII. 17
Lanjutan

No.	Ligan Uji	Δ G (kkal/ mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/ alkyl	
64	*3-Hydroxy-3-phenylpropanoic acid*	-6,6	ASP 863, SER 783	LEU 785, MET 774, LEU 796	PHE 864 (Pi-Pi T-shaped)
65	*Selina-3,11-dien-6α-ol*	-6,6	-	ARG 756, ALA 763, LEU 755, LEU 866	PHE 731 (Pi-Sigma)
66	*4-Hydroxy-3,5-dimethoxybenzoic acid*	-6,5	ASP 863	VAL 734, ALA 751, LEU 726, LEU 852, LEU 800	SER 728 MET 801 (Carbon Hydrogen Bond), VAL 734 LEU 852 (Pi-Sigma)
67	*Linalool*	-6,4	SER 783	MET 774, PHE 864, LEU 785, ALA 771, LEU 796	
68	*cis-Cadin-4-en-7-ol*	-6,3	GLU 766	ARG 756, ALA 763, PHE 731	PHE 731 (Pi-Sigma)
69	*Pentadienoic acid*	-5,4	SER 783, ASP 863	LEU 796, LEU 785, ALA 771	
70	*(E)-4,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	-	-	-	-

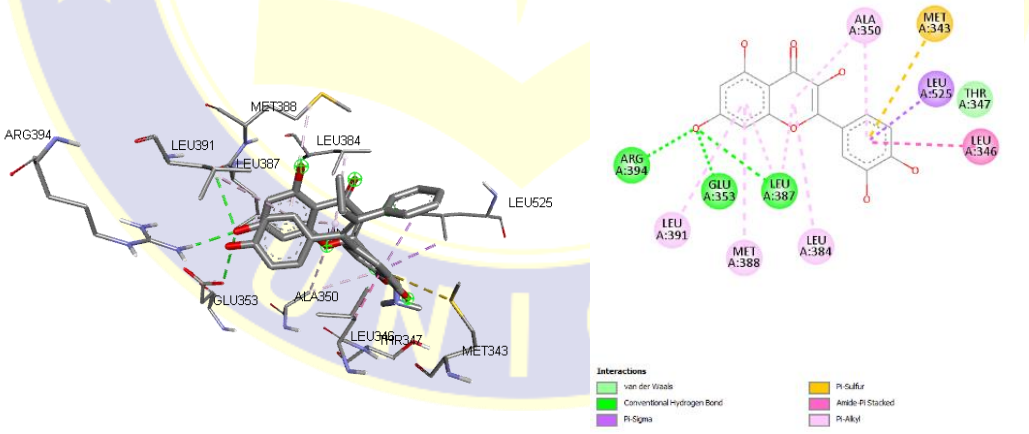
LAMPIRAN 16

VISUALISASI HASIL SIMULASI *MOLECULAR DOCKING* LIGAN ALAMI, LIGAN PEMBANDING DAN SENYAWA TERBAIK



(a) (b)

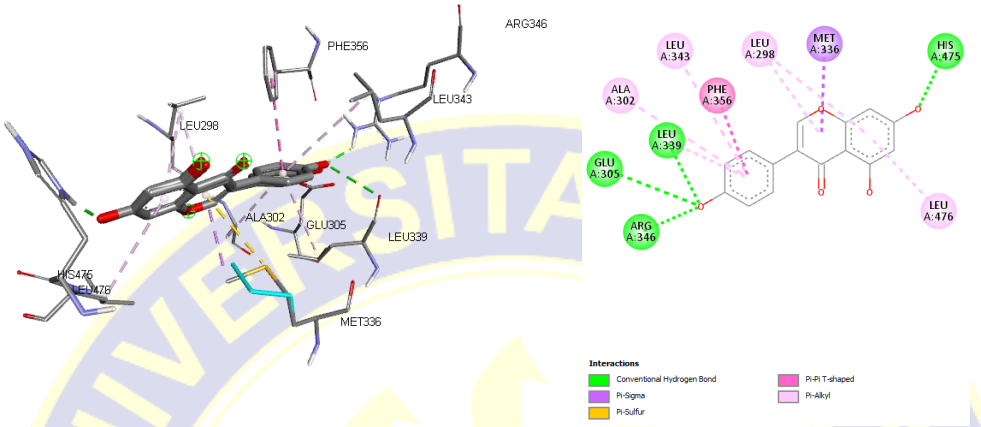
Gambar VII. 32 Visualisasi struktur 3D (a) dan 2D (b) ligan alami 4-Hydroxytamoxifen terhadap ER-α



(a) (b)

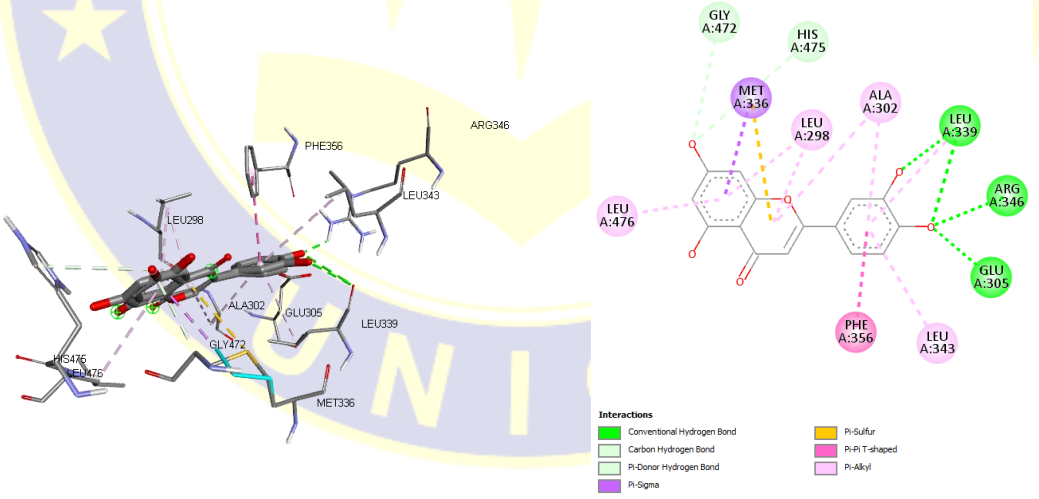
Gambar VII. 33 Visualisasi struktur 3D (a) dan 2D (b) ligan Quercetin terhadap ER-α

LAMPIRAN 16
(LANJUTAN)



(a) (b)

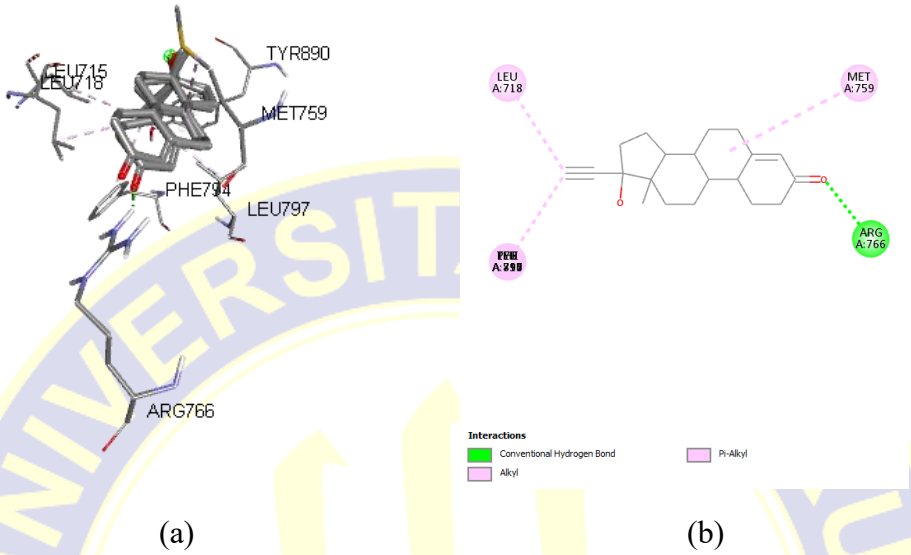
Gambar VII. 34 Visualisasi struktur 3D (a) dan 2D (b) ligan alami Genistein terhadap ER-β



(a) (b)

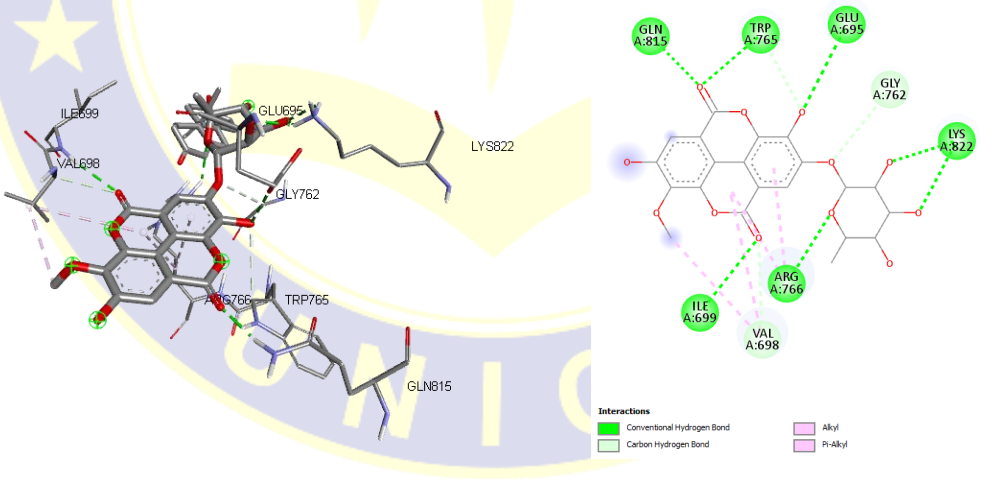
Gambar VII. 35 Visualisasi struktur 3D (a) dan 2D (b) ligan Luteolin terhadap ER- β

LAMPIRAN 16
(LANJUTAN)



(a) (b)

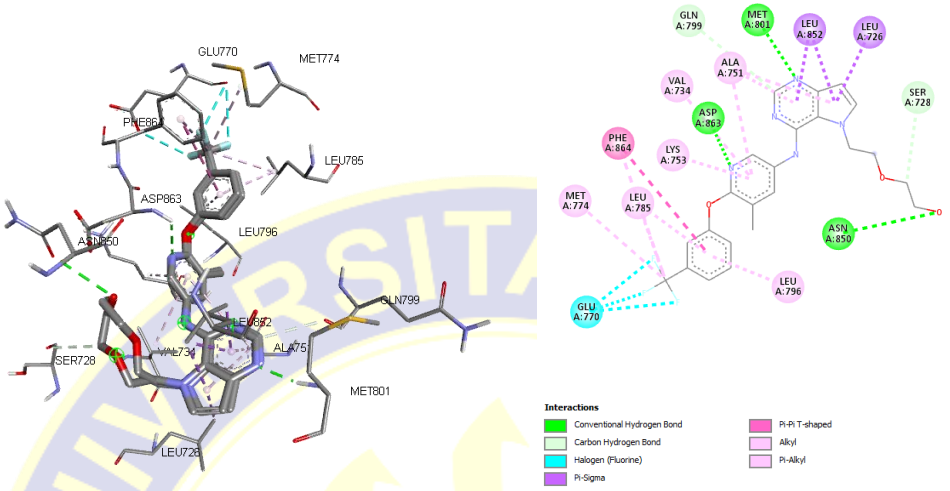
Gambar VII. 36 Visualisasi struktur 3D (a) dan 2D (b) ligan alami Norethindrone terhadap Progesteron



(a) (b)

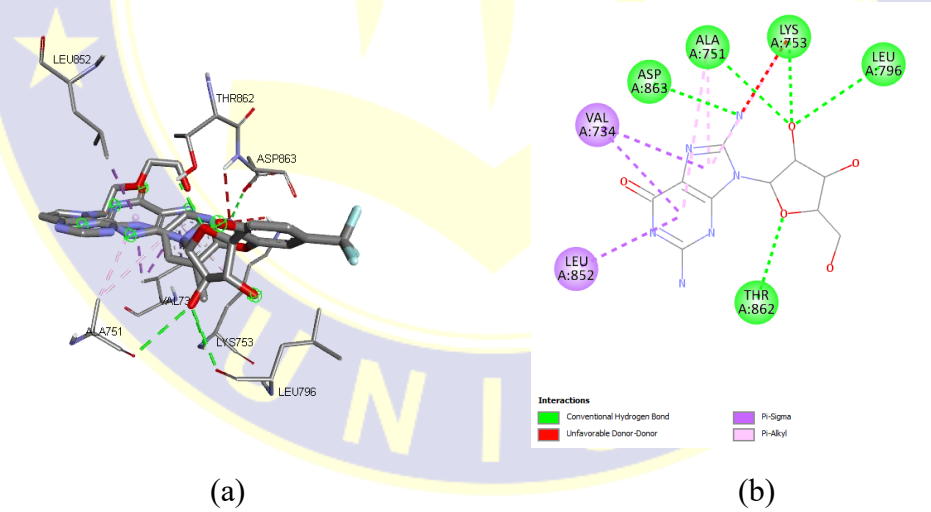
Gambar VII. 37 Visualisasi struktur 3D (a) dan 2D (b) ligan 3-O-Methylellagic acid-4′-O-α-L-rhamnopyranoside terhadap Progesteron

LAMPIRAN 16
(LANJUTAN)



(a) (b)

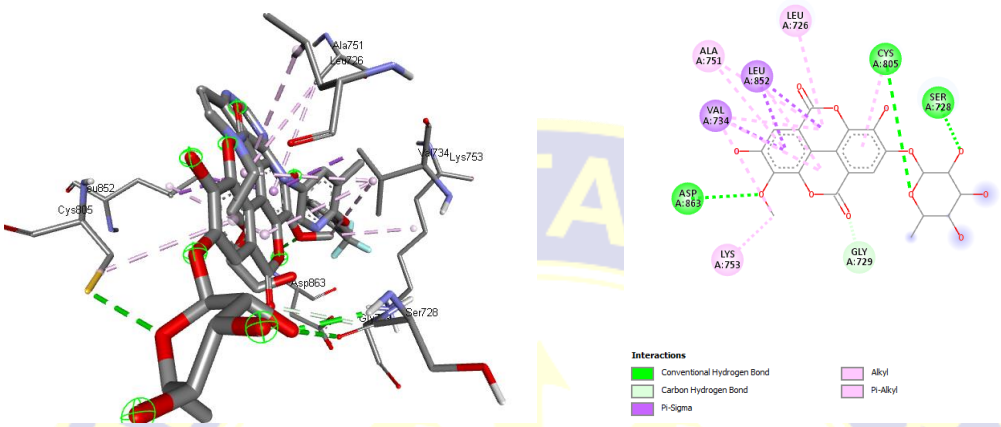
Gambar VII. 38 Visualisasi struktur 3D (a) dan 2D (b) ligan alami O3Q terhadap HER2



(a) (b)

Gambar VII. 39 Visualisasi struktur 3D (a) dan 2D (b) ligan ligan pembanding Trastuzumab terhadap HER2

LAMPIRAN 16
(LANJUTAN)



(a) (b)

Gambar VII. 40 Visualisasi struktur 3D (a) dan 2D (b) ligan 3-O-Methylellagic acid-4′-O-α-L-rhamnopyranoside terhadap HER2

LAMPIRAN 17

HASIL PREDIKSI *DRUGLIKENESS*

Tabel VII. 18
Hasil Prediksi *Druglikeness*

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
1	Cleistocalyxic acid A	470	2	4	6.27	Tidak Memenuhi
2	Cleistocalyxic acid B	500	2	5	6.24	Tidak Memenuhi
3	Cleistocalyxic acid C	472	3	4	6.20	Tidak Memenuhi
4	Cleistocalyxic acid D	500	2	5	6.53	Tidak Memenuhi
5	Cleistocalyxolide B	504	4	6	3.82	Tidak Memenuhi
6	Cleistocalyxic acid H	516	3	6	5.21	Tidak Memenuhi
7	Actinidic acid	486	4	5	4.95	Memenuhi
8	Cleistocalyxic acid I	502	5	6	3.92	Tidak Memenuhi
9	Cleistocalyxic acid J	516	4	6	4.58	Tidak Memenuhi
10	Cleistocalyxic acid K	500	4	6	4.13	Tidak Memenuhi
11	Ursolic acid	456	2	3	7.089	Tidak Memenuhi
12	Corosolic acid	472	3	4	6.060	Tidak Memenuhi
13	Asiatic acid	488	4	5	5.033	Tidak Memenuhi
14	2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid	504	5	6	4	Tidak Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
15	*2α,3β-Dihydroxy-24-nor-urs-4(23),12-dien-28-oic acid*	472	3	4	6.060	Tidak Memenuhi
16	*β-Sitosterol*	414	1	1	8.024	Tidak Memenuhi
17	*Betulinic acid*	456	2	3	7.089	Tidak Memenuhi
18	*Alphitolic acid*	472	3	4	6.060	Tidak Memenuhi
19	*Oleanolic acid*	456	2	3	7.23	Tidak Memenuhi
20	*Maslinic acid*	472	3	4	6.20	Tidak Memenuhi
21	*3-O-trans-p-Coumaroyl maslinic acid*	312	5	6	-0.05	Memenuhi
22	*3-O-cis-p-Coumaroyl maslinic acid*	312	5	6	-0.05	Memenuhi
23	*Arjunolic acid*	488	4	5	5.17	Tidak Memenuhi
24	*Cleistocalyxic acid E*	504	5	6	4.15	Tidak Memenuhi
25	*Cleistocalyxic acid F*	518	4	6	4.80	Tidak Memenuhi
26	*Cleistocalyxic acid G*	502	4	6	4.35	Tidak Memenuhi
27	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	298	2	4	3.62	Memenuhi
28	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	312	2	5	3.12	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
29	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	328	3	6	2.83	Memenuhi
30	*3'-Formyl-6',4-dihydroxy-2'-methoxy-5'-methylchalcone 4'-O-β-D-glucopyranoside*	490	4	11	0.51	Tidak Memenuhi
31	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	284	2	4	3.31	Memenuhi
32	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	312	5	6	-0.05	Memenuhi
33	*Kaempferol*	286	4	6	2.30	Memenuhi
34	*Quercetin*	302	5	7	2.011	Tidak Memenuhi
35	*Tamarixetin*	316	4	7	2.31	Memenuhi
36	*Myricetin-3'-methylether 3-O-β-D-galactopyranoside*	480	9	13	-1.02	Tidak Memenuhi
37	*Myricetin-3'-methylether*	332	5	8	1.80	Tidak Memenuhi
38	*Gossypetin-8,3'-dimethylether-3-O-β-D-galactoside*	312	5	6	-0.05	Tidak Memenuhi
39	*Luteolin*	286	4	6	2.12	Memenuhi
40	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	296	1	4	3.63	Memenuhi
41	*(2S)-8-Formyl-6-methylnaringenin*	314	3	6	2.63	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
42	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	476	5	11	0.20	Tidak Memenuhi
43	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	312	1	5	3.23	Memenuhi
44	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	312	1	5	3.23	Memenuhi
45	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	298	1	4	3.72	Memenuhi
46	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	284	1	4	3.41	Memenuhi
47	*(2S)-8-methylpinocembrin*	270	2	4	3.11	Memenuhi
48	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	298	1	4	3.72	Memenuhi
49	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	284	2	4	3.42	Memenuhi
50	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	314	2	5	2.83	Memenuhi
51	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	300	3	5	2.39	Memenuhi
52	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	296	1	4	3.63	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
53	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	462	5	12	-1.59	Tidak Memenuhi
54	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	372	6	9	-0.49	Tidak Memenuhi
55	*(trans)-4-Hydroxy-5-(2-hydroxypropan-2-yl)-2-methylcyclopent-2-en-1-one*	112	1	2	0.12	Memenuhi
56	*4-Hydroxy-2,2,5-trimethylcyclopent-4-ene-1,3-dione*	154	1	3	0.99	Memenuhi
57	*4'-Dihydrophaseic acid*	444	6	10	-1.49	Tidak Memenuhi
58	*Pentadienoic acid*	98	1	2	0.81	Memenuhi
59	*4-Hydroxybenzoic acid*	138	2	3	1.090	Memenuhi
60	*Methyl 3,4,5-trihydroxybenzoate*	184	3	5	0.59	Memenuhi
61	*4-Hydroxy-3,5-dimethoxybenzoic acid*	198	2	5	1.11	Memenuhi
62	*Cinnamic acid*	148	1	2	1.78	Memenuhi
63	*Cleistoperlone A*	594	2	8	6.057	Tidak Memenuhi
64	*Operculatol A*	432	1	4	6.080	Tidak Memenuhi
65	*1-Tetratriacontanol*	312	5	6	-0.05	Tidak Memenuhi
66	*3-Hydroxy-3-phenylpropanoic acid*	166	2	3	1.19	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
67	*Tetrahydrofurfuryl acetate*	144	0	3	0.73	Memenuhi
68	*β-Pinene*	136	0	0	2.99	Memenuhi
69	*Myrcene*	136	0	0	3.47	Memenuhi
70	*Limonene*	136	0	0	3.31	Memenuhi
71	*(Z)-β-Ocimene*	136	0	0	3.47	Memenuhi
72	*(E)-β-Ocimene*	136	0	0	3.47	Memenuhi
73	*Rosefuran*	150	0	1	3.096	Memenuhi
74	*Linalool*	154	1	1	2.67	Memenuhi
75	*6-Methyl-3,5-heptadien-2-one*	124	0	1	2.097	Memenuhi
76	*allo-Ocimene*	136	0	0	3.47	Memenuhi
77	*(Z)-Epoxy ocimene (=(Z)-MyrOxide)*	152	0	1	2.68	Memenuhi
78	*(E)-Epoxy ocimene (= (E)-Myroxide)*	152	0	1	2.68	Memenuhi
79	*Naphthalene*	126	0	0	2.84	Memenuhi
80	*(3Z)-Octenyl acetate*	170	0	2	2.68	Memenuhi
81	*(3E)-Octenyl acetate*	170	0	2	2.68	Memenuhi
82	*Cyclosativene*	204	0	0	3.96	Memenuhi
83	*α-Copaene*	204	0	0	4.27	Memenuhi
84	*Geranyl acetate*	196	0	2	3.24	Memenuhi
85	*(E)-Caryophyllene*	204	0	0	4.50	Memenuhi
86	*β-Copaene*	204	0	0	4.27	Memenuhi
87	*Aromadendrene*	204	0	0	4.27	Memenuhi
88	*α-Humulene*	204	0	0	5.035	Tidak Memenuhi
89	*γ-Muurolene*	204	0	0	4.58	Memenuhi
90	*β-Selinene*	204	0	0	4.72	Memenuhi
91	*γ-Cadinene*	204	0	0	4.58	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
92	*(E)-Nerolidol*	222	1	1	4.39	Memenuhi
93	*Spathulenol*	220	1	1	3.38	Memenuhi
94	*Caryophyllene oxide*	220	0	1	3.94	Memenuhi
95	*Humulene epoxide I*	220	0	1	4.25	Memenuhi
96	*Humulene epoxide II*	220	0	1	4.25	Memenuhi
97	*Selina-6-en-4β-ol*	222	1	1	3.92	Memenuhi
98	*Caryophylla-4(12),8(13)-dien-5β-ol*	220	1	1	3.69	Memenuhi
99	*Selina-3,11-dien-6α-ol*	220	1	1	3.69	Memenuhi
100	*Selin-11-en-4α-ol*	222	1	1	3.92	Memenuhi
101	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	220	1	1	3.69	Memenuhi
102	*γ-Gurjunene*	204	0	0	4.58	Memenuhi
103	*δ-Cadinene*	204	0	0	4.72	Memenuhi
104	*cis-Cadin-4-en-7-ol*	222	1	1	3.77	Memenuhi
105	*p-Cymene*	134	0	0	3.12	Memenuhi
106	*Rosefuran epoxide*	166	0	2	2.31	Memenuhi
107	*α-Terpineol*	154	1	1	2.50	Memenuhi
108	*α-Terpinyl acetate*	196	0	2	3.074	Memenuhi
109	*cis-4-Caranone*	152	0	1	2.26	Memenuhi
110	*β-Oplopenone*	220	0	1	3.84	Memenuhi
111	*α-Amorphene*	204	0	0	4.58	Memenuhi
112	*α-Muurolene*	204	0	0	4.58	Memenuhi
113	*α-Cadinene*	204	0	0	4.58	Memenuhi
114	*τ-Cadinol*	222	1	1	3.77	Memenuhi
115	*τ-Muurolol*	222	1	1	3.77	Memenuhi
116	*α-Muurolol (= δ-Cadinol)*	312	5	6	-0.05	Memenuhi
117	*α-Cadinol*	222	1	1	3.77	Memenuhi
118	*1-epi-Cubenol*	222	1	1	3.77	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII. 18
Lanjutan

No	Ligan Uji	BM g/mol (<500)	Donor H (<5)	Akseptor H (<10)	Log P (<5)	Keterangan
119	*β-Calacorene*	200	0	0	4.54	Memenuhi
120	*p-Mentha-1,5-dien-8-ol*	152	1	1	2.28	Memenuhi
121	*α-Pinene oxide*	152	0	1	2.21	Memenuhi
122	*Globulol*	222	1	1	3.46	Memenuhi
123	*Viridiflorol*	222	1	1	3.46	Memenuhi
124	*α-Pinene*	136	0	0	2.99	Memenuhi
125	*Guaiol*	222	1	1	3.92	Memenuhi
126	*α-Calcorene*	200	0	0	4.54	Memenuhi
127	*β-Calacorene*	200	0	0	4.54	Memenuhi

LAMPIRAN 18

HASIL PREDIKSI ADMET

Tabel VII. 19
Hasil Prediksi Profil Farmakokinetik dan Tokisitas

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
1	Cleistocalyxic acid A	96.71	21.24	100	Non Mutagen	Positif
2	Cleistocalyxic acid B	97.22	21.24	97.68	Non Mutagen	Positif
3	Cleistocalyxic acid C	94.28	21.28	100	Non Mutagen	Positif
4	Cleistocalyxic acid D	97.22	21.25	98.75	Non Mutagen	Negatif
5	Cleistocalyxolide B	86	21.21	93.44	Non Mutagen	Negatif
6	Cleistocalyxic acid H	94.88	20.98	95.69	Non Mutagen	Positif
7	Actinidic acid	91.62	20.97	94.22	Mutagen	Positif
8	Cleistocalyxic acid I	86.28	20.87	90.39	Mutagen	Positif
9	Cleistocalyxic acid J	91.84	20.92	90.28	Mutagen	Positif
10	Cleistocalyxic acid K	91.21	20.89	89.97	Mutagen	Positif
11	Ursolic acid	95.99	21.86	100	Non Mutagen	Positif
12	Corosolic acid	94.28	21.26	99.22	Non Mutagen	Positif
13	Asiatic acid	91.24	20.98	96.45	Non Mutagen	Positif
14	2α,3β,11α,23-Tetrahydroxyurs-12-en-28-oic acid	85.17	20.87	91.92	Non Mutagen	Positif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
15	*2α,3β-Dihydroxy-24-nor-urs-4(23),12-dien-28-oic acid*	94.28	21.26	99.22	Non Mutagen	Positif
16	*β-Sitosterol*	100	52.37	100	Non Mutagen	Positif
17	*Betulinic acid*	95.99	21.86	100	Mutagen	Negatif
18	*Alphitolic acid*	94.28	21.26	100	Mutagen	Negatif
19	*Oleanolic acid*	95.99	21.89	100	Non Mutagen	Positif
20	*Maslinic acid*	94.28	21.28	100	Non Mutagen	Positif
21	*3-O-trans-p-Coumaroyl maslinic acid*	95.53	21.90	100	Non Mutagen	Positif
22	*3-O-cis-p-Coumaroyl maslinic acid*	95.53	21.91	100	Non Mutagen	Positif
23	*Arjunolic acid*	91.23	20.98	97.05	Non Mutagen	Positif
24	*Cleistocalyxic acid E*	85.14	20.87	92.20	Non Mutagen	Positif
25	*Cleistocalyxic acid F*	91.40	20.95	91.64	Non Mutagen	Positif
26	*Cleistocalyxic acid G*	90.36	20.89	91.22	Non Mutagen	Positif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
27	*2',4'-Dihydroxy-6'-methoxy-3',5'-dimethylchalcone*	93.24	20.13	91.52	Non Mutagen	Negatif
28	*3'-Formyl-4',6'-dihydroxy-2'-methoxy-5'-methylchalcone*	93.60	21.04	89.60	Mutagen	Negatif
29	*3'-Formyl-4',6',4-trihydroxy-2'-methoxy-5'-methylchalcone*	88.91	19.87	88.59	Mutagen	Positif
30	*3'-Formyl-6',4-dihydroxy-2'-methoxy-5'-methylchalcone 4'-O-β-D-glucopyranoside*	77.08	5.08	61.70	Non Mutagen	Positif
31	*2',4'-Dihydroxy-3'-methyl-6'-methoxychalcone*	93.04	18.44	92.06	Mutagen	Negatif
32	*2,2',4'-Trihydroxy-6'-methoxy-3',5'-dimethylchalcone*	89.44	20.62	91.26	Non Mutagen	Negatif
33	*Kaempferol*	79.44	9.58	89.61	Mutagen	Negatif
34	*Quercetin*	63.48	3.41	93.24	Mutagen	Negatif
35	*Tamarixetin*	78.35	4.94	82.77	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
36	*Myricetin-3'-methylether 3-O-β-D-galactopyranoside*	5.29	7.42	62.40	Non Mutagen	Negatif
37	*Myricetin-3'-methylether*	60.34	0.70	86.62	Mutagen	Negatif
38	*Gossypetin-8,3'-dimethylether-3-O-β-D-galactoside*	0.36	6.79	18.58	Non Mutagen	Positif
39	*Luteolin*	79.43	4.54	99.72	Mutagen	Negatif
40	*7-Hydroxy-5-methoxy-6,8-dimethylflavone*	95.62	32.11	90.96	Mutagen	Negatif
41	*(2S)-8-Formyl-6-methylnaringenin*	87.22	14.87	92.69	Mutagen	Negatif
42	*(2S)-8-Formyl-6-methylnaringenin 7-O-β-D-glucopyranoside*	61.33	4.56	63.35	Non Mutagen	Positif
43	*(2S)-8-Formyl-5-hydroxy-7-methoxy-6-methylflavanone*	96.39	14.02	89.28	Mutagen	Negatif
44	*(2S)-6-Formyl-8-methyl-7-O-methylpinocembrin*	96.39	16.22	89.03	Mutagen	Negatif
45	*(2S)-7-Hydroxy-5-methoxy-6,8-dimethylflavanone*	95.57	32.51	93.47	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
46	*(2S)-7-Hydroxy-5-methoxy-8-methylflavanone*	95.54	23.16	93.86	Mutagen	Negatif
47	*(2S)-8-methylpinocembrin*	92.57	5.07	97.89	Mutagen	Negatif
48	*(2S)-5-Hydroxy-7-methoxy-6,8-dimethylflavanone*	95.57	32.51	92.76	Mutagen	Negatif
49	*(2S)-5,7-Dihydroxy-6,8-dimethylflavanone*	92.78	10.26	97.38	Mutagen	Negatif
50	*(2S)-2,7-Dihydroxy-5-methoxy-6,8-dimethylflavanone*	93.33	16.11	88.58	Non Mutagen	Negatif
51	*(2S,3S)-2,3-trans-5,7-Dihydroxy-6,8-dimethyldihydroflavonol*	88.67	12.11	89.43	Mutagen	Negatif
52	*7-Hydroxy-5-methoxy-6,8-dimethylisoflavone*	95.62	31.41	89.59	Mutagen	Negatif
53	*3-O-Methylellagic acid-4'-O-α-L-rhamnopyranoside*	34.07	17.43	59.59	Non Mutagen	Negatif
54	*1-[(2-Methylbutyryl)-phloroglucinyl]-β-D-glucopyranoside*	23.63	2.51	59.30	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
55	*(trans)-4-Hydroxy-5-(2-hydroxypropan-2-yl)-2-methylcyclopent-2-en-1-one*	92.36	19.03	89.46	Mutagen	Negatif
56	*4-Hydroxy-2,2,5-trimethylcyclopent-4-ene-1,3-dione*	88.90	20.07	100	Mutagen	Negatif
57	*4'-Dihydrophaseic acid*	24.26	5.15	32.40	Non Mutagen	Positif
58	*Pentadienoic acid*	93.10	20.52	0	Mutagen	Negatif
59	*4-Hydroxybenzoic acid*	88.14	20.31	8.04	Mutagen	Negatif
60	*Methyl 3,4,5-trihydroxybenzoate*	69.75	18.32	88.44	Mutagen	Negatif
61	*4-Hydroxy-3,5-dimethoxybenzoic acid*	82.03	18.83	69.77	Mutagen	Negatif
62	*Cinnamic acid*	97.84	21.03	60.85	Mutagen	Negatif
63	*Cleistoperlone A*	95.76	27.64	90.40	Non Mutagen	Negatif
64	*Operculatol A*	96.45	47.68	95.30	Non Mutagen	Negatif
65	*1-Tetratriacontanol*	100	52.19	99.83	Non Mutagen	Positif
66	*3-Hydroxy-3-phenylpropanoic acid*	90.76	20.63	41.32	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
67	*Tetrahydrofurfuryl acetate*	95.68	46.10	74.81	Mutagen	Positif
68	*β-Pinene*	100	23.49	100	Mutagen	Negatif
69	*Myrcene*	100	23.63	100	Mutagen	Negatif
70	*Limonene*	100	23.63	100	Mutagen	Negatif
71	*(Z)-β-Ocimene*	100	23.63	100	Mutagen	Positif
72	*(E)-β-Ocimene*	100	23.63	100	Mutagen	Positif
73	*Rosefuran*	100	38.21	100	Mutagen	Positif
74	*Linalool*	100	29.35	100	Mutagen	Negatif
75	*6-Methyl-3,5-heptadien-2-one*	100	21.16	44.12	Mutagen	Positif
76	*allo-Ocimene*	100	23.45	98.87	Mutagen	Positif
77	*(Z)-Epoxy ocimene (=(Z)-MyrOxide)*	100	30.46	62.85	Mutagen	Positif
78	*(E)-Epoxy ocimene (= (E)-Myroxide)*	100	30.47	62.86	Mutagen	Positif
79	*Naphthalene*	100	23.44	100	Mutagen	Positif
80	*(3Z)-Octenyl acetate*	100	43.81	100	Mutagen	Positif
81	*(3E)-Octenyl acetate*	100	43.81	100	Mutagen	Positif
82	*Cyclosativene*	100	22.30	100	Mutagen	Negatif
83	*α-Copaene*	100	23.63	100	Non Mutagen	Negatif
84	*Geranyl acetate*	100	44.51	100	Non Mutagen	Positif
85	*(E)-Caryophyllene*	100	23.63	100	Mutagen	Negatif
86	*(3E)-Octenyl acetate*	100	43.81	100	Mutagen	Positif
87	*β-Copaene*	100	23.49	100	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
88	*Aromadendrene*	100	23.50	100	Mutagen	Negatif
89	*α-Humulene*	100	23.63	100	Non Mutagen	Positif
90	*γ-Muurolene*	100	23.64	100	Mutagen	Negatif
91	*β-Selinene*	100	23.49	100	Mutagen	Negatif
92	*α-Selinene*	100	23.63	100	Mutagen	Negatif
93	*γ-Cadinene*	100	23.63	100	Mutagen	Negatif
94	*(E)-Nerolidol*	100	26.61	100	Non Mutagen	Negatif
95	*Spathulenol*	100	54.42	82.89	Mutagen	Positif
96	*Caryophyllene oxide*	100	56.35	90.85	Mutagen	Positif
97	*Humulene epoxide I*	100	52.27	100	Mutagen	Positif
98	*Humulene epoxide II*	100	52.28	100	Mutagen	Positif
99	*Selina-6-en-4β-ol*	100	55.68	100	Mutagen	Positif
100	*Caryophylla-4(12),8(13)-dien-5β-ol*	100	45.87	98.74	Mutagen	Negatif
101	*Selina-3,11-dien-6α-ol*	100	40.81	100	Mutagen	Positif
102	*Selin-11-en-4α-ol*	100	55.68	86.28	Mutagen	Negatif
103	*(E)-trans-α-Bergamota-2,10-dien-12-ol*	100	23.50	100	Non Mutagen	Positif
104	*γ-Gurjunene*	100	23.64	100	Mutagen	Negatif
105	*δ-Cadinene*	100	23.64	100	Mutagen	Positif
106	*cis-Cadin-4-en-7-ol*	100	55.41	100	Mutagen	Positif
107	*p-Cymene*	100	23.43	100	Mutagen	Positif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 19
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaC0-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity Mouse
108	*Rosefuran epoxide*	100	41.38	76.19	Mutagen	Positif
109	*α-Terpineol*	100	50.81	23.42	Mutagen	Negatif
110	*α-Terpinyl acetate*	100	37.76	98.54	Mutagen	Negatif
111	*cis-4-Caranone*	100	37.76	66.70	Mutagen	Negatif
112	*β-Oplopenone*	100	48.89	95.34	Mutagen	Negatif
113	*α-Amorphene*	100	23.63	100	Mutagen	Positif
114	*α-Muurolene*	100	23.63	100	Mutagen	Positif
115	*α-Cadinene*	100	23.63	100	Mutagen	Positif
116	*τ-Cadinol*	100	55.41	100	Mutagen	Negatif
117	*τ-Muurolol*	100	55.41	100	Mutagen	Negatif
118	*α-Muurolol (= δ-Cadinol)*	100	55.41	100	Mutagen	Negatif
119	*α-Cadinol*	100	55.41	100	Mutagen	Negatif
120	*1-epi-Cubenol*	100	55.41	100	Mutagen	Positif
121	*β-Calacorene*	100	23.46	100	Mutagen	Negatif
122	*p-Mentha-1,5-dien-8-ol*	100	50.72	30.56	Mutagen	Negatif
123	*α-Pinene oxide*	100	57.96	100	Mutagen	Positif
124	*Globulol*	100	54.57	100	Mutagen	Negatif
125	*Viridiflorol*	100	54.58	100	Non Mutagen	Negatif
126	*α-Pinene*	100	23.63	100	Mutagen	Negatif
127	*Guaiol*	100	55.38	100	Mutagen	Negatif

Keterangan :

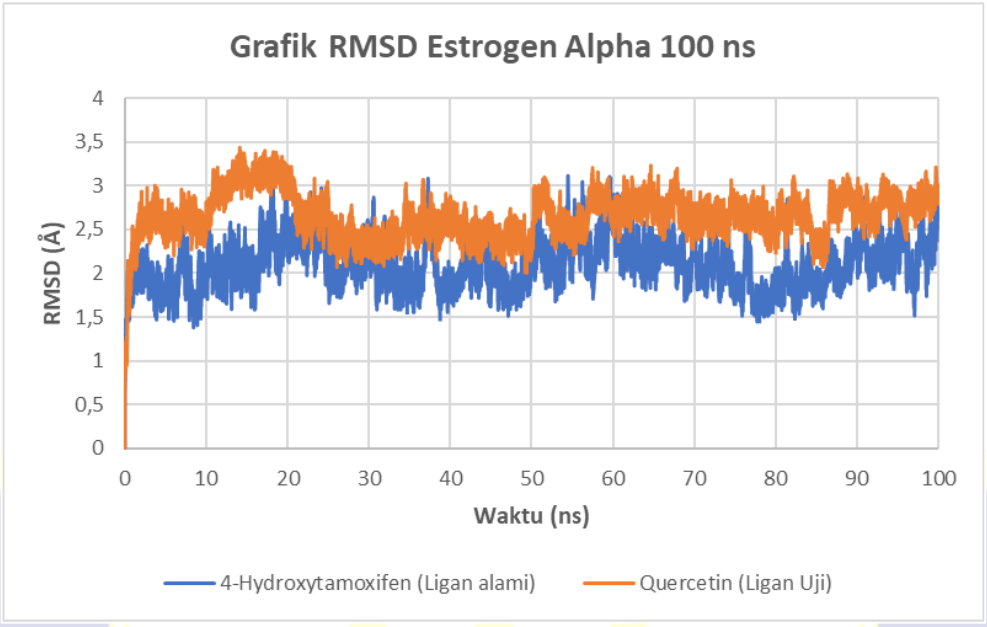
HIA (%)
70-100 : Terserap baik
20-70 : Cukup terserap
<20 : Kurang terserap

CaCo-2 (nm sec)
>70 : Permeabilitas tinggi
4-70 : Permeabilitas sedang
<4 : Permeabilitas rendah

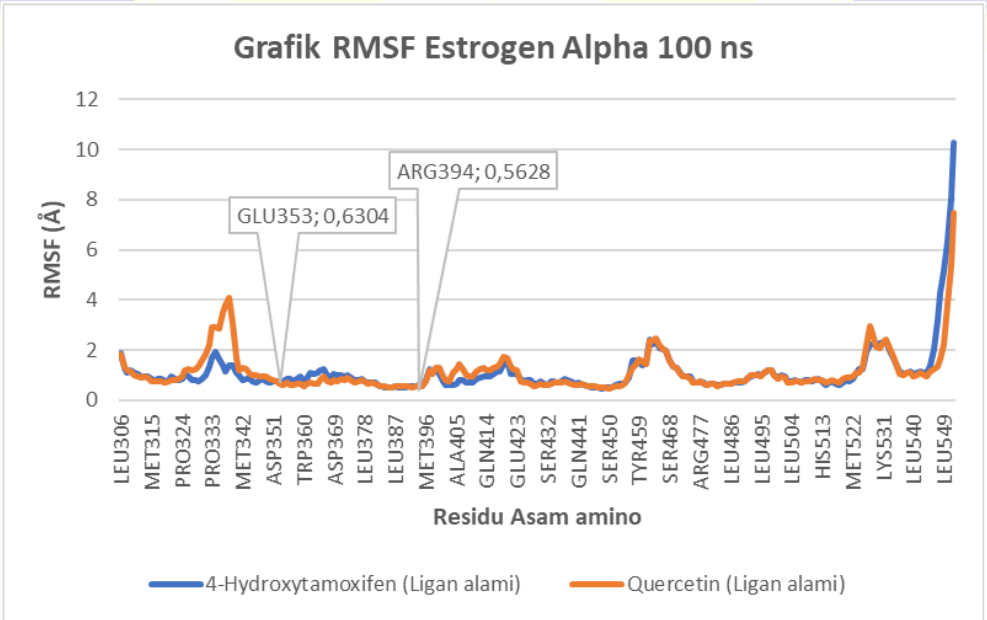
PPB (%)
>90 : Terikat kuat
<90 : Terikat lemah

LAMPIRAN 19

HASIL SIMULASI *MOLECULAR DYNAMIC*



Gambar VII. 41 Grafik nilai RMSD kompleks ligan-reseptor ER- α



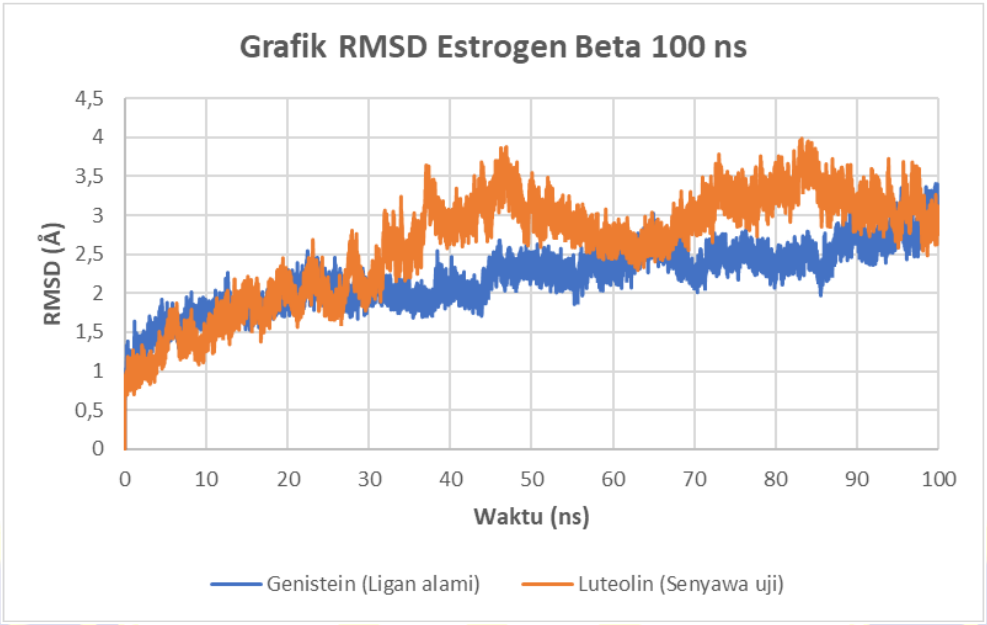
Gambar VII. 42 Grafik nilai RMSF kompleks ligan-reseptor ER- α

LAMPIRAN 19
(LANJUTAN)

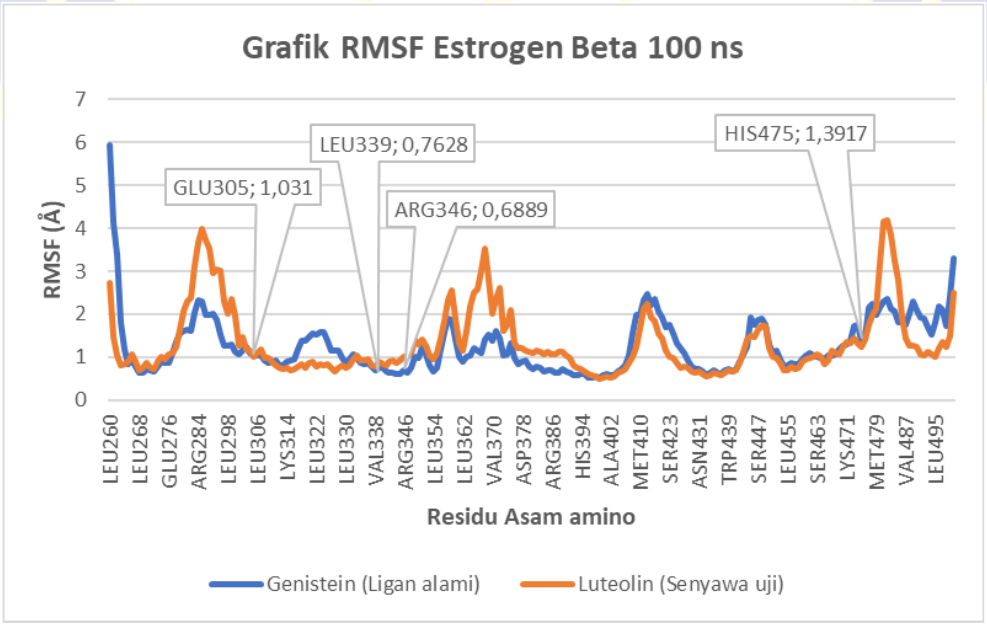
Tabel VII. 20
Hasil MMGBSA Reseptor ER-α

No	Komponen Energi (kkal/mol)	Reseptor ER-α	
		4-Hydroxytamoxifen	**Quercetin**
1	Interaksi Van der Waals (VdW)	-49.3197	-12.6498
2	Energi Elektrostatik (EEL)	140.6719	13.7315
3	Kontribusi Elektrostatik terhadap Energi Bebas Solvasi (EGB)	-124.2451	-8.8579
4	Kontribusi Non-polar terhadap Energi Bebas Solvasi (ESURF)	-7.2703	-2.0753
5	ΔGgas (VdW+EEL)	91.3523	1.0817
6	ΔGsolv (EGB + ESURF)	-131.5154	-10.9332
7	ΔGTOTAL (VdW + EEL + EGB + ESURF)	-40.1631	-9.8515

LAMPIRAN 19
(LANJUTAN)



Gambar VII. 43 Grafik nilai RMSD kompleks ligan-reseptor ER-β



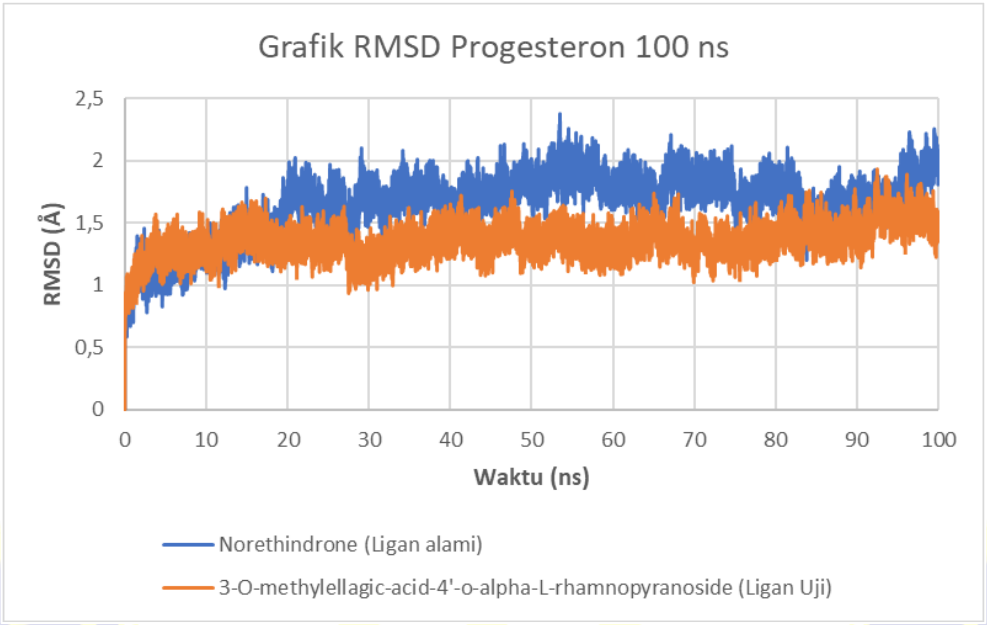
Gambar VII. 44 Grafik nilai RMSF kompleks ligan-reseptor ER-β

LAMPIRAN 19
(LANJUTAN)

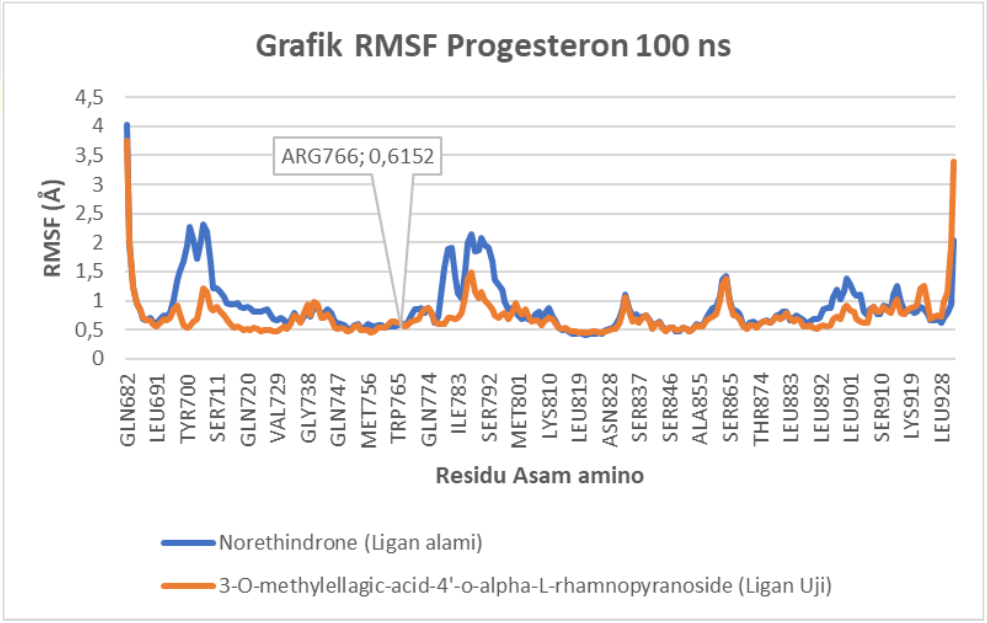
Tabel VII. 21
Hasil MMGBSA Reseptor ER-β

No	Komponen Energi (kkal/mol)	Reseptor ER-β	
		Genistein	**Luteolin**
1	Interaksi Van der Waals (VdW)	-22.7621	-30.4724
2	Energi Elektrostatik (EEL)	-234.6349	-8.4717
3	Kontribusi Elektrostatik terhadap Energi Bebas Solvasi (EGB)	254.0302	20.5513
4	Kontribusi Non-polar terhadap Energi Bebas Solvasi (ESURF)	-4.5020	-4.5922
5	ΔGgas (VdW+EEL)	-257.3970	-38.9441
6	ΔGsolv (EGB + ESURF)	249.5282	15.9592
7	ΔGTOTAL (VdW + EEL + EGB + ESURF)	-7.8688	-22.9849

LAMPIRAN 19
(LANJUTAN)



Gambar VII. 45 Grafik nilai RMSD kompleks ligan-reseptor Progesteron



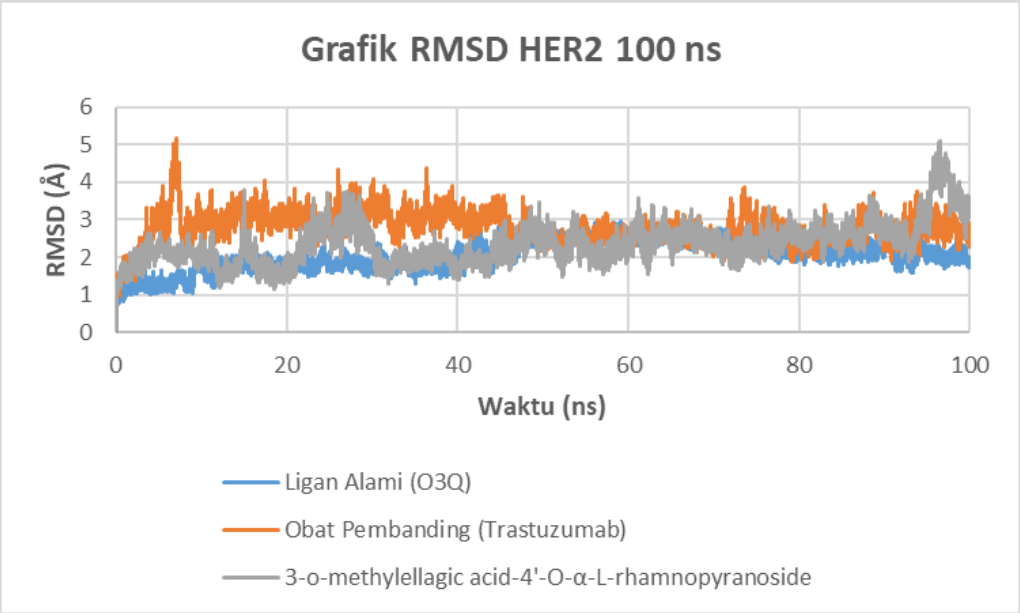
Gambar VII. 46 Grafik nilai RMSF kompleks ligan-reseptor Progesteron

LAMPIRAN 19
(LANJUTAN)

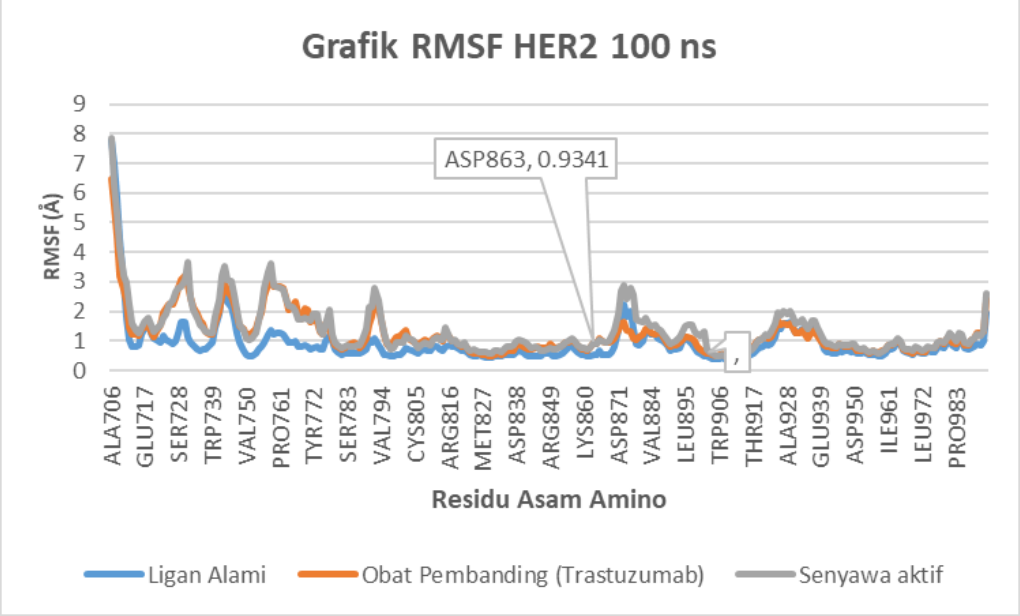
Tabel VII. 22
Hasil MMGBSA Reseptor Progesteron

No	Komponen Energi (kkal/mol)	Reseptor Progesteron	
		Norethindorne	**3-O-methylellagic_acid_4'-O-alpha-L-rhamnopyranoside**
1	Interaksi Van der Waals (VdW)	-39.5353	-45.0738
2	Energi Elektrostatik (EEL)	-141.9033	-161.3086
3	Kontribusi Elektrostatik terhadap Energi Bebas Solvasi (EGB)	123.3994	162.6270
4	Kontribusi Non-polar terhadap Energi Bebas Solvasi (ESURF)	-5.4817	-6.1906
5	ΔGgas (VdW+EEL)	-181.4385	-206.3824
6	ΔGsolv (EGB + ESURF)	117.9177	156.4363
7	ΔGTOTAL (VdW + EEL + EGB + ESURF)	-63.5208	-49.9461

LAMPIRAN 19
(LANJUTAN)



Gambar VII. 47 Grafik nilai RMSD kompleks ligan-reseptor HER2



Gambar VII. 48 Grafik nilai RMSF kompleks ligan-reseptor HER2

LAMPIRAN 19
(LANJUTAN)

Tabel VII. 23
Hasil MMGBSA Reseptor HER2

No	Komponen Energi (kkal/mol)	Reseptor HER2		
		O3Q	**Trastuzumab**	**3-O-methylellagic_acid_4'-O-alpha-L-rhamnopyranoside**
1	Interaksi Van der Waals (VdW)	-64.6942	-10.1164	-49.7416
2	Energi Elektrostatik (EEL)	-52.1238	-359.3462	-259.2820
3	Kontribusi Elektrostatik terhadap Energi Bebas Solvasi (EGB)	65.4422	359.2802	266.8933
4	Kontribusi Non-polar terhadap Energi Bebas Solvasi (ESURF)	-8.1367	-2.0111	-5.4443
5	ΔGgas (VdW+EEL)	-116.8180	-369.4626	-309.0236
6	ΔGsolv (EGB + ESURF)	57.3055	357.2691	261.4490
7	ΔGTOTAL (VdW + EEL + EGB + ESURF)	-59.5125	-12.1935	-47.5746

DAFTAR RIWAYAT HIDUP

I. IDENTITAS DIRI



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Agama : Islam

Kewarganegaraan : Indonesia

Status : Mahasiswa

Alamat : Kp. Sawah Lega RT 003/ RW 006 Desa Parakan Kecamatan Samarang Kabupaten Garut Jawab Barat Indonesia 44151

Telepon : 0895361179516

Email : anidaalmalia15@gmail.com

II. RIWAYAT PENDIDIKAN

Jenjang Pendidikan	Nama Sekolah/Perguruan Tinggi	Tahun Masuk	Tahun Lulus
SD/MI	SDN Parakan 1	2008	2014
SMP/MTs	SMP KHZ Musthafa Sukamanah	2014	2017
Pesantren	KHZ Musthafa Sukamanah	2014	2017
SMA/MA/SMK	SMKN 1 Garut	2017	2020
Perguruan Tinggi	Universitas Garut	2020	2024

III. PENGALAMAN ORGANISASI

1. Badan Eksekutif Mahasiswa sebagai wakil Sekretaris Departemen Entrepreneurship (2021-2022)