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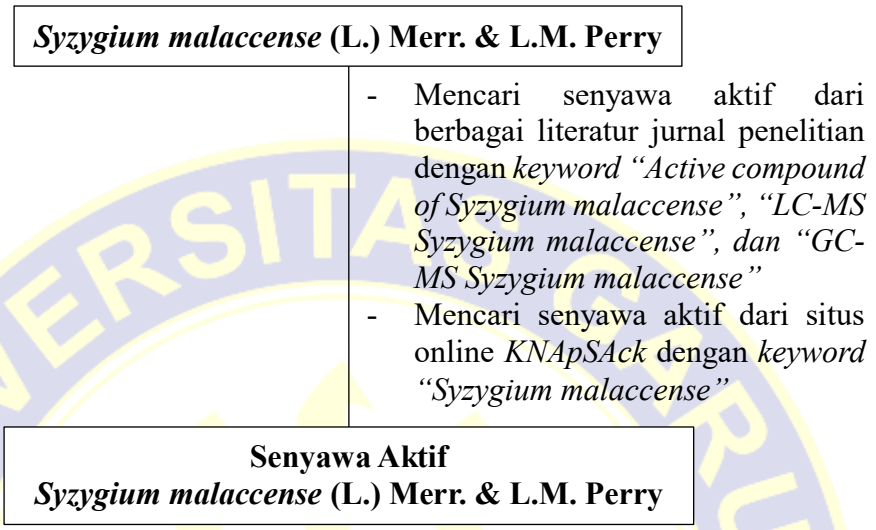
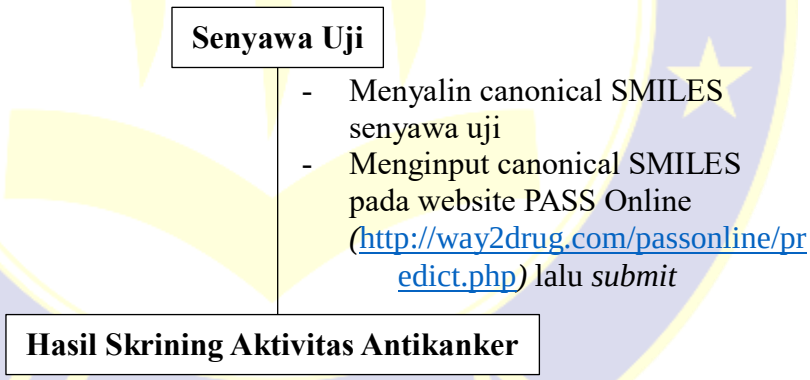
LAMPIRAN 1

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

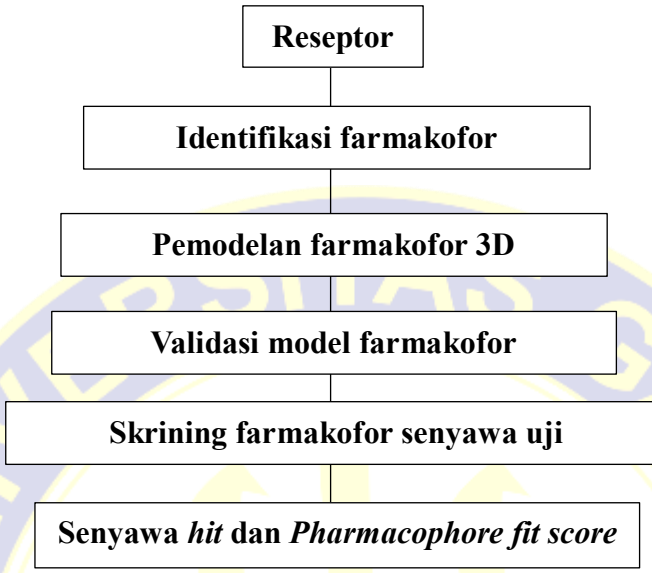


Gambar VII. 1 Alur penelitian pencarian senyawa aktif



Gambar VII. 2 Alur penelitian skrining aktivitas antikanker

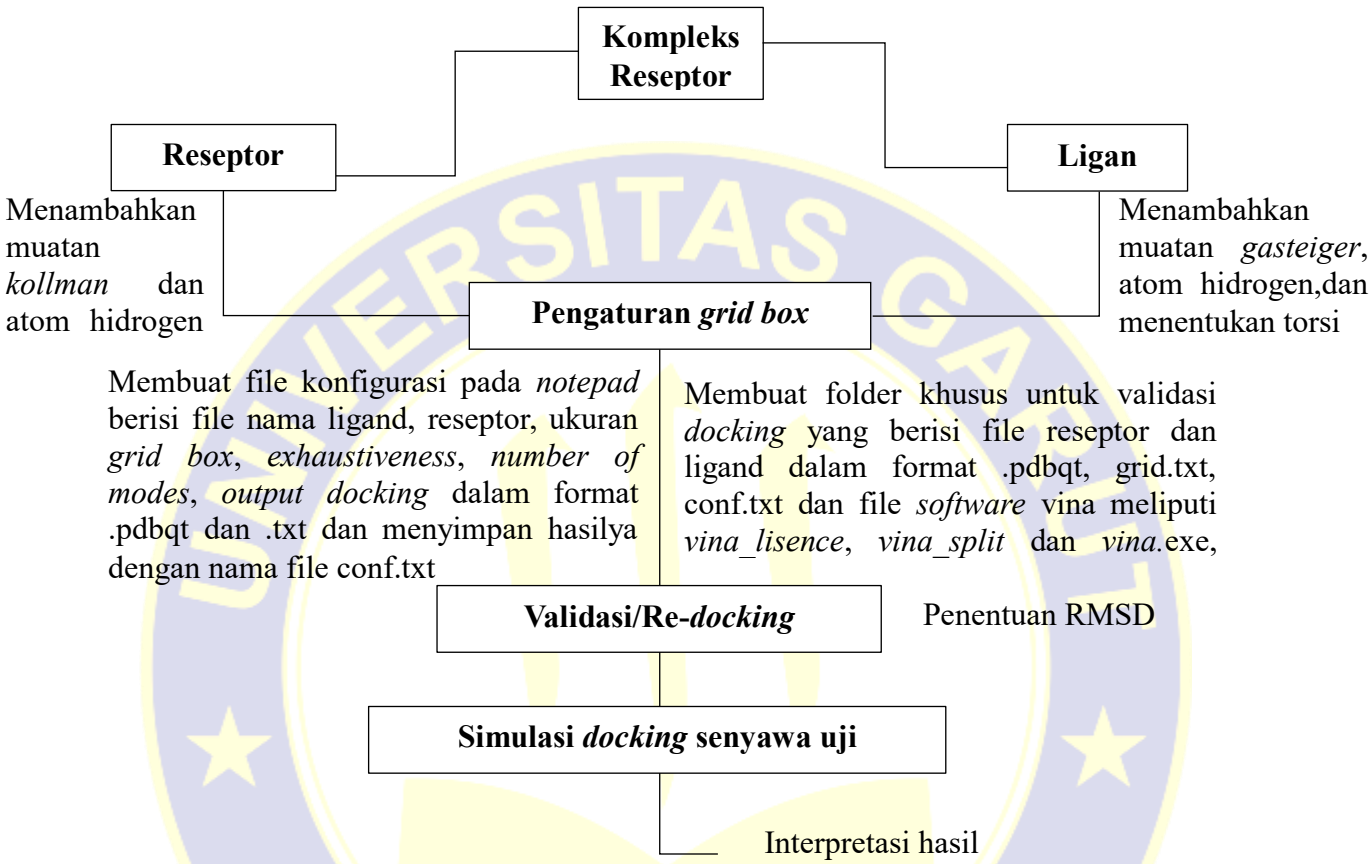
LAMPIRAN 1
(LANJUTAN)



Gambar VII. 3 Alur penelitian studi farmakofor

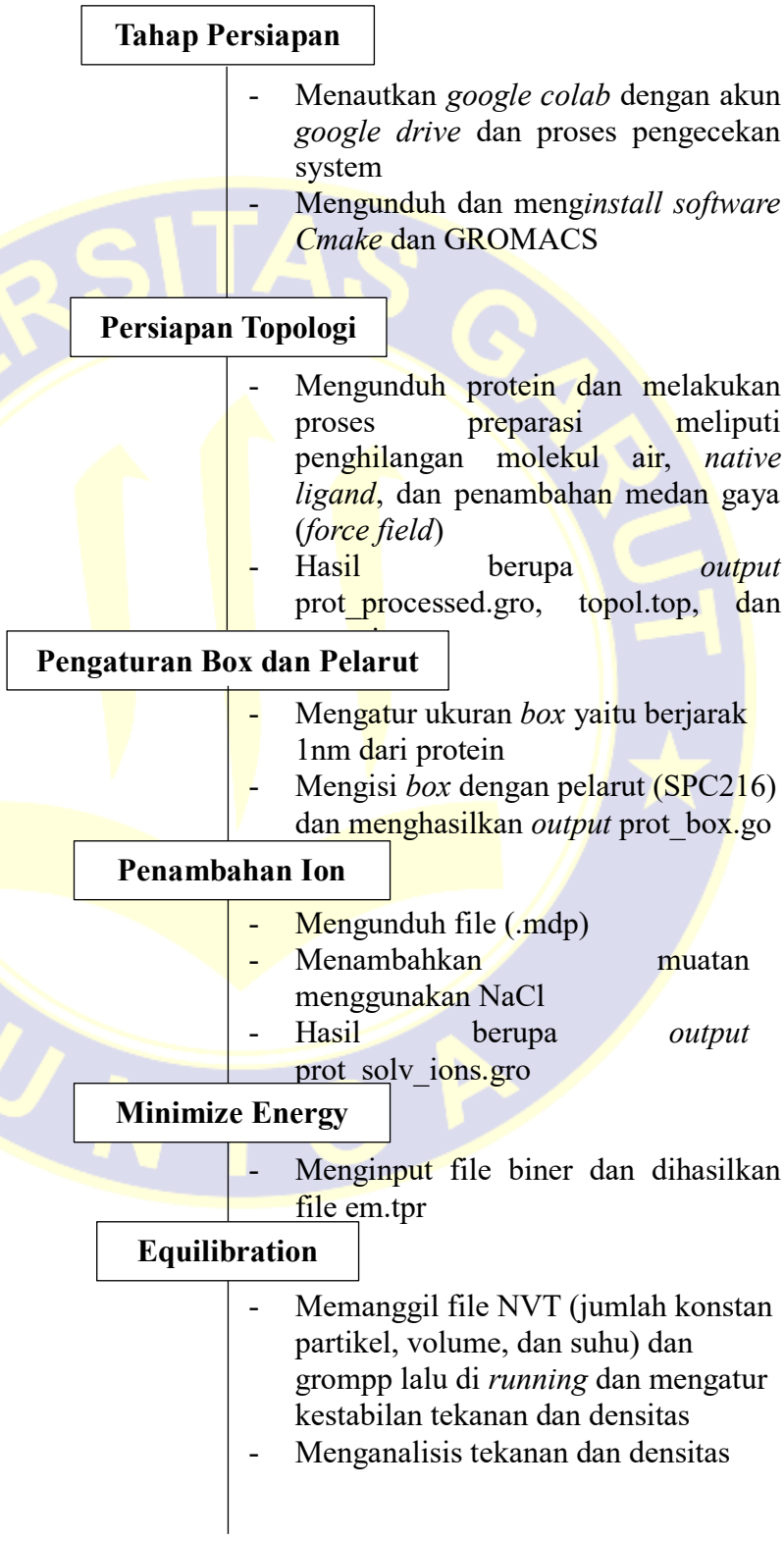
LAMPIRAN 2

ALUR SIMULASI *MOLECULAR DOCKING*, SIMULASI *MOLECULAR DYNAMIC,* DAN RUTE SINTESIS

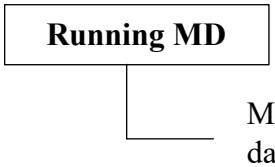


Gambar VII. 4 Alur penelitian simulasi *molecular docking*

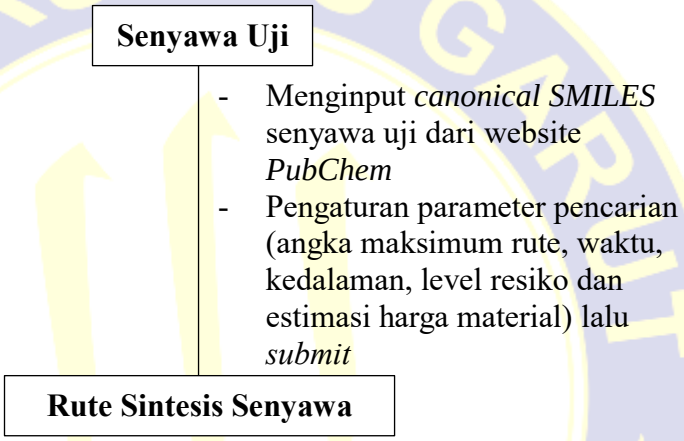
LAMPIRAN 2
(LANJUTAN)



LAMPIRAN 2
(LANJUTAN)



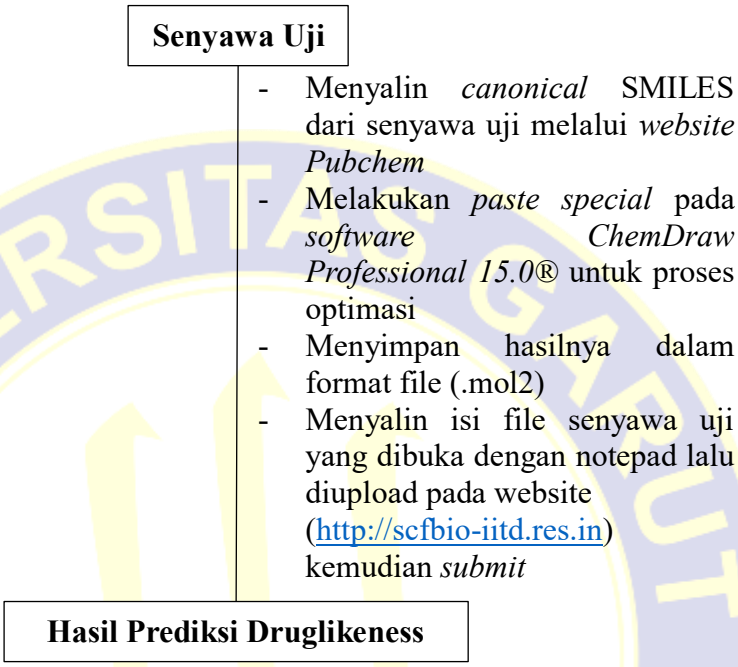
Gambar VII. 5 Alur penelitian simulasi *molecular dynamic*



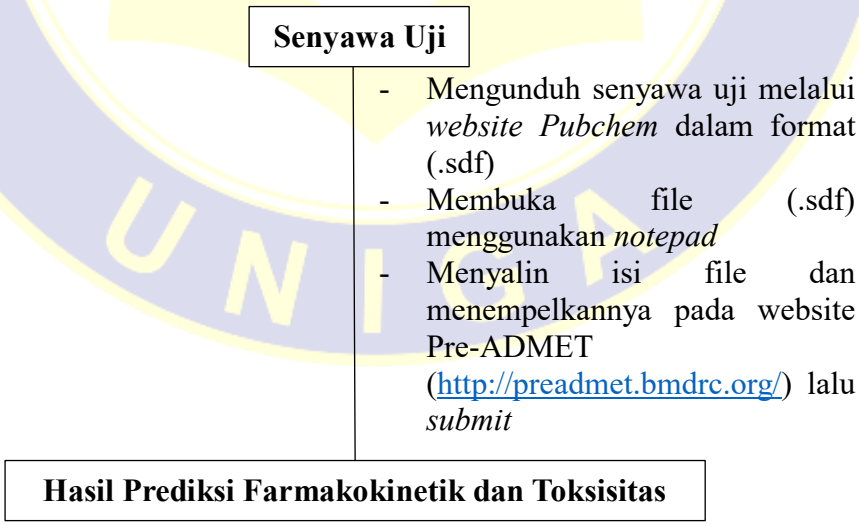
Gambar VII. 6 Alur penelitian prediksi rute sintesis senyawa

LAMPIRAN 3

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



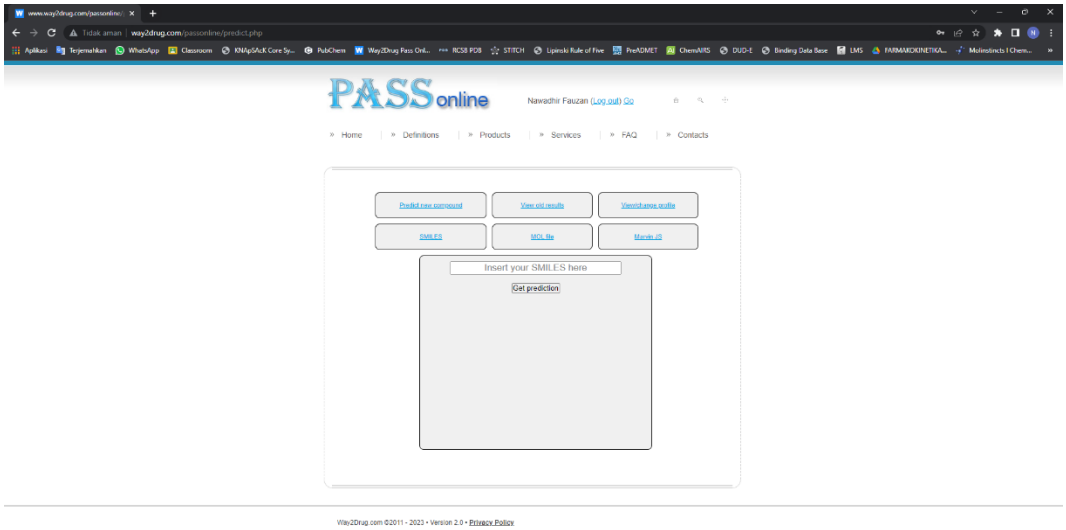
Gambar VII. 7 Alur penelitian prediksi *Lipinki's Rule of Five (Druglikenes)*



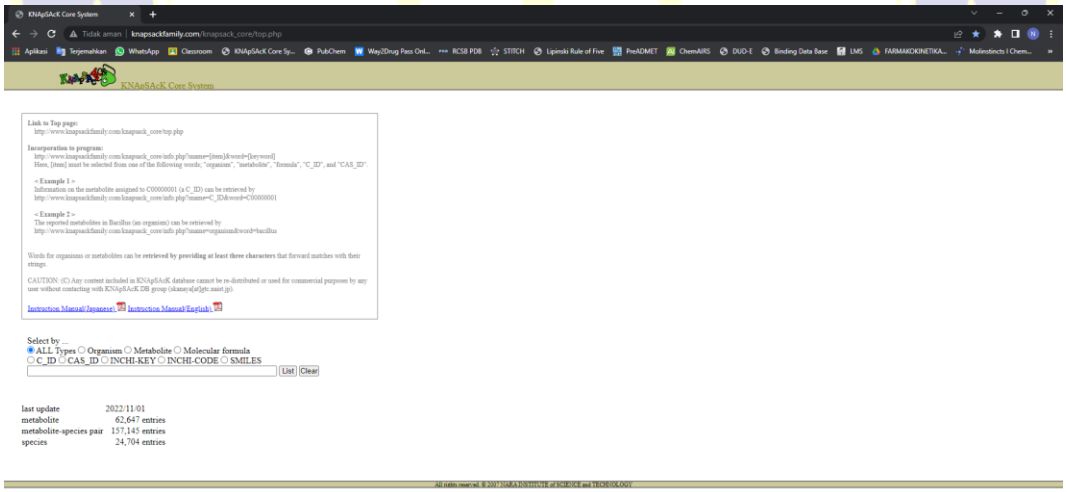
Gambar VII. 8 Alur penelitian prediksi farmakokinetik dan toksisitas

LAMPIRAN 4

SITUS DAN APLIKASI

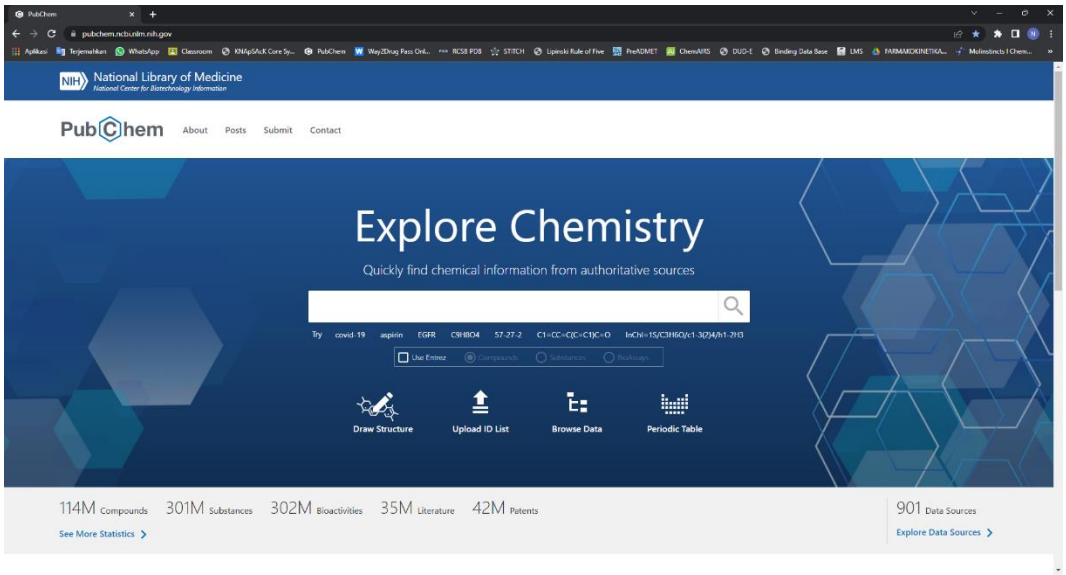


Gambar VII. 9 Tampilan situs *PASS Online*

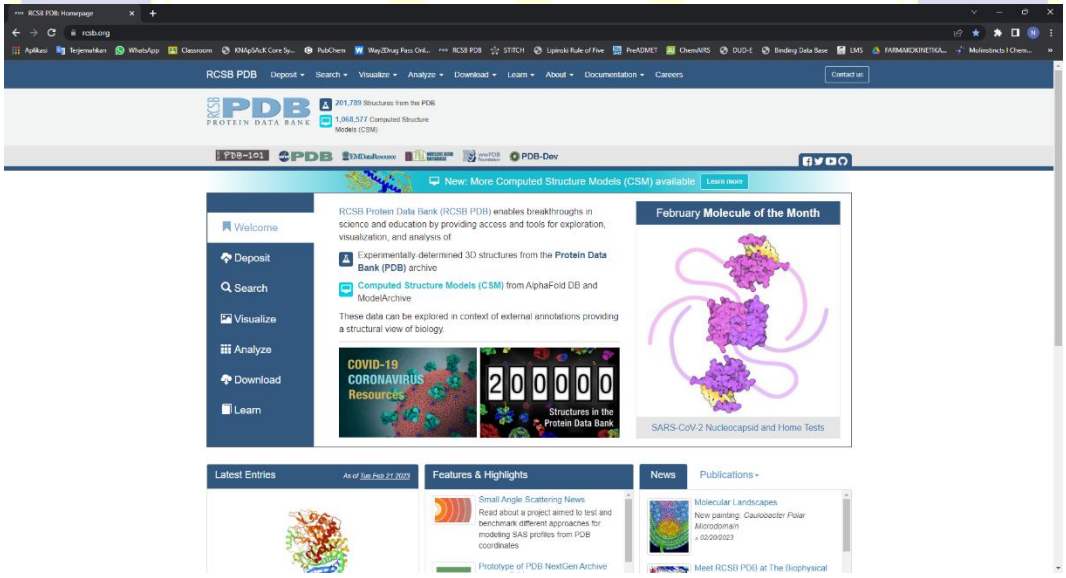


Gambar VII. 10 Tampilan situs *KNApSacK*

LAMPIRAN 4
(LANJUTAN)

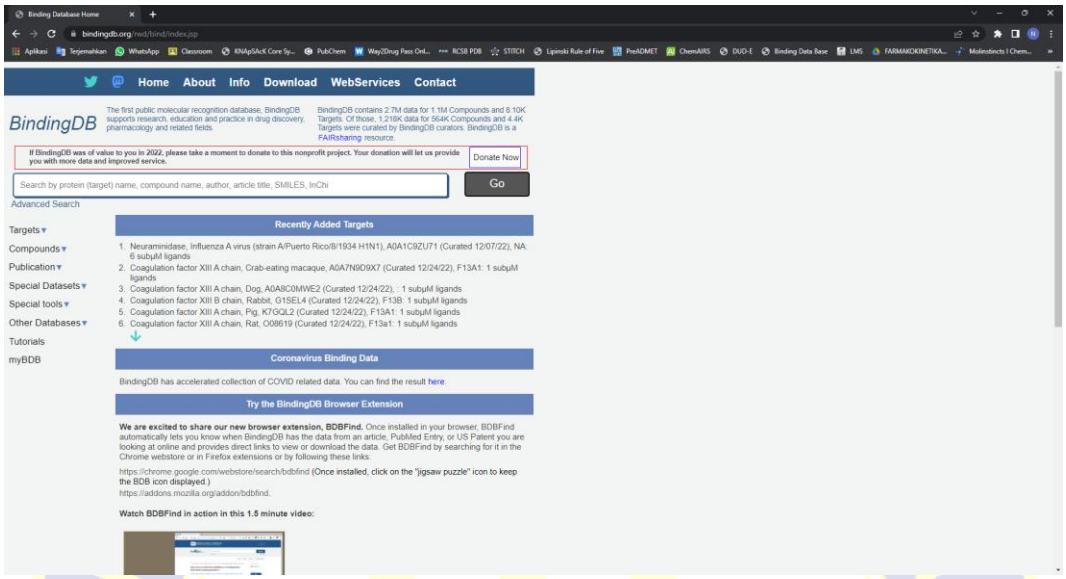


Gambar VII. 11 Tampilan situs *Pubchem*

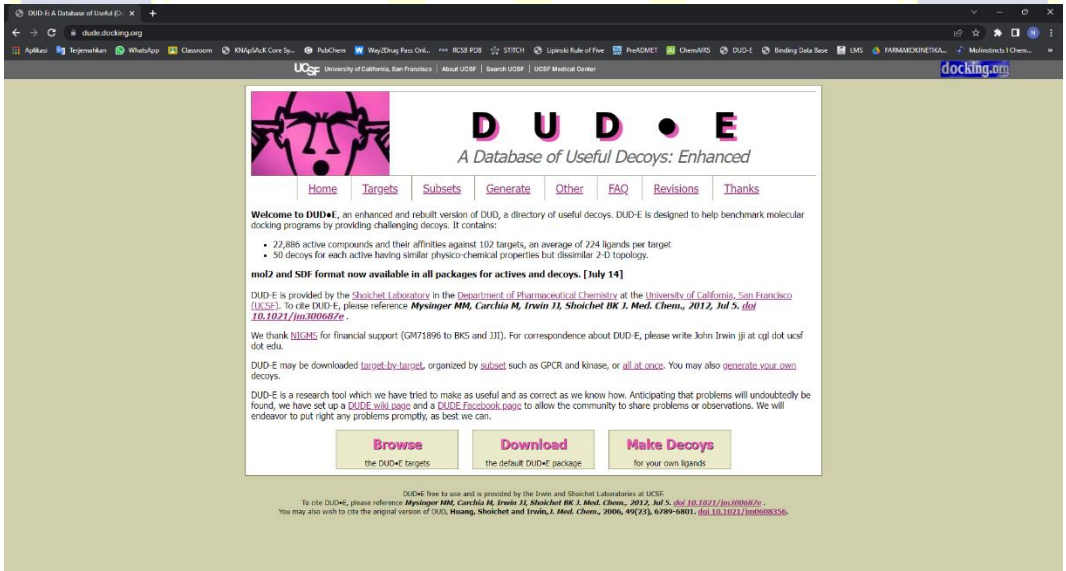


Gambar VII. 12 Tampilan situs *Protein Data Bank*

LAMPIRAN 4
(LANJUTAN)

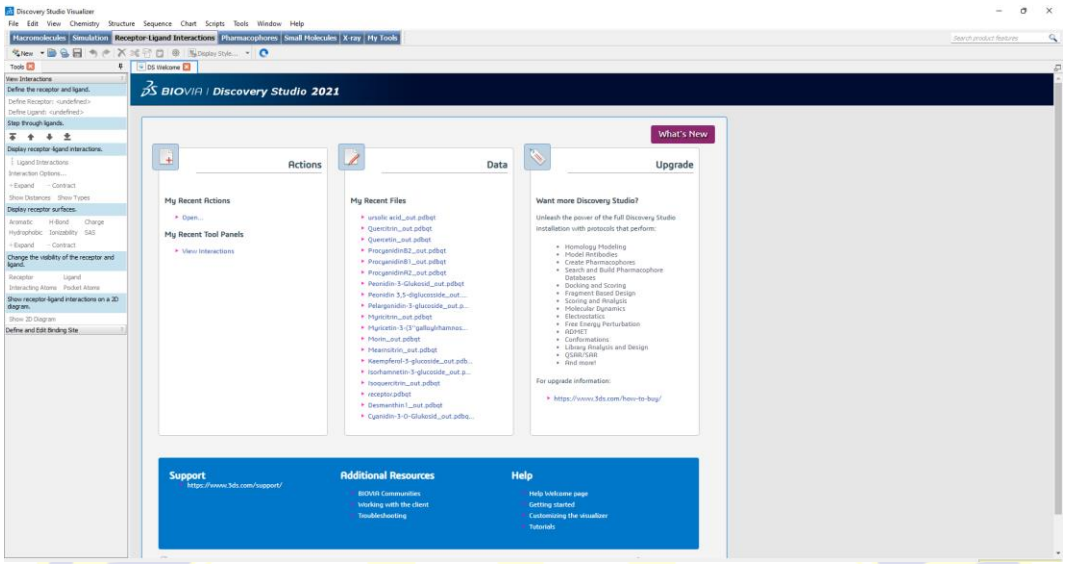


Gambar VII. 13 Tampilan situs *Binding Data Base*

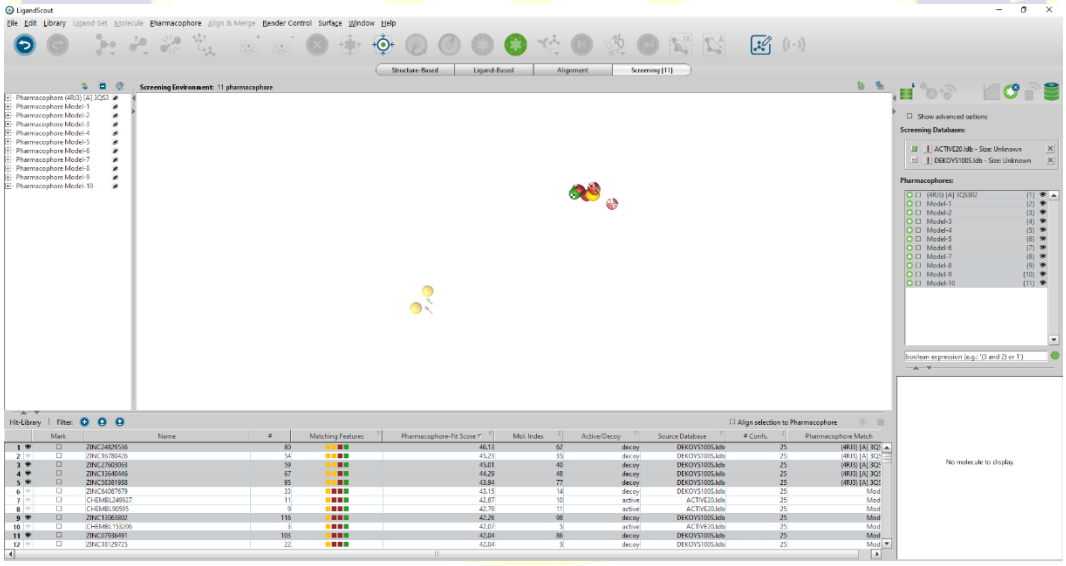


Gambar VII. 14 Tampilan situs *DUD-E*

LAMPIRAN 4
(LANJUTAN)



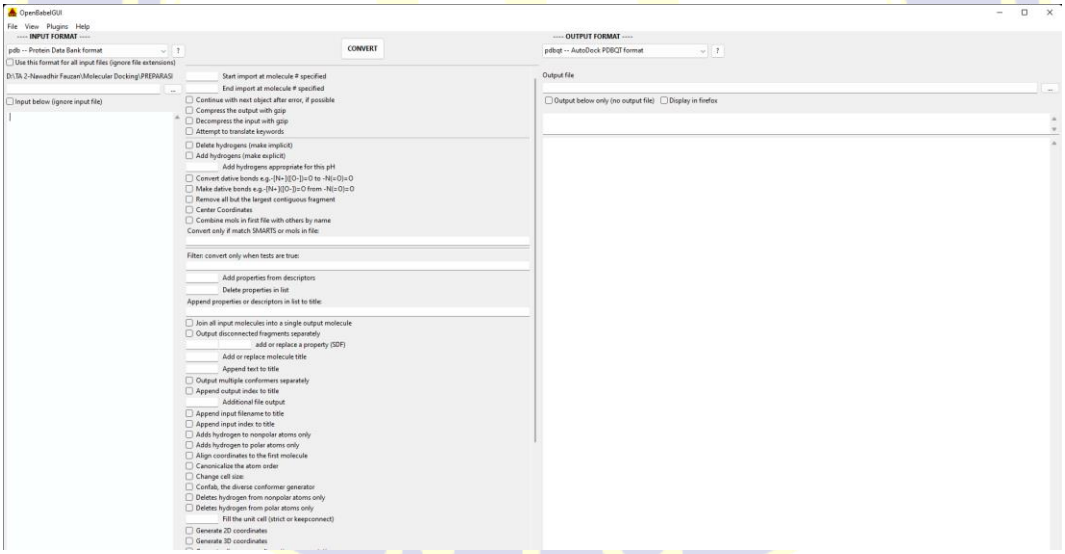
Gambar VII. 15 Tampilan *software Discovery Studio Visualizer*



Gambar VII. 16 Tampilan *software LigandScout*

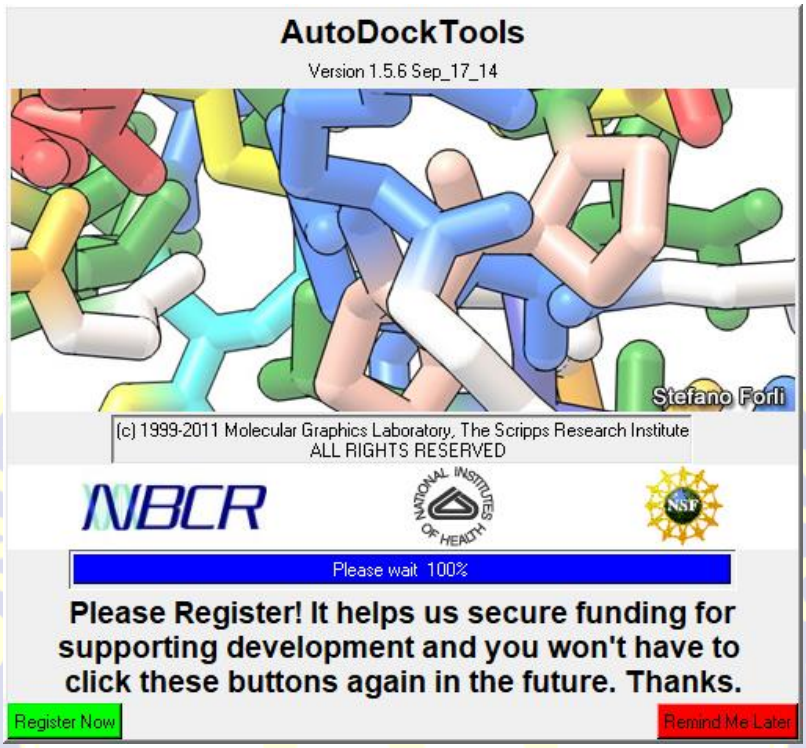
LAMPIRAN 4
(LANJUTAN)

Gambar VII. 17 Tampilan *software Marvin Sketch*

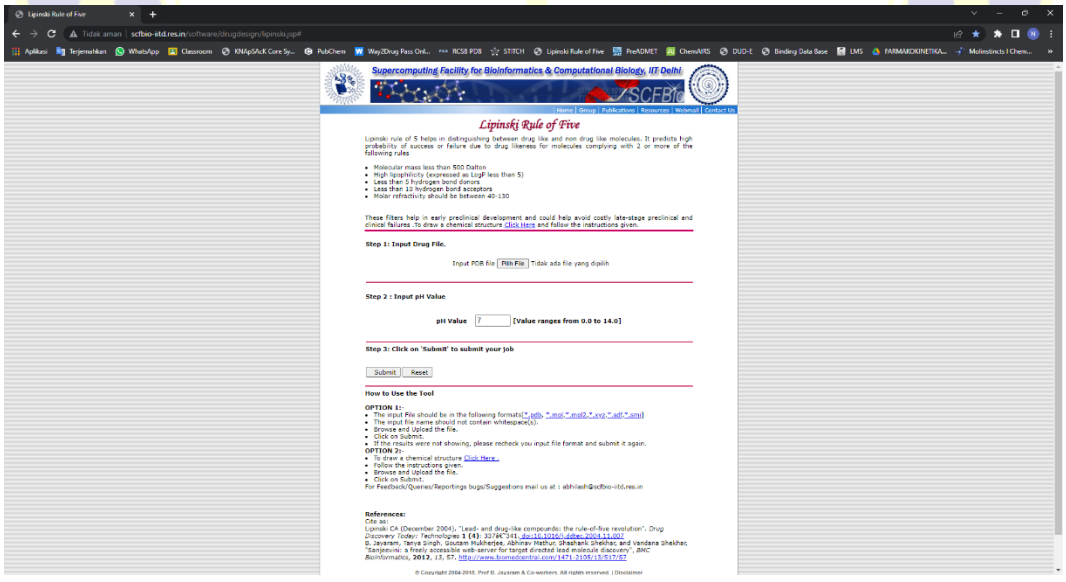


Gambar VII. 18 Tampilan *software Open Babel*

LAMPIRAN 4
(LANJUTAN)

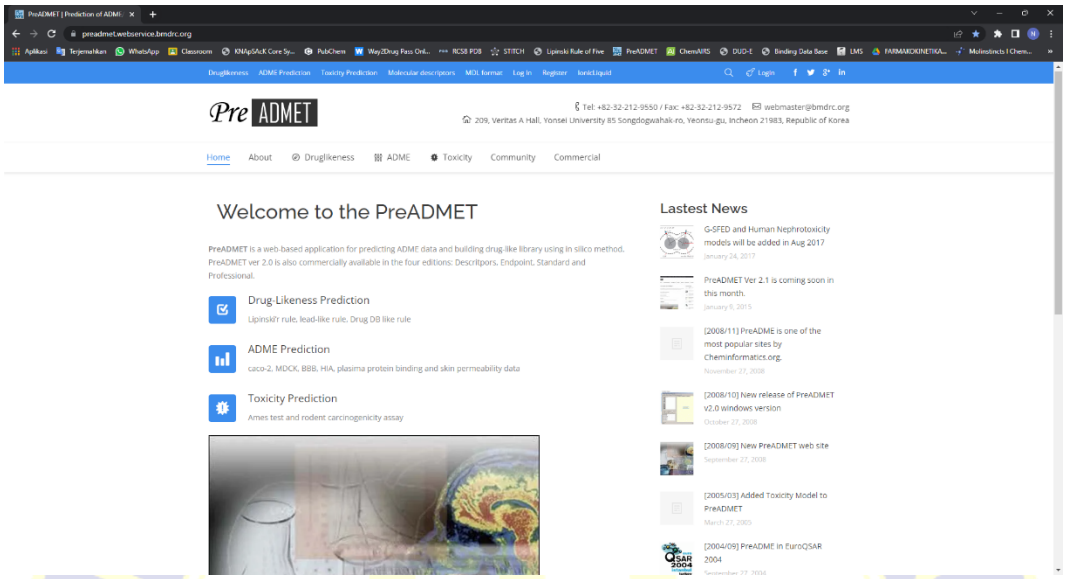


Gambar VII. 19 Tampilan *software AutodockTools*



Gambar VII. 20 Tampilan *situs Lipinski Rule of Five*

LAMPIRAN 4
(LANJUTAN)

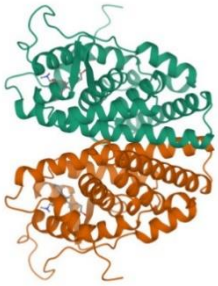
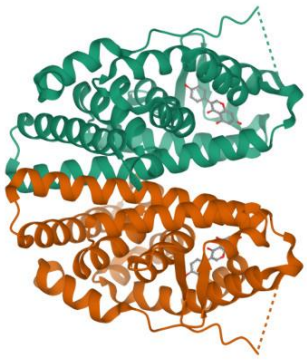


Gambar VII. 21 Tampilan situs *PreADMET*

LAMPIRAN 5

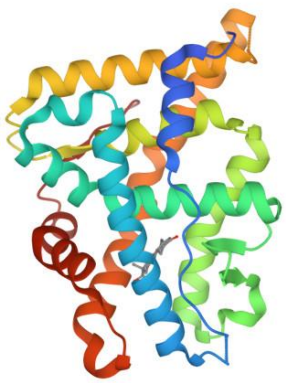
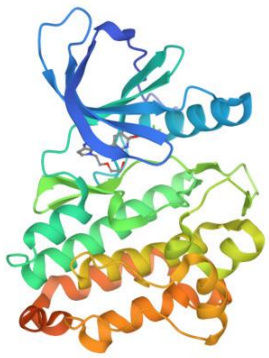
STRUKTUR 3D RESEPTOR

Tabel VII. 1
Struktur 3D Reseptor

ID PDB	STRUKTUR KOMPLEKS
3ERT	
1QKM	

LAMPIRAN 5
(LANJUTAN)

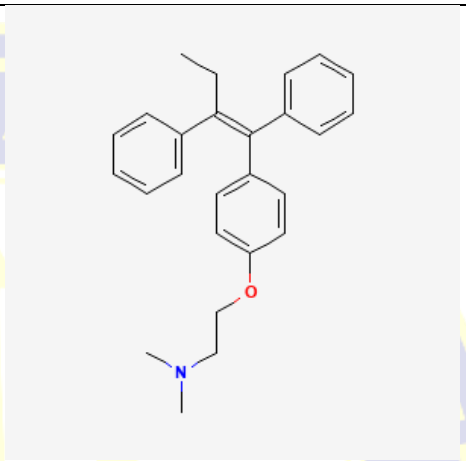
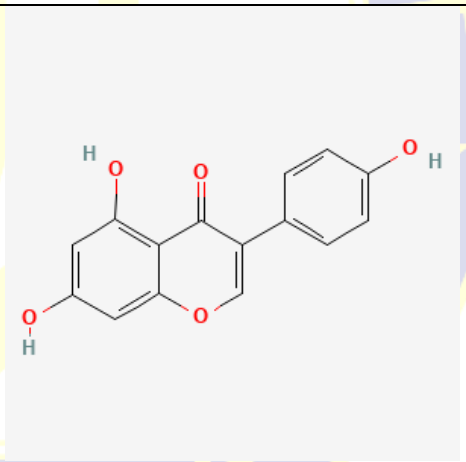
Tabel VII. 1
Lanjutan

ID PDB	STRUKTUR KOMPLEKS
1SQN	
3PP0	

LAMPIRAN 6

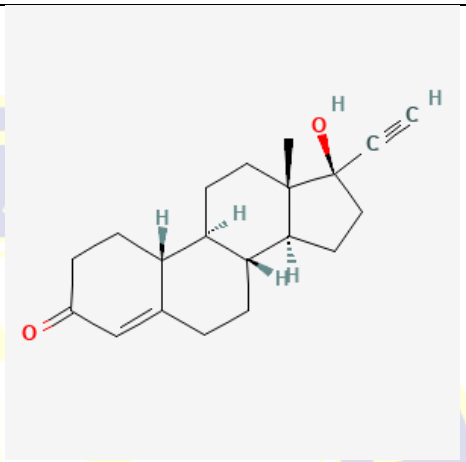
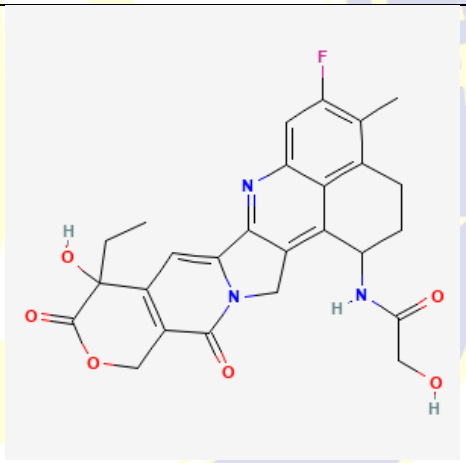
STRUKTUR 2D LIGAN PEMBANDING

Tabel VII. 2
Struktur 3D Ligan Pembanding

NAMA LIGAN PEMBANDING	STRUKTUR SENYAWA
4-Hidroxytamoxifen	
Genistein	

LAMPIRAN 6
(LANJUTAN)

Tabel VII.2
Lanjutan

NAMA LIGAN PEMBANDING	STRUKTUR SENYAWA
Norethindrone	
Trastuzumab	

LAMPIRAN 7

HASIL PENCARIAN SENYAWA

Tabel VII. 3
Daftar Senyawa Aktif

No.	Bagian Tanaman	Senyawa	CID	Referensi
1.	Minyak daun	*α-thujene*	17868	[10]
2.	Minyak daun	*(+)-α-pinene*	82227	[10]
3.	Minyak daun	*camphene*	6616	[10]
4.	Minyak daun	*(-)-β-pinene*	440967	[10]
5.	Minyak daun	*myrcene*	31253	[10]
6.	Minyak daun	*α-phellandrene*	7460	[10]
7.	Minyak daun	*α-terpinene*	7462	[10]
8.	Minyak daun	*p-cymene*	7463	[10]
9.	Minyak daun	*limonene*	22311	[10]
10.	Minyak daun	*(Z)-β-ocimene*	5320250	[10]
11.	Minyak daun	*(E)-β-ocimene*	5281553	[10]

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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
12.	Minyak daun	*γ-terpinene*	7461	[10]
13.	Minyak daun	*terpinolene*	11463	[10]
14.	Minyak daun	*linalool*	6549	[10]
15.	Minyak daun	*α-fenchol*	439711	[10]
16.	Minyak daun	*isopulegol*	170833	[10]
17.	Minyak daun	*borneol*	64685	[10]
18.	Minyak daun	*terpinen-4-ol*	11230	[10]
19.	Minyak daun	*α-terpineol*	17100	[10]
20.	Minyak daun	*isopulegyl acetate*	94579	[10]
21.	Minyak daun	*α-cubebene*	442359	[10]
22.	Minyak daun	*citronellyl acetate*	9017	[10]

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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
23.	Minyak daun	*α-copaene*	19725	[10]
24.	Minyak daun	*β-elemene*	6918391	[10]
25.	Minyak daun	*(-)-β-caryophyllene*	5281515	[10]
26.	Minyak daun	*aromadendrene*	91354	[10]
27.	Minyak daun	*α-humulene*	5281520	[10]
28.	Minyak daun	*allo-aromadendrene*	42608158	[10]
29.	Minyak daun	*γ-muurolene*	12313020	[10]
30.	Minyak daun	*β-selinene*	442393	[10]
31.	Minyak daun	*α-selinene*	10856614	[10]
32.	Minyak daun	*α -muurolene*	12306047	[10]
33.	Minyak daun	*δ-amorphene*	12306059	[10,11]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
34.	Minyak daun	*δ-cadinene*	441005	[10]
35.	Minyak daun	*cadina-1,4-diene*	6427091	[10]
36.	Minyak daun	*(-)-caryophyllene oxide*	1742210	[10]
37.	Minyak daun	*Myltayl-4(12)-ene*	12721294	[11]
38.	Minyak daun	*Viridiflorol*	11996452	[11]
39.	Minyak daun	*(2E,6E)-Farnesyl acetate*	638500	[11]
40.	Minyak daun	*2-pentadecanone*	61303	[11]
41.	Minyak daun	*α-cadinol*	10398656	[10,12]
42.	Ekstrak methanol daun	*ursolic acid*	64945	[12]
43.	Ekstrak methanol daun	*β-sitosterol*	222284	[12]

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(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
44.	Minyak atsiri daun	*hexanoic acid*	8892	[12]
45.	Minyak atsiri daun	*methyl salicylate*	4133	[12]
46.	Minyak atsiri daun	*3-hexen-1-ol*	5284503	[12]
47.	Minyak atsiri daun dan buah	*1-octen-3-ol*	18827	[12,13]
48.	Minyak atsiri daun dan buah	*n-hexadecanoic acid*	985	[12]
49.	Minyak atsiri daun	*2-hexenal*	5281168	[12]
50.	Minyak atsiri daun	*3-buten-2-one*	6570	[12]

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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
51.	Minyak atsiri daun	*1-hexanol*	8103	[12,13]
52.	Minyak atsiri daun	*phytol*	5280435	[11,12]
53.	Minyak atsiri daun	*acetic acid*	176	[12]
54.	Minyak atsiri daun	*azulene*	9231	[12]
55.	Minyak atsiri daun	*2-octen-1-ol*	5318599	[12]
56.	Minyak atsiri buah	*9-octadecynoic acid*	68167	[12]
57.	Minyak atsiri buah	*(Z,Z)-9-12-octadecadien-1-ol*	5365682	[12]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
58.	Minyak atsiri buah	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	5284507	[12]
59.	Minyak atsiri buah	*tetradecanoic acid*	11005	[12]
60.	Minyak atsiri buah	*2-ethylhexyl p-methoxycinnamate*	5355130	[12]
61.	Minyak atsiri buah	*2-phenylethanol*	6054	[12]
62.	Minyak atsiri buah	*(E)-2-octen-1-ol*	5318599	[12]
63.	Minyak atsiri buah	*benzyl benzoate*	2345	[12]
64.	Buah	*p-Coumaric acid*	637542	[14–16]
65.	Buah	*Benzoic acid*	243	[14,15]
66.	Buah	*(-)-Epicatechin gallate*	107905	[14,15]
67.	Buah	*(+)-Catechin*	9064	[14–16]

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(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
68.	Buah	*(-)-Epicatechin*	72276	[14–16]
69.	Buah	*Procyanidin A2*	124025	[14,15]
70.	Buah	*Procyanidin B1*	11250133	[14,15]
71.	Buah	*Procyanidin B2*	122738	[14,15]
72.	Buah	*Isoquercitrin*	5280804	[14,15]
73.	Buah	*Quercetin*	5280343	[14–16]
74.	Buah	*Rutin*	5280805	[14–16]
75.	Buah	*Cyanidin-3,5-O-diglucoside*	441688	[14]
76.	Buah	*Cyanidin-3-O-glucoside*	441667	[14]
77.	Buah	*Cyanidin 3-glucoside*	4481259	[15,17]
78.	Buah	*Peonidin 3-glucoside*	443654	[15,17]
79.	Buah	*Peonidin 3,5-diglucoside*	44256843	[15]
80.	Buah	*Pelargonidin 3-glucoside*	443648	[15]
81.	Ekstrak methanol buah	*Isorhamnetin 3-glucoside*	5318645	[15]
82.	Buah	*Kaempferol 3-glucoside*	5282102	[15]

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(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
83.	Buah	*Quercitrin*	5280459	[15]
84.	Buah	*Myricetin*	5281672	[15]
85.	Buah	*Morin*	5281670	[15]
86.	Buah	*(-)-Epigallocatechin gallate*	65064	[15]
87.	Buah	*Ellagic acid*	5281855	[15]
88.	Buah	*t-Cinnamic acid*	444539	[15]
89.	Buah	*Gallic acid*	370	[15]
90.	Buah	*Chlorogenic acid*	1794427	[15]
91.	Ekstrak daun	*Vanillic acid*	8468	[16]
92.	Ekstrak daun	*Caffeic acid*	689043	[16]
93.	Ekstrak daun	*Ferulic acid*	445858	[16]
94.	Ekstrak daun	*pentyllic acid*	338	[16]
95.	Ekstrak methanol kulit batang	*Pinocembrin*	68071	[18]

LAMPIRAN 7
(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
96.	Ekstrak methanol kulit batang	*8-Methylpinocembrin*	6453244	[18]
97.	Ekstrak methanol kulit batang	*Uvangoletin*	6483649	[18]
98.	Ekstrak methanol kulit batang	*Stercurensin*	11778601	[18]
99.	Ekstrak methanol kulit batang	*2',4'-Dihydroxy-6'-methoxy-3'-methyldihydrochalcone*	10085385	[18]
100.	Ekstrak methanol kulit batang	*Aurentiacin*	11472044	[18]

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(LANJUTAN)

Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
101.	Ekstrak methanol kulit batang	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	10424762	[18]
102.	Ekstrak methanol kulit batang	*Epigallocatechin gallate*	65064	[18]
103.	Ekstrak methanol kulit batang	*Myricitrin*	5281673	[18]
104.	Ekstrak methanol kulit batang	*Mearnsitrin*	6918652	[18]
105.	Ekstrak methanol kulit batang	*Desmanthin 1*	44259450	[18]

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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
106.	Ekstrak methanol kulit batang	*Myricetin-3-(3"galloylrhamnoside)*	44259451	[18]
107.	Buah	*Acetaldehyde*	177	[13]
108.	Buah	*Ethanol*	702	[13]
109.	Buah	*1-Propanol*	1031	[13]
110.	Buah	*Diacetyl*	650	[13]
111.	Buah	*Ethyl acetate*	8857	[13]
112.	Buah	*Isobutanol*	6560	[13]
113.	Buah	*3-Methylbutanal*	11552	[13]
114.	Buah	*1-Butanol*	263	[13]
115.	Buah	*1-Penten-3-ol*	12020	[13]
116.	Buah	*3-Methyl-2-butanone*	11251	[13]
117.	Buah	*Isoamyl alcohol*	31260	[13]
118.	Buah	*2-Methyl-1-butanol*	8723	[13]
119.	Buah	*1H-Pyrrole*	8027	[13]
120.	Buah	*Pyridine*	1049	[13]
121.	Buah	*1-Pentanol*	6276	[13]
122.	Buah	*(Z)-2-Pentenol*	5364919	[13]
123.	Buah	*3-Methyl-2-buten-1-ol*	11173	[13]
124.	Buah	*2,3-Butanediol*	262	[13]
125.	Buah	*Toluene*	1140	[13]

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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
126.	Buah	*Hexanal*	6184	[13]
127.	Buah	*2-Furfural*	7362	[13]
128.	Buah	*Ethyl (E)-2-butenoate*	429065	[13]
129.	Buah	*(E)-2-Hexanal*	5281168	[13]
130.	Buah	*(Z)-3-Hexanol*	12178	[13]
131.	Buah	*Isoamyl acetate*	31276	[13]
132.	Buah	*2-Heptanone*	8051	[13]
133.	Buah	*Ethylbenzene*	7500	[13]
134.	Buah	*Heptanal*	8130	[13]
135.	Buah	*2-Acetylfuran*	14505	[13]
136.	Buah	*Pentyl acetate*	12348	[13]
137.	Buah	*γ-Butyrolactone*	7302	[13]
138.	Buah	*Pentanoic acid*	7991	[13]
139.	Buah	*α-Pinene*	6654	[13]
140.	Buah	*Ethyl 3-hydroxybutanoate*	62572	[13]
141.	Buah	*(E)-2-Heptenal*	5283316	[13]
142.	Buah	*Benzaldehyde*	240	[13]
143.	Buah	*5-Methyl-2-furfural*	12097	[13]
144.	Buah	*1-Heptanol*	8129	[13]
145.	Buah	*β-Pinene*	14896	[13]
146.	Ekstrak methanol kulit batang	*(+)-6,8-Dimethyl-5methoxypinocembrin*	-	[18]

LAMPIRAN 7
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Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
147.	Minyak esensial daun	*Menthone*	26447	[75]
148.	Minyak esensial daun	*α-Ylangene*	442409	[75]
149.	Minyak esensial daun	*Sibirene*	14167644	[75]
150.	Minyak esensial daun	*gamma – Elemene*	6432312	[75]
151.	Minyak esensial daun	*gamma – Patchoulene*	521302	[75]
152.	Minyak esensial daun	*Trans-sesquisabinene hydrate*	6428444	[75]
153.	Minyak esensial daun	*Spathulenol*	92231	[75]

LAMPIRAN 7
(LANJUTAN)

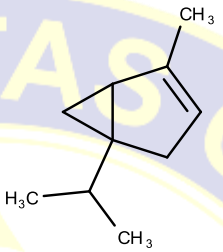
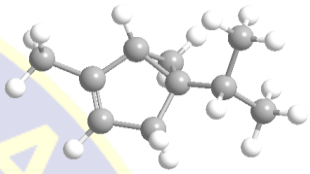
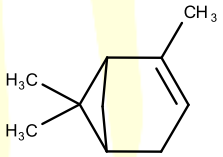
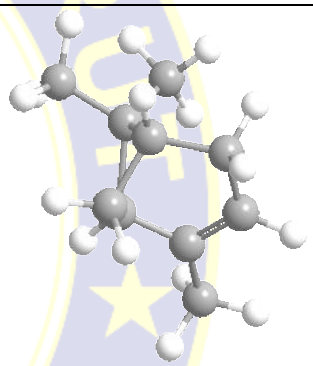
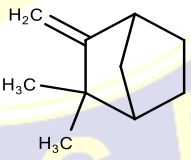
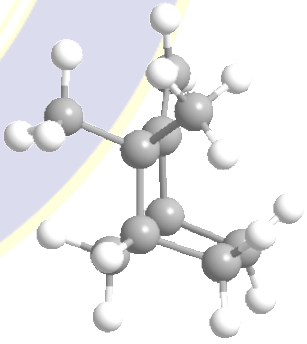
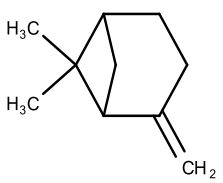
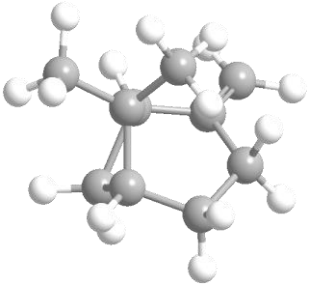
Tabel VII. 3
Lanjutan

No.	Bagian Tanaman	Senyawa	CID	Referensi
154.	Minyak esensial daun	*Guaiol*	227829	[75]
155.	Minyak esensial daun	*Mustakone*	12313013	[75]

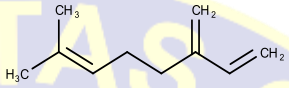
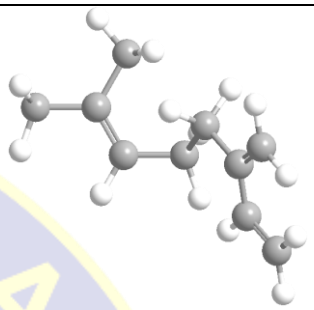
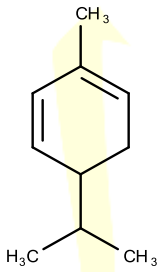
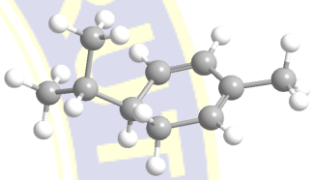
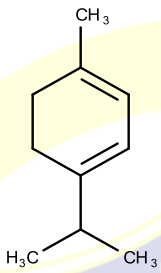
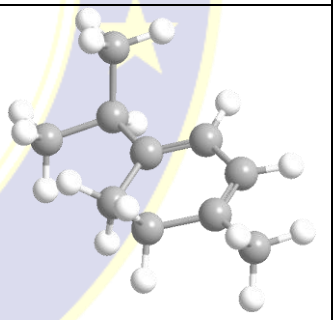
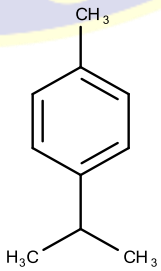
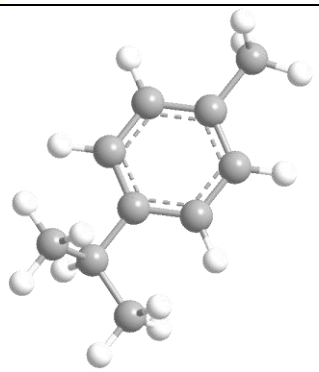
LAMPIRAN 8

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.	*α-thujene*	$C_{10}H_{16}$		
2.	*(+)-α-pinene*	$C_{10}H_{16}$		
3.	*camphene*	$C_{10}H_{16}$		
4.	*(-)-β-pinene*	$C_{10}H_{16}$		

LAMPIRAN 8
(LANJUTAN)
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
5.	*myrcene*	$C_{10}H_{16}$		
6.	*α-phellandrene*	$C_{10}H_{16}$		
7.	*α-terpinene*	$C_{10}H_{16}$		
8.	*p-cymene*	$C_{10}H_{14}$		

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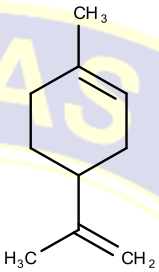
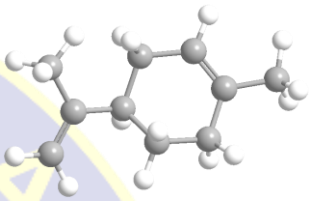
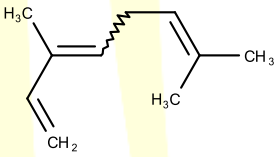
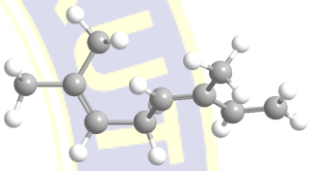
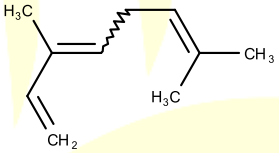
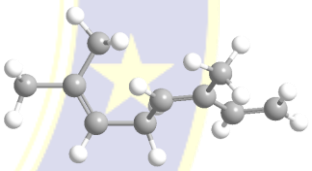
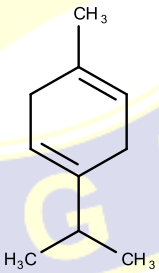
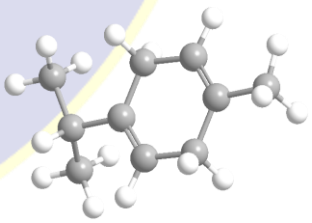
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
9.	*limonene*	$C_{10}H_{16}$		
10.	*(Z)-β-ocimene*	$C_{10}H_{16}$		
11.	*(E)-β-ocimene*	$C_{10}H_{16}$		
12.	*γ-terpinene*	$C_{10}H_{16}$		

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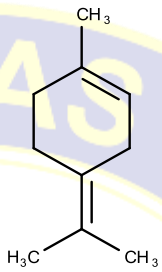
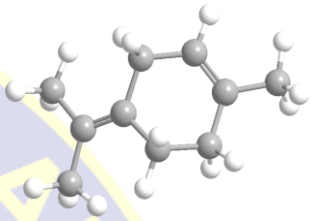
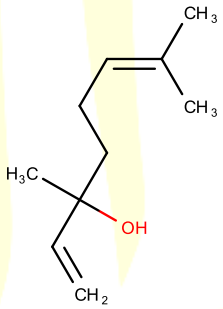
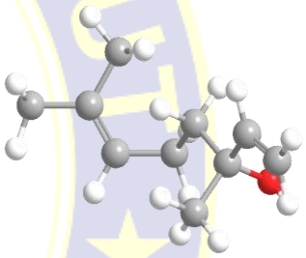
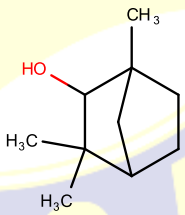
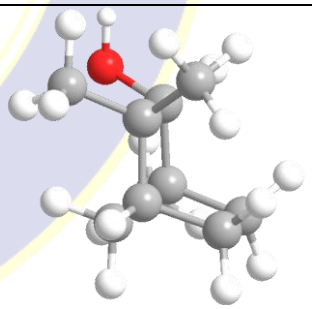
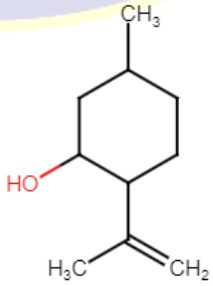
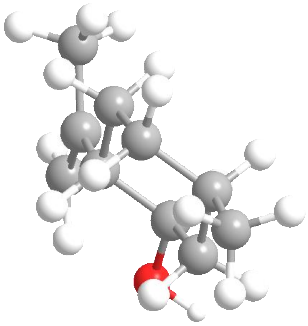
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
13.	*terpinolene*	$C_{10}H_{16}$		
14.	*linalool*	$C_{10}H_{18}O$		
15.	*α-Fenchol*	$C_{10}H_{18}O$		
16.	*isopulegol*	$C_{10}H_{18}O$		

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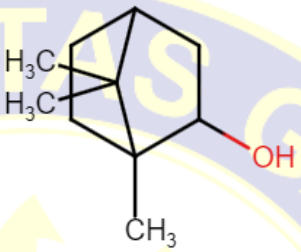
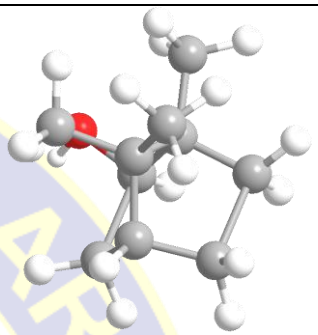
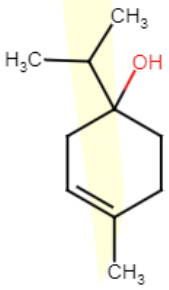
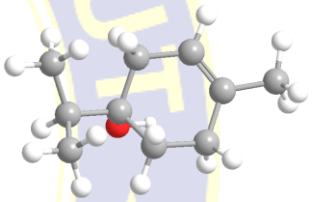
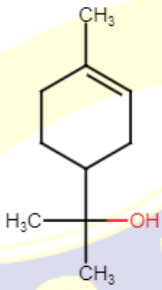
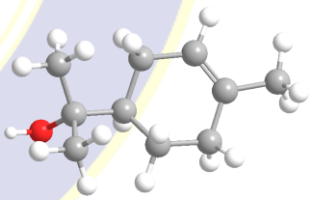
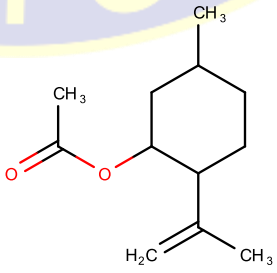
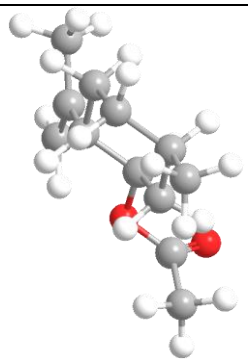
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
17.	*borneol*	$C_{10}H_{18}O$		
18.	*terpinen-4-ol*	$C_{10}H_{18}O$		
19.	*α-terpineol*	$C_{10}H_{18}O$		
20.	*Isopulegyl acetate*	$C_{12}H_{20}O_2$		

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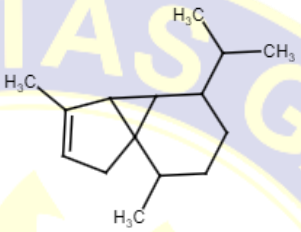
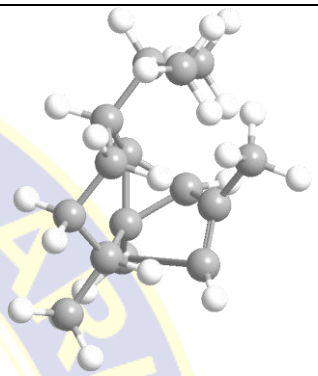
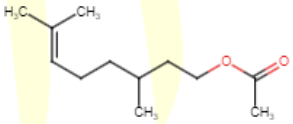
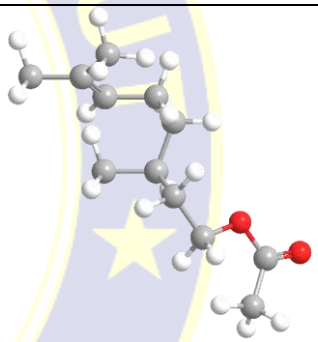
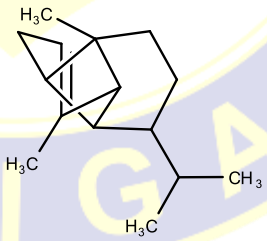
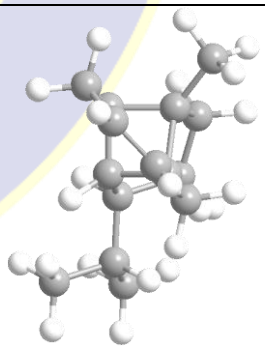
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
21.	*α-cubebene*	$C_{15}H_{24}$		
22.	*citronellyl acetate*	$C_{12}H_{22}O_2$		
23.	*α-copaene*	$C_{15}H_{24}$		

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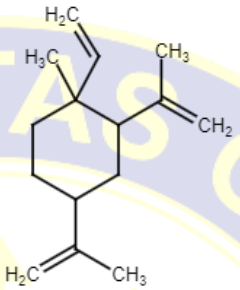
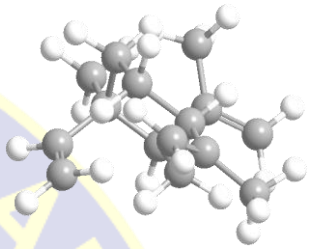
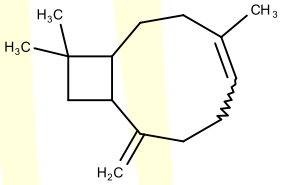
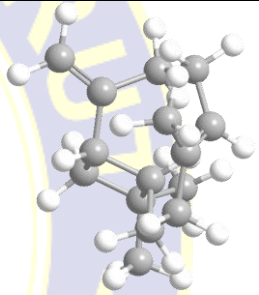
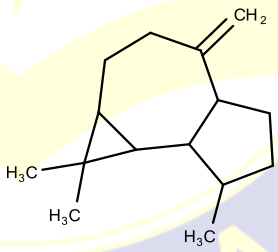
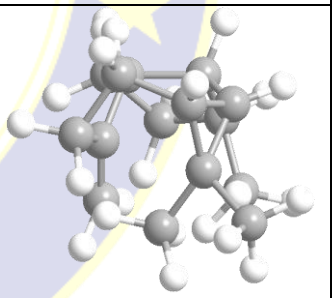
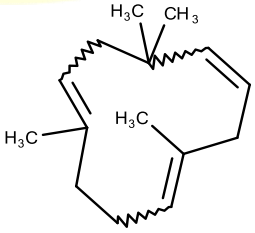
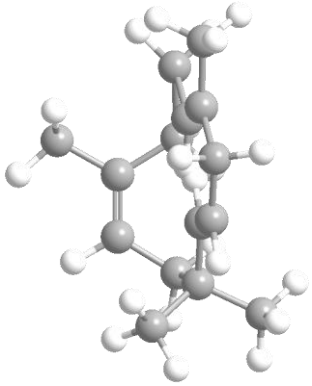
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
24.	*β-elemene*	$C_{15}H_{24}$		
25.	*(-)-β-caryophyllene*	$C_{15}H_{24}$		
26.	*aromadendrene*	$C_{15}H_{24}$		
27.	*α-humulene*	$C_{15}H_{24}$		

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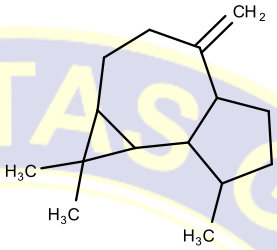
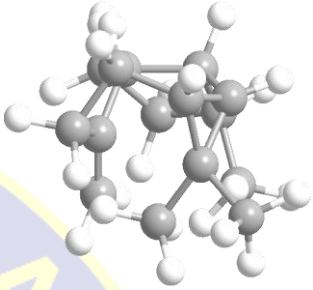
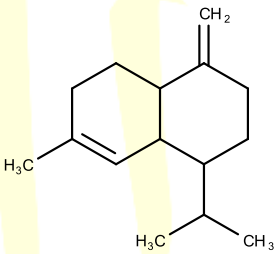
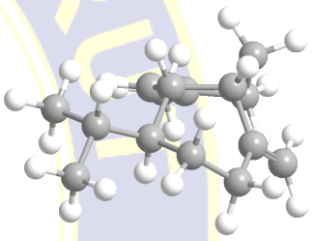
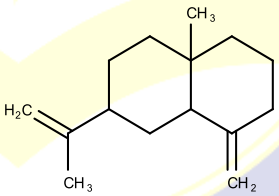
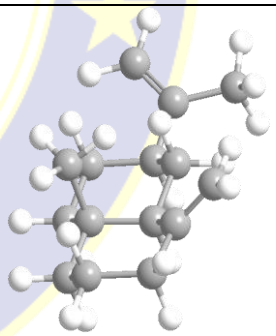
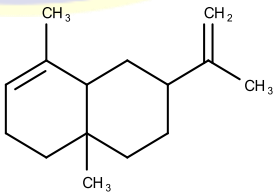
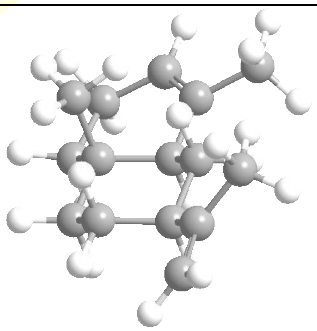
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
28.	*allo-aromadendrene*	$C_{15}H_{24}$		
29.	*γ-muurolene*	$C_{15}H_{24}$		
30.	*β-selinene*	$C_{15}H_{24}$		
31.	*α-selinene*	$C_{15}H_{24}$		

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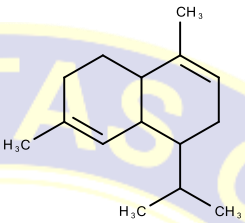
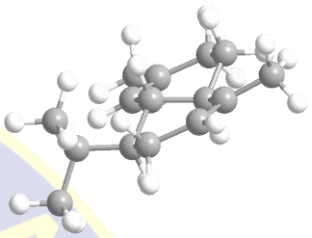
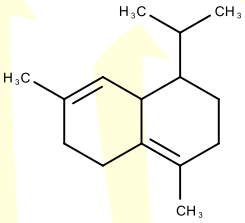
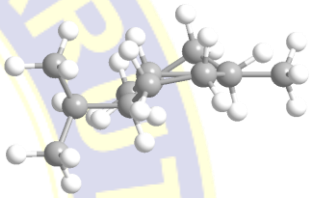
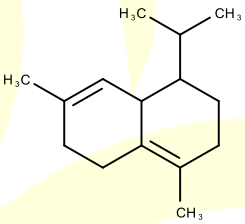
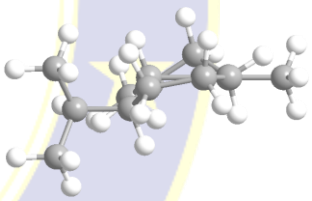
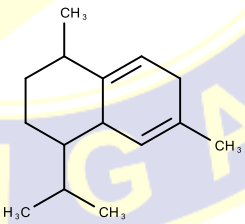
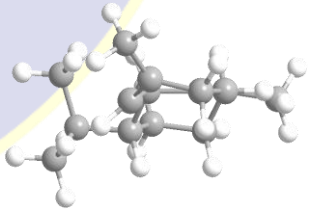
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
32.	*a-muurolene*	$C_{15}H_{24}$		
33.	*δ-amorphene*	$C_{15}H_{24}$		
34.	*δ-cadinene*	$C_{15}H_{24}$		
35.	*cadina-1,4-diene*	$C_{15}H_{24}$		

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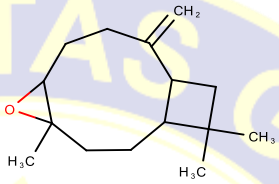
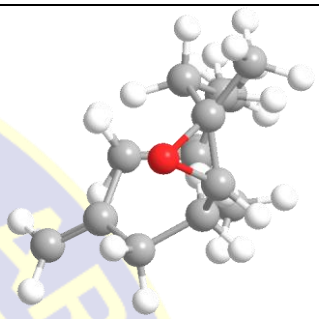
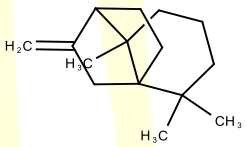
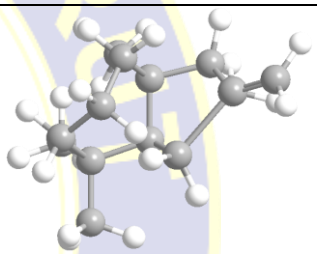
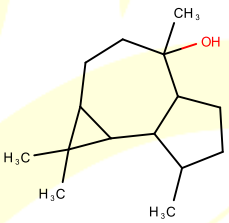
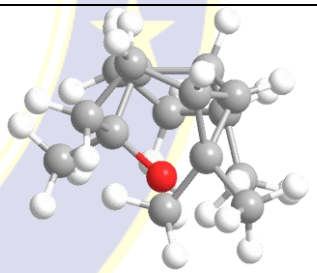
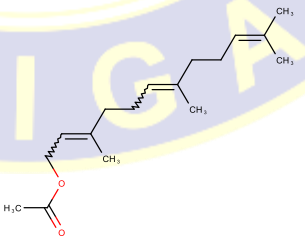
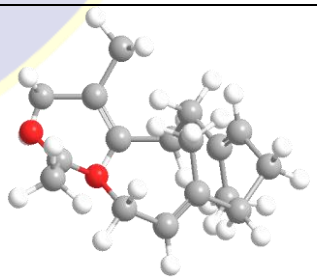
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
36.	*(-)-caryophyllene oxide*	$C_{15}H_{24}O$		
37.	*Myltayl-4(12)-ene*	$C_{15}H_{24}$		
38.	*Viridiflorol*	$C_{15}H_{26}O$		
39.	*(2E,6E)-Farnesyl acetate*	$C_{17}H_{28}O_2$		

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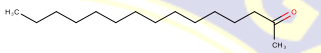
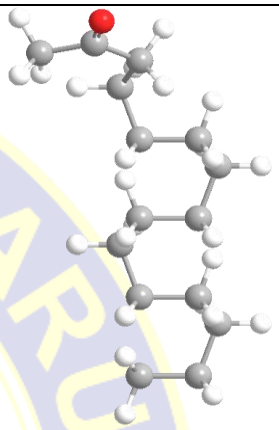
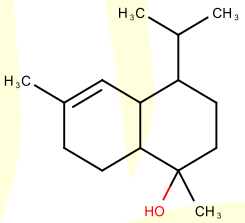
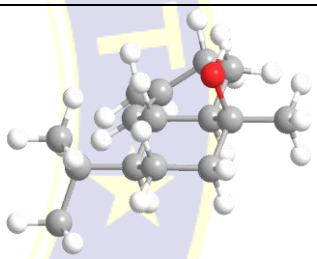
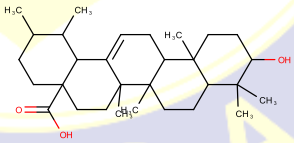
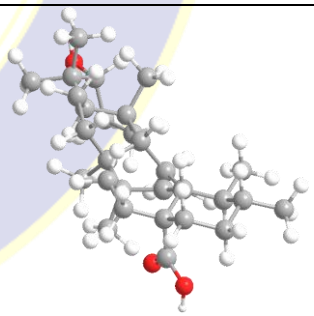
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
40.	*2-pentadecanone*	$C_{15}H_{30}O$		
41.	*α-cadinol*	$C_{15}H_{26}O$		
42.	*ursolic acid*	$C_{30}H_{48}O_3$		

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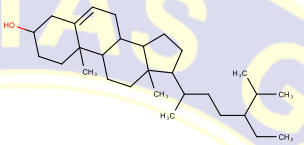
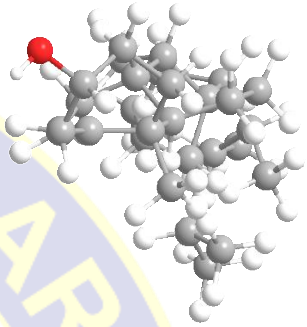
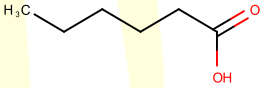
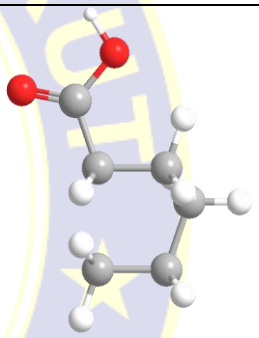
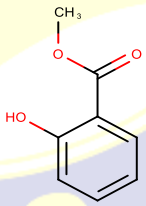
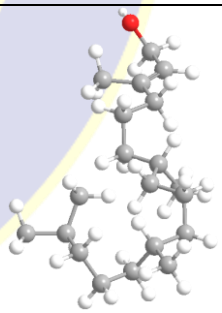
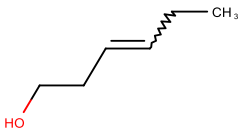
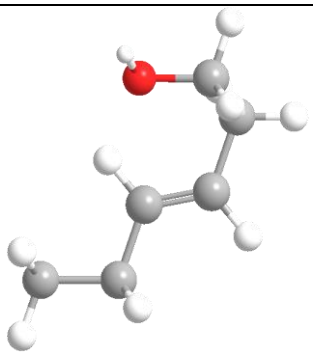
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
43.	*β-sitosterol*	$C_{29}H_{50}O$		
44.	*hexanoic acid*	$C_6H_{12}O_2$		
45.	*methyl salicylate*	$C_8H_8O_3$		
46.	*3-hexen-1-ol*	$C_6H_{12}O$		

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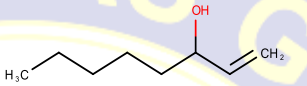
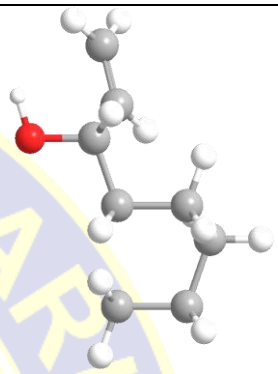
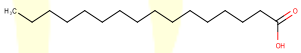
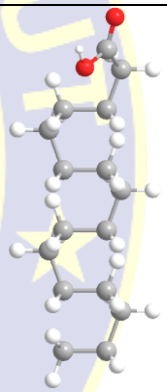
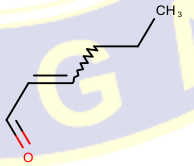
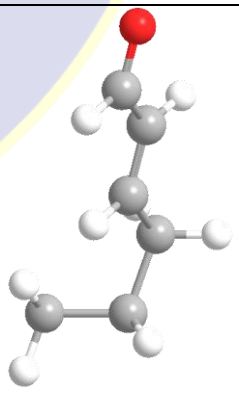
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
47.	*1-octen-3-ol*	$C_8H_{16}O$		
48.	*n-hexadecanoic acid*	$C_{16}H_{32}O_2$		
49.	*2-hexenal*	$C_6H_{10}O$		

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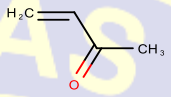
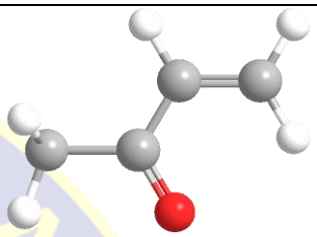
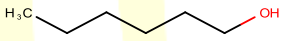
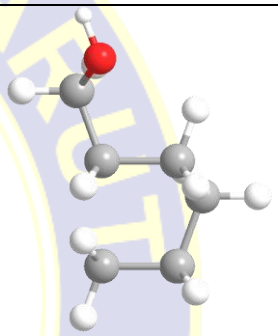
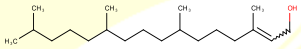
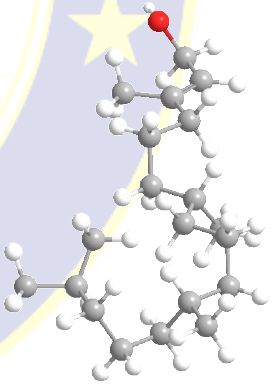
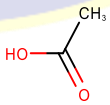
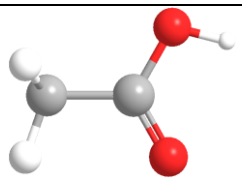
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
50.	*3-buten-2-one*	C_4H_6O		
51.	*1-hexanol*	$C_6H_{14}O$		
52.	*phytol*	$C_{20}H_{40}O$		
53.	*acetic acid*	$C_2H_4O_2$		

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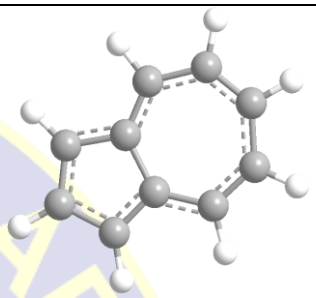
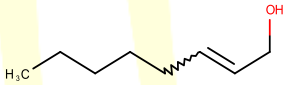
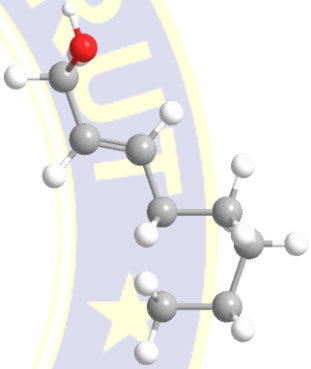
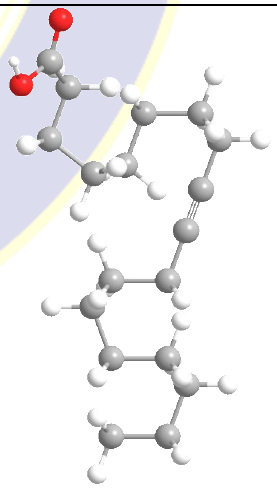
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
54.	*azulene*	$C_{10}H_8$		
55.	*2-octen-1-ol*	$C_8H_{16}O$		
56.	*9-octadecynoic acid*	$C_{18}H_{32}O_2$		

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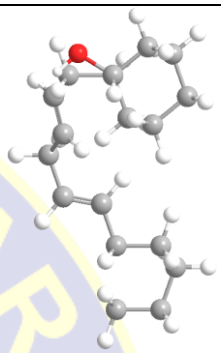
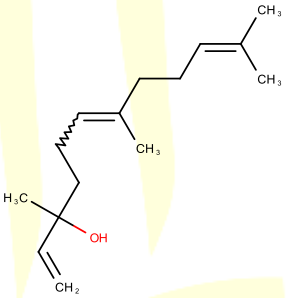
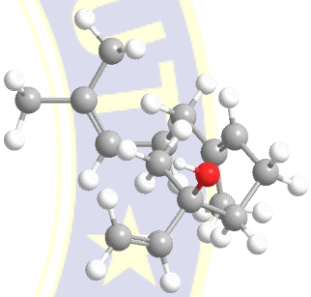
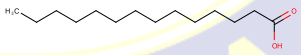
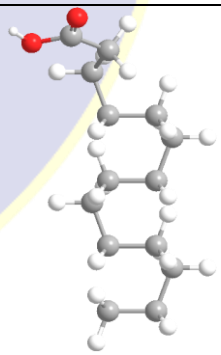
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
57.	*(Z,Z)-9-12-octadecadien-1-ol*	$C_{18}H_{34}O$		
58.	*(E)-3,7,11-trimethyl-1,6,10-dodecatrien-3-ol*	$C_{15}H_{26}O$		
59.	*tetradecanoic acid*	$C_{14}H_{28}O_2$		

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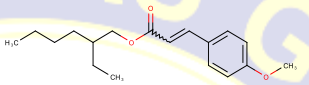
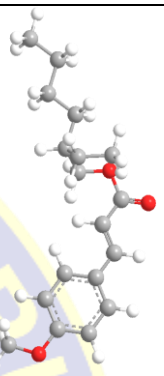
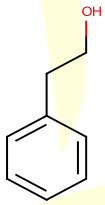
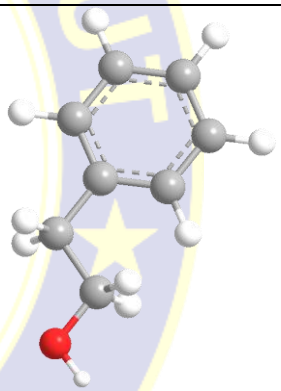
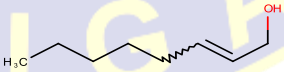
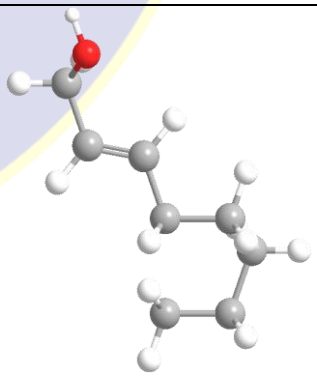
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
60.	*2-ethylhexyl p-methoxycinnamate*	$C_{18}H_{26}O_3$		
61.	*2-phenylethanol*	$C_8H_{10}O$		
62.	*(E)-2-octen-1-ol*	$C_8H_{16}O$		

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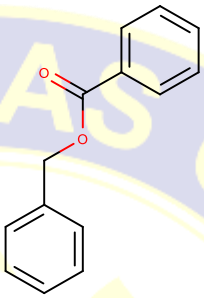
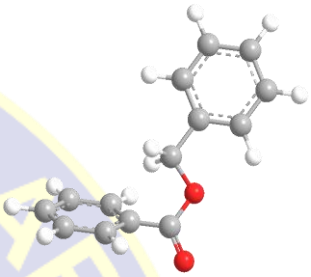
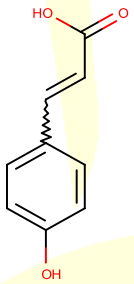
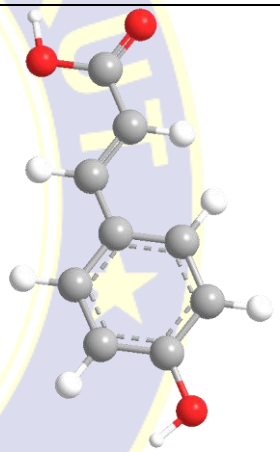
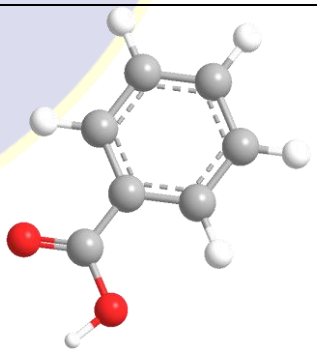
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
63.	*benzyl benzoate*	$C_{14}H_{12}O_2$		
64.	*p-Coumaric acid*	$C_9H_8O_3$		
65.	*Benzoic acid*	$C_7H_6O_2$		

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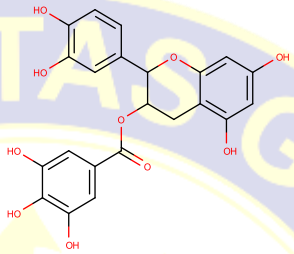
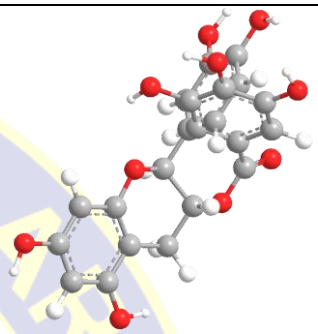
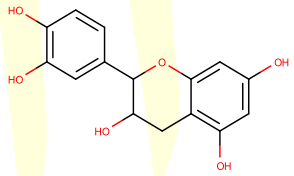
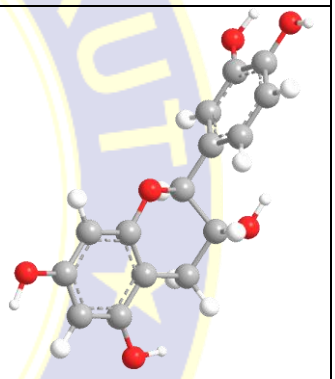
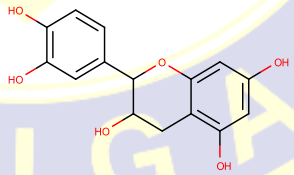
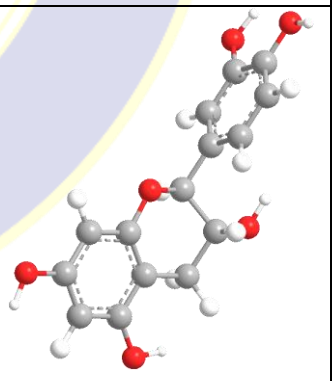
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
66.	*(-)-Epicatechin gallate*	$C_{22}H_{18}O_{10}$		
67.	*(+)-Catechin*	$C_{15}H_{14}O_6$		
68.	*(-)-Epicatechin*	$C_{15}H_{14}O_6$		

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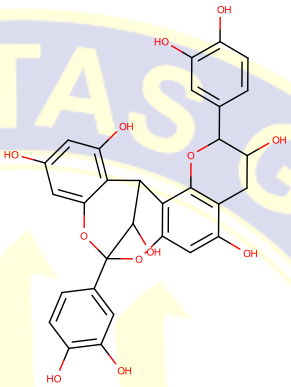
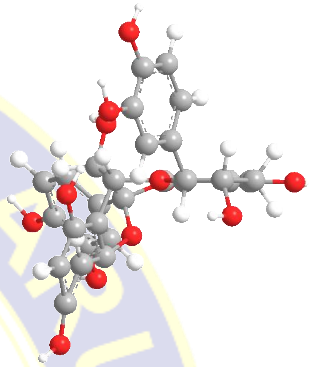
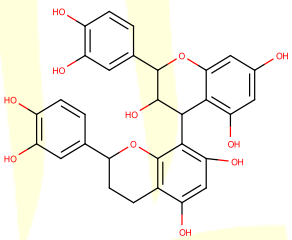
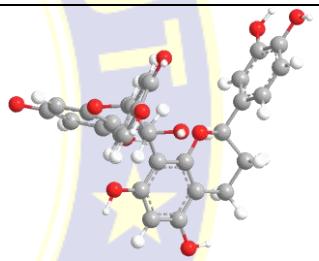
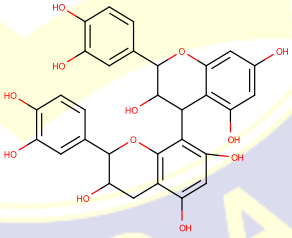
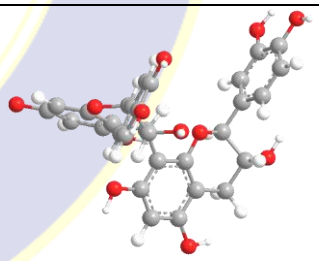
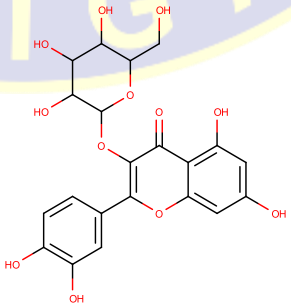
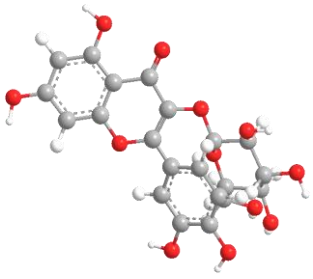
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
69.	*Procyanidin A2*	$C_{30}H_{24}O_{12}$		
70.	*Procyanidin B1*	$C_{30}H_{26}O_{12}$		
71.	*Procyanidin B2*	$C_{30}H_{26}O_{12}$		
72.	*Isoquercitrin*	$C_{21}H_{20}O_{12}$		

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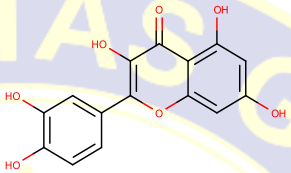
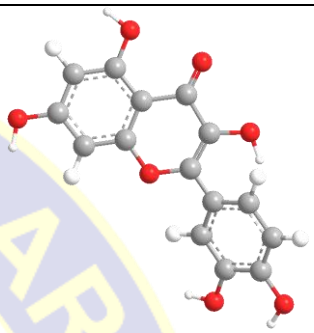
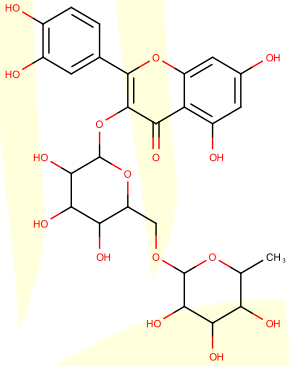
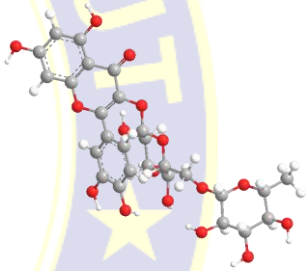
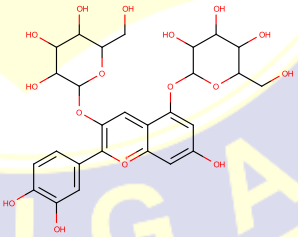
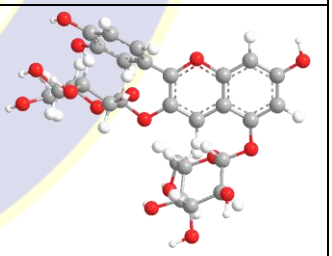
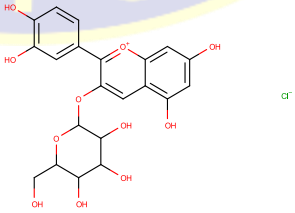
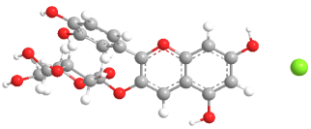
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
73.	*Quercetin*	$C_{15}H_{10}O_7$		
74.	*Rutin*	$C_{27}H_{30}O_{16}$		
75.	*Cyanidin-3,5-O-diglucoside*	$C_{27}H_{31}O_{16}^{+}$		
76.	*Cyanidin-3-O-glucoside*	$C_{21}H_{21}ClO_{11}$		

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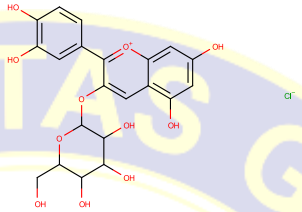
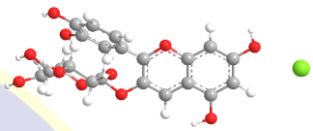
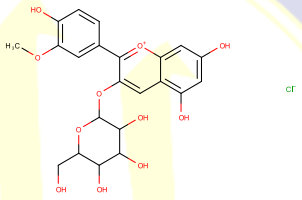
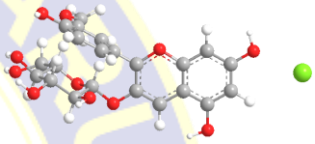
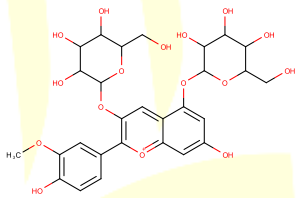
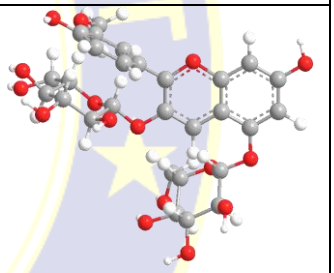
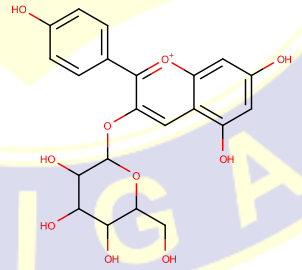
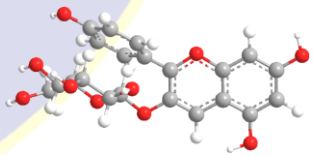
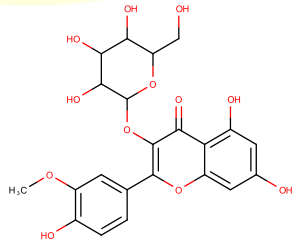
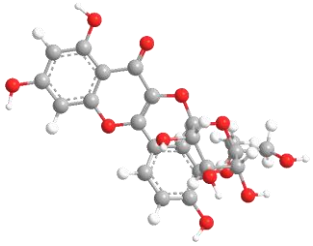
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
77.	*Cyanidin 3-glucoside*	$C_{21}H_{21}ClO_{11}$		
78.	*Peonidin 3-glucoside*	$C_{22}H_{23}ClO_{11}$		
79.	*Peonidin 3,5-diglucoside*	$C_{28}H_{33}O_{16}^{+}$		
80.	*Pelargonidin 3-glucoside*	$C_{21}H_{21}O_{10}^{+}$		
81.	*Isorhamnetin 3-glucoside*	$C_{22}H_{22}O_{12}$		

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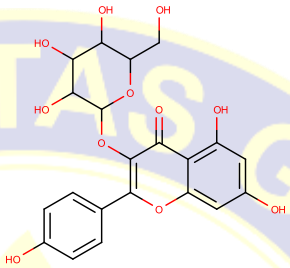
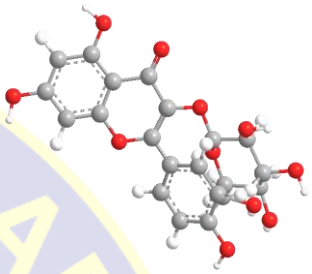
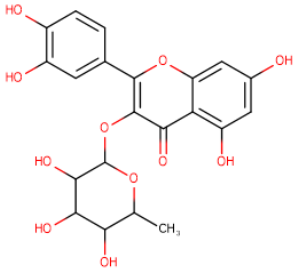
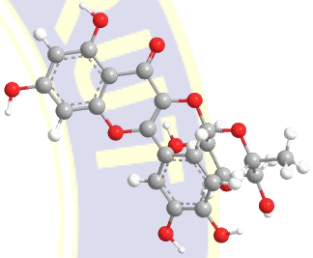
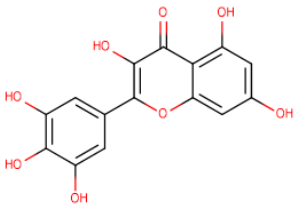
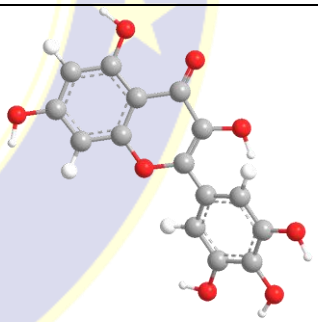
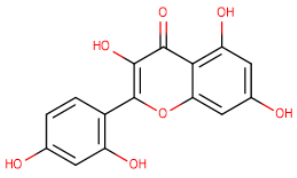
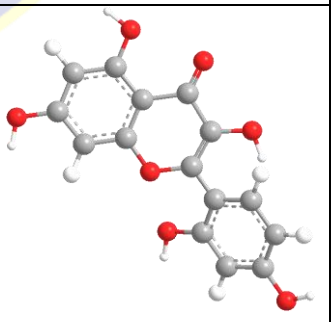
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
82.	*Kaempferol 3-glucoside*	$C_{21}H_{20}O_{11}$		
83.	*Quercitrin*	$C_{21}H_{20}O_{11}$		
84.	*Myricetin*	$C_{15}H_{10}O_8$		
85.	*Morin*	$C_{15}H_{10}O_7$		

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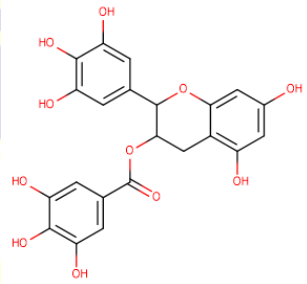
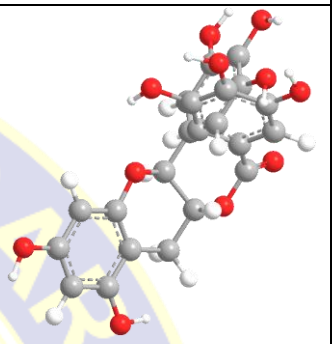
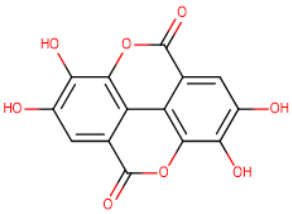
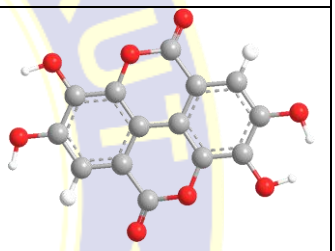
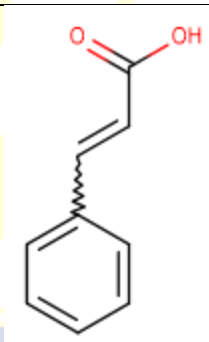
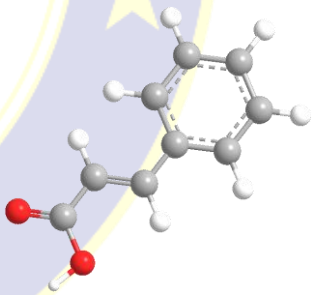
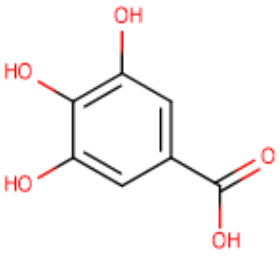
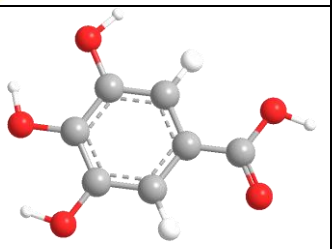
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
86.	*(-)-Epigallocatechin gallate*	$C_{22}H_{18}O_{11}$		
87.	*Ellagic acid*	$C_{14}H_6O_8$		
88.	*t-Cinnamic acid*	$C_9H_8O_2$		
89.	*Gallic acid*	$C_7H_6O_5$		

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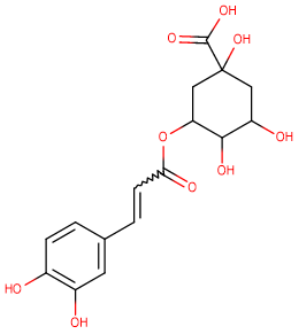
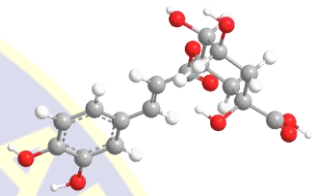
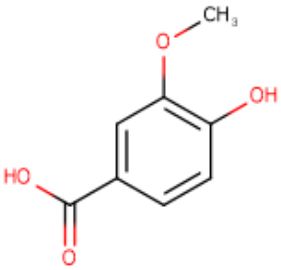
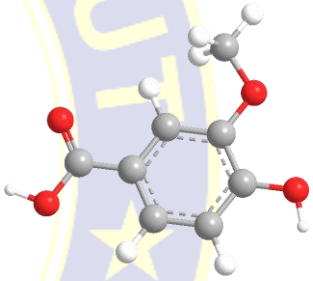
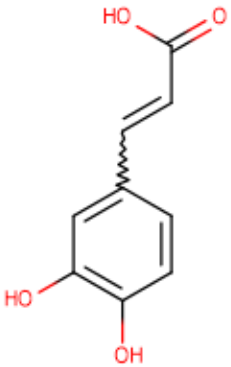
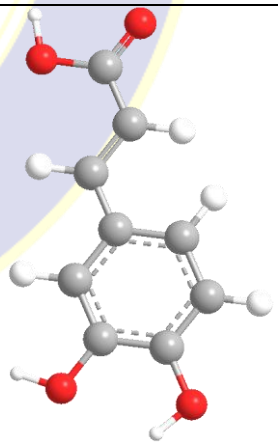
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
90.	*Chlorogenic acid*	$C_{16}H_{18}O_9$		
91.	*Vanillic acid*	$C_8H_8O_4$		
92.	*Caffeic acid*	$C_9H_8O_4$		

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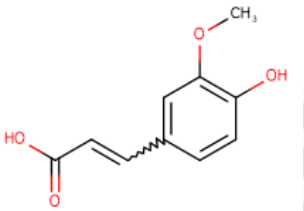
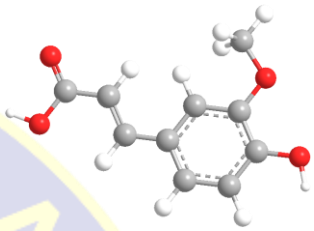
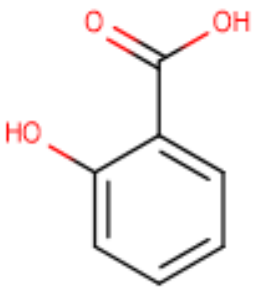
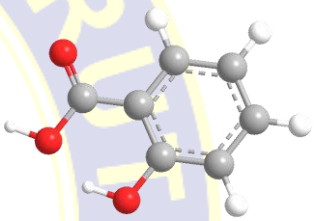
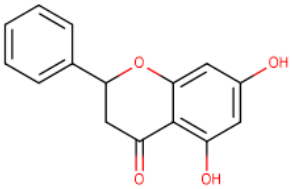
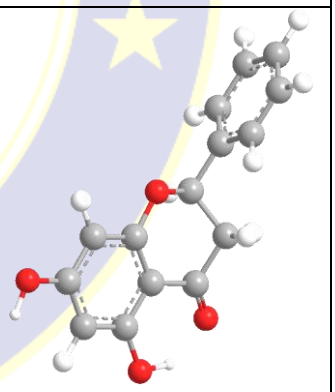
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
93.	*Ferulic acid*	$C_{10}H_{10}O_4$		
94.	*Salicylic acid*	$C_7H_6O_3$		
95.	*Pinocembrin*	$C_{15}H_{12}O_4$		

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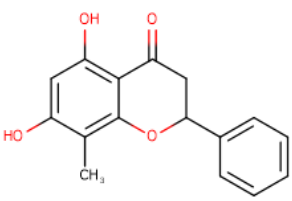
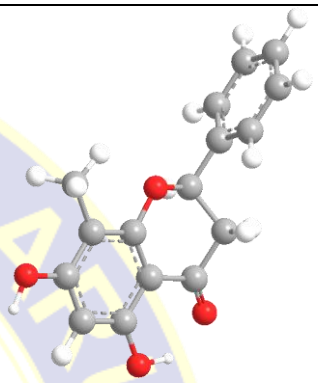
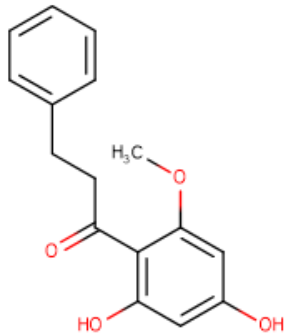
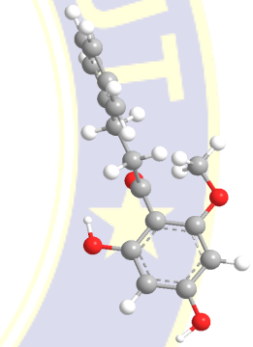
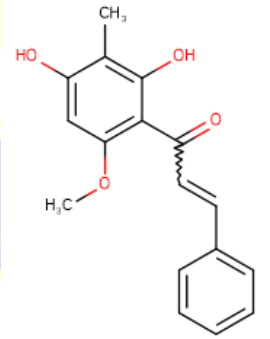
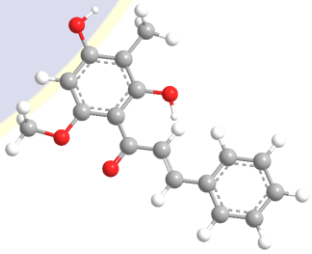
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
96.	*8-Methylpinocembrin*	$C_{16}H_{14}O_4$		
97.	*Uvangoletin*	$C_{16}H_{16}O_4$		
98.	*Stercurensin*	$C_{17}H_{16}O_4$		

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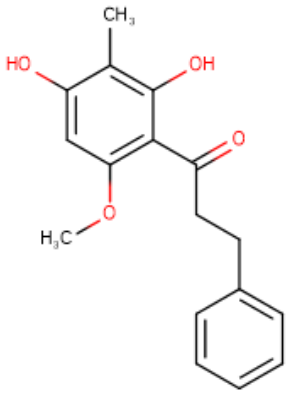
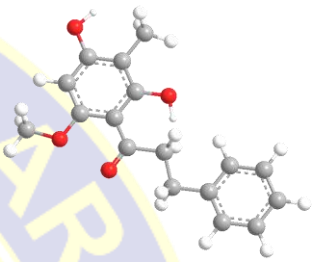
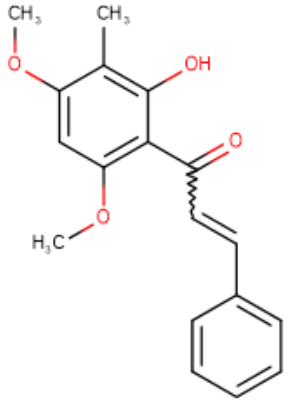
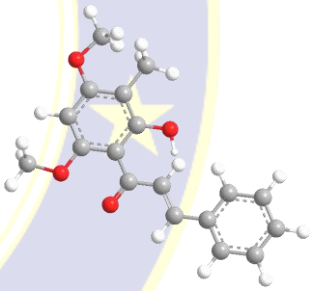
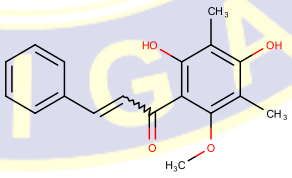
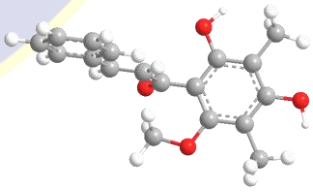
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
99.	*2',4'-Dihydroxy-6'-methoxy-3'-methyldihydrochalcone*	$C_{17}H_{18}O_4$		
100.	*Aurentiacin*	$C_{18}H_{18}O_4$		
101.	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	$C_{18}H_{18}O_4$		

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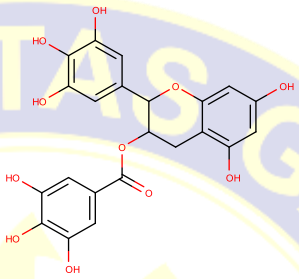
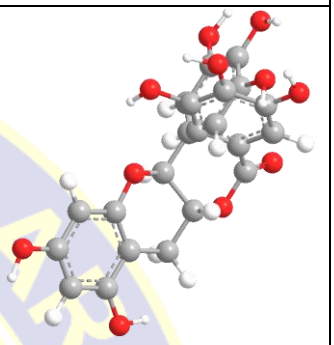
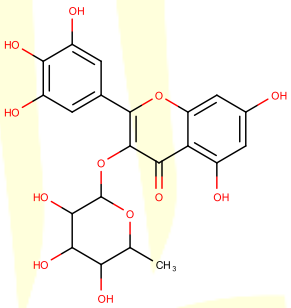
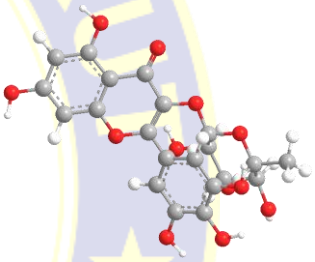
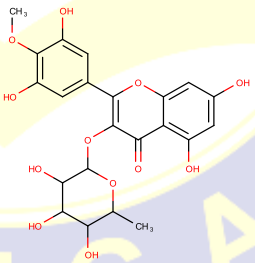
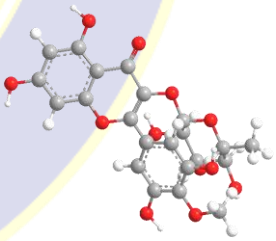
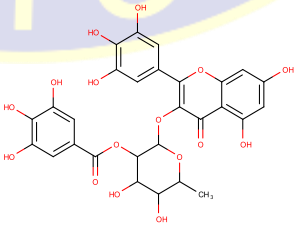
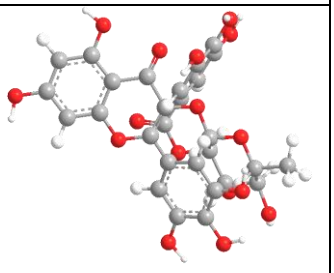
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
102.	*Epigallocatechin gallate*	$C_{22}H_{18}O_{11}$		
103.	*Myricitrin*	$C_{21}H_{20}O_{12}$		
104.	*Mearnsitrin*	$C_{22}H_{22}O_{12}$		
105.	*Desmanthin 1*	$C_{28}H_{24}O_{16}$		

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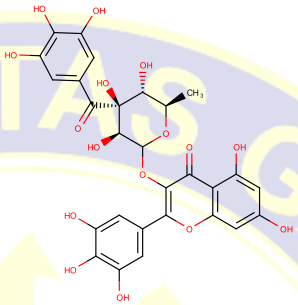
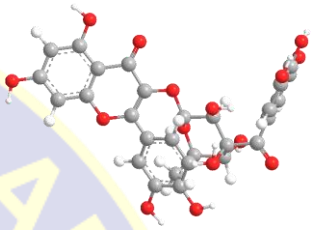
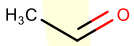
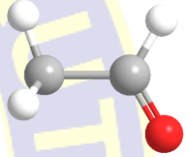
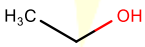
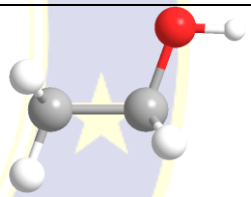
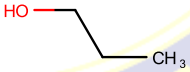
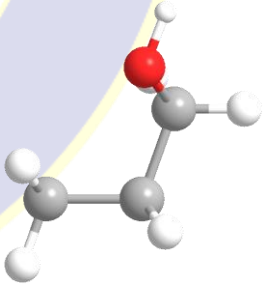
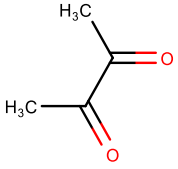
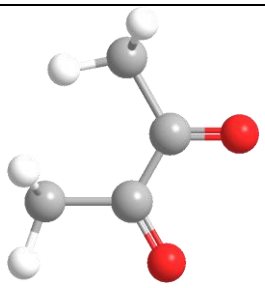
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
106.	*Myricetin-3-(3"galloylrhamnoside)*	$C_{28}H_{24}O_{16}$		
107.	*Acetaldehyde*	C_2H_4O		
108.	*Ethanol*	C_2H_6O		
109.	*1-Propanol*	C_3H_8O		
110.	*Diacetyl*	$C_4H_6O_2$		

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Tabel VII.4
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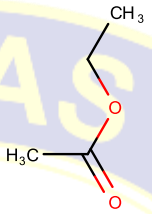
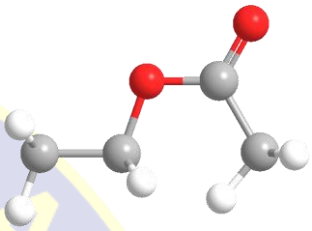
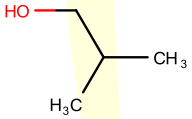
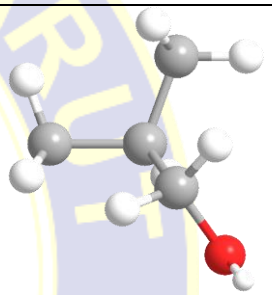
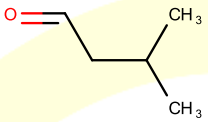
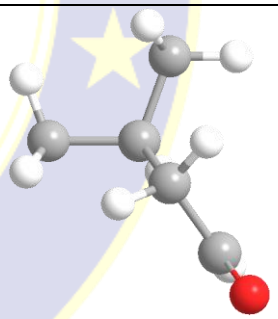
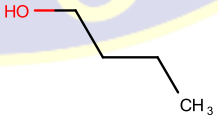
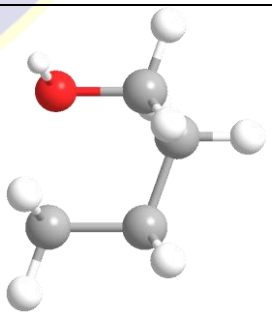
No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
111.	*Ethyl acetate*	$C_4H_8O_2$		
112.	*Isobutanol*	$C_4H_{10}O$		
113.	*3-Methylbutanal*	$C_5H_{10}O$		
114.	*1-Butanol*	$C_4H_{10}O$		

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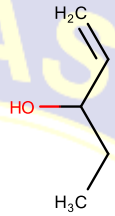
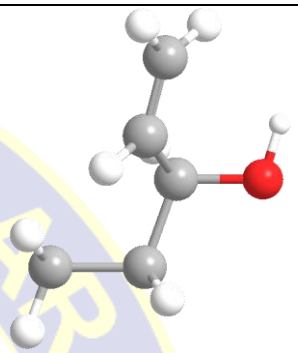
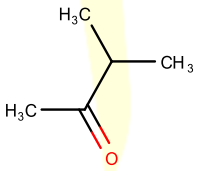
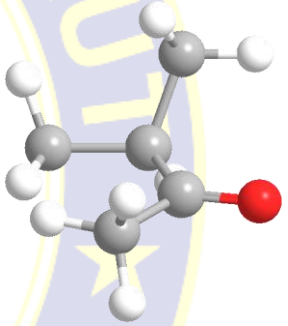
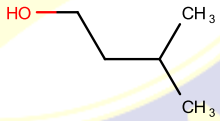
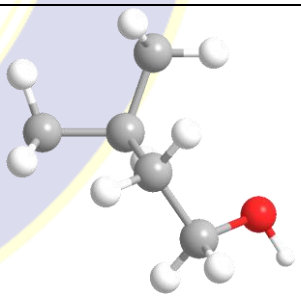
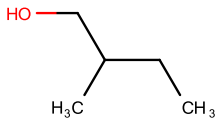
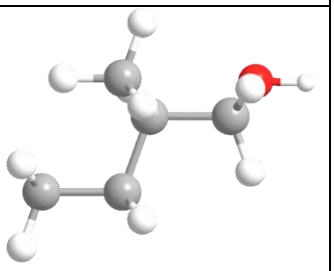
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
115.	*1-Penten-3-ol*	$C_5H_{10}O$		
116.	*3-Methyl-2-butanone*	$C_5H_{10}O$		
117.	*Isoamyl alcohol*	$C_5H_{12}O$		
118.	*2-Methyl-1-butanol*	$C_5H_{12}O$		

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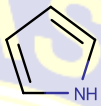
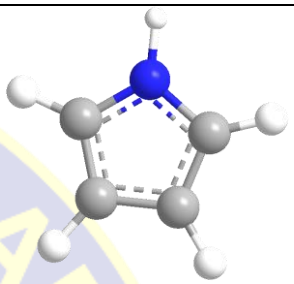
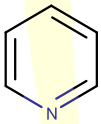
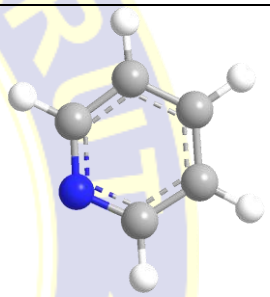
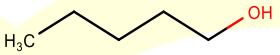
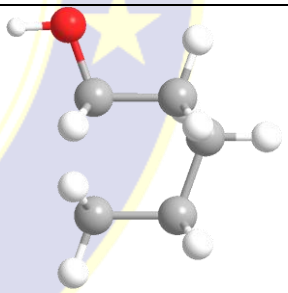
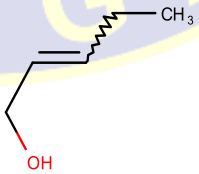
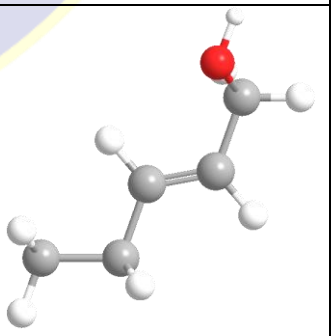
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
119.	*1H-Pyrrole*	C_4H_5N		
120.	*Pyridine*	C_5H_5N		
121.	*1-Pentanol*	$C_5H_{12}O$		
122.	*(Z)-2-Pentenol*	$C_5H_{10}O$		

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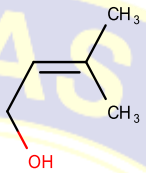
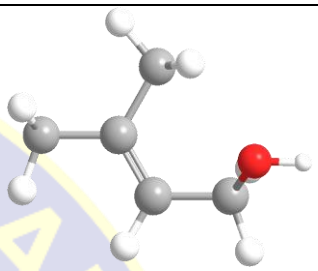
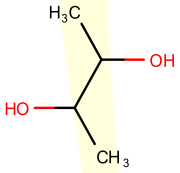
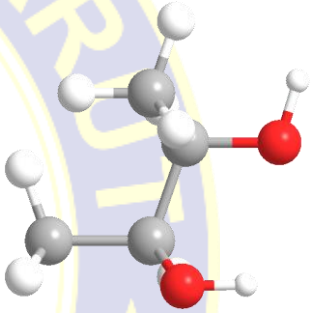
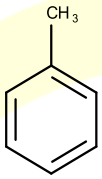
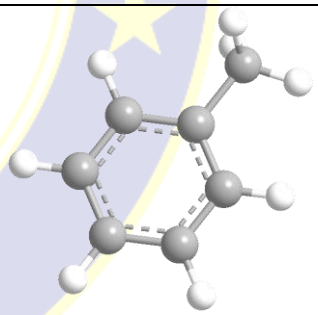
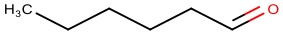
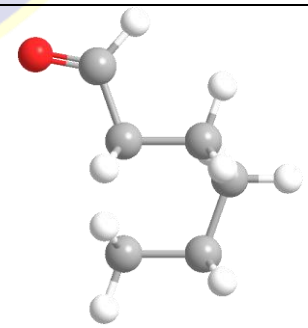
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
123.	*3-Methyl-2-buten-1-ol*	$C_5H_{10}O$		
124.	*2,3-Butanediol*	$C_4H_{10}O_2$		
125.	*Toluene*	C_7H_8		
126.	*Hexanal*	$C_6H_{12}O$		

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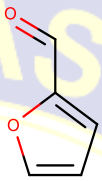
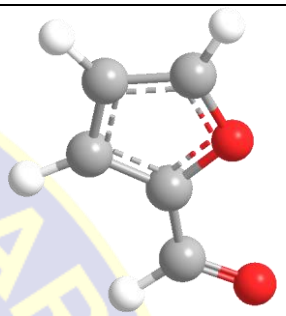
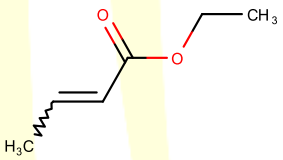
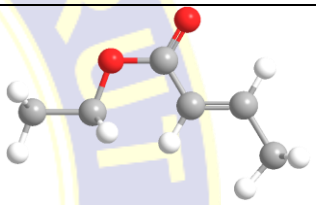
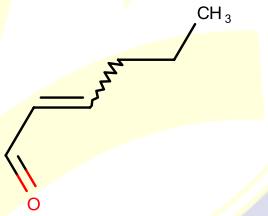
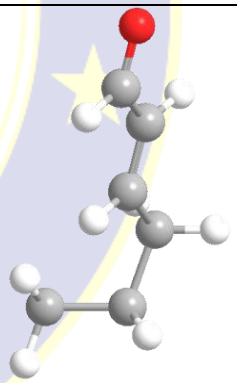
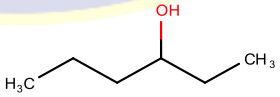
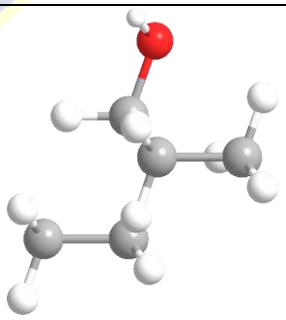
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
127.	*2-Furfural*	$C_5H_4O_2$		
128.	*Ethyl (E)-2-butenoate*	$C_6H_{10}O_2$		
129.	*(E)-2-Hexanal*	$C_6H_{10}O$		
130.	*(Z)-3-Hexanol*	$C_6H_{14}O$		

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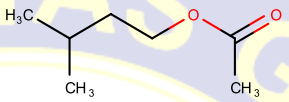
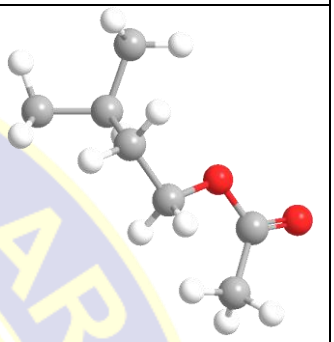
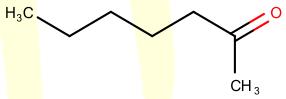
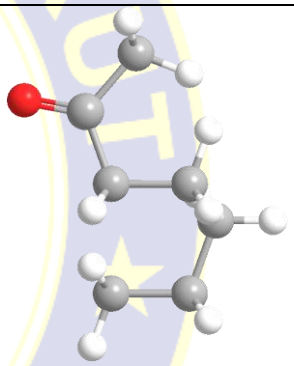
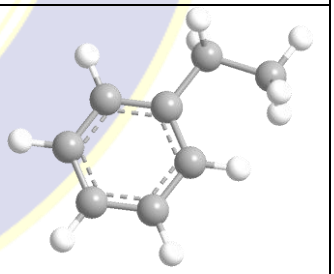
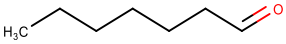
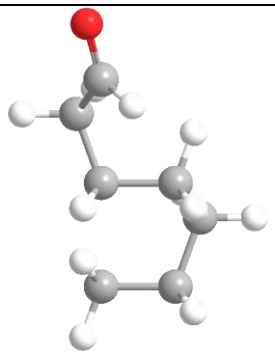
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
131.	*Isoamyl acetate*	$C_7H_{14}O_2$		
132.	*2-Heptanone*	$C_7H_{14}O$		
133.	*Ethylbenzene*	C_8H_{10}		
134.	*Heptanal*	$C_7H_{14}O$		

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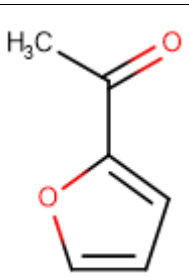
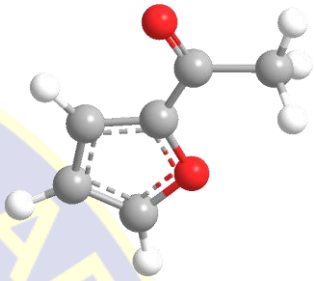
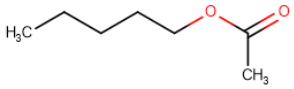
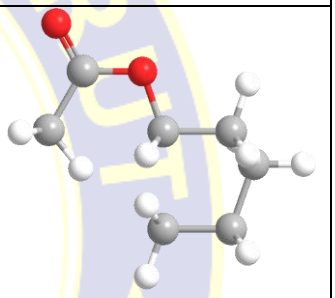
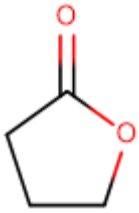
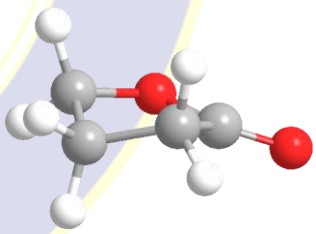
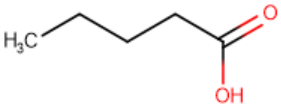
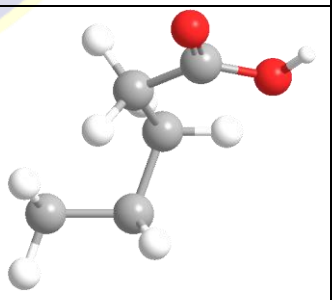
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
135.	*2-Acetylfuran*	$C_6H_6O_2$		
136.	*Pentyl acetate*	$C_7H_{14}O_2$		
137.	*γ-Butyrolactone*	$C_4H_6O_2$		
138.	*Pentanoic acid*	$C_5H_{10}O_2$		

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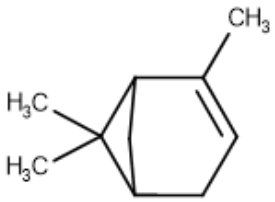
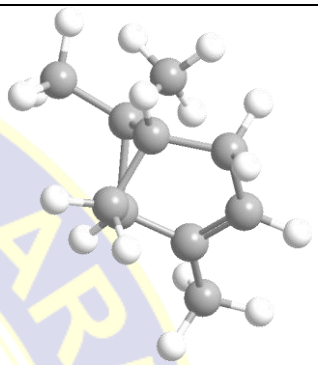
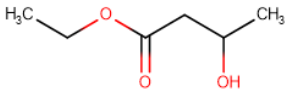
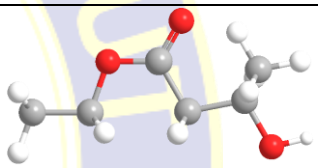
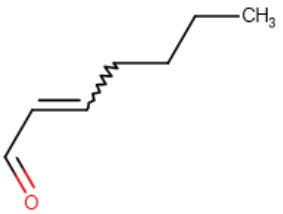
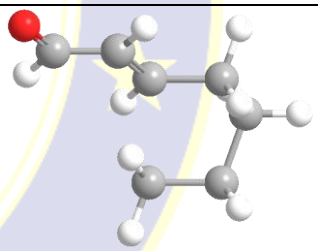
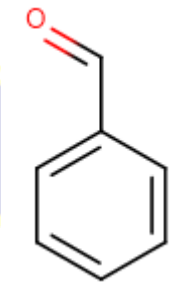
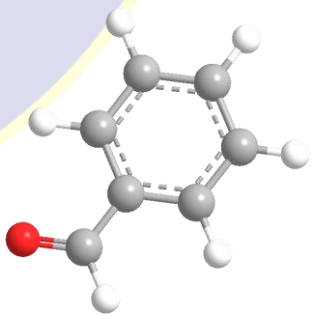
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
139.	*α-Pinene*	$C_{10}H_{16}$		
140.	*Ethyl 3-hydroxybutanoate*	$C_6H_{12}O_3$		
141.	*(E)-2-Heptenal*	$C_7H_{12}O$		
142.	*Benzaldehyde*	C_7H_6O		

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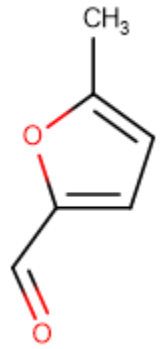
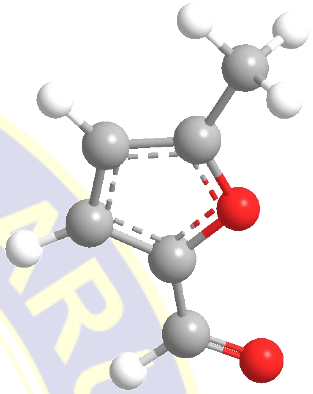
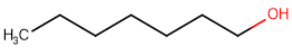
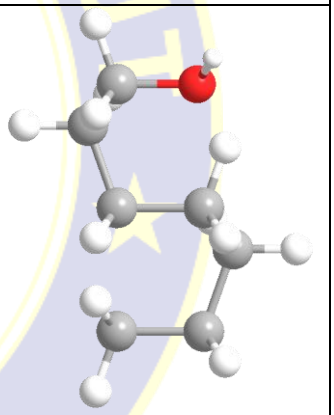
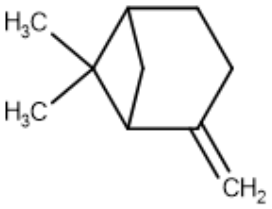
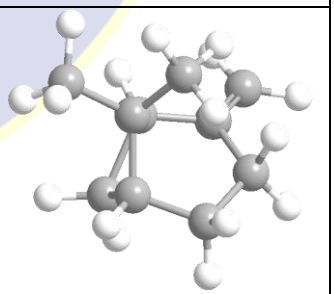
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
143.	*5-Methyl-2-furfural*	$C_6H_6O_2$		
144.	*1-Heptanol*	$C_7H_{16}O$		
145.	*β-Pinene*	$C_{10}H_{16}$		

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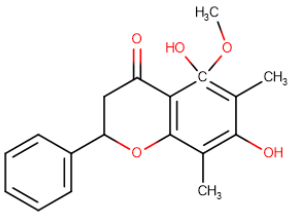
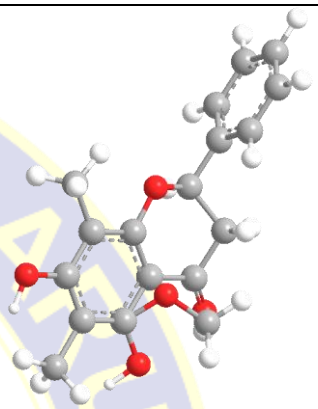
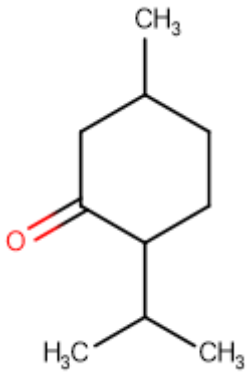
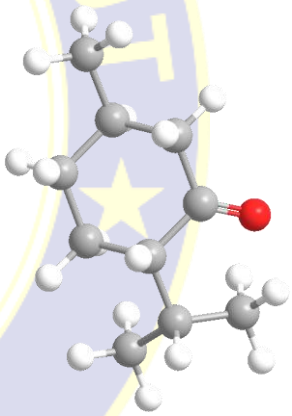
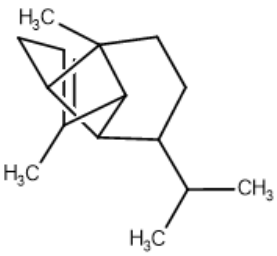
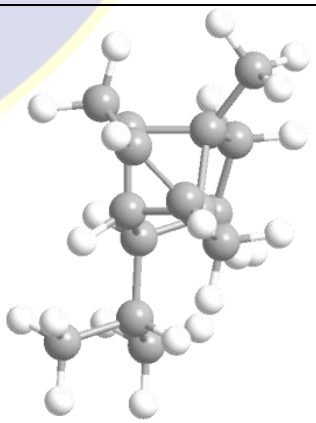
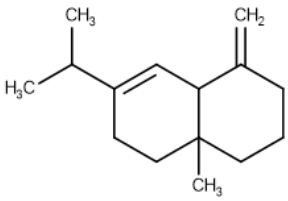
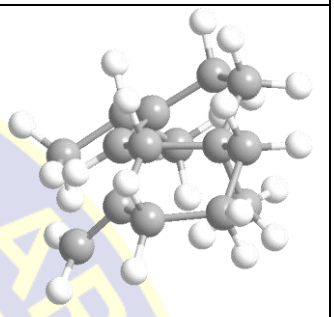
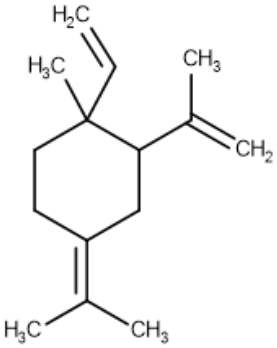
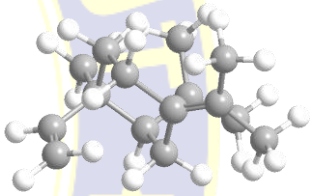
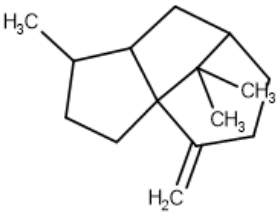
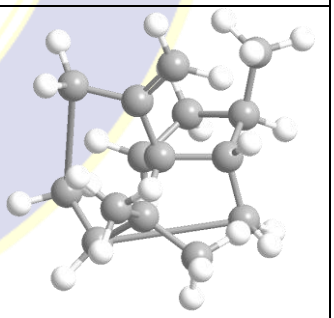
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
146.	*(+)-6,8-Dimethyl-5methoxypinocembrin*	$C_{10}H_{16}$		
147.	*Menthone*	$C_{10}H_{18}O$		
148.	*a – Ylangene*	$C_{15}H_{24}$		

LAMPIRAN 8
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
149.	*Sibirene*	$C_{15}H_{24}$		
150.	*gamma – Elemene*	$C_{15}H_{24}$		
151.	*gamma – Patchoulene*	$C_{15}H_{24}$		

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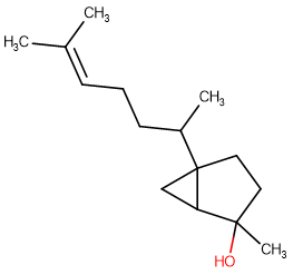
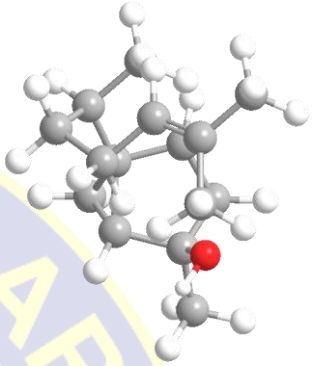
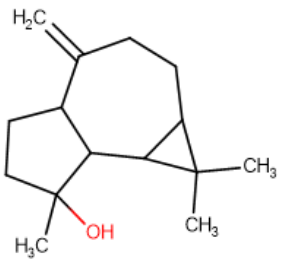
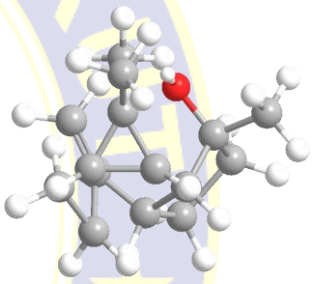
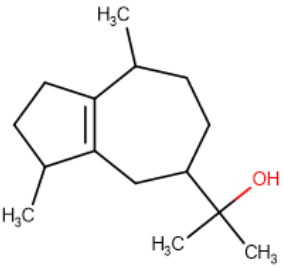
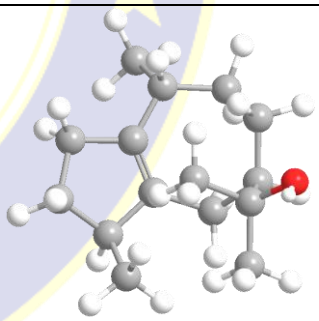
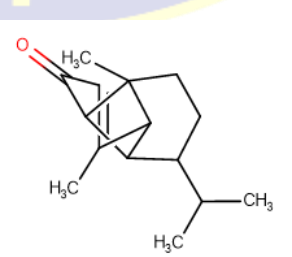
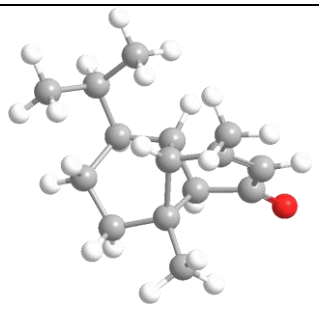
Tabel VII.4
Lanjutan

No.	Nama Senyawa	Rumus Molekul	Struktur 2D	Struktur 3D
152.	*Trans-sesquisabinene hydrate*	$C_{15}H_{26}O$		
153.	*Spathulenol*	$C_{15}H_{24}O$		
154.	*Guaiol*	$C_{15}H_{26}O$		
155.	*Mustakone*	$C_{15}H_{22}O$		

LAMPIRAN 9

HASIL SKRINING AKTIVITAS ANTIKANKER PAYUDARA

Tabel VII. 5
Hasil Skrining Aktivitas Antikanker Payudara

No.	Senyawa	Pa	Pi	Aktivitas *Antineoplastic*
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	*Desmanthin 1*	0,636	0,008	*Antineoplastic (breast cancer)*
5	*Pinocembrin*	0,629	0,009	*Antineoplastic (breast cancer)*
6	*Mearnsitrin*	0,610	0,010	*Antineoplastic (breast cancer)*
7	*β-selinene*	0,603	0,010	*Antineoplastic (breast cancer)*
8	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	0,600	0,010	*Antineoplastic (breast cancer)*
9	*Aurentiacin*	0,589	0,011	*Antineoplastic (breast cancer)*
10	*Stercurensin*	0,583	0,012	*Antineoplastic (breast cancer)*
11	*8-Methylpinocembrin*	0,579	0,012	*Antineoplastic (breast cancer)*
12	*Myricetin*	0,578	0,012	*Antineoplastic (breast cancer)*
13	*Quercetin*	0,577	0,012	*Antineoplastic (breast cancer)*
14	*isopulegyl acetate*	0,563	0,013	*Antineoplastic (breast cancer)*
15	*(2E,6E)-Farnesyl acetate*	0,562	0,014	*Antineoplastic (breast cancer)*
16	*Morin*	0,556	0,014	*Antineoplastic (breast cancer)*
17	*Quercitrin*	0,555	0,014	*Antineoplastic (breast cancer)*
18	*Myricitrin*	0,555	0,014	*Antineoplastic (breast cancer)*
19	*(-)-Epigallocatechin gallate*	0,541	0,015	*Antineoplastic (breast cancer)*
20	*Epigallocatechin gallate*	0,541	0,015	*Antineoplastic (breast cancer)*
21	*Rutin*	0,536	0,016	*Antineoplastic (breast cancer)*
22	*Isorhamnetin 3-glucoside*	0,531	0,016	*Antineoplastic (breast cancer)*
23	*(-)-Epicatechin gallate*	0,528	0,016	*Antineoplastic (breast cancer)*

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Tabel VII.5
Lanjutan

No.	Senyawa	Pa	Pi	Aktivitas *Antineoplastic*
24	*(-)-β-caryophyllene*	0,527	0,016	*Antineoplastic (breast cancer)*
25	*α-selinene*	0,521	0,017	*Antineoplastic (breast cancer)*
26	*Limonene*	0,515	0,018	*Antineoplastic (breast cancer)*
27	*Isoquercitrin*	0,502	0,019	*Antineoplastic (breast cancer)*
28	*(-)-caryophyllene oxide*	0,494	0,019	*Antineoplastic (breast cancer)*
29	*Myricetin-3-(3"galloylrhamnoside)*	0,493	0,020	*Antineoplastic (breast cancer)*
30	*Kaempferol 3-glucoside*	0,490	0,020	*Antineoplastic (breast cancer)*
31	*(+)-Catechin*	0,486	0,020	*Antineoplastic (breast cancer)*
32	*(-)-Epicatechin*	0,486	0,020	*Antineoplastic (breast cancer)*
33	*Ferulic acid*	0,467	0,023	*Antineoplastic (breast cancer)*
34	*isopulegol*	0,462	0,023	*Antineoplastic (breast cancer)*
35	*Myltayl-4(12)-ene*	0,460	0,023	*Antineoplastic (breast cancer)*
36	*Ursolic acid*	0,416	0,029	*Antineoplastic (breast cancer)*
37	*Procyanidin A2*	0,411	0,030	*Antineoplastic (breast cancer)*
38	*Procyanidin B1*	0,406	0,031	*Antineoplastic (breast cancer)*
39	*Caffeic acid*	0,399	0,032	*Antineoplastic (breast cancer)*
40	*p-Coumaric acid*	0,394	0,033	*Antineoplastic (breast cancer)*
41	*Chlorogenic acid*	0,391	0,033	*Antineoplastic (breast cancer)*
42	*citronellyl acetate*	0,373	0,037	*Antineoplastic (breast cancer)*
43	*Procyanidin B2*	0,366	0,038	*Antineoplastic (breast cancer)*
44	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	0,359	0,040	*Antineoplastic (breast cancer)*
45	*γ-Butyrolactone*	0,352	0,041	*Antineoplastic (breast cancer)*
46	*2',4'-Dihydroxy-6'-methoxy-3'- methyldihydrochalcone*	0,320	0,050	*Antineoplastic (breast cancer)*

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Tabel VII.5
Lanjutan

No.	Senyawa	Pa	Pi	Aktivitas *Antineoplastic*
47	*3-Methyl-2-buten-1-ol*	0,318	0,050	*Antineoplastic (breast cancer)*
48	*t-Cinnamic acid*	0,300	0,055	*Antineoplastic (breast cancer)*
49	*Vanillic acid*	0,298	0,055	*Antineoplastic (breast cancer)*
50	*β-elemene*	0,290	0,058	*Antineoplastic (breast cancer)*
51	*Uvangoletin*	0,274	0,063	*Antineoplastic (breast cancer)*
52	*gamma – Elemene*	0,264	0,066	*Antineoplastic (breast cancer)*
53	*Linalool*	0,259	0,068	*Antineoplastic (breast cancer)*
54	*Borneol*	0,259	0,068	*Antineoplastic (breast cancer)*
55	*Benzaldehyde*	0,256	0,069	*Antineoplastic (breast cancer)*
56	*α-humulene*	0,254	0,070	*Antineoplastic (breast cancer)*
57	*Mustakone*	0,227	0,081	*Antineoplastic (breast cancer)*
58	*Ethyl (E)-2-butenoate*	0,223	0,083	*Antineoplastic (breast cancer)*
59	*Sibirene*	0,221	0,084	*Antineoplastic (breast cancer)*
60	*2-ethylhexyl p-methoxycinnamate*	0,219	0,085	*Antineoplastic (breast cancer)*
61	*Terpinolene*	0,218	0,085	*Antineoplastic (breast cancer)*
62	*Trans-sesquisabinene hydrate*	0,218	0,085	*Antineoplastic (breast cancer)*
63	*Ellagic acid*	0,216	0,086	*Antineoplastic (breast cancer)*
64	*Ethyl acetate*	0,214	0,087	*Antineoplastic (breast cancer)*
65	*Methyl salicylate*	0,202	0,093	*Antineoplastic (breast cancer)*
66	*3-buten-2-one*	0,194	0,098	*Antineoplastic (breast cancer)*
67	*α-copaene*	0,186	0,103	*Antineoplastic (breast cancer)*
68	*α -Ylangene*	0,186	0,103	*Antineoplastic (breast cancer)*
69	*Aromadendrene*	0,184	0,105	*Antineoplastic (breast cancer)*
70	*Allo-aromadendrene*	0,184	0,105	*Antineoplastic (breast cancer)*

LAMPIRAN 9
(LANJUTAN)

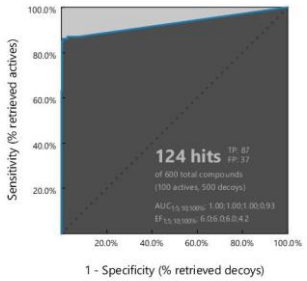
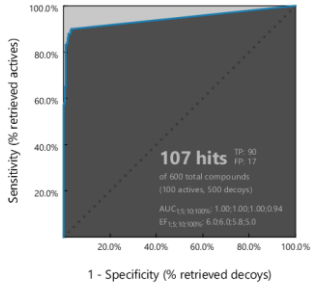
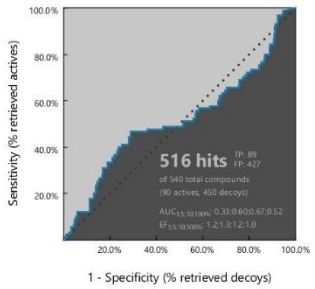
Tabel VII.5
Lanjutan

No.	Senyawa	Pa	Pi	Aktivitas *Antineoplastic*
71	*Phytol*	0,179	0,108	*Antineoplastic (breast cancer)*
72	*3-hexen-1-ol*	0,178	0,109	*Antineoplastic (breast cancer)*
73	*Gallic acid*	0,176	0,110	*Antineoplastic (breast cancer)*
74	*γ-muurolene*	0,167	0,119	*Antineoplastic (breast cancer)*
75	*(-)-β-pinene*	0,163	0,124	*Antineoplastic (breast cancer)*
76	*β-Pinene*	0,163	0,124	*Antineoplastic (breast cancer)*
77	*Pentyl acetate*	0,161	0,126	*Antineoplastic (breast cancer)*
78	*α-Fenchol*	0,154	0,134	*Antineoplastic (breast cancer)*
79	*β-sitosterol*	0,153	0,134	*Antineoplastic (breast cancer)*
80	*Spathulenol*	0,144	0,144	*Antineoplastic (breast cancer)*

LAMPIRAN 10

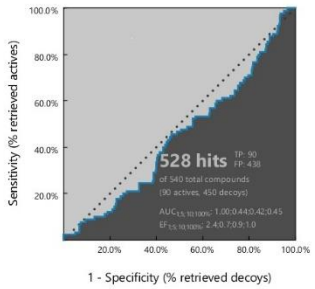
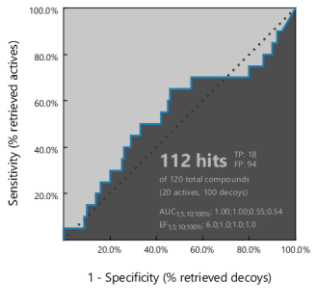
HASIL STUDI FARMAKOFOR

Tabel VII. 6
Hasil Validasi Farmakofor

Reseptor	ROC Curve	AUC	GH Score
ER-α		0,93	0,69
ER-β		0,94	0,83
Progesteron		0,45	0,02

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 6
Lanjutan

Reseptor	ROC Curve	AUC	GH Score
Progesteron		0,52	0,01
HER2		0,52	0,02

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 7
Hasil Skrining Farmakofor Ligan Uji Terhadap Reseptor ER-α

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*Cyanidin-3,5-O-diglucosid*	63.97
2	*Quercitrin*	63.49
3	*Peonidin 3,5-diglucosside*	60.95
4	*Pelargonidin-3-glucoside*	60.74
5	*Procyanidin B2*	60.64
6	*Peonidin-3-Glukosid*	60.64
7	*Procyanidin B1*	60.58
8	*Cyanidin-3-O-Glukosid*	60.56
9	*Cyanidin 3-glucoside*	60.54
10	*Procyanidin A2*	60.37
11	*2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone*	56.26
12	*Stercurensin*	55.47
13	*Kaempferol-3-glucoside*	53.19
14	*Isorhamnetin-3-glucoside*	53.11
15	*Isoquercitrin*	53.04
16	*(-)-Epicatechin*	53.00
17	*Quercetin*	52.93
18	*(+)-Catechin*	52.88
19	*Morin*	52.71
20	*Myricitrin*	52.43
21	*Chlorogenic Acid*	51.98
22	*Myricetin-3-(3''galloylrhamnoside)*	51.95

LAMPIRAN 10
(LANJUTAN)

Tabel VII. 7
Lanjutan

No.	Ligan Uji	*Pharmacophore-Fit Score*
23	*Mearnsitrin*	50.96
24	*(-)-Epicatechin gallate*	50.71
25	*Desmanthin1*	50.53
26	*Rutin*	50.24
27	*Ursolic Acid*	44.60

Tabel VII. 8
Hasil Studi Farmakofor Terhadap Reseptor ER-β

No.	Ligan Uji	*Pharmacophore-Fit Score*
1	*Chlorogenic Acid*	57.94
2	*Morin*	57.40
3	*(-)-Epicatechin gallate*	57.08
4	*Kaempferol-3-glucoside*	57.03
5	*Procyanidin B2*	56.34
6	*Isoquercitrin*	55.91
7	*Cyanidin-3,5-O-diglucosid*	55.90
8	*Pelargonidin-3-glucoside*	54.37
9	*Peonidin-3-Glukosid*	54.18
10	*(+)-Catechin*	54.04
11	*Cyanidin 3-glucoside*	53.96
12	*Isorhamnetin-3-glucoside*	46.72
13	*Quercetin*	46.62
14	*(-)-Epicatechin*	46.61
15	*Cyanidin-3-O-Glukosid*	46.28

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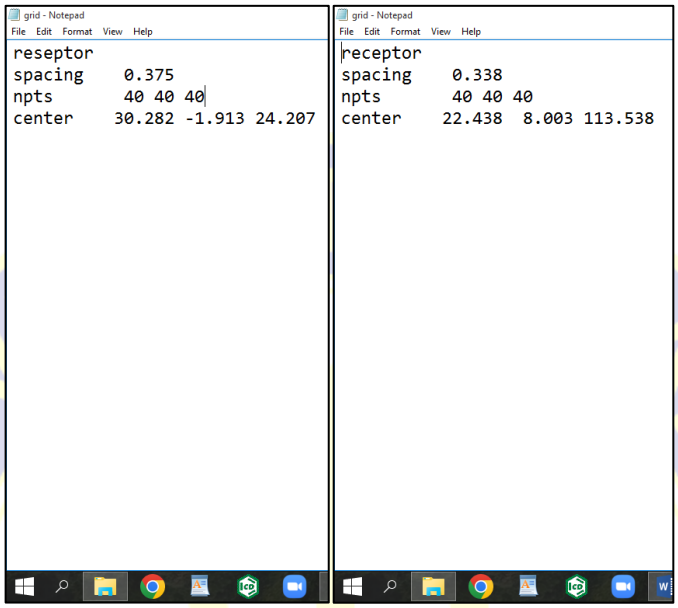
(LANJUTAN)

Tabel VII. 8
Lanjutan

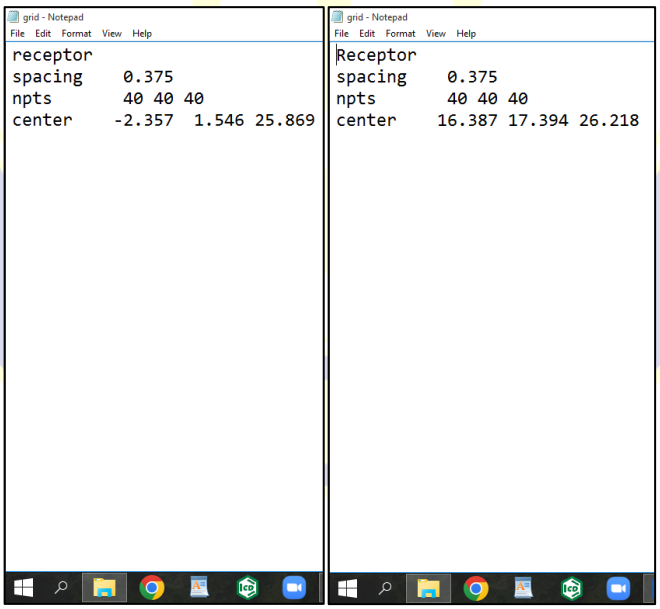
No.	Ligan Uji	*Pharmacophore-Fit Score*
16	*Procyanidin A2*	46.22
17	*Quercitrin*	46.09
18	*Procyanidin B1*	46.01
19	*Rutin*	45.81
20	*Peonidin 3,5-diglucosside*	45.46
21	*Myricitrin*	44.54
22	*Mearnsitrin*	44.37
23	*Ursolic Acid*	44.15
24	*Desmanthin 1*	43.97
25	*Myricetin-3-(3''galloylrhamnoside)*	43.67

LAMPIRAN 11

GRID-BOX VALIDASI *DOCKING*



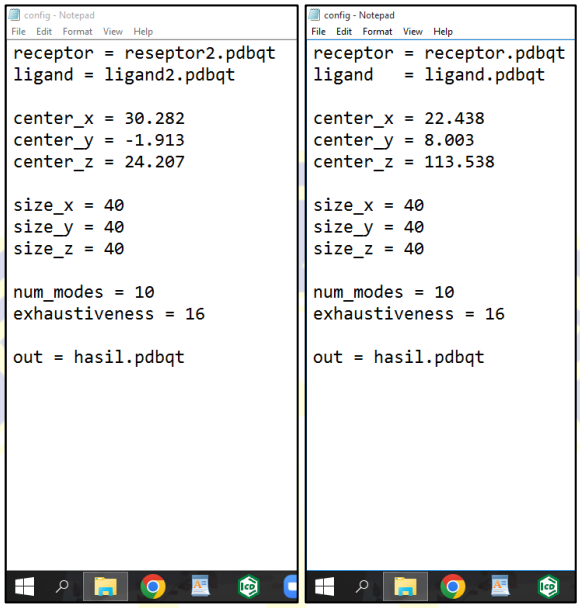
Gambar VII. 22 *Grid-box* validasi ER-α dan ER-β



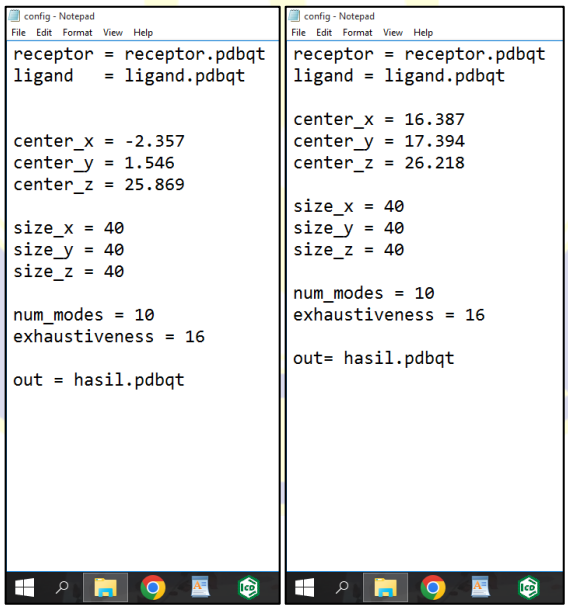
Gambar VII. 23 *Grid-box* validasi PR dan HER2

LAMPIRAN 12

CONFIG DOCKING



Gambar VII. 24 *Config* ER-α dan ER-β



Gambar VII. 25 *Config* PR dan HER2

LAMPIRAN 13

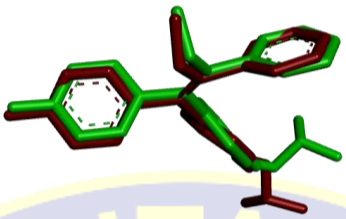
HASIL VALIDASI *DOCKING*

Tabel VII. 9 Hasil Validasi *Docking*

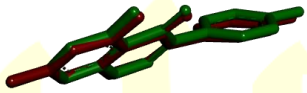
PDB ID	Grid Center			Grid Box			RMSD	Keterangan
	X	Y	Z	X	Y	Z		
3ERT	30.282	-1.913	24.207	40	40	40	1.1162 Å	Valid
1QKM	22.438	8.003	113.538	40	40	40	0,2799 Å	
1SQN	-2.357	1.546	25.869	40	40	40	0.3846 Å	
3PP0	16.387	17.394	26.218	40	40	40	0,6678 Å	

LAMPIRAN 14

VISUALISASI TUMPANG TINDIH HASIL VALIDASI *DOCKING*

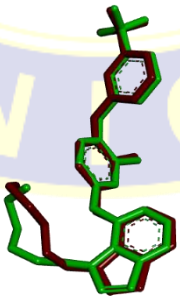


Gambar VII. 26 Visualisasi tumpang tindih validasi *docking* ER-α



Gambar VII. 27 Visualisasi tumpang tindih validasi *docking* ER-β

Gambar VII. 28 Visualisasi tumpang tindih validasi *docking* PR



Gambar VII. 29 Visualisasi tumpang tindih validasi *docking* HER2

LAMPIRAN 15

HASIL SIMULASI *MOLECULAR DOCKING*

Tabel VII. 10
Hasil *Molecular Docking* terhadap ER-α dan Analisis Residu Asam Amino

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
1	*Ligan Alami 4OHT (Pembanding)*	-9.684	ARG 394, GLU 353	LEU 387, LEU 391, LEU 346, MET 421, ALA 350, LEU 525, MET 388	-
2	*Procyanidin A2*	-11.166	CYS 530	ALA 350, LYS 529, VAL 533, LEU 536	LEU 536 (Pi-Sigma), TRP 383 (Pi-Pi Stacked)
3	*Procyanidin B1*	-10.393	LEU 525, CYS 530, ASP 351	LYS 529, LEU 536, VAL 533, LEU 525	TRP 383 (Pi-Pi Stacked)
4	*Procyanidin B2*	-10.207	MET 343, THR 347, CYS 530	ALA 350, LYS 529, VAL 533, LEU 536, LEU 525	LEU 525, LEU 536 (Pi-Sigma), ASP 351 (Pi-Anion), MET 523 (Pi-Sulfur), LEU 346 (Amide-Pi Stacked)
5	*Ursolic Acid*	-10.103	-	-	-
6	*Rutin*	-10.057	VAL 534, LEU 536, THR 347, MET 522, CYS 530	MET 522	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 10
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
7	*Desmanthin1*	-9.832	LEU 536, CYS 530, ASP 351, MET 522	LYS 529, LEU 525, LEU 536	LEU 536 (Pi-Sigma), TYR 526 (Van der Waals), TRP 383 (Pi-Pi Stacked), MET 522 (Pi-Sulfur), LEU 525 (Amide-Pi- Stacked)
8	*Cyanidin-3,5-O-diglucosid*	-9.579	LEU 536, MET 522, THR 347	MET 522, LEU 525	PRO 535 (Carbon Hidrogen Bond), LEU 525 (Pi-sigma)
9	*Quercitrin*	-9.510	THR 347	LEU 525	LEU 525, LEU 536 (Pi-Sigma), ASP 351 (Carbon Hidrogen Bond)
10	*Myricetin-3-(3"galloylrhamnoside)*	-9.486	CYS 530, THR 347, TRP 383, LEU 536	LEU 525, MET 522	-
11	*Mearnsitrin*	-9.280	-	ALA 350, MET 343, LEU 525	LEU 525 (Pi-Sigma), ASP 351 (Carbon Hidrogen Bond)
12	*(-)-Epicatechin gallate*	-9.176	THR 347, CYS 530, LEU 536	LYS 529	LEU 525, VAL 533 (Pi-Sigma)
13	*Peonidin 3,5-diglucosside*	-9.157	GLU 380, TYR 537, LEU 536, THR 347	MET 522, LEU 525	LEU 525 (Pi-sigma), ASP 351 (Carbon Hidrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 10
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
14	*Kaempferol-3-glucoside*	-8.985	VAL 534, CYS 530	MET 522	LEU 525 (Pi-Sigma), TYR 526 (Pi-Pi T-Shaped)
15	*Myricitrin*	-8.980	THR 347	LEU 525	LEU 525 (Pi-Sigma), ASP 351 (Carbon Hidrogen Bond)
16	*Quercetin*	-8.840	ARG 394, GLU 353, LEU 387	ALA 350, LEU 384, MET 388, LEU 391	LEU 525 (Pi-Sigma), THR 347 (Van der Waals), MET 343 (Pi-Sulfur), LEU 346 (Amide-Pi Stacked)
17	*Morin*	-8.799	ARG 394, GLU 353, MET 343	LEU 391, ALA 350, LEU 387, LEU 384, MET 388	LEU 525 (Pi-Sigma), MET 343 (Pi-Sulfur)
18	*Isoquercitrin*	-8.744	VAL 534, MET 522, THR 347	MET 522	LEU 525 (Pi-Sigma), TYR 526 (Pi-Pi T-Shaped)
19	*(-)-Epicatechin*	-8.713	GLU 353, LYS 449, TRP 393	PRO 324, ARG 394	ILE 326 (Pi-Sigma), GLU 323 (Pi-Anion)
20	*Pelargonidin-3-glucoside*	-8.701	CYS 530, VAL 534	MET 522	LEU 525 (Pi-sigma), TYR 526 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 10
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
21	*Cyanidin-3-O-Glukosid*	-8.514	CYS 530, VAL 534, LEU 536,	MET 522	LEU 525 (Pi-sigma), TYR 526 (Pi-Pi T-shaped)
22	*Peonidin-3-Glukosid*	-8.495	ASP 351	MET 522, LEU 525	LEU 525 (Pi-sigma), TRP 383 (Pi-Pi T-shaped), ASP 351 (Carbon Hidrogen Bond)
23	*Cyanidin 3-glucoside*	-8.460	CYS 530, MET 522	MET 522, LEU 525, LEU 536	MET 522 (Pi-Sulfur), TRP 383 (Pi-Pi T-shaped)
24	*Isorhamnetin-3-glucoside*	-8.272	VAL 534, MET 522, THR 347	MET 522	LEU 525 (Pi-Sigma), ASP 351 (Carbon Hidrogen Bond), TYR 526 (Pi-Pi T-Shaped)
25	*Chlorogenic Acid*	-8.229	GLU 353, ASP 351	LEU 525, ALA 350	MET 343 (Pi-Sulfur)
26	*(+)-Catechin*	-7.969	ARG 394, GLU 353, LEU 387, HIS 524	LEU 525, MET 421, LEU 346, LEU 391	PHE 404 (Pi-Pi T-shaped), GLY 521 (Carbon Hidrogen Bond)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 10
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
27	*2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone*	-7.710	-	LEU 387, ALA 350, LEU 525, ILE 424	THR 347 (Van der Waals), MET 343, MET 421 (Pi-Sulfur), LEU 346 (Amide-Pi Stacked)
28	*Stercurensin*	-7.649	-	LEU 525, ALA 350, LEU 384	LEU 384 (Pi-sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Hasil *Molecular Docking* terhadap ER-β dan Analisis Residu Asam Amino

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
1	Ligan Alami Genistein (Pembanding)	-10,5	ARG 346, GLU 305, LEU 339, HIS 475	LEU 339, ALA 302, LEU 343, LEU 298, LEU 476	MET 336 (Pi-Sigma), PHE 356 (Pi-Pi-T-shaped)
2	Rutin	-10,6	ARG 346, GLU 305, LYS 401, GLU 276, TYR 397, HIS 279, TRP 345, HIS 394	VAL 280, PRO 277, ARG 346,	HIS 394, GLU 276, GLU 305, (Carbon Hidrogen Bond), ILE 355 (Pi-Sigma), TRP 345 (Pi-Pi Stacked)
3	*Procyanidin B1*	-10,4	TRP 345, LYS 401, PRO 358	ARG 346, PRO 277, ILE 355, PRO 358	HIS 279, PRO 277 (Carbon Hidrogen Bond, Pi-Donor Hidrogen Bond), ARG 346, HIS 279 (Pi-Cation), TRP 345 (Pi-Pi T-shaped)
4	*Myricetin-3-(3''galloylrhamnoside)*	-10,2	ARG 346, TRP 345, ASP 249, HIS 279, PHE 356, VAL 280, PRO 278	ARG 346, PRO 358, ALA 357	PRO 358 (Carbon Hidrogen Bond), VAL 280 (Pi-Donor Hidrogen Bond), ARG 346, ASP 349 (Pi-Cation), HIS 279 (Pi-Anion), ILE 355 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
5	*Procyanidin B2*	-10,0	ARG 346, PRO 358, ASP 349, TRP 345, GLU 276	ARG 346, ILE 355, PRO 358, PRO 277	GLU 276 (Pi-Anion), ARG 346, HIS 279 (Pi-Cation) ,TRP 345 (Pi-Pi T-shaped), GLY 342 (Carbon Hidrogen Bond)
6	*Procyanidin A2*	-9,9	GLU 305, LYS 401	ARG 346	TRP 345, GLY 342 (Carbon Hidrogen Bond), ARG 346, HIS 279 (Pi-Cation), HIS 394, GLU 276 (Pi-Anion), PRO 277 (Pi-Sigma),
7	*Myricitrin*	-9,2	GLU 305, VAL 280, HIS 279, TRP 345	ARG 346, PRO 277	ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
8	*Quercitrin*	-9,1	GLU 305, VAL 280, HIS 279, TRP 345	ARG 346, PRO 277	ARG 346 (Carbon Hidrogen Bond), ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
9	*Morin*	-9,0	ARG 346, GLU 305, VAL 280	ARG 346, PRO 277	HIS 279, GLY 342 (Carbon Hidrogen Bond, Pi-Donor Hidrogen Bond), ARG 346 (Pi-Cation), GLU 305 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
10	*Quercetin*	-9,0	GLU 305, VAL 280, TRP 345	ARG 346, PRO 277	HIS 279 (Carbon Hidrogen Bond, Pi-Donor Hidrogen Bond), ARG 346 (Pi-Cation), GLU 305 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
11	*Mearnsitrin*	-8,9	GLU 305, VAL 280, HIS 279, TRP 345	ARG 346, PRO 277, LEU 273	ARG 346, (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
12	*Desmanthin1*	-8,6	ARG 346, TRP 345, HIS 394, ASP 349, ILE 348, HIS 350, PRO 277	ARG 346	ASP 349 (Pi-Anion), ILE 355 (Pi-Sigma), HIS 279 (Pi-Pi T-shaped), PRO 358 (Carbon Hidrogen Bond), HIS 279 (Pi-Donor Hidrogen Bond)
13	*(-)-Epicatechin*	-8,5	ARG, 346, GLU 305, HIS 279	PRO 277	HIS 279 (Pi-Pi T-shaped), ARG 346 (Pi-Cation), GLY 342 (Carbon Hidrogen Bond), PRO 358 (Carbon Hidrogen Bond)
14	*(-)-Epicatechin gallate*	-8,5	GLU 305, VAL 280, ARG 346, TRP 345, GLU 276	PRO 277, ARG 346	HIS 279 (Carbon Hidrogen Bond), ARG 346 (Pi-Cation)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
15	*Cyanidin-3,5-O-diglucosid*	-8,5	TRP 345, PRO 277, HIS 279, PRO 278, VAL 280,	ARG 346, PRO 358	ARG 346 (Carbon Hidrogen Bond), TRP 345 (Pi-Donor Hidrogen Bond), PRO 277 (Carbon Hidrogen Bond), ILE 355 (Pi-Sigma), HIS 279 (Pi-Cation), ARG 346 (Pi-Cation)
16	*(+)-Catechin*	-8,3	ARG 346, GLU 305, VAL 280,TRP 345, GLY 342	-	ARG 346 (Pi-Cation), GLU 276 (Pi-Cation), PRO 358 (Carbon Hidrogen Bond)
17	*Isoquercitrin*	-8,1	GLU 305, VAL 280, HIS 279, TRP 345	ARG 346, PRO 277	ARG 346 (Pi-Cation), ARG 346 (Carbon Hidrogen Bond), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
18	*Cyanidin-3-O-Glukosid*	-8,0	GLU 305, TRP 345, HIS 279	ARG 346, PRO 277	ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
19	*Isorhamnetin-3-glucoside*	-8,0	VAL 280, PRO 278, TRP 345	ALA 357, PRO 358	PRO 358 (Carbon Hidrogen Bond), GLU 276, TRP 345 (Pi-Donor Hidrogen Bond), ARG 346, HIS 279 (Pi-Cation), ILE 355 (Pi-Sigma)
20	*Kaempferol-3-glucoside*	-8,0	GLU 305, VAL 280, HIS 279, TRP 345	ARG 346, PRO 277	ARG 346 (Carbon Hidrogen Bond), ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
21	*Peonidin 3,5-diglucosside*	-8,0	VAL 280, PRO 277, TRP 345	ARG 346, PRO 358	HIS 394 (Carbon Hidrogen Bond, Pi-Donor Hidrogen Bond), ILE 355 (Pi-Sigma), HIS 279, ARG 346 (Pi-Cation)

LAMPIRAN 15
(LANJUTAN)

Tabel VII. 11
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
22	*Chlorogenic Acid*	-7,7	TRP 345, GLU 276, VAL 280, HIS 279	PRO 277	GLU 305 (Pi-Anion), PRO 277 (Carbon Hidrogen Bond), HIS 279 (Carbon Hidrogen Bond)
23	*Pelargonidin-3-glucoside*	-7,7	GLU 305, VAL 280, TRP 345, HIS 279	PRO 277	ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
24	*Cyanidin 3-glucoside*	-7,6	GLU 276, HIS 279, TRP 345	ILE 355, ARG 346	PRO 278 (Carbon Hidrogen Bond), PRO 358 (Carbon Hidrogen Bond), HIS 394 (Carbon Hidrogen Bond), HIS 279 (Pi-Cation)
25	*Peonidin-3-Glukosid*	-7,6	GLU 305, TRP 345, HIS 279	ARG 346, PRO 277	ARG 346 (Pi-Cation), GLU 276 (Pi-Anion), HIS 279 (Pi-Pi T-shaped)
26	*Ursolic Acid*	-7,6	-	-	PRO 358 (Carbon Hidrogen Bond)

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Tabel VII. 12
Hasil *Molecular Docking* Terhadap Reseptor Progesteron dan Analisis Residu Asam Amino

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
1	Ligan Alami	-12,0	ARG 766	MET 759, LEU 718, LEU 715, PHE 794, LEU 797, TYR 890	-
2	*Quercetin*	-9,9	ARG 766, GLN 725, ASN 719, MET 756	CYS 891, LEU 718, MET 759, LEU 763	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)
3	*Procyanidin A2*	-9,8	ARG 724, ASP 697, LYS 731, ILE 694	PRO 696, ARG 724, ILE 699, LYS 731	TYR 700 (Pi-Pi Stacked)
4	*(+)-Catechin*	-9,6	GLN 725, MET 759	LEU 763, MET 759, CYS 891	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)
5	*8-Methylpinocembrin*	-9,6	-	MET 759, LEU 718, LEU 763	PHE 778 (Pi-Pi T-Shaped)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
6	*Morin*	-9,6	ARG 766, GLN 725, MET 759, MET 891, MET 756	LEU 718, LEU 763	PHE 778 (Pi-Pi T-Shaped)
7	*(-)-Epigallocatechin gallate*	-9,5	GLN 815, TRP 765, LYS 882	PRO 696, ARG 766	ARG 766, HIS 770 (Pi-Cation), GLU 695 (Unforable Acceptor-Acceptor)
8	*Epigalocatechin Gallate*	-9,5	GLN 815, TRP 765, LYS 882	PRO 696, ARG 766	ARG 766, HIS 770 (Pi-Cation), GLU 695 (Unforable Acceptor-Acceptor)
9	*(-)-Epicatechin gallate*	-9,4	GLN 815, TRP 765, LYS 882	PRO 696, ARG 766	LYS 769 (Carbon Hydrogen Bond), ARG 766, HIS 770 (Pi-Cation)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
10	*(-)-Epicatechin*	-9,4	ARG 766, GLN 725, ASN 719, MET 756	LEU 718, CYS 891, LEU 763, MET 759	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)
11	*Procyanidin B2*	-9,4	THR 894, ASN 893, SER 796, THR 800, GLU 791	LEU 889, LEU 797	TYR 890 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond)
12	*Desmanthin 1*	-9,1	TYR 700, HIS 770, GLN 815	PRO 780, VAL 698, ARG 766	GLY 762, TRP 765, HIS 770, ARG 766, VAL 698 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), GLU 695 (Pi-Cation, Pi-Anion), TRP 765 (Pi-Pi T-Shaped)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
13	*Myricetin*	-9,1	HIS 770, LYS 822, LEU 758, GLN 815	PRO 696, ARG 766	ARG (Pi-Cation), TRP 765 (Pi-Pi T-Shaped)
14	*Procyanidin B1*	-9,1	ASN 893, SER 792, TYR 890	LEU 889	SER 792, SER 793 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), GLU 791 (Pi-Anion), TYR 890, SER 792 (Pi-Pi T-Shaped, Amide-Pi Stacked)
15	*Ellagic acid*	-9,0	ILE 699, LYS 822, ASP 697, SER 728, LEU 758	PRO 696	GLY 762, TRP 765 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), GLU 695 (Pi-Cation), ARG 766 (Pi-Anion), PRO 696 (Pi-Sigma)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
16	*Myricitrin*	-9,0	ILE 699, GLN 815, LYS 822, HIS 770	PRO 696, LYS 769	VAL 698, LYS 769 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), ARG 766 (Pi-Cation), TRP 765 (Pi-Pi T-Shaped)
17	*Pinocembrin*	-9,0	-	MET 759, LEU 763, LEU 718, CYS 891	PHE 778 (Pi-Pi T-Shaped)
18	*Rutin*	-9,0	VAL 698, ILE 699, HIS 770, GLN 815, LYS 769, TRP 765, MET 692	PRO 696, ILE 699	LYS 769 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), GLU 695 (Pi-Anion), MET 692 (Sulfur X, Pi-Sulfur)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
19	*Isoquercitrin*	-8,9	LYS 822, GLN 815, TRP 765, HIS 770	PRO 696	ARG 766, ASP 697 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), GLU 695 (Pi-Anion)
20	*Kaempferol 3-glucoside*	-8,7	VAL 698, ILE 699, HIS 770, GLN 815	PRO 696, ILE 699	ARG 766 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), GLU 695 (Pi-Anion), MET 692 (Sulfur X, Pi-Sulfur)
21	*Quercitrin*	-8,7	ILE 699, LYS 822, GLN 815	PRO 696, ARG 766, LYS 769	LYS 769, VAL 698 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), TRP 765 (Pi-Pi T-Shaped)
22	*ursolic acid*	-8,7	TYR 700	-	ARG 724 (Carbon Hydrogen Bond)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
23	*Chlorogenic acid*	-8,6	ARG 766, GLN 725, MET 759	LEU 763, MET 759	MET 801 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)
24	*Mearnsitrin*	-8,6	ILE 699, LYS 822, HIS 770, GLN 815	PRO 696, LYS 769	LYS 769, VAL 698 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), ARG 766 (Pi-Cation), TRP 765 (Pi-Pi t-Shaped)
25	*Uvangoletin*	-8,6	ARG 766, GLN 725, MET 759, LEU 718	LEU 887, CYS 891, LEU 763, MET 759	LEU 797 (Pi-Sigma), PHE 778 (Pi-Pi T-Shaped)
26	*2',4'-Dihydroxy-6'-methoxy-3'-methyldihydrochalcone*	-8,5	-	CYS 891, MET 759, LEU 763	PHE 778 (Pi-Pi T-Shaped)
27	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	-8,5	-	CYS 891, MET 759, LEU 763, LEU 721	MET 756 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
28	*Isorhamnetin 3-glucoside*	-8,5	ASP 697, VAL 698, ILE 699, HIS 770, GLN 815	PRO 696	ARG 766 (Carbon Hydrogen Bond), ARG 766 (Pi-Cation), GLU 695 (Pi-Anion), MET 692 (Sulfur X, Pi-Sulfur), PRO 696 (Pi-Sigma)
29	*Beta Seline*	-8,3	-	MET 759, PHE 778, LEU 763, LEU 718, LEU 721	-
30	*Stercurensin*	-8,3	-	LEU 797, MET 756, MET 759, LEU 721	LEU 887, THR 894, CYS 891 (Carbon Hydrogen Bond), CYS 891 (Pi-Sulfur), TYR 890, PHE 778 (Pi-Pi T-Shaped)
31	*alpha seline*	-8,2	-	LEU 718, LEU 763, MET 759, PHE 778	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
32	*Beta Sitosterol*	-8,2	-	ILE 699, PRO 696, VAL 729, LYS 822, LEU 758, HIS 770, LYS 769	-
33	*Aurentiacin*	-8,1	THR 894	LEU 763, MET 759, PHE 905, LEU 715	ASN 719 (Carbon Hydrogen Bond), MET 756, CYS 891 (Pi-Sulfur), PHE 778 (Pi-Pi T-Shaped)
34	*Myricetin-3-(3''galloylrhamnoside)*	-8,1	SER 796, SER 793, ASN 893, GLN 886	LEU 901	SER 793 (Carbon Hydrogen Bond, Pi-Donor Hydrogen Bond), GLU 791 (Pi-Anion), TYR 890 (Pi-Pi T-Shaped)
35	*Mustakone*	-8,0	-	LEU 721, MET 801, PHE 778, LEU 718, LEU 797, PHE 794	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
36	*Myltayl-4(12)-ene*	-8,0	-	PHE 778, CYS 891, LEU 718	-
37	*alpha-ylangene*	-7,9	-	LEU 718, LEU 763, MET 801, VAL 760	-
38	*Sibirene*	-7,9	-	LEU 718	-
39	*(-)-Beta Caryophyllene*	-7,8	-	LEU 718, PHE 905, CYS 891	-
40	*alpha-copaene*	-7,8	-	LEU 763, MET 801, PHE 778, MET 759, MET 909, LEU 718	-
41	*Gamma-Muurolene*	-7,8	-	MET 801, LEU 718, PHE 794, LEU 797, PHE 778, MET 759, LEU 721	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
42	*(-)-caryophyllene oxide*	-7,7	GLN 725	PHE 778, LEU 718, MET 759	-
43	*allo-aromadendrene*	-7,7	-	LEU 718, LEU 797, MET 801, VAL 760, LEU 887, MET 756	-
44	*alpha-humulene*	-7,7	-	LEU 718	-
45	*aromadendrene*	-7,7	-	LEU 778, LEU 718, MET 759, MET 801, VAL 760, LEU 763, LEU 887	-
46	*Spathulenol*	-7,6	-	LEU 763, MET 759, PHE 778, MET 756	-
47	*Trans-sesquisabinene hydrate*	-7,6	THR 894	LEU 718, PHE 778, LEU 763, MET 759	CYS 891 (Carbon Hydrogen Bond)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
48	*(2E,6E)-Farnesyl acetate*	-7,5	ARG 766	LEU 718, TYR 890, LEU 887, LEU 797, CYS 891, MET 756	-
49	*gamma – Elemene*	-7,5	-	LEU 718	-
50	*2-ethylhexyl p-methoxycinnamate*	-7,3	GLN 725	LEU 715, PHE 905, TYR 890, LEU 718, MET 759, LEU 763, LEU 721, PHE 778	GLN 725 (Carbon Hydrogen Bond), PHE 778 (Pi-Pi T-Shaped)
51	*Beta Elemene*	-7,2		LEU 721, PHE 778	
52	*Ferulic acid*	-7,1	ILE 699, LYS 882	PHE 818, PRO 696	GLU 695 (Carbon Hydrogen Bond)
53	*Caffeic acid*	-7,0	ILE 699, LYS 822	PRO 696	-
54	*Gallic acid*	-6,7	SER 757, THR 829, TYR 753, HIS 888	VAL 884	HIS 881 (Carbon Hydrogen Bond, Pi-Cation), HIS 888 (Pi-Cation)

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
55	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	-6,6	GLN 725	CYS 891, LEU 715, TYR 890, LEU 718, PHE 778	-
56	*p-Coumaric acid*	-6,6	ARG 766, GLN 725, MET 759	LEU 721, LEU 763	PHE 778 (Pi-Pi T-Shaped)
57	*isopulegyl acetate*	-6,4		LEU 718	
58	*Vanillic acid*	-6,2	LYS 822, ASP 697	PRO 696, PHE 818	GLU 695 (Carbon Hydrogen Bond)
59	*borneol*	-6,1		LEU 718	-
60	*isopulegol*	-6,1	LEU 718	LEU 721, PHE 778, LEU 715, PHE 794, LEU 797, TYR 890	-
61	*t-Cinnamic acid*	-6,1	GLN 725		LEU 718 (Pi-Sigma)
62	*citronellyl acetate*	-6,0	ARG 766, GLN 725	MET 759, LEU 718, PHE 778, TYR 890, LEU 715, LEU 797, PHE 794	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
63	*terpinolene*	-6,0	-	PHE 794, TYR 890, LEU 797, LEU 715, LEU 721, PHE 778	LEU 718 (Pi-Sigma)
64	*alpha-fenchol*	-5,9	MET 801	LEU 718, MET 759	-
65	*phytol*	-5,9	GLU 695	ARG 766, VAL 698, VAL 729, MET 759, PRO 696	-
66	*(-)-β-pinene*	-5,8	-	TYR 890, LEU 718, CYS 891, PHE 905, LEU 715	-
67	*Beta Pinene*	-5,8	-	MET 756, LEU 718, LEU 797, LEU 715, TYR 890, LEU 887	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
68	*limonene*	-5,7	-	LYS 885, HIS 888, VAL 925, ILE 920, PRO 927, HIS 881	-
69	*linalool*	-5,7	GLN 725	PHE 778, MET 801, PHE 794, LEU 797, LEU 718	-
70	*methyl salicylate*	-5,7	THR 829, SER 757	ILE 920	HIS 881 (Carbon Hydrogen Bond, Pi-Cation), HIS 888 (Carbon Hydrogen Bond, Pi-Pi T-Shaped), TYR 753 (Carbon Hydrogen Bond)
71	*E-Beta-Ocimene*	-5,5	-	LEU 721, LEU 763, PHE 778, MET 801, LEU 718, LEU 797, PHE 794	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
72	*myrcene*	-5,5	-	LEU 763, VAL 760, MET 759, MET 801, PHE 778, LEU 718	-
73	*Z-Beta-Ocimene*	-5,5	-	LEU 763, LEU 721, PHE 778, MET 801, LEU 718, LEU 797, PHE 794	-
74	*Benzaldehyde*	-5,0	-	LEU 718, MET 759, LEU 721	PHE 778 (Pi-Pi T-Shaped)
75	*Ethyl (E)-2-butenoate*	-4,7	ARG 766	LEU 887, LEU 763, MET 801, VAL 760	-
76	*Pentyl acetate*	-4,5	ARG 766, GLN 725	LEU 718, LEU 721, PHE 778	-

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Tabel VII.12
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
77	*3-hexen-1-ol*	-4,4	MET 759	LEU 763, PHE 778, MET 759, MET 756, MET 801, VAL 760, LEU 887	-
78	*3-Methyl-2-buten-1-ol*	-4,0	MET 756	MET 759, PHE 778, LEU 763	-
79	*Ethyl acetate*	-3,9	ARG 766, GLN 725	LEU 721, PHE 778, LEU 718	-
80	*Gamma-Butyrolactone*	-3,9	ARG 766, GLN 725	-	-
81	*3-buten-2-one*	-3,6	ARG 766, GLN 725	-	-

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Tabel VII. 13
Hasil *Molecular Docking* terhadap HER2 dan Analisis Residu Asam Amino

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
1	*Trastuzumab*	-7,8	ASP 863, ALA 751, LYS 753, LEU 796, THR 862	-	-
2	*Ligan Alami (O3Q)*	-11,4	ASP 863, MET 801	ALA 751, VAL 734, LYS 753, LEU 785, MET 774, LEU 796, PHE 864	GLN 779, ASP 863 (Carbon Hydrogen Bond), GLU 770 (Halogen (Fluorine)), LEU 852, LEU 726 (Pi-Sigma), PHE 864 (Pi-Pi T-shaped)
3	*Ellagic acid*	-10,4	ASP 863, CYS 805	ALA 751, LEU 726, CYS 805, LEU 852, VAL 734	GLY 729, GLY 804 (Carbon Hydrogen Bond), LEU 852, THR 862, VAL 734 (Pi-Sigma)

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Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
4	*Myricetin*	-10,3	ASP 863, LYS 753, MET 801, ALA 751, LEU 796	LEU 726, VAL 734, LEU 852, ALA 751, LYS 753	GLY 804 (Carbon Hydrogen Bond), LEU 852, THR 798, VAL 734 (Pi-Sigma)
5	*Procyanidin B1*	-10,3	ASN 758, ARG 844, ARG 868, LYS 762, SER 760	ARG 756, ALA 763, LEU 755	ASN 758 (Carbon Hydrogen Bond), GLY 882 (Pi-Cation)
6	*(+)-Catechin*	-9,9	GLU 770	LEU 796, MET 774, LEU 785, LYS 753, ALA 751	PHE 864 (Pi-Pi T-shaped), VAL 734 (Pi-Sigma)
7	*(-)-Epicatechin*	-9,9	-	LYS 753, LEU 796, LEU 852	GLY 729 (Carbon Hydrogen Bond), VAL 734 (Pi-Sigma)

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Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
8	*Morin*	-9,9	ASP 863, LYS 753, MET 801	LEU 726, ALA 751, VAL 734, LYS 753, LEU 852	LEU 852, VAL 734, THR 798 (Pi-Sigma)
9	*Quercetin*	-9,9	ASP 863, MET 801	LEU 726, ALA 751, VAL 734, LYS 753, LEU 852, ASP 863	GLY 804 (Carbon Hydrogen Bond), LEU 852, THR 798, VAL 734 (Pi-Sigma)
10	*Pinocembrin*	-9,8	-	LEU 796, LYS 753, ALA 751, LEU 726	GLY 729 (Carbon Hydrogen Bond), VAL 734, LEU 852 (Pi-Sigma)
11	*Procyanidin A2*	-9,8	ASN 758, ARG 844, GLU 766	ARG 756	ALA 879 (Carbon Hydrogen Bond), ARG 868, GLY 882 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Amide-Pi Stacked)

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Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
12	*Rutin*	-9,6	ASN 758, ARG 756, LYS 883, SER 760	ILE 767, LEU 755	THR 759 (Carbon Hydrogen Bond), ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)
13	*8-Methylpinocembrin*	-9,5	LEU 726	ALA 751, LYS 753, VAL 734	GLY 804, GLY 727 (Carbon Hydrogen Bond)
14	*ursolic acid*	-9,5	PHE 731, ILE 886, LYS 887	-	-
15	*Myricitrin*	-9,4	ARG 756, SER 760, LYS 762	LEU 755, ILE 767	ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)

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Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
16	*Procyanidin B2*	-9,4	ASN 758, GLU 770, GLU 766, ARG 868, LYS 762	ARG 756, ALA 763	LYS 762 (Carbon Hydrogen Bond), GLY 882 (Pi-Cation), PHE 731 (Pi-Pi T Shaped)
17	*Mearnsitrin*	-9,3	ARG 756, SER 760, LYS 762	LEU 755, ILE 767, ALA 879	GLY 882 (Carbon Hydrogen Bond), ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)
18	*Quercitrin*	-9,3	ASN 758, ARG 868, ARG 756, LYS 762, SER 760	LEU 755, ARG 756	PHE 731 (Pi-Pi Stacked)

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Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
19	*Epigalocatechin Gallate*	-9,2	ASN 758, ARG 756, ARG 868	LEU 755, ALA 763, ARG 756	GLY 865, LYS 762 (Carbon Hydrogen Bond), GLU 766 (Pi-Anion), LYS 762 (Pi-Cation), ARG 756 (Pi-Sigma), PHE 731 (Pi-Pi Stacked)
20	*(-)-Epigallocatechin gallate*	-9,1	ASN 758, ARG 756, ARG 868	LEU 755, ALA 763, ARG 756	GLY 865, LYS 762 (Carbon Hydrogen Bond), GLU 766 (Pi-Anion), LYS 762 (Pi-Cation), ARG 756 (Pi-Sigma), PHE 731 (Pi-Pi Stacked)
21	*Desmanthin 1*	-9,1	ARG 756, LYS 762, TYR 877, LYS 883	LEU 755, ARG 756	ARG 844, ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
22	*(-)-Epicatechin gallate*	-9,0	ASN 758, ARG 756, ARG 868	LEU 755, ALA 763, ARG 756	GLY 865 (Carbon Hydrogen Bond), GLU 766 (Pi-Anion), ARG 756 (Pi-Sigma), PHE 731 (Pi-Pi Stacked)
23	*2',4'-Dihydroxy-6'-methoxy-3'-methyldihydrochalcone*	-9,0	THR 862	LEU 796, LYS 753, ALA 751, VAL 734, LEU 726, LEU 852	LEU 852 (Pi-Sigma)
24	*aromadendrene*	-8,9	-	ALA 751, LEU 726, LEU 852, VAL 734	-
25	*Chlorogenic acid*	-8,9	CYS 805, LEU 726, SER 728, LEU 796, LYS 753	VAL 734, ALA 751, LYS 753	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik Pi-alkyl/alkyl	Interaksi lain
26	*Myricetin-3-(3''galloylrhamnoside)*	-8,9	ARG 756, LYS 883, LYS 762	LEU 755, ILE 767	GLY 882 (Carbon Hydrogen Bond), ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)
27	*2-ethylhexyl p-methoxycinnamate*	-8,7	-	LEU 796, PHE 864, ALA 771, LEU 785, ALA 751, LEU 726	ASP 863 (Carbon Hydrogen Bond), LEU 852, VAL 734 (Pi-Sigma)
28	*Aurentiacin*	-8,7	ASP 863	ALA 751, VAL 734, LEU 852, LEU 726, CYS 805, LEU 785, LEU 796	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
29	*Isoquercitrin*	-8,7	ARG 756, ASN 758, SER 760	LEU 755	ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)
30	*Isorhamnetin 3-glucoside*	-8,7	ARG 756, ASN 758, SER 760, LYS 762	LEU 755	GLY 882 (Carbon Hydrogen Bond), ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked)
31	*Uvangoletin*	-8,6	ASP 863, THR 862	ALA 751, LEU 726, VAL 734, LEU 852, LEU 796, LYS 753	LEU 852 (Pi-Sigma)
32	*Kaempferol 3-glucoside*	-8,5	ARG 756, ASN 758, SER 760	LEU 755	ARG 868 (Pi-Cation), PHE 731 (Pi-Pi Stacked, Pi-Pi T Shaped)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
33	*Stercurensin*	-8,4	GLU 770	LEU 852, ALA 751, LYS 753, LEU 796	LEU 785, THR 862, VAL 734 (Pi-Sigma)
34	*(2E,6E)-Farnesyl acetate*	-8,3	SER 783	LEU 726, ALA 751, VAL 734, LEU 852, LYS 753	ASP 863 (Carbon Hydrogen Bond)
35	*Beta Sitosterol*	-8,3	-	ARG 756, ALA 763, PHE 731, ILE 767, LEU 775	-
36	*alpha seline*	-8,2	-	LEU 852, LEU 726, CYS 805, VAL 734	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
37	*phytol*	-8,2	CYS 805	LEU 785, ALA 771, LEU 796, MET 774, PHE 864, LYS 753, VAL 734, ALA 751, LEU 726, LEU 852	-
38	*alpha-copaene*	-8,1	-	LEU 755, ALA 763, ARG 756, LEU 866, PHE 731	PHE 731 (Pi-Sigma)
39	*alpha-ylangene*	-8,1	-	LEU 866, ALA 763, PHE 731, ARG 756, LEU 755	PHE 731 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
40	*Beta Seline*	-7,9	-	LEU 755, ARG 756, PHE 731, ALA 763	-
41	*Gamma-Muurolene*	-7,9	-	LEU 726, ALA 751, VAL 734, LEU 852	-
42	*(-)-caryophyllene oxide*	-7,6	-	ALA 763, PHE 731	-
43	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	-7,6	THR 862	VAL 734, LEU 852, LYS 753, LEU 785, MET 774, LEU 796, PHE 864, ALA 771	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
44	*allo-aromadendrene*	-7,6	-	ALA 751, LEU 852, LYS 753, VAL 734	-
45	*Spathulenol*	-7,6	ARG 868, GLU 766	ARG 756, LEU 755, ALA 763, PHE 731	PHE 731 (Pi-Sigma)
46	*Gallic acid*	-7,4	THR 862, GLU 770	LEU 785, LEU 796	PHE 864 (Pi-Pi T-shaped)
47	*(-)-Beta Caryophyllene*	-7,3	-	VAL 734, LEU 726	-
48	*Caffeic acid*	-7,3	THR 862, ASP 863	LEU 796, LYS 753	-
49	*Ferulic acid*	-7,3	ASP 863, THR 862	VAL 734, LYS 753, LEU 796	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
50	*Sibirene*	-7,3		CYS 805, VAL 734, LEU 852, ALA 751, LEU 726	
51	*Trans-sesquisabinene hydrate*	-7,3	-	LYS 753, VAL 734, LEU 726, LEU 852	-
52	*alpha-humulene*	-7,2	-	ARG 756, ALA 763, PHE 731	-
53	*Vanillic acid*	-7,2	ASP 863, GLU 770, SER 783	LYS 753, MET 774, LEU 785	PHE 864 (Pi-Pi T Shaped)
54	*isopulegol*	-7,0	SER 783	VAL 734, LYS 753, LEU 796, PHE 864, LEU 785, MET 774	-

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
55	*Mustakone*	-7,0	-	ALA 763, ARG 756, LEU 866, PHE 731	PHE 731 (Pi-Sigma)
56	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	-6,9	SER 760	ALA 763, LEU 755, ILE 767	-
57	*citronellyl acetate*	-6,9	ASP 863, SER 783	VAL 734, ALA 751, LYS 753	-
58	*isopulegyl acetate*	-6,8	-	ALA 751, LYS 753, VAL 734	-
59	*methyl salicylate*	-6,7	SER 783, ASP 863	LEU 785, MET 774	LEU 796 (Carbon Hydrogen Bond), PHE 864 (Pi-Pi T Shaped)
60	*p-Coumaric acid*	-6,7	ASP 863	LEU 852, ALA 751	VAL 734 (Pi-Sigma)
61	*t-Cinnamic acid*	-6,6	ASP 863	LEU 852, ALA 751	VAL 734 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
62	*terpinolene*	-6,5	-	ALA 751, LYS 753, VAL 734	LEU 852, VAL 734 (Pi-Sigma)
63	*Beta Elemene*	-6,4	-	ARG 756, ALA 763, PHE 731, ILE 767	-
64	*E-Beta-Ocimene*	-6,4	-	LYS 753, LEU 796, LEU 785, ALA 771	-
65	*Z-Beta-Ocimene*	-6,4	-	LYS 753, LEU 796, LEU 785, ALA 771	-
66	*linalool*	-6,3	SER 783	MET 774, PHE 864, LEU 785, ALA 771, LEU 796	-
67	*(-)-β-pinene*	-6,2	-	ALA 763, LEU 866	PHE 731 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
68	*Beta Pinene*	-6,2	-	ALA 763, LEU 866, PHE 731	PHE 731 (Pi-Sigma)
69	*Myltayl-4(12)-ene*	-6,2	-	ALA 763, PHE 731	PHE 731 (Pi-Sigma)
70	*myrcene*	-6,2	-	LYS 753, LEU 796, LEU 785, ALA 771, ILE 767	-
71	*gamma – Elemene*	-6,1	-	PHE 731, ARG 756, ALA 763	-
72	*limonene*	-6,1	-	LEU 866, ALA 763, PHE 731	PHE 731 (Pi-Sigma)
73	*alpha-fenchol*	-6,0	SER 783	LYS 753, LEU 796	-
74	*borneol*	-5,7	ARG 868, GLY 865	ALA 763	PHE 731 (Pi-Sigma)

LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
75	*Benzaldehyde*	-5,4	ASP 863, SER 783	LEU 785, LEU 796, MET 774	PHE 864 (Pi-Sigma)
76	*Pentyl acetate*	-5,4	SER 783	LEU 796, PHE 864, ALA 771, LEU 785, MET 774	-
77	*3-hexen-1-ol*	-5,1	SER 783	PHE 864, ALA 771, LEU 785, MET 774, LEU 796	-
78	*Ethyl (E)-2-butenoate*	-5,0	-	LEU 785, LEU 796, MET 774, LYS 753	-
79	*3-Methyl-2-buten-1-ol*	-4,6	SER 783	PHE 864, LEU 785, MET 774, LEU 796	-
80	*Gamma-Butyrolactone*	-4,4	ASP 863, SER 783	-	-

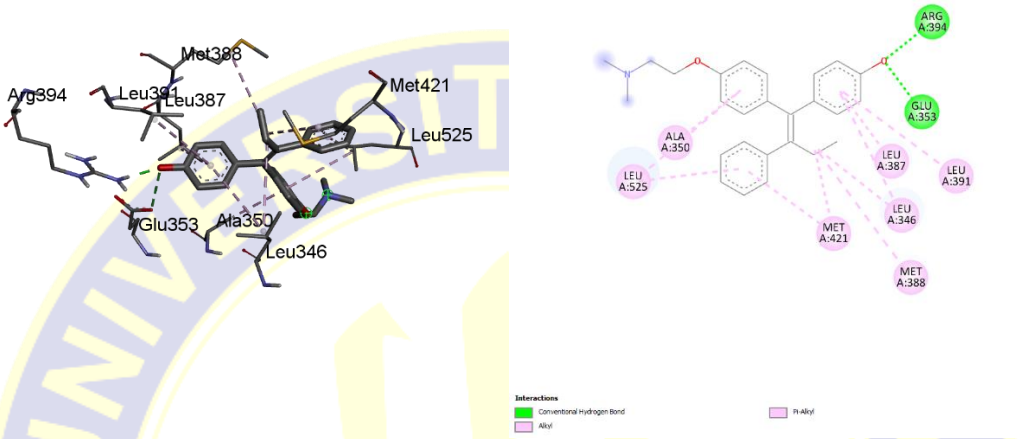
LAMPIRAN 15
(LANJUTAN)

Tabel VII.13
Lanjutan

No.	Ligan Uji	ΔG (kkal/mol)	Ikatan Hidrogen	Interaksi Hidrofobik	Interaksi lain
				Pi-alkyl/alkyl	
81	*Ethyl acetate*	-3,9	-	LEU 785, MET 744	-
82	*3-buten-2-one*	-3,8	-	-	-

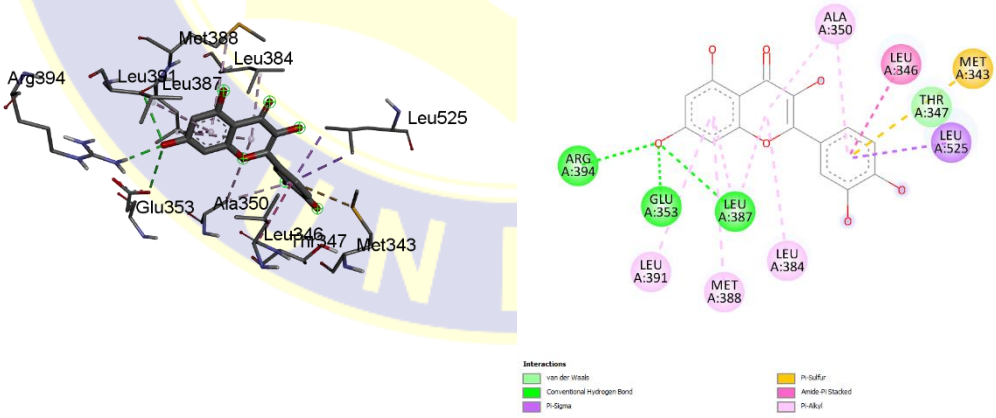
LAMPIRAN 16

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



(a) (b)

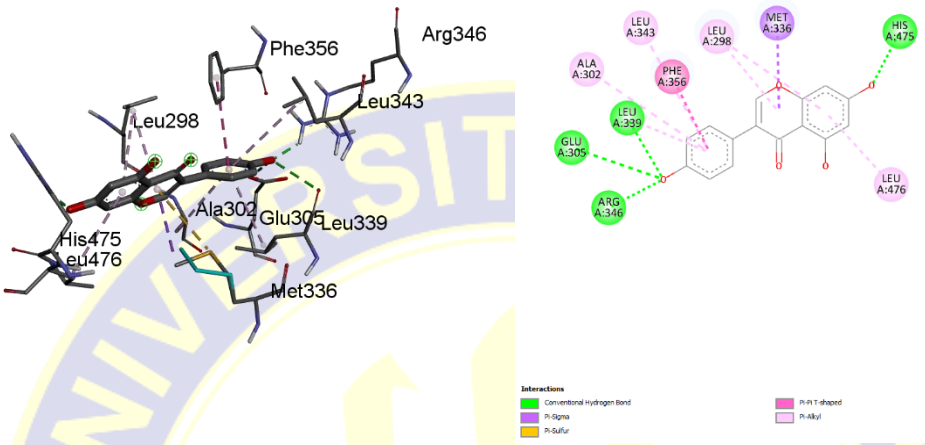
Gambar VII. 30 Visualisasi struktur 3D (a) dan 2D (b) ligan alami *4-Hydroxytamoxifen* terhadap ER-α



(a) (b)

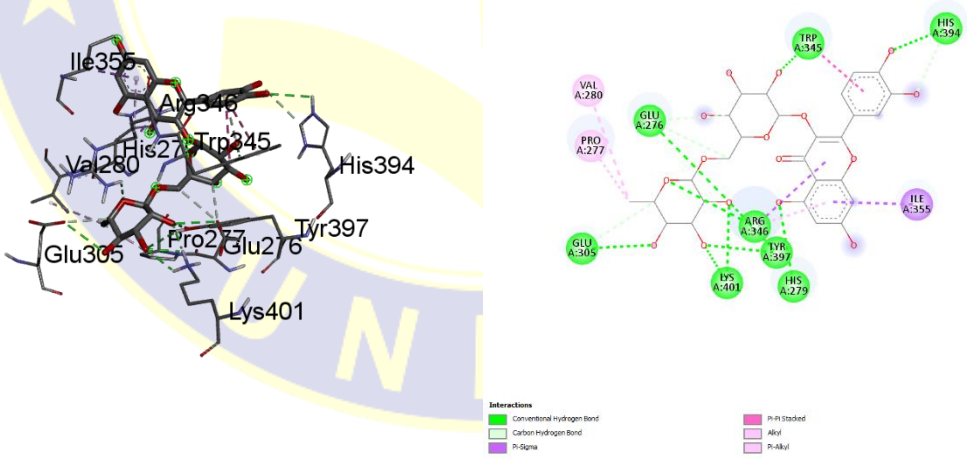
Gambar VII. 31 Visualisasi struktur 3D (a) dan 2D (b) ligan *Quercetin* terhadap ER-α

LAMPIRAN 16
(LANJUTAN)



(a) (b)

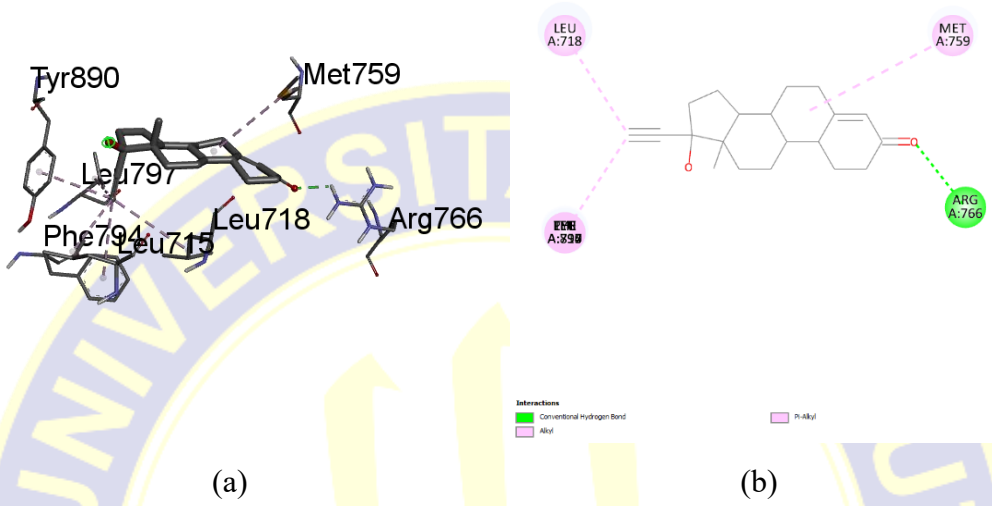
Gambar VII. 32 Visualisasi struktur 3D (a) dan 2D (b) ligan alami *Genistein* terhadap ER-β



(a) (b)

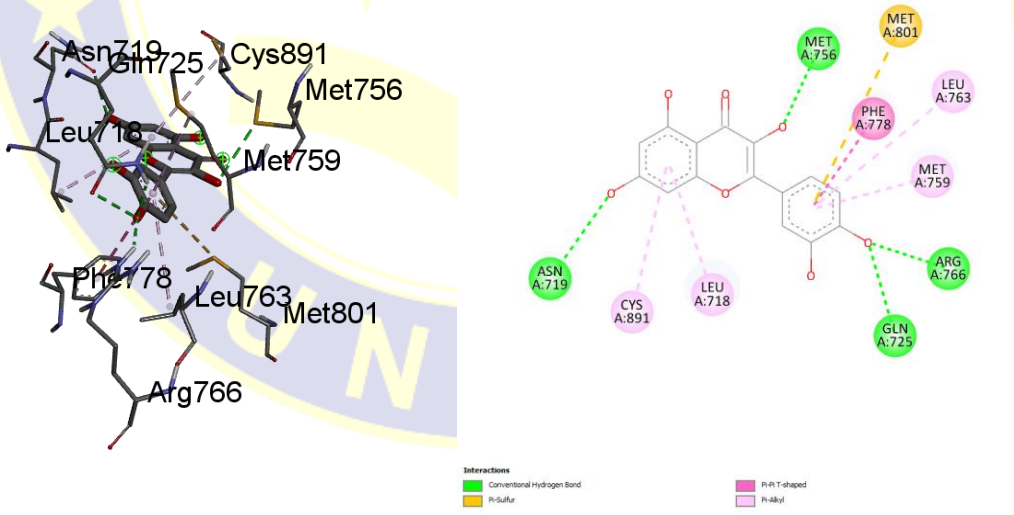
Gambar VII. 33 Visualisasi struktur 3D (a) dan 2D (b) ligan *Rutin* terhadap ER-β

LAMPIRAN 16
(LANJUTAN)



(a) (b)

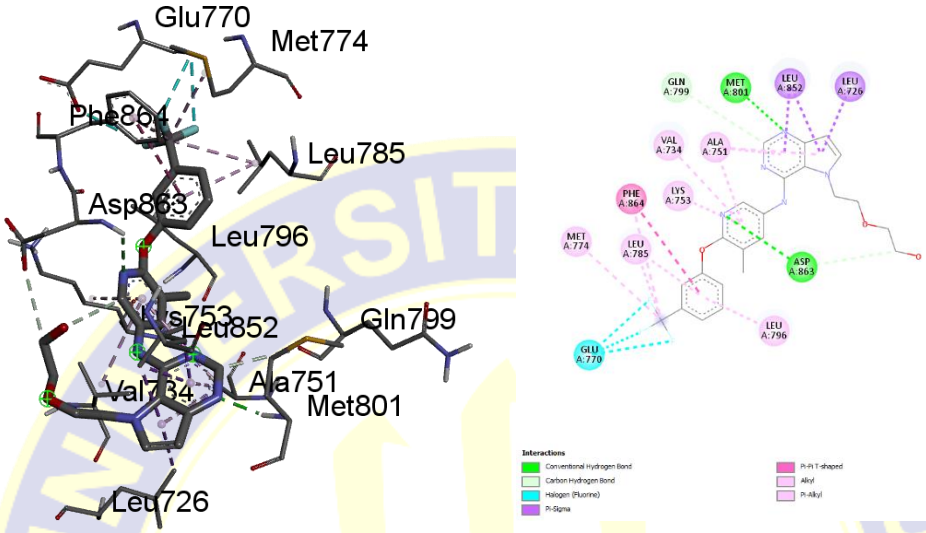
Gambar VII. 34 Visualisasi struktur 3D (a) dan 2D (b) ligan alami *Norethindrone* terhadap Progesteron



(a) (b)

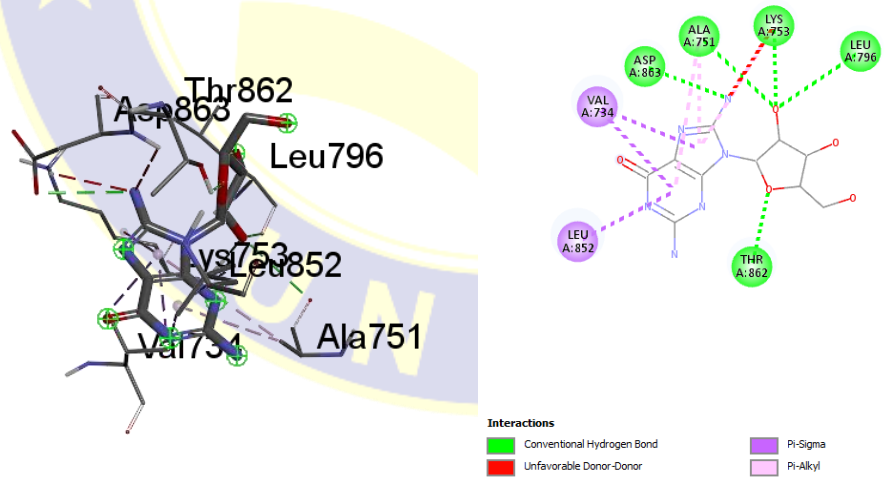
Gambar VII. 35 Visualisasi struktur 3D (a) dan 2D (b) ligan *Quercetin* terhadap Progesteron

LAMPIRAN 16
(LANJUTAN)



(a) (b)

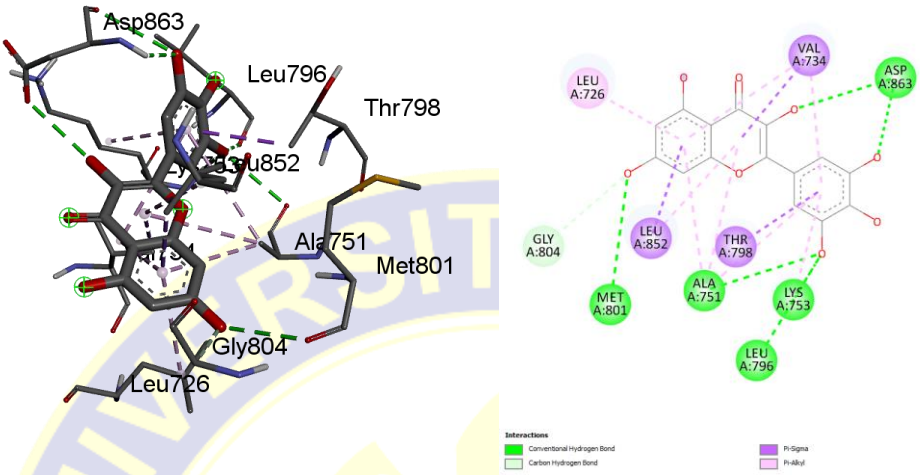
Gambar VII. 36 Visualisasi struktur 3D (a) dan 2D (b) ligan alami O3Q terhadap HER2



(a) (b)

Gambar VII. 37 Visualisasi struktur 3D (a) dan 2D (b) ligan pembanding Trastuzumab terhadap HER2

LAMPIRAN 16
(LANJUTAN)



(a) (b)

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

LAMPIRAN 17

HASIL PREDIKSI *DRUGLIKENESS*

Tabel VII. 14
Hasil Prediksi *Druglikeness*

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
1	*4-Hydroxytamoxifen*	358	0	2	0,73	Memenuhi
2	*Genistein*	260	0	5	-1,3	Memenuhi
3	*Norethindrone*	272	0	2	0,19	Memenuhi
4	*O3Q*	474,5	0	8	0,23	Memenuhi
5	*Trastuzumab*	284	0	11	0	Tidak Memenuhi
6	*Cyanidin-3,5-O-diglucosid*	580	0	16	-3,69	Tidak Memenuhi
7	*Quercitrin*	428	0	11	0	Tidak Memenuhi
8	*Peonidin 3,5-diglucosside*	592	0	16	-1,77	Tidak Memenuhi
9	*Pelargonidin-3-glucoside*	412	0	10	-2,19	Tidak Memenuhi
10	*Procyanidin B2*	552	0	12	-0,71	Tidak Memenuhi
11	*Peonidin-3-Glukosid*	475	0	11	0	Tidak Memenuhi
12	*Procyanidin B1*	552	0	12	0	Tidak Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
13	*Cyanidin-3-O-Glukosid*	463	0	11	-1,28	Tidak Memenuhi
14	*Cyanidin 3-glucoside*	463	0	11	-1,28	Tidak Memenuhi
15	*Procyanidin A2*	552	0	12	-2,83	Tidak Memenuhi
16	*2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone*	268	0	4	0,57	Memenuhi
17	*Stercurensin*	268	0	4	0,57	Memenuhi
18	*Kaempferol-3-glucoside*	428	0	11	0	Tidak Memenuhi
19	*Isorhamnetin-3-glucoside*	456	0	12	0	Tidak Memenuhi
20	*Isoquercitrin*	444	0	12	0	Tidak Memenuhi
21	*(-)-Epicatechin*	276	0	6	-1,56	Memenuhi
22	*Quercetin*	292	0	7	0	Memenuhi
23	*(+)-Catechin*	276	0	6	-1,56	Memenuhi
24	*Morin*	292	0	7	0	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
25	*Myricitrin*	444	0	12	0	Tidak Memenuhi
26	*Chlorogenic Acid*	336	0	9	0	Memenuhi
27	*Myricetin-3-(3''galloylrhamnoside)*	592	0	16	0	Tidak Memenuhi
28	*Mearnsitrin*	456	0	12	0	Tidak Memenuhi
29	*(-)-Epicatechin gallate*	424	0	10	-2,88	Tidak Memenuhi
30	*Desmanthin1*	592	0	16	0	Tidak Memenuhi
31	*Rutin*	580	0	16	0	Tidak Memenuhi
32	*Ursolic Acid*	408	0	3	0,42	Memenuhi
33	*(-)-Beta Caryophyllene*	180	0	0	1,56	Memenuhi
34	*(-)-β-pinene*	120	0	0	0,84	Memenuhi
35	*(-)-caryophyllene oxide*	196	0	1	1,12	Memenuhi
36	*(-)-Epigallocatechin gallate*	440	0	11	-3,4	Tidak Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
37	*(2E,6E)-Farnesyl acetate*	236	0	2	0	Memenuhi
38	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	196	0	1	0	Memenuhi
39	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	280	0	4	0,18	Memenuhi
40	*2-ethylhexyl p-methoxycinnamate*	264	0	3	0,79	Memenuhi
41	*3-buten-2-one*	64	0	1	-0,15	Memenuhi
42	*3-hexen-1-ol*	88	0	1	0,23	Memenuhi
43	*3-Methyl-2-buten-1-ol*	76	0	1	-0,07	Memenuhi
44	*8-Methylpinocembrin*	256	0	4	-0,31	Memenuhi
45	*allo-aromadendrene*	180	0	0	1,64	Memenuhi
46	*alpha-copaene*	180	0	0	1,09	Memenuhi
47	*alpha-fenchol*	136	0	1	0,06	Memenuhi
48	*alpha-humulene*	180	0	0	0	Memenuhi
49	*alpha seline*	180	0	0	0	Memenuhi
50	*alpha-ylangene*	180	0	0	1,09	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
51	*aromadendrene*	180	0	0	1,64	Memenuhi
52	*Aurentiacin*	280	0	4	0,73	Memenuhi
53	*Benzaldehyde*	100	0	1	0,16	Memenuhi
54	*Beta Pinene*	120	0	0	0,84	Memenuhi
55	*Beta Seline*	180	0	0	0,82	Memenuhi
56	*Beta Sitosterol*	364	0	1	1,77	Memenuhi
57	*Beta Elemene*	180	0	0	1,06	Memenuhi
58	*borneol*	136	0	1	0,06	Memenuhi
59	*Caffeic acid*	172	0	4	-2,52	Memenuhi
60	*citronellyl acetate*	176	0	2	0,21	Memenuhi
61	*E-Beta-Ocimene*	120	0	0	0	Memenuhi
62	*Ellagic acid*	296	0	8	-1,93	Memenuhi
63	*Epigalocatechin Gallate*	440	0	11	-3,4	Tidak Memenuhi
64	*Ethyl (E)-2-butenoate*	104	0	2	-0,25	Memenuhi
65	*Ethyl acetate*	80	0	2	-0,27	Memenuhi
66	*Ferulic acid*	184	0	4	-1,47	Memenuhi
67	*Gallic acid*	164	0	5	-2,96	Memenuhi
68	*gamma – Elemene*	180	0	0	0	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
69	*Gamma-Butyrolactone*	80	0	2	-0,41	Memenuhi
70	*Gamma-Muurolene*	180	0	0	1,64	Memenuhi
71	*isopulegol*	136	0	1	9,47	Tidak Memenuhi
72	*isopulegyl acetate*	176	0	2	0,58	Memenuhi
73	*limonene*	120	0	0	1,02	Memenuhi
74	*linalool*	136	0	1	0,09	Memenuhi
75	*methyl salicylate*	144	0	3	-0,23	Memenuhi
76	*Mustakone*	196	0	1	0	Memenuhi
77	*Myltayl-4(12)-ene*	180	0	0	0,58	Memenuhi
78	*myrcene*	120	0	0	0	Memenuhi
79	*Myricetin*	308	0	8	-2,29	Memenuhi
80	*p-Coumaric acid*	156	0	3	-2,09	Memenuhi
81	*Pentyl acetate*	116	0	2	-0,34	Memenuhi
82	*phytol*	256	0	1	0	Memenuhi
83	*Pinocembrin*	244	0	4	-0,36	Memenuhi
84	*Sibirene*	180	0	0	0,74	Memenuhi
85	*Spathulenol*	196	0	1	0,84	Memenuhi
86	*t-Cinnamic acid*	140	0	2	-1,26	Memenuhi

LAMPIRAN 17
(LANJUTAN)

Tabel VII.14
Lanjutan

No.	Ligan Uji	BM(g/mol)	Donor H	Akseptor H	Log P	Keterangan
87	*terpinolene*	120	0	0	1,02	Memenuhi
88	*Trans-sesquisabinene hydrate*	196	0	1	0	Memenuhi
89	*Uvangoletin*	256	0	4	0	Memenuhi
90	*Vanillic acid*	160	0	4	-1,48	Memenuhi
91	*Z-Beta-Ocimene*	120	0	0	0	Memenuhi

LAMPIRAN 18

HASIL PREDIKSI ADMET

Tabel VII. 15
Hasil Prediksi Profil Farmakokinetik dan Toksisitas

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
1	*4-Hydroxytamoxifen*	97,17*	47,76**	100*	Non Mutagen	Negatif
2	*Genistein*	88,12*	5,74**	89,73**	Mutagen	Negatif
3	*Norethindrone*	95, 75*	29,58**	100*	Non Mutagen	Positif
4	*O3Q*	95,56*	36,18**	90,99*	Non Mutagen	Negatif
5	*Trastuzumab*	12,85***	7,46**	5,89**	Mutagen	Negatif
6	*Cyanidin-3,5-O-diglucosid*	2,16***	3,23***	47,73**	Non Mutagen	Negatif
7	*Quercitrin*	24,94**	7,37**	64,95**	Non Mutagen	Negatif
8	*Peonidin 3,5-diglucosside*	4,27***	3,83***	29,76**	Non Mutagen	Negatif
9	*Pelargonidin-3-glucoside*	39,14**	6,59**	77,6**	Non Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
10	*Procyanidin B2*	19,51***	13,67**	100*	Non Mutagen	Negatif
11	*Peonidin-3-Glukosid*	35,22**	6,84**	65,4**	Non Mutagen	Negatif
12	*Procyanidin B1*	19,51***	13,67**	100*	Non Mutagen	Negatif
13	*Cyanidin-3-O-Glukosid*	19,72***	5,92**	79,61**	Non Mutagen	Positif
14	*Cyanidin 3-glucoside*	19,72***	5,92**	79,61**	Non Mutagen	Negatif
15	*Procyanidin A2*	35,29**	9,23**	100*	Non Mutagen	Negatif
16	*2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone*	92,76*	18,49**	96,08*	Mutagen	Negatif
17	*Stercurensin*	93,03*	18,43**	92,06*	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
18	*Kaempferol-3-glucoside*	25,17**	11,14**	57,57**	Non Mutagen	Negatif
19	*Isorhamnetin-3-glucoside*	21,6**	9,93**	47,83**	Non Mutagen	Negatif
20	*Isoquercitrin*	11,77***	9,43**	59,15**	Non Mutagen	Negatif
21	*(-)-Epicatechin*	66,7**	0,65***	100*	Mutagen	Negatif
22	*Quercetin*	63,48**	3,41***	93,23*	Mutagen	Negatif
23	*(+)-Catechin*	66,7**	0,65***	100*	Mutagen	Negatif
24	*Morin*	63,49**	17,1**	91,62*	Mutagen	Negatif
25	*Myricitrin*	11,64***	6,14**	65,37**	Non Mutagen	Negatif
26	*Chlorogenic Acid*	20,42**	18,71**	41,96**	Mutagen	Positif
27	*Myricetin-3-(3''galloylrhamnoside)*	4,07***	7,47**	100*	Non Mutagen	Positif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
28	*Mearnsitrin*	21,45**	6,21**	55,6**	Non Mutagen	Negatif
29	*(-)-Epicatechin gallate*	40,58**	13,21**	100*	Non Mutagen	Negatif
30	*Desmanthin1*	4,07***	13,67**	100*	Non Mutagen	Positif
31	*Rutin*	2,86***	7,91**	43, 89**	Non Mutagen	Negatif
32	*Ursolic Acid*	95,99*	21,86**	100*	Non Mutagen	Positif
33	*(-)-Beta Caryophyllene*	100*	23,63**	100*	Mutagen	Negatif
34	*(-)-β-pinene*	100*	23,49**	100*	Mutagen	Negatif
35	*(-)-caryophyllene oxide*	100*	56,34**	90,84*	Mutagen	Positif
36	*(-)-Epigallocatechin gallate*	20,71**	12,04**	100*	Non Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
37	*(2E,6E)-Farnesyl acetate*	100*	55,05**	100*	Non Mutagen	Positif
38	*(E)-3,7,11- trimethyl-1,6,10-dodecatrien-3-ol*	100*	26,61**	100*	Non Mutagen	Negatif
39	*2',4'-Dihydroxy-6'-methoxy-3',5'-Dimethylchalcone*	93,23*	20,13**	91,52*	Non Mutagen	Negatif
40	*2-ethylhexyl p-methoxycinnamate*	98,76*	55,98**	94,07*	Non Mutagen	Positif
41	*3-buten-2-one*	100*	30,44**	62,78**	Mutagen	Negatif
42	*3-hexen-1-ol*	100*	25,12**	87,64**	Mutagen	Negatif
43	*3-Methyl-2-buten-1-ol*	100*	21,72**	81,16**	Mutagen	Negatif
44	*8-Methylpinocembrin*	95,57*	5,06**	97,89*	Mutagen	Negatif
45	*allo-aromadendrene*	100*	23,49**	100*	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
46	*alpha-copaene*	100*	23,63**	100*	Non Mutagen	Negatif
47	*alpha-fenchol*	100*	24,23**	100*	Mutagen	Negatif
48	*alpha-humulene*	100*	23,63**	100*	Non Mutagen	Positif
49	*alpha seline*	100*	23,63**	100*	Mutagen	Negatif
50	*alpha-ylangene*	100*	23,63**	100*	Non Mutagen	Negatif
51	*aromadendrene*	100*	23,49**	100*	Mutagen	Negatif
52	*Aurentiacin*	95,62*	36,48**	90,50*	Mutagen	Negatif
53	*Benzaldehyde*	100*	21,87**	4,50**	Mutagen	Negatif
54	*Beta Pinene*	100*	23,49**	100*	Mutagen	Negatif
55	*Beta Seline*	100*	23,49**	100*	Mutagen	Negatif
56	*Beta Sitosterol*	100*	52,37**	100*	Non Mutagen	Positif
57	*Beta Elemene*	100*	23,49**	100*	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
58	*borneol*	100*	24,23**	100*	Mutagen	Negatif
59	*Caffeic acid*	82,30*	21,10**	40,29**	Mutagen	Negatif
60	*citronellyl acetate*	100*	44,81**	100*	Non Mutagen	Positif
61	*E-Beta-Ocimene*	100*	23,63**	100*	Mutagen	Positif
62	*Ellagic acid*	61,39**	20,48**	88,40**	Mutagen	Negatif
63	*Epigalocatechin Gallate*	20,71**	12,04**	100*	Non Mutagen	Negatif
64	*Ethyl (E)-2-butenoate*	100*	50,49**	96,52*	Mutagen	Positif
65	*Ethyl acetate*	99,78*	37,20**	79,98**	Mutagen	Positif
66	*Ferulic acid*	90,60*	21,11**	50,41**	Mutagen	Negatif
67	*Gallic acid*	53,69**	13,84**	65,38**	Mutagen	Negatif
68	*gamma – Elemene*	100*	23,49**	100*	Mutagen	Negatif
69	*Gamma-Butyrolactone*	99,78*	20,78**	78,40**	Mutagen	Negatif
70	*Gamma-Muurolene*	100*	23,63**	100*	Mutagen	Negatif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
71	*isopulegol*	100*	38,71	100*	Mutagen	Negatif
72	*isopulegyl acetate*	100*	53,74**	99,14*	Mutagen	Positif
73	*limonene*	100*	23,63**	100*	Mutagen	Negatif
74	*linalool*	100*	29,35**	100*	Mutagen	Negatif
75	*methyl salicylate*	93,05*	20,78**	44,29**	Mutagen	Negatif
76	*Mustakone*	100*	40,02**	100*	Mutagen	Positif
77	*Myltayl-4(12)-ene*	100*	23,49**	81,32**	Mutagen	Negatif
78	*myrcene*	100*	23,63**	100*	Mutagen	Negatif
79	*Myricetin*	40,96**	0,99***	96,78*	Mutagen	Negatif
80	*p-Coumaric acid*	92,09*	21,10**	63,05**	Mutagen	Positif
81	*Pentyl acetate*	100*	52,87**	95,17*	Mutagen	Positif
82	*phytol*	100*	37,62**	100*	Non Mutagen	Positif
83	*Pinocembrin*	92,35*	2,47***	98,45*	Mutagen	Negatif
84	*Sibirene*	100*	23,64**	100*	Mutagen	Negatif
85	*Spathulenol*	100*	54,42**	82,88**	Mutagen	Positif

LAMPIRAN 18
(LANJUTAN)

Tabel VII. 15
Lanjutan

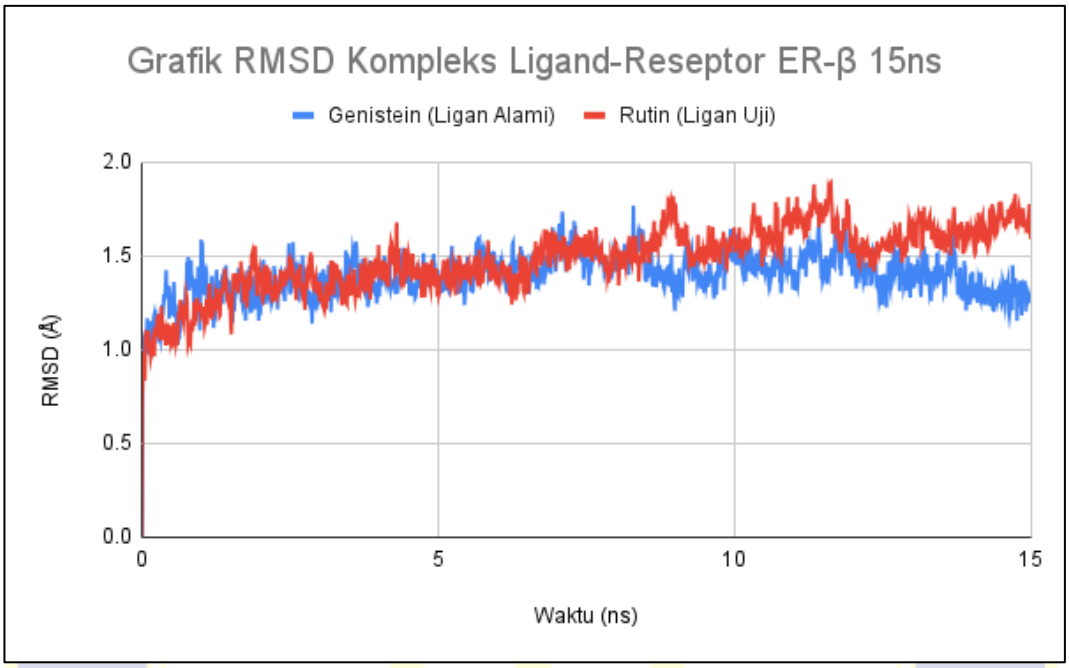
No.	Ligan Uji	Absorpsi		Distribusi	Toksisitas dan Mutagenitas	
		HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
86	*t-Cinnamic acid*	97,84*	21,03**	60,85**	Mutagen	Negatif
87	*terpinolene*	100*	23,63**	93,16*	Mutagen	Positif
88	*Trans-sesquisabinene hydrate*	100*	21,21**	100*	Mutagen	Positif
89	*Uvangoletin*	92,55*	16,01**	96,38*	Mutagen	Negatif
90	*Vanillic acid*	85,36*	19,93***	52,10**	Mutagen	Negatif
91	*Z-Beta-Ocimene*	100*	23,63**	100*	Mutagen	Positif

Keterangan:

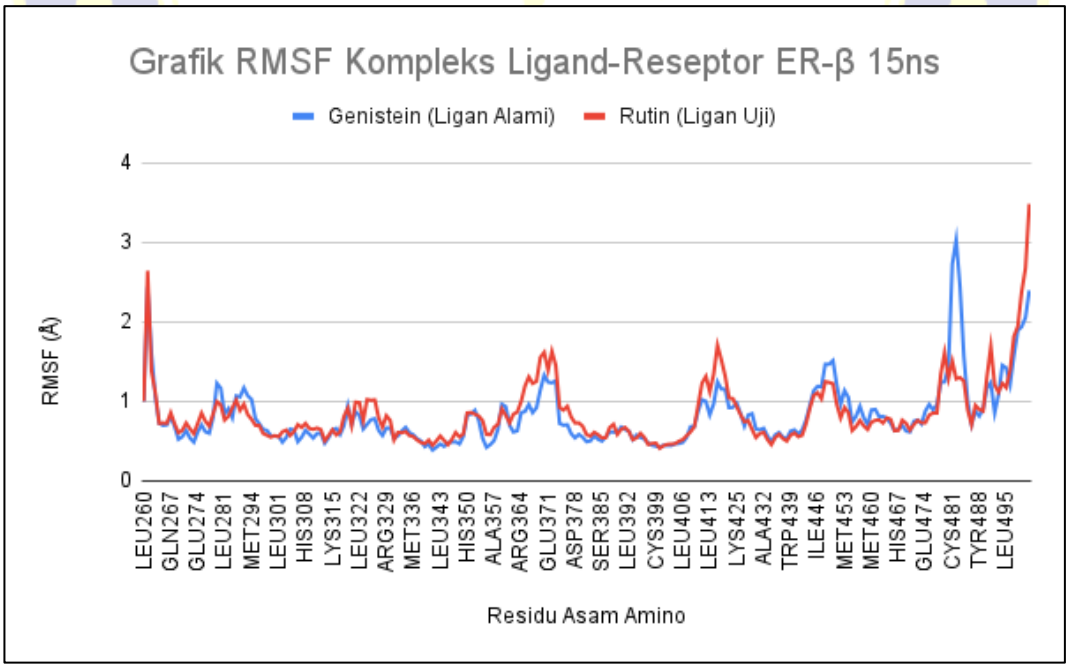
HIA (%)	CaCo-2 (nm sec)	PPB (%)
70-100 : Terserap baik (*)	>70 : Permeabilitas tinggi (*)	>90 : Terikat kuat (*)
20-70 : Cukup terserap (**)	4-70 : Permeabilitas sedang (**)	<90 : Terikat lemah (**)
< 20 : Kurang terserap (***)	<4 : Permeabilitas rendah (***)	

LAMPIRAN 19

HASIL SIMULASI *MOLECULAR DYNAMIC*

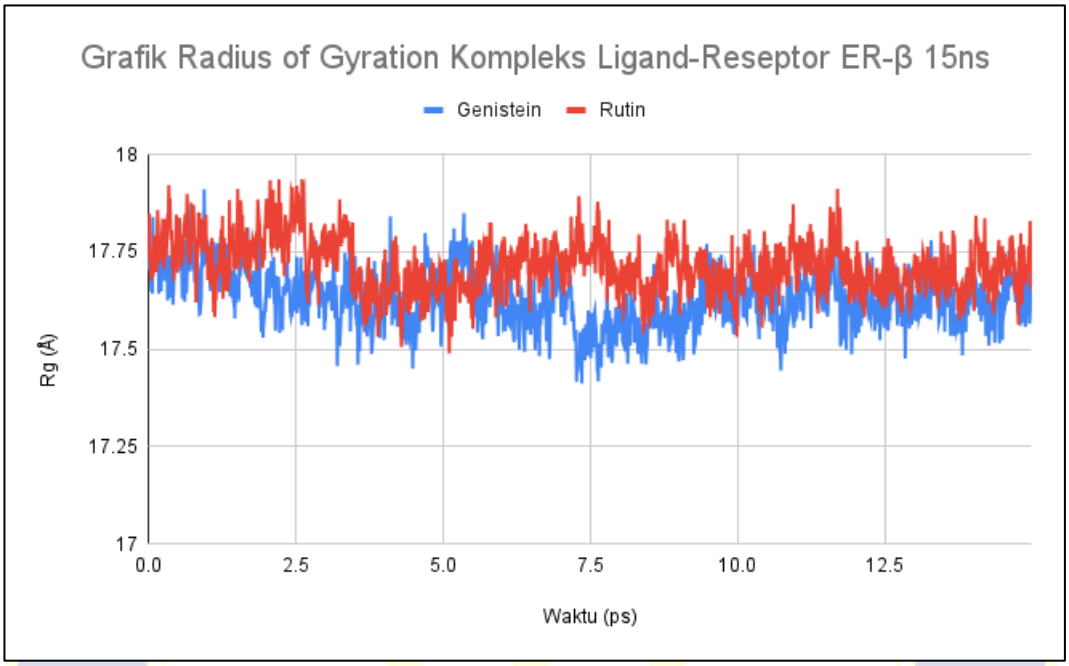


Gambar VII. 39 Grafik nilai RMSD kompleks ligan-reseptor ER-β

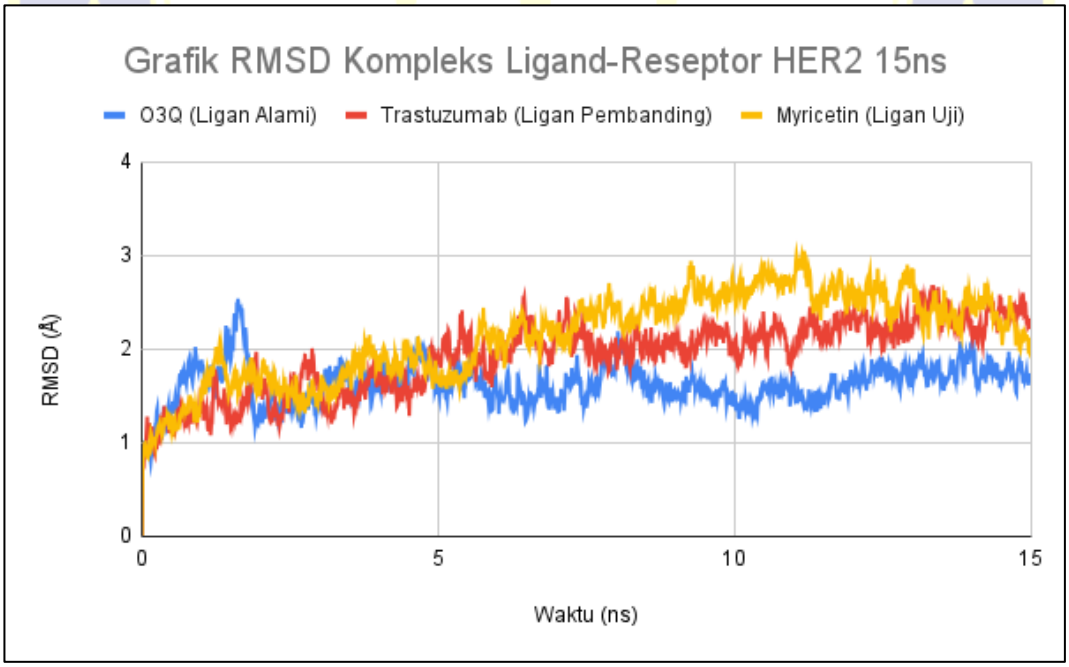


Gambar VII. 40 Grafik nilai RMSF kompleks ligan-reseptor ER-β

LAMPIRAN 19
(LANJUTAN)

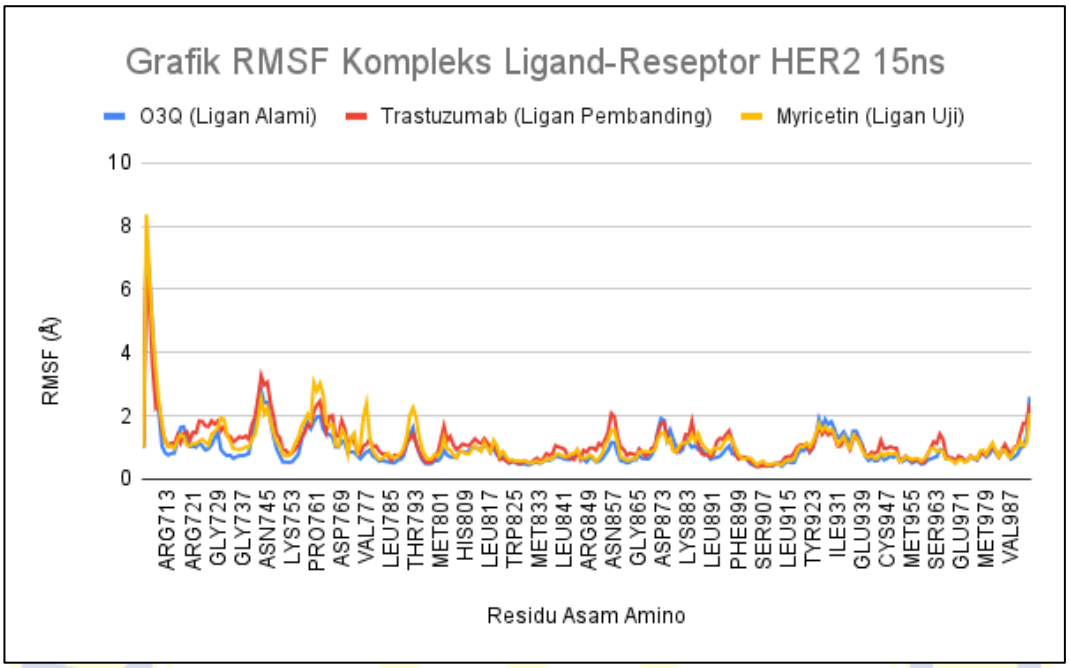


Gambar VII. 41 Grafik nilai RG kompleks ligan-reseptor ER-β

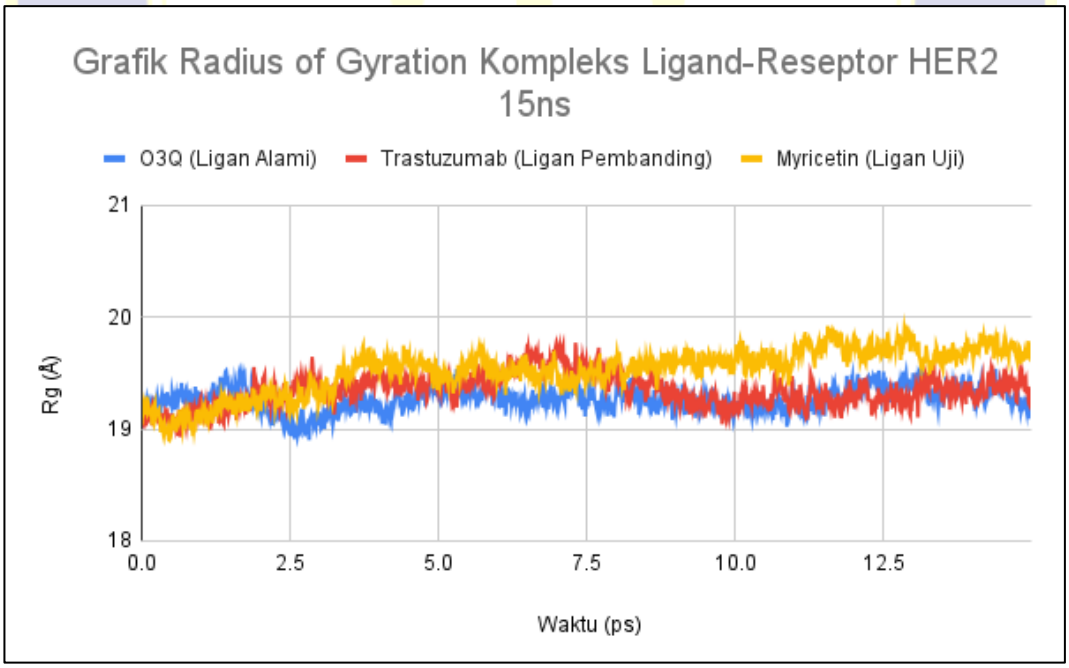


Gambar VII. 42 Grafik nilai RMSD kompleks ligan-reseptor HER2

LAMPIRAN 19
(LANJUTAN)



Gambar VII. 43 Grafik nilai RMSF kompleks ligan-reseptor HER2



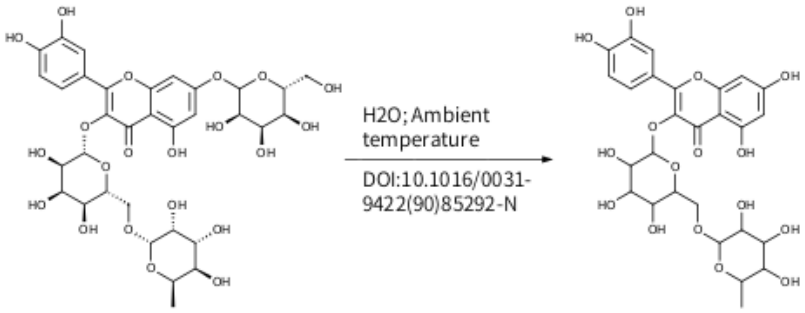
Gambar VII. 44 Grafik nilai RG kompleks ligan-reseptor HER2

LAMPIRAN 20

HASIL PREDIKSI RUTE SINTESIS

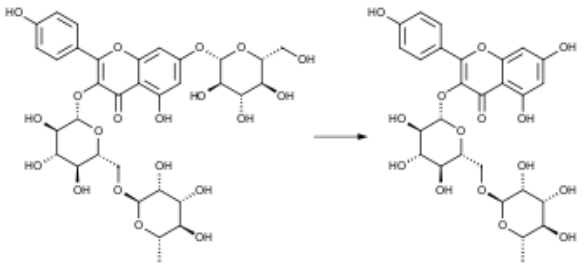
Export Route	3a0d0b59-5a7a-eb9d-4fc9-2c1eb0fef7b7_R001

Scheme



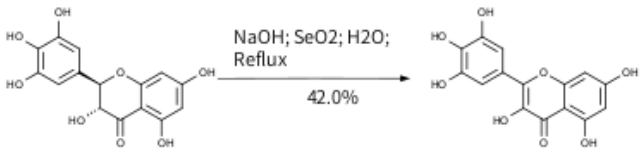
1a Target Compound

Information_3a0d0b59-5a7a-eb9d-4fc9-2c1eb0fef7b7_R001 View in ChemAIRS

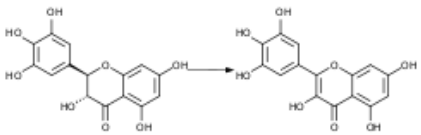
ID	Target Compound
ReferenceRXN	
Yield(%)	N/A
Similarity(%)	100
Conditions	H2O; Ambient temperature
Procedures	N/A
References	Phytochemistry; vol. 29; 11; (1990); p. 3643 - 3647
DOI	10.1016/0031-9422(90)85292-N

Gambar VII. 45 Prediksi rute sintesis senyawa *Rutin*

LAMPIRAN 20
(LANJUTAN)

Export Route	3a0d0b70-7647-3339-968e-71645ebd640d_R004
Scheme	 1a Target Compound

Information_3a0d0b70-7647-3339-968e-71645ebd640d_R004 View in ChemAIRS

ID	Target Compound
ReferenceRXN	
Yield(%)	42
Similarity(%)	100
Conditions	NaOH; SeO2; H2O; Reflux
Procedures	(1) Dihydromyricetin (45 g) is dissolved in 300 ml of deionized water, and then heated to reflux to dissolve. Sodium hydroxide (10 g) aqueous solution (40 ml) is slowly added. After the addition, thesolution is in a reflux state. Heat for 15 minutes.(2) Slowly add selenium dioxide (15 g) aqueous solution (60 ml). After the addition, stir at reflux temperature for 90 minutes. After the reaction is completed, the reaction is slowly cooled to 20-30 C.(3) 5M hydrochloric acid was added to adjust the pH to 4-5, and stirred for 30 minutes. Rotary steamed to 3-5 times the volume of dihydromyricetin, stirred at 10-20 C for 2 to 3 hours, and filtered.(4) The filter cake is added with an aqueous ethanol solution (80%, 200 ml) and beaten for 1 to 2 hours, filtered, and the filter cake is washed with the aqueous ethanol solution. The filter cake is collected and dried to obtain a red selenium elementary solid with a yield of 95% and a purity greater than 99%.(5) Combine the organic phases, spin dry until there is no ethanol taste, a large amount of solids precipitate, filter, and rinse the filter cake with an aqueous ethanol solution (10%) to obtain 19 g of yellow solid,

Gambar VII. 46 Prediksi rute sintesis senyawa *Myricetin*

DAFTAR RIWAYAT HIDUP

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II. RIWAYAT PENDIDIKAN

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SMP	SMPN 2 Leles	2013	2016
SMA	SMAN 2 Garut	2016	2019
Perguruan Tinggi	Universitas Garut	2019	2023

III. PENGALAMAN ORGANISASI

-

EDITOR DECISION FOR THE SUBMITTED JOURNAL

Fwd: [Pharmaciana] Editor Decision
1 pesan

Meilia Suherman <meilia.suherman@uniga.ac.id> Sab, 14 Okt 2023 pukul 7:18 AM
Kepada: nawadhirfauzan34@gmail.com

---------- Forwarded message ---------
From: **Riska Prasetiawati** <riska@uniga.ac.id>
Date: Wed, 11 Oct 2023, 04:42
Subject: Fwd: [Pharmaciana] Editor Decision
To: <meilia.suherman@uniga.ac.id>

---------- Forwarded message ---------
From: **Prof.Dr. apt. Nurkhasanah Mahfudh,M.Si** <nurkhasanah@pharm.uad.ac.id>
Date: Tue, Oct 10, 2023, 12:49
Subject: [Pharmaciana] Editor Decision
To: Mrs Riska Prasetiawati <riska@uniga.ac.id>

Mrs Riska Prasetiawati:

We have reached a decision regarding your submission to Pharmaciana, "In Silico Study: Secondary Metabolites from Malay Apple (Syzygium malaccense (L.) Merr. & L.M. Perry) as Potential Breast Cancer Treatments".

Our decision is to: Accept Submission

Prof.Dr. Nurkhasanah Mahfudh,M.Si.,Apt
Fakultas Farmasi, Universitas Ahmad Dahlan
ibufathan@yahoo.com

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http://www.journal.uad.ac.id/index.php/Pharmaciana

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DOI: 10.12928/pharmaciana.xxxx.xxxx

In Silico Study: Secondary Metabolites from Malay Apple (*Syzygium malaccense* (L.) Merr. & L.M. Perry) as Potential Breast Cancer Treatments

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Submitted :..... Reviewed :..... Accepted:.....

ABSTRACT

Breast cancer has the highest prevalence of all cancers. Breast cancer has overtaken lung cancer as the leading cause of global cancer incidence in 2020, accounting for 2,261,419 new cases, or 11.7% of all new cancer cases worldwide (Globocan, 2020). Among the efforts that can be done are efforts to find breast cancer medications that are safe and selective for the treatment and prevention of cancer, particularly those derived from medicinal plants. The Malay apple (*Syzygium malaccense* (L.) Merr. & L.M. Perry) is one plant that has been extensively examined and proved to have an antiproliferative effect (Rabeta et al., 2013). The pharmacophore modelling, molecular docking, and molecular dynamic approach was conducted on 155 active compounds of Malay apple to alpha and beta estrogen receptors. With a fit score of 45.81, rutin was potentially selective for ER-β receptors, molecular docking to ER-β obtained that rutin was predicted to have breast cancer activity with a free binding energy value of -10.6 kcal /mol with better conformation and affinity compared to native ligand (genistein), and bound to essential amino acids as anticancer breast at ARG 346, GLU 305, and molecular dynamics simulations show that the compound has good stability when binding to the receptor. In silico ADMET prediction from rutin showed outcomes that match the requirements for the candidate drug. However, rutin cannot be turned into oral dosage form because the Lipinski rule of five factors, but it can adjust the dosage form to reach the receptor. Furthermore, rutin can be isolated, optimized, and developed as a therapeutic candidate for the treatment of breast cancer that targets the ER-β receptor.

Keywords: breast cancer, *Syzygium malaccense*, in silico study, virtual screening

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INTRODUCTION

Cancer is a disease that develops as a result of abnormal cell proliferation in body tissues. Cancer is a disease that kills many people in Indonesia and around the world. Breast cancer has the highest prevalence of all cancers. According to the Global Burden Cancer (Globocan) report, there were 65,858 new cases of breast cancer in 2020, representing 16.6% of the total 396,914 new cases of cancer in Indonesia (Globocan, 2020), whereas at the global level, breast cancer has become the leading cause of new cancer cases in 2020, accounting for 2.261,419 new cases, or 11.7% of the total number of new cancer cases worldwide (Sung et al., 2021).

Breast cancer therapy is still being developed due to the numerous side effects it produces, such as chemotherapy, which frequently leads to failure due to the low selectivity of anticancer medications. As a result, the identification of novel anticancer potential is critical in order to overcome this adverse effect of existing cancer medications, one of which is natural medicine.

Since ancient times, traditional herbal treatment has been regarded as an alternate strategy to treating and dealing with various disorders. Malay apple is one of the plants that has been actively researched in the search for new medication candidates. Malay apple (*Syzygium malaccense* (L.) Merr. & L.M. Perry) has high antioxidants activity, it has the potential to improve human health. Rabeta et al. (2013) discovered that malay apple methanol extract had an antiproliferative impact on Michigan Cancer Foundation-7 (MCF-7) cells with 79% viability and IC_{50} = 632.3 g/ml (Rabeta et al., 2013). However, in vitro tests have not revealed an active anti-cancer compound in the breast, so further research is required.

Various new drug developments, including the in silico method, are being used to accelerate the discovery of anti-breast cancer drugs. Because they are supported by good computational techniques and also shorten the time in the drug discovery process, in silico methods for developing new drugs are growing rapidly. Based on earlier research, the experiment was developed to look for anti-breast cancer candidates by studying active compounds in malay apple utilizing in silico methodologies. As a result, it can be utilized as the first-line treatment for breast cancer, particularly in Indonesia.

MATERIALS AND METHOD

Materials

155 structures of secondary metabolites of malay apple were obtained from the site https://pubchem.ncbi.nlm.nih.gov. The breast cancer receptor (PDB ID 3ERT for ER-α and PDB ID 1QKM for ER-β receptor-ligand complex) were downloaded from the https://rcsb.org site in PDB format. **Hardware:** ASUS A456U notebook (operating system: Microsoft Windows 10 Pro and Ubuntu 17.04), 64-bit; Memory: 4GB; Processor: Intel Core i5-7200U, Personal Computer (operating system: Ubuntu 16.04 LTS, Xeon Processor, 16 GB Memory). **Software:** Discovery Studio Visualizer® Version 2021 freeware, MarvinSketch Version 17.2.13® freeware, Autodock Tools 1.5.6® freeware, Autodock Vina 1.1.2® freeware, KNApSAck (http://www.knapsackfamily.com/KNApSAcK/), PASS (Prediction of Activity Spectra for Substances) Online (http://way2drug.com/passonline/predict.php), Liganscout 4.4.9 30 days free trial. **Website:** PreADMET (http://preadmet.bmdrc.org/), PubChem (http://pubchem.ncbi.nlm.nih.gov), Lipinski's Rule of Five (http://www .scfbio-iitd.res.in/software/drugdesign/lipinski.jsp), and the Protein Data Bank (PDB) (https://www.rscb.org/), Google Colabolatory, OpenMM.

Method

Compound Library Selection and Ligand Preparation

The compound of malay apple obtained through various library sources and based on search results using the KNApSAcK online database site (http://www.knapsackfamily.com/KNApSAcK/)

Screening Activity

The malay apple compound was examined for anti-breast cancer activity using the PASS Online prediction site.

Geometry Optimization

The shape of the 3D molecular structure of secondary metabolites contained in malay apple was carried out on geometric optimization using MarvinSketch Version 17.2.13® freeware with the semi-empirical AM1 method.

Lipinski's Rule of Five Testing

In this study, the ligands or molecules evaluated were secondary metabolites of malay apple. Ligands were redrawn in ChemDraw® Ultra 12.0 and energy was minimized in Chem3D® Pro 12.0 before being stored in.pdb format. Following preparation, the compound's physicochemical properties were determined using Lipinski's Rule of Five.

Pre-ADMET Testing

The tests conducted seek to examine the first characteristics of pharmacokinetics, such as absorption, distribution, and metabolism, as well as toxicity testing, such as mutagenic and carcinogenic qualities of substances. Testing is done out using a specific program that is carried out online on the http:// preadme.bmdrc.kr/ site. After drawing the structure of the test substance, click submit for analysis. The collected results are data in.pdb format.

Pharmacophore Modeling

Pharmacophore modeling was used to find and extract potential interactions between ligand-receptor complexes. Liganscout 4.4 30 days free trial software was used to conduct the tests. The first stage involves preparing target receptors from the PDB, standard compounds from the binding data base, active compounds and decoy compounds from DUD-E (Database of Useful Decoys Enhanced). The pharmacophore of the receptor was then identified, and the pharmacophore model was validated, yielding the ROC (Receiver Operating Characteristic) curve, which displayed the hit molecule and the AUC (Area Under Curve) value. Following the validation stage, the test ligands were screened to generate a list of hit compounds and pharmacophore fit scores.

Protein Selection and Preparation

Receptors downloaded via PDB website (https://www.rscb.org/) with PDB ID 3ERT for ER-α and PDB ID 1QKM for ER-β receptor, receptor-ligand complex separated and prepared using Autodock Tools® software, then validated and a scoring function to calculate the binding affinity using Autodock Vina®.

Molecular Docking

The docking method was validated by redocking native ligands on the ER-α and ER-β receptors. Molecular docking is performed with previously validated parameters. Canonical SMILES of the test compound were obtained from the Pubchem website (http://pubchem.ncbi.nlm.nih.gov) then the optimization process was carried out, then the docking process was carried out using Autodock Tools 4.2.6® freeware and visualization was carried out using the Discovery Studio Visualizer® freeware. The improved 3D-ligand structures were then bound to the active sites of ER-α and ER-β. ΔG (Gibbs free energy), inhibition constant, and interaction poses were calculated from the results.

Molecular Dynamics Simulation

Molecular dynamics simulations were performed using open MM software on the complex between ER-β receptor and the ligand with the lowest binding energy based on molecular docking

experiments. Begin by creating a protein topology and a ligand topology. The ff19SB force field was used to add the ligand topology, and the GAFF2 force field with the TIP3P water model was used to add the receptor topology then equilibration and production for 15 ns.

RESULT AND DISCUSSION

Screening Compound

Based on literature investigations from related journals and screening for active compounds of Syzygium malaccense (L.) Merr. & L.M. Perry, 155 active compounds were discovered and employed in this study.

Screening of Anti-Breast Cancer Activity

The active compound of malay apple was screened for anti-breast cancer activity, and 80 out of 155 compounds were predicted to have anti-breast cancer activity. The goal of this screening is to make early predictions about the test substance as anti-breast cancer activity. The metrics employed in the PASS Online prediction findings include Activity, the value of Pa (Probability activity), and Pi (Probability inactivity), which indicate the test compound's likelihood or opportunity value in creating the expected biological activity.

Pharmacophore Validation

Pharmacophore validation was performed using LigandScout 4.4.5 software to determine the suitability of the pharmacophore model for use in screening the test chemicals. A decent pharmacophore model can detect the majority of active drugs as well as a few decoy molecules. Ten pharmacophore models were created from a database of 200 chemicals and will be validated. Validation was performed using 100 active compound databases and 500 decoy compound databases obtained from the DUD-E site. The pharmacophore model is stated to be valid if the AUC-ROC value is greater than 0.7 or 70%; in other words, an AUC-ROC value near to one is considered good and is believed to be capable of distinguishing between active and decoy compounds.(Hamzah et al., 2014; Moussa et al., 2021; Suherman et al., 2020). The AUC-ROC results of active ligands in ER-α demonstrate that 124 hit compounds were acquired with an AUC value of 0.93 or 93% out of a total of 600 active and decoy compounds, whereas in ER-β, 107 of the total active and decoy compounds were 600 compounds. A good hit score can also be determined by the GH Score (Goodness of Hit Score), which is another validation metric. A good hit score can also be determined by the GH Score, which is another validation metric. The following computations yield the GH Score:

$$GH = [(Ha4/HtA)\,(3A+Ht)\;x\;(1-(Ht-Ha)/D-A)]$$

D = Total *molecules in database*
A = Total *number of actives in database*
Ht = Total *Hits*
Ha = *Active Hits*

The GH Score calculation yielded a score of 0.81 or 81% for the active ligand ER-α, while it was 0.94 or 94% for ER- β. So it is said that pharmacophore modeling based on active ligands on ER-α and ER-β is legitimate and can be utilized to screen pharmacophore on test ligands. (**Figure 1)**

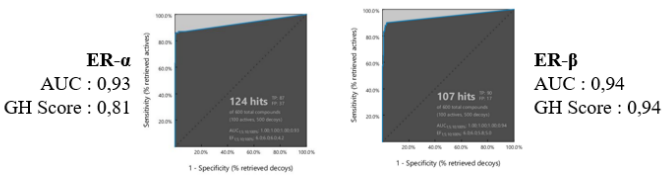

Figure 1. Pharmacophore Validation Results

Pharmacophore Modelling

The pharmacophore research of the test compounds against ER-α and ER-β yielded 27 and 25 hit compounds, respectively, as well as their pharmacophore fit-scores (**Tables 1 and 2**). Pharmacopore tests revealed that it had similar pharmacological action to the reference ligand and that it can be further evaluated in molecular docking simulations.

Table 1. Pharmacophore Study Results Against ER-α

No.	Compound	Pharmacophore-Fit Score
1	Cyanidin-3,5-O-diglucosid	63.97
2	Quercitrin	63.49
3	Peonidin 3,5-diglucosside	60.95
4	Pelargonidin-3-glucoside	60.74
5	Procyanidin B2	60.64
6	Peonidin-3-Glukosid	60.64
7	Procyanidin B1	60.58
8	Cyanidin-3-O-Glukosid	60.56
9	Cyanidin 3-glucoside	60.54
10	Procyanidin A2	60.37
11	2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone	56.26
12	Stercurensin	55.47
13	Kaempferol-3-glucoside	53.19
14	Isorhamnetin-3-glucoside	53.11
15	Isoquercitrin	53.04
16	(-)-Epicatechin	53.00
17	Quercetin	52.93
18	(+)-Catechin	52.88
19	Morin	52.71
20	Myricitrin	52.43
21	Chlorogenic Acid	51.98
22	Myricetin-3-(3"galloylrhamnoside)	51.95
23	Mearnsitrin	50.96
24	(-)-Epicatechin gallate	50.71
25	Desmanthin1	50.53
26	Rutin	50.24
27	Ursolic Acid	44.60

Table 2. Pharmacophore Study Results Against ER-β

No.	Compound	Pharmacophore-Fit Score
1	Chlorogenic Acid	57.94
2	Morin	57.40
3	(-)-Epicatechin gallate	57.08
4	Kaempferol-3-glucoside	57.03
5	Procyanidin B2	56.34
6	Isoquercitrin	55.91
7	Cyanidin-3,5-O-diglucosid	55.90
8	Pelargonidin-3-glucoside	54.37
9	Peonidin-3-Glukosid	54.18
10	(+)-Catechin	54.04
11	Cyanidin 3-glucoside	53.96
12	Isorhamnetin-3-glucoside	46.72
13	Quercetin	46.62
14	(-)-Epicatechin	46.61
15	Cyanidin-3-O-Glukosid	46.28
16	Procyanidin A2	46.22
17	Quercitrin	46.09
18	Procyanidin B1	46.01
19	Rutin	45.81
20	Peonidin 3,5-diglucosside	45.46
21	Myricitrin	44.54
22	Mearnsitrin	44.37
23	Ursolic Acid	44.15
24	Desmanthin 1	43.97
25	Myricetin-3-(3"galloylrhamnoside)	43.67

Docking Validation

Docking parameter validation occurs prior to the docking process for the test ligands. The docking parameter is considered valid if it can re-docking the native ligand that has been withdrawn from the native ligand or the ligand complex to its original position with an RMSD value less than 2 Å (Astuty & Komari, 2022). The RMSD values obtained from re-docking native ligands are shown in **Table 3**. The RMSD values were declared valid and ready for use in molecular docking simulations of the test compounds. **Figure 2** depicts the docking parameter validation findings.

Figure 2. Superimposition of the X-ray crystal structure (green) and docked conformation (pink) (left : 3ERT, right : 1QKM)

Table 3. Size of grid center, grid box and RMSD values from docking validation results

PDB ID	Grid Center			Grid Box (Å)			Exhaustiveness	RMSD
	X	Y	Z	X	Y	Z		
3ERT	30.282	-1.913	24.207	40	40	40	16	1.1162 Å
1QKM	22.438	8.003	113.538	40	40	40	16	0,2799 Å

Molecular Docking Simulation

The docking of malay apple compounds revealed that the 6 test compounds (Procyanidin A2, Procyanidin B1, Procyanidin B2, Ursolic Acid, Rutin, and Desmanthin1) had lower binding free energy than the native ligand (4OHT), although none of the complexes between malay apple compounds and ER-α had interactions with essential amino acid residues. Quercetin is the test compound that has the same amino acid interaction as the native ligand but does not have a lower binding free energy value than the native ligand. (**Figure 3**). In ER-β, rutin has a lower binding free energy (G) than the native ligand (Genistein). The molecular docking results between rutin and ER-β reveal the presence of hydrogen interactions residues surrounding the cavity at the catalytic site (ARG 346 and GLU 305) (**Figure 4**).

Table 4. Results of Molecular Docking of ER-α and analysis of linked amino acid residues

No.	Compound	ΔG (kcal/mol)	Hydrogen Interaction
1	Procyanidin A2	-11.166	CYS 530
2	Procyanidin B1	-10.393	LEU 525, CYS 530, ASP 351
3	Procyanidin B2	-10.207	MET 343, THR 347, CYS 530
4	Ursolic Acid	-10.103	-
5	Rutin	-10.057	VAL 534, LEU 536, THR 347, MET 522, CYS 530
6	Desmanthin1	-9.832	LEU 536, CYS 530, ASP 351, MET 522
7	**Native Ligan (4OHT)**	**-9.684**	**ARG 394, GLU 353**
8	Cyanidin-3,5-O-diglucosid	-9.579	LEU 536, MET 522, THR 347
9	Quercitrin	-9.510	THR 347
10	Myricetin-3-(3"galloylrhamnoside)	-9.486	CYS 530, THR 347, TRP 383, LEU 536
11	Mearnsitrin	-9.280	-
12	(-)-Epicatechin gallate	-9.176	THR 347, CYS 530, LEU 536
13	Peonidin 3,5-diglucosside	-9.157	GLU 380, TYR 537, LEU 536, THR 347
14	Kaempferol-3-glucoside	-8.985	VAL 534, CYS 530
15	Myricitrin	-8.980	THR 347
16	Quercetin	-8.840	**ARG 394, GLU 353**, LEU 387
17	Morin	-8.799	**ARG 394, GLU 353,** MET 343
18	Isoquercitrin	-8.744	VAL 534, MET 522, THR 347
19	(-)-Epicatechin	-8.713	GLU 353, LYS 449, TRP 393
20	Pelargonidin-3-glucoside	-8.701	CYS 530, VAL 534
21	Cyanidin-3-O-Glukosid	-8.514	CYS 530, VAL 534, LEU 536,
22	Peonidin-3-Glukosid	-8.495	ASP 351
23	Cyanidin 3-glucoside	-8.460	CYS 530, MET 522

No.	Compound	ΔG (kcal/mol)	Hydrogen Interaction
24	Isorhamnetin-3-glucoside	-8.272	VAL 534, MET 522, THR 347
25	Chlorogenic Acid	-8.229	GLU 353, ASP 351
26	(+)-Catechin	-7.969	**ARG 394, GLU 353**, LEU 387, HIS 524
27	2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone	-7.710	-
28	Stercurensin	-7.649	-

Table 5. Results of Molecular Docking of ER-β and analysis of linked amino acid residues

No.	Compound	ΔG (kcal/mol)	Hydrogen Interaction
1	**Rutin**	**-10,6**	**ARG 346, GLU 305,** LYS 401, GLU 276, TYR 397, HIS 279, TRP 345, HIS 394
2	**Native Ligand (Genistein)**	**-10,5**	**ARG 346, GLU 305,** LEU 339, HIS 475
3	Procyanidin B1	-10,4	TRP 345, LYS 401, PRO 358
4	Myricetin-3-(3"galloylrhamnoside)	-10,2	**ARG 346**, TRP 345, ASP 249, HIS 279, PHE 356, VAL 280, PRO 278
5	Procyanidin B2	-10,0	**ARG 346,** PRO 358, ASP 349, TRP 345, GLU 276
6	Procyanidin A2	-9,9	**GLU 305**, LYS 401
7	Myricitrin	-9,2	**GLU 305**, VAL 280, HIS 279, TRP 345
8	Quercitrin	-9,1	**GLU 305**, VAL 280, HIS 279, TRP 345
9	Morin	-9,0	**ARG 346, GLU 305**, VAL 280
10	Quercetin	-9,0	**GLU 305**, VAL 280, TRP 345
11	Mearnsitrin	-8,9	**GLU 305,** VAL 280, HIS 279, TRP 345
12	Desmanthin1	-8,6	**ARG 346,** TRP 345, HIS 394, ASP 349, ILE 348, HIS 350, PRO 277
13	(-)-Epicatechin	-8,5	**ARG, 346, GLU 305,** HIS 279
14	(-)-Epicatechin gallate	-8,5	**GLU 305**, VAL 280, **ARG 346,** TRP 345, GLU 276
15	Cyanidin-3,5-O-diglucosid	-8,5	TRP 345, PRO 277, HIS 279, PRO 278, VAL 280,
16	(+)-Catechin	-8,3	**ARG 346, GLU 305,** VAL 280,TRP 345, GLY 342
17	Isoquercitrin	-8,1	**GLU 305,** VAL 280, HIS 279, TRP 345
18	Cyanidin-3-O-Glukosid	-8,0	**GLU 305,** TRP 345, HIS 279
19	Isorhamnetin-3-glucoside	-8,0	VAL 280, PRO 278, TRP 345
20	Kaempferol-3-glucoside	-8,0	**GLU 305**, VAL 280, HIS 279, TRP 345
21	Peonidin 3,5-diglucosside	-8,0	VAL 280, PRO 277, TRP 345
22	Chlorogenic Acid	-7,7	TRP 345, GLU 276, VAL 280, HIS 279
23	Pelargonidin-3-glucoside	-7,7	**GLU 305**, VAL 280, TRP 345, HIS 279
24	Cyanidin 3-glucoside	-7,6	GLU 276, HIS 279, TRP 345

No.	Compound	ΔG (kcal/mol)	Hydrogen Interaction
25	Peonidin-3-Glukosid	-7,6	**GLU 305**, TRP 345, HIS 279
26	Ursolic Acid	-7,6	-

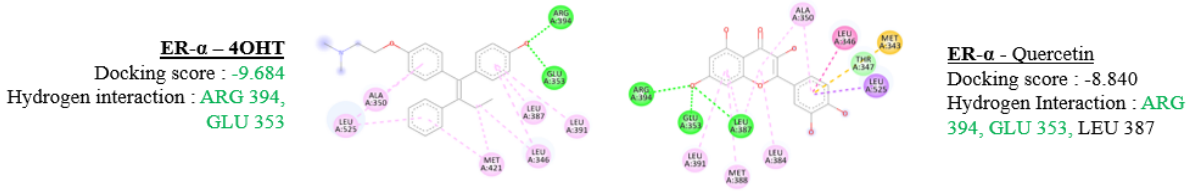

Figure 3. Results of ER-α docking with natural ligands and Quercetin

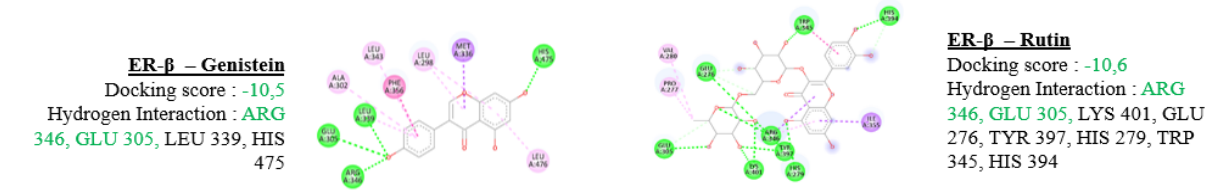

Figure 4. Results of ER-β docking with natural ligands and Rutin

Lipinski's Rule of Five Analysis, Pharmacokinetics and Toxicity

The online portal http://scfbio-iitd.res.in is used to forecast the potential of the tested molecule to be employed as a medication candidate in oral dosage forms (Lipinsi's Rule of Five). This prediction was produced using Lipinski's Rule of Five, which indicates that the molecular weight (BM) should not exceed 500 Daltons since a high molecular weight will alter the concentration of substances absorbed on the surface of the intestinal epithelium. The rule also states that the partition coefficient (Log P) should not be greater than 5, because a higher partition coefficient indicates that a compound has hydrophobic properties, which causes it to stay longer in the lipid bilayer membrane and cause the compound to become toxic, whereas a lower partition coefficient indicates that the compound is hydrophilic, which makes it difficult for the compound to penetrate the lipid bilayer membrane. Furthermore, hydrogen donor bonds must be fewer than 5 and bond acceptors must be no more than 10, because hydrogen donors and acceptors can absorb. The high number of hydrogen bonds influences the passive migration of molecules from the hydrophilic phase into the lipid bilayer membrane (Az-Zahra et al., 2022).

The HIA (Human Intestinal Absorption) and Caco2 value parameters are used to predict the pharmacokinetic absorption profile, while the distribution parameter is PPB (Plasma Protein Binding). HIA is a measure that describes absorption prediction in the human gut. If the HIA value is in the range 0-20%, it indicates a low level of absorption or poorly absorbed, HIA 20-70% indicates a sufficient amount of absorption, and HIA 70-100% indicates a high level of absorption or well absorbed (Sagitasa et al., 2021). Caco2 is an in vitro cell model that is used to predict drug absorption through the intestinal epithelium as measured by the permeability level (nm/sec), where a permeability value of <4 nm/sec indicates the compound is hydrophilic, 4-70 nm/sec indicates the permeability level of the compound which is moderate, which means the compound is neither too hydrophilic nor lipophilic, permeability >70 nm/sec indicates the compound is lipophilic (Suherman

et al., 2020). The PPB (Protein Plasma Binding) value, which is the distribution level of chemical binding to proteins in plasma, is used to predict the pharmacokinetic distribution profile. A PPB value of 90% indicates that the molecule is poorly linked to plasma proteins, whereas a PPB value more than 90% suggests that the drug is highly bound to plasma proteins. The higher the compound's affinity for plasma proteins, the better the compound's distribution (Nusantoro & Fadlan, 2020). The Ames and carcinogenicity test parameters are used to predict toxicity. The Ames test is a method for determining the qualities of a test compound based on its mutagenic and carcinogenic capabilities, which are known due to the test compound's chemical structure. A positive Ames test result suggests that the substance is mutagenic and may be carcinogenic; therefore, a carcinogenicity prediction is performed to confirm (Hartanti et al., 2022). Table 7 shows the results of Lipinski's Rule of Five Analysis, Pharmacokinetics and Toxicity Analysis.

Molecular Dynamic Simulation

Molecular Dynamic (MD) simulations were performed on the best docking compounds to determine the stability of the binding relationship between the test ligand and receptor under physiological settings (Chairunisa et al., 2023). The simulation was ran for 15ns using Open MM software and Google colab, which was linked to Google Drive.

The RMSD, RMSF, and RG values were produced and assessed based on the results of research conducted on the best compound obtained in the molecular docking simulation, namely the molecule Rutin on the ER-β receptor. The Rutin test ligand complex against the ER-β receptor had an average RMSD fluctuation value of 1.48 with the highest fluctuation of 1.89, while analysis of the RMSD value of the native ligand Genistein against the ER-β receptor resulted in an average RMSD fluctuation value of 1.39 with the highest fluctuation of 1.89. According to the results of the RMSD study, the test ligand Rutin and the native ligand Genistein have a stable conformation since the average RMSD value is 5, although the test ligand Rutin has a 0.09 higher average value than the native ligand Genistein (Elfita et al., 2023). According to the RMSF graph (shown in Figure 6), the results obtained for the Routine test ligand were amino acid residues that experienced high fluctuations, namely ASP 261, VAL 370, ALA 420, and MET 479, whereas high fluctuations occurred in the residues for the native ligand Genistein. ASP 261, GLN 450, and LYS 482 are amino acids. High fluctuations suggest that a conformational change has occurred, causing the bond in the binding site to become unstable and inactive. According to the low fluctuation of amino acid residues, the amino acid residues that experienced low fluctuations in the Routine test ligand were MET 295, LEU 298, GLU 305, MET 336, LEU 339, and ARG 346, while low fluctuations occurred in acid amino LEU 298, GLU 305, MET 336, LEU 339, ARG 346, MET 295, and ILE 376 in the native ligand Genistein. Low fluctuations imply that the amino acid residues can bind stably and actively participate in the binding area. Both the test ligand complex and the native ligand can bind stably, although the native ligand Genistein is more stable than the conventional test ligand because low amino acid residues fluctuate more (Elfita et al., 2023). According to the RG value (shown in Figure 7), the test ligand Rutin and the native ligand Genistein had the same RG value at the start of the simulation. As the simulation progressed, there was an increase in fluctuation in the test ligand Routine, which indicated protein unfolding, but after that there was stability until the simulation ended, whereas there was a decrease in fluctuation in the native ligand Genistein, which indicated protein folding and lasted until the simulation ended. The RG analysis results demonstrate that both the Routin test ligand and the natural Genistein ligand are stable during the simulation procedure, although the natural Genistein ligand is more stable than the rutin. Figure 5 shows the RMSD, RMSF, and Radyus of Gyration Graph for 1QKM 15ns Ligand-Receptor Complex

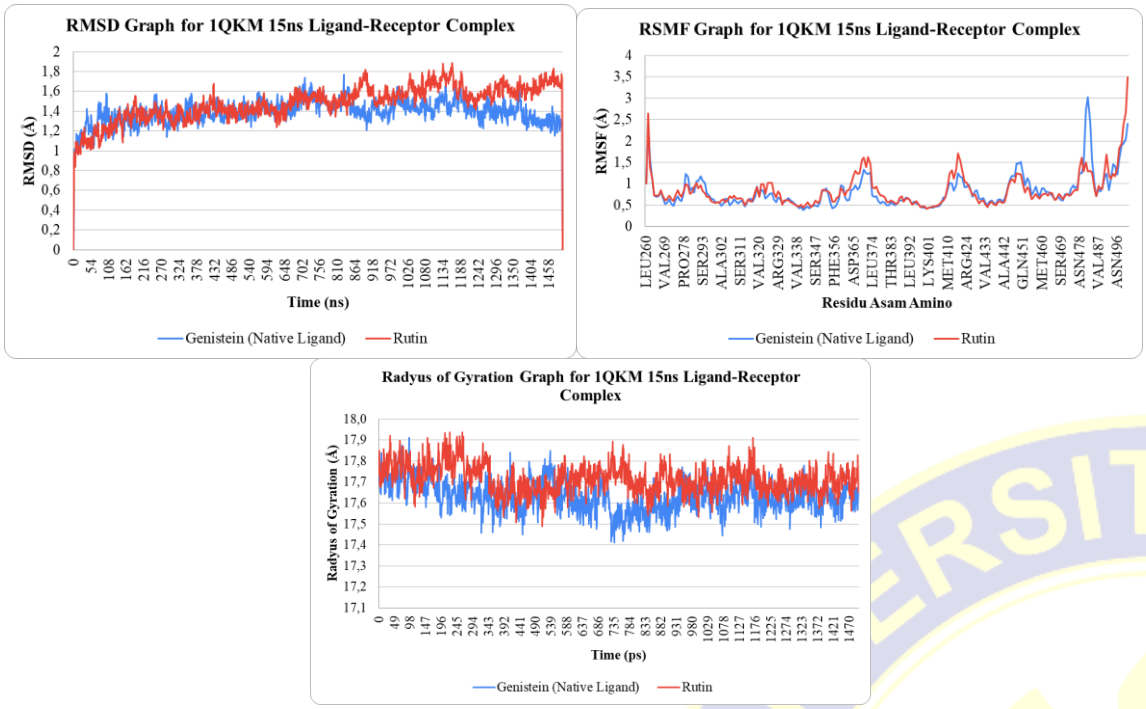

Figure 5. RMSD, RMSF, and Radyus of Gyration Graph for 1QKM 15ns Ligand-Receptor Complex

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Table 6. Results of Lipinski's Rule of Five Analysis, Pharmacokinetics and Toxicity Analysis

No.	Compound	Lipinski's Rule of Five Analysis				Pharmacokinetics and Toxicity Analysis				
						Absorption		Distribution	Toxicity	
		MW(g/mol)	H Donor	H Acceptor	Log P	HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
1	Cyanidin-3,5-O-diglucosid	580	0	16	-3,69	2,16***	3,23***	47,73**	Non Mutagen	Negative
2	Quercitrin	428	0	11	0	24,94**	7,37**	64,95**	Non Mutagen	Negative
3	Peonidin 3,5-diglucosside	592	0	16	-1,77	4,27***	3,83***	29,76**	Non Mutagen	Negative
4	Pelargonidin-3-glucoside	412	0	10	-2,19	39,14**	6,59**	77,6**	Non Mutagen	Negative
5	Procyanidin B2	552	0	12	-0,71	19,51***	13,67**	100*	Non Mutagen	Negative
6	Peonidin-3-Glukosid	475	0	11	0	35,22**	6,84**	65,4**	Non Mutagen	Negative
7	Procyanidin B1	552	0	12	0	19,51***	13,67**	100*	Non Mutagen	Negative
8	Cyanidin-3-O-Glukosid	463	0	11	-1,28	19,72***	5,92**	79,61**	Non Mutagen	Positive
9	Cyanidin 3-glucoside	463	0	11	-1,28	19,72***	5,92**	79,61**	Non Mutagen	Negative
10	Procyanidin A2	552	0	12	-2,83	35,29**	9,23**	100*	Non Mutagen	Negative
11	2',4'-Dihydroxy-6'-Methoxy-3-Methyldihidrochalcone	268	0	4	0,57	92,76*	18,49**	96,08*	Mutagen	Negative
12	Stercurensin	268	0	4	0,57	93,03*	18,43**	92,06*	Mutagen	Negative

No.	Compound	Lipinski's Rule of Five Analysis				Pharmacokinetics and Toxicity Analysis				
						Absorption		Distribution	Toxicity	
		MW(g/mol)	H Donor	H Acceptor	Log P	HIA (%)	CaCO-2 Cell (nm sec)	Plasma Protein Binding (%)	Ames Test	Carsinogenity
13	Kaempferol-3-glucoside	428	0	11	0	25,17**	11,14**	57,57**	Non Mutagen	Negative
14	Isorhamnetin-3-glucoside	456	0	12	0	21,6**	9,93**	47,83**	Non Mutagen	Negative
15	Isoquercitrin	444	0	12	0	11,77***	9,43**	59,15**	Non Mutagen	Negative
16	(-)-Epicatechin	276	0	6	-1,56	66,7**	0,65***	100*	Mutagen	Negative
17	Quercetin	292	0	7	0	63,48**	3,41***	93,23*	Mutagen	Negative
18	(+)-Catechin	276	0	6	-1,56	66,7**	0,65***	100*	Mutagen	Negative
19	Morin	292	0	7	0	63,49**	17,1**	91,62*	Mutagen	Negative
20	Myricitrin	444	0	12	0	11,64***	6,14**	65,37**	Non Mutagen	Negative
21	Chlorogenic Acid	336	0	9	0	20,42**	18,71**	41,96**	Mutagen	Positive
22	Myricetin-3-(3"galloylrhamnoside)	592	0	16	0	4,07***	7,47**	100*	Non Mutagen	Positive
23	Mearnsitrin	456	0	12	0	21,45**	6,21**	55,6**	Non Mutagen	Negative
24	(-)-Epicatechin gallate	424	0	10	-2,88	40,58**	13,21**	100*	Non Mutagen	Negative
25	Desmanthin1	592	0	16	0	4,07***	13,67**	100*	Non Mutagen	Positif
26	Rutin	580	0	16	0	2,86***	7,91**	43, 89**	Non Mutagen	Negative
27	Ursolic Acid	408	0	3	0,42	95,99*	21,86**	100*	Non Mutagen	Positive

Information:

HIA (%):	**CaCo-2 (nm sec):**	**PPB (%):**
70-100 is well absorbed	>70 high permeability	>90 tightly bound
20-70 absorbed enough	4-70 medium permeability	<90 weakly bound
<20 poorly adsorbed	<4 low permeability	

CONCLUSION

The results of in silico testing through pharmacophore modeling, molecular docking, molecular dynamic and ADMET prediction showed that rutin has the potential to be a therapeutic candidate for the treatment of breast cancer that targets the ER- β receptor. The pharmacophore study results show that the Rutin compound has a fitscore value of 45.81%, molecular docking simulations show a Gibbs free energy (G) value of Rutin of -10.6 kcal/mol, which is lower than the comparison ligand, and molecular dynamics simulations show that the compound has good stability when binding to the receptor. However, rutin cannot be turned into oral dosage form because the Lipinski rule of five factors, but it can adjust the dosage form to reach the receptor. Furthermore, rutin can be isolated, optimized, and developed as a therapeutic candidate for the treatment of breast cancer that targets the ER-β receptor.

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