

## DAFTAR PUSTAKA

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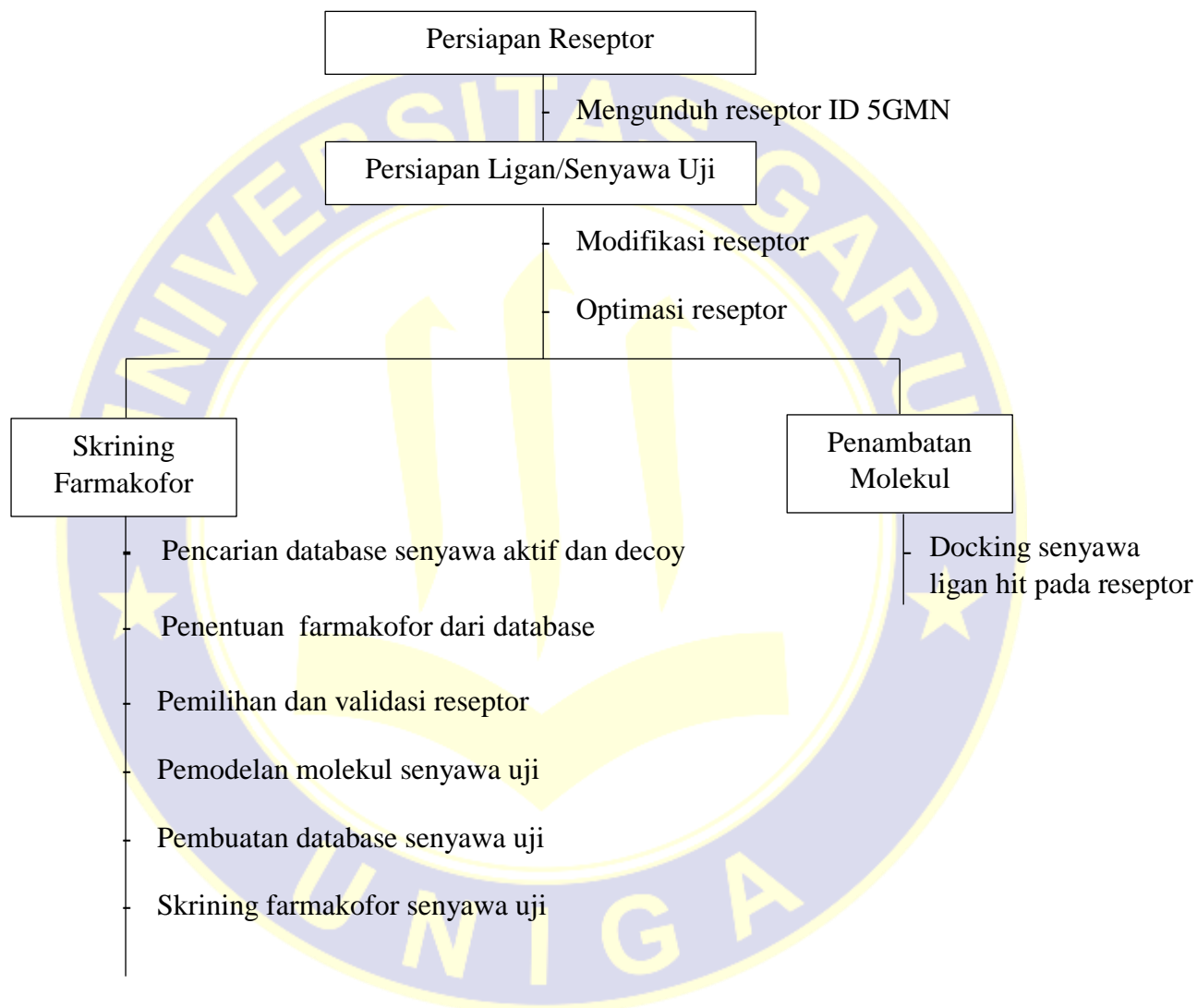
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## LAMPIRAN 1

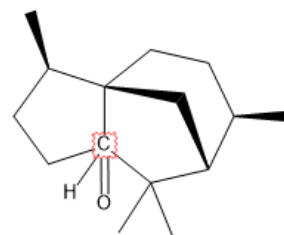
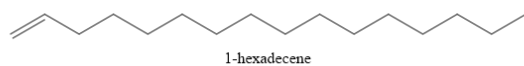
### ALUR PENELITIAN SKRINING FARMAKOFOR

### DAN PENAMBATAN MOLEKUL



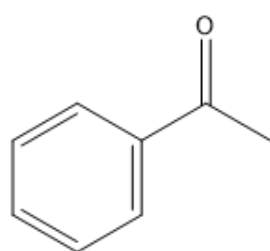
## LAMPIRAN 2

## SENYAWA UJI

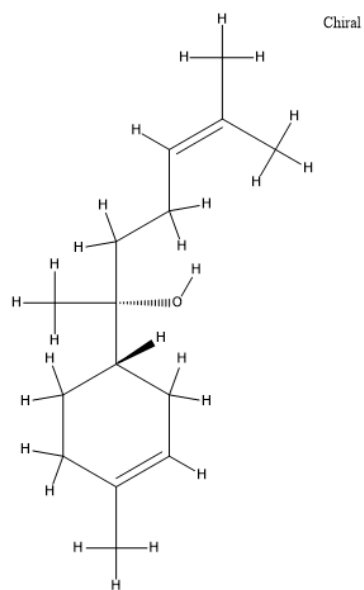


5-cedranone

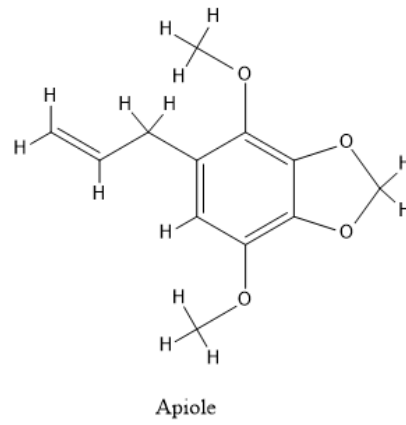
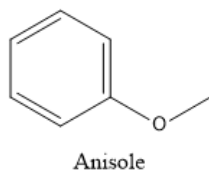
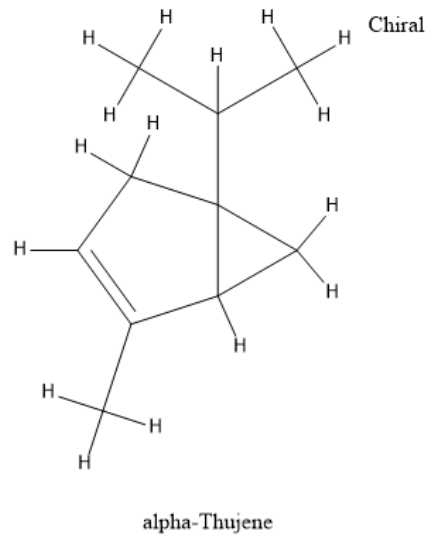
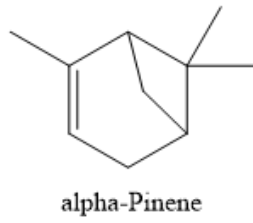
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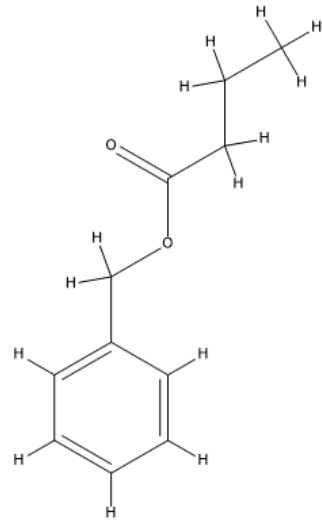
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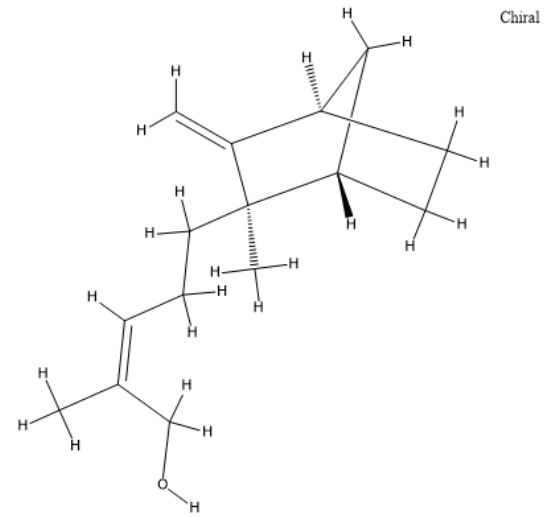
alpha-bisabolol

**LAMPIRAN 2  
(LANJUTAN)**

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(LANJUTAN)**

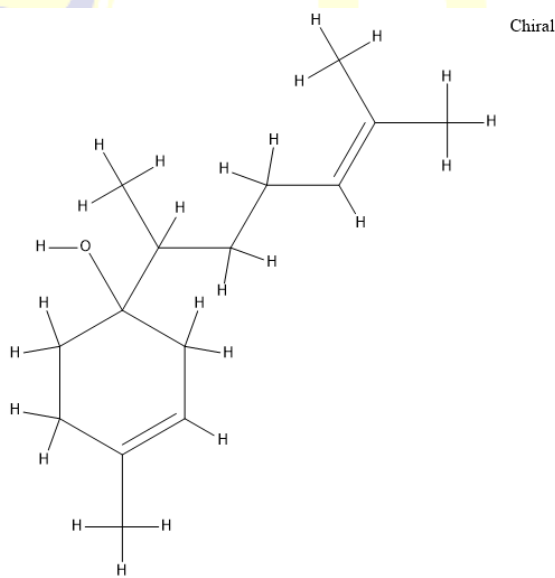


Benzyl butyrate



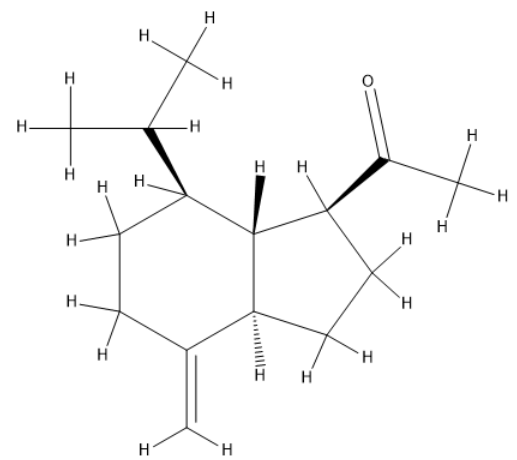
Chiral

beta cis santalol



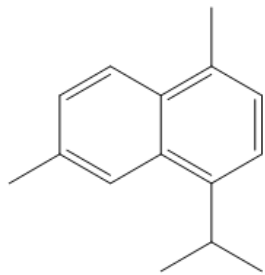
Chiral

beta-Bisabolol

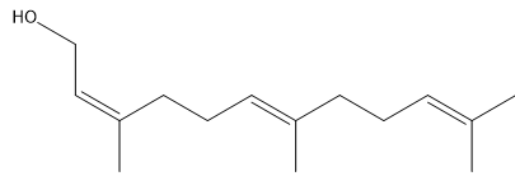


Chiral

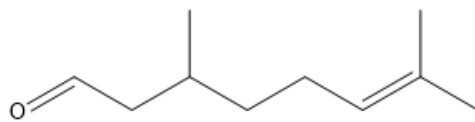
beta-Oplopenone

**LAMPIRAN 2  
(LANJUTAN)**

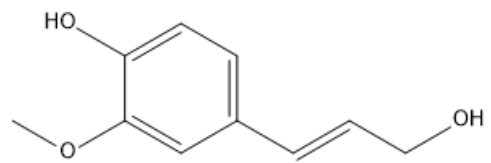
Cadalene



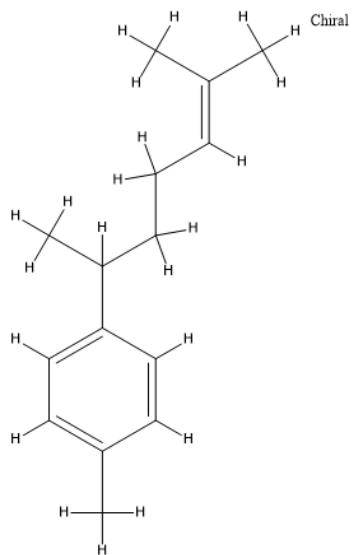
cis-farnesol



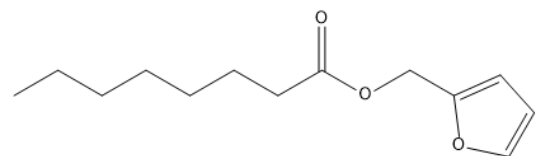
Citronellal



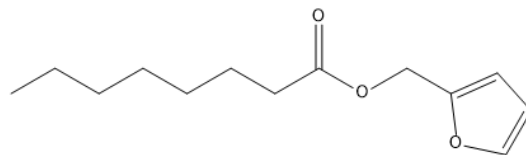
coniferyl alcohol



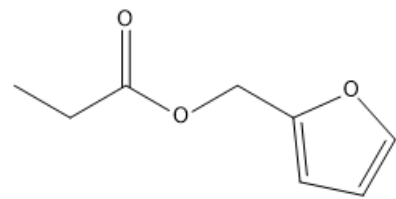
Curcumene



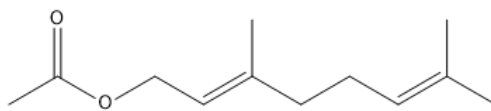
furfuryl octanoate

**LAMPIRAN 2  
(LANJUTAN)**

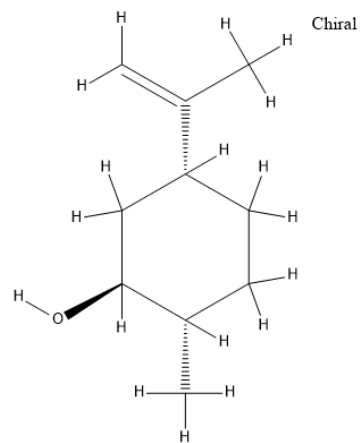
furfuryl octanoate



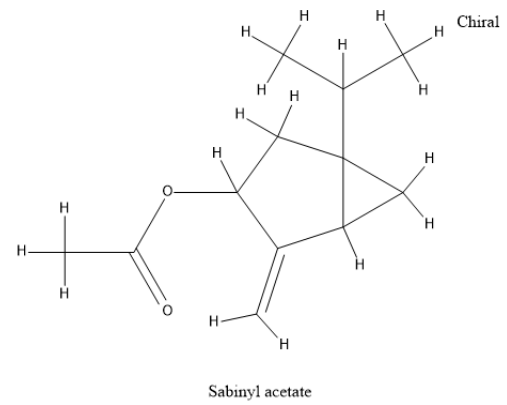
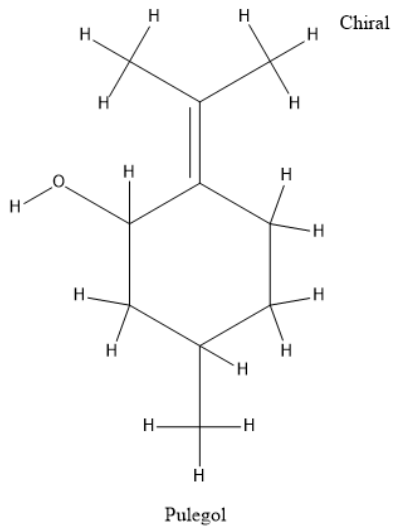
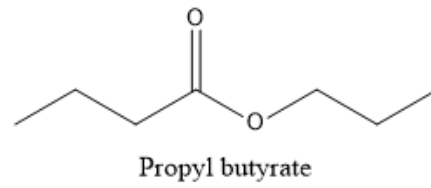
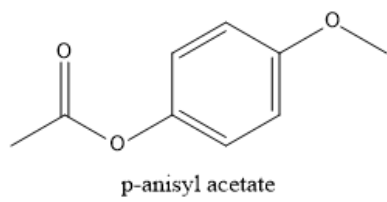
Furfuryl propionate



Geranyl acetate



Iso-dihydrocarveol

**LAMPIRAN 2  
(LANJUTAN)**

UNIGA

**LAMPIRAN 2  
(LANJUTAN)**



Tridecanol



## LAMPIRAN 3

**Tabel V.1**  
 Hasil Sifat Ligan Berdasarkan Aturan *Lipinski's Rule Of Five*

No	Senyawa/Ligan Uji	Donor Hidrogen <5	Akseptor Hidrogen <10	Bobot molekul	Log P	Memenuhi/Tidak Memenuhi Syarat
1.	1-hexadecene	0	0	224,432	6,2	Tidak Memenuhi
2.	5-cedranone	0	1	220,356	3,6	Memenuhi
3.	Acetophenone	0	1	120,151	1,6	Memenuhi
4.	Alpha-bisabolol	1	1	222,372	4,2	Memenuhi
5.	Alpha-Pinene	0	0	136,238	2,9	Memenuhi
6.	Alpha-Thujene	0	0	136,238	2,9	Memenuhi
7.	Anisole	0	1	108,140	1,6	Memenuhi
8.	Apiole	0	2	222,240	3,0	Memenuhi
9.	Benzyl butyrate	0	1	178,231	2,2	Memenuhi
10.	Beta-Bisabolol	1	1	222,372	4,2	Memenuhi
11.	Beta-Oplophenone	1	1	220,356	3,8	Memenuhi
12.	Cadalene	0	0	198,309	4,5	Memenuhi
13.	Cis-farnesol	1	1	222,372	4,3	Memenuhi
14.	Citronellal	0	1	154,253	2,9	Memenuhi
15.	Coniferyl alcohol	2	3	180,203	1,4	Memenuhi
16.	Curcumene	0	0	202,341	4,8	Memenuhi
17.	Ethyl vanillin	1	3	166,176	1,6	Memenuhi
18.	Furfuryl octanoate	0	1	224,300	3,9	Memenuhi
19.	Furfuryl propionate	0	1	154,165	1,4	Memenuhi
20.	Geranyl acetate	0	1	196,290	3,2	Memenuhi
21.	Iso-dihydrocarveol	1	1	154,253	2,3	Memenuhi

## LAMPIRAN 3

(LANJUTAN)

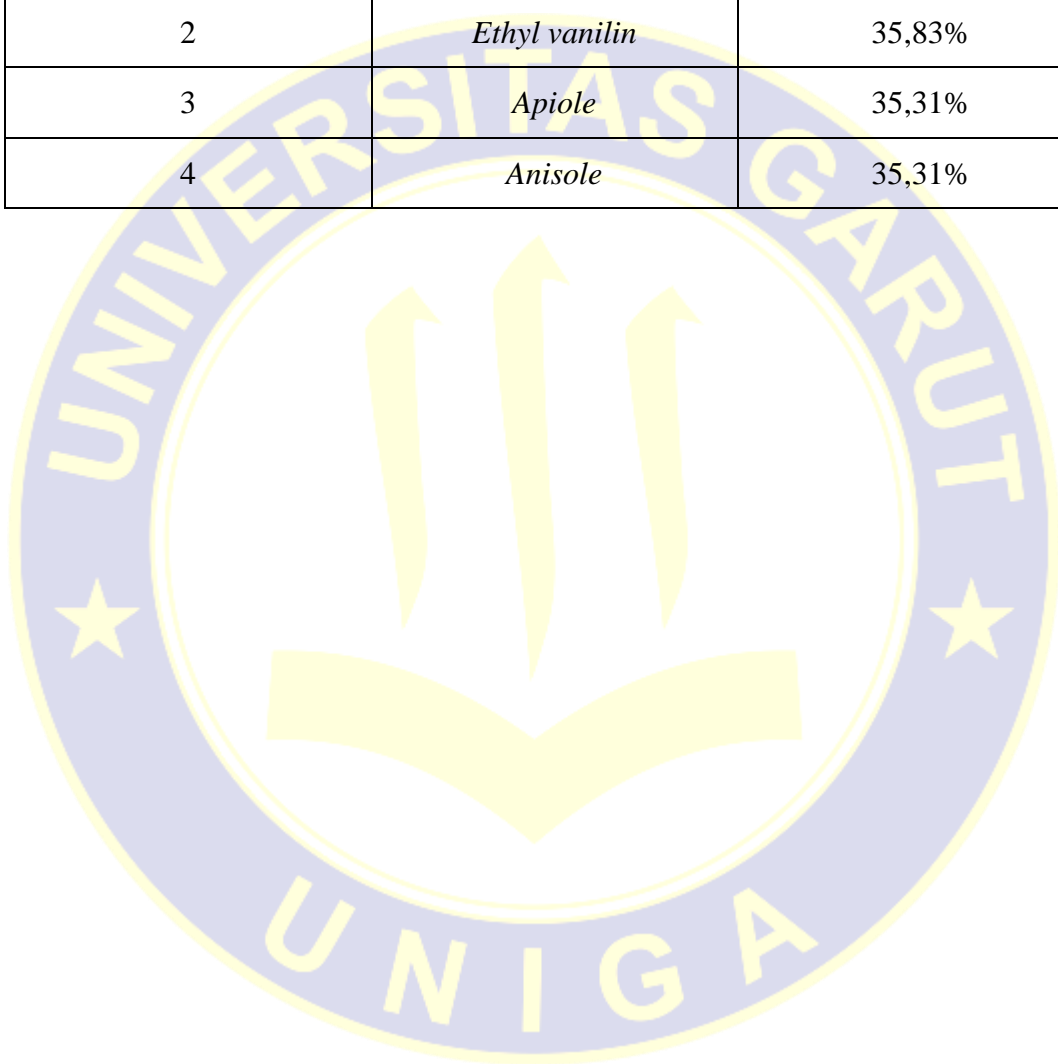
Tabel V.1  
Lanjutan

No	Senyawa/Ligan Uji	Donor Hidrogen <5	Akseptor Hidrogen <10	Bobot molekul	Log P	Memenuhi/Tidak Memenuhi Syarat
22.	Oplopanone	1	2	238,371	3,0	Memenuhi
23.	P-anisyl acetate	1	2	180,203	1,4	Memenuhi
24.	Propyl butyrate	0	1	130,187	1,7	Memenuhi
25.	Pulegol	1	1	154,253	2,5	Memenuhi
26.	Sabinyl acetate	0	1	194,274	2,5	Memenuhi
27.	Trans-farnesol	1	1	222,372	4,3	Memenuhi
28.	Tridecanol	1	1	200,366	1,7	Memenuhi

**LAMPIRAN 4**

**Tabel V.2**  
Hasil Skrining Senyawa Uji

<b>No</b>	<b>Senyawa</b>	<b>Fit Score</b>
1	<i>Conyferyl alcohol</i>	36,83%
2	<i>Ethyl vanilin</i>	35,83%
3	<i>Apiole</i>	35,31%
4	<i>Anisole</i>	35,31%



## LAMPIRAN 5

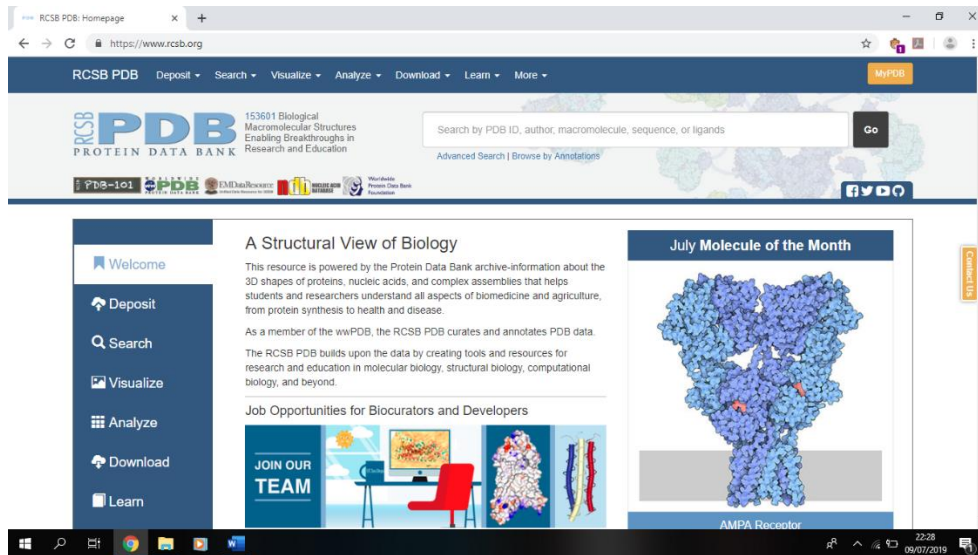
**Tabel V.3**  
Validasi Penambatan Ulang Ligan Polmacoxib Pada Sisi Aktif Enzim  
*Cyclooxygenase-2 (COX-2)*

SENYAWA	INTERAKSI HIDROGEN	INTERAKSI HIDROFOBIAK	RM SD (Å)	ΔG (kkal /mol)
Ligan Standar (Polmacoxib)	HOH598A HOH604A HOH576A THR198A	LEU197A THR199A VAL121A LEU140A VAL134A ILE91A PHE130A	2,4	-8,50
Ligan Pembanding (Celecoxib)	HOH598A THR198A THR199A	LEU203A VAL134A PHE130A ILE91A VAL121A LEU197A EU203A	6,56	-8,20

## LAMPIRAN 6

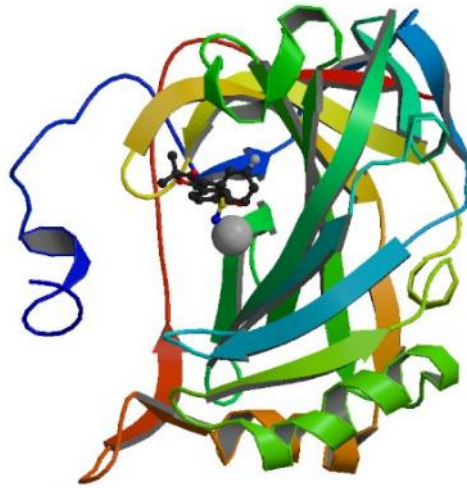
**Tabel V.4**  
Hasil Simulasi Docking

NO	SENYAWA	$\Delta G$ (kcal/mol)	INTERAKSI	Ki ( $\mu M$ )
1.	Celecoxib	-7,30	Ikatan Hidrogen : THR198A, THR199A, HOH576A Ikatan Hidrofobik: PHE130A, LEU140A, ILE91A, VAL121A, LEU197A	4,42
2.	Conyferyl Alcohol	- 6,10	Ikatan Hidrogen : THR198A, THR199A Ikatan Hidrofobik: LEU197A, LEU140A, VAL121A, VAL142A	3,36
3.	Ethyl Vanilin	-4,90	Ikatan Hidrogen : THR198A, HOH604A, HOH576A Ikatan Hidrofobik: LEU140A, VAL121A, THR199A, LEU197A	2,54
4.	Apiole	-5,70	Ikatan Hidrogen : THR198A, THR199A Ikatan Hidrofobik: LEU197A, VAL121A	6,60
5.	Anisole	-5,80	Ikatan Hidrogen : THR198A, THR199A, HOH598A Ikatan Hidrofobik: VAL121A, LEU197A	5,57

**LAMPIRAN 7****SITUS RSCB *PROTEIN DATA BANK*****Gambar IV.1** Situs RSCB *protein data bank*

**LAMPIRAN 8****STRUKTUR CYCLOOXYGENASE-2 (COX-2) (PDB ID: 5GMN)**

x

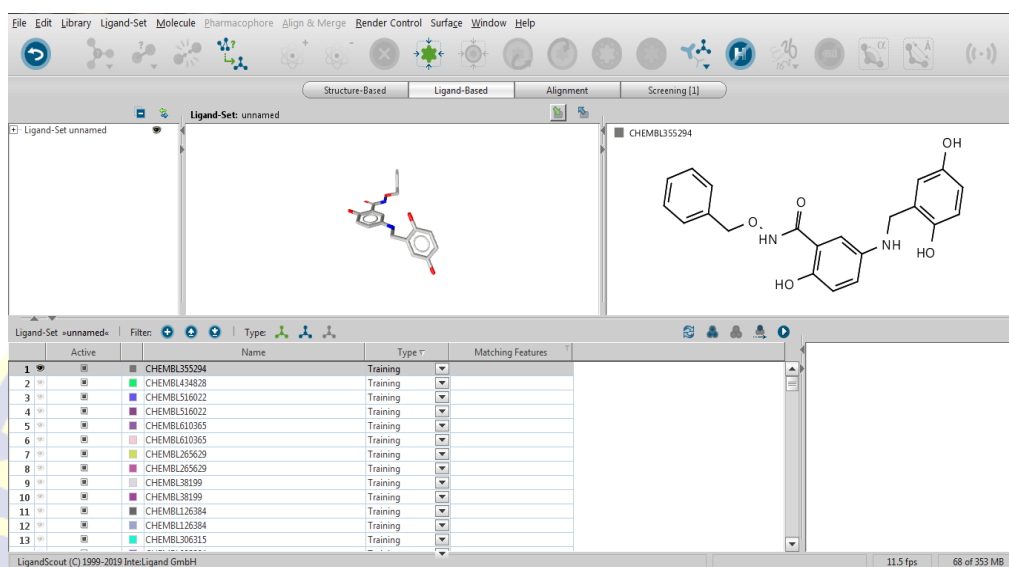


**Gambar V.2** Struktur Cyclooxygenase-2 (COX-2) (PDB ID: 5GMN)

[ Sumber: diunduh dari <http://www.rcsb.org/structure/5GMN> ]

## LAMPIRAN 9

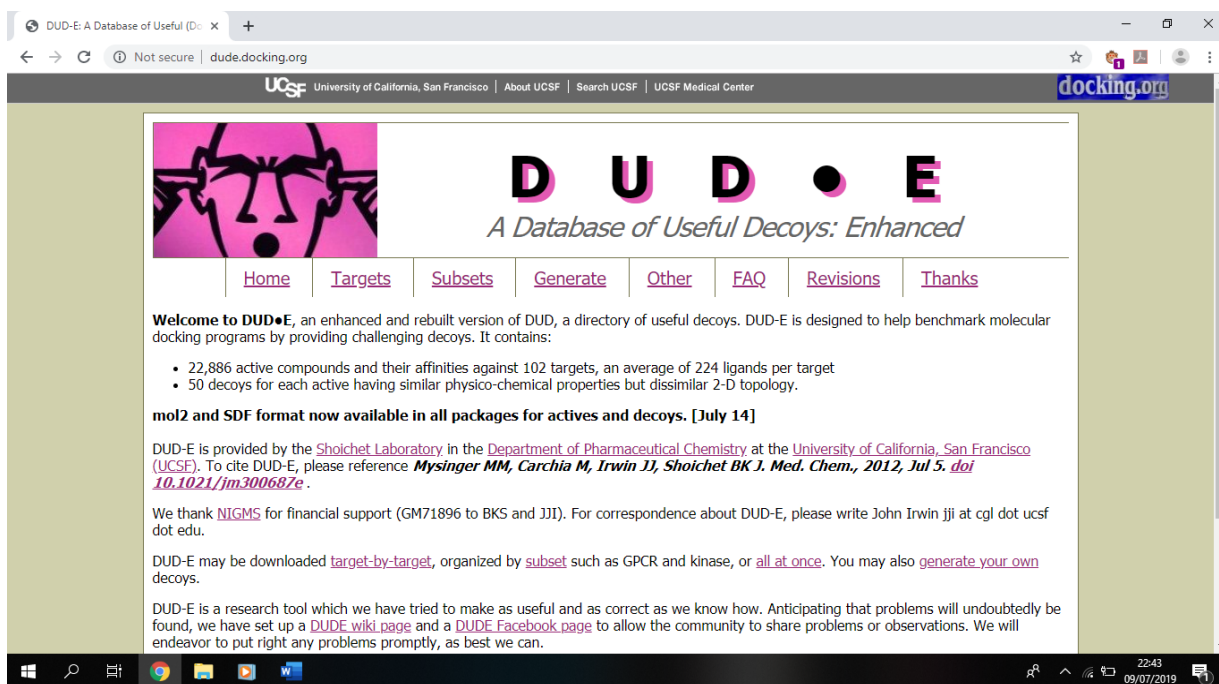
### APLIKASI LIGANDSCOUT



Gambar IV.3 Aplikasi *LigandScout*

## LAMPIRAN 10

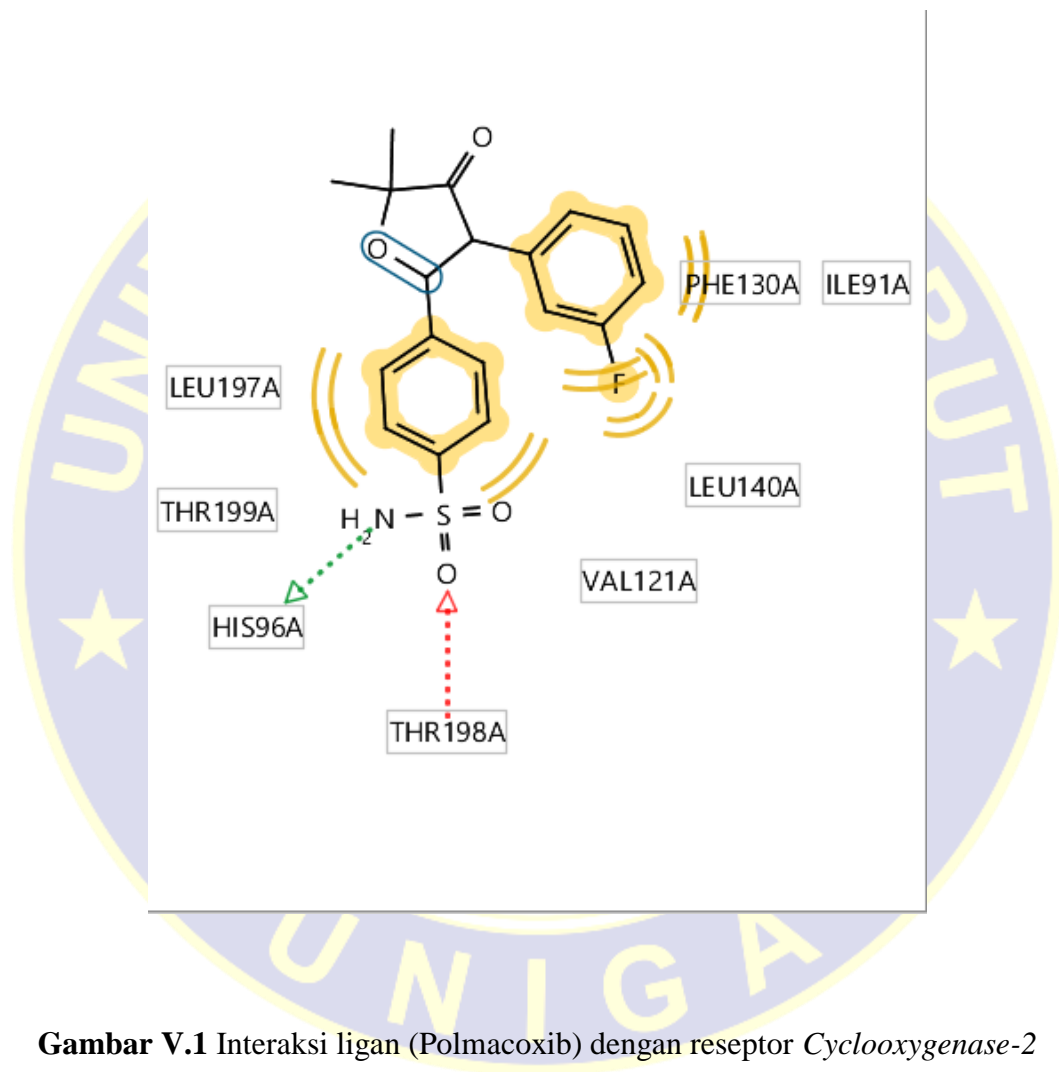
## SITUS DUD.E



Gambar IV.4 Situs Dud.e

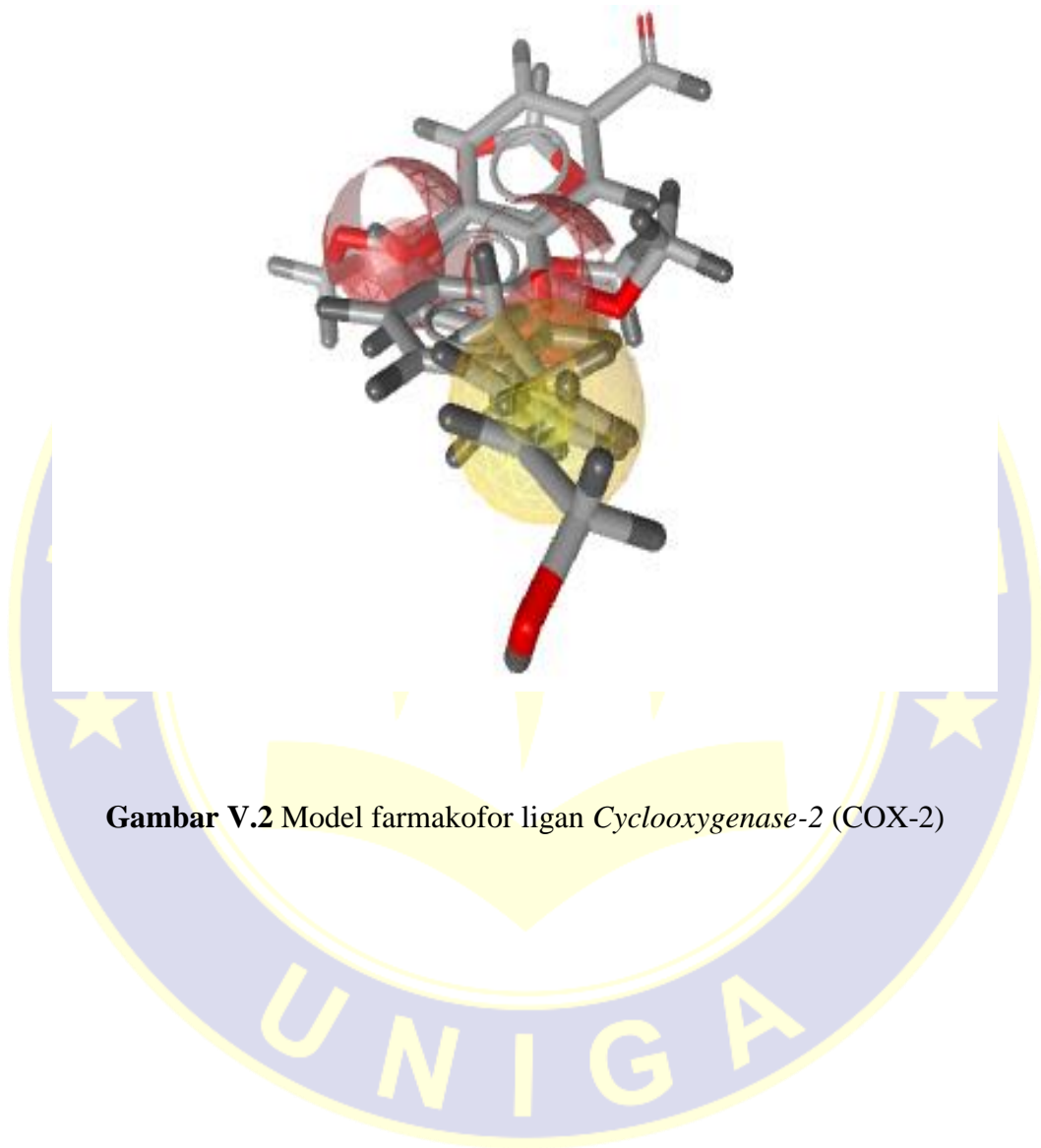
## LAMPIRAN 11

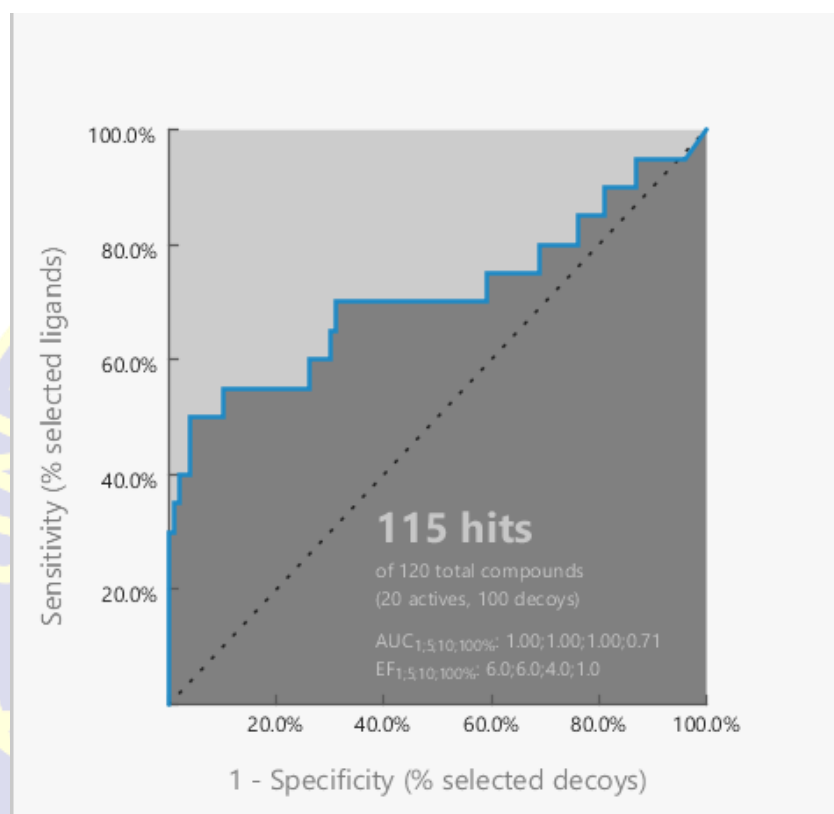
## INTERAKSI LIGAN (POLMACOXIB) DENGAN RESEPTOR

*CYCLOOXYGENASE-2 (COX-2)*

**Gambar V.1** Interaksi ligan (Polmacoxib) dengan reseptor *Cyclooxygenase-2* (COX-2)

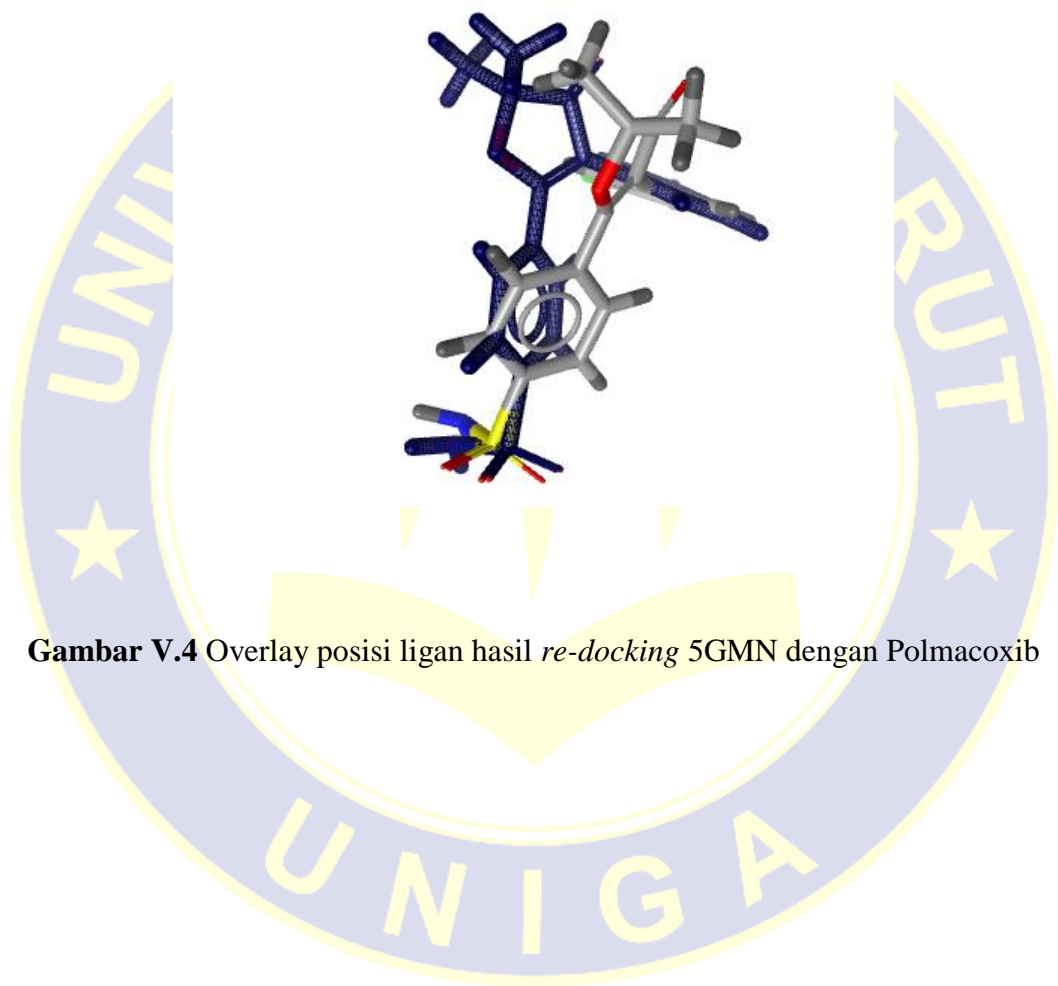
## LAMPIRAN 12

MODEL FARMAKOFOR LIGAN *CYCLOOXYGENASE-2* (COX-2)

**LAMPIRAN 13****ROC CURVE****Gambar V.3 ROC Curve**

[ Divisualisasi menggunakan *LigandScout 4.4* ]

**LAMPIRAN 14**  
**OVERLAY POSISI LIGAN HASIL *RE-DOCKING* 5GMN DENGAN**  
**POLMACOXIB**



**Gambar V.4** Overlay posisi ligan hasil *re-docking* 5GMN dengan Polmacoxib

**DAFTAR RIWAYAT HIDUP**

1. Nama : Dwi Damia Khoirunnisa
2. Tempat, Tanggal Lahir : Garut, 16 Mei 1996
3. Jenis Kelamin : Perempuan
4. Alamat : Perum Bumi Cimanganten Asri blok G5:02,  
Kec. Tarogong Kaler, Kel. Rancabango, Kab.  
Garut, Prov. Jawa Barat, Indonesia
5. Nama Orang Tua
  - a. Ayah : Sumardin S.Pd, M.Pd (Alm)
  - b. Ibu : Yayah S.Pd.I
6. Saudara Kandung : Pratiwi Nurul Khojimah (Kakak)  
Tri Abdillah Kamal Arramadhan (Adik)
7. Riwayat Pendidikan
  - a. Sekolah Dasar : SDIT Persis Tarogong Garut (2002-2008)
  - b. SMP/Sederajat : Pondok Pesantren Darussalam Garut (2008-2011)
  - c. SMA/Sederajat : MAN 1 Garut (2011-2014)
  - d. Perguruan Tinggi : Universitas Garut (2015-2020)