

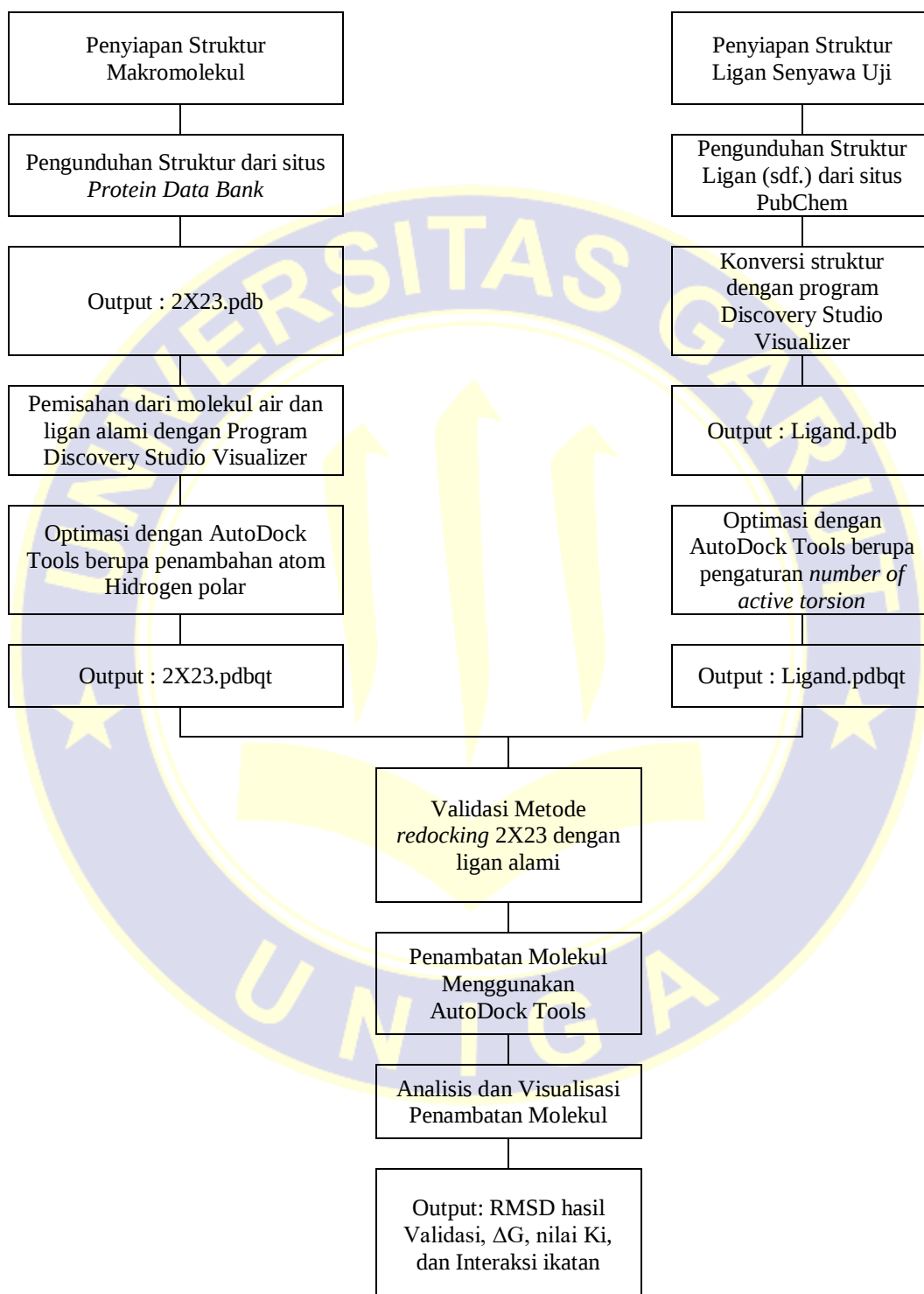
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LAMPIRAN 1

ALUR PENELITIAN

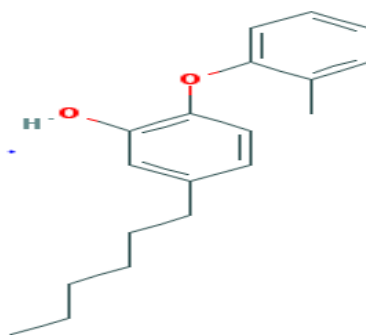


Gambar IV.1 Alur Penelitian

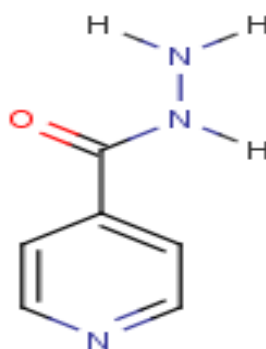
LAMPIRAN 2**RESEPTOR**

Gambar IV.2 Enzim InhA PDB ID 2X23

LAMPIRAN 3
SENYAWA LIGAN

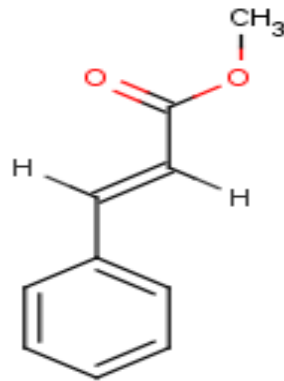


Gambar IV.3 Ligan alami dari Inhibitor Enzim Inh A dengan kode 2X23

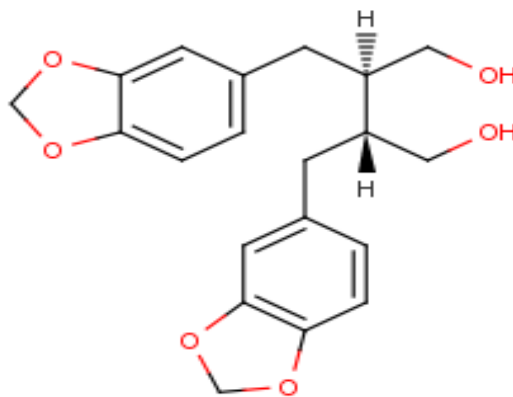


Gambar IV.4 Ligan Senyawa Pembanding Isoniazid

**LAMPIRAN 3
(LANJUTAN)**

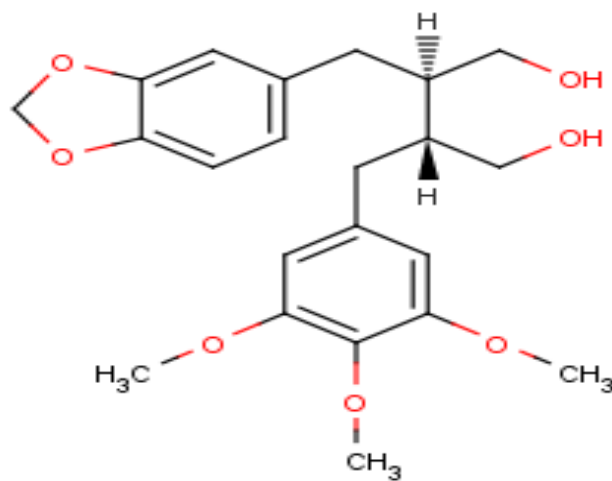


Gambar IV.5 Asam sinamat

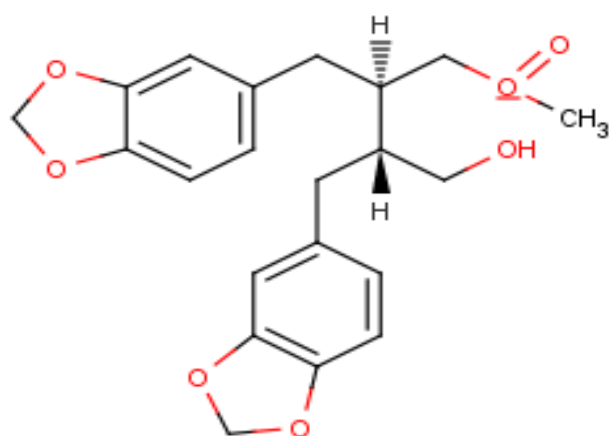


Gambar IV.6 Dihidrokubebin

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(LANJUTAN)**

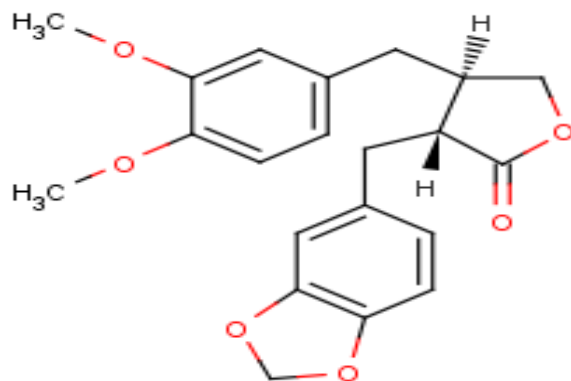


Gambar IV.7 Dihidroklusin

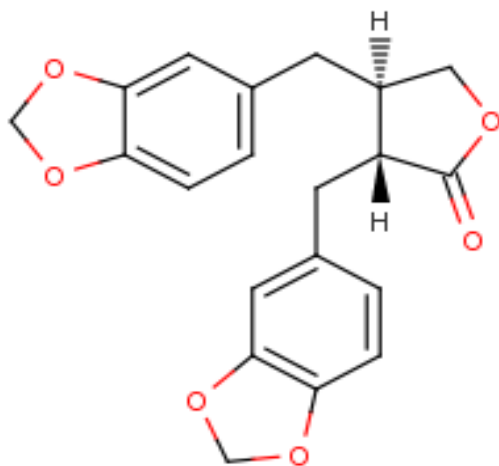


Gambar IV.8 Hemiarisensin

LAMPIRAN 3 (LANJUTAN)

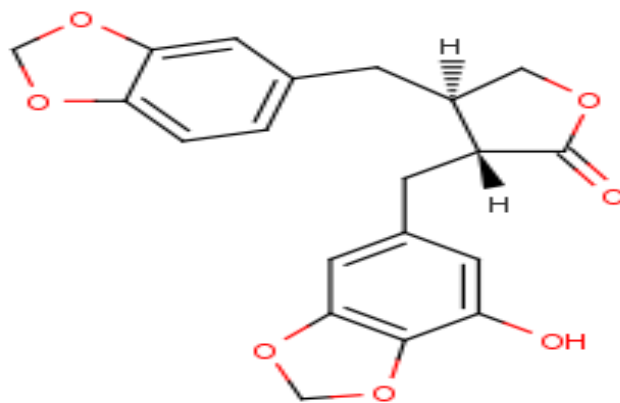


Gambar IV.9 (2R,3R)-2-(3'',4''-Metilen dioksibenzil)-3-(3',4'-dimetoksibenzil)butirolakton

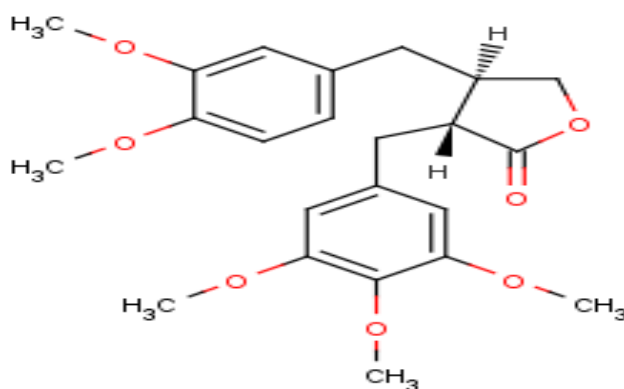


Gambar IV.10 Hinokinin

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(LANJUTAN)**

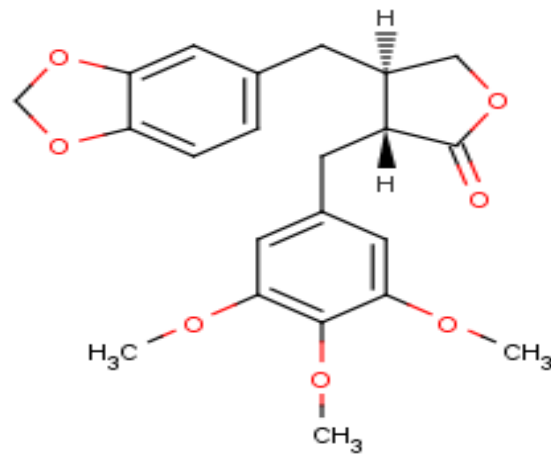


Gambar IV.11 5''-Metoksihinokinin

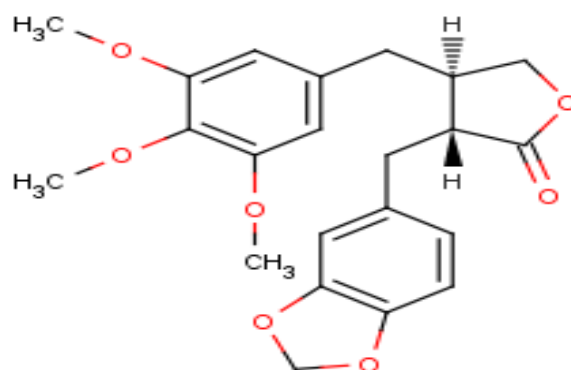


Gambar IV.12 Tujaplikatin trimetil eter

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(LANJUTAN)**

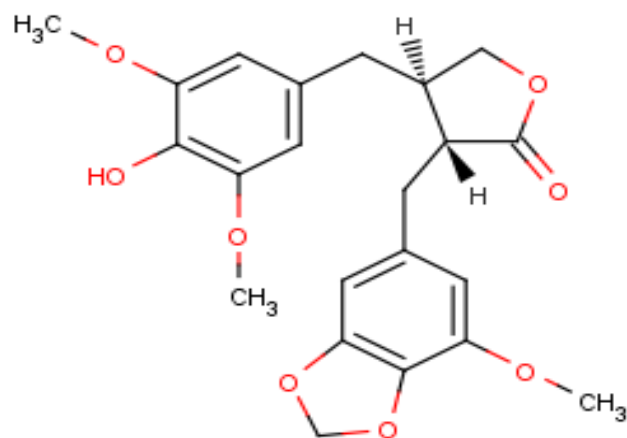


Gambar IV.13 Yatein

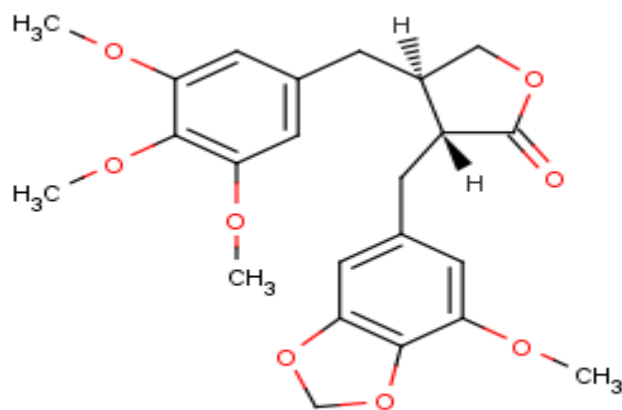


Gambar IV.14 Isoyatein

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(LANJUTAN)**

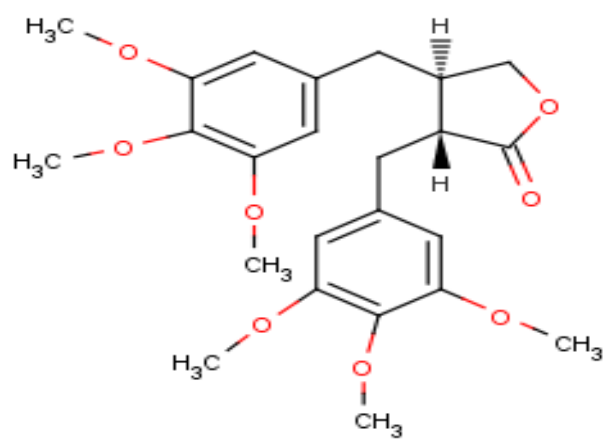


Gambar IV.15 (8R,8'R)-4-Hidroksi-kubebinon

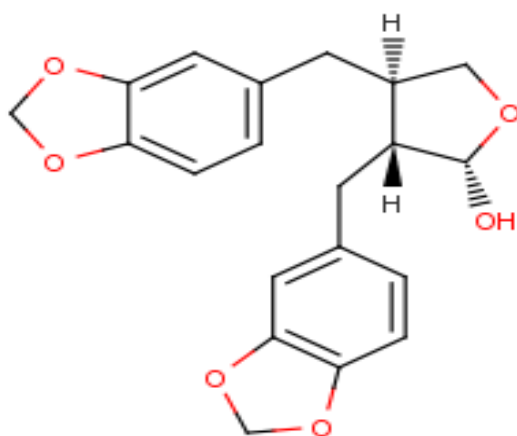


Gambar IV.16 Kubebinon

**LAMPIRAN 3
(LANJUTAN)**

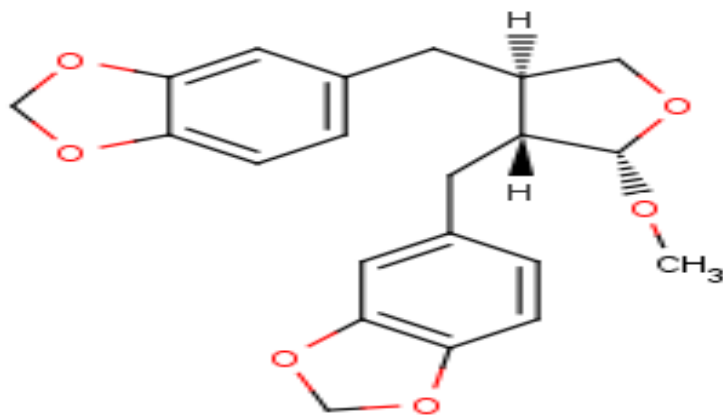


Gambar IV.17 Kubebininolida

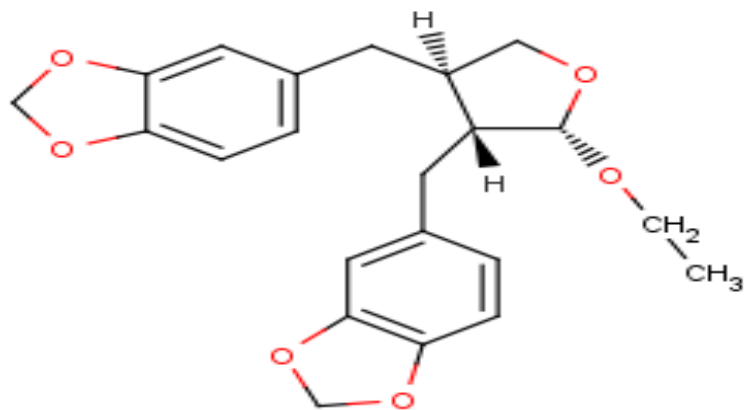


Gambar IV.18 Kubebin

**LAMPIRAN 3
(LANJUTAN)**

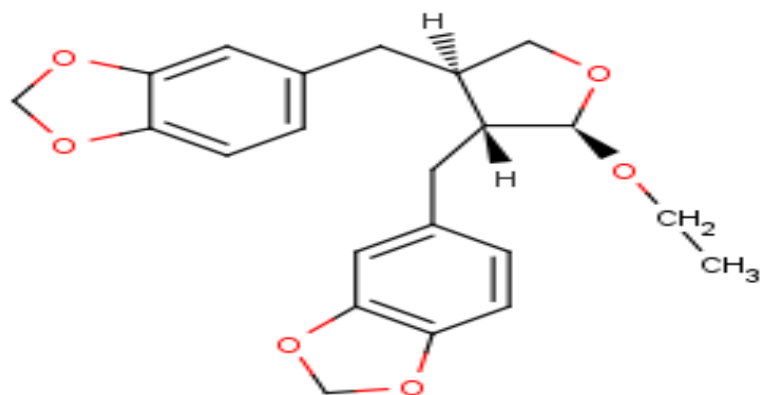


Gambar IV.19 α -Metil kubebin

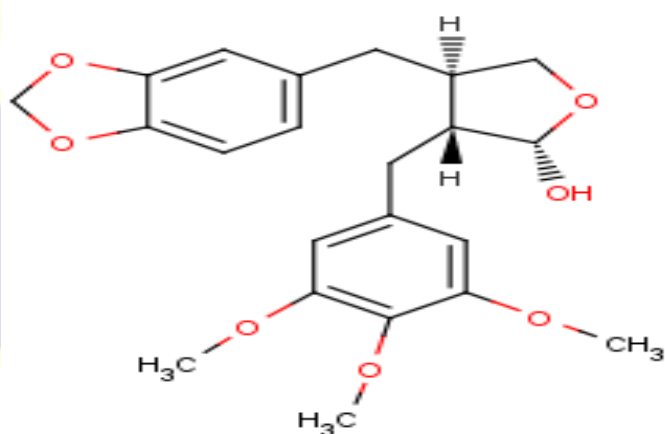


Gambar IV.20 α -O-Etilkubebin

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(LANJUTAN)**

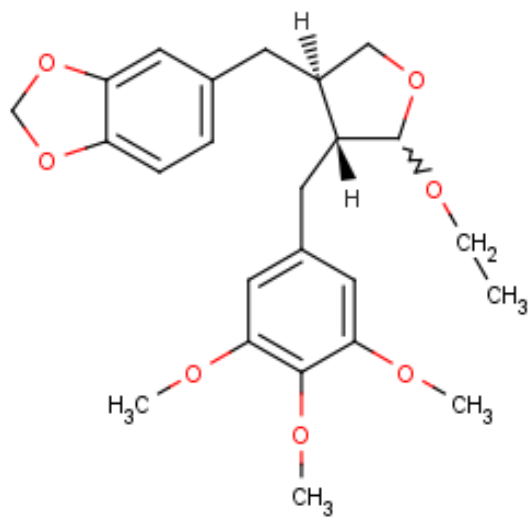


Gambar IV.21 β -O-Etilkubebin

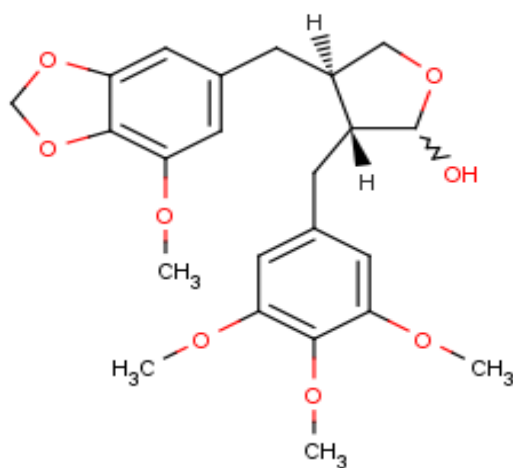


Gambar IV.22 Klusin

**LAMPIRAN 3
(LANJUTAN)**

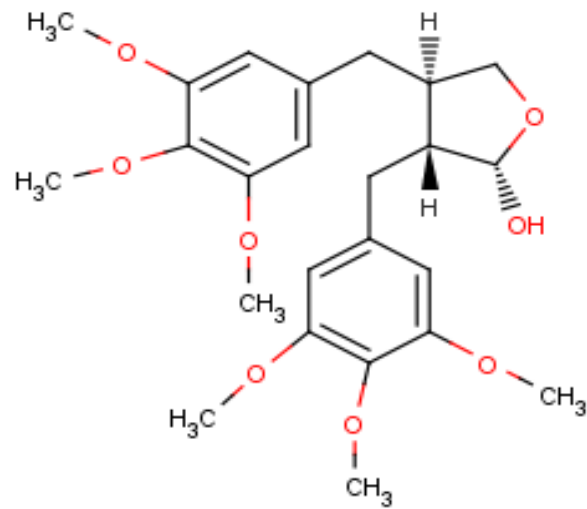


Gambar IV.23 Etoksiklusin

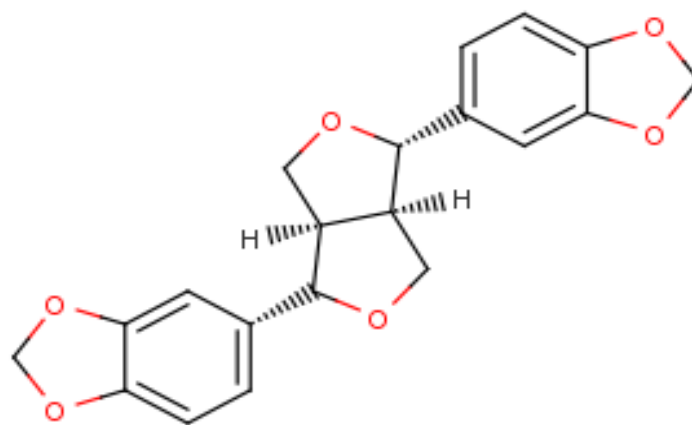


Gambar IV.24 5-Metoksiklusin

**LAMPIRAN 3
(LANJUTAN)**

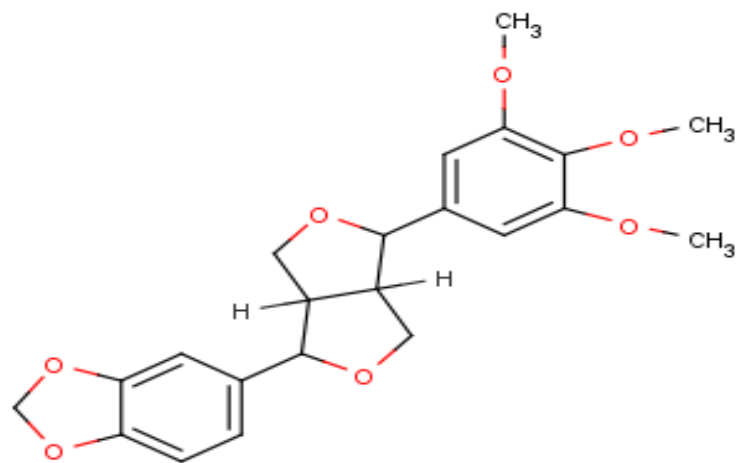


Gambar IV.25 Kubebinin

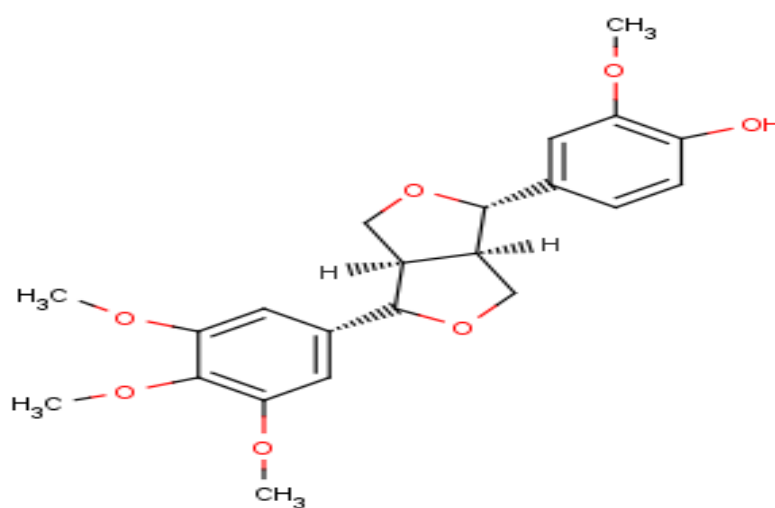


Gambar IV.26 Sesamin

**LAMPIRAN 3
(LANJUTAN)**

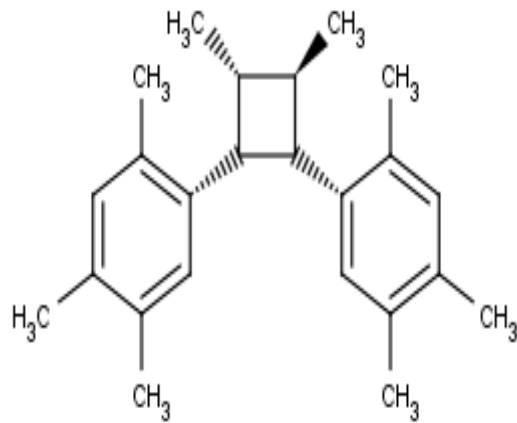


Gambar IV.27 Askantin

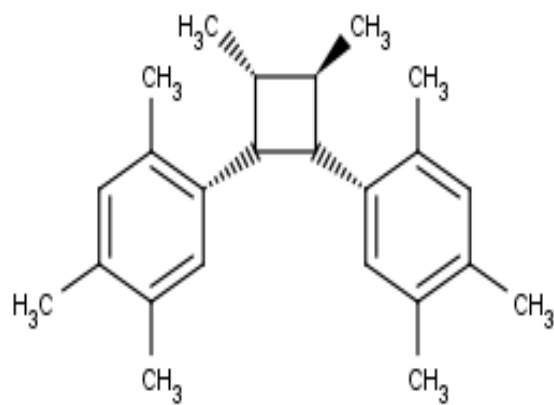


Gambar IV.28 Medioresinol

**LAMPIRAN 3
(LANJUTAN)**

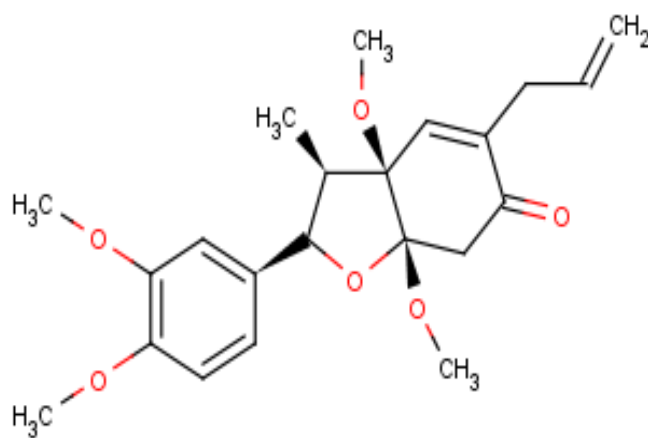


Gambar IV.29 Heterotropin

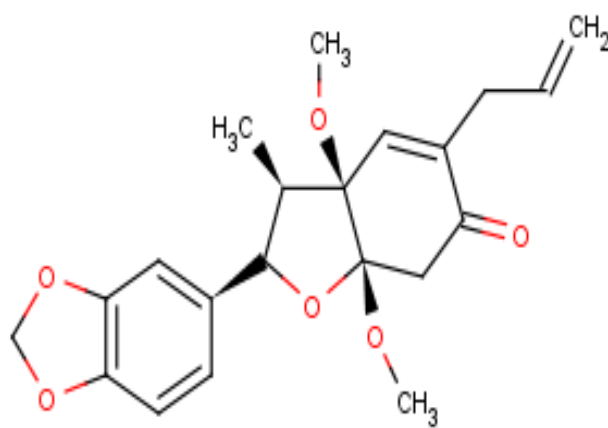


Gambar IV.30 Magnosalin

**LAMPIRAN 3
(LANJUTAN)**

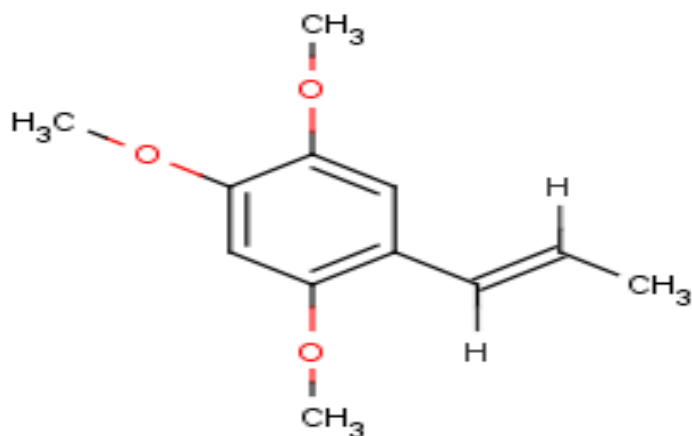


Gambar IV.31 Piperenon

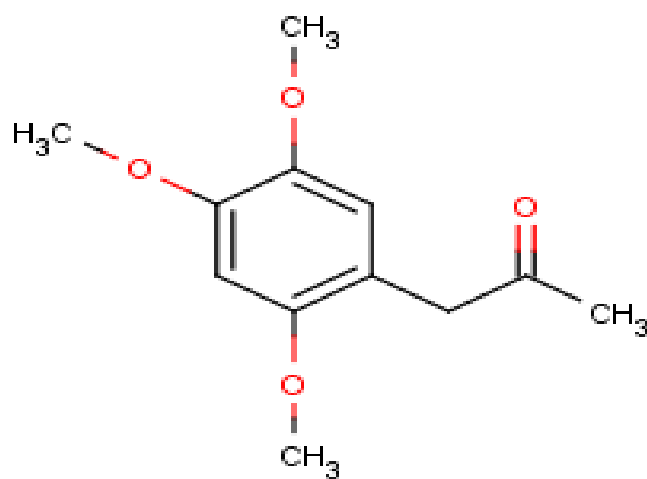


Gambar IV.32 Kadsurin-A

**LAMPIRAN 3
(LANJUTAN)**

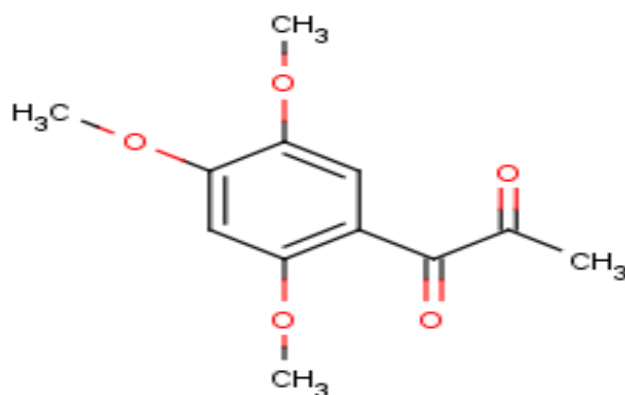


Gambar IV.33 α -Asaron

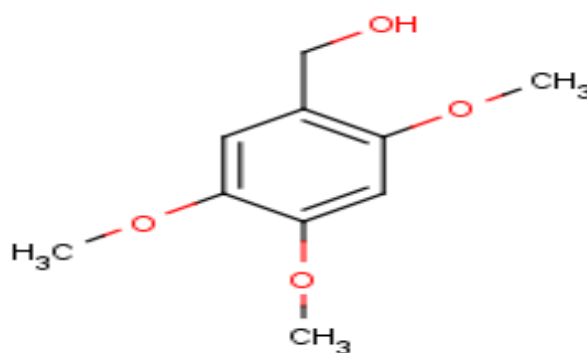


Gambar IV.34 2,4,5-Trimetoksi fenilaseton

**LAMPIRAN 3
(LANJUTAN)**

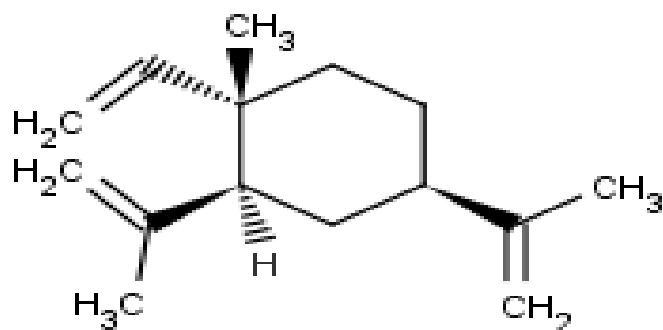


Gambar IV.35 1-(2,4,5-Trimetoksifenil)- 1,2-propandion

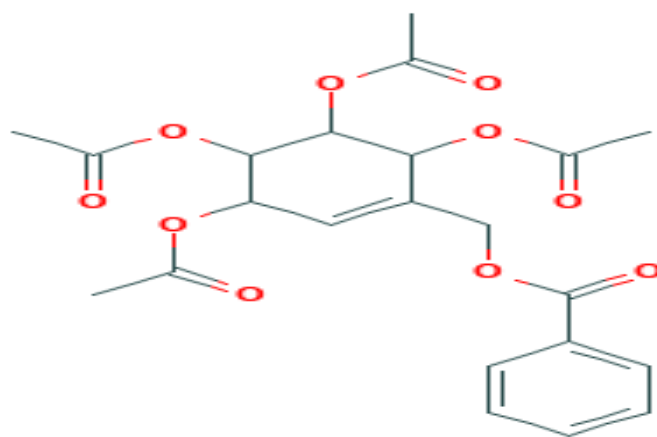


Gambar IV.36 2,4,5-Trimetoksi benzalhida

**LAMPIRAN 3
(LANJUTAN)**

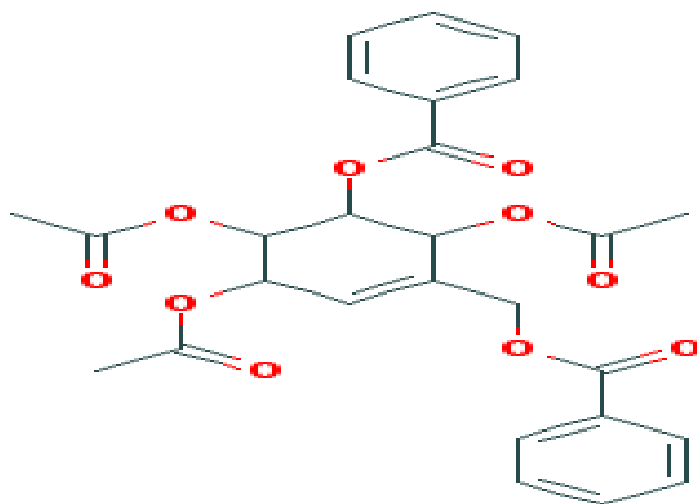


Gambar IV.37 β -Elemen

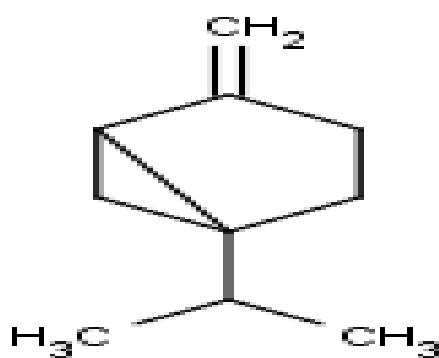


Gambar IV.38 Piperenol C

**LAMPIRAN 3
(LANJUTAN)**

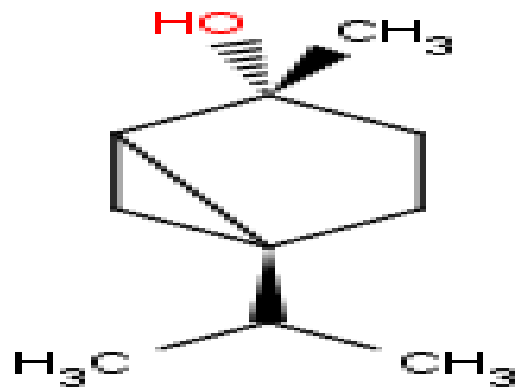


Gambar IV.39 Piperenol A

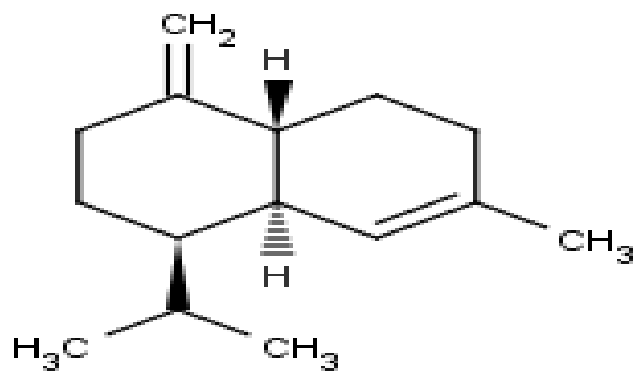


Gambar IV.40 Sabinen

LAMPIRAN 3
(LANJUTAN)

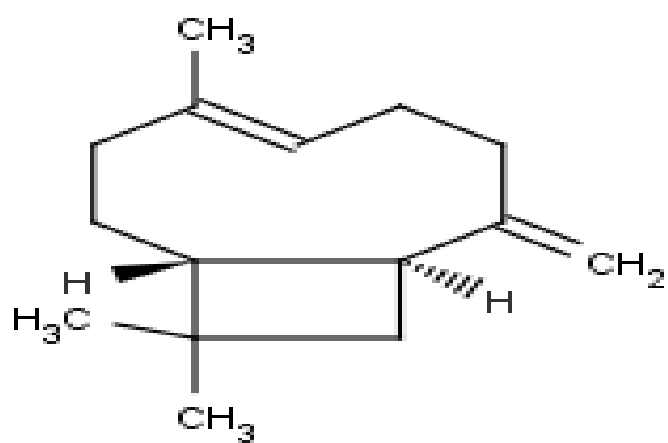


Gambar IV.41 Trans-Sabinen hidrat

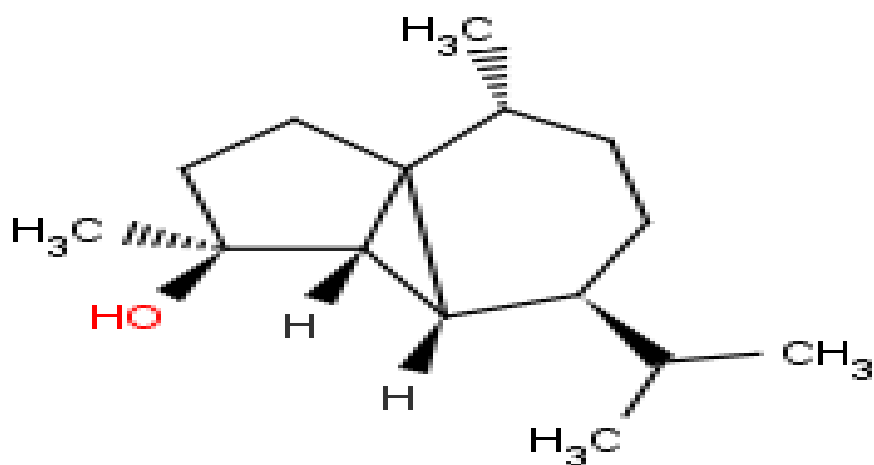


Gambar IV.42 γ-Kadinen

LAMPIRAN 3
(LANJUTAN)

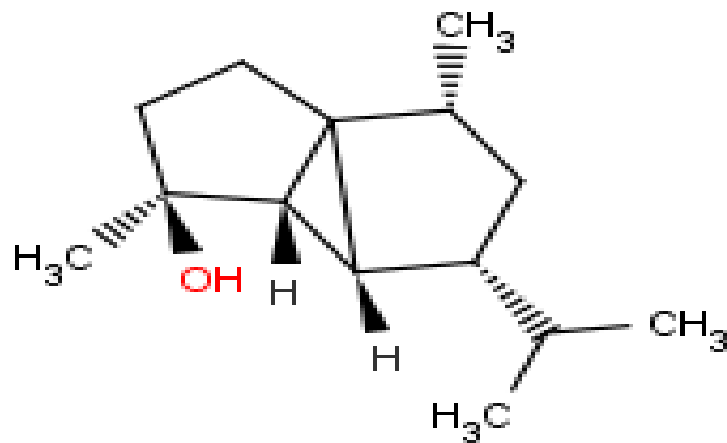


Gambar IV.43 β -Kariofilen

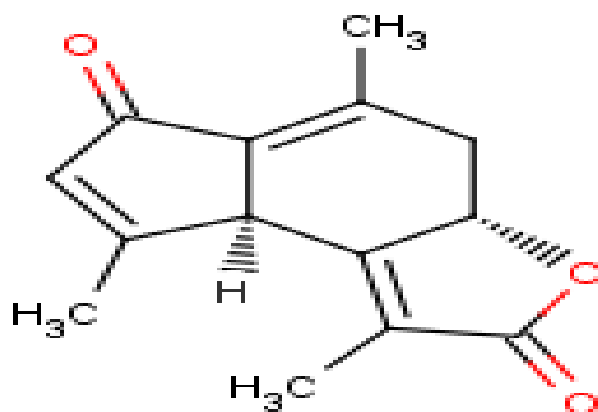


Gambar IV.44 Kubebol

LAMPIRAN 3
(LANJUTAN)

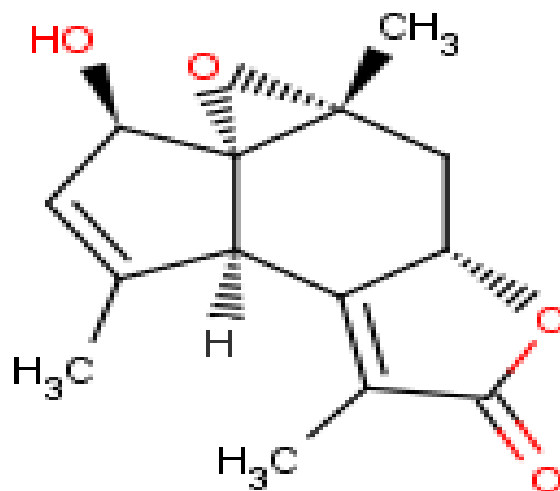


Gambar IV.45 Epikubebol



Gambar IV46 (5 α ,8 α)-2-okso-1(10) 3,7(11)-guaiaatrien-12,8-olida

LAMPIRAN 3
(LANJUTAN)



Gambar IV.47 (1 α ,2 β ,5 α ,8 α ,10 α)-1,10-Epoksi-2-hidroksi-3,7(11)-guaiaadien-12,8-olida

LAMPIRAN 4

HASIL VALIDASI METODE

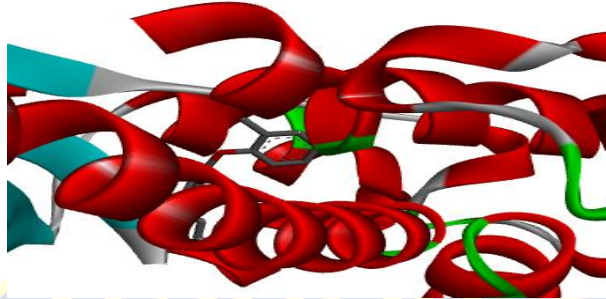
CLUSTERING HISTOGRAM						
Clus	Lowest	Run	Mean	Num	Histogram	
-ter	Binding		Binding	in		
Rank	Energy		Energy	Clus	5	10 15 20 25 30 35
					:	:
1	-8.15	68	-8.15	100	#####	

Number of multi-member conformational clusters found = 1, out of 100 runs.

RMSD TABLE						
Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	68	-8.15	0.00	0.66	RANKING
1	2	55	-8.15	0.01	0.66	RANKING
1	3	4	-8.15	0.01	0.66	RANKING
1	4	51	-8.15	0.03	0.66	RANKING
1	5	82	-8.15	0.01	0.66	RANKING
1	6	80	-8.15	0.02	0.66	RANKING
1	7	8	-8.15	0.02	0.66	RANKING
1	8	64	-8.15	0.02	0.66	RANKING
1	9	29	-8.15	0.02	0.66	RANKING

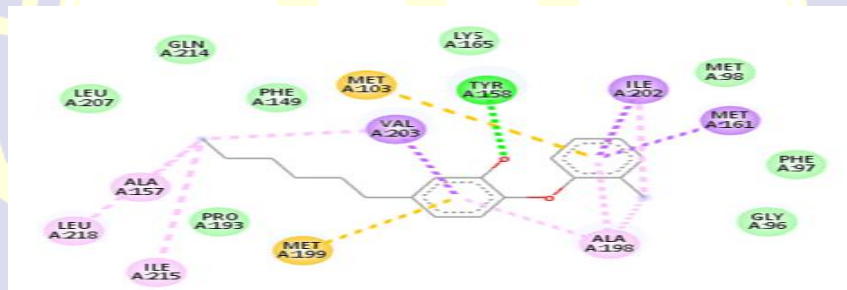
Gambar V.1 Hasil validasi metode dengan re-docking Enzim InhA PDB ID 2X23

LAMPIRAN 4 (LANJUTAN)



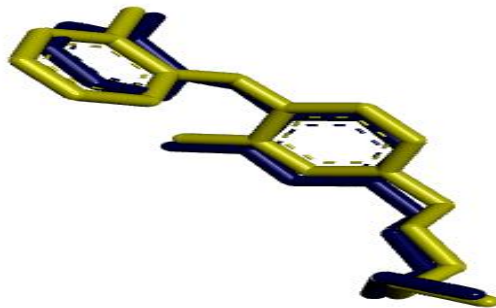
Gambar V.2 Interaksi hasil validasi metode dengan re-docking InhA PDB ID

2X23



Gambar V.3 Visualisasi interaksi Inh A 2X23 dengan ligan alami

**LAMPIRAN 4
(LANJUTAN)**



Gambar V.4 Hasil visualisasi tumpang tindih ligan alami dengan hasil kristalografi sinar-X (biru) dengan ligan hasil re-docking (kuning)

LAMPIRAN 5

LIPINSKI'S RULE OF FIVE SENYAWA TUMBUHAN KEMUKUS**Tabel V.1***Lipinski's Rule of Five Senyawa Tumbuhan Kemukus*

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Refractory Molar
1	Asam sinamat	148	1,78	1	2	43,11
2	Dihidrokubebin	358	2,15	2	6	93,69
3	Dihidroklusin	404	2,44	2	7	107,22
4	Hemiarisensin	400	2,72	1	7	103,24
5	(2R,3R)-2(3'',4''- Metilendioksibenzil)-3- (3',4'- dimetoksibenzil)butirol akton	350	1,22	0	6	77,06
6	Hinokinin	354	2,72	0	6	90,48
7	5-Metoksihinokinin	384	2,73	0	7	97,03
8	Tujaplikatin trimetil eter	390	1,99	0	7	84,62
9	Yatein	400	3,01	0	7	104
10	Isoyatein	400	3,01	0	7	104
11	(8R,8'R)-4-Hidroksi- kubebinon	394	1,16	0	8	83,96
12	Kubebinon	406	1,70	0	8	85,71
13	Kubebinolida	446	3,31	0	8	117,54
14	Kubebin	356	2,51	1	6	91,48
15	α -Metilkubebin	370	3,16	0	6	96,27
16	α -O-Etilkubebin	362	1,30	0	6	79,64
17	β -O-Etilkubebin	362	1,30	0	6	79,64
18	Klusin	402	2,81	1	7	105
19	Etoksiklusin	402	2,06	0	7	87,19

**LAMPIRAN 5
(LANJUTAN)**

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Refractory Molar
20	5-Metoksiklusin	406	1,70	0	8	85,71
21	Kubebinin	448	3,10	1	8	118,54
22	Sesamin	354	3,22	0	6	89,49
23	Askantin	400	3,52	0	7	103,02
24	Medioresinol	388	3,20	2	7	103,03
25	Heterotropan	416	4,89	0	6	116
26	Magnosalin	416	4,89	0	6	116
27	Piperenon	388	3,61	0	6	104,54
28	Kadsurin-A	372	3,32	0	6	97,55
29	α -Asaron	208	2,72	0	3	60,80
30	2,4,5- Trimetoksifenilaseton	208	0,96	0	4	44,60
31	1-(2,4,5- Trimetoksifenil)-1,2- propandion	224	1,01	0	5	49,04
32	2,4,5- Trimetoksibenzaldehida	184	0,87	0	4	38,39
33	Piperenol C	448	1,51	0	10	107,02
34	Piperenol A	384	1,09	3	7	98,47
35	Sabinen	136	2,99	0	0	43,75
36	<i>Trans</i> -Sabinen hidrat	136	0,35	0	1	35,57
37	γ -Kadinen	204	4,58	0	0	66,67
38	β -Elemen	204	4,75	0	0	68,76
39	β -Kariofilen	204	4,72	0	0	66,74
40	Kubebol	222	3,46	1	1	65,99
41	Epikubebol	186	0,73	0	1	48,36
42	(5 α ,8 α)-2-okso- 1(10),3,7(11)- guaiatrien-12,8-olida	217	0,36	0	3	52,38
43	(1 α ,2 β ,5 α ,8 α ,10 α)-1,10- Epoksi-2-hidroksi- 3,7(11)-guaiadien-12,8- olida	233	0,14	0	4	53,24

LAMPIRAN 6

HASIL PENAMBATAN MOLEKUL (*MOLECULAR DOCKING*)

Tabel V.2

Hasil *Molecular Docking* Senyawa Ligan alami 2X23, Isoniazid dan Tumbuhan Kemukus.

No	Ligan	ΔG (Kkal/mol)	Konstanta inhibisi (nM)
1	Ligan alami	-8,15	7,8
2	Isoniazid	-4,56	4,52
3	Asam sinamat	-5,11	1,79
4	Dihidrokubebin	-6,78	0,10
5	Dihidroklusin	-4,94	2,38
6	Hemiarisensin	-5,97	0,41
7	(2R,3R)-2-(3'',4''-Metilendioksibenzil)-3-(3',4'-dimetoksibenzil)butirolakton	-8,82	3,42
8	Hinokinin	-8,25	8,92
9	5-Metoksihinokinin	-8,93	2,82
10	Tujaplikatin trimetil eter	-6,01	0,39
11	Yatein	-6,96	0,73
12	Isoyatein	-6,62	0,14
13	(8R,8'R)-4-Hidroksi-kubebinon	-5,92	0,45
14	Kubebinon	-4,78	3,15
15	Kubebinolida	-4,19	8,16
16	Kubebin	-8,60	4,96
17	α -Metilkubebin	-8,55	5,38
18	α -O-Etilkubebin	-9,04	2,38
19	β -O-Etilkubebin	-8,46	6,29

**LAMPIRAN 6
(LANJUTAN)**

No	Ligan	ΔG (Kkal/mol)	Konstanta inhibisi (nM)
20	Klusin	-8,68	4,32
21	Etoksiklusin	-5,19	1,58
22	5-Metoksiklusin	-8,27	8,72
23	Kubebinin	-1,48	0,82
24	Sesamin	-8,91	2,93
25	Askantin	-7,90	0,16
26	Medioresinol	-5,28	1,34
27	Heterotropan	-2,39	1,78
28	Magnosalin	+0,9	8,79
29	Piperenon	-4,65	3,88
30	Kadsurin-A	-7,86	1,75
31	α -Asaron	-4,85	2,76
32	2,4,5-Trimetoksi fenilaseton	-4,93	2,43
33	1-(2,4,5-Trimetoksifenil)-1,2-propandion	-5,40	3,43
34	2,4,5-Trimetoksi benzaldehida	-5,27	1,36
35	Piperenol C	-6,68	1,27
36	Piperenol A	-8,13	5,35
37	Sabinen	-5,58	0,81
38	<i>Trans</i> -Sabinen hidrat	-5,86	0,50
39	γ -Kadinen	-8,12	1,11
40	β -Elemen	-7,25	4,84
41	β -Kariofilen	-8,45	6,40

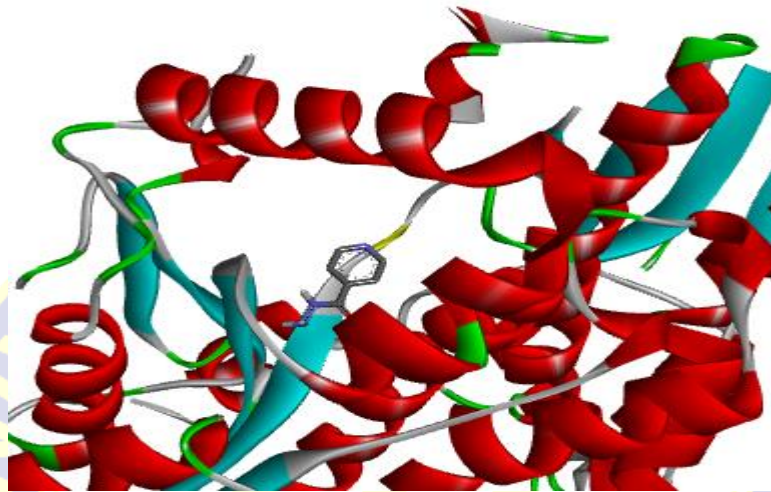
**LAMPIRAN 6
(LANJUTAN)**

No	Ligan	ΔG (Kkal/mol)	Konstanta inhibisi (nM)
42	Kubebol	-7,68	2,34
43	Epikubebol	-7,16	5,68
44	(5 α ,8 α)-2-okso-1(10),3,7911)-guaiatrien-12,8-olida	-7,98	1,42
45	(1 α ,2 β ,5 α ,8 α ,10 α)-1,10-Epoksi-2-hidroksi-3,7(11)-guaiadien-12,8-olida	-8,06	1,24

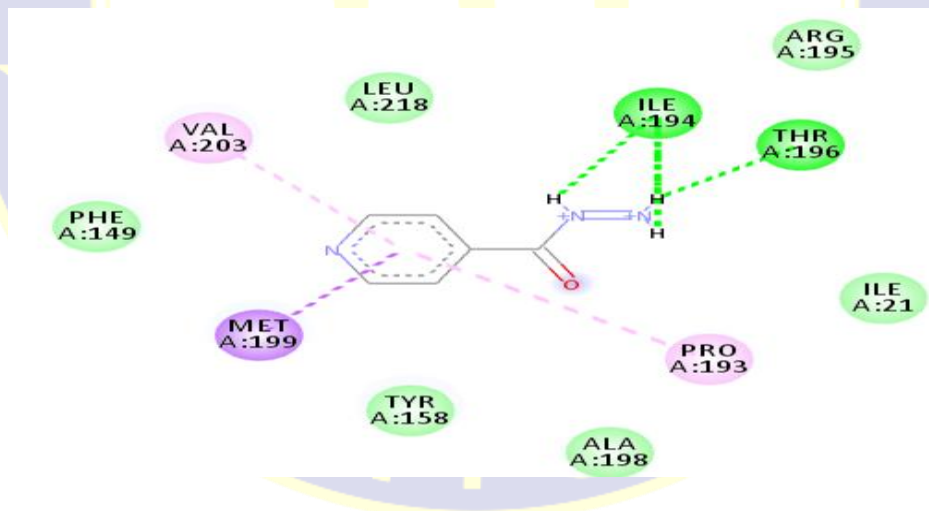
LAMPIRAN 7

INTERAKSI SENYAWA ISONIAZID TERHADAP RESEPTOR ENZIM

InhA

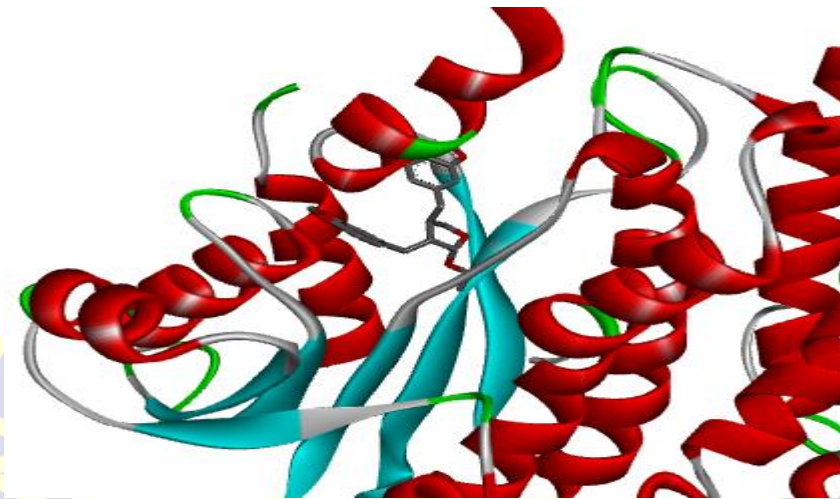


Gambar V.5 Interaksi senyawa Isoniazid dengan Enzim InhA

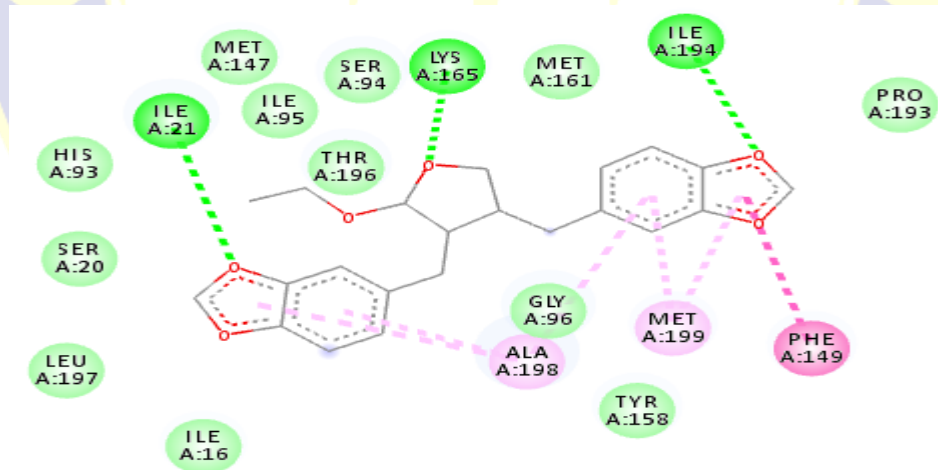


Gambar V.6 Visualisasi interaksi senyawa Isoniazid dengan Enzim InhA

LAMPIRAN 8

INTERAKSI SENYAWA α -O-ETILKUBEKIN TERHADAP ENZIM InhA

Gambar V.7 Interaksi senyawa α -O-Etilkubebine dengan Enzim InhA



Gambar V.8 Visualisasi interaksi senyawa α -O-Etilkubebine dengan Enzim InhA

LAMPIRAN 9

INTERAKSI IKATAN HIDROGEN DAN RESIDU ASAM AMINO

Tabel V.3

Hasil Analisis Ikatan Hidrogen dan Residu Asam Amino yang Terlibat

No	Senyawa	Jumlah ikatan hidrogen	Residu Asam Amino
1	Ligan alami	1	TYR158
2	Isoniazid	2	ILE194, THR196
3	Asam sinamat	1	ILE194
4	Dihidrokubebin	2	TYR158, ILE21
5	Dihidroklusin	-	
6	Hemiarisensin	1	ASP148
7	(2R,3R)-2-(3'',4''-Metilendioksibenzil)-3-(3',4'-dimetoksibenzil)butirolakton	1	ILE202
8	Hinokinin	2	ILE194, THR196
9	5-Metoksihinokinin	-	
10	Tujaplikatin trimetil eter	-	
11	Yatein	2	THR196, LYS165
12	Isoyatein	1	VAL203
13	(8R,8'R)-4-Hidroksi-kubebinon	1	ILE21
14	Kubebinon	1	MET98
15	Kubebinolida	1	ILE194
16	Kubebin	-	
17	α -Metil kubebin	1	THR196
18	α -O-Etilkubebin	3	ILE194, LYS165, ILE21
19	β -O-Etilkubebin	1	LYS165
20	Klusin	2	GLY192, ILE194
21	Etoksiklusin	-	
22	5-Metoksiklusin	-	
23	Kubebinin	-	
24	Sesamin	-	

**LAMPIRAN 9
(LANJUTAN)**

No	Senyawa	Jumlah ikatan hidrogen	Residu Asam Amino
25	Askantin	-	
26	Medioresinol	2	PRO156, LYS165
27	Heterotropan	-	
28	Magnosalin	1	ILE194
29	Piperenon	-	
30	Kadsurin-A	1	LYS165
31	α -Asaron	-	
32	2,4,5-Trimetoksifenilaseton	-	
33	1-2(2,4,5-Trimetoksifenil)-1,2-propandion	-	
34	2,4,5-Trimetoksi-benzaldehida	1	THR196
35	Piperenol C	-	
36	Piperenol A	1	TYR158
37	Sabinen	-	
38	<i>Trans</i> -Sabinen hidrat	1	ILE194
39	γ -Kadinen	-	
40	β -Elemen	-	
41	β -Kariofilen	-	
42	Kubebol	-	
43	Epikubebol	-	
44	(5 α ,8 α)-2-okso-1(10),3,7(11)-guaiatrien-12,8-olida	2	ILE194, LYS165
45	(1 α ,2 β ,5 α ,8 α ,10 α)-1,10-Epoksi-2-hidroksi-3,7(11)-guaiadien-12,8-olida	1	ALA191

LAMPIRAN 10

HASIL UJI PRE-ADME

Tabel V.4

Hasil Uji Pre-ADME Senyawa Ligan Alami 2X23, Isoniazid dan Tumbuhan Kemukus

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	Protein Plasma Binding (%)
1	Ligan alami	31,99	97,61	100
2	Isoniazid	19,50	87,11	1,607
3	Asam sinamat	31,56	96,55	53,55
4	Dihidrokubebin	23,39	93,83	86,26
5	Dihidroklusin	31,56	93,33	85,00
6	Hemiarisensin	25,09	94,42	82,78
7	(2R,3R)-2-(3'',4''-Metilendioksibenzil)-3-(3',4'-dimetoksibenzil)butirolakton	48,69	98,36	88,88
8	Hinokinin	39,68	98,46	89,20
9	5''-Metoksihinokinin	43,56	98,89	88,19
10	Tujaplikatin trimetil eter	54,77	98,79	87,43
11	Yatein	50,94	98,86	87,86
12	Isoyatein	50,97	98,86	87,86
13	(8R,8'R)-4-Hidroksi-kubebinon	34,52	96,98	86,98
14	Kubebinon	52,54	86,94	99,14
15	Kubebinolida	55,44	99,17	86,34
16	Kubebin	34,95	96,20	87,17
17	α-Metil kubebin	55,09	97,83	88,42

LAMPIRAN 10
(LANJUTAN)

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	<i>Protein Plasma Binding (%)</i>
18	α -O-Etilkubebin	56,92	97,71	89,12
19	β -O-Etilkubebin	57,60	97,47	94,10
20	Klusin	48,23	96,68	85,40
21	Etoksiklusin	57,56	98,09	87,76
22	5-Metoksiklusin	50,55	97,14	84,01
23	Kubebinin	54,50	97,14	83,06
24	Sesamin	57,02	97,95	83,12
25	Askantin	57,52	98,37	79,90
26	Medioresinol	55,27	96,54	78,66
27	Heterotropen	23,25	100	100
28	Magnosalin	232,25	100	100
29	Piperenon	56,43	98,38	84,34
30	Kadsurin-A	55,65	98,49	84,86
31	α -Asaron	58,10	100	93,39
32	2,4,5-Trimetoksifenilaseton	41,65	97,80	55,43
33	1-(2,4,5-Trimetoksifenil)- 1,2-propandion	17,57	95,59	60,33
34	2,4,5-Trimetoksi benzaldehida	43,38	93,87	76,83
35	Piperenol C	18,76	87,54	65,66
36	Piperenol A	16,34	90,56	83,46
37	Sabinen	23,49	100	60,97
38	<i>Trans</i> -Sabinen hidrat	49,55	100	35,94
39	γ -Kadinen	23,63	100	100

LAMPIRAN 10
(LANJUTAN)

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	<i>Protein Plasma Binding (%)</i>
40	β -Elemen	23,49	100	100
41	β -Kariofilen	23,63	100	100
42	Kubebol	55,50	100	94,61
43	Epikubebol	54,57	100	100
44	(5 α ,8 α -2-okso-1(10),3,7(11)- guaiatrien-12,8-olida	23,18	94,87	82,85
45	(1 α ,2 β ,5 α ,8 α ,10 α)-1,10-Epoksi- 2-hidroksi-3,7(11)-guaiadien- 12,8-olida	22,50	98,23	91,92

Keterangan :

%HIA : 70-100% well absorbed, 20-70% moderately absorbed, 0-20% poorly absorbed.

In Vitro caco-2 cell permeability : > 70 higher permeability, 4-70 medium permeability, < 40 low permeability

% PPB : > 90% strongly bound, <90% weakly bound

LAMPIRAN 11

HASIL UJI TOKSISITAS

Tabel V.5

Hasil Prediksi Toksisitas Senyawa Ligan alami 2X23, Isoniazid dan Tumbuhan Kemukus

No	Senyawa Ligan	Kroes TTC decision tree
1	Ligan alami (TCU)	1
2	Isoniazid	2
3	Asam sinamat	1
4	Dihidrokubebin	1
5	Dihidroklusin	2
6	Hemiarisensin	1
7	(2R,3R)-2-(3'',4''-Metilendioksibenzil)-3-(3',4'-dimetoksibenzil)butirolakton	1
8	Hinokinin	1
9	5''-Metoksihinokinin	1
10	Tujaplikatin trimetil eter	1
11	Yatein	1
12	Isoyatein	1
13	(8R,8'R)-4-Hidroksi-kubebinon	1
14	Kubebinon	1
15	Kubebinolida	1
16	Kubebin	1
17	α -Metil kubebin	1
18	α -O-Etilkubebin	1
19	β -O-Etilkubebin	1
20	Klusin	1
21	Etoksiklusin	1

LAMPIRAN 11
(LANJUTAN)

No	Senyawa Ligan	Kroes TTC decision tree
22	5-Metoksiklusin	1
23	Kubebinin	1
24	Sesamin	1
25	Askantin	1
26	Medioresinol	1
27	Heterotropen	1
28	Magnosalin	1
29	Piperenon	2
30	Kadsurin-A	2
37	Sabinen	1
38	<i>Trans</i> -Sabinen hidrat	1
39	γ -Kadinen	2
40	β -Elemen	1
41	β -Kariofilen	1
42	Kubebol	1
43	Epikubebol	1
44	(5 α ,8 α)-2-okso-1(10),3,7(11)-guaiatrien-12,8-olida	2
45	(1 α ,2 β ,5 α ,8 α ,10 α)-1,10-Epoksi-2-hidroksi-3,7(11)-guaiadien-12,8-olida	1

Kroes TTC decision tree :

1 = Aman

2 = Resiko dapat diabaikan