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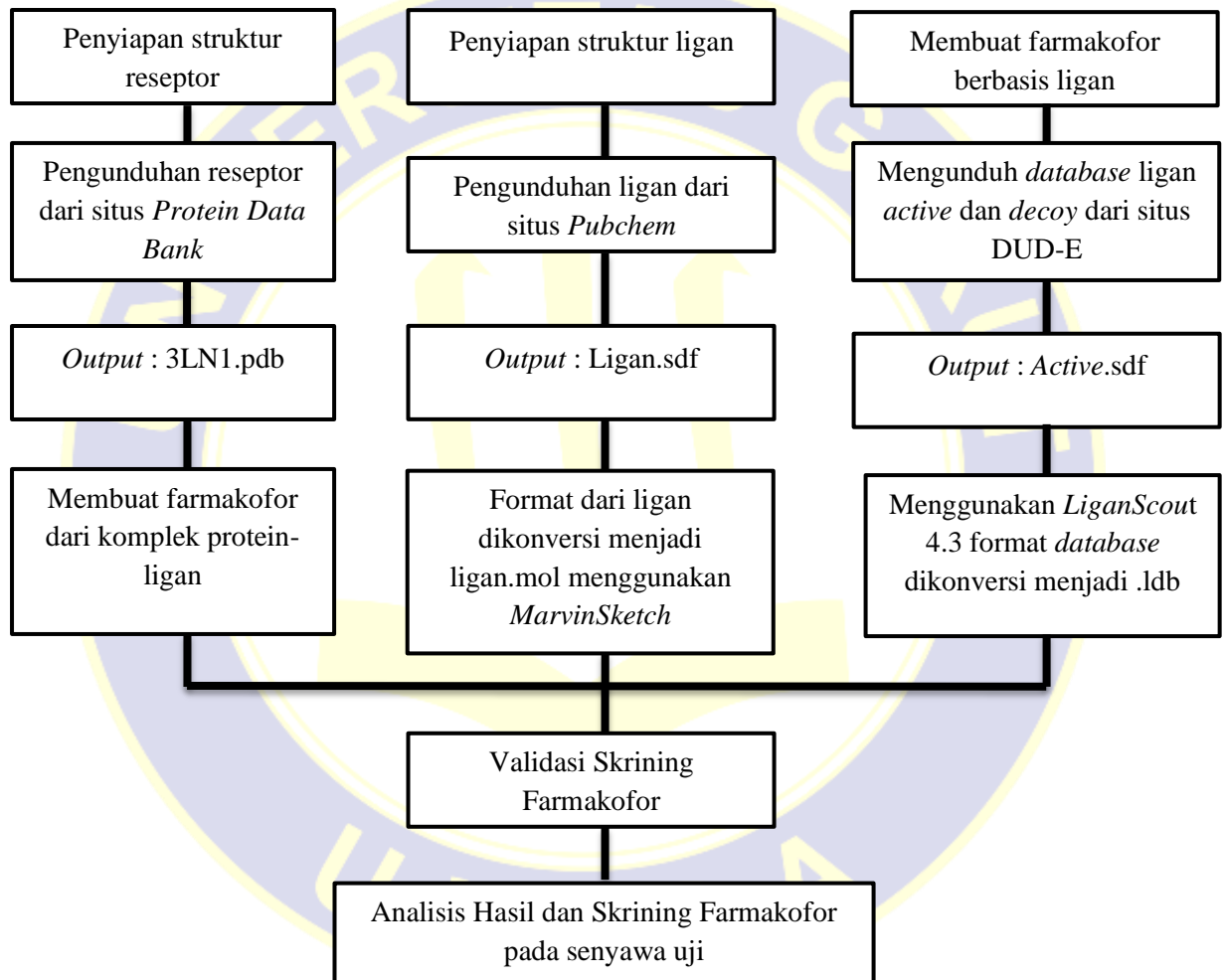
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LAMPIRAN 1

ALUR PENELITIAN SKRINING FARMAKOFOR

Tabel IV.1

Alur Penelitian Skrining Farmakofor

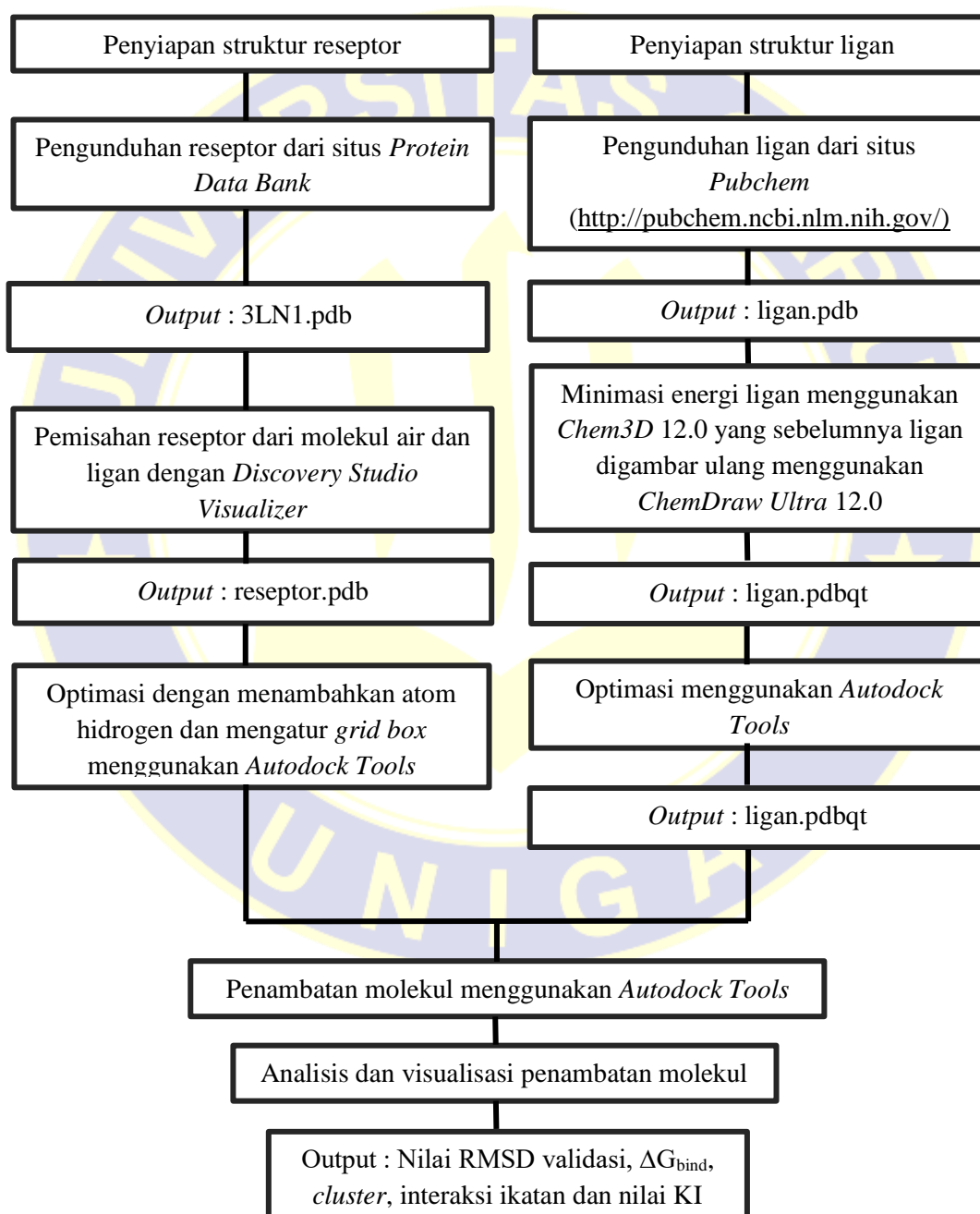


LAMPIRAN 2

ALUR PENELITIAN *MOLECULAR DOCKING*

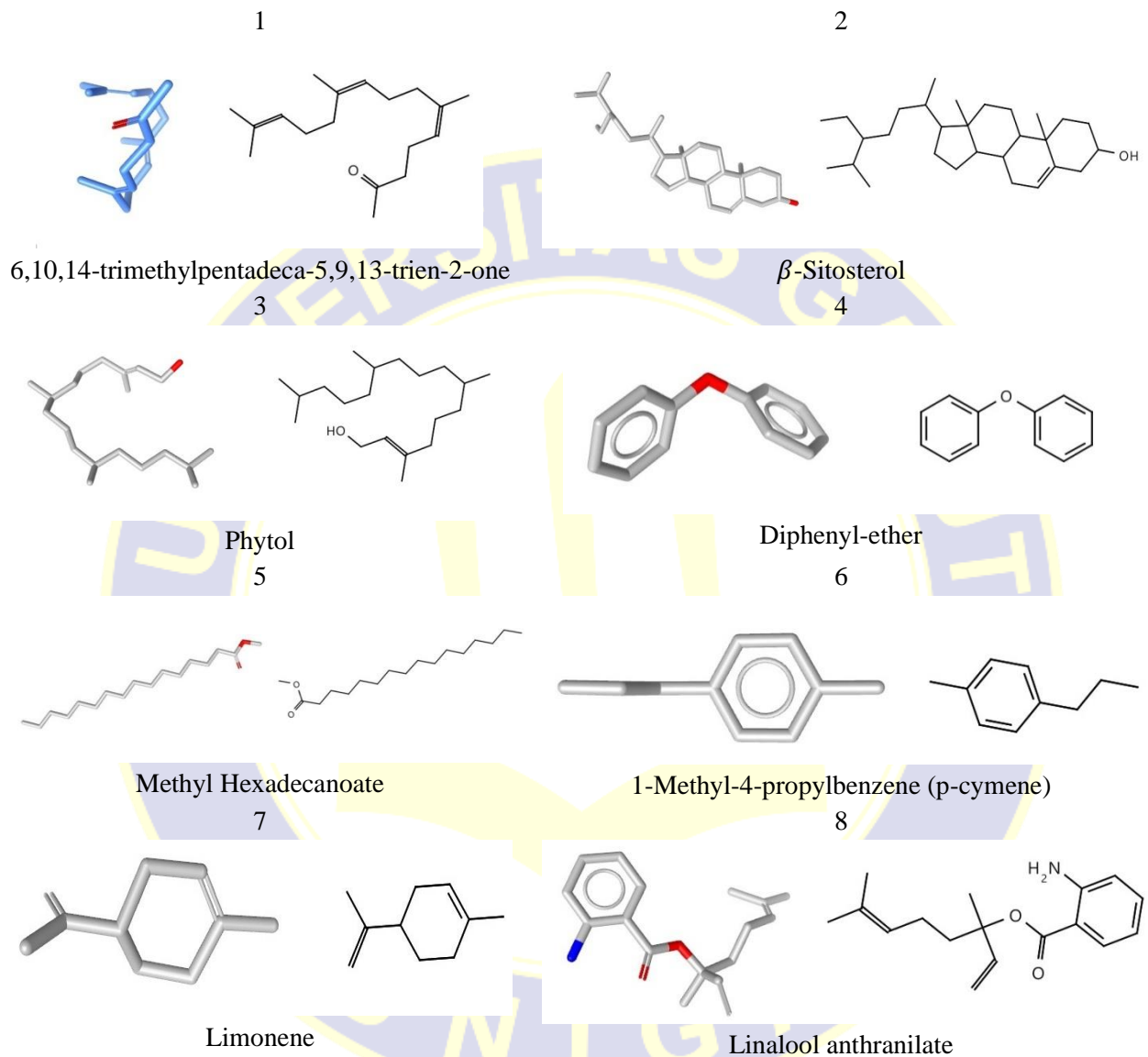
Tabel IV.1

Alur Penelitian Molecular Docking



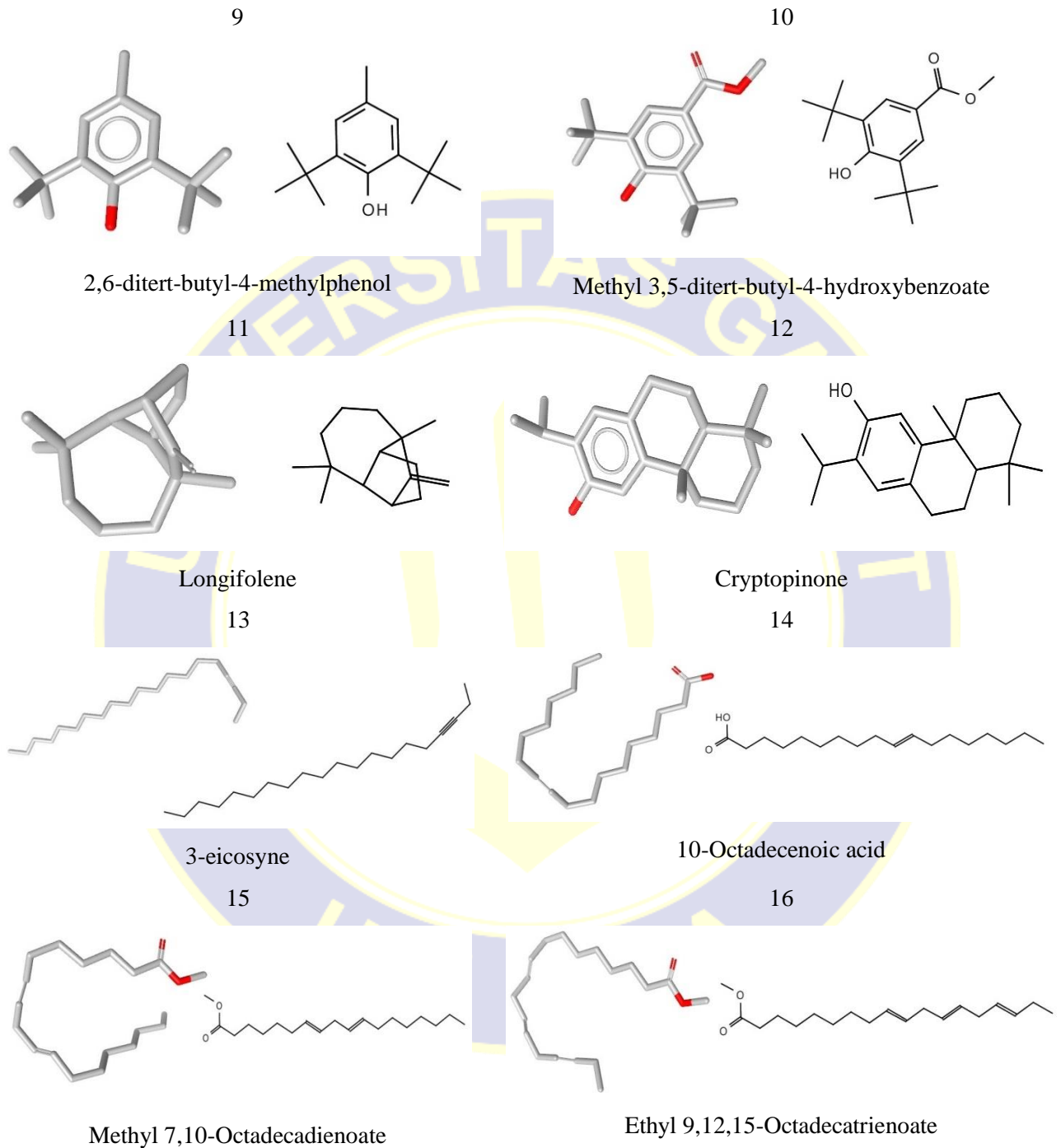
LAMPIRAN 3

STRUKTUR 3D DAN 2D SENYAWA DAUN ASAM JAWA

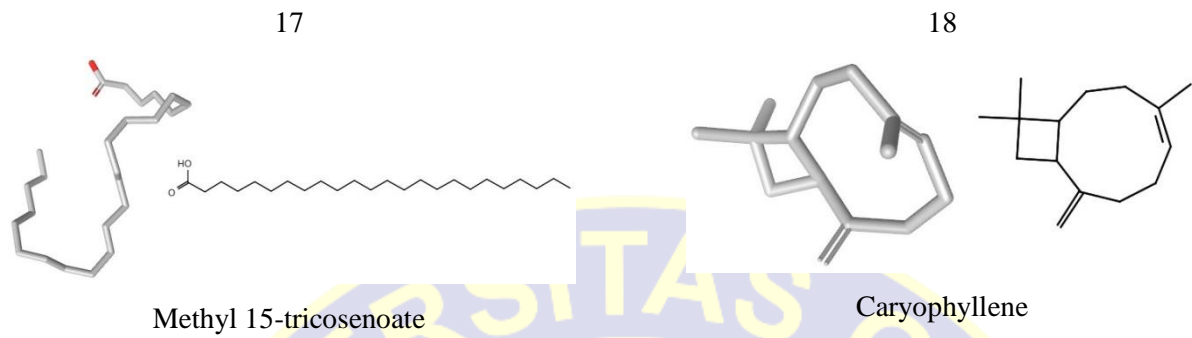


Gambar IV.1 Struktur kimia kandungan senyawa aktif dalam daun asam jawa (*Tamarindus indica* L.)

LAMPIRAN 3 (LANJUTAN)



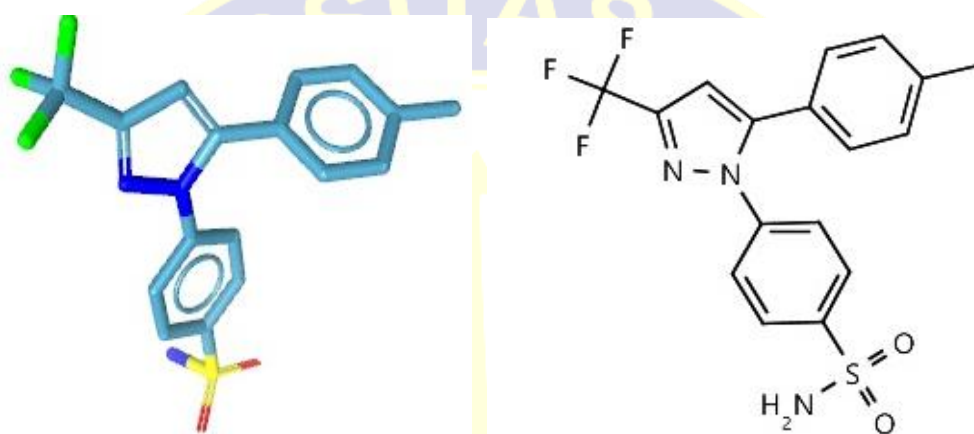
Gambar IV.1 Struktur kimia kandungan senyawa aktif dalam daun asam jawa (*Tamarindus indica* L.)

**LAMPIRAN 3
(LANJUTAN)**

Gambar IV.1 Struktur kimia kandungan senyawa aktif dalam daun asam jawa
(*Tamarindus indica* L.)

LAMPIRAN 4

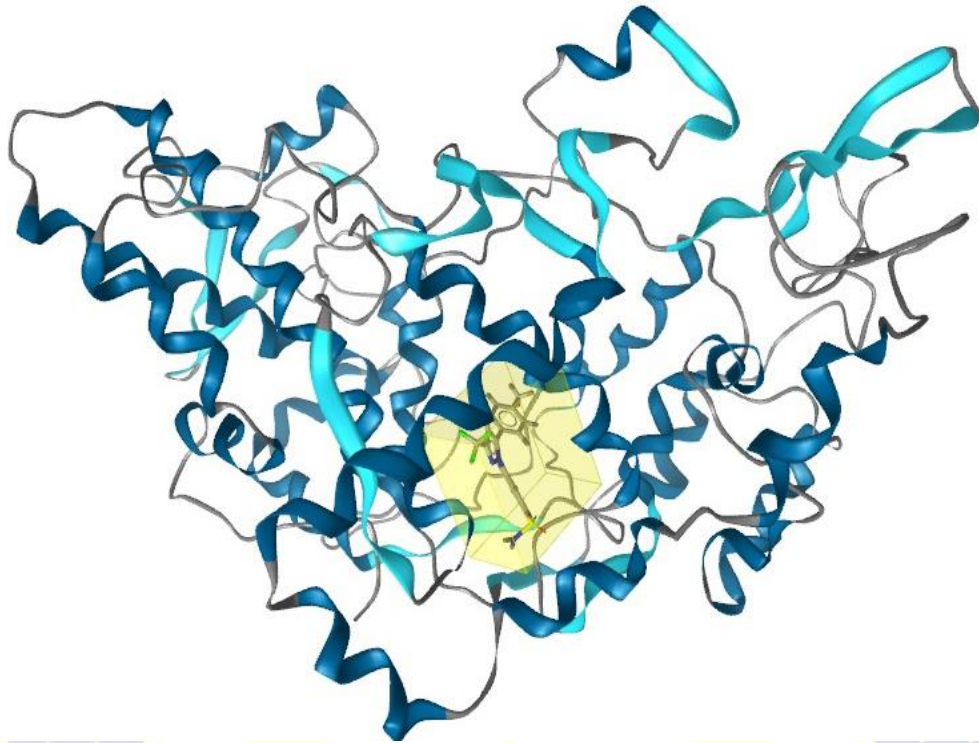
STRUKTUR 3D DAN 2D LIGAN ALAMI CELECOXIB



Gambar IV.2 Struktur kimia ligan alami Celecoxib

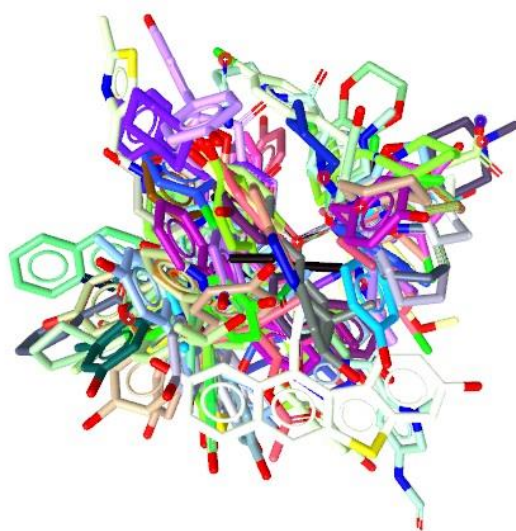
LAMPIRAN 5

STRUKTUR 3D RESEPTOR SIKLOOKSIGENASE-2

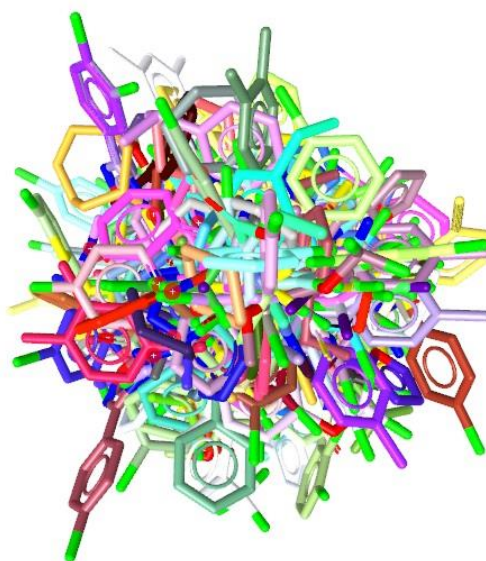


Gambar IV.3 Struktur tiga dimensi (3D) reseptor Siklooksigenase-2

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LAMPIRAN 6**STRUKTUR 3D DATABASE *ACTIVE* DAN *DECOY***

Gambar IV.4 Kumpulan struktur tiga dimensi senyawa *active* yang didapatkan dari situs *DUD-E*



Gambar IV.5 Kumpulan struktur tiga dimensi senyawa *decoy* yang didapatkan dari situs *DUD-E*

LAMPIRAN 7

SITUS *PROTEIN DATA BANK*



Gambar IV.6 Tampilan situs *Protein Data Bank* (PDB) sebagai tempat pengunduhan reseptor.

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LAMPIRAN 8

SITUS PUBCHEM

The screenshot shows the main interface of the PubChem website. At the top, there is a dark blue header with the NIH logo and the text "U.S. National Library of Medicine National Center for Biotechnology Information". Below this is a white navigation bar with the PubChem logo and links for "About", "Blog", "Submit", "Contact", and "PubChem Periodic Table and Element pages Read More >". The main content area has a dark blue background with the heading "Explore Chemistry" and the subtext "Quickly find chemical information from authoritative sources". A search bar is prominently displayed. Below the search bar, there are several suggested search terms: "Try aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)/n1-2H3". There are four icons representing different functions: "Draw Structure", "Upload ID List", "Browse Data", and "Periodic Table". At the bottom of the main content area, there is a statistics bar showing "96M Compounds", "235M Substances", "265M Bioactivities", "30M Literature", "3M Patents", and "681 Data Sources". There are also links for "See More Statistics >" and "Explore Data Sources >".

Gambar IV.7 Tampilan utama situs *PubChem* sebagai tempat pengunduhan beberapa senyawa dalam format .pdb

LAMPIRAN 9

SITUS DUD-E



UCSF University of California, San Francisco | About UCSF | Search UCSF | UCSF Medical Center docking.org

D U D • E

A Database of Useful Decoys: Enhanced

[Home](#) | [Targets](#) | [Subsets](#) | [Generate](#) | [Other](#) | [FAQ](#) | [Revisions](#) | [Thanks](#)

Welcome to **DUD-E**, an enhanced and rebuilt version of DUD, a directory of useful decoys. DUD-E is designed to help benchmark molecular docking programs by providing challenging decoys. It contains:

- 22,886 active compounds and their affinities against 102 targets, an average of 224 ligands per target
- 50 decoys for each active having similar physico-chemical properties but dissimilar 2-D topology.

mol2 and SDF format now available in all packages for actives and decoys. [July 14]

DUD-E is provided by the [Shoichet Laboratory](#) in the [Department of Pharmaceutical Chemistry](#) at the [University of California, San Francisco \(UCSF\)](#). To cite DUD-E, please reference [Mysinger MM, Carchia M, Irwin JJ, Shoichet BK. *J. Med. Chem.*, 2012, Jul 5. doi:10.1021/jm300687z](#).

We thank [NIGMS](#) for financial support (GM71896 to BKS and JJI). For correspondence about DUD-E, please write John Irwin jji at cgl dot ucsf dot edu.

DUD-E may be downloaded [target-by-target](#), organized by [subset](#) such as GPCR and kinase, or [all at once](#). You may also [generate your own](#) decoys.

DUD-E is a research tool which we have tried to make as useful and as correct as we know how. Anticipating that problems will undoubtedly be found, we have set up a [DUD-E help page](#) and a [DUD-E feedback page](#) to allow the community to share problems or observations. We will endeavor to put right any problems promptly, as best we can.

Browse **Download** **Make Decoys**
the DUD-E targets the default DUD-E package for your own ligands

DUD-E free to use and is provided by the Irwin and Shoichet Laboratories at UCSF.
To cite DUD-E, please reference: [Mysinger MM, Carchia M, Irwin JJ, Shoichet BK. *J. Med. Chem.*, 2012, Jul 5. doi:10.1021/jm300687z](#).
You may also wish to cite the original version of DUD. [Huang, Shoichet and Irwin, *J. Med. Chem.*, 2006, 49\(23\), 6789-6801. doi:10.1021/jm0608356](#).

Gambar IV.8 Tampilan utama situs *DUD-E* sebagai tempat pengunduhan senyawa *active* dan *decoy* dalam format *.sdf*

LAMPIRAN 10

SITUS LIPINSKI RULE OF FIVE



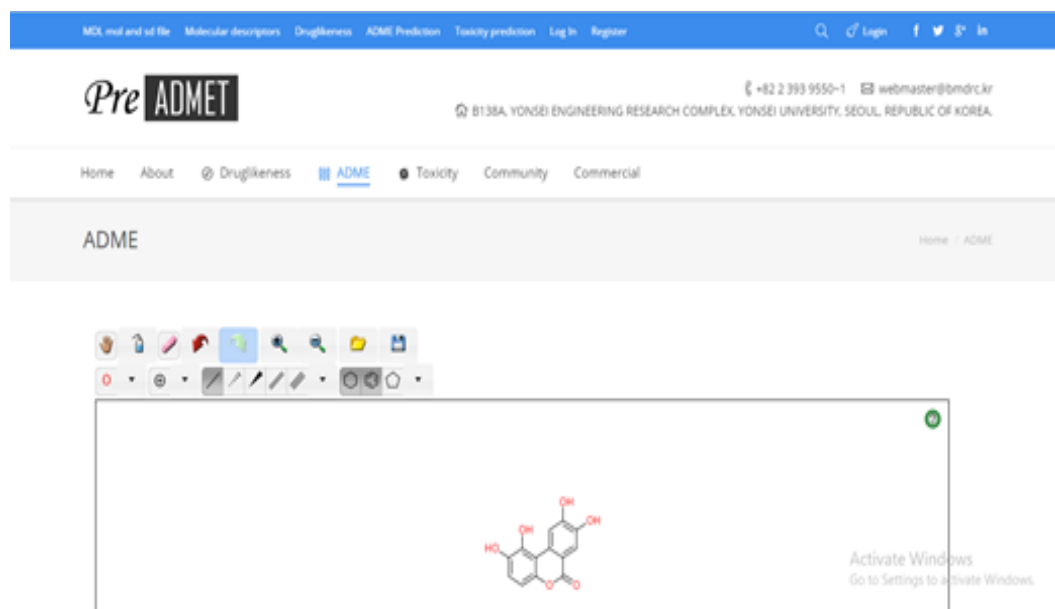
The screenshot shows the web interface for the Lipinski Rule of Five tool. At the top, it features the logo of the Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi (SCFBIC). The main heading is "Lipinski Rule of Five". Below this, a paragraph explains that the rule helps distinguish between drug-like and non-drug-like molecules. A bulleted list of five rules is provided: molecular mass less than 500 Carbon, high lipophilicity (LogP less than 5), less than 5 hydrogen bond donors, less than 10 hydrogen bond acceptors, and molar refractivity between 40-130. A note states that these filters help in early preclinical development. The interface is divided into three steps: Step 1: Input Drug File, with a text input field and a "Choose File" button; Step 2: Input pH Value, with a text input field containing "7" and a note that the value ranges from 0.0 to 14.0; and Step 3: Click on "Submit" to submit your job, with "Submit" and "Reset" buttons. A "How to Use the Tool" section at the bottom provides a note about file formats: "The input file should be in the following formats: *.sdf, *.mol, *.mol2, *.xyz, *.cif, *.mol".

Gambar IV.9 Tampilan situs *Lipinski rule of five* untuk pengujian sifat fisikokimia

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LAMPIRAN 11

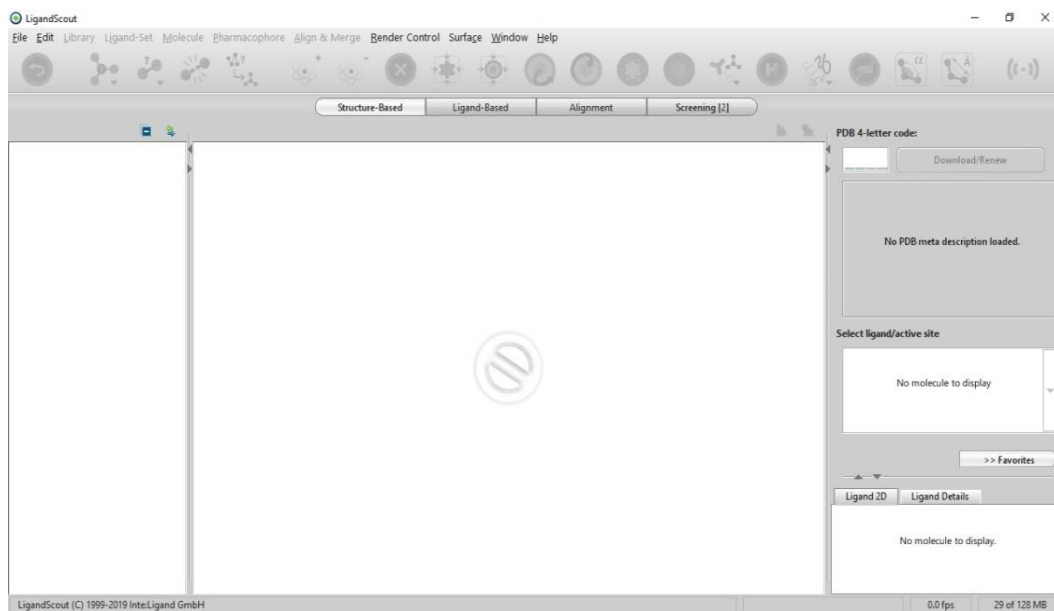
SITUS PREAMMET



Gambar IV.10 Tampilan situs *PreADMET*

LAMPIRAN 12

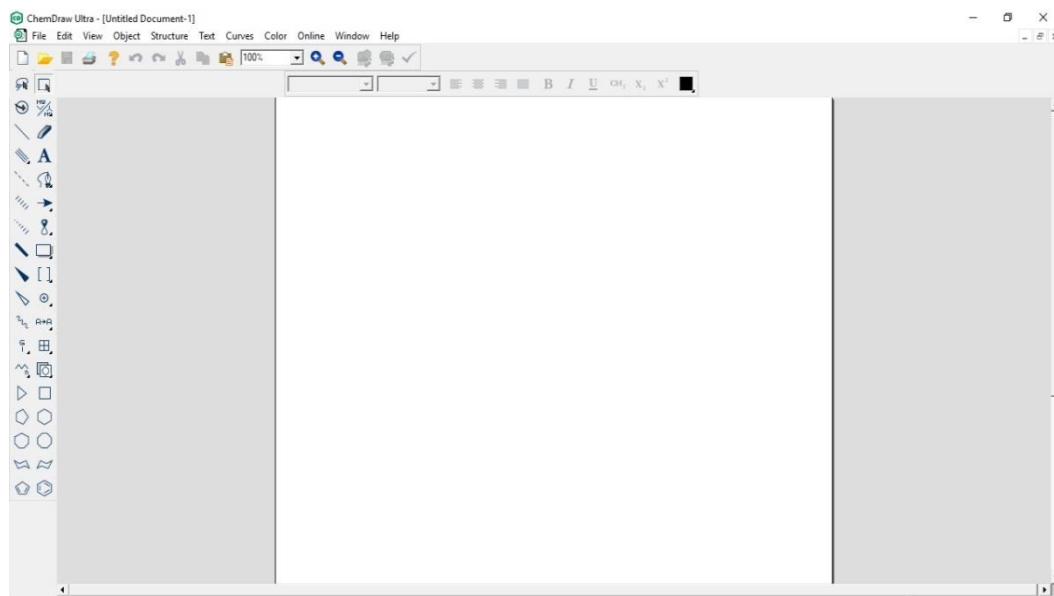
PERANGKAT LUNAK LIGANDSCOUT 4.3



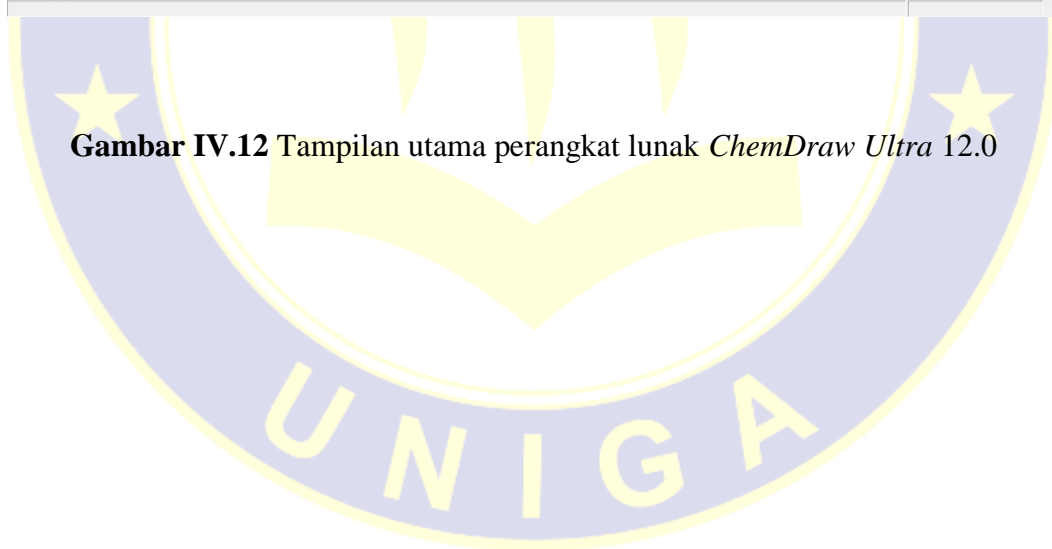
Gambar IV.11 Tampilan utama perangkat lunak *LigandScout* 4.3

LAMPIRAN 13

PERANGKAT LUNAK CHEMDRAW ULTRA 12.0

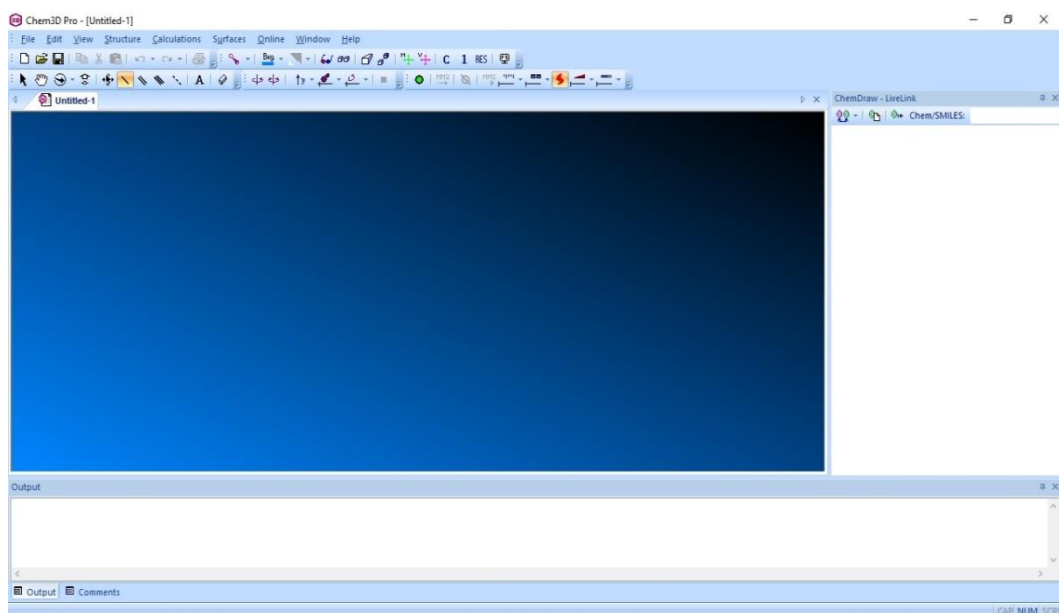


Gambar IV.12 Tampilan utama perangkat lunak *ChemDraw Ultra 12.0*

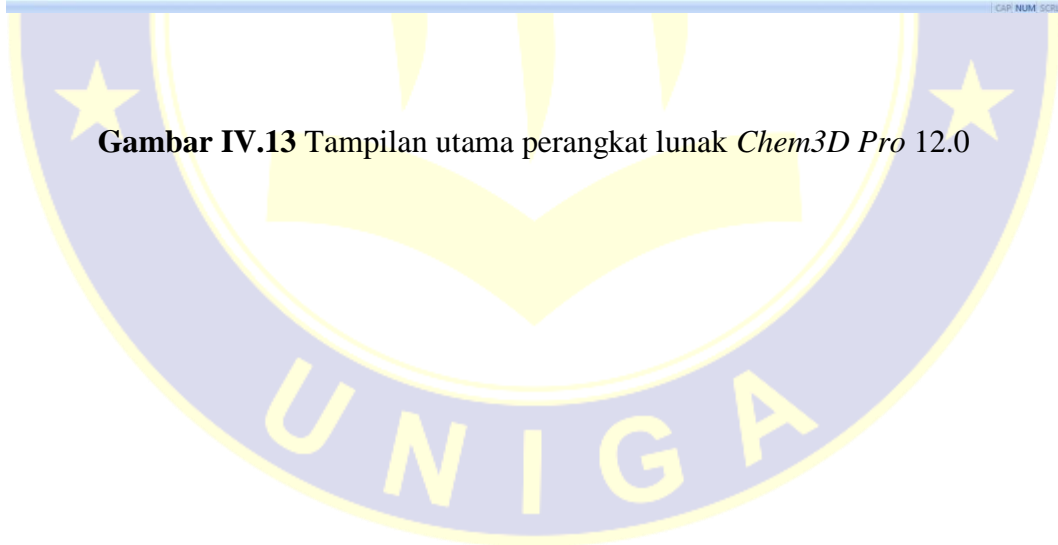


LAMPIRAN 14

PERANGKAT LUNAK CHEM3D PRO 12.0

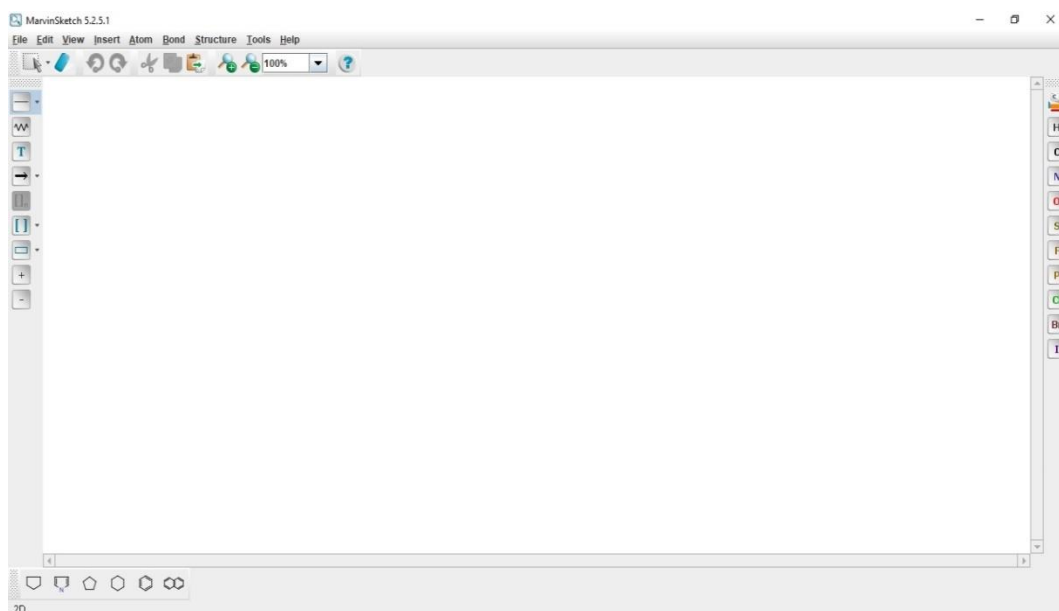


Gambar IV.13 Tampilan utama perangkat lunak *Chem3D Pro 12.0*



LAMPIRAN 15

PERANGKAT LUNAK MARVINSKETCH

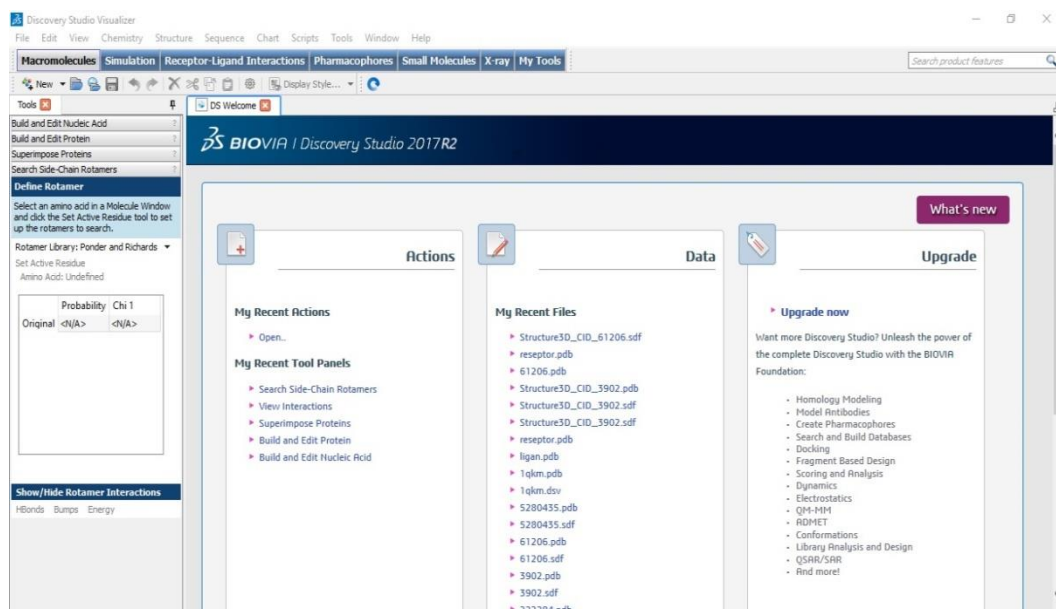


Gambar IV.14 Tampilan perangkat lunak *MarvinSketch*

LAMPIRAN 16

PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER

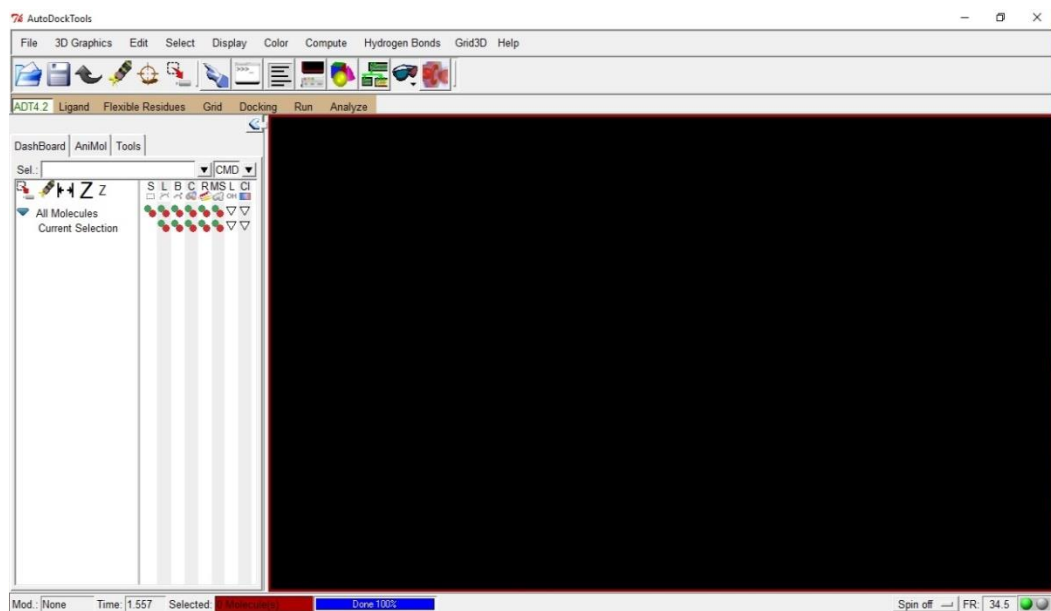
2017 CLIENT



Gambar IV.15 Tampilan utama perangkat lunak *Discovery Studio Visualizer*

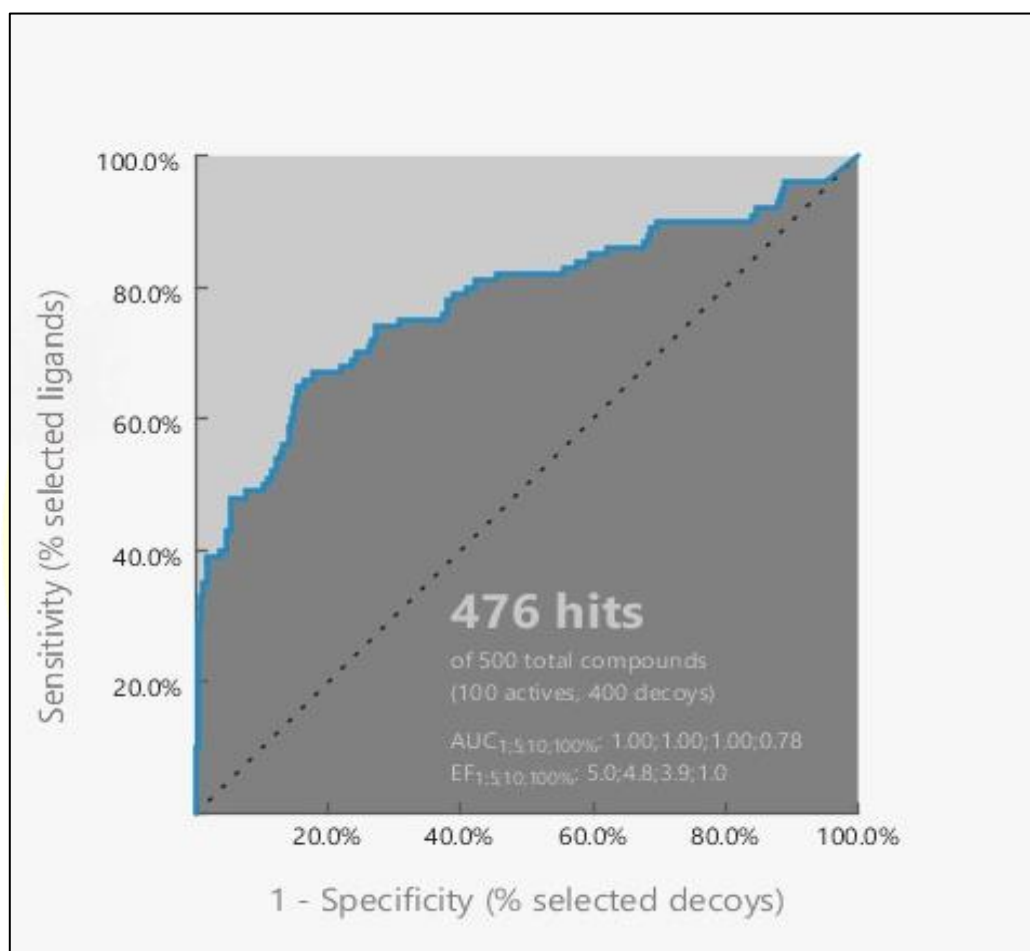
LAMPIRAN 17

PERANGKAT LUNAK AUTODOCK TOOLS



Gambar IV.16 Tampilan perangkat lunak *AutoDock Tools* sebagai tempat penambatan molekul antara ligan dengan reseptor

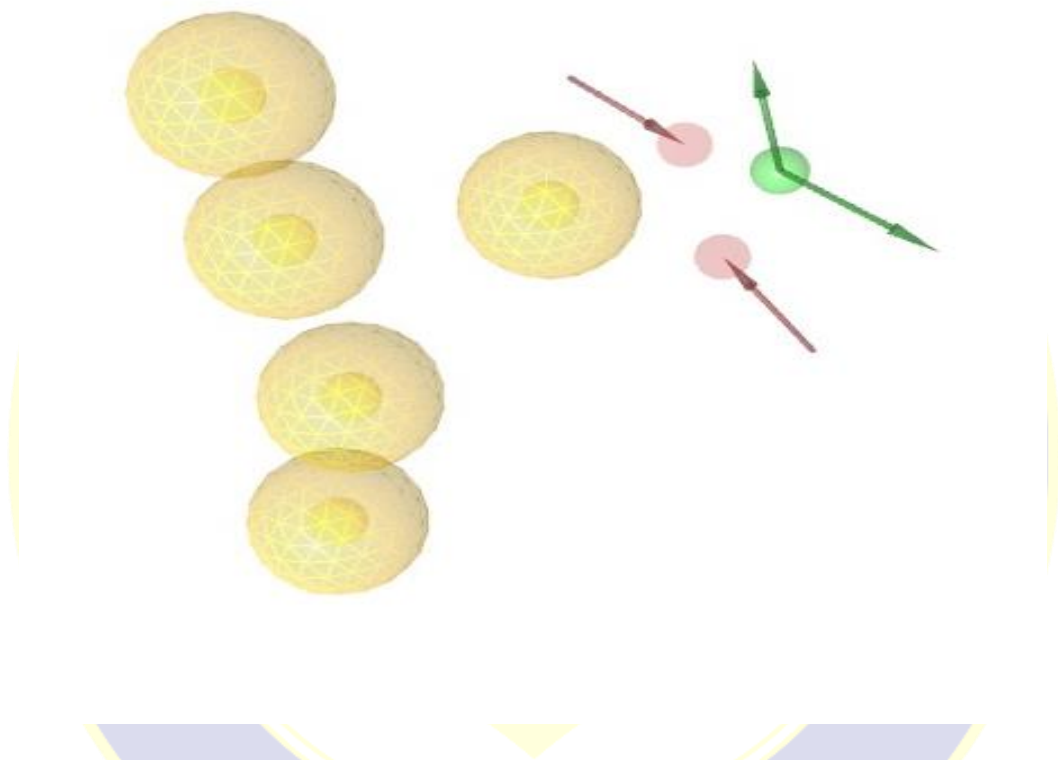
LAMPIRAN 18
KURVA VALIDASI SKRINING FARMAKOFOR
(KURVA *ROC*)



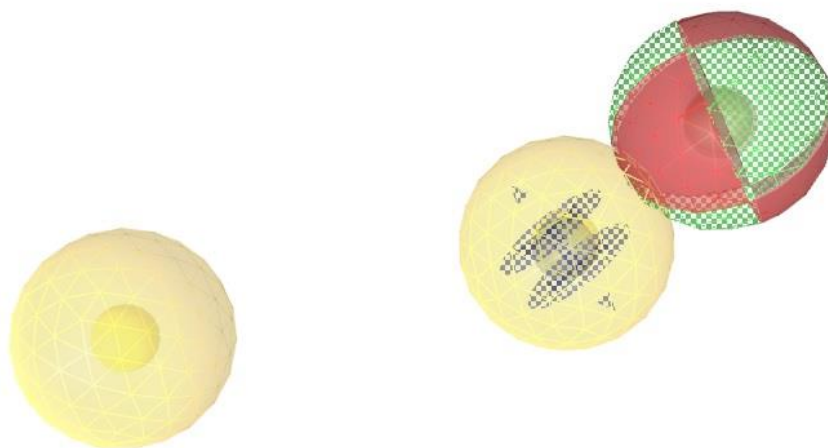
Gambar V.1 Kurva validasi (kurva *ROC*) model farmakofor

LAMPIRAN 19

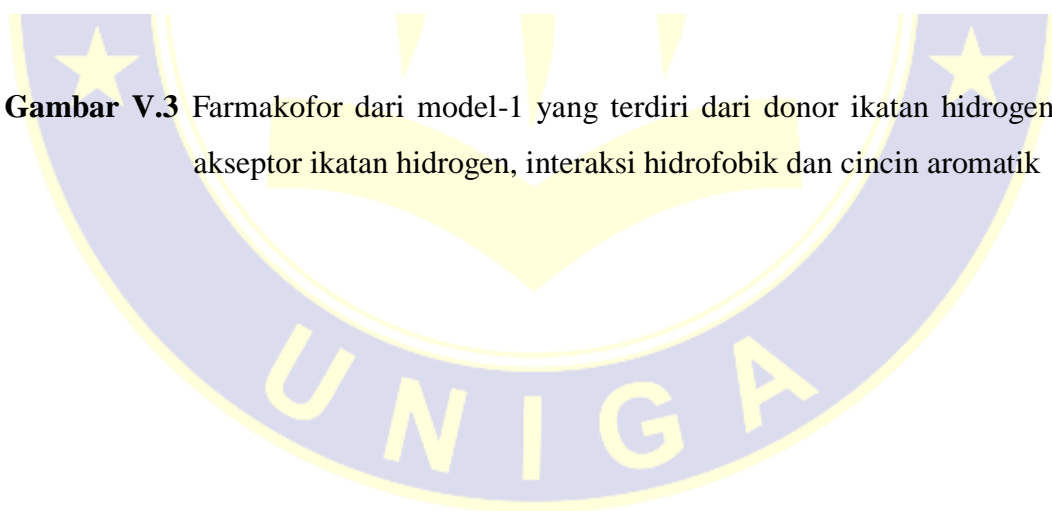
FARMAKOFOR RESEPTOR SIKLOOKSIGENASE-2



Gambar V.2 Farmakofor dari reseptor Siklooksigenase-2 yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen dan interaksi hidrofobik

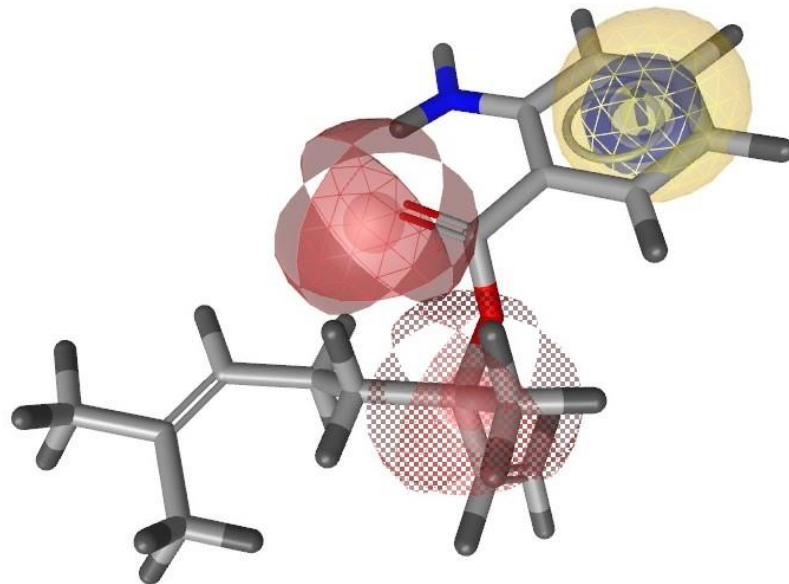
LAMPIRAN 20**FARMAKOFOR MODEL 1 (MODEL TERBAIK)**

Gambar V.3 Farmakofor dari model-1 yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen, interaksi hidrofobik dan cincin aromatik



LAMPIRAN 21

HASIL SKRINING FARMAKOFOR




Farmakofor model-1 hit dengan Linalool

Gambar V.4 Hasil Skrining Farmakofor Senyawa Daun Asam Jawa (*Tamarindus indica* L.)

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**LAMPIRAN 21
(LANJUTAN)**

Tabel V.1

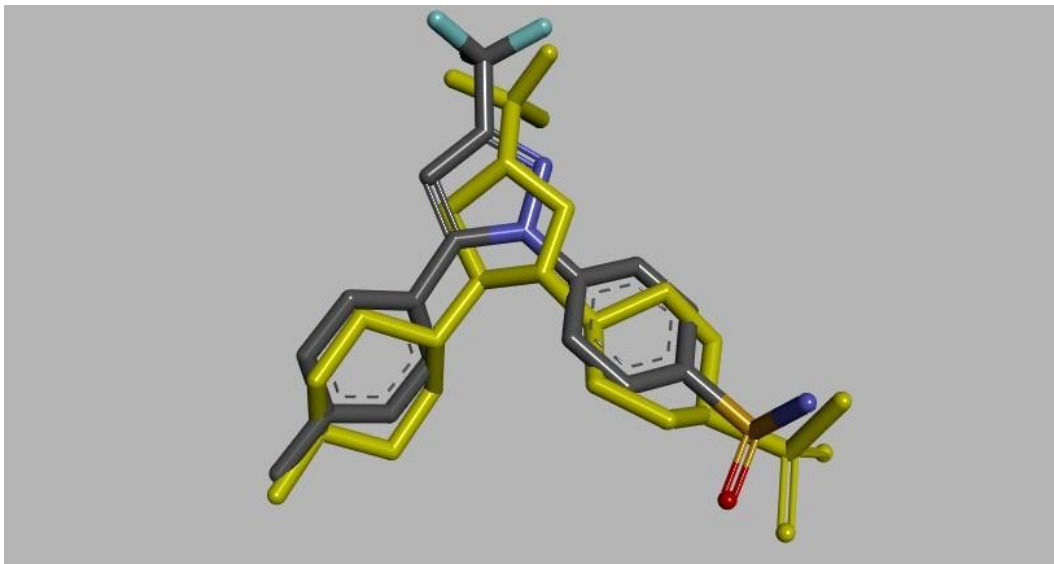
No	Nama Senyawa	Pharmacophore Depiction	Pharmacophore Fit Score
1	Linalool		52.11

Hasil Skrining Farmakofor Senyawa Daun Asam Jawa (*Tamarindus indica* L.)

Keterangan: warna kuning = interaksi hidrofobik
warna merah = akseptor ikatan hidrogen
warna hijau = donor ikatan hidrogen

LAMPIRAN 22

VALIDASI METODE RESEPTOR SIKLOOKSIGENASE-2



Gambar V.5 Visualisasi tumpang tindih ligan alami Celecoxib (warna abu gelap) dengan ligan hasil *redocking* (warna kuning)

Tabel V.2

Hasil validasi metode dengan *redocking* ligan alaminya didapatkan nilai RMSD < 2.4 Å yaitu 0.863 Å menunjukkan validitas metode dan reseptor yang sudah valid

Kode PDB	Grid Box	Tingkat Validasi	Validasi		Ikatan Energi (kkal/mol)
			RMSD Cluster (Å)	RMSD Reference (Å)	
3LN1	X: 77.870 Y: -15.391 Z: -7.855	2.500.000	0.00	0.863	-7.98

LAMPIRAN 23

HASIL PENAMBATAN MOLEKUL LIGAN ALAMI

DAN SENYAWA UJI

Tabel V.3

Hasil penambatan molekul berdasarkan nilai energi ikatan (ΔG) beserta nilai konstanta inhibisi (KI) dan residu asam aminonya

No	Senyawa/Ligan Uji	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI
Ligan Alami					
	Ligan Alami Celecoxib	-7.98	8	ILE503, GLN178, PHE504, HIS75, TYR371, SER339, ARG449.106	62.85 nM
Senyawa Aktif Asam Jawa (<i>Tamarindus indica</i> L.)					
1	6,10,14- trimethylpentadeca- 5,9,13-trien-2-one	-6.01	1	ARG346	55.48 nM
2	Phytol	-7.11	2	GLU305, ARG346	64.15. nM
3	β -Sitosterol	-6.92	1	GLU305	69.67 nM
4	Diphenyl-ether	-5.40	-	-	52.25 nM
5	Methyl Hexadecanoate	-6.26	1	ARG346	58.76 nM

LAMPIRAN 23 (LANJUTAN)

Tabel V.3

Hasil penambatan molekul berdasarkan nilai energi ikatan (ΔG) beserta nilai konstanta inhibisi (KI) dan residu asam aminonya

No	Senyawa/Ligan Uji	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI
6	1-Methyl-4-propylbenzene (p-cymene)	-6.48	-	-	96.22 nM
7	Limonene	-5.91	-	-	96.3 nM
8	Linalool anthranilate	-9,21	1	TYR371	62.41 nM
9	2,6-ditert-butyl-4-methylphenol	-5.75	1	LEU298	52.07 nM
10	Methyl 3,5-ditert-butyl-4-hydroxybenzoate	-6.11	1	LEU298	11.14 nM
11	Longifolene	-6.99	-	-	21.4 nM
12	Cryptopinone	-8.21	1	SER339	89.13 nM
13	3-eicosyne	-6.78	-	-	51.99 nM
14	10-Octadecenoic acid	-6.12	2	GLU305, ARG346	63.09 nM

**LAMPIRAN 23
(LANJUTAN)**

Tabel V.3

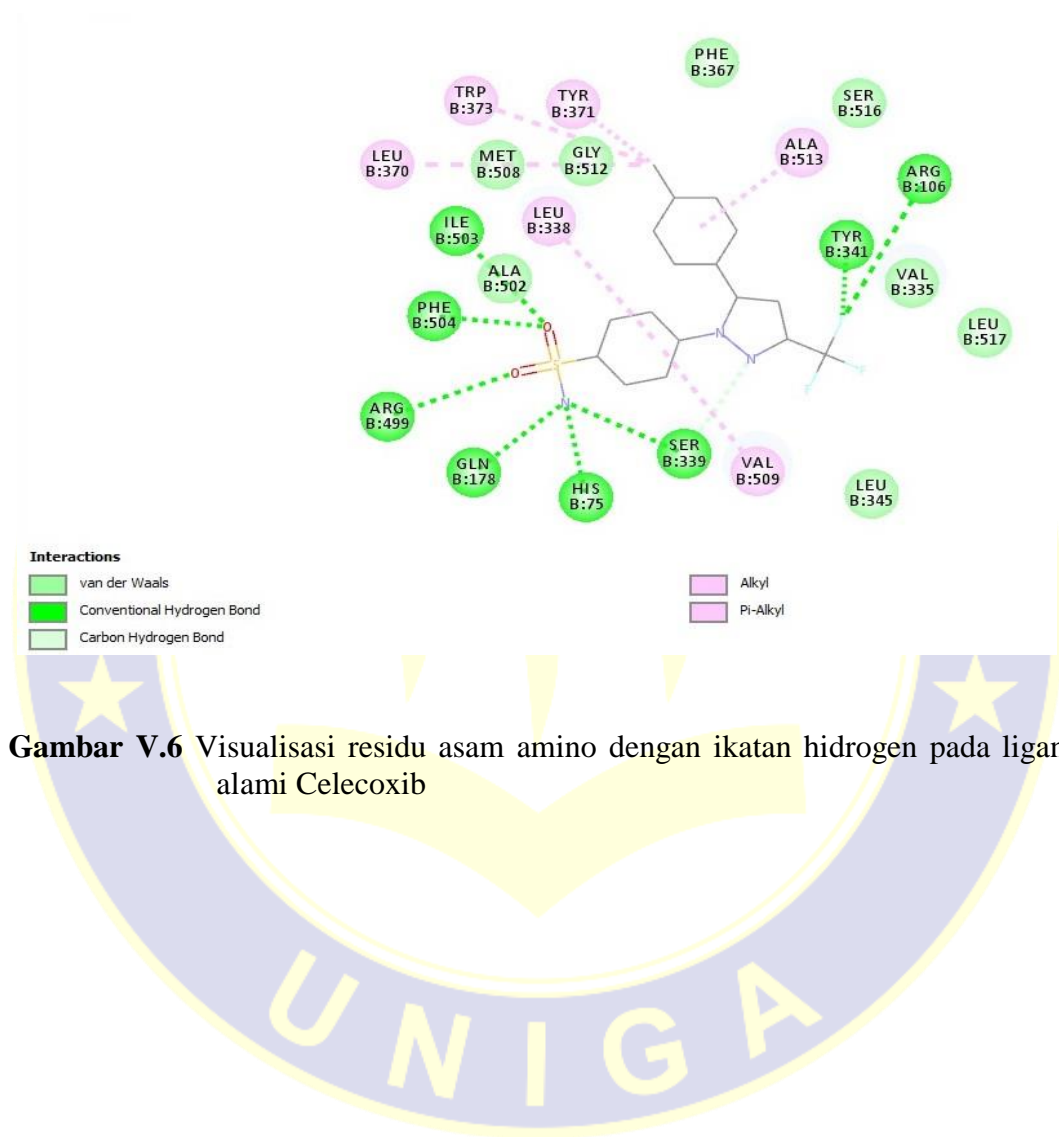
Hasil penambatan molekul berdasarkan nilai energi ikatan (ΔG) beserta nilai konstanta inhibisi (KI) dan residu asam aminonya

No	Senyawa/Ligan Uji	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI
15	Methyl 7,10- Octadecadienoate	-6.96	1	HIS475	41.26 nM
16	Ethyl 9,12,15- Octadecatrienoate	-6.58	1	ARG346	72.28 nM
17	Methyl 15- tricosenoate	-5.44	-	-	63.55 nM
18	Caryophyllene	-6.15	-	-	41.07 nM

LAMPIRAN 24

VISUALISASI PENAMBATAN MOLEKUL CELECOXIB

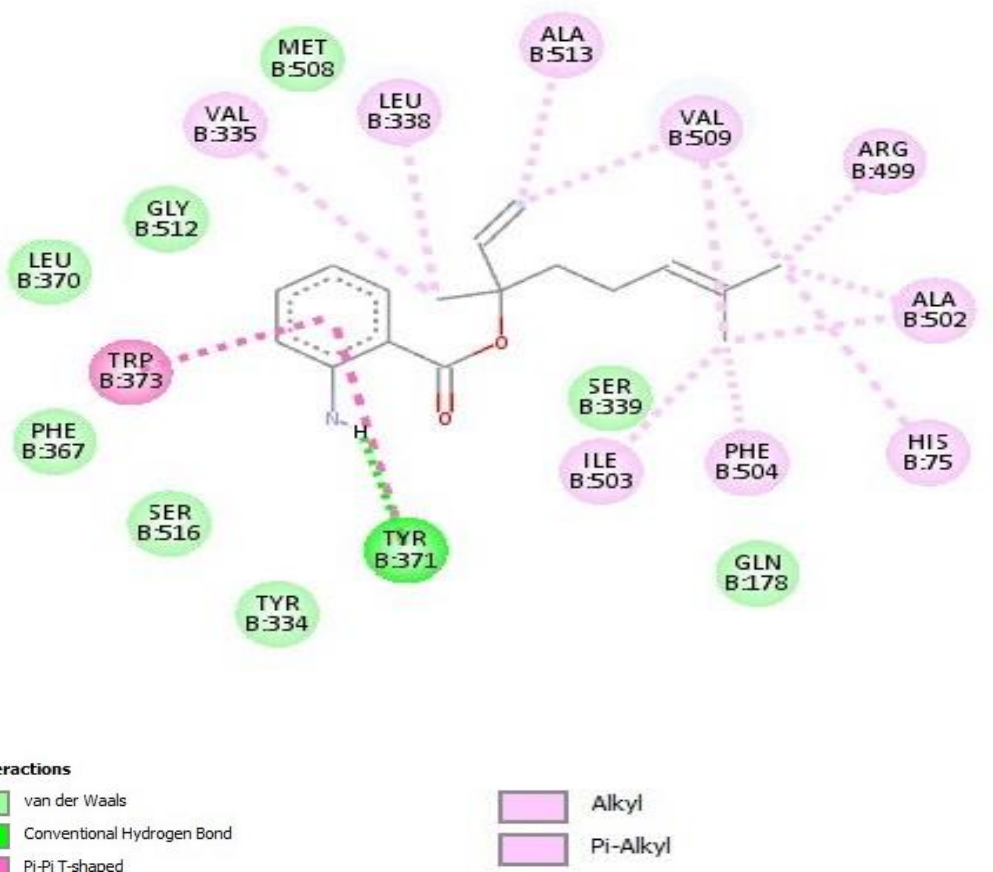
DENGAN RESEPTOR



Gambar V.6 Visualisasi residu asam amino dengan ikatan hidrogen pada ligan alami Celecoxib

LAMPIRAN 25

VISUALISASI HASIL PENAMBATAN LINALOOL DENGAN
RESEPTOR SIKLOOKSIGENASE-2



Gambar V.7 Visualisasi residu asam amino dengan ikatan hidrogen pada Linalool

LAMPIRAN 26

SIFAT FISIKOKIMIA SENYAWA DAUN ASAM JAWA

BERDASARKAN *LIPINSKI'S RULE OF FIVE*

Tabel V.4

Data sifat fisikokimia senyawa uji berdasarkan *Lipinski's rule of five*

No	Senyawa/Ligan Uji	Donor Hidrogen	Akseptor Hidrogen	Bobot molekul	Log P	Memenuhi/Tidak Memenuhi Syarat
1	6,10,14-trimethylpentadeca-5,9,13-trien-2-one	0	1	262.437	5.77 5	Tidak memenuhi
2	β -Sitosterol	1	1	414.718	8.02 5	Tidak memenuhi
3	Phytol	1	1	296.539	6.36 4	Tidak memenuhi
4	Diphenyl-ether	0	0	170.211	3.47 9	Memenuhi
5	Methyl Hexadecanoate	0	1	270.457	5.64 1	Tidak memenuhi
6	1-Methyl-4-propylbenzene (p-cymene)	0	0	134.222	2.94 8	Memenuhi
7	Limonene	0	0	136.238	3.30 9	Memenuhi
8	Linalool anthranilate	1	1	273.376	3.88 5	Memenuhi
9	2,6-ditert-butyl-4-methylphenol	1	1	220.356	4.29 6	Memenuhi

**LAMPIRAN 26
(LANJUTAN)**

Tabel V.4

Data sifat fisikokimia senyawa uji berdasarkan *Lipinski's rule of five*

No	Senyawa/Ligan Uji	Donor Hidrogen	Akseptor Hidrogen	Bobot molekul	Log P	Memenuhi/Tidak Memenuhi Syarat
10	Methyl 3,5-ditert-butyl-4-hydroxybenzoate	1	2	264.365	3.542	Memenuhi
11	Longifolene	0	0	204.357	4.415	Memenuhi
12	Cryptopinone	1	1	286.459	5.546	Tidak memenuhi
13	3-eicosyne	0	0	278.524	7.351	Tidak memenuhi
14	10-Octadecenoic acid	0	2	282.468	6.109	Tidak memenuhi
15	Methyl 7,10-Octadecadienoate	0	1	294.479	5.973	Tidak memenuhi
16	Ethyl 9,12,15-Octadecatrienoate	0	1	292.463	5.749	Tidak memenuhi
17	Methyl 15-tricosenoate	0	2	368.646	8.673	Tidak memenuhi
18	Caryophyllene	0	0	204.357	4.725	Memenuhi

- Syarat:
1. BM < 500 mg/mol
 2. Log P < 5
 3. Donor Hidrogen < 5
 4. Akseptor Hidrogen < 10

LAMPIRAN 27

HASIL UJI PREADME (ABSORPSI DAN DISTRIBUSI)

Tabel V.5

Data hasil pengujian *PreADME* pada ke 18 senyawa aktif daun asam jawa
(*Tamarindus indica* L.)

No	Nama Senyawa	Caco-2 cell (nm ^{sec-1})	HIA (%)	Protein Plasma Binding
1	6,10,14-trimethylpentadeca- 5,9,13-trien-2-one	56.6804 ^b	100.00 ^a	100.00 ^a
2	β -Sitosterol	52.3734 ^b	100.00 ^a	100.00 ^a
3	Phytol	38.7817 ^b	100.00 ^a	100.00 ^a
4	Diphenyl-ether	22.5539 ^b	100.00 ^a	100.00 ^a
5	Methyl Hexadecanoate	45.8362 ^b	100.00 ^a	100.0 ^a
6	1-Methyl-4-propylbenzene (p- cymene)	23.4336 ^b	100.00 ^a	100.0 ^a
7	Limonene	23.6317 ^b	100.00 ^a	100.00 ^a
8	Linalool anthranilate	37.4763 ^b	96.005494 ^a	95.05476 ^a
9	2,6-ditert-butyl-4-methylphenol	45.9116 ^b	100.00 ^a	100.00 ^a
10	Methyl 3,5-ditert-butyl-4- hydroxybenzoate	22.8946 ^b	95.001042 ^a	100.00 ^a
11	Longifolene	23.4939 ^b	100.00 ^a	92.352757 ^a
12	Cryptopinone	44.363 ^b	100.00 ^a	100.00 ^a
13	3-eicosyne	22.518 ^b	100.00 ^a	100.00 ^a
14	10-Octadecenoic acid	28.1906 ^b	98.436935 ^a	100.00 ^a
15	Methyl 7,10-Octadecadienoate	47.1151 ^b	100.00 ^a	100.00 ^a

LAMPIRAN 27 (LANJUTAN)

Tabel V.5

Data hasil pengujian *PreADME* pada ke 18 senyawa aktif daun asam jawa
(*Tamarindus indica* L.)

No	Nama Senyawa	Caco-2 cell (nm ^{sec-1})	HIA (%)	Protein Plasma Binding
16	Ethyl 9,12,15- Octadecatrienoate	47.0406 ^b	100.00 ^a	100.00 ^a
17	Methyl 15-tricosenoate	35.2315 ^b	98.083030 ^a	100.00 ^a
18	Caryophyllene	23.6315 ^b	100.00 ^a	100.00 ^a

Klasifikasi: *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 28

HASIL UJI TOKSISITAS

Tabel V.6

Data hasil pengujian toksisitas yang dilihat dari potensi mutagen dan karsinogen dari ke 18 senyawa uji

No	Nama Senyawa	Toksisitas	Karsinogenisitas
1	6,10,14-trimethylpentadeca-5,9,13-trien-2-one	Non-mutagen	Positif
2	β -Sitosterol	Non-mutagen	Negatif
3	Phytol	Non-mutagen	Negatif
4	Diphenyl-ether	Mutagen	Positif
5	Methyl Hexadecanoate	Non-mutagen	Positif
6	1-Methyl-4-propylbenzene (p-cymene)	Mutagen	Negatif
7	Limonene	Mutagen	Positif
8	Linalool anthranilate	Non-mutagen	Positif
9	2,6-ditert-butyl-4-methylphenol	Non-mutagen	Negatif
10	Methyl 3,5-ditert-butyl-4-hydroxybenzoate	Non-mutagen	Negatif
11	Longifolene	Mutagen	Positif
12	Cryptopinone	Non-mutagen	Positif
13	3-eicosyne	Non-mutagen	Positif
14	10-Octadecenoic acid	Mutagen	Positif
15	Methyl 7,10-Octadecadienoate	Non-mutagen	Positif
16	Ethyl 9,12,15-Octadecatrienoate	Non-mutagen	Positif
17	Methyl 15-tricosenoate	Non-mutagen	Positif
18	Caryophyllene	Mutagen	Positif