DAFTAR PUSTAKA

1. Kurniyawan, E. H. Narrative Review: Terapi Komplementer Alternatif Akupresur dalam Menurunkan Tingkat Nyeri. *NurseLine J.* **1**, 246–256 (2016).
2. Public, G. & Priority, H. Pain as a Global Public Health Priority Pain as a Global Public Health Priority. *BMC Public Health* 0–11 (2011) doi:10.1186/1471-2458-11-770.
3. Rahardja.K., T. T. &. *Obat-Obat Penting Khasiat, Penggunaan, dan Efek-Efek Sampingnya*. (PT Elex Media Komputindo, 2007).
4. Katzung, BG., Masters, S.B.dan Trevor, A. J. *Farmakologi Dasar & Klinik*. (Buku Kedokteran EGC, 2014).
5. Yulianti, S. Inventarisasi Tanaman Obat di Arboretum (Bukit 1) Kecamatan Samarang Kabupaten Garut. Fakultas MIPA. Universitas Garut. (2015).
6. Ávila-Peña, D., Peña, N., Quintero, L. & Suárez-Roca, H. Antinociceptive activity of Syzygium jambos leaves extract on rats. *J. Ethnopharmacol.* **112**, 380–385 (2007).
7. Bonfanti, G. *et al.* Syzygium jambos and Solanum guaraniticum show similar antioxidant properties but induce different enzymatic activities in the brain of rats. *Molecules* **18**, 9179–9194 (2013).
8. IT IS (Integrated Taxonomic Information System). *Syzygium Jambos (L.) Alston*. https://www.itis.gov/servlet/SingleRpt/SingleRpt?search_topic=TSN&sear

ch_value=505420 (2011).

9. Heyne, K. *Tumbuhan Berguna Indonesia jilid III*. (1987).

10. Morton, J. Rose Apple (J.) Fruitr of Warm Climates. in 383–386 (1987).

11. Devakumar, J., Keerthana, V. & Sudha, S. S. Identification of bioactive compounds by gas chromatography-mass spectrometry analysis of Syzygium jambos (L.) collected from Western Ghats region Coimbatore, Tamil Nadu. *Asian J. Pharm. Clin. Res.* **10**, 364–369 (2017).

12. Sharma, R., Kishore, N., Hussein, A. & Lall, N. Antibacterial and anti-inflammatory effects of Syzygium jambos L. (Alston) and isolated compounds on acne vulgaris. *BMC Complement. Altern. Med.* **13**, 1–10 (2013).

13. Suwandi, D. W., Perdana, F., Garut, F. M. & No, J. J. Jurnal Ilmiah Farmako Bahari ANTIHYPERURICEMIA ACTIVITY OF ETHANOL EXTRACT AND GUAVA LEAF FRACTIONS IN SWISS WEBSTER MALE FRAKSI-FRAKSI DAUN JAMBU MAWAR PADA MENCIT. 35–44 (2018).

14. Handayani, S., Wirasutisna, K. & Insanu, M. Penapisan Fitokimia Dan Karakterisasi Simplisia Daun Jambu Mawar (Syzygium jambos Alston) Selpida. *Jf Fik Uinam* **5**, 177–179 (2017).

15. Al-hawshabi, O. S. S. Syzygium jambos (L.) Alston (Myrtaceae), a new record introduced to the flora of Yemen. *J. Biol. Earth Sci.* **4**, 52–56 (2014).

16. Mamahit, P., Wuisan, J. & Anindita, P. S. Efektifitas Ekstrak Daun Jambu Mawar (Syzigium jambos L. alston) MENGHAMBAT PERTUMBUHAN

Streptococcus mutans SECARA IN VITRO. *Pharmacon* **5**, 53–58 (2016).

17. Mutschler. *Dinamika Obat Terjemahan Widiyanto M.B A.S. Ranti*. (Penerbit ITB, 1991).
18. Yulinah, E., D. *ISO Farmakoterapi*. (PT. ISFI, 2008).
19. Guyton, A. C. *Fisiologi Manusia dan Mekanisme Penyakit*. (Buku Kedokteran EGC, 1990).
20. Denise R. Ferrier, PhD., Richard A. Harvey, P. *Lippincott's Illustrated Reviews Biochemistry*.
21. Susanti R, F. F. *Teknologi Enzim*. (CV. Andi Offset, 2017).
22. Fessenden RJ, F. J. *Kimia Organik jilid II*. (Erlangga, 1986).
23. Syamsudin, M. B. *Famakologi Molekuler; mekanisme kerja obat pada tingkat molekul*. (Buku Kedokteran EGC, 2014).
24. Sarker, S. dan N. L. *Kimia Untuk Mahasiswa Farmasi Bahan Kimia Organik, Alam dan Umum.* (Pustaka Belajar, 2009).
25. Muchtaridi & Yusuf, M. Teori dan Praktek Penambatan Molekul (Molecular Docking). in 15-16p, 37-38pp (Univeristas Padjadjaran Press, 2018).
26. Rose, P. W. *et al.* The RCSB Protein Data Bank: New resources for research and education. *Nucleic Acids Res.* **41**, 475–482 (2013).
27. Wang, Y. *et al.* PubChem's BioAssay database. *Nucleic Acids Res.* **40**, (2012).
28. A., N. Introduction to the Discovery Studio Visualizer Introduction. http://www.adrianomartinelli.it/Fondamenti/Tutorial_0.pdf.
29. Morris G M, S David, E. M. *Autodock Version 4.2*.

30. Nursamsiar, Ibrahim S, H. T. D. Absorption, Distribution and Toxicity Prediction of Curculigoside A and its Derivatives. doi:10.2991/iccst-15.2015.7.

31. Suppercomputing Facility for Bionformatic & Computational Biologi. Lipinski's Rule Of Five. http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp.

32. Situs Protein Data Bank (PDB) [Serial Online]. https://www.rcsb.org/.

33. Situs PubChem [Serial Online]. https://pubchem.ncbi.nlm.nih.gov/.

34. Situs Pre-ADMET [Serial Online]. https://preadmet.bmdrc.kr/adme/.

35. Situs Lipinski's Rule Of Five [Serial Online]. http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp.

36. Muttaqin, F. Z. Molecular Docking and Molecular Dynamic Studies of Stilbene Derivative Compounds As Sirtuin-3 (Sirt3) Histone Deacetylase Inhibitor on Melanoma Skin Cancer and Their Toxicities Prediction. *J. Pharmacopolium* **2**, 112–121 (2019).

37. Marcio F, Giminez B G, S. M. S. Evaluation of Blocbuster Drugs Under The Rule of Five. doi: 10.1691/ph.2010.9733.

LAMPIRAN 1

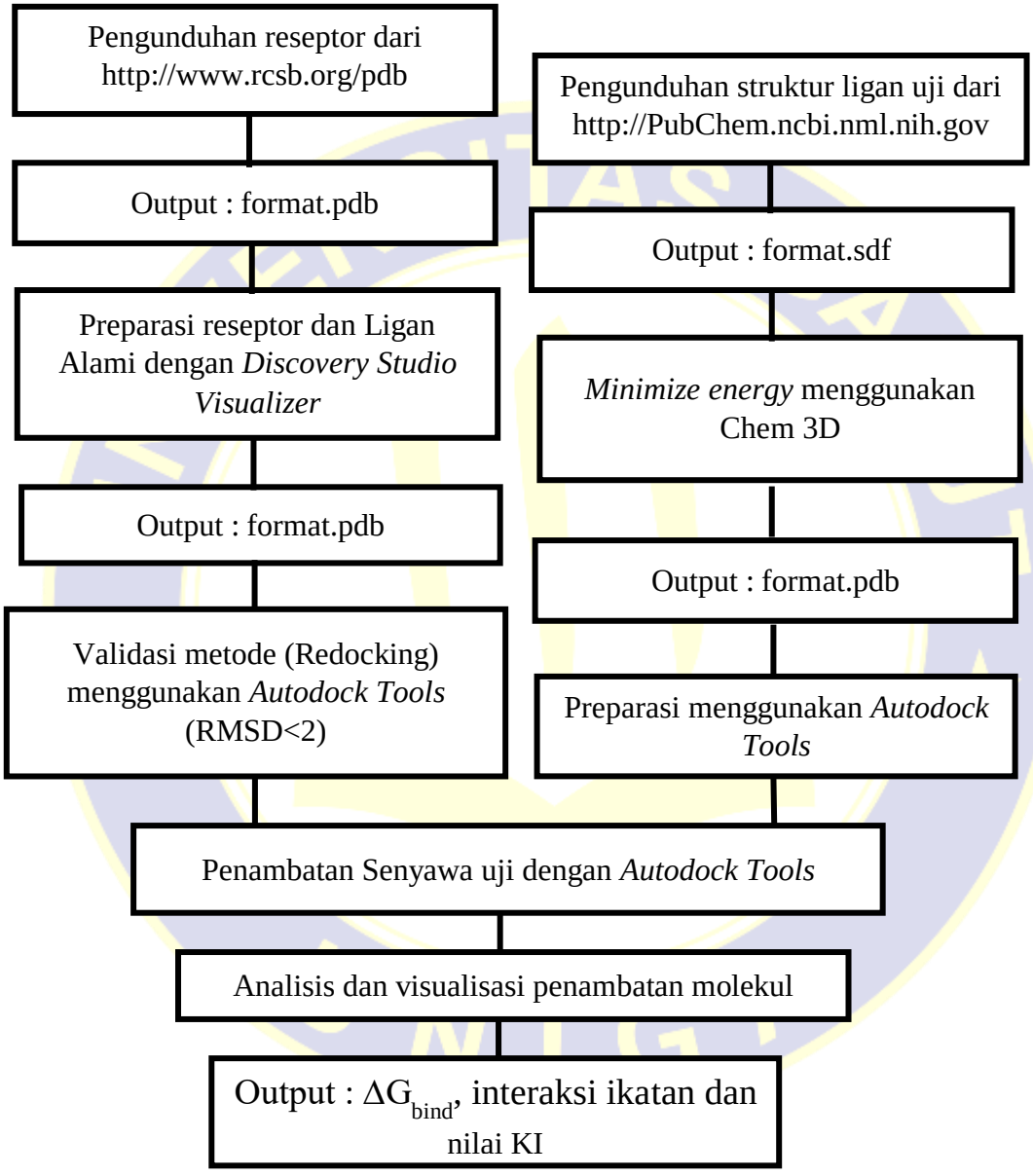
DAUN JAMBU MAWAR

Gambar II.2 Tanaman Daun Jambu Mawar

Sumber: https://pixabay.com/id/photos/rosenpfel-buah-buahan-pohon-daun-93629/

LAMPIRAN 2

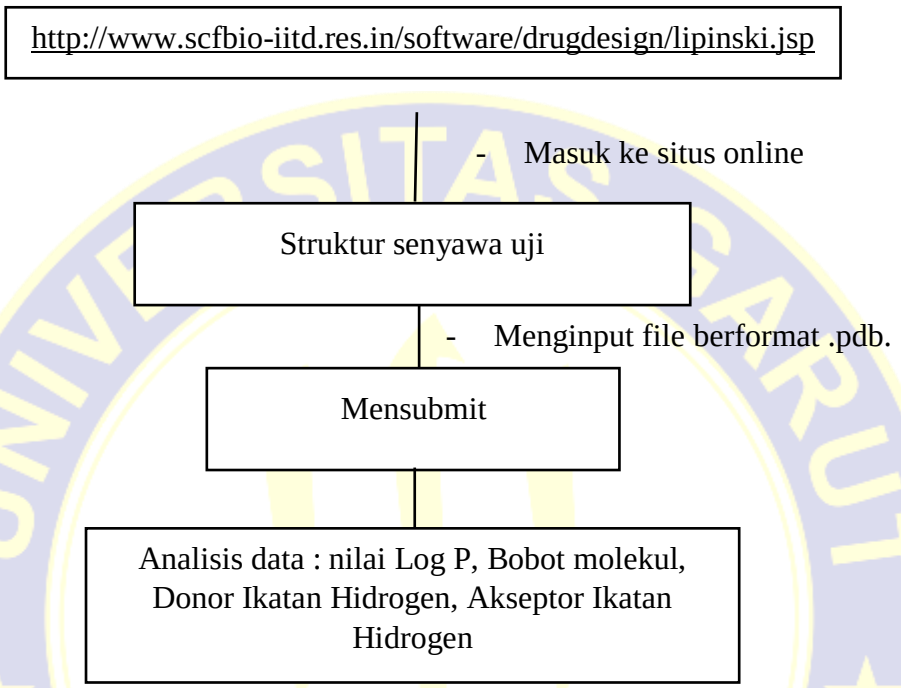
ALUR PENELITIAN



Gambar IV.1 Alur Penelitian Penambatan Molekul

LAMPIRAN 2
(LANJUTAN)

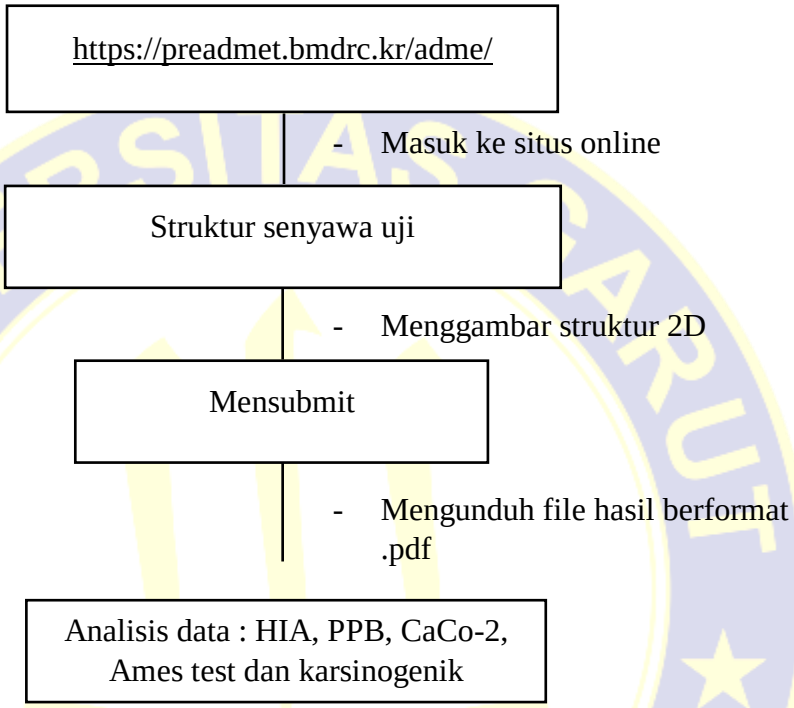
ALUR PENELITIAN



Gambar IV.2 Analisis *Lipinski's Rule of Five*

LAMPIRAN 2
(LANJUTAN)

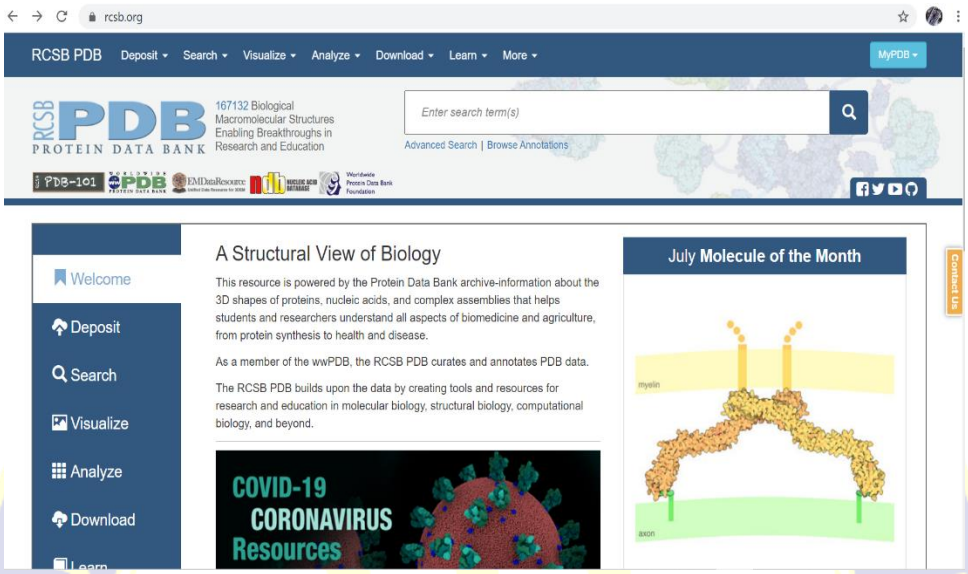
ALUR PENELITIAN



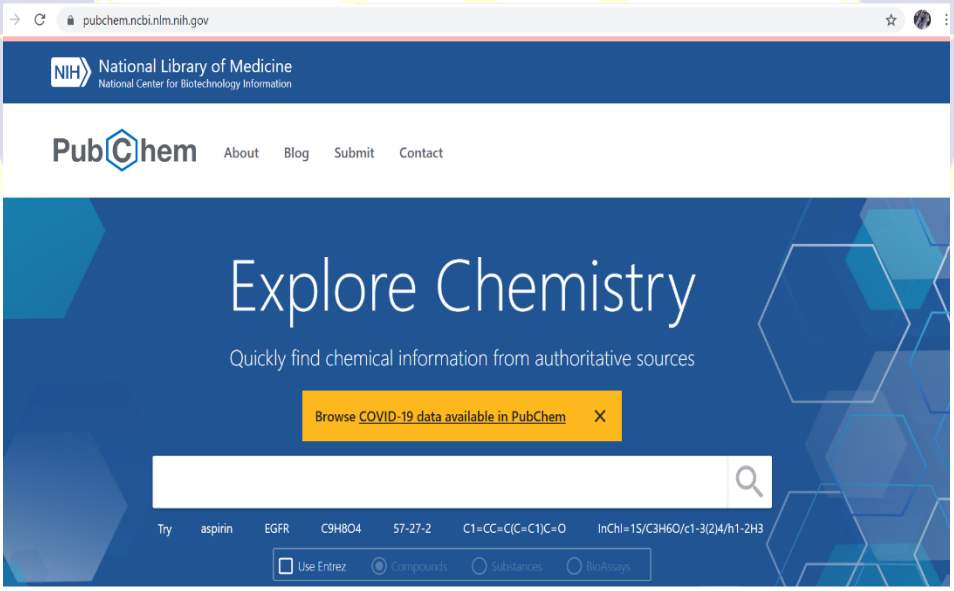
Gambar IV.3 Analisis *pre-ADME* dan Toksisitas

LAMPIRAN 3

SITUS DAN APLIKASI

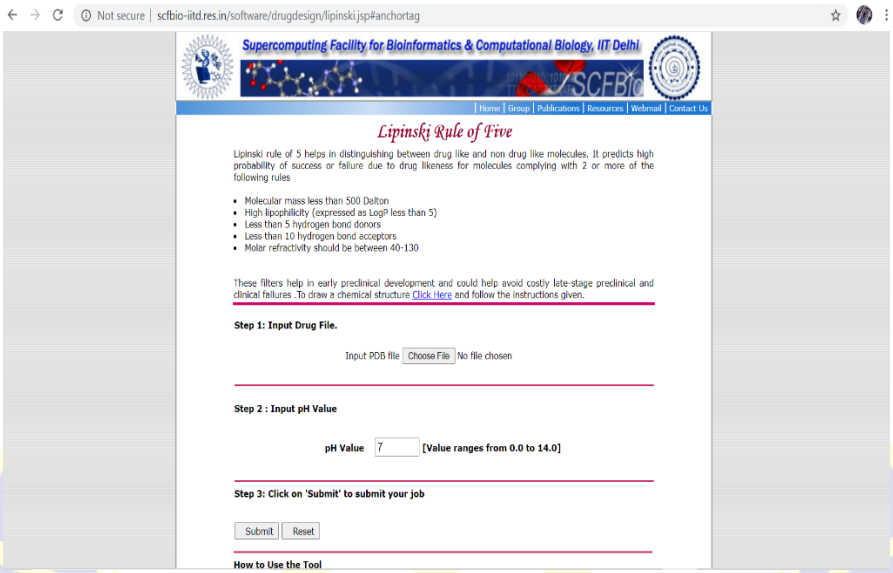


Gambar IV.4 Tampilan situs *Protein Data Bank* (PDB)

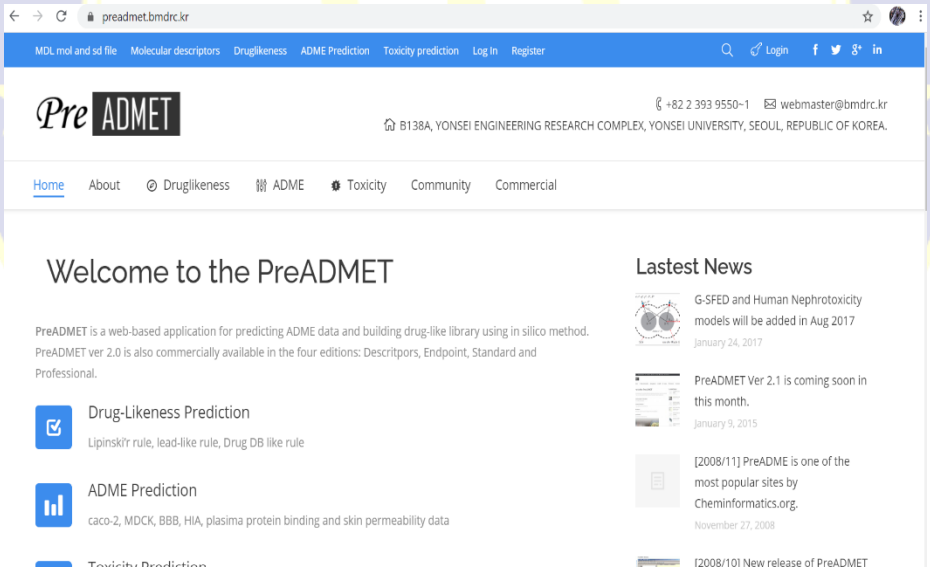


Gambar IV.5 Tampilan situs *Pubchem*

LAMPIRAN 3
(LANJUTAN)

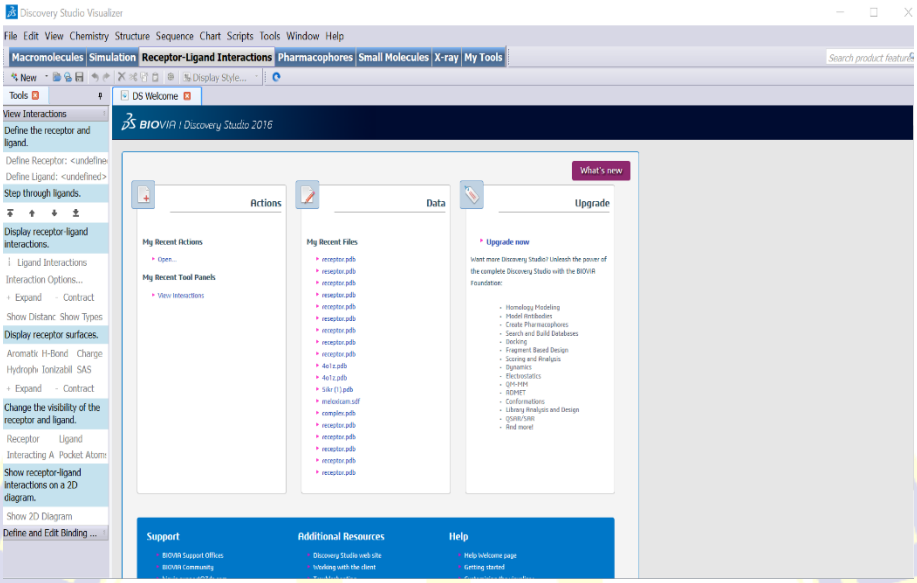


Gambar IV.6 Tampilan situs *Lipinski's Rule of Five*

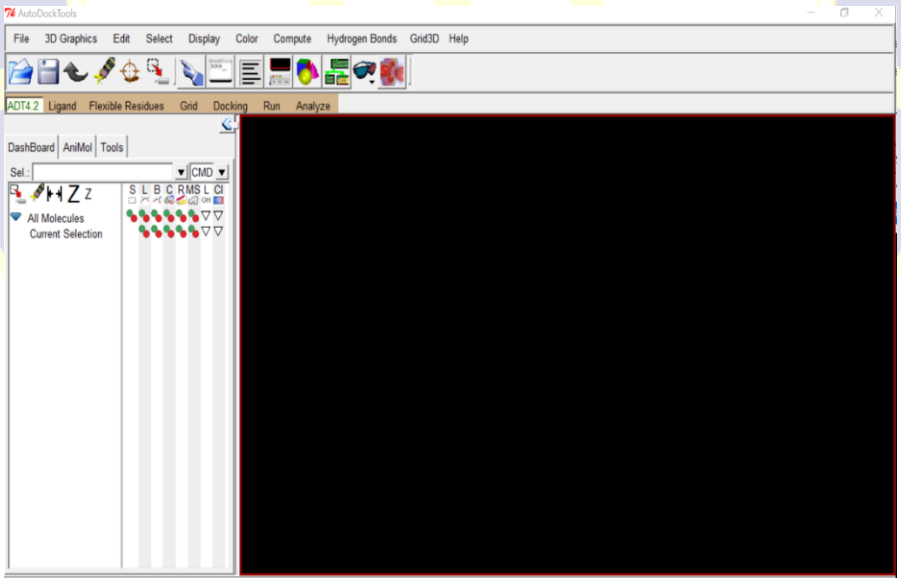


Gambar IV.7 Tampilan situs Pre*ADMET*

LAMPIRAN 3
(LANJUTAN)

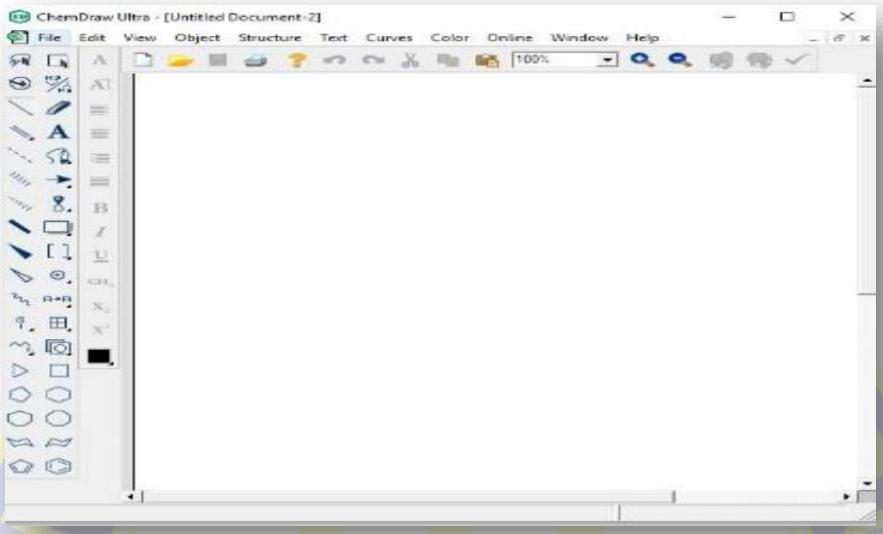


Gambar IV.8 Tampilan aplikasi *Discovery Studio Visualizer*®



Gambar IV.9 Tampilan aplikasi *AutoDock Tools*®

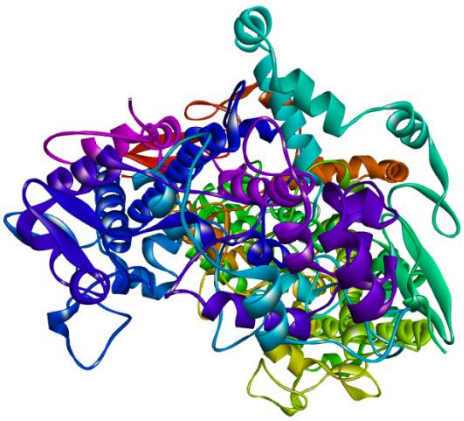
LAMPIRAN 3
(LANJUTAN)



Gambar IV.10 Tampilan aplikasi *Chemdraw Office*®

LAMPIRAN 4

STRUKTUR 3D RESEPTOR



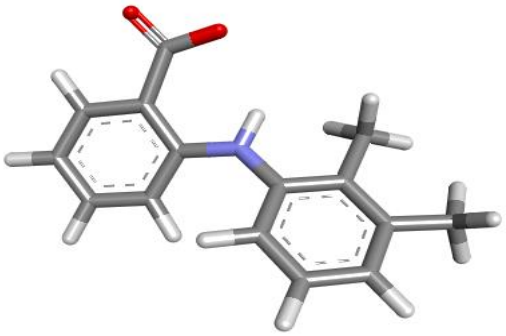
Gambar IV.11 COX-1 (kode 4O1Z)

Gambar IV.12 COX-2 (kode 5IKR)

LAMPIRAN 5

LIGAN ALAMI

Gambar IV.13 Ligan Alami Reseptor COX-1 Complex With Meloxicam

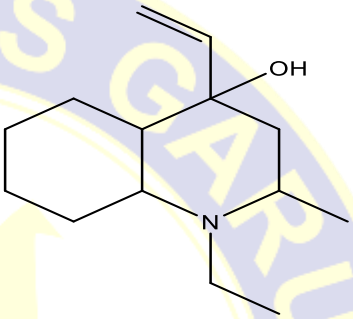
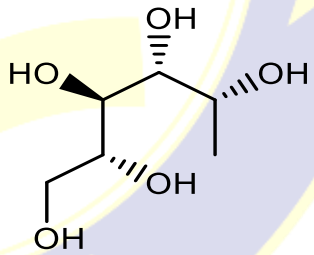
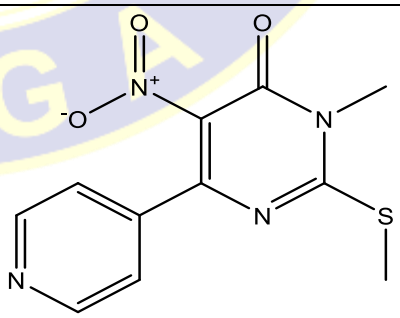


Gambar IV.14 Ligan Alami Reseptor COX-2 (Asam Mefenamat)

LAMPIRAN 6

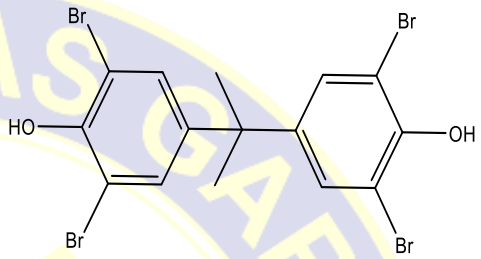
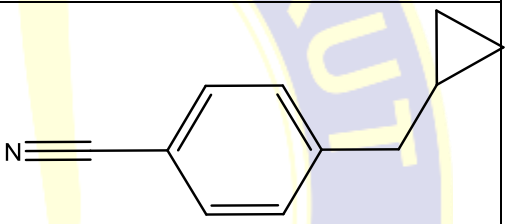
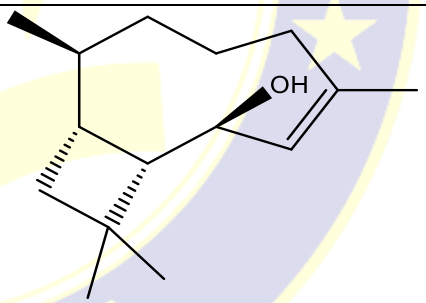
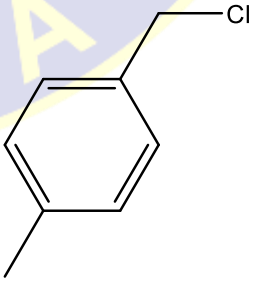
STRUKTUR 2D LIGAN UJI

Tabel IV.1
Senyawa Daun Jambu Mawar (*Syzygium Jambos* .L. Alston)

No.	Nama Senyawa	Struktur
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	

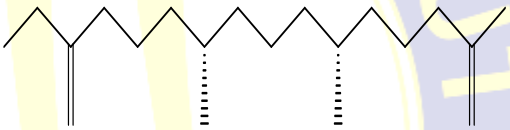
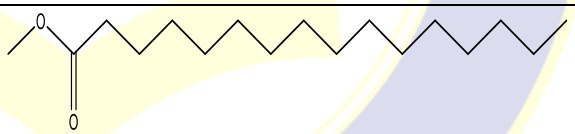
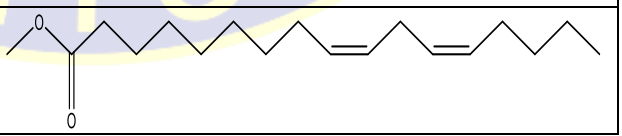
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
5.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	
6.	4-Cyclopropyl methyl benzonitrile	
7.	Caryophyllen alcohol	
8.	4-Methylbenzyl chloride	

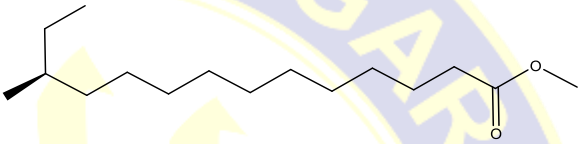
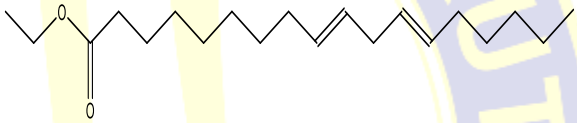
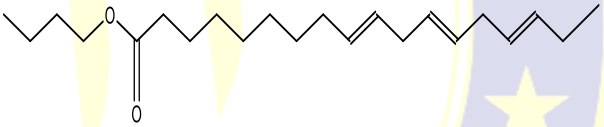
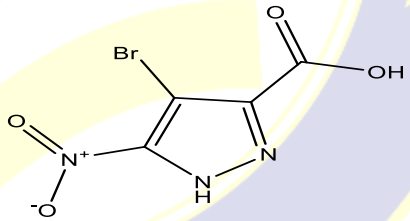
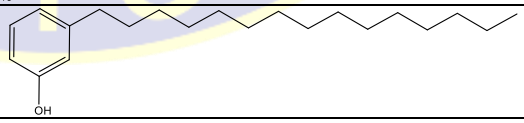
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
9.	Methyl 18-fluorooctadecanoate	
10.	E-15-Heptadecenal	
11.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	
12.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	
13.	Hexadecanoic acid, methyl ester	
14.	Pentadecanoic acid	
15.	Methyl-9,12-heptadecadienoate	

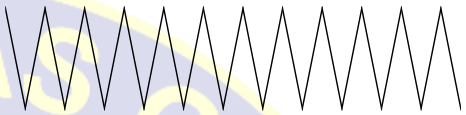
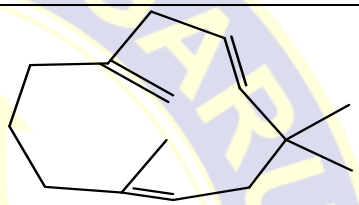
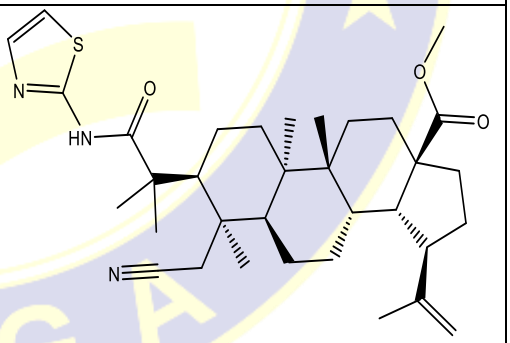
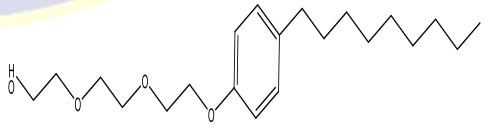
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
16.	5,9,12-octadecatrienoic acid	
17.	Methyl-12-methyltetradecanoic	
18.	Ethyl-9,12-octadecadienoate	
19.	Butyl-9,12,15-octadecatrienoate	
20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	
21.	1-O-hexadecylglycerol - bis-trimethylsi	
22.	3-Pentadecylphenol	

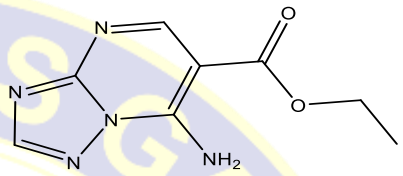
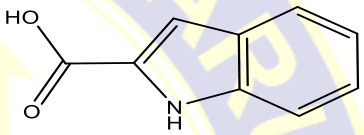
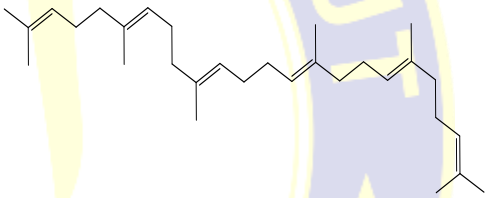
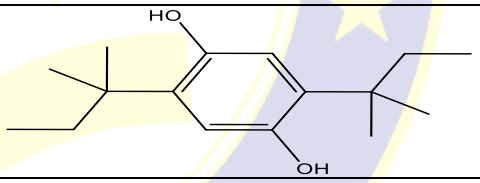
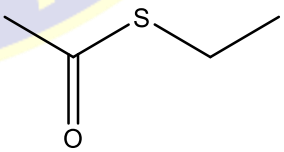
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
23.	N-Tetracosane	
24.	beta.-Humulene	
25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	
26.	methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	
27.	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	

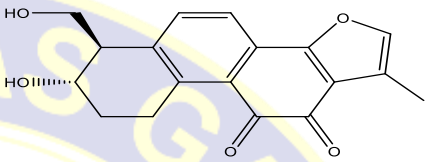
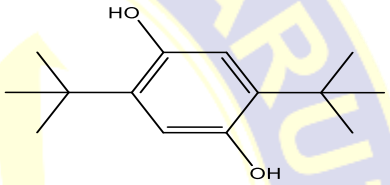
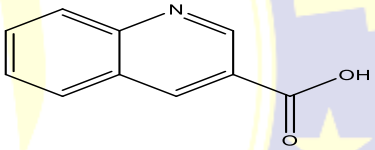
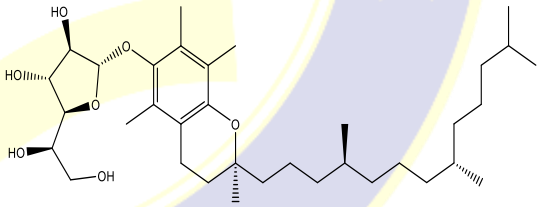
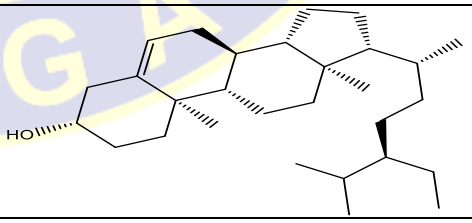
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
28.	Ethyl 7-amino [1,2,4] triazolo[1,5-a] pyrimidine-6-carboxylate	
29.	1H-Indole-2-carboxylic acid	
30.	2,6,10,14,18,22-Tetracosahexaene	
31.	2,5-Di-tert-amylhydroquinone	
32.	7-Hexadecenal	
33.	S-Ethyl ethanethioate	

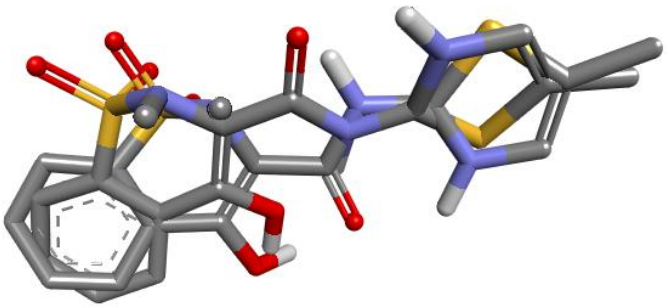
LAMPIRAN 6
(LANJUTAN)

Tabel IV.1
Lanjutan

No.	Nama Senyawa	Struktur
34.	Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9-tetrahydro-7-hydroxy-6-(hydroxymethyl)-1-methyl- (Przewaquinone F)	
35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	
36.	Quinoline-3-carboxylic acid	
37.	alpha.-Tocopherol-.beta.-D-mannoside	
38.	Stigmast-5-en-3-ol	

LAMPIRAN 7

VALIDASI METODE

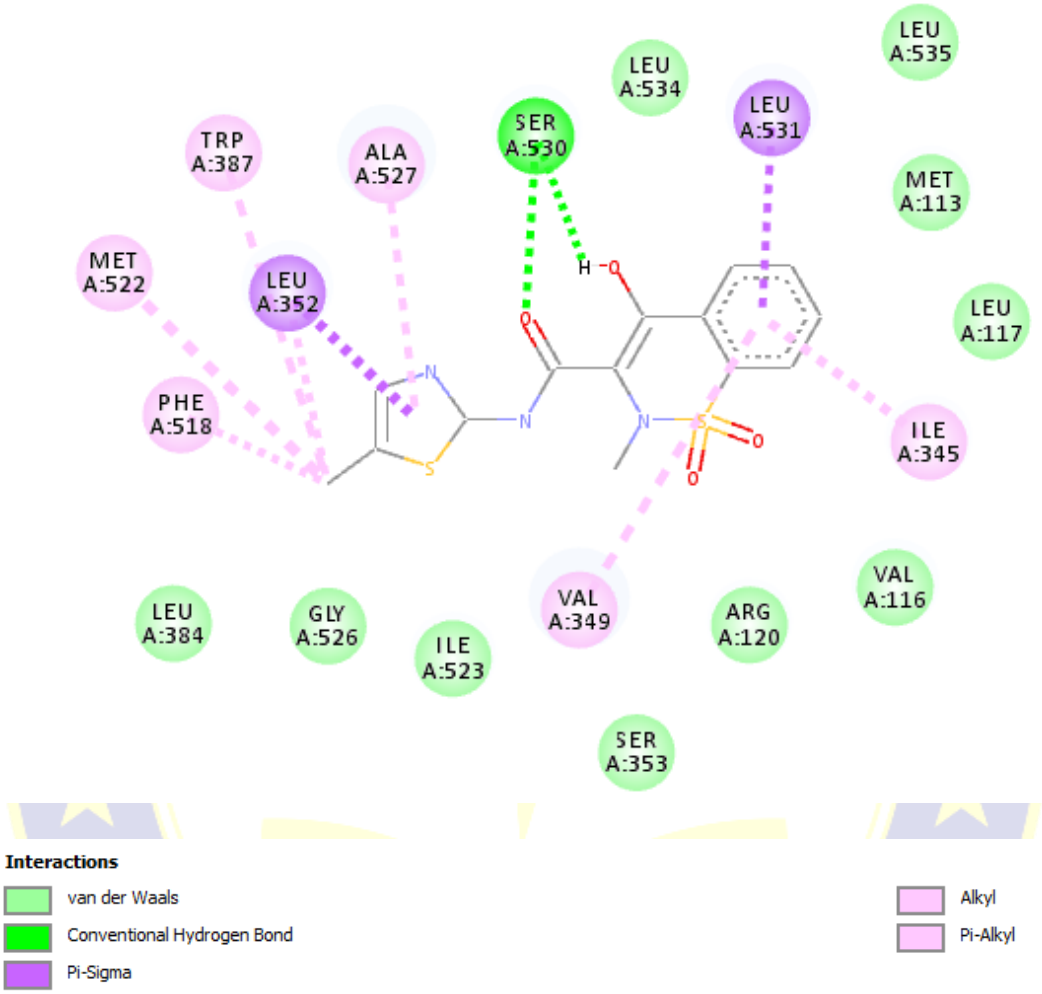


Gambar V.1 Hasil visualisasi tumpang tindih ligan alami (Meloxicam) dengan reseptor cox-1 dari hasil kristalografi sinar X dengan ligan hasil *redocking*

Tabel V.1 *Grid Box, RMSD,* dan Nilai Energi Ikatan Ligan alami

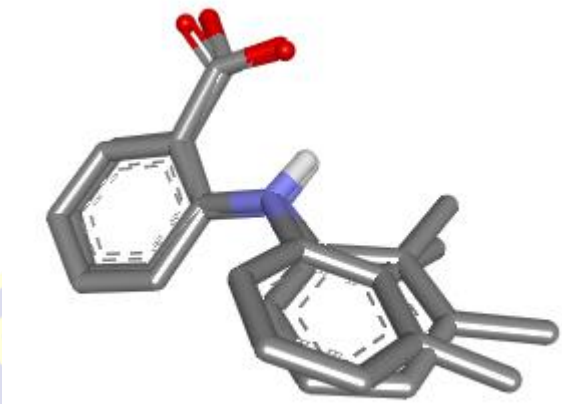
Kode Reseptor	**Grid Box**	**RMSD(Å)**	**ΔG (kkal/mol)**	**Konstanta Inhibisi (µM)**
4OIZ (Meloxicam)	X: 251.485 Y: 107.183 Z: 4.561	1.253	-8.74	0.391

LAMPIRAN 7
(LANJUTAN)



Gambar V.2 Hasil visualisasi interaksi ligan alami (meloxicam) dengan reseptor *cyclooxygenase-1*

LAMPIRAN 7
(LANJUTAN)

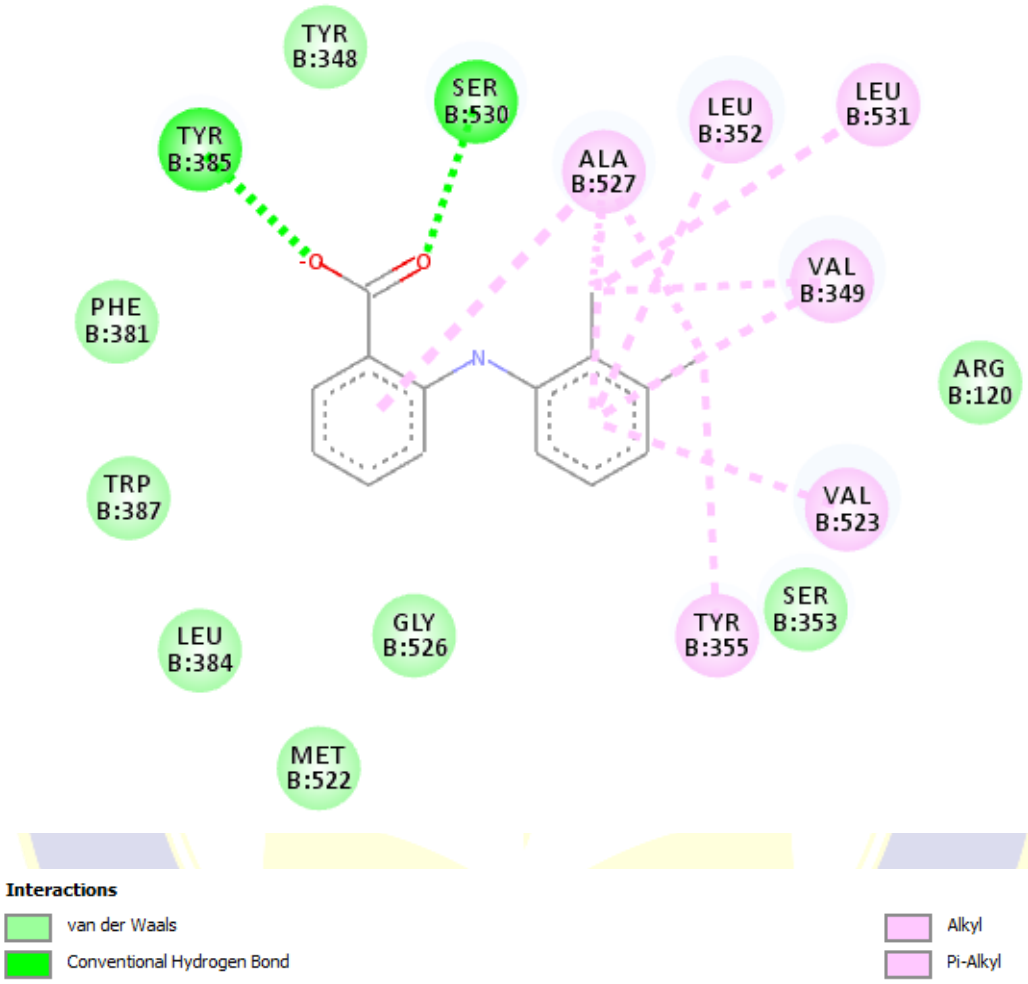


Gambar V.3 Hasil visualisasi tumpang tindih ligan alami (asam mefenamat) dengan reseptor cox-2 dari hasil kristalografi sinar X dengan ligan hasil *redocking*

Tabel V.2 *Grid Box*, *RMSD*, dan Nilai Energi Ikatan Ligan alami

Kode Reseptor	**Grid Box**	**RMSD(Å)**	**ΔG (kkal/mol)**	**Konstanta Inhibisi (µM)**
5IKR (Asam Mefenamat)	X: 40.741 Y: 38.189 Z: 85.878	0.536	-7.25	4.86

LAMPIRAN 7
(LANJUTAN)



Gambar V.4 Hasil visualisasi interaksi ligan alami (asam mefenamat) dengan reseptor *cyclooxygenase-2*

LAMPIRAN 8

HASIL PENAMBATAN MOLEKUL

Tabel V.3
Nilai Energi Ikatan dari Ligan Alami dan Senyawa Uji
pada enzim *Cyclooxygenase* -1

No.	Senyawa/Ligan	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Meloxicam	-8.74	1	SER530	0.391
Ligan Uji					
1.	4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	-6.49	1	ALA527	17.47
2.	Glucitol,6-O-nonyl	-4.20	-	-	838.
3.	1-Deoxy-d-mannitol	-2.05	2	ALA527 SER 530	31.450
4.	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-6.47	1	TYR355	17.99
5.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-8.30	2	SER 530 TYR385	0.824
6.	4-Cyclopropyl methyl benzonitrile	-5.92	-	-	46.06
7.	Caryophyllen alcohol	-7.67	2	ARG120 TYR355	2.37
8.	4-Methylbenzyl chloride	-5.11	-	-	180.51
9.	Methyl 18-fluorooctadecanoate	-6.20	1	TYR385	28.73

LAMPIRAN 8
(LANJUTAN)

Tabel V.3
Lanjutan

No.	Senyawa/Ligan	ΔG kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Meloxicam	-8.74	1	SER530	0.391
Ligan Uji					
10.	E-15-Heptadecenal	-6.57	1	SER530	15.27
11.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	-8.14	-	-	1.09
12.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-7.90	1	GLY526	1.63
13.	Hexadecanoic acid, methyl ester (palmitic acid)	-6.10	2	SER530 TYR385	33.67
14.	Pentadecanoic acid	-6.49	2	ARG120 TYR355	17.44
15.	Methyl-9,12-heptadecadienoate	-6.76	-	-	11.04
16.	5,9,12-octadecatrienoic acid	-8.22	2	ARG 120 TYR355	0.940
17.	Tetradecanoic acid, 12-methyl-, methyl ester	-6.38	1	ARG120	21.02
18.	Ethyl-9,12-octadecadienoate	-7.31	1	SER530	4.38
19.	Butyl-9,12,15-octadecatrienoate	-7.28	-	-	4.63

LAMPIRAN 8
(LANJUTAN)

Tabel V.3
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Meloxicam	-8.74	1	SER530	0.391
Ligan Uji					
20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-5.07	2	TYR 355 ARG120	193.67
21.	1-O-hexadecylglycerol -bis-trimethylsi	-5.74	2	SER530 ALA527	62.13
22.	3-Pentadecylphenol	-7.84	1	MET522	1.79
23.	N-Tetracosane	-7.65	-	-	2.45
24.	beta.-Humulene	-7.41	-	-	3.72
25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	-7.80	1	TYR385	1.92
26.	methyl (4R,9R,10R,15R)-4- (cyanomethyl) -4,9,10-trimethyl-3- [2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	-1.19	1	-	134.270
27.	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-6.21	1	MET522	28.02
28.	Ethyl 7-amino [1,2,4] triazolo[1,5-a] pyrimidine-6-carboxylate (, 7-amino-, ethyl ester)	-4.70	2	MET522 ILE523	357.03
29.	1H-Indole-2-carboxylic acid	-5.91	1	TYR355	46.85

LAMPIRAN 8
(LANJUTAN)

Tabel V.3
Lanjutan

No.	Senyawa/Ligan	(ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Meloxicam	-8.74	1	SER530	0.391
Ligan Uji					
30.	2,6,10,14,18,22-Tetracosahexaene	-9.62	-	-	0.089
31.	2,5-Di-tert-amylhydroquinone(79-74-3;(Santouar A)	-6.85	1	ALA527	9.52)
32.	7-Hexadecenal	-6.54	-	-	16.08
33.	S-Ethyl ethanethioate	-3.46	1	SER530	2.920
34.	Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9-tetrahydro-7-hydroxy-6-(hydroxymethyl)-1-methyl-(Przewaquinone F)	-8.27	2	ILE523 VAL349	0.872
35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-7.20	2	SER530 ILE523	5.27
36.	Quinoline-3-carboxylic acid	-6.19	3	ALA527 ARG120 TYR355	29.21

LAMPIRAN 8
(LANJUTAN)

Tabel V.3
Lanjutan

No.	Senyawa/Ligan	(ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Meloxicam	-8.74	1	SER530	0.391
Ligan Uji					
37.	alpha.-Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2- (4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)	-11.58	-	-	0.032
38.	Stigmast-5-en-3-ol	-0.58	1	GLY526	374.480

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Nilai Energi Ikatan dari Ligan Alami dan Senyawa Uji
pada enzim *Cyclooxygenase* -2

No.	Senyawa/Ligan	(ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SER 530 TYR 385	4.86
Ligan Uji					
1.	4-Quinolinol, 4-ethenyl-1-ethyldecahydro-2-methyl	-6.81	2	SER530 VAL523	10.14
2.	Glucitol,6-O-nonyl	-3.93	1	ARG120	1310
3.	1-Deoxy-d-mannitol	-2.80	3	VAL523 MET522 ALA527	8890
4.	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-6.09	1	SER530	34.29
5.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-7.99	-	-	1.40
6.	4-Cyclopropyl methyl benzonitrile	-6.19	-	-	29.18

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SER530 TYR385	4.86
Ligan Uji					
7.	Caryophyllen alcohol	-8.29	1	VAL523	0.843
8.	4-Methylbenzyl chloride	-4.88	-	-	265.31
9.	Methyl 18-fluorooctadecanoate	-6.37	2	ARG120 TYR355	21.59
10.	E-15-Heptadecenal	-6.41	2	ARG120 TYR355	19.98
11.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	-7.49	-	-	3.23
12.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-7.43	2	SER530 ALA527	3.57
13.	Hexadecanoic acid, methyl ester (palmitic acid)	-6.31	2	ARG120 TYR355	23.78

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SER530 TYR385	4.86
Ligan Uji					
14.	Pentadecanoic acid	-6.62	2	ARG120 TYR355	14.12
15.	Methyl-9,12-heptadecadienoate	-6.69	1	ARG120	12.57
16.	5,9,12-octadecatrienoic acid	-7.68	1	TYR355	2.33
17.	Tetradecanoic acid, 12-methyl-, methyl ester	-6.04	2	ARG120 TYR 355	37.15
18.	Ethyl-9,12-octadecadienoate	-7.26	2	ARG120 TYR355	4.79
19.	Butyl-9,12,15-octadecatrienoate	-7.53	1	SER530	3.02
20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-4.63	2	VAL523 MET522	0.405

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SERB530 TYR385	4.86
Ligan Uji					
21.	1-O-hexadecylglycerol - bis-trimethylsi	-4.74	1	SER530	337.42
22.	3-Pentadecylphenol	-7.85	2	ARG120 TYR 355	1,76
23.	N-Tetracosane	-7.19	-	-	5.34
24.	beta.-Humulene	-8.06	-	-	1.23
25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	-8.06	2	ARG120 TYR355	1,23
26.	methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3- [2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	+10.58	2	ARG120 ALA527	-
27.	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-6.57	2	SER530 VAL 523	15.27

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SER530 TYR385	4.86
Ligan Uji					
28.	Ethyl 7-amino[1,2,4] triazolo[1,5-a] pyrimidine-6-carboxylate(, 7-amino-, ethyl ester)	-4.97	2	SER530 MET 522	227.70
29.	1H-Indole-2-carboxylic acid	-5.63	2	TYR385 SER530	0.075
30.	2,6,10,14,18,22-Tetracosahexaene	-9.88	-	-	0.056
31.	2,5-Di-tert-amylhydroquinone (79-74-3;(Santouar A)	-7.30	2	SER530 VAL523	4,44
32.	(Z)-7-Hexadecenal	-6.52		ARG120 TYR 355	0.016
33.	S-Ethyl ethanethioate	-3.35	1	TYR385	3530
34.	Phenanthro (1,2-b) furan-10,11-dione,6,7,8,9-tetrahydro-7-hydroxy-6-(hydroxymethyl)-1-methyl-	-8.20	2	TYR355 SER530	0.973

LAMPIRAN 8
(LANJUTAN)

Tabel V.4
Lanjutan

No.	Senyawa/Ligan	ΔG (kkal/mol)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
Ligan Alami					
	Asam Mefenamat	-7.25	2	SER530 TYR385	4.86
Ligan Uji					
35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-6.53	2	SER530 VAL523	16.38
36.	Quinoline-3-carboxylic acid	-6.26	-	-	25.68
37.	Alpha -Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)	-10.50	-	-	0.020
38	Stigmast-5-en-3-ol	+6.89	2	SER530 GLY 526	-

LAMPIRAN 9

HASIL PENGUJIAN *LIPINSKI'S RULE OF FIVE*

Tabel V.5
Sifat Fisikokimia yang Berdasarkan Aturan *Lipinski's Rule of Five*

Senyawa/Ligan	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul (Dalton)	Log P	Memenuhi Syarat/ tidak
Caryophyllen alcohol	1	1	222	3,77	Memenuhi syarat
3,7,11,15Tetramethyl-2-hexadecen-1-ol	1	1	296	6,36	Tidak memenuhi
5,9,12-octadecatrienoic acid	1	2	278	5,66	Tidak memenuhi
Ethyl-9,12-octadecadienoate	0	2	308	6,36	Tidak memenuhi
Butyl-9,12,15-octadecatrienoate	0	2	334	6,91	Tidak memenuhi
3-Pentadecylphenol	1	1	304	7,02	Tidak memenuhi
Methyl (Z)-5,11,14,17-eicosatetraenoate	0	2	318	6,30	Tidak memenuhi
2,5-Di-tert-amylhydroquinone	2	2	250	4,47	Memenuhi syarat
Przewaquinone F	2	5	312	1,36	Memenuhi syarat

LAMPIRAN 9
(LANJUTAN)

Tabel V.5
Lanjutan (keterangan tabel)

Keterangan : Massa molekul kurang dari 500 Dalton

LogP kurang dari 5

Donor ikatan hidrogen kurang dari 5

Akseptor ikatan hidrogen kurang dari 10

LAMPIRAN 10

HASIL PENGUJIAN PreADME

Tabel V.6
Uji PreADME (Absorpsi dan Distribusi**)**

Senyawa/Ligan	Absorpsi		Distribusi
	CaCO-2 Cell (nm Sec-1)	HIA (%)	Protein Plasma Binding (%)
Caryophyllen alcohol	22.2	100	100
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	23.40	100	100
5,9,12-octadecatrienoic acid	27.97	98.27	100
Ethyl-9,12-octadecadienoate	57.09	100	100
Butyl-9,12,15-octadecatrienoate	47.92	100	100
3-Pentadecylphenol	56.03	100	100
Methyl (Z)-5,11,14,17-eicosatetraenoate	49.45	100	100
2,5-Di-tert-amylhydroquinone	28.22	91.57	100
Przewaquinone F	21.12	94.52	89.51

LAMPIRAN 10
(LANJUTAN)

Tabel V.6
Lanjutan (keterangan tabel)

Keterangan :

% *Human Intestinal Absorbsi* (% HIA) = (a)70-100% *well absorbed*

(b) 20-70% *moderately absorbed*

(c) 0-20% *poorly absorbed*

In Vitro Caco-2 *cell permeability* (nm sec-1) = (a) >70 *higher permeability*

(b) 4-70 *medium permeability*

(c) <4 *low permeability*

Plasma protein binding = (a) >90 *strongly bound*

(b) < 90% *weakly bound*

LAMPIRAN 11

HASIL PENGUJIAN TOKSISITAS

Tabel V.7
Uji Toksisitas

Senyawa/Ligan	Ames Test	Karsinogenik
	Mutagen / Non-Mutagen	**(-) / (+)**
Caryophyllen alcohol	Mutagen	+
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	Non-mutagen	+
5,9,12-octadecatrienoic acid	Mutagen	+
Ethyl-9,12-octadecadienoate	Non-mutagen	+
Butyl-9,12,15-octadecatrienoate	Non-mutagen	+
3-Pentadecylphenol	Non-mutagen	+
Methyl (Z)-5,11,14,17-eicosatetraenoate	Mutagen	+
2,5-Di-tert-amyl hydroquinone	Non-mutagen	-
Przewaquinone F	Mutagen	+