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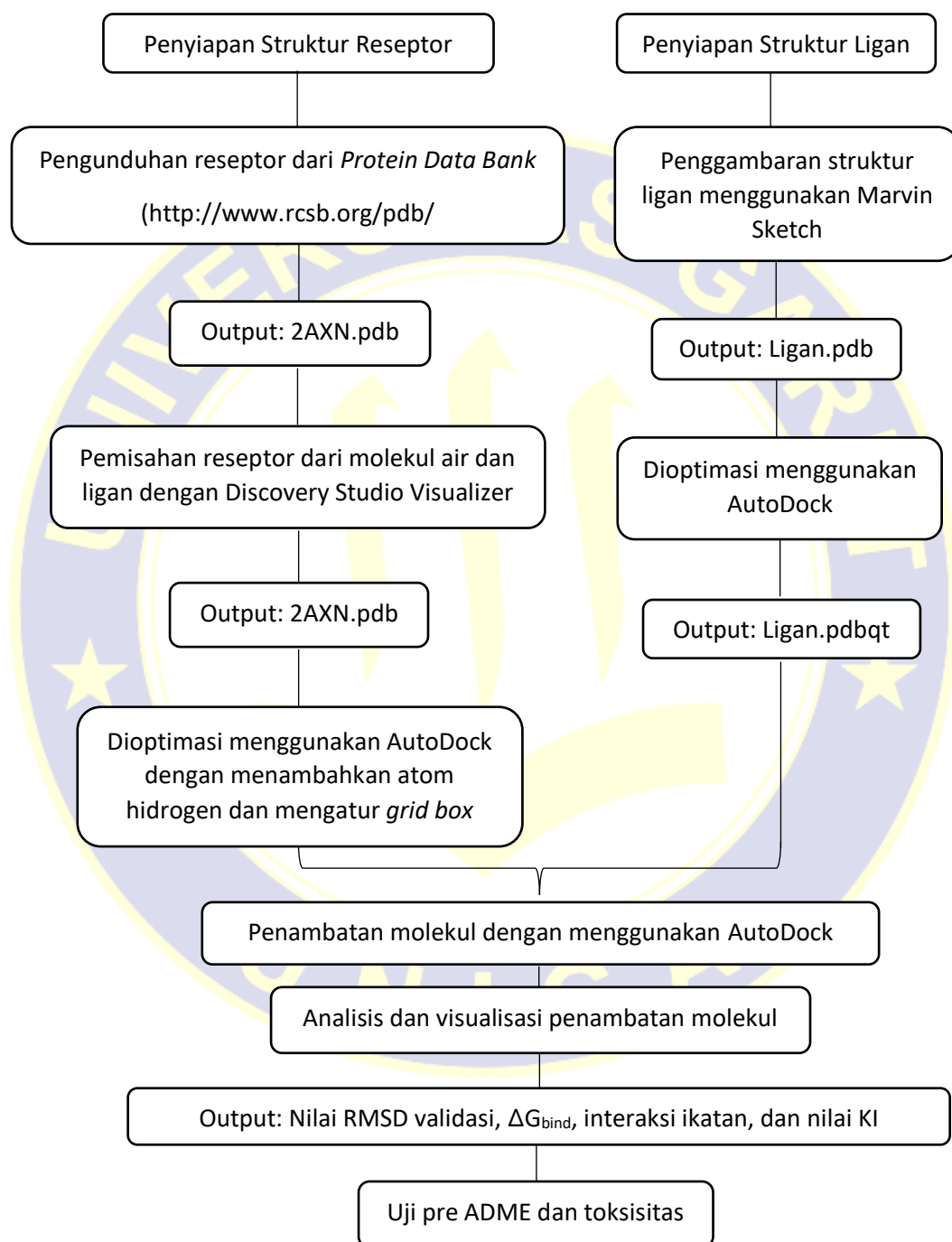
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LAMPIRAN 1

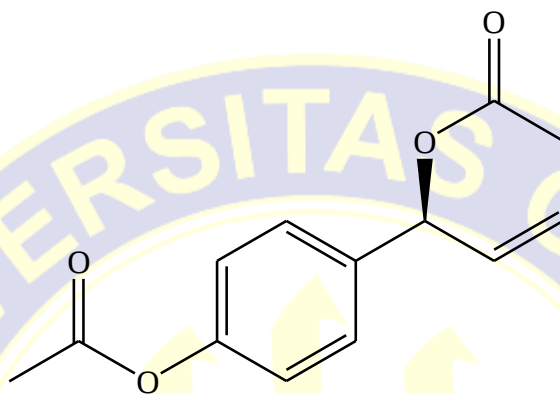
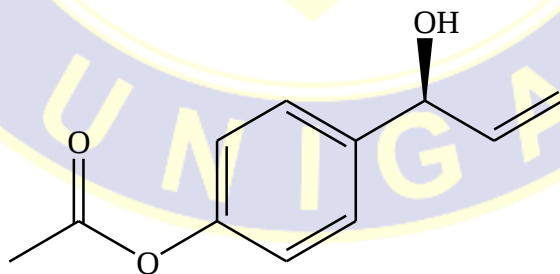
ALUR PENELITIAN



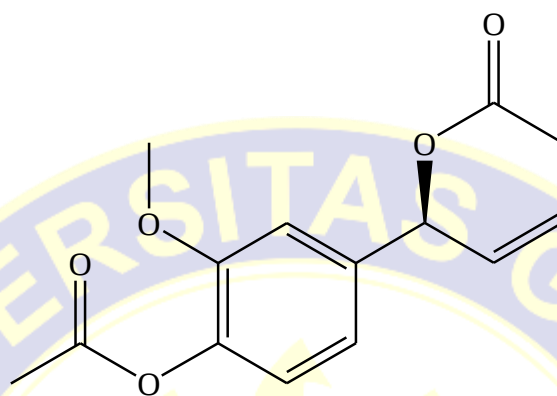
Gambar V.1 Alur penelitian penambatan molekul

LAMPIRAN 2

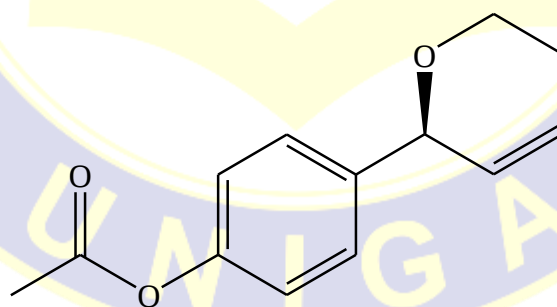
SENYAWA TURUNAN FENILPROPANOID

**Gambar V.2** 1'S-1'-Acetoxychavicol acetate (ACA)**Gambar V.3** 1'S-1'-Hydroxychavicol acetate

**LAMPIRAN 2
(LANJUTAN)**

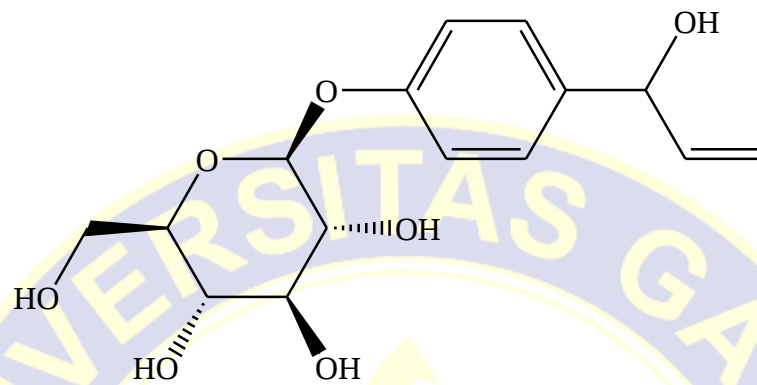


Gambar V.4 1'S-1'-Acetoxyeugenol acetate

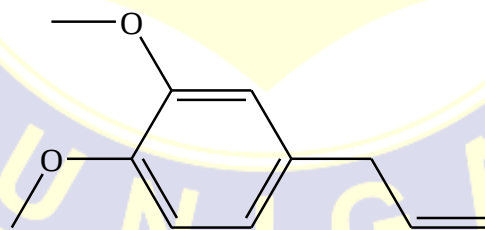


Gambar V.5 1'S-1'-Ethoxy chavicol acetate

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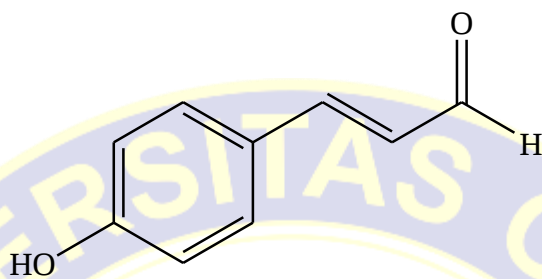


Gambar V.6 Chavicol *beta*-D-glucopyranoside

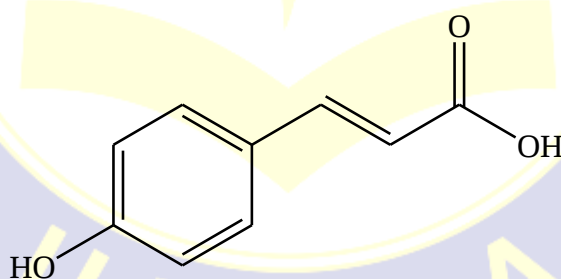


Gambar V.7 Methyleugenol

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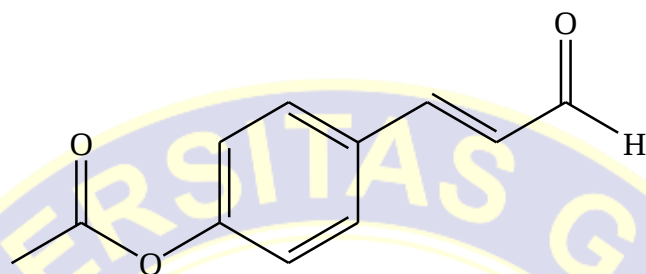


Gambar V.8 *trans-p*-Hydroxycinnamaldehyde

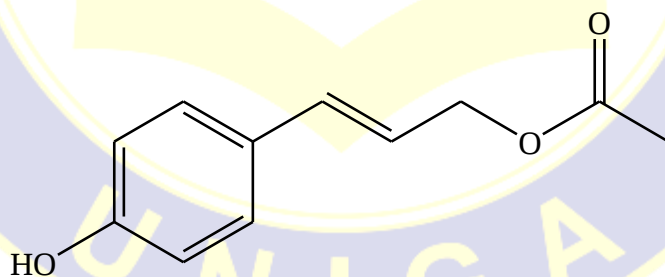


Gambar V.9 *trans-p*-Hydroxycinnamic acid

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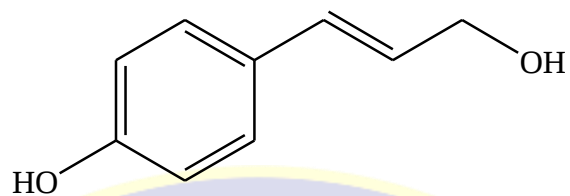


Gambar V.10 *trans-p*-Hydroxycinnamaldehyde acetate

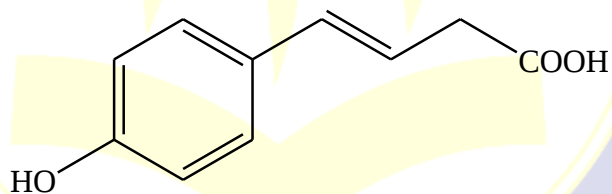


Gambar V.11 *p*-Hydroxycinnamyl acetate

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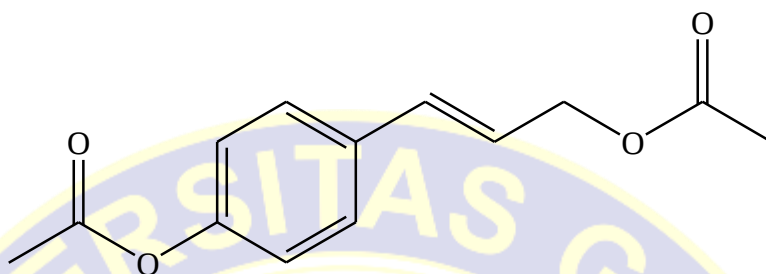


Gambar V.12 *trans-p*-Coumaryl alcohol

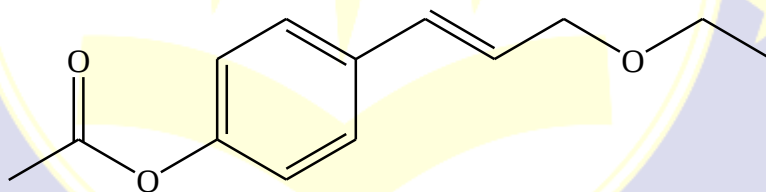


Gambar V.13 *trans-p*-Coumaric acid

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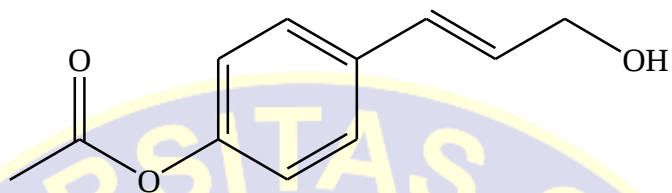


Gambar V.14 *trans-p*-Coumaryl diacetate

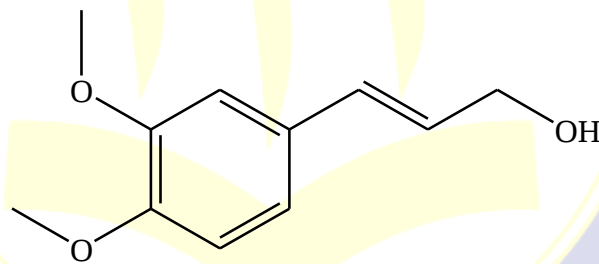


Gambar V.15 (*E*)-4-Acetoxy cinnamyl ethyl ether

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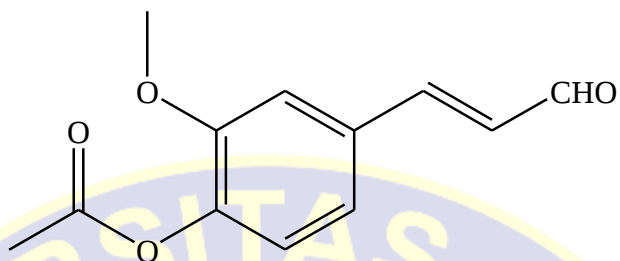


Gambar V.16 (*E*)-4-Acetoxy cinnamyl alcohol

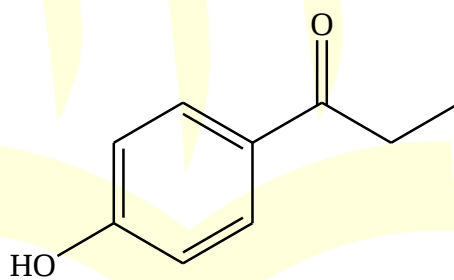


Gambar V.17 *trans*-3,4-dimethoxycinnamyl alcohol

**LAMPIRAN 2
(LANJUTAN)**

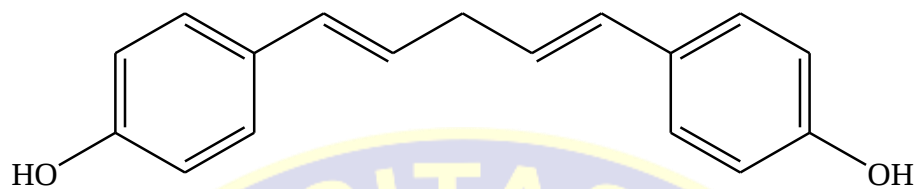


Gambar V.18 2-propenal, 3-[4-(acetyloxy)-3-methoxyphenyl]

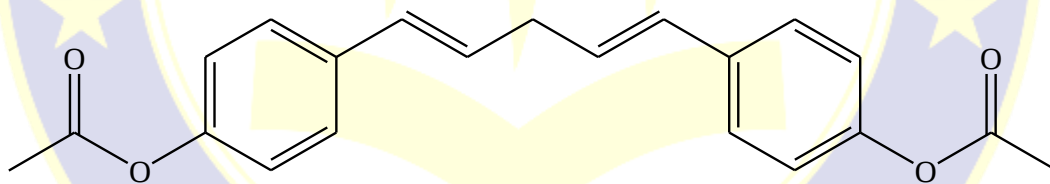


Gambar V.19 1-(4-hydroxyphenyl)-1-propanone

**LAMPIRAN 2
(LANJUTAN)**

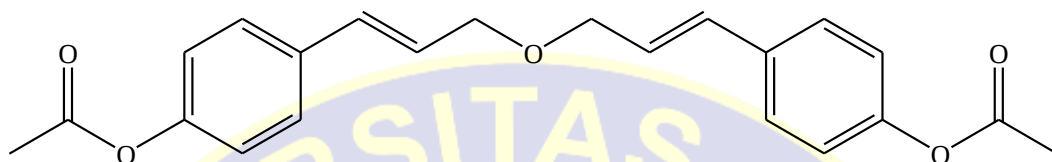


Gambar V.20 [di(*p*-hydroxy-cis-styryl)] methane

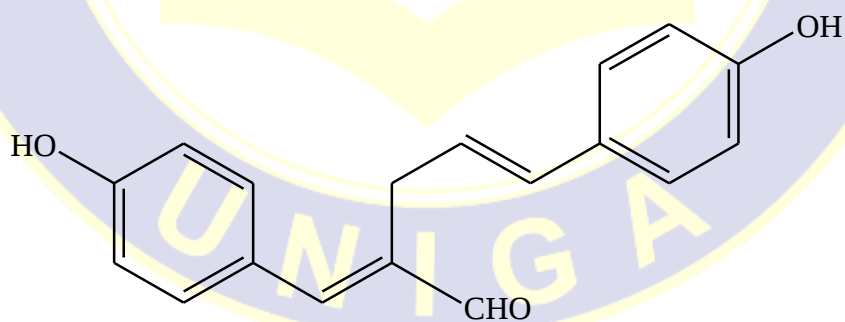


Gambar V.21 [di-(*p*-acetoxy-cis-styryl)] methane

**LAMPIRAN 2
(LANJUTAN)**

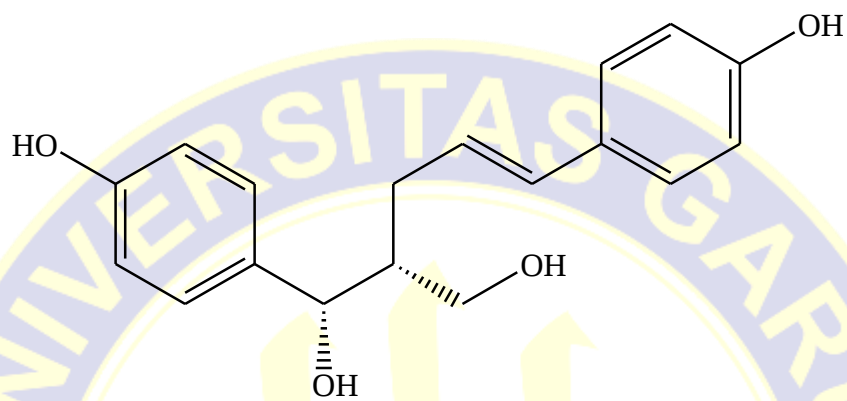


Gambar V.22 4, 4'[(2*E*,2'*E*)-bis(prop-2-ene)-1,1'-oxy]diphenyl-7,7'-diacetate

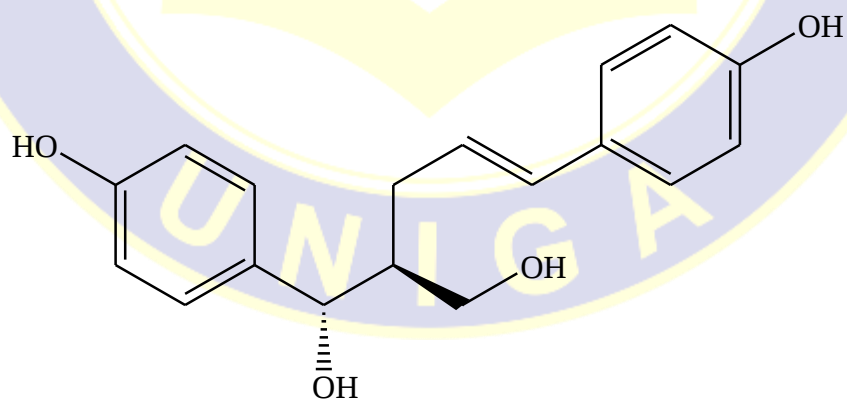


Gambar V.23 Galanganal

**LAMPIRAN 2
(LANJUTAN)**

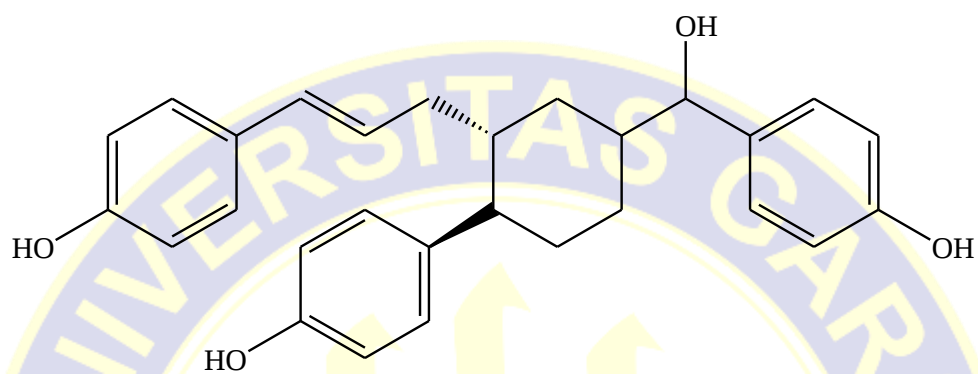


Gambar V.24 Galanganol A

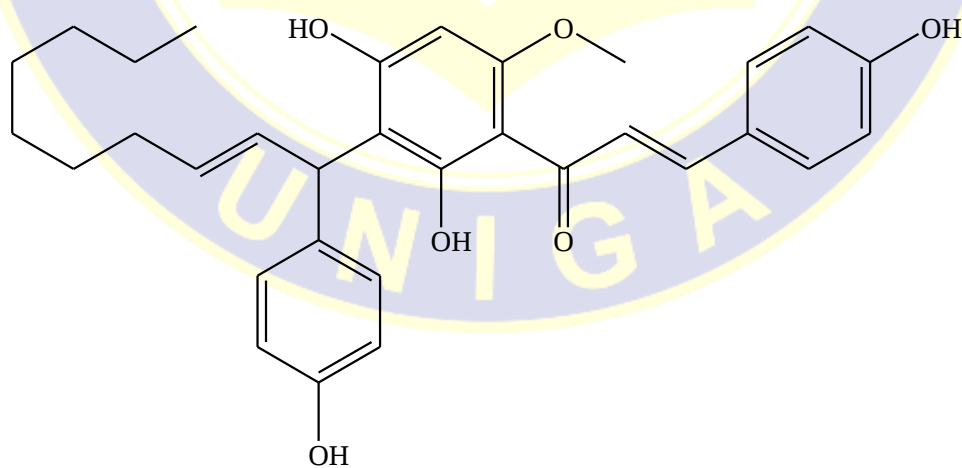


Gambar V.25 Galanganol B

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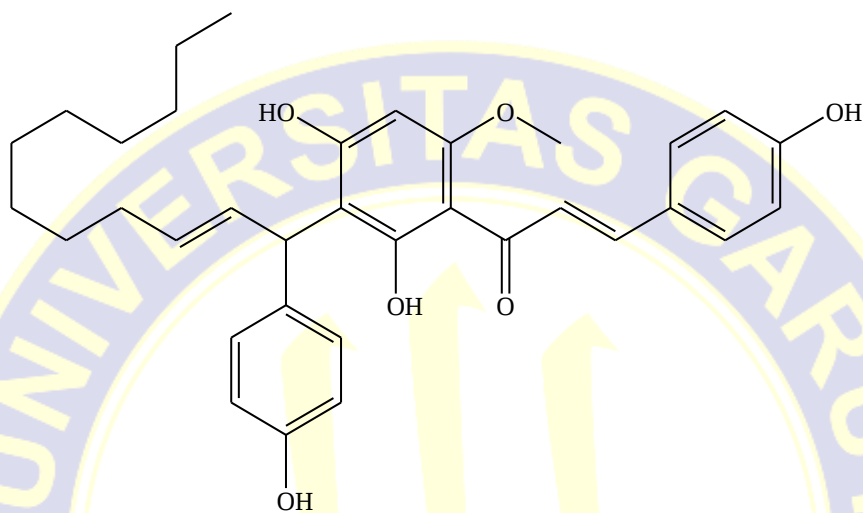


Gambar V.26 Galanganol C

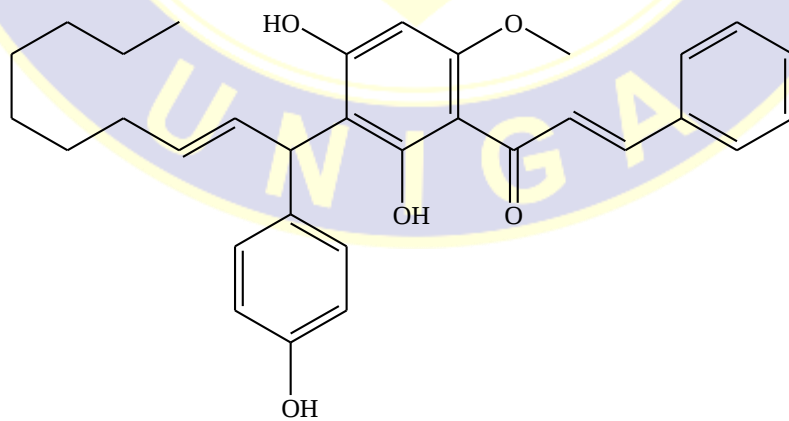


Gambar V.27 Galanganones A

**LAMPIRAN 2
(LANJUTAN)**



Gambar V.28 Galanganones B



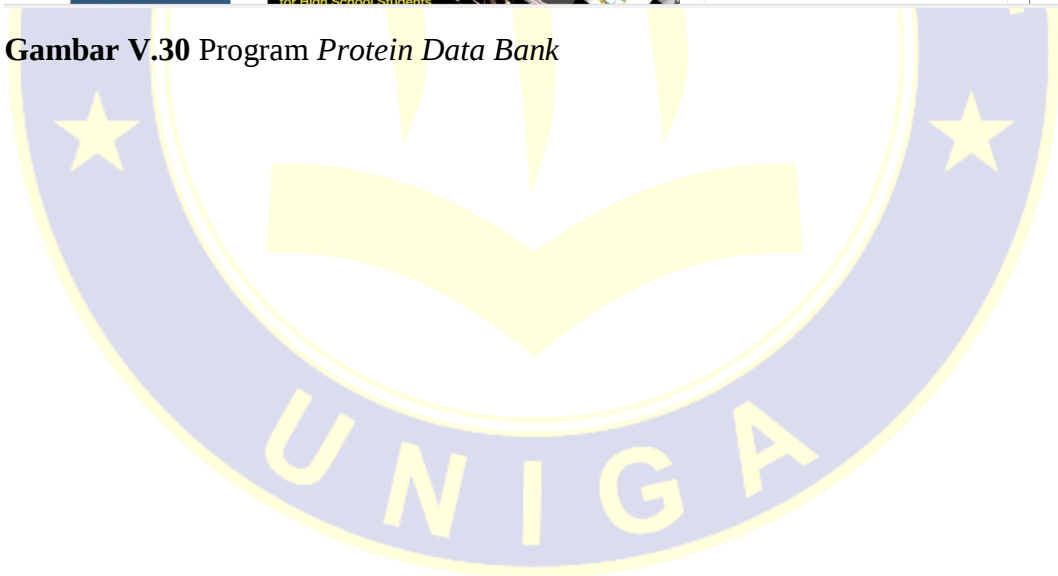
Gambar V.29 Galanganones C

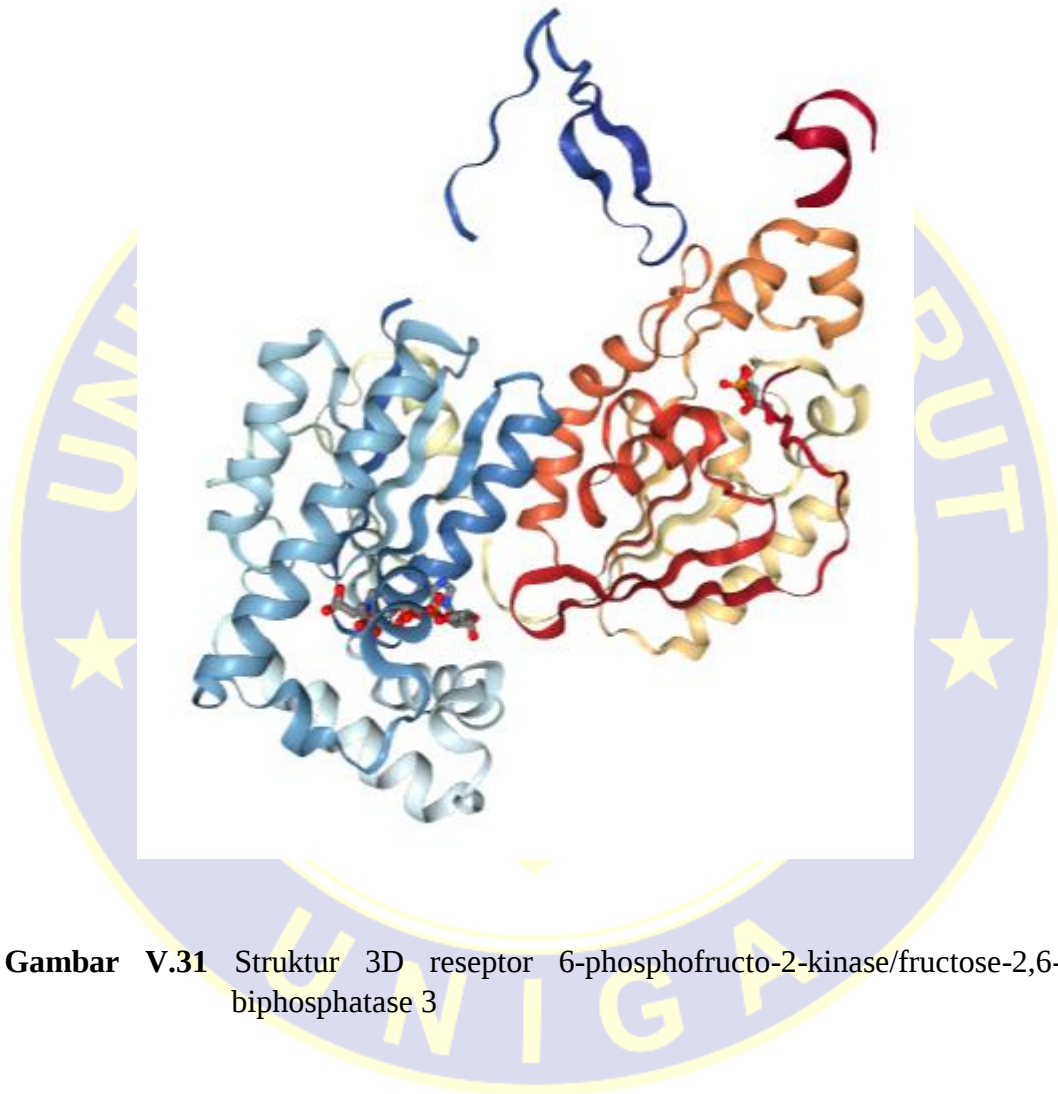
LAMPIRAN 3

SITUS *PROTEIN DATA BANK*

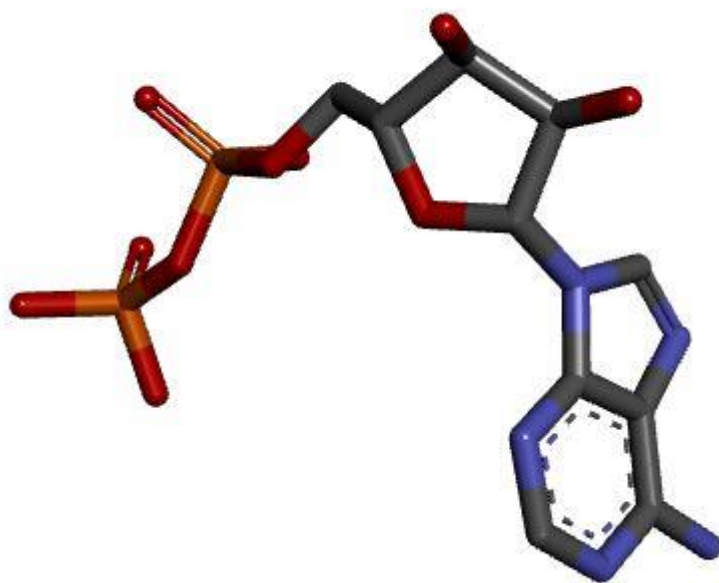


Gambar V.30 Program *Protein Data Bank*



LAMPIRAN 4**STRUKTUR 3D RESEPTOR PFKFB3**

Gambar V.31 Struktur 3D reseptor 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 3

LAMPIRAN 5**LIGAN ALAMI**

Gambar V.32 Ligan alami Adenosin Difosfat

LAMPIRAN 6

SITUS PUBCHEM

Secure | <https://pubchem.ncbi.nlm.nih.gov/compound/119104>

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1'-Acetoxychavicol acetate

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STRUCTURE VENDORS PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID: 119104

Chemical Names: 1'-Acetoxychavicol acetate; 52946-22-2; 1'-Acetoxychavicol; UNII-SQV3080A2Q; CHEBI:469; 1'S-1'-Acetoxychavicol acetate More...

Molecular Formula: C13H14O4

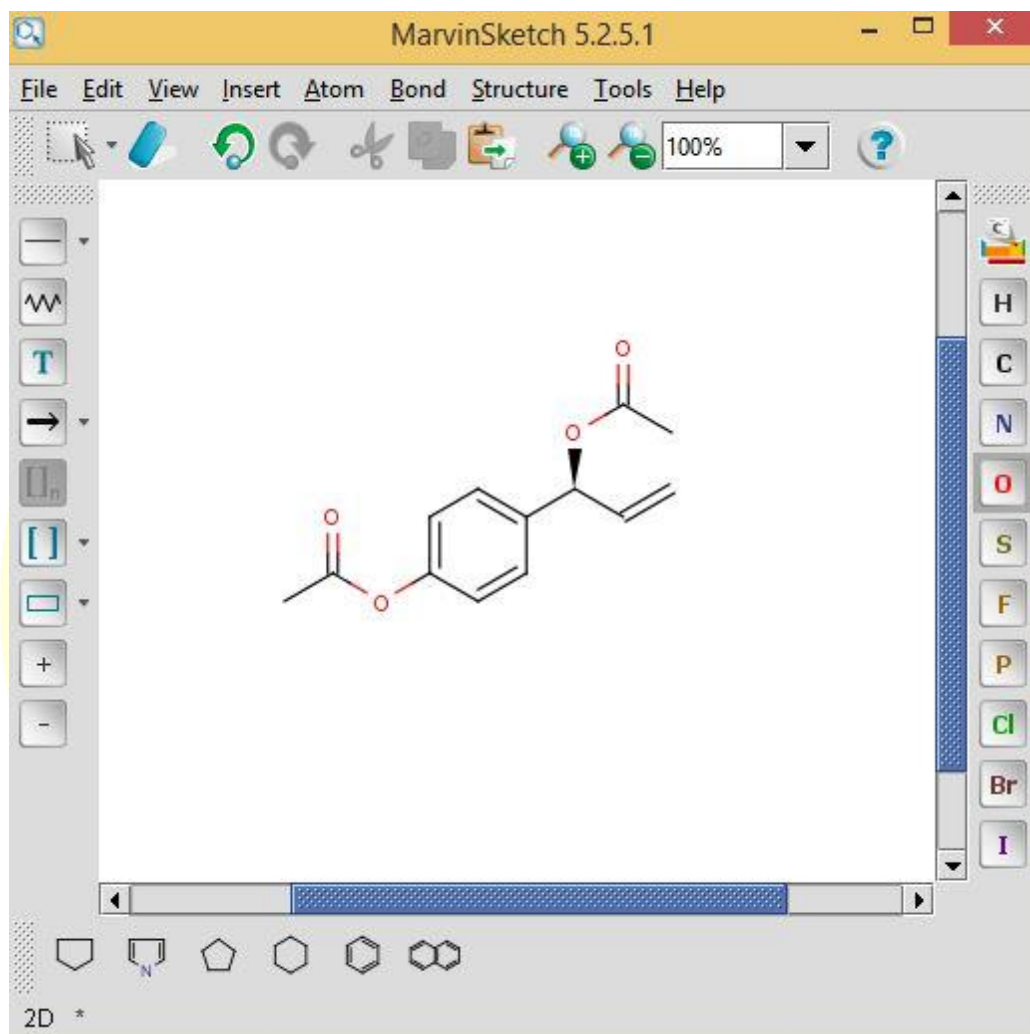
Molecular Weight: 234.251 g/mol

InChI Key: JAMQIUWGGBSIKZ-ZDUSSCGKSA-N

Substance Registry: FDA UNII

Gambar V.33 Tampilan situs Pubchem untuk senyawa 1'-Acetoxychavicol acetate

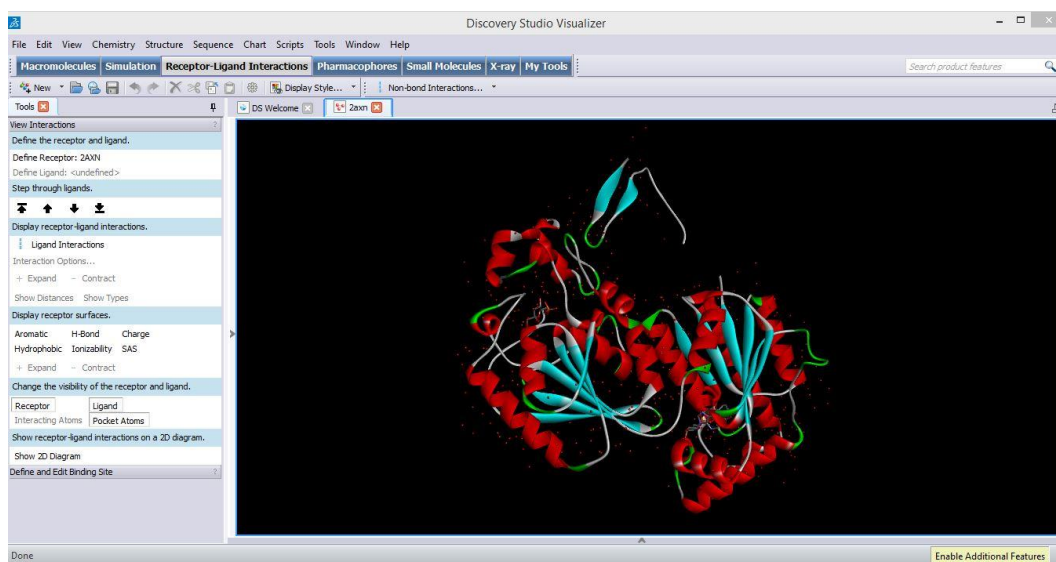
LAMPIRAN 7
PERANGKAT LUNAK MARVINSKETCH



Gambar V.34 Tampilan program MarvinSketch

LAMPIRAN 8

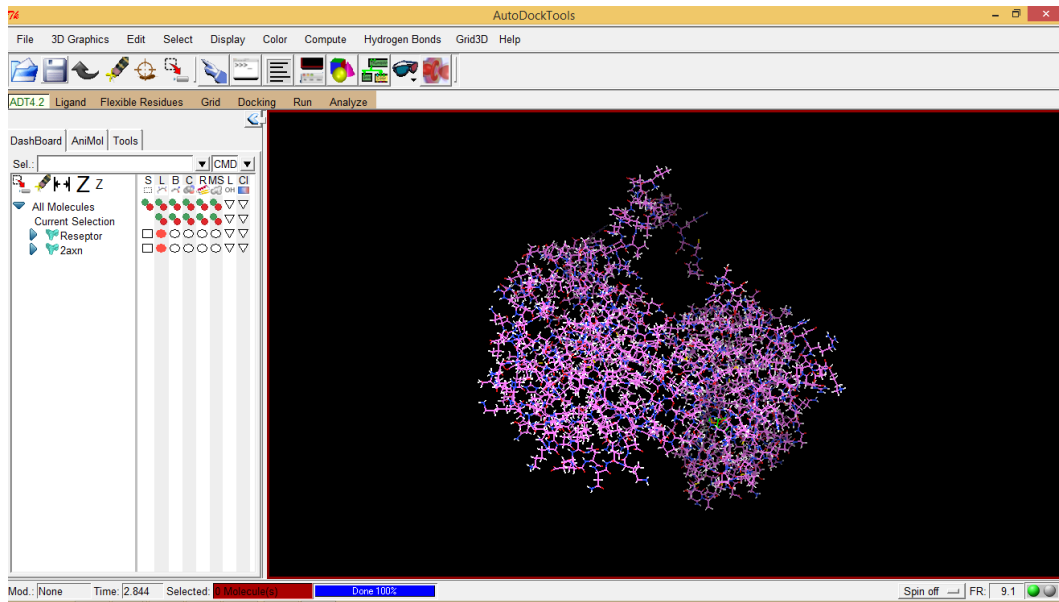
PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER



Gambar V.35 Tampilan program Discovery Studio Visualizer

LAMPIRAN 9

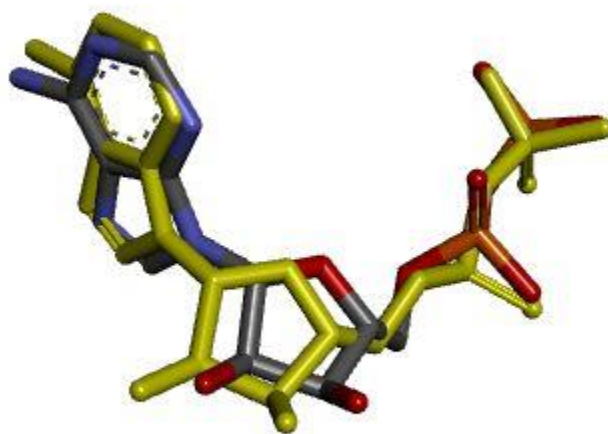
PERANGKAT LUNAK AUTODOCK TOOLS



Gambar V.36 Tampilan program AutoDock Tools

LAMPIRAN 10

VALIDASI METODE



Gambar V.37 Visualisasi tumpang tindih ligan alami 2AXN (Merah-Abu-Biru) dengan ligan hasil *redocking* (kuning)

Tabel V.1

Grid Box, RMSD, Nilai Ikatan Energi, Ligan Alami, dan Temozolomid

Kode PDB	Grid Box	RMSD	Ikatan Energi Temozolomid (kkal/mol)	Ikatan Energi Ligan Alami (kkal/mol)
2AXN	X : -9,824 Y : 47,857 Z : 8,679	0,804Å	-5,90	-16,13

LAMPIRAN 11
SIFAT FISIKOKIMIA 5 LIPINSKI

Tabel V.2
 Sifat Fisikokimia Senyawa Turunan Fenilpropanoid Berdasarkan Aturan 5 Lipinski

No.	Senyawa Uji	Ikatan Hidrogen		Bobot Molekul (g/mol)	Log P	Molar Refractivity
		Donor	Aseptor			
1.	1'S-1'-Acetoxychavicol acetate (ACA)	0	4	234	2,40	62,45
2.	1'S-1'-Hydroxychavicol acetate	1	3	192	1,83	52,91
3.	1'S-1'-Acetoxyeugenol acetate	0	5	264	2,41	69,00
4.	1'S-1'-Ethoxy chavicol acetate	0	3	220	2,88	62,31
5.	Chavicol <i>beta</i> -D-glucopyranoside	4	6	296	-0,41	74,74
6.	Methyleugenol	0	2	178	2,43	53,45
7.	<i>trans-p</i> -Hydroxycinnamaldehyde	1	2	148	1,60	43,20
8.	<i>trans-p</i> -Hydroxycinnamic acid	2	3	164	1,49	44,78
9.	<i>trans-p</i> -Hydroxycinnamaldehyde acetate	0	3	190	1,82	52,85
10.	<i>p</i> -Hydroxycinnamyl acetate	1	3	192	1,97	55,77
11.	<i>trans-p</i> -Coumaryl alcohol	2	2	150	1,39	44,23
12.	<i>trans-p</i> -Coumaric acid	2	3	164	1,49	44,50
13.	<i>trans-p</i> -Coumaric diacetate	0	4	234	2,19	63,42
14.	(<i>E</i>)-4-Acetoxy cinnamyl ethyl ether	0	3	220	2,66	63,28

**LAMPIRAN 11
(LANJUTAN)**

Tabel V.2

Sifat Fisikokimia Senyawa Turunan Fenilpropanoid Berdasarkan Aturan 5 Lipinski

No.	Senyawa Uji	Ikatan Hidrogen		Bobot Molekul (g/mol)	Log P	Molar Refractivity
		Donor	Aseptor			
15.	(<i>E</i>)-4-Acetoxy cinnamyl alcohol	1	3	192	1,62	53,87
16.	<i>trans</i> -3,4-dimethoxycinnamyl alcohol	1	3	194	1,71	55,67
17.	2-propenal, 3-[4-(acetyloxy)-3-methoxyphenyl]	0	4	220	1,83	59,40
18.	1-(4-hydroxyphenyl)-1-propane	1	2	150	1,98	42,73
19.	[di-(<i>p</i> -hydroxy- <i>cis</i> -styryl)] methane	2	2	252	4,21	78,89
20.	[di-(<i>p</i> -acetoxy- <i>cis</i> -styryl)] methane	0	4	336	4,65	98,19
21.	4, 4'[(2 <i>E</i> ,2' <i>E</i>)-bis(prop-2-ene)-1,1'-oxy]-diphenyl-7,7'-diacetate	0	5	366	4,28	104,39
22.	Galanganal	2	3	280	3,78	83,91
23.	Galanganol A	4	4	300	2,84	85,40
24.	Galanganol B	4	4	300	2,84	85,40
25.	Galanganol C	4	5	432	4,33	123,22
26.	Galanganones A	4	6	516	7,46	150,26
27.	Galanganones B	4	6	560	8,97	165,88
28.	Galanganones C	3	5	502	7,73	148,65

LAMPIRAN 12

NILAI IKATAN ENERGI DAN RESIDU ASAM AMINO

Tabel V.3
 Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji

No.	Ligan/Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1.	Ligan Alami	-16,13	6	TYR49, GLY46, ALA44, THR48, TYR424, ARG45	151×10^{-3}
2.	Temozolomid	-5,90	7	VAL217, ASP216, LYS168, SER152, ARG45, VAL153, VAL214	14360
3.	1'S-1'-Acetoxychavicol acetate (ACA)	-8,72	3	ARG45, LYS47, GLY46	405
4.	1'S-1'-Hydroxychavicol acetate	-8,53	3	ARG45, LYS47, LYS168	558
5.	1'S-1'-Acetoxyeugenol acetate	-6,80	3	ASN163, ASP216, VAL217	4070
6.	1'S-1'Ethoxy chavivol acetate	-8,49	3	ARG45, LYS47, GLY46	598
7.	Chavicol <i>beta</i> -D-glucopyranoside	-7,61	3	ASN163, ALA423, GLU166	2660

LAMPIRAN 12
(LANJUTAN)

Tabel V.3

Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji

No.	Ligan/Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
8.	Methyleugenol	-5,73	1	LYS168	62880
9.	<i>trans-p</i> -Hydroxycinnamaldehyde	-6,42	2	ARG45, LYS47	19520
10.	<i>trans-p</i> -Hydroxycinnamic acid	-9,37	3	ARG45, ALA44, LYS47	134
11.	<i>trans-p</i> -Hydroxycinnamaldehyde acetate	-8,19	5	ARG45, ALA44, GLY46, THR48, ASN163	995
12.	<i>p</i> -Hydroxycinnamyl acetate	-7,43	3	ARG45, GLY46, THR48	3600
13.	<i>trans-p</i> -Coumaryl alcohol	-6,50	3	ARG45, LYS47, GLY46	149
14.	<i>trans-p</i> -Coumaric acid	-9,31	2	ARG45, LYS47	17140
15.	<i>trans-p</i> -Coumaryl diacetate	-8,72	5	ARG45, GLY46, LYS47, THR48, ASN163	405
16.	(<i>E</i>)-4-Acetoxy cinnamyl ethyl ether	-8,44	3	ARG45, LYS47, GLY46	646
17.	(<i>E</i>)-4-Acetoxy cinnamyl alcohol	-8,37	4	ARG45, LYS47, GLY46, ASN163	737
18.	<i>trans</i> -3,4-dimethoxycinnamyl alcohol	-7,05	3	ARG45, LYS47, GLY46	6850

**LAMPIRAN 12
(LANJUTAN)**

Tabel V.3
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji

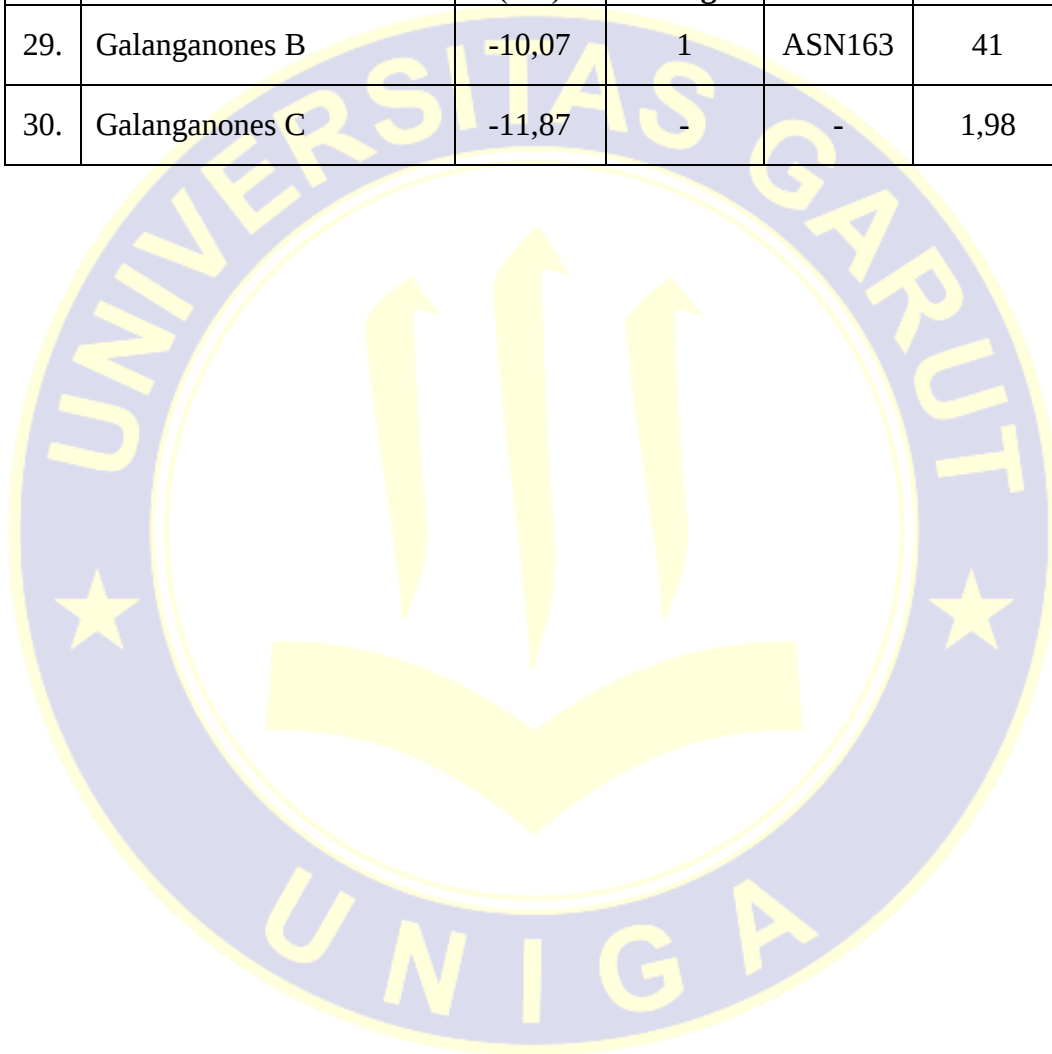
No.	Ligan/Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
19.	2-propenal, 3-[4-(acetyloxy)-3-methoxyphenyl]	-7,32	4	ASN163, LYS47, GLY46, THR48	4310
20.	1-(4-hydroxyphenyl)-1-propanone	-6,21	3	ARG45, LYS47, ALA44	28080
21.	[di-(<i>p</i> -hydroxy- <i>cis</i> -styryl)] methane	-9,20	3	LYS168, THR48, VAL217	179
22.	[di- <i>p</i> -acetoxy- <i>cis</i> -styryl)] methane	-12,33	4	ARG45, LYS47, GLY46, SER152	0,95
23.	4, 4'[(2 <i>E</i> , 2' <i>E</i>)-bis(prop-2-ene)-1,1'-oxy]-diphenyl-7,7'-diacetate	-12,66	3	ARG45, GLY46, VAL217	0,99
24.	Galanganal	-10,04	2	THR48, VAL217	43
25.	Galanganol A	-10,15	4	ALA44, LYS168, ASN163, VAL217	36
26.	Galanganol B	-10,19	4	LYS168, ASN163, THR48, VAL217	33
27.	Galanganol C	-12,69	3	LYS168, ALA44, VAL217	0,92
28.	Galanganones A	-12,57	3	LYS47, THR48, VAL217	0,99

LAMPIRAN 12
(LANJUTAN)

Tabel V.3

Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji

No.	Ligan/Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
29.	Galanganones B	-10,07	1	ASN163	41
30.	Galanganones C	-11,87	-	-	1,98



LAMPIRAN 13

UJI PREADME

Tabel V.4

Uji PreADME (Absorpsi dan Distribusi) Senyawa Turunan Fenilpropanoid dan Obat Pembeding

No.	Ligan	Absorpsi			Distribusi
		Blood Brain Barrier	Caco-2 cell (nm sec ⁻¹)	HIA (%)	Protein Plasma Binding (%)
1.	Temozolomid	0,12 ^b	20,07 ^b	64,65 ^b	58,35 ^b
2.	1'S-1'-Acetoxychavicol acetate (ACA)	0,018 ^c	44,24 ^b	98,24 ^a	74,94 ^b
3.	1'S-1'-Hydroxychavicol acetate	6,33 ^a	45,77 ^b	100 ^a	100 ^a
4.	1'S-1'-Acetoxyeugenol acetate	0,017 ^c	49,74 ^b	97,48 ^a	75,66 ^b
5.	1'S-1'-Ethoxy chavicol acetate	0,04 ^c	57,00 ^b	99,12 ^a	86,21 ^b
6.	Chavicol <i>beta</i> -D-glucopyranoside	0,08 ^c	1,43 ^c	75,34 ^a	66,07 ^b
7.	Methyleugenol	1,11 ^b	58,09 ^b	100 ^a	100 ^a
8.	<i>trans-p</i> -Hydroxycinnamaldehyde	0,69 ^b	21,29 ^b	94,71 ^a	62,87 ^b
9.	<i>trans-p</i> -Hydroxycinnamic acid	0,69 ^b	21,11 ^b	92,09 ^a	63,06 ^b
10.	<i>trans-p</i> -Hydroxycinnamaldehyde acetate	0,02 ^c	26,55 ^b	98,04 ^a	74,14 ^b
11.	<i>p</i> -Hydroxycinnamyl acetate	0,11 ^b	24,11 ^b	94,57 ^a	69,32 ^b
12.	<i>trans-p</i> -Coumaryl alcohol	1,67 ^b	21,18 ^b	89,68 ^a	39,18 ^b
13.	<i>trans-p</i> -Coumaric acid	0,69 ^b	21,11 ^b	92,09 ^a	63,06 ^b

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Uji PreADME (Absorpsi dan Distribusi) Senyawa Turunan Fenilpropanoid dan Obat Pembanding

No.	Ligan	Absorpsi			Distribusi
		Blood Brain Barrier	Caco-2 cell (nm sec ⁻¹)	HIA (%)	Protein Plasma Binding (%)
14.	<i>trans-p</i> -Coumaric diacetate	0,11 ^b	37,53 ^b	97,83 ^a	73,61 ^b
15.	(<i>E</i>)-4-Acetoxy cinnamyl ethyl ether	0,03 ^c	57,59 ^b	99,12 ^a	72,98 ^b
16.	(<i>E</i>)-4-Acetoxy cinnamyl alcohol	0,08 ^c	24,03 ^b	94,77 ^a	62,49 ^b
17.	<i>trans</i> -3,4-dimethoxycinnamyl alcohol	0,64 ^b	44,16 ^b	95 ^a	50,11 ^b
18.	2-propenal, 3-[4-(acetyloxy)-3-methoxyphenyl]	0,03 ^c	33,82 ^b	97,54 ^a	65,95 ^b
19.	1-(4-hydroxyphenyl)-1-propane	0,58 ^b	18,61 ^b	94,31 ^a	10,79 ^b
20.	[di-(<i>p</i> -hydroxy- <i>cis</i> -styryl)] methane	7,09 ^a	27,95 ^b	93,47 ^a	100 ^a
21.	[di-(<i>p</i> -acetoxy- <i>cis</i> -styryl)] methane	0,06 ^c	51,17 ^b	97,44 ^a	91,62 ^a
22.	4, 4'[(2 <i>E</i> ,2' <i>E</i>)-bis(prop-2-ene)-1,1'-oxy]-diphenyl-7,7'-diacetate	1,20 ^b	26,75 ^b	98,88 ^a	98,15 ^a
23.	Galanganal	2,85 ^a	21,71 ^b	93,52 ^a	99,03 ^a
24.	Galanganol A	1,29 ^b	20,48 ^b	85,74 ^a	82,21 ^b
25.	Galanganol B	1,29 ^b	20,48 ^b	85,74 ^a	82,21 ^b
26.	Galanganol C	3,10 ^a	21,20 ^b	87,27 ^a	85,13 ^b
27.	Galanganones A	6,99 ^a	23,00 ^b	92,59 ^a	100 ^a

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.4

Uji PreADME (Absorpsi dan Distribusi) Senyawa Turunan Fenilpropanoid dan Obat Pembanding

No.	Ligan	Absorpsi			Distribusi
		Blood Brain Barrier	Caco-2 cell (nm sec ⁻¹)	HIA (%)	Protein Plasma Binding (%)
28.	Galanganones B	8,54 ^a	25,67 ^b	93,31 ^a	100 ^a
29.	Galanganones C	8,84 ^a	29,99 ^b	94,69 ^a	100 ^a

Klasifikasi: BBB: >2,0 *high absorption to CNS* (a), 0,1-2,0 *middle absorption to CNS* (b), <0,1 *low absorption to CNS* (c); *In Vitro Caco-2 cell permeability* (nm sec⁻¹): >70 *higher permeability* (a), 4-70 *medium permeability* (b), <4 *low permeability* (c); %*human intestinal absorption* (%HIA): 70-100% *well absorbed* (a), 20-70% *moderately absorbed* (b), 0-20% *poorly absorbed* (c); %*plasma protein binding*: >90% *strongly bound* (a), <90% *weakly bound* (b).

LAMPIRAN 14

UJI TOKSISITAS

Tabel V.5

Uji Toksisitas Senyawa Turunan Fenilpropanoid dan Obat Pembanding

No.	Ligan	Mutagenik	Karsinogenik
1.	Temozolomid	Mutagen	Positif
2.	1'S-1'-Acetoxychavicol acetate (ACA)	Mutagen	Positif
3.	1'S-1'-Hydroxychavicol acetate	Mutagen	Positif
4.	1'S-1'-Acetoxyeugenol acetate	Mutagen	Positif
5.	1'S-1'-Ethoxy chavicol acetate	Mutagen	Negatif
6.	Chavicol <i>beta</i> -D-glucopyranoside	Mutagen	Negatif
7.	Methyleugenol	Mutagen	Positif
8.	<i>trans</i> - <i>p</i> -Hydroxycinnamaldehyde	Mutagen	Negatif
9.	<i>trans</i> - <i>p</i> -Hydroxycinnamic acid	Mutagen	Positif
10.	<i>trans</i> - <i>p</i> -Hydroxycinnamaldehyde acetate	Mutagen	Positif
11.	<i>p</i> -Hydroxycinnamyl acetate	Mutagen	Negatif
12.	<i>trans</i> - <i>p</i> -Coumaryl alcohol	Mutagen	Negatif
13.	<i>trans</i> - <i>p</i> -Coumaric acid	Mutagen	Positif
14.	<i>trans</i> - <i>p</i> -Coumaric diacetate	Mutagen	Negatif
15.	(<i>E</i>)-4-Acetoxy cinnamyl ethyl ether	Mutagen	Negatif
16.	(<i>E</i>)-4-Acetoxy cinnamyl alcohol	Mutagen	Negatif

**LAMPIRAN 14
(LANJUTAN)**

Tabel V.5
Uji Toksisitas Senyawa Turunan Fenilpropanoid dan Obat Pembanding

No.	Ligan	Mutagenik	Karsinogenik
17.	<i>trans</i> -3,4-dimethoxycinnamyl alcohol	Mutagen	Negatif
18.	2-propenal, 3-[4-(acetyloxy)-3-methoxyphenyl]	Mutagen	Positif
19.	1-(4-hydroxyphenyl)-1-propane	Mutagen	Negatif
20.	[di-(<i>p</i> -hydroxy- <i>cis</i> -styryl)] methane	Mutagen	Negatif
21.	[di-(<i>p</i> -acetoxy- <i>cis</i> -styryl)] methane	Mutagen	Positif
22.	4, 4'[(2 <i>E</i> ,2' <i>E</i>)-bis(prop-2-ene)-1,1'-oxy]-diphenyl-7,7'-diacetate	Mutagen	Negatif
23.	Galanganal	Non-mutagen	Negatif
24.	Galanganol A	Non-mutagen	Negatif
25.	Galanganol B	Non-mutagen	Negatif
26.	Galanganol C	Non-mutagen	Negatif
27.	Galanganones A	Non-mutagen	Positif
28.	Galanganones B	Non-mutagen	Positif