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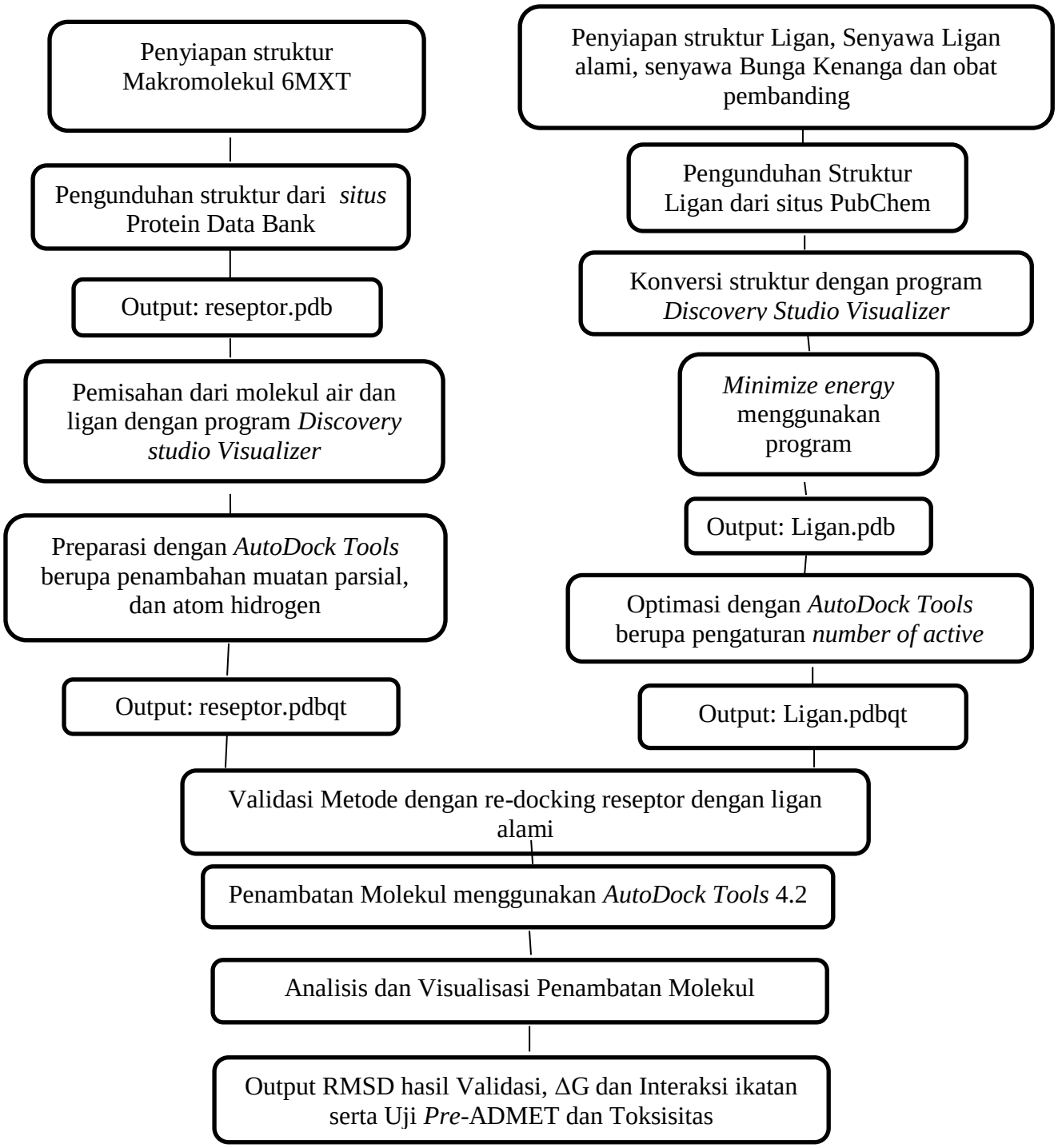
LAMPIRAN 1

ALUR PENELITIAN



Gambar V.1 Alur penelitian

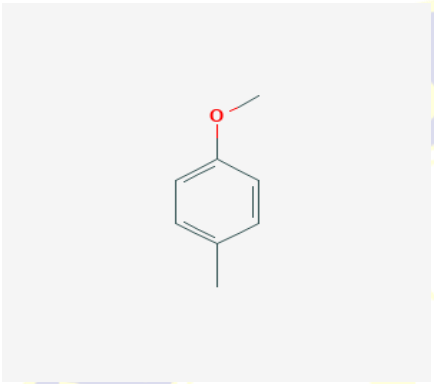
LAMPIRAN 2

TANAMAN BUNGA KENANGA (*Canangium odorata(Lam) hook.F. & Thomson)*

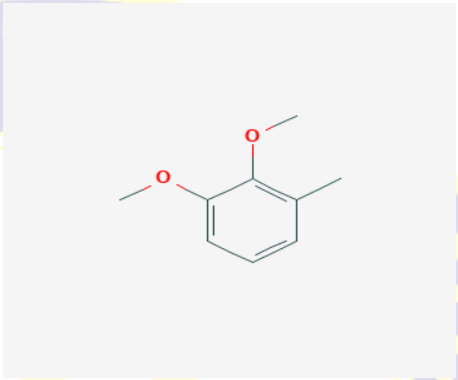
Gambar V.2 Tanaman bunga kenanga

LAMPIRAN 3

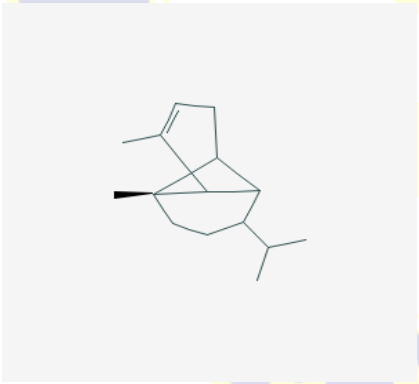
SENYAWA BUNGA KENANGA



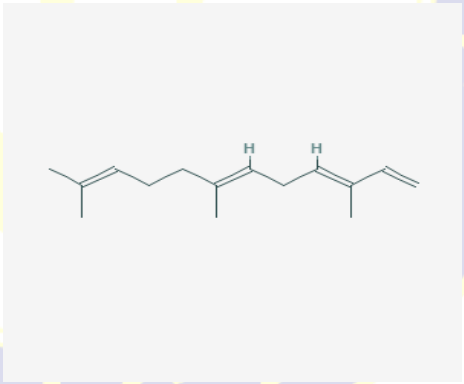
1-methoxy-4-methylbenzene



2,3-dimethoxytoluen



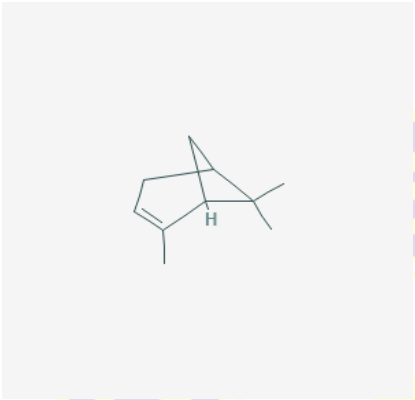
Alpha copaene



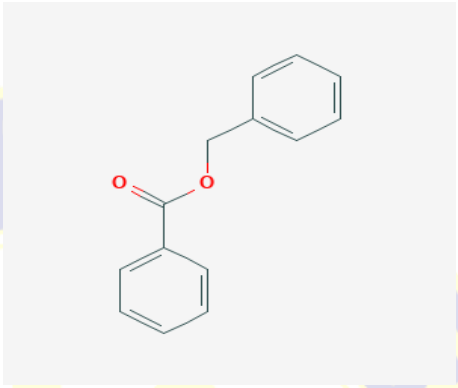
Alpha farnesene

LAMPIRAN 3

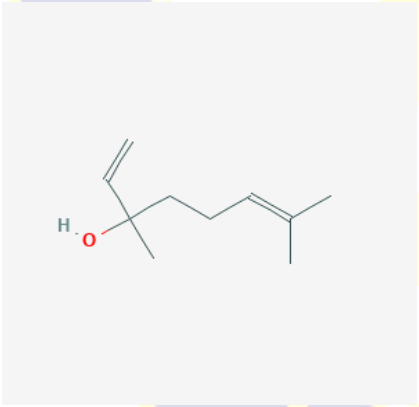
LANJUTAN 1



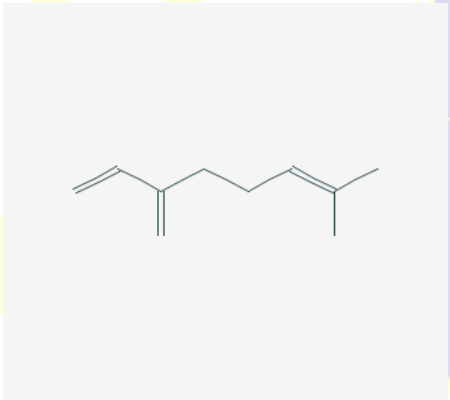
Alpha pinene



Benzyl benzoate



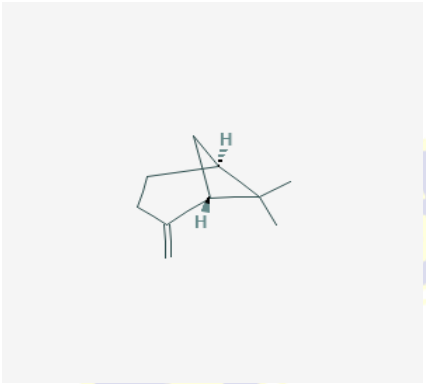
Beta linalool



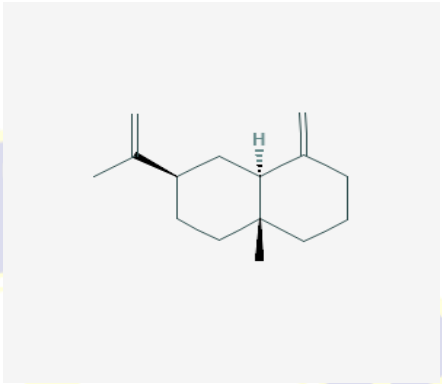
Beta myrcene

LAMPIRAN 3

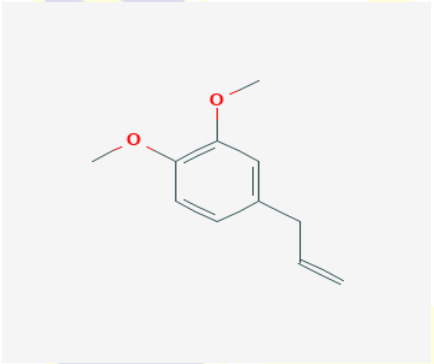
LANJUTAN 2



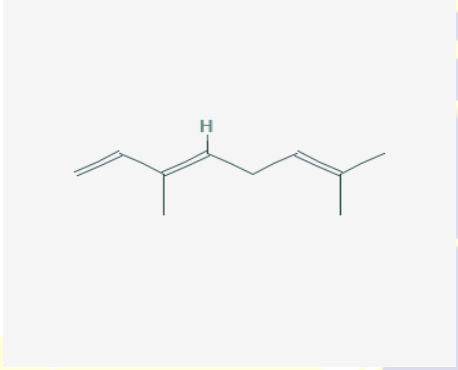
Beta pinene



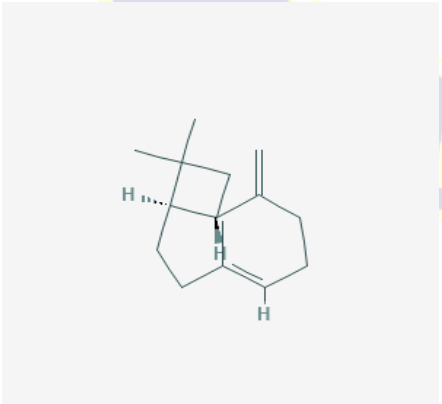
Beta silenene



Methyleugenol



Transbetaocimen



Trans-caryophyllene

Gambar V.3 Struktur 2D senyawa bunga kenanga

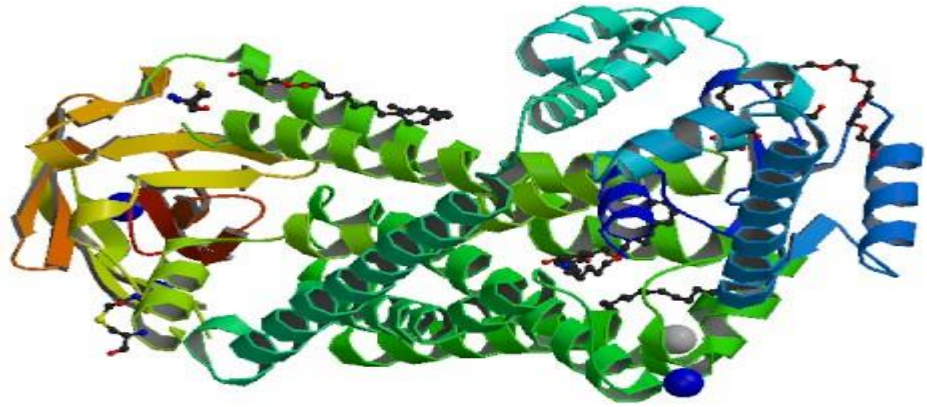
LAMPIRAN 4

SITUS *PROTEIN DATA BANK*

Gambar V.4 Program situs *protein data bank*

LAMPIRAN 5

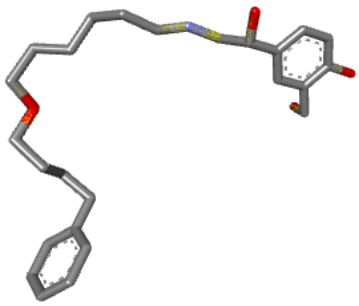
STRUKTUR 3D RESEPTOR



Gambar V.5 Struktur 3D reseptor Salmeterol (6MXT)

LAMPIRAN 6

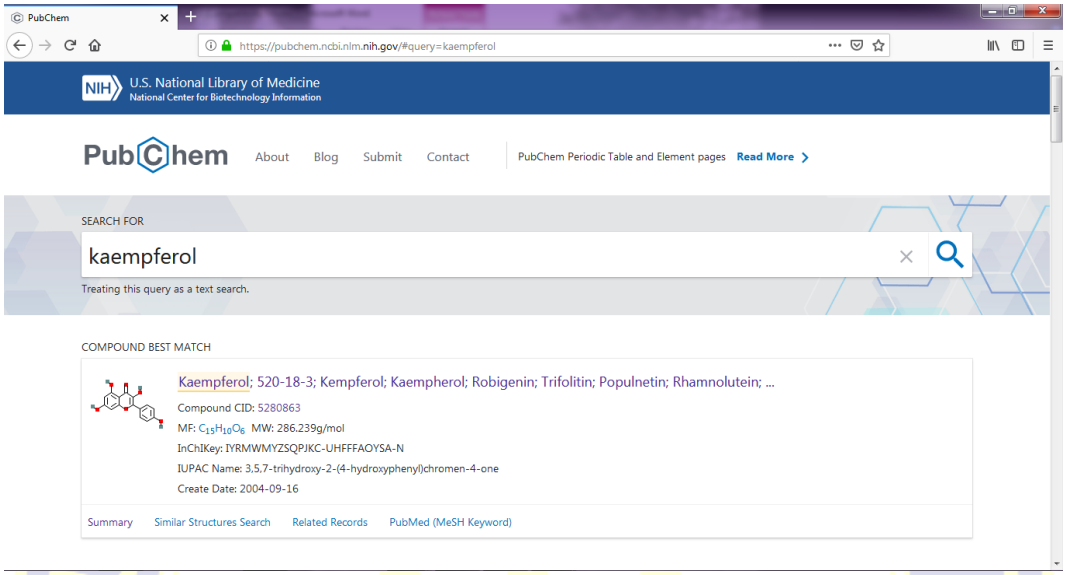
LIGAN ALAMI 6MXT



Gambar V.6 Ligan alami dari reseptor 6MXT

LAMPIRAN 7

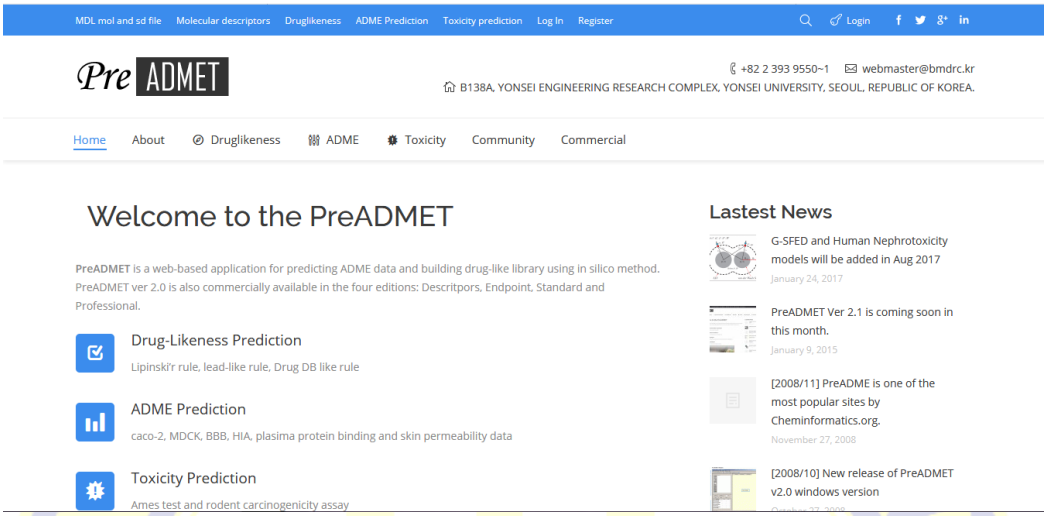
SITUS PUBCHEM



Gambar V.7 Situs pubchem

LAMPIRAN 8

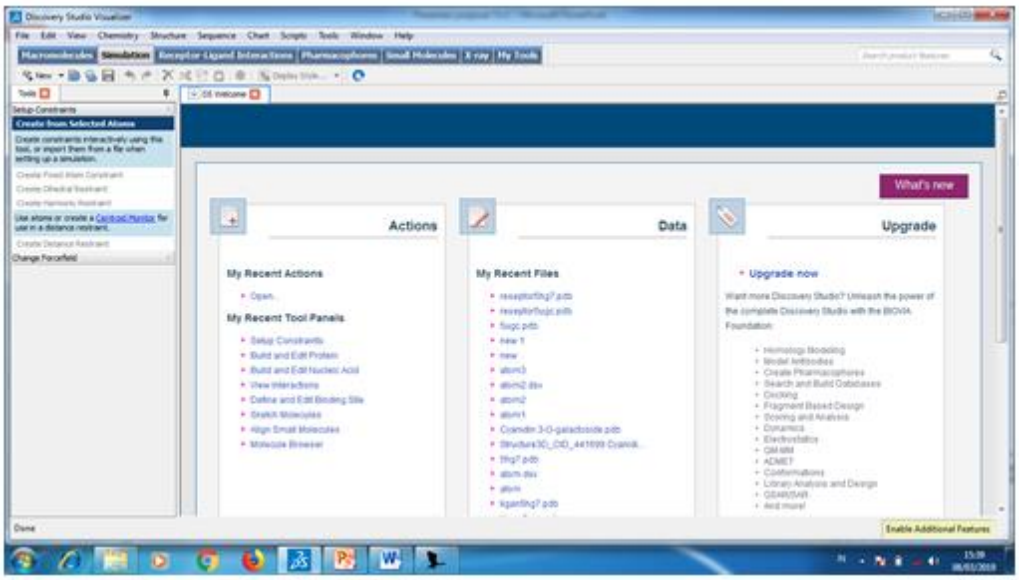
SITUS PRE-ADMET



Gambar V.8 Situs preADMET

LAMPIRAN 9

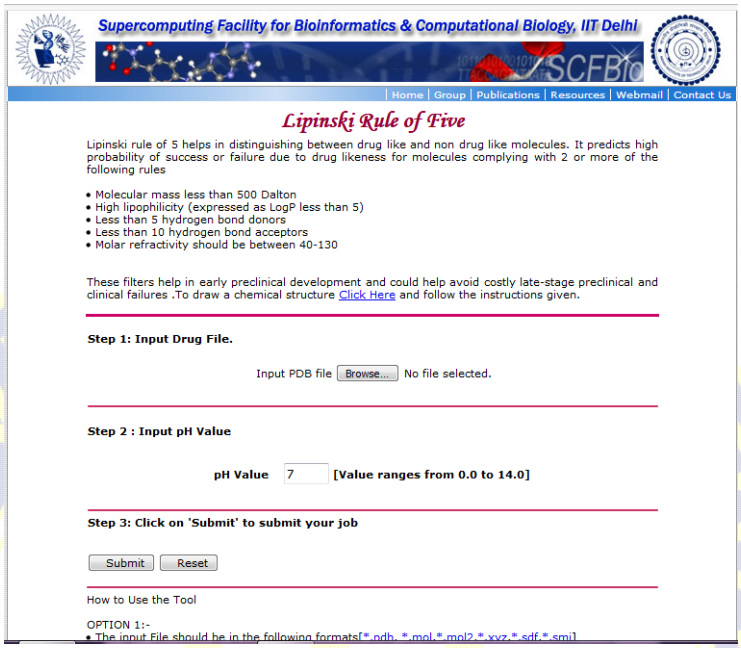
PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER



Gambar V.9 Tampilan program Discovery Studio Visualizer

LAMPIRAN 10

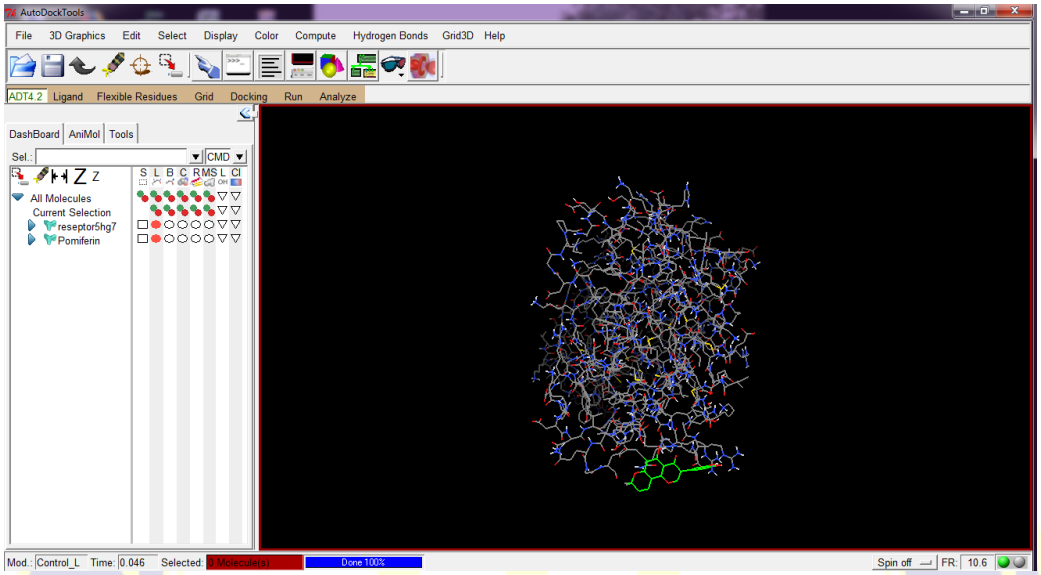
SITUS LIPINSKI'S RULE OF FIVE



Gambar V.10 Situs lipinski's rule of five

LAMPIRAN 11

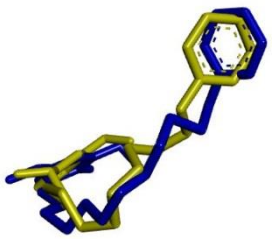
PERANGKAT LUNAK AUTODOCK TOOLS



Gambar V.11 Tampilan program Autodock Tools

LAMPIRAN 12

VALIDASI METODE



Gambar V.12 Visualisasi tumpang tindih ligan alami 6MXT (biru) dengan ligan hasil *redocking* (kuning)

Tabel V.1
Grid Box, RMSD, Nilai Ikatan Energi, dan Validasi Metode Ligan Alami

Kode PDB	Grid Box	RMSD	Ikatan Energi Salbutamol (kkal/mol)	Ikatan Energi Ligan Alami (kkal/mol
6MXT	X: -9,426 Y: -3,116 Z: 38,18	1,051 Å	-8,50	-10,33

LAMPIRAN 13
SIFAT FISIKOKIMIA 5 LIPINSKI

Tabel V.2
Sifat Fisikokimia Senyawa Bunga Kenanga Berdasarkan Aturan 5 Lipinski

No.	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	AkseptorHidrogen	Refractory Molar	Ket
1	1-metoksi-4-metil benzene	122	2	0	1	40,73	Memenuhi
2	2,3-dimetoxytoluen	152	2,01	0	2	44,28	Memenuhi
3	Alpha Copaene	220	3,38	1	1	65,97	Memenuhi
4	Alpha Farnesene	204	5,2	0	0	70,99	Memenuhi
5	Alpha Pinene	136	2,99	0	0	43,75	Memenuhi
6	Benzil Benzoat	121	3,04	0	2	62	Memenuhi
7	Beta linalool	154	2,66	1	1	49,48	Memenuhi
8	Beta Mircen	136	3,47	0	0	48	Memenuhi
9	Beta Pinene	136	2,99	0	0	43,75	Memenuhi
10	Beta Silenene	204	4,72	0	0	66,74	Memenuhi
11	Metil Eugenol	194	1,64	0	3	52,98	Memenuhi
12	Trans Beta Ocimen	136	3,47	0	0	48	Memenuhi
13	Trans Cariopilene	204	4,72	0	0	66,74	Memenuhi

Syarat : 1. BM <500 mg/mol
2. Log P <5
3. Donor Hidrogen <5
4. Akseptor Hidrogen <10
5. *Molar Refrectory* antara 40-130

LAMPIRAN 14

HASIL PENAMBATAN MOLEKUL

Tabel V.3

Hasil Penambatan Molekuler Senyawa Bunga Kenanga (6MXT)

No.	Ligan	ΔG (kkal/mol)	Konstanta inhibisi (nM)
1	Ligan alami	-10,33	26,98
2	Salbutamol	-8,50	583,50
3	1-methoxy-4-methylbenzene	-4,76	322230
4	2,3-dimethoxytoluen	-4,68	370240
5	Alpha copaene	-7,72	2180
6	Alpha farnesene	-6,93	8370
7	Alpha pinene	-5,72	64430
8	Benzyl benzoate	-7,30	4460

LAMPIRAN 14
(LANJUTAN)

No.	Ligan	ΔG (kkal/mol)	Konstanta inhibisi (nM)
9	Beta linalool	-5,52	90660
10	Beta myrcene	-4,94	239170
11	Beta pinene	-5,68	68060
12	Beta silenene	-7,63	2540
13	Methyleugenol	-5,23	146990
14	Transbetaocimen	-5,17	162060
15	Trans-caryophyllene	-6,87	9250

LAMPIRAN 15

INTERAKSI IKATAN HIDROGEN DAN RESIDU ASAM AMINO

Tabel V.4

Hasil Analisis Ikatan Hidrogen dan Residu Asam Amino yang Terlibat (6MXT)

No.	Senyawa	Jumlah ikatan hidrogen	Residu asam amino
1	Ligan alami	6 (ASP1113,ASP1192, ASN1312, SER1207, SER1203,PHE1193)	VAL1117, VAL1114, TYR1306,ASP1192, PHE1290, HIS1206
2	Salbutamol	6 (ASP1113, ASN1312, ASN1293, SER1203, SER1207, TYR1316)	VAL1114, PHE1193, PHE1290
3	1-methoxy-4-methylbenzene	1 (SER1207)	VAL1117, VAL1114, ALA1200, SER1204, SER1203, THR1195, THR1118, TYR1199, PHE1193, PHE1290, ASN1293

LAMPIRAN 15

(LANJUTAN)

No.	Senyawa	Jumlah ikatan hidrogen	Residu asam amino
4	2,3-dimethoxytoluen	0	VAL1117, VAL1114, ALA1200, SER1204, SER1203, THR1195
5	Alpha copaene	0	VAL1117, VAL1114, ALA1200, TYR119, TYR1308, PHE1193, PHE 1289, PHE 1290
6	Alpha farnesene	0	THR1110, TYR1308, VAL1114, HIS1093
7	Alpha pinene	0	SER1203, SER1204, SER1207, ASN1293, ALA1200, VAL1114
8	Benzyl benzoate	1 (ASN1312)	THR1110, THR1118, TRP1109, VAL1114, VAL1117
9	Beta linalool	2 (ASP1113, ASN1312)	SER1203, SER1204,

LAMPIRAN 15

(LANJUTAN)

No.	Senyawa	Jumlah ikatan hidrogen	Residu asam amino
10	Beta myrcene	0	SER1203, SER1204
11	Beta pinene	0	SER1203, SER1207
12	Beta silenene	0	SER1203, SER1204, SER1207, ASN1293
13	Methyleugenol	0	SER1203, ASN1312
14	Transbetaocimen	0	ASN1312, ASP1113
15	Trans-caryophyllene	0	ASP1113

LAMPIRAN 16

UJI PREADME

Tabel V.5

Uji PreADME (Absorpsi dan Distribusi) Senyawa Bunga Kenanga dan Obat Pembanding

No	Senyawa	Caco-2 (nm.sec^{-1})	HIA (%)	*Protein Plasma Binding (%)*
1	Salbutamol	19,30	75,95	13,36
2	1-methoxy-4-methylbenzene	29,44	96,47	100
3	2,3-dimethoxytoluen	57,55	100	100
4	Alpha copaene	23,01	100	100
5	Alpha farnesene	23,41	100	100
6	Alpha pinene	57,50	100	100
7	Benzyl benzoate	38,50	100	90,65
8	Beta linalool	29,35	100	100
9	Beta myrcene	23,63	100	100
10	Beta pinene	22,35	100	100

LAMPIRAN 16
(LANJUTAN)

.

No	Senyawa	Caco-2 (nm.sec^{-1})	HIA (%)	*Protein Plasma Binding (%)*
11	Beta silenene	23,50	100	100
12	Methyleugenol	58,09	100	100
13	Transbetaocimen	23,63	100	100
14	Trans-caryophyllene	23,53	100	100

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, < 4 low permeability.
% PPB = 90% strongly bond, < 90% weakly bond.

LAMPIRAN 17

UJI TOKSISITAS

Tabel V.6
Uji Toksisitas Senyawa Bunga Kenanga dan Obat Pembanding

No	Senyawa Ligan	Kroes TTC decision tree
1	Salbutamol	1
2	1-methoxy-4-methylbenzene	1
3	2,3-dimethoxytoluen	1
4	Alpha copaene	1
5	Alpha farnesene	1
6	Alpha pinene	1
7	Benzyl benzoate	1
8	Beta linalool	1
9	Beta myrcene	1
10	Beta pinene	1

LAMPIRAN 17
(LANJUTAN)

No	Senyawa Ligan	Kroes TTC decision tree
11	Beta silenene	1
12	Methyleugenol	1
13	Transbetaocimen	1
14	Trans-caryophyllene	1

Kroes TTC decision tree :
1 = Substance would not be expected to be a safety concern
2 = Negligible risk (low probability of a life-time cancer risk greater than in 10^6)
3 = Risk assesment requires compound-specific toxicity data