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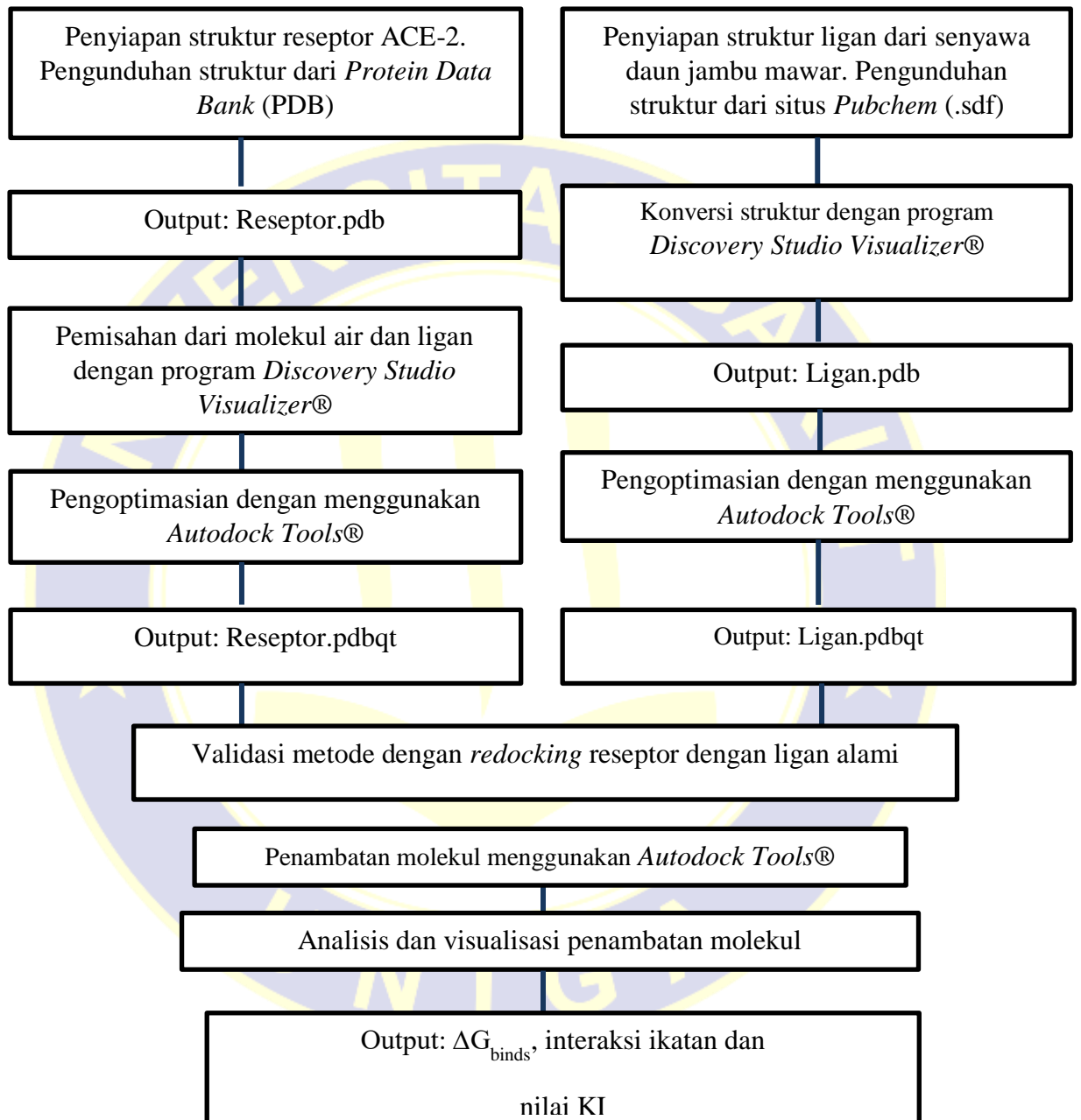
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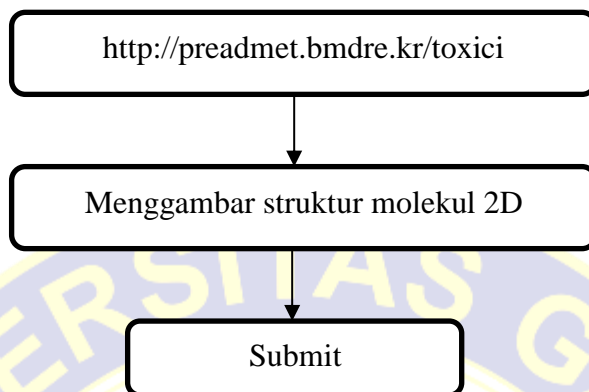
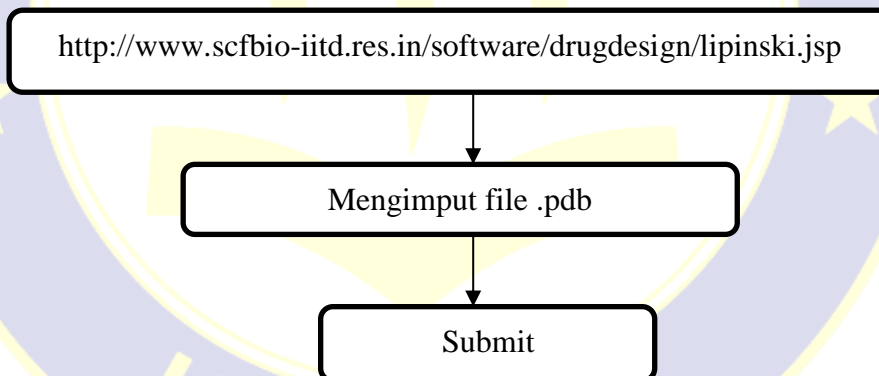
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LAMPIRAN 1

ALUR PENELITIAN



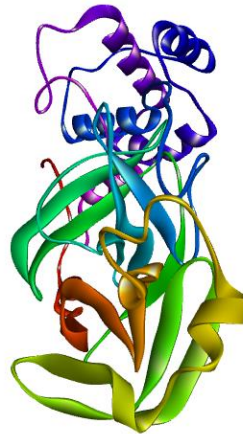
Gambar I.1 Alur Penelitian

LAMPIRAN 1**(LANJUTAN)****Gambar I.2** Analisis *Pre-ADME* dan Toksisitas**Gambar I.3** Analisis *Lipinski's Rule of Five*

LAMPIRAN 2**TANAMAN DAUN JAMBU MAWAR**

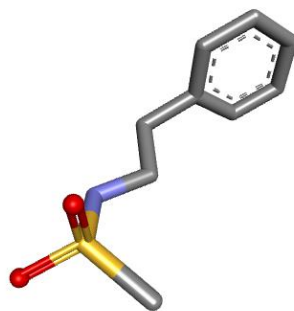
Gambar II.1 Tanaman Daun Jambu Mawar (*Syzygium Jambos* (L.) Alston)

LAMPIRAN 3
STRUKTUR 3D RESEPTOR



Gambar III.1 Enzim Mpro (*Main Protease*) (PDB ID 5R7Y)

LAMPIRAN 4
STRUKTUR LIGAN ALAMI

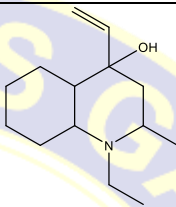
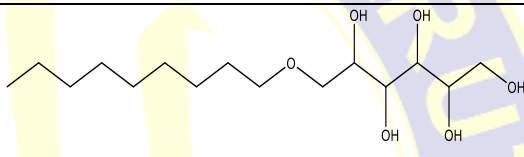
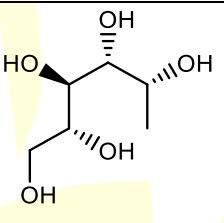
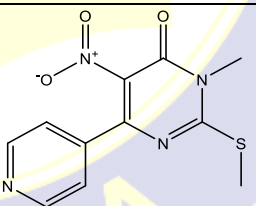
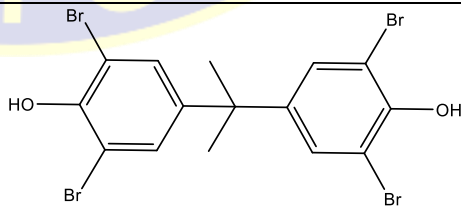


Gambar III.2 Ligan Alami Enzim Mpro (N-(2-phenylethyl)methanesulfonamide)

LAMPIRAN 5

STRUKTUR 2D SENYAWA UJI

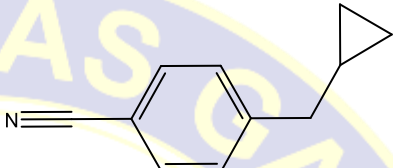
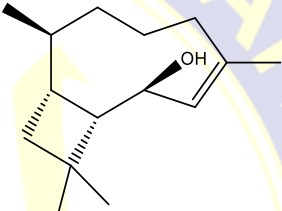
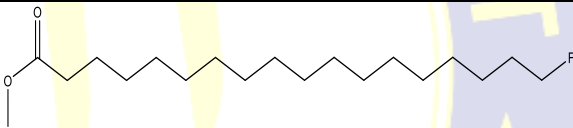
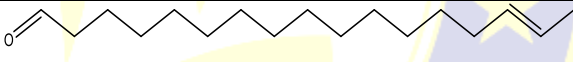
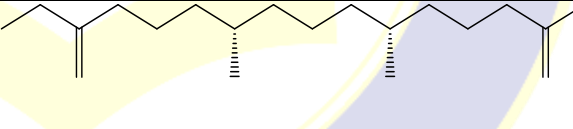

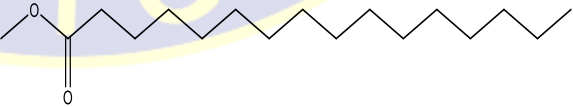
Tabel I.1 Struktur Senyawa Uji

No.	Senyawa	Struktur 2D Senyawa
1	4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	
2	Glucitol,6-O-nonyl	
3	1-Deoxy-d-mannitol	
4	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	
5	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	

LAMPIRAN 5

(LANJUTAN)

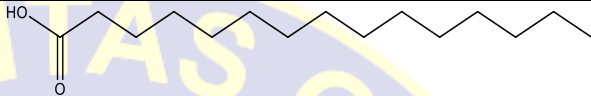
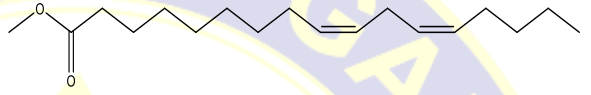
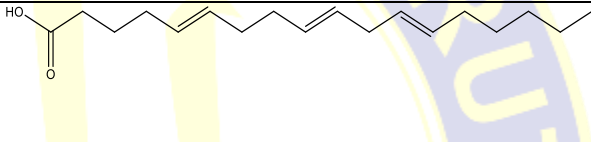
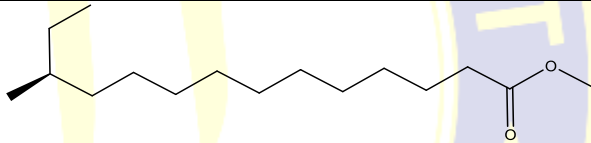
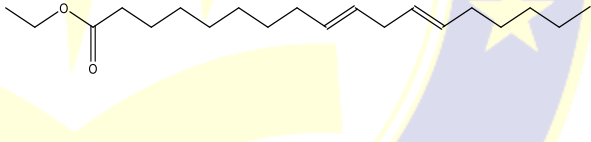

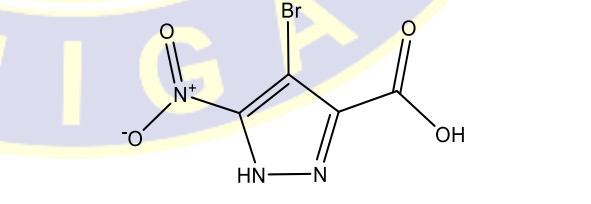
Tabel I.2 Struktur Senyawa Uji

No.	Senyawa	Struktur 2D Senyawa
6	4-Cyclopropyl methylbenzonitrile	
7	Caryophyllen alcohol	
8	Methyl 18-fluoro octadecanoate	
9	E-15-Heptadecenal	
10	2,6,10-trimethyl, 14- ethylene-14-pentadecne	
11	3,7,11,15-Tetramethyl- 2-hexadecen-1-ol	
12	Hexadecanoic acid, methyl ester (palmitic acid)	

LAMPIRAN 5

(LANJUTAN)


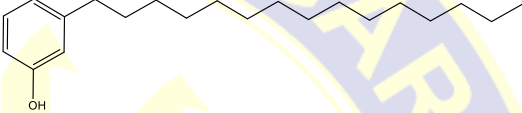
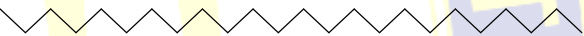

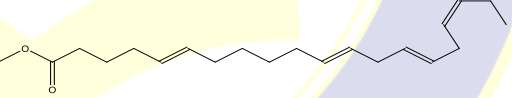
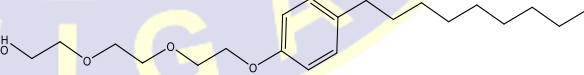
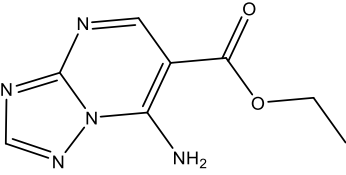
Tabel I.3 Struktur Senyawa Uji

No.	Senyawa	Struktur 2D Senyawa
13	Pentadecanoic acid	
14	Methyl-9,12-heptadecadienoate	
15	5,9,12-octadecatrienoic acid	
16	Methyl 12-methyl tetradecanoate	
17	Ethyl-9,12-octadecadienoate	
18	Butyl-9,12,15-octadecatrienoate	
19	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	

LAMPIRAN 5

(LANJUTAN)

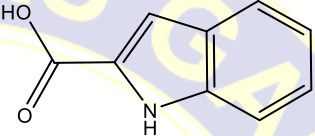
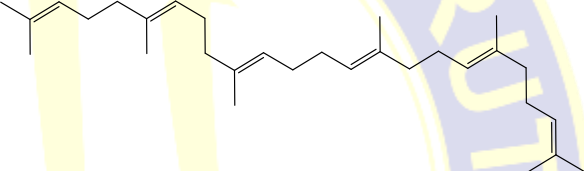
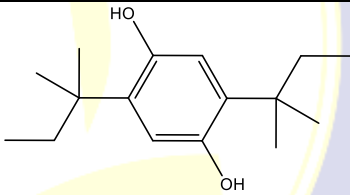
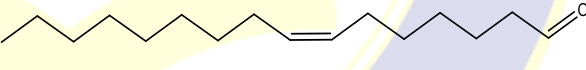
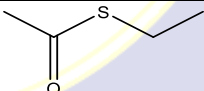
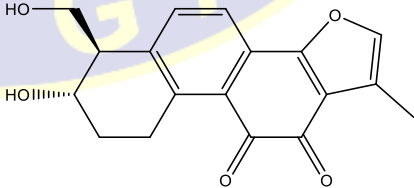
Tabel I.4 Struktur Senyawa Uji

No.	Senyawa	Struktur 2D Senyawa
20	1-O-hexadecylglycerol - bis-trimethylsi	
21	3-Pentadecylphenol	
22	N-Tetracosane	
23	beta.-Humulene	
24	Methyl (Z)-5,11,14,17- eicosatetraenoate	
25	2-[2-[2-(4- nonylphenoxy) ethoxy] ethoxy] ethanol	
26	Ethyl 7- amino[1,2,4]triazolo[1,5- -a] pyrimidine-6- carboxylate	

LAMPIRAN 5

(LANJUTAN)

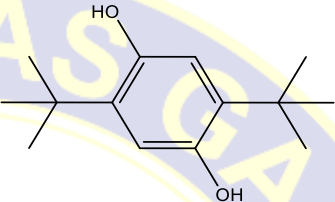
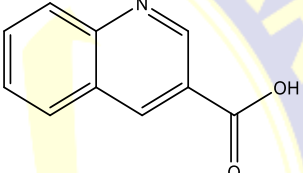
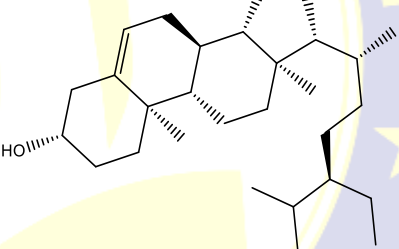
Tabel I.5 Struktur Senyawa Uji

No.	Senyawa	Struktur 2D Senyawa
27	1H-Indole-2-carboxylic acid	
28	2,6,10,14,18,22-Tetracosahexaene	
29	2,5-Di-tert-amylhydroquinone	
30	(Z)-7-Hexadecenal	
31	S-Ethyl ethanethioate	
32	Phenanthro (1,2-b) furan-10,11-dione, 6,7,8,9-tetrahydro-7-hydroxy-6-(hydroxy methyl)-1-methyl-	

LAMPIRAN 5

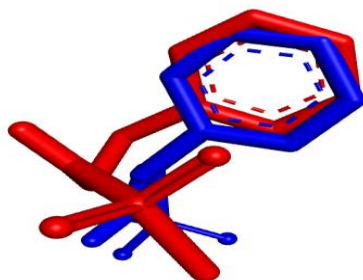
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Tabel I.6 Struktur Senyawa Uji

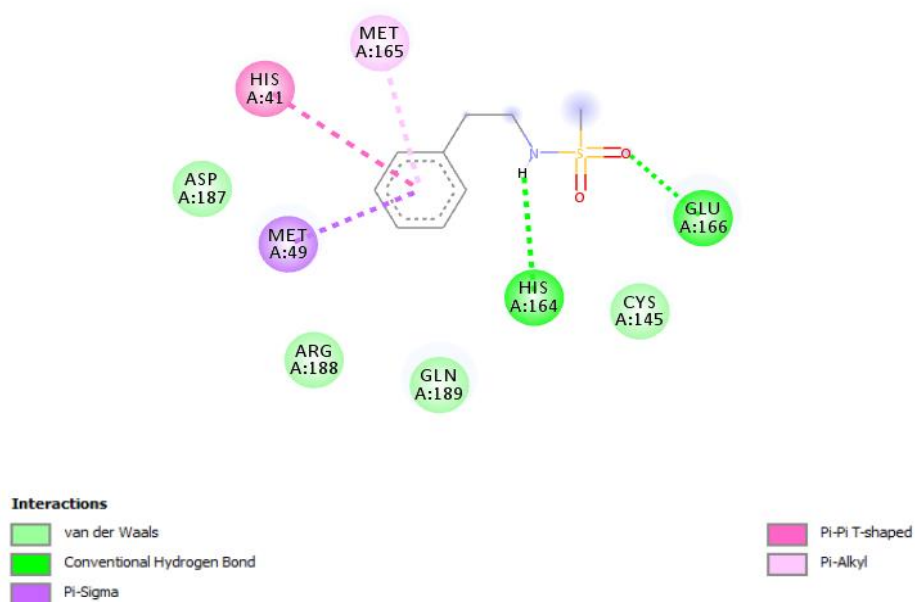
No.	Senyawa	Struktur 2D Senyawa
33	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	
34	Quinoline-3-carboxylic acid	
35	Stigmast-5-en-3-ol	

LAMPIRAN 6

VALIDASI METODE



Gambar IV.1 Hasil visualisasi tumpang tindih ligan alami Enzim Mpro dari hasil kristalografi sinar-X (Merah) dengan ligan hasil *redocking* (biru)



Gambar IV.2 Hasil visualisasi interaksi ligan alami dengan Enzim Mpro

LAMPIRAN 6**(LANJUTAN)****Tabel II.1** *Grid Box, RMSD, Nilai Ikatan Energi dan Nilai Konstanta Inhibisi*

Ligan Alami

Kode Reseptor	Grid Box			RMSD (Å)	Ikatan Energi Bebas (kcal/mol)	Konstanta Inhibisi (nM)
	Size	Center	Spacing			
5R7Y	X : 20 Y : 22 Z : 24	X : 10.301 Y : -2.386 Z : 24.735	0.375 Å	1.510 Å	-4.77	321.51

LAMPIRAN 7

HASIL PENAMBATAN MOLEKUL

Tabel III.1 Hasil Penambatan Molekul dari Ligan Alami dan Senyawa Uji

Senyawa/Ligan	Ikatan Energi (ΔG) kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami Enzim Mpro(N-(2-phenylethyl) methanesulfonamide)	-4.77	1	HIS164, GLU166	321.51
Caryophyllen alcohol	-5.52	-	-	89.88
beta.-Humulene	-5.35	-	-	119.50
2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-5.33	-	-	124.71
2,5-Di-tert-amylhydroquinon	-5.25	-	-	142.32
Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9 tetrahydro-7-hydroxy-6 (5hydroxyl methyl)-1-methyl	-5.21	-	-	152.60
4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	-5.09	2	HIS164, GLU166	186.67
1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-4.84	-	-	284.12
3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-4.62	-	-	408.59

LAMPIRAN 7

(LANJUTAN)

Tabel III.2 Hasil Penambatan Molekul dari Ligan Alami dan Senyawa Uji

Senyawa/Ligan	Ikatan Energi (ΔG) kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Stigmast-5-en-3-ol	-4.47	-	-	530.41
3-Pentadecylphenol	-4.46	-	-	542.09
2,6,10-trimethyl, 14-ethylene-14-pentadecne	-4.36	-	-	631.73
4-Cyclopropyl methylbenzotrile	-4.11	-	-	967.54
2,6,10,14,18,22-Tetracosahexaene	-4.03	-	-	1.12
Methyl 12-methyl tetradecanoate	-4.00	-	-	1.16
Ethyl 7-amino[1,2,4]triazolo [1,5-a] pyrimidine-6-carboxylate	-3.96	1	GLN127	1.25
Methyl-9,12-heptadecadienoat	-3.84	-	-	1.52
1H-Indole-2-carboxylic acid	-3.80	-	-	1.64
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-3.67	-	-	2.04
Methyl (Z)-5,11,14,17-eicosatetraenoate	-3.67	-	-	2.04
E-15-Heptadecenal	-3.61	-	-	2.25
(Z)-7-Hexadecenal	-3.53	-	-	2.60
Ethyl-9,12-octadecadienoate	-3.38	-	-	3.04

LAMPIRAN 7

(LANJUTAN)

Tabel III.3 Hasil Penambatan Molekul dari Ligan Alami dan Senyawa Uji

Senyawa/Ligan	Ikatan Energi (ΔG) kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Butyl-9,12,15-octadecatrienoate	-3.35	-	-	3.50
Hexadecanoic acid, methyl ester (palmitic acid)	-3.31	-	-	3.76
5,9,12-octadecatrienoic acid	-3.15	-	-	4.94
N-Tetracosane	-2.87	-	-	7.92
4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-2.76	-	-	9.44
S-Ethyl ethanethioate	-2.68	-	-	10.82
2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-2.62	-	-	12.01
Pentadecanoic acid	-2.61	-	-	12.29
Quinoline-3-carboxylic acid	-2.54	-	-	2.53
Methyl 18-fluoro octadecanoate	-2.52	1	GLN107	14.21
1-O-hexadecylglycerol - bis-trimethylsi	-2.21	-	-	23.85
1-Deoxy-d-mannitol	-2.00	1	LYS5	34.34
Glucitol,6-O-nonyl	-1.52	2	GLN127, GLU290	77.26

LAMPIRAN 8

HASIL PENGUJIAN *LIPINSKI'S RULE OF FIVE*

Tabel IV.1 Sifat Fisikokimia Senyawa yang Terkandung dalam Daun Jambu

Mawar Berdasarkan 5 Aturan *Lipinski's Rule of Five*

Senyawa	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/ Tidak
Caryophyllen alcohol	1	1	222	3.78	Memenuhi
beta.-Humulene	0	0	204	5.03	Tidak Memenuhi
2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	2	2	540	6.47	Tidak Memenuhi
2,5-Di-tert-amylhydroquinon	2	2	250	4.47	Memenuhi
Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9 tetrahydro-7-hydroxy-6 (6hydroxyl methyl)-1-methyl-	2	5	312	1.36	Memenuhi
4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	1	2	223	2.58	Memenuhi
1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	2	2	222	3.69	Memenuhi

LAMPIRAN 8

(LANJUTAN)

Tabel IV.2 Sifat Fisikokimia Senyawa yang Terkandung dalam Daun JambuMawar Berdasarkan 5 Aturan *Lipinski's Rule of Five*

Senyawa	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/ Tidak
3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	0	6	278	1.22	Tidak Memenuhi
Stigmast-5-en-3-ol	1	1	414	8.02	Tidak Memenuhi
3-Pentadecylphenol	1	1	304	7.02	Tidak Memenuhi
2,6,10-trimethyl, 14-ethylene-14-pentadecne	0	0	278	7.31	Tidak Memenuhi
4-Cyclopropyl methylbenzonitrile	0	1	157	2.51	Tidak Memenuhi
2,6,10,14,18,22-Tetracosahexaen	0	0	410	10.60	Tidak Memenuhi
Methyl 12-methyl tetradecanoate	0	2	256	5.11	Tidak Memenuhi
Ethyl 7-amino[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate	2	6	207	-0.11	Memenuhi
Methyl-9,12-heptadecadienoat	0	2	280	5.58	Tidak Memenuhi
1H-Indole-2-carboxylic acid	2	2	161	1.86	Memenuhi

LAMPIRAN 8

(LANJUTAN)

Tabel IV.3 Sifat Fisikokimia Senyawa yang Terkandung dalam Daun JambuMawar Berdasarkan 5 Aturan *Lipinski's Rule of Five*

Senyawa	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/ Tidak Memenuhi
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1	1	296	6.36	Tidak Memenuhi
Methyl (Z)-5,11,14,17-eicosatetraenoat	0	2	318	6.30	Tidak Memenuhi
E-15-Heptadecenal	0	1	252	5.83	Tidak Memenuhi
(Z)-7-Hexadecenal	0	1	238	5.44	Tidak Memenuhi
Ethyl-9,12-octadecadienoat	0	2	308	6.36	Tidak Memenuhi
Butyl-9,12,15-octadecatrienoat	0	2	334	6.91	Tidak Memenuhi
Hexadecanoic acid, methyl ester (palmitic acid)	0	2	270	5.64	Tidak Memenuhi
5,9,12-octadecatrienoic acid	1	2	278	5.66	Tidak Memenuhi
N-Tetracosane	0	0	338	9.61	Tidak Memenuhi
4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	2	5	235	0.78	Memenuhi
S-Ethyl ethanethioate	0	1	104	1.28	Tidak Memenuhi

LAMPIRAN 8

(LANJUTAN)

Tabel IV.4 Sifat Fisikokimia Senyawa yang Terkandung dalam Daun JambuMawar Berdasarkan 5 Aturan *Lipinski's Rule of Five*

Senyawa	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/ Tidak
2-[2-[2-(4-nonylphenoxy)ethoxy]ethoxy]ethanol	1	1	354	4.38	Memenuhi
Pentadecanoic acid	1	2	242	5.61	Tidak Memenuhi
Quinoline-3-carboxylic acid	1	3	173	1.93	Memenuhi
Methyl 18-fluoro octadecanoate	0	2	316	6.37	Tidak Memenuhi
1-O-hexadecylglycerol - bis-trimethylsi	2	3	316	4.84	Memenuhi
1-Deoxy-d-mannitol	5	5	166	-2.56	Memenuhi
Glucitol,6-O-nonyl	5	6	308	0.18	Memenuhi

Keterangan :

Donor Ikatan Hidrogen : ≤ 5 Akseptor Ikatan Hidrogen : ≤ 10 Bobot Molekul : ≤ 500 g/molLog P : ≤ 5

LAMPIRAN 9

HASIL PENGUJIAN *PreADME*Tabel V.1 Uji *PreADME* (Absorpsi dan Distribusi)

Senyawa	Absorpsi		Distribusi
	Caco-2 cell (nm sec-1)	HIA (%)	Protein Plasma Binding (%)
Caryophyllen alcohol	46.23	100.0	100.0
beta.-Humulene	23.49	100.0	100.0
2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	39.77	95.35	100.0
2,5-Di-tert-amylhydroquinon	28.68	90.51	85.52
Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9 tetrahydro-7-hydroxy-6 (65ydroxyl methyl)-1-methyl-	21.12	94.53	89.51
4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	41.53	99.51	47.59
1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	23.98	90.84	100.0
3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	19.53	87.33	62.63
Stigmast-5-en-3-ol	23.40	100.0	100.0
3-Pentadecylphenol	56.03	100.0	100.0
2,6,10-trimethyl, 14-ethylene-14-pentadecne	23.27	100.0	100.0

LAMPIRAN 9

(LANJUTAN)

Tabel V.2 Uji *PreADME* (Absorpsi dan Distribusi)

Senyawa	Absorpsi		Distribusi
	Caco-2 cell (nm sec-1)	HIA (%)	Protein Plasma Binding (%)
4-Cyclopropyl methylbenzotrile	12.92	100.0	87.98
2,6,10,14,18,22- Tetracosahexaen	23.40	100.0	100.0
Methyl 12-methyl tetradecanoate	41.95	100.0	100.0
Ethyl 7- amino[1,2,4]triazolo[1,5-a] pyrimidine-6-carboxylate	20.29	81.19	33.31
Methyl-9,12-heptadecadienoat	46.43	100.0	100.0
1H-Indole-2-carboxylic acid	20.40	88.49	36.91
3,7,11,15-Tetramethyl-2- hexadecen-1-ol	37.63	100.0	100.0
Methyl (Z)-5,11,14,17- eicosatetraenoat	48.15	100.0	100.0
E-15-Heptadecenal	49.75	100.0	100.0
(Z)-7-Hexadecenal	23.19	100.0	100.0

LAMPIRAN 9

(LANJUTAN)

Tabel V.3 Uji *PreADME* (Absorpsi dan Distribusi)

Senyawa	Absorpsi		Distribusi
	Caco-2 cell (nm sec-1)	HIA (%)	Protein Plasma Binding (%)
Ethyl-9,12-octadecadienoat	57.11	100.0	100.0
Butyl-9,12,15-octadecatrienoat	57.26	100.0	100.0
Hexadecanoic acid, methyl ester (palmitic acid)	45.84	100.0	100.0
5,9,12-octadecatrienoic acid	27.97	98.27	100.0
N-Tetracosane	22.19	100.0	100.0
4-bromo-5-nitro-1h-pyrazole-3- carboxylic acid	17.33	57.21	17.60
S-Ethyl ethanethioate	21.67	100.0	76.65
2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	40.05	95.50	93.14
Pentadecanoic acid	25.04	98.11	100.0
Quinoline-3-carboxylic acid	20.97	97.90	86.62

LAMPIRAN 9

(LANJUTAN)

Tabel V.4 Uji *PreADME* (Absorpsi dan Distribusi)

Senyawa	Absorpsi		Distribusi
	Caco-2 cell (nm sec-1)	HIA (%)	Protein Plasma Binding (%)
Methyl 18-fluoro octadecanoate	49.11	100.0	100.0
1-O-hexadecylglycerol - bis-trimethylsi	49.14	91.38	100.0
1-Deoxy-d-mannitol	0.95	46.33	15.49
Glucitol,6-O-nonyl	0.89	42.95	78.89

Keterangan : HIA (*Human Intestinal Absorpsi*) = 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*

Plasma Protein Binding = > 90% *strongly bound*

< 90% *weakly bound*

LAMPIRAN 10

HASIL PENGUJIAN TOKSISITAS

Tabel VI.1 Uji Toksisitas

Senyawa	Ames Test	Karsinogenik
	Mutagen / Non Mutagen	(-) / (+)
Caryophyllen alcohol	Mutagen	Positif
beta.-Humulene	Mutagen	Positif
2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	Non- Mutagen	Negatif
2,5-Di-tert-amylhydroquinon	Non-Mutagen	Negatif
Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9 tetrahydro-7-hydroxy-6 (69droxyl methyl)-1-methyl-	Mutagen	Positif
4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	Mutagen	Negatif
1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	Non- Mutagen	Negatif
3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	Mutagen	Negatif
Stigmast-5-en-3-ol	Non- Mutagen	Positif
3-Pentadecylphenol	Non- Mutagen	Positif
2,6,10-trimethyl, 14-ethylene-14-pentadecne	Non- Mutagen	Negatif
4-Cyclopropyl methylbenzonitrile	Mutagen	Negatif

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(LANJUTAN)

Tabel VI.2 Uji Toksisitas

Senyawa	Ames Test	Karsinogenik
	Mutagen / Non Mutagen	(-) / (+)
2,6,10,14,18,22-Tetracosahexaen	Mutagen	Negatif
Methyl 12-methyl tetradecanoate	Non-Mutagen	Positif
Ethyl 7-amino[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylate	Mutagen	Negatif
Methyl-9,12-heptadecadienoat	Non- Mutagen	Positif
1H-Indole-2-carboxylic acid	Mutagen	Negatif
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	Non- Mutagen	Positif
Methyl (Z)-5,11,14,17-eicosatetraenoat	Non-Mutagen	Positif
E-15-Heptadecenal	Non- Mutagen	Positif
(Z)-7-Hexadecenal	Non-Mutagen	Positif
Ethyl-9,12-octadecadienoat	Non- Mutagen	Positif
Butyl-9,12,15-octadecatrienoat	Non- Mutagen	Positif
Hexadecanoic acid, methyl ester (palmitic acid)	Non- Mutagen	Positif
5,9,12-octadecatrienoic acid	Mutagen	Positif
N-Tetracosane	Non- Mutagen	Positif

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(LANJUTAN)

Tabel VI.3 Uji Toksisitas

Senyawa	Ames Test	Karsinogenik
	Mutagen / Non Mutagen	(-) / (+)
4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	Mutagen	Negatif
S-Ethyl ethanethioate	Mutagen	Negatif
2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	Mutagen	Negatif
Pentadecanoic acid	Non- Mutagen	Negatif
Quinoline-3-carboxylic acid	Mutagen	Negatif
Methyl 18-fluoro octadecanoate	Non- Mutagen	Positif
1-O-hexadecylglycerol - bis-trimethylsi	Non-Mutagen	Negatif
1-Deoxy-d-mannitol	Mutagen	Negatif
Glucitol,6-O-nonyl	Non- Mutagen	Negatif

DAFTAR RIWAYAT HIDUP

DATA PRIBADI



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- Pelatihan Kimia *Atomic Absorption Spectrophotometer* (AAS) dan *Fourier Transform Infra Red* (FTIR)

