

DAFTAR PUSTAKA

1. Dewi GAT, Hendrati LY. Analisis risiko kanker payudara berdasar riwayat pemakaian kontrasepsi hormonal dan usia menarche. *Jurnal Berkala Epidemiologi*. 2013;14p.
2. Kementerian Kesehatan Republik Indonesia. Bulan Peduli Kanker Payudara. *Info DATIN* ISSN 2442-7659. 2016. 2p.
3. World Health Organization. International Agency for Research on Cancer. 2018. 876:99–100p.
4. Suparman Erna, Suparman Eddy. Peran Estrogen dan Progesteron Terhadap Kanker Payudara. :141–8p.
5. P. Soemitro, Monty dan Kusumadjayanti N. *Berani Deteksi Dini: Hindari Kanker Payudara*. 1st ed. Qanita; 2018. 11–142p.
6. Hussain F, Rana Z, Shafique H, Malik A, Hussain Z. Phytopharmacological potential of different species of *Morus alba* and their bioactive phytochemicals: A review. *Asian Pacific Journal of Tropical Biomedicine* [serial online]. 2017;7(10):950–6p. DOI: 10.1016/j.apjtb.2017.09.015.
7. Khaira YN, Ramadhania ZM. Kandungan Senyawa Kimia Murbei Hitam (*Morus nigra* L.) dan efek farmakologinya. 2008;16:247–50p.
8. Zelova H, Hanakova Z, Cermakova Z, et al. Evaluation of Anti-Inflammatory Activity of Prenylated Substances Isolated from *Morus alba* and *Morus nigra*. *Journal of Natural Products*. 2013. DOI: 10.1021/np401025f.
9. CABI. *Risk Assessment for Morus nigra L: Invasive Species Compendium*. 2016.
10. Isnan W, Muin N. *Tanaman Murbei Sumber Daya Hutan Multi Manfaat*. 2015;111–2p.
11. Prasetiawati R, Zamri A, Barliana MI, Muchtaridi M. In silico predictive for modification of chalcone with pyrazole derivatives as a novel therapeutic compound for targeted breast cancer treatment. 2019;9(02):20–8p.
12. Zheng ZP, Cheng KW, Zhu Q, Wang XC, Lin ZX, Wang M. Tyrosinase inhibitory constituents from the roots of *Morus nigra*: A structure-activity relationship study. *Journal of Agricultural and Food Chemistry*.

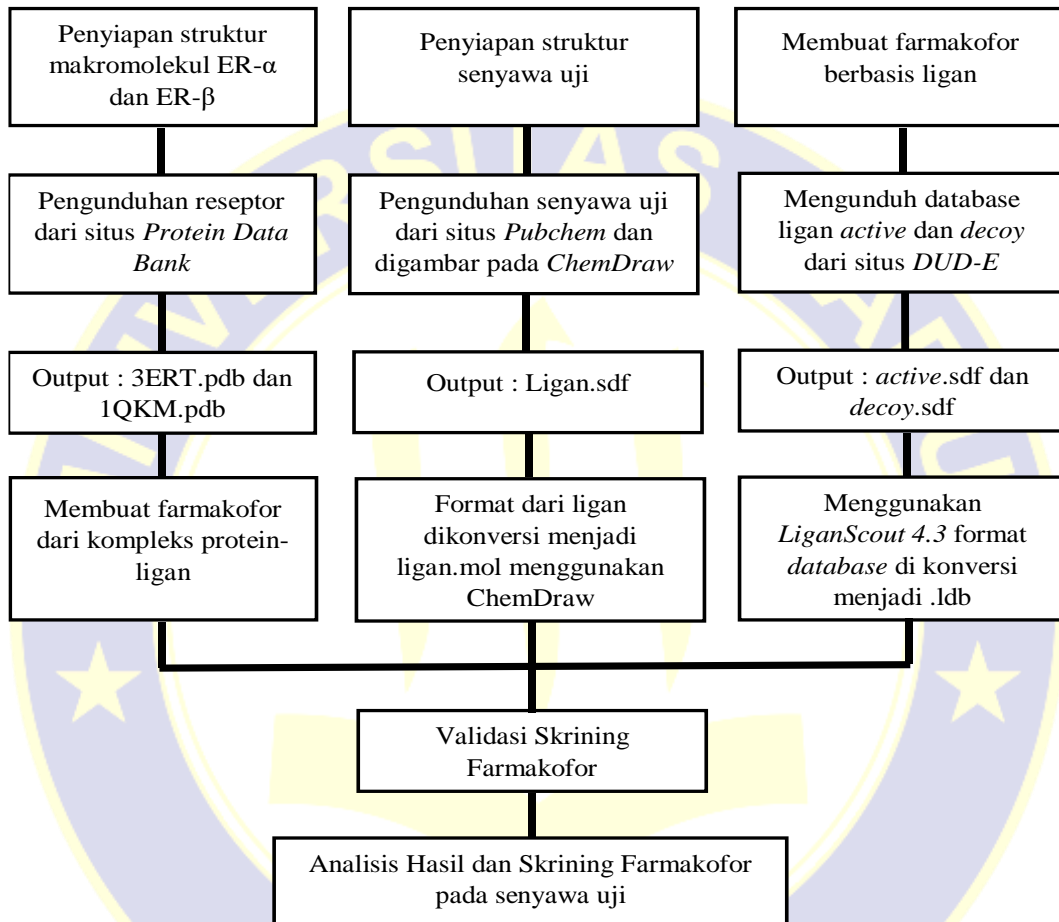
2010;58(9):5371–2.

13. Tortora GJ, Derrickson B. Principles of Anatomy dan Physiology [Internet]. 15th ed. United States: Pearson; 2013. 1085p.
14. Rochmawati L. Kanker Payudara [Internet]. Ginekologi. 2009 [cited 2019 Jun 5]. Available from: <https://lusa.afkar.id/kanker-payudara-ca-mammae?responsive=true>
15. Fei J, Zhou L, Liu T, Tang X. Pharmacophore Modeling, Virtual Screening, and Molecular Docking Studies for Discovery of Novel Akt2 Inhibitors. International Journal of Medical Sciences. 2013;10:265-75p.
16. Richard AH, Pamela CC. Farmakologi. 4th ed. Jakarta: EGC; 2016. 570p.
17. Wulandari E, Hendarmin LA. Integrasi Biokimia dalam Modul Kedokteran [Internet]. Jakarta: Fakultas Kedokteran dan Ilmu Kesehatan UIN Syarif Hidayatullah; 2010. 62, 69, 72p. Available from: <http://repository.uinjkt.ac.id/dspace/handle/123456789/38256>
18. Satyajit DS, Lutfun N. Kimia Untuk Mahasiswa Farmasi. Yogyakarta: Pustaka Pelajar; 2009. 37-40p.
19. Muchtaridi, Yanuar, A., Megantara, S., & Purnomo H. Kimia medisinal: dasar-dasar dalam perancangan obat. Pertama. Jakarta: Prenadamedia Group; 2018. 52-54, 193p.
20. Hamzah N, Najib A, Thahir N, Misqawati I. Studi farmakofor reseptor COX-2 sebagai anti inflamasi. JF FIK UINAM. 2015;2(3):99–107p.
21. Yanuar A. Penambatan Molekular Praktek dan Aplikasi pada Virtual Screening. Jakarta: Fakultas Farmasi Universitas Indonesia; 2012.
22. Suppercomputing Facility for Bioinformatic and Computational Biologi [Internet]. Lipinski Rule Of Five. Available from: <http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp>
23. Situs Pre-ADMET [Internet]. Available from: <https://preadmet.bmdrc.kr/adme/>
24. Nursamsiar, Ibrahim S, Tjahjono DH. Absorption, Distribution and Toxicity Prediction of Curculigoside A and its Derivative. 2015.
25. Muchtaridi, Yusuf M. Teori dan Praktek Penambatan Molekul (Molekular Docking). Bandung: Unpad Press; 2018. 37-38p.

26. Wang Y, Xiao J, O Tugba. PubChem's BioAssay Database. 2011.
27. Mysinger MM, Carchia M, Irwin, JJ, Shoichet BK. Directory of Useful Decoys, Enhanced (DUD-E): Better Ligands and Decoys for Better Benchmarking. *J Med Chem* 55(14); 2012. 6582-94p.
28. Inte:Ligand. Advanced Molecular Design [Internet]. Inte:Ligand. 2018. Available from: <http://www.inteligand.com/>
29. Yang SY. Pharmacophore Modeling and Applications in Drug Discovery: Challenges and Recent Advances. *Drug Discov Today*. 2010;444-450p.
30. A Nomartinelli. Introduction to The Discovery Studio Visualizer.
31. Evans DA. History of the Harvard ChemDraw Project. *Angew Chemie Int Ed* 53; 2014. 11140-5p.
32. Morris GM, S David, E Michael. AutoDock Version 4.2. 2014; Available from: http://autodock.scripps.edu/faqs-help/manual/autodock-4-2-user-guide/AutoDock4.2.6_UserGuide.pdf.
33. Inte:Ligand. Creating a pharmacophore from a single protein-ligand complex. *Comp A J Comp Educ*. :1-8p. 38

LAMPIRAN 1

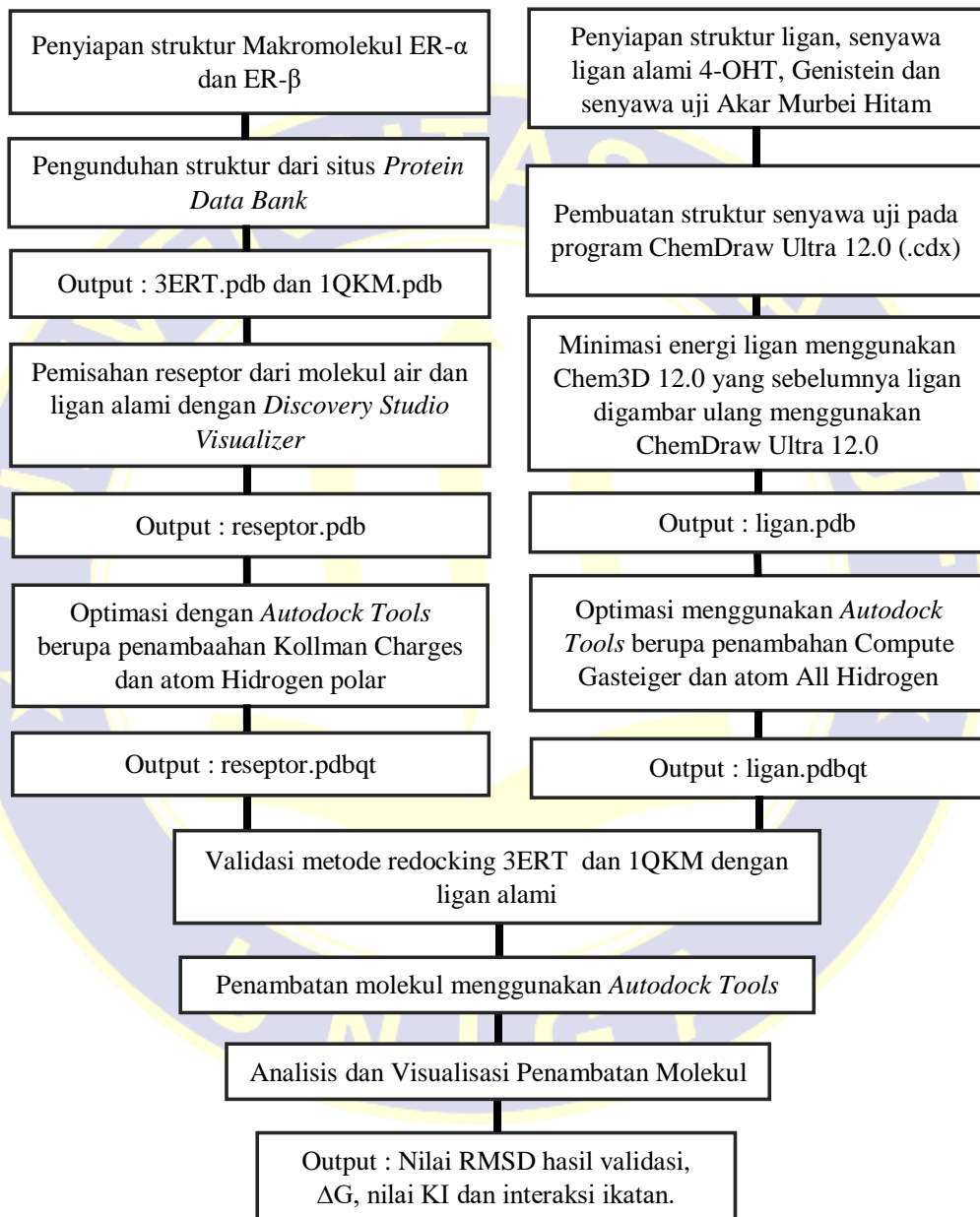
ALUR PENELITIAN *SKRINING* FARMAKOFOR



Gambar IV.1 Alur Penelitian *Skrining* Farmakofor

LAMPIRAN 2

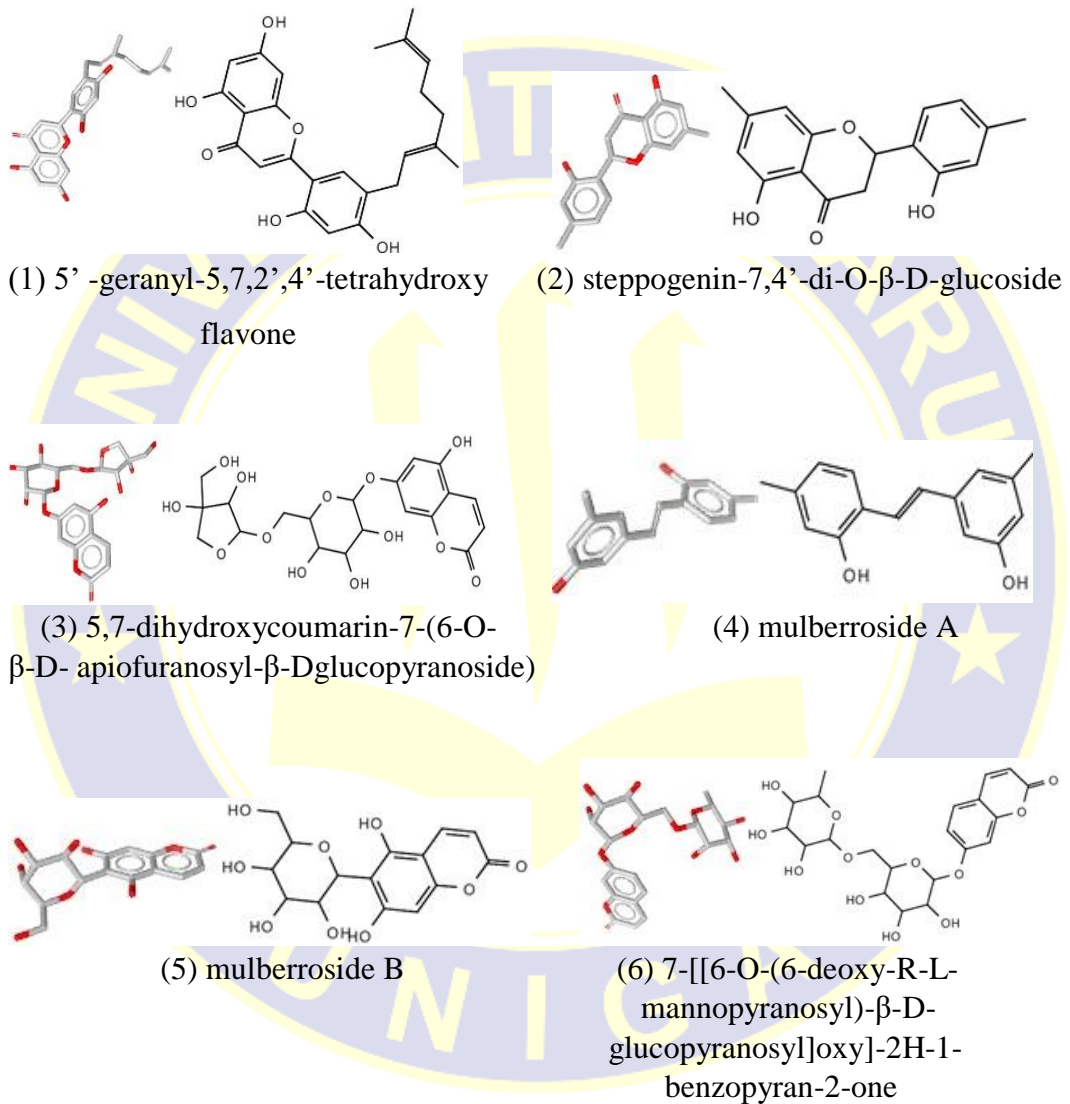
ALUR PENELITIAN *MOLECULAR DOCKING*



Gambar IV.2 Alur Penelitian *Molecular Docking*

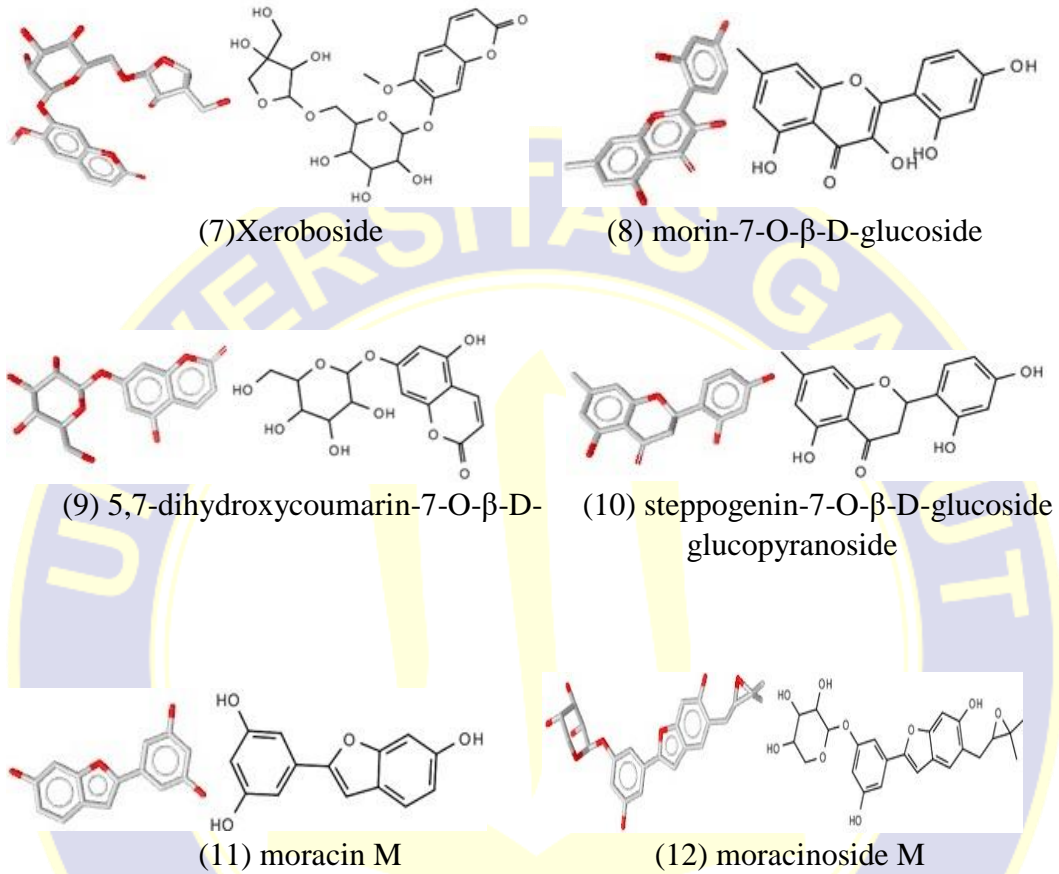
LAMPIRAN 3

STRUKTUR 3D DAN 2D SENYAWA AKAR MURBEI HITAM



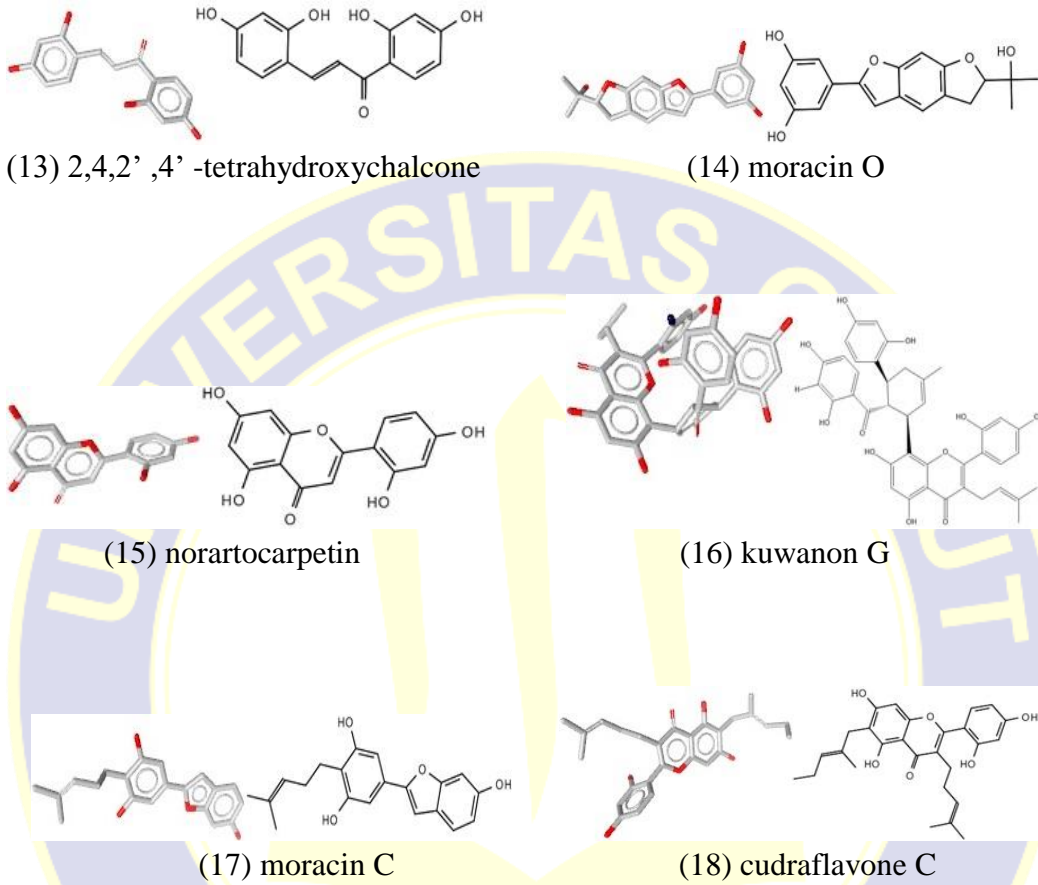
Gambar IV.3 Struktur 3D dan 2D kandungan senyawa aktif dalam akar murbei hitam (*Morus nigra* L.)

**LAMPIRAN 3
(LANJUTAN)**



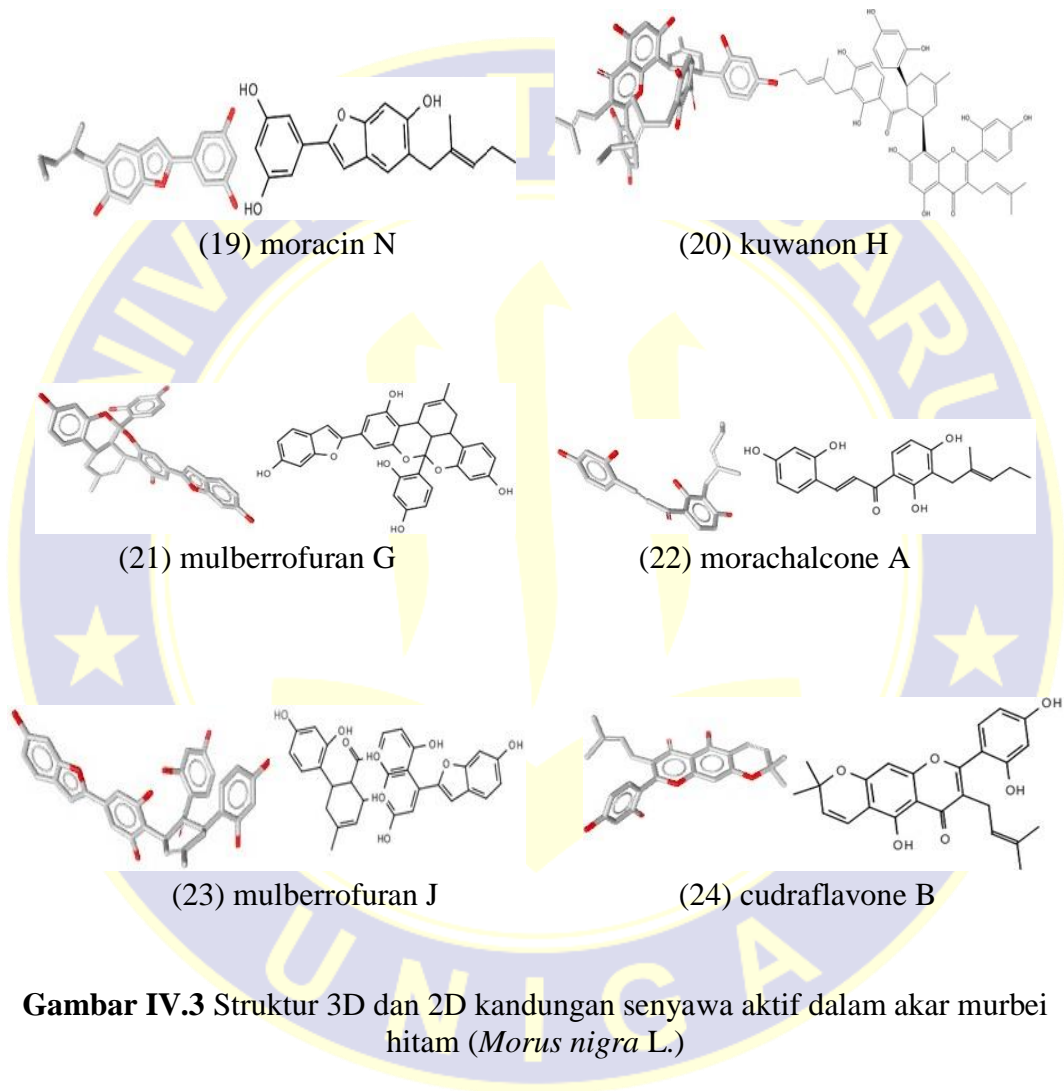
Gambar IV.3 Struktur 3D dan 2D kandungan senyawa aktif dalam akar murbei hitam (*Morus nigra* L.)

LAMPIRAN 3 (LANJUTAN)

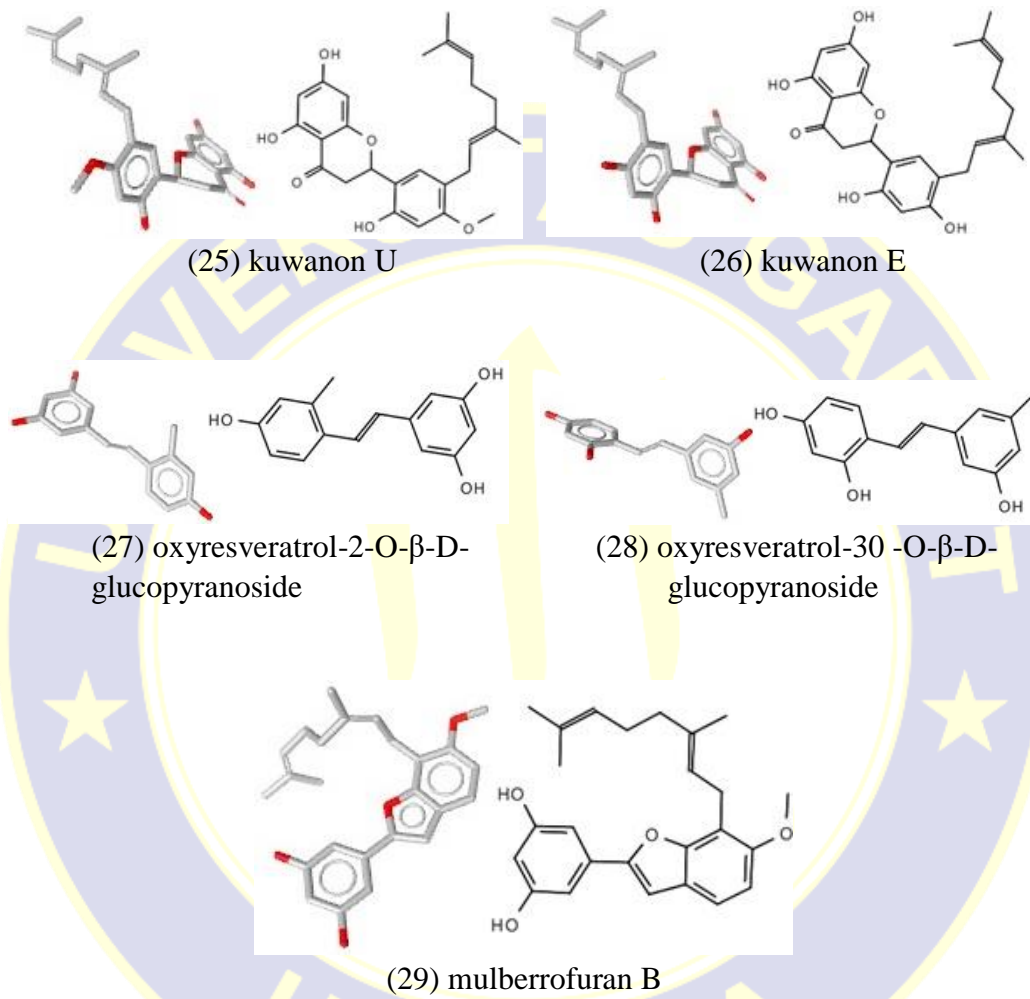


Gambar IV.3 Struktur 3D dan 2D kandungan senyawa aktif dalam akar murbei hitam (*Morus nigra* L.)

**LAMPIRAN 3
(LANJUTAN)**



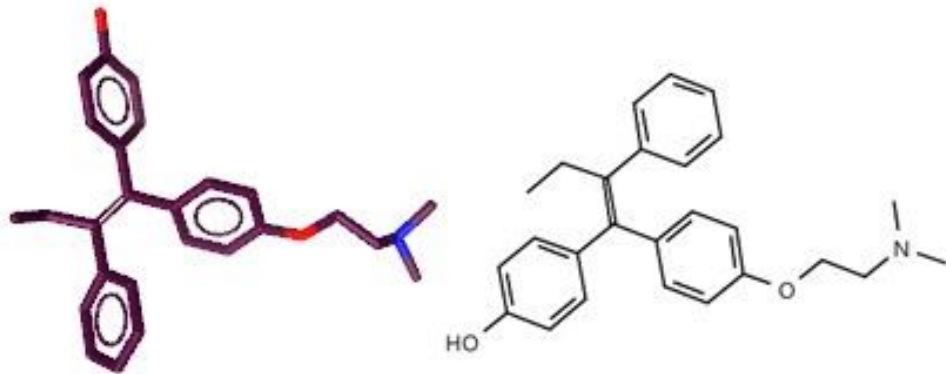
**LAMPIRAN 3
(LANJUTAN)**



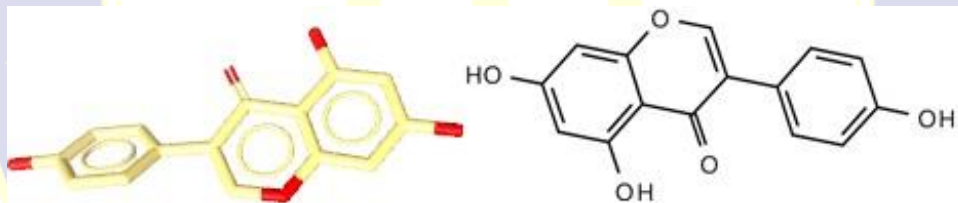
Gambar IV.3 Struktur 3D dan 2D kandungan senyawa aktif dalam akar murbei hitam (*Morus nigra* L.)

LAMPIRAN 4

STRUKTUR 3D DAN 2D LIGAN ALAMI



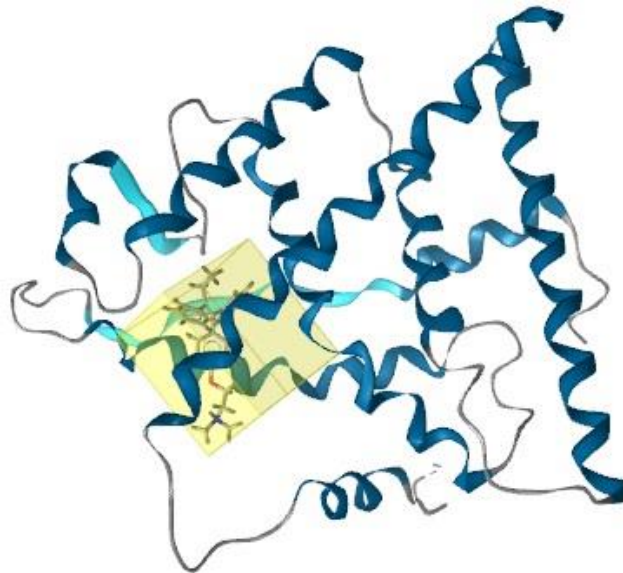
Gambar IV.4 Struktur kimia ligan alami 4-Hydroxytamoxifen



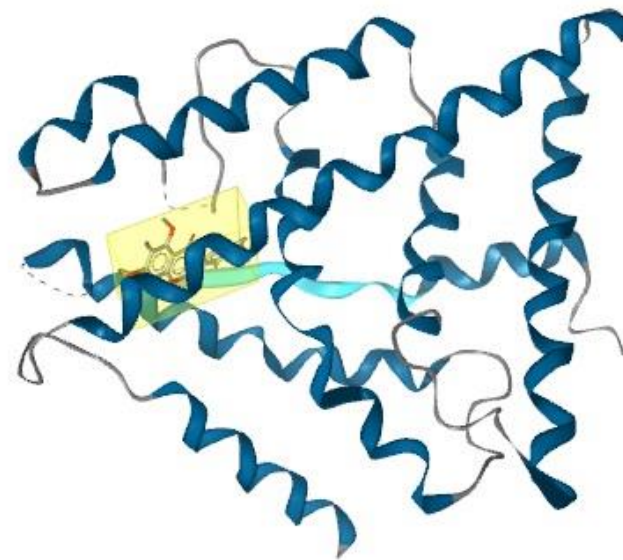
Gambar IV.5 Struktur kimia ligan alami Genistein

LAMPIRAN 5

STRUKTUR 3D RESEPTOR



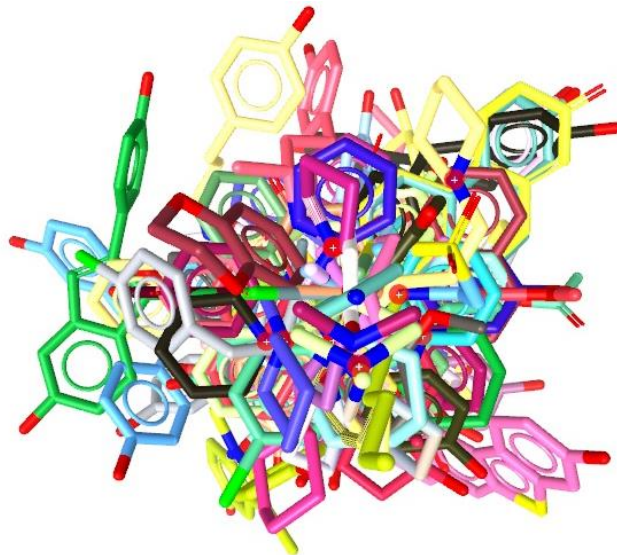
Gambar IV.6 Struktur 3D estrogen receptor alpha (ER- α)



Gambar IV.7 Struktur 3D estrogen receptor beta (ER- β)

LAMPIRAN 6

STRUKTUR 3D *DATABASE ACTIVE DAN DECOY*

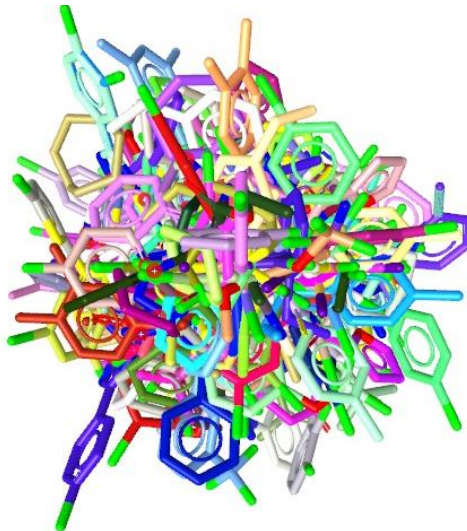


Gambar IV.8 Kumpulan struktur tiga dimensi senyawa *active ER- α* yang didapatkan dari situs DUD-E

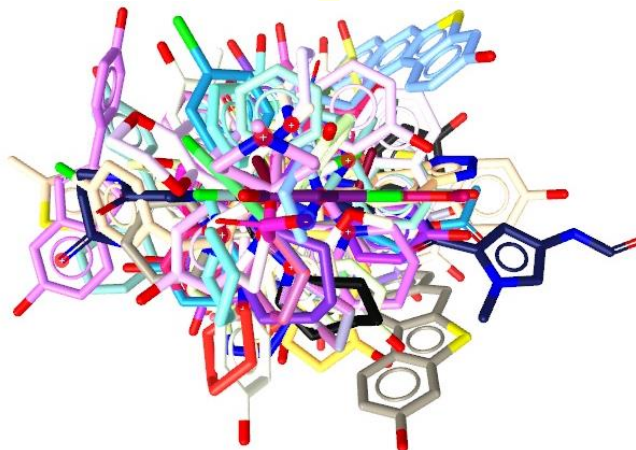


Gambar IV.9 Kumpulan struktur tiga dimensi senyawa *decoy ER- α* yang didapatkan dari situs DUD-E

**LAMPIRAN 6
(LANJUTAN)**



Gambar IV.10 Kumpulan struktur tiga dimensi senyawa *active* ER- β yang didapatkan dari situs DUD-E



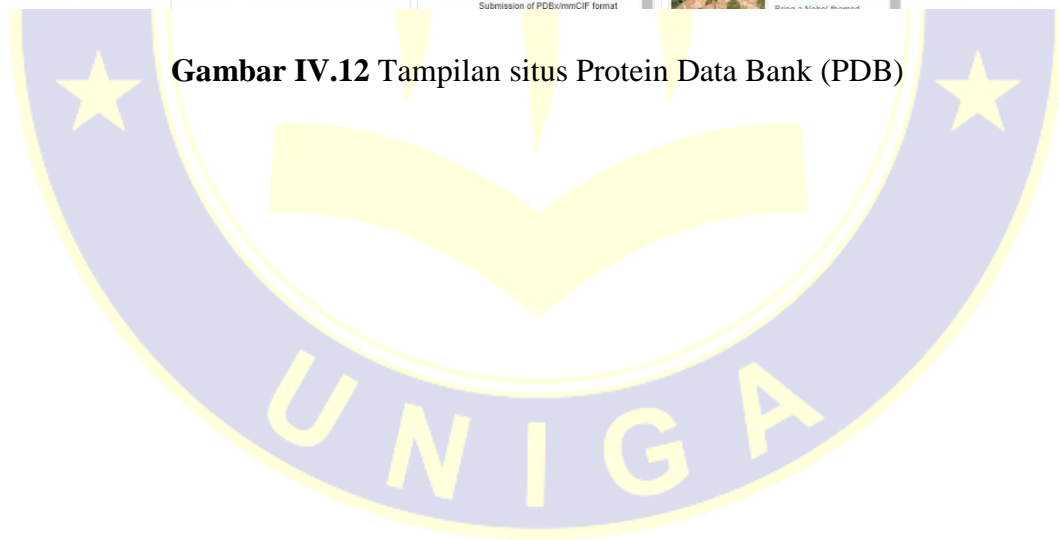
Gambar IV.11 Kumpulan struktur tiga dimensi senyawa *decoy* ER- β yang didapatkan dari situs DUD-E

LAMPIRAN 7

SITUS PROTEIN DATA BANK



Gambar IV.12 Tampilan situs Protein Data Bank (PDB)

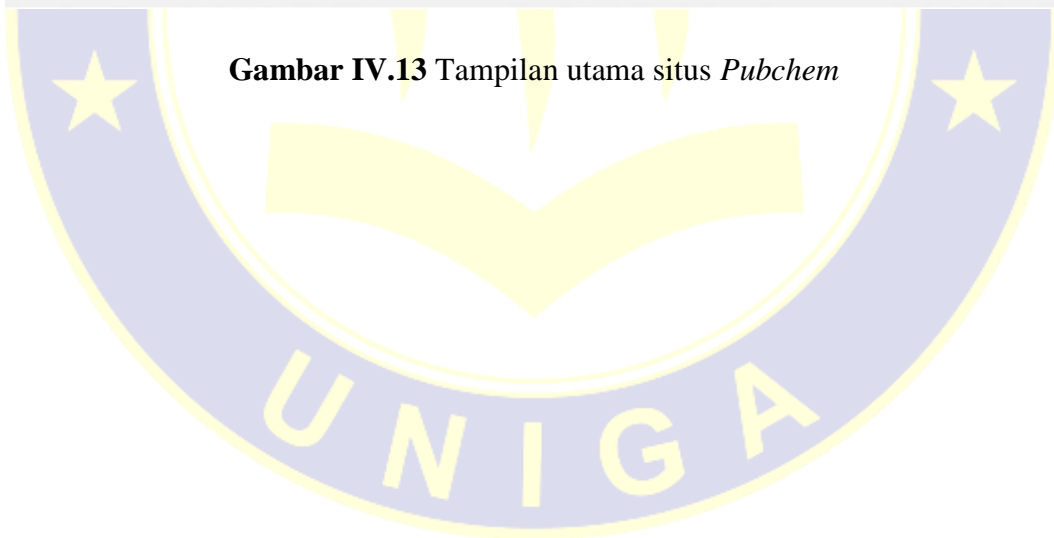


LAMPIRAN 8

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, with a magnifying glass icon on the right. 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)/h1-2H3". Underneath these suggestions are four icons representing different functions: "Draw Structure" (a chemical structure), "Upload ID List" (an upload arrow), "Browse Data" (a grid icon), and "Periodic Table" (a periodic table icon). At the bottom of the main content area, there is a light grey bar with statistics: "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.13 Tampilan utama situs *Pubchem*



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 H, Irwin JJ, Shoichet BK J. Med. Chem., 2012, Jul 5, doi 10.1021/jm300687e](#).

We thank [NIH/NS](#) for financial support (GM71896 to BKS and JJI). For correspondence about DUD-E, please write John Irwin jji at cgi 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 wiki page](#) and a [DUD-E Facebook page](#) to allow the community to share problems or observations. We will endeavor to put right any problems promptly, as best we can.

[Browse](#) the DUD-E targets

[Download](#) the default DUD-E package

[Make Decoys](#) 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 H, Irwin JJ, Shoichet BK J. Med. Chem., 2012, Jul 5, doi 10.1021/jm300687e](#).
You may also wish to cite the original version of DUD: [Wuang, Shoichet and Irwin, J. Med. Chem., 2006, 49\(23\), 6789-6801, doi 10.1021/jm060835e](#).

Gambar IV.14 Tampilan utama situs DUD-E

LAMPIRAN 10

SITUS *LIPINSKI'S RULE OF FIVE*



The screenshot shows the web interface for the Lipinski Rule of Five tool. At the top, it identifies the Supercomputing Facility for Bioinformatics & Computational Biology at IIT Delhi. The main heading is "Lipinski Rule of Five". Below this, a paragraph explains the tool's purpose: "Lipinski rule of 5 helps in distinguishing between drug like and non-drug like molecules. It predicts high probability of success or failure due to drug likeness for molecules complying with 2 or more of the following rules".

- Molecular mass less than 500 Dalton
- High lipophilicity (expressed as LogP less than 5)
- Less than 5 hydrogen bond donors
- Less than 10 hydrogen bond acceptors
- Molar refractivity should be between 40-130

Below the list, a note states: "These filters help in early preclinical development and could help avoid costly late-stage preclinical and clinical failures. To draw a chemical structure [Click Here](#) and follow the instructions given."

The interface is divided into three steps:

Step 1: Input Drug File.
Input PDB file: No file chosen.

Step 2: Input pH Value.
pH Value: [Value ranges from 0.0 to 14.0]

Step 3: Click on 'Submit' to submit your job.

How to Use the Tool

OPTION 1:

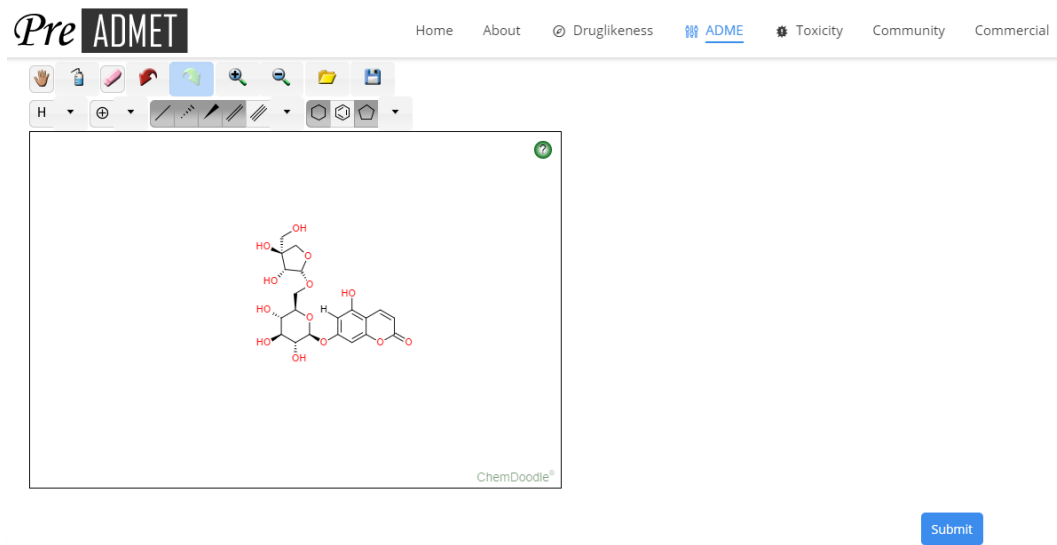
- The input file should be in the following formats: *.pdb, *.mol, *.mol2, *.sdf, *.cif, *.mol2

At the bottom right, there is a watermark for "UNIGA" (Universitas Negeri Gorontalo) and a Windows activation notice.

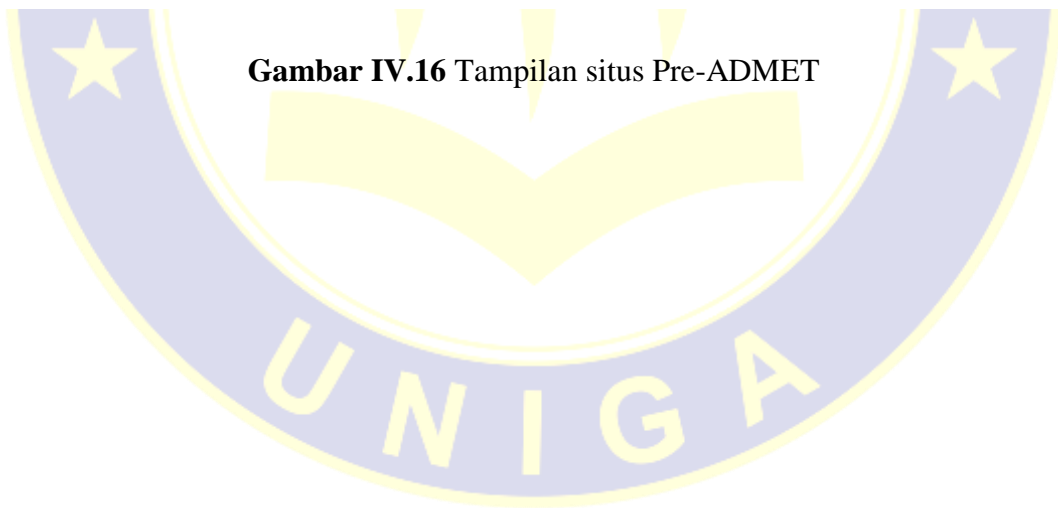
Gambar IV.15 Tampilan situs *Lipinski's rule of five*

LAMPIRAN 11

SITUS PRE-ADMET

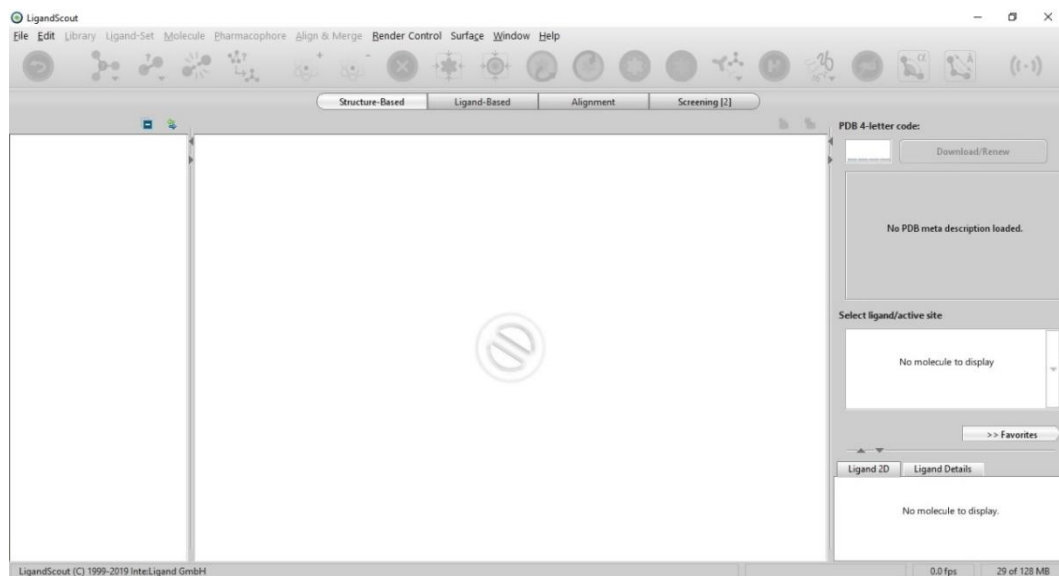


Gambar IV.16 Tampilan situs Pre-ADMET



LAMPIRAN 12

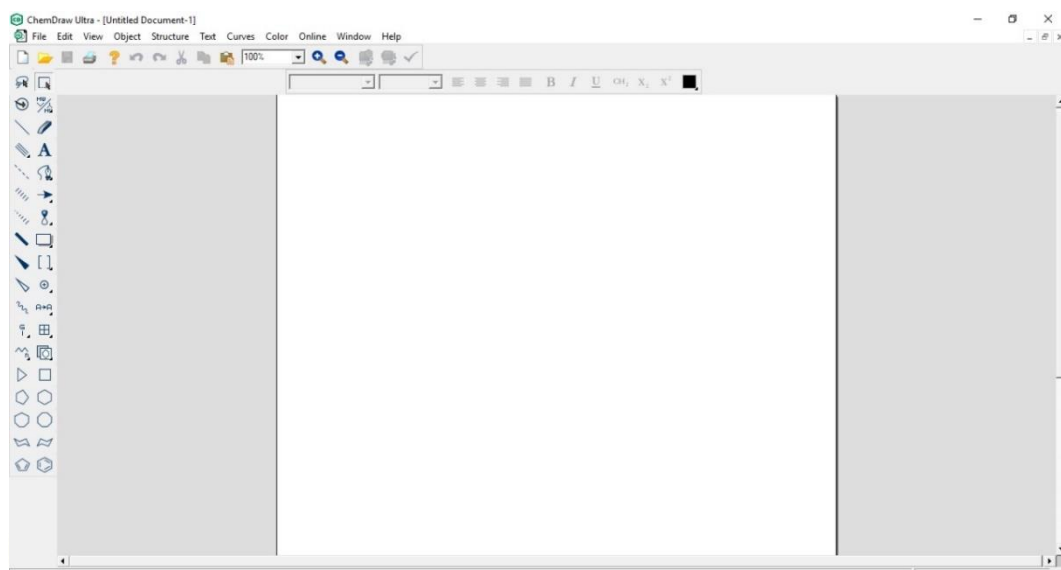
PERANGKAT LUNAK *LIGANDSCOUT* 4.3



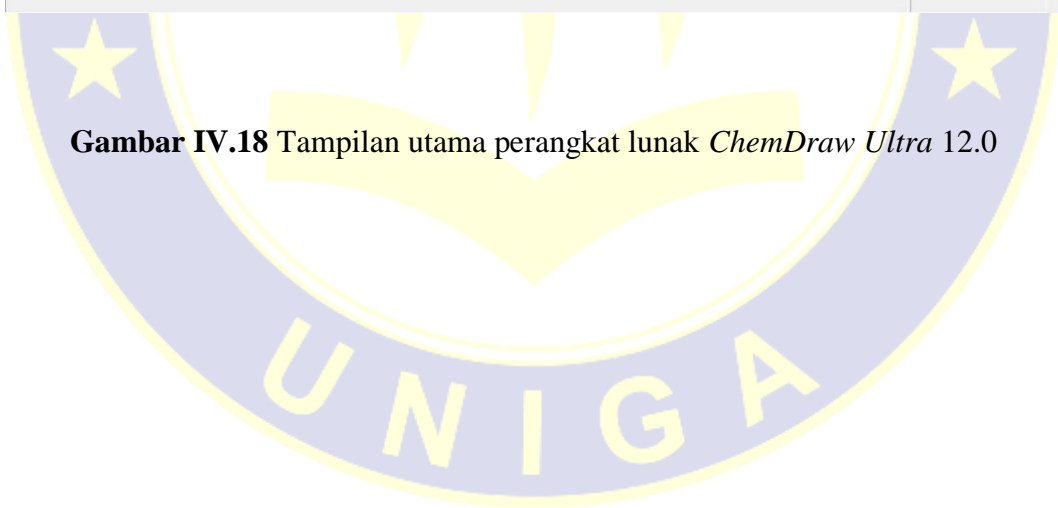
Gambar IV.17 Tampilan utama perangkat lunak *LiganScout* 4.3

LAMPIRAN 13

PERANGKAT LUNAK *CHEMDRAW ULTRA 12.0*

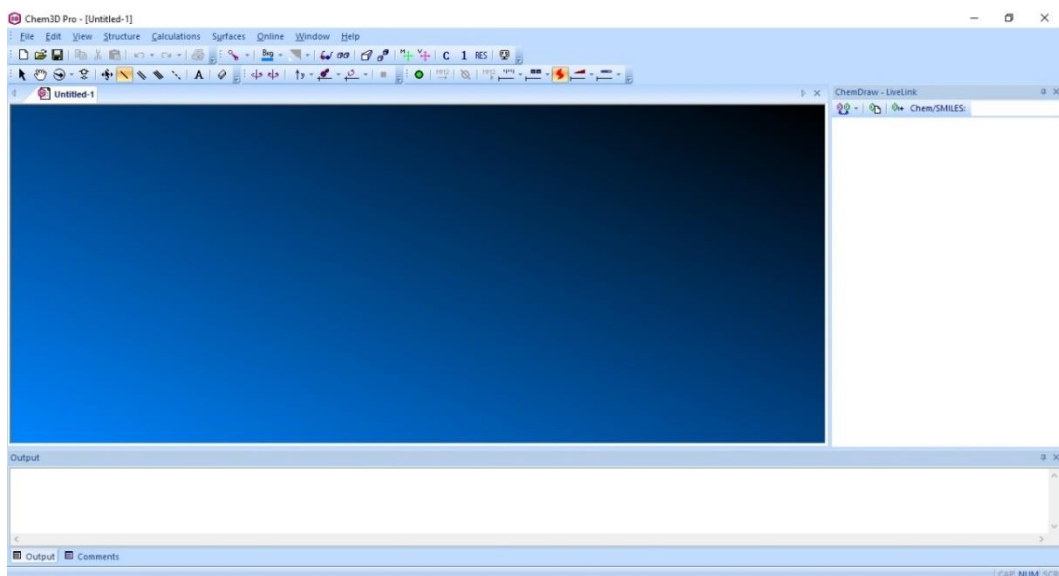


Gambar IV.18 Tampilan utama perangkat lunak *ChemDraw Ultra 12.0*

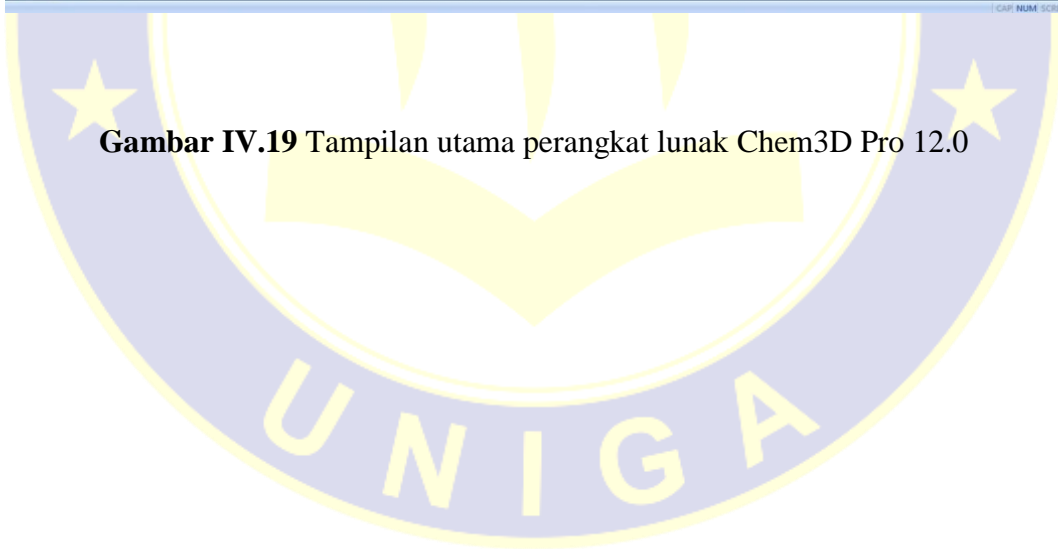


LAMPIRAN 14

PERANGKAT LUNAK CHEM3D PRO 12.0

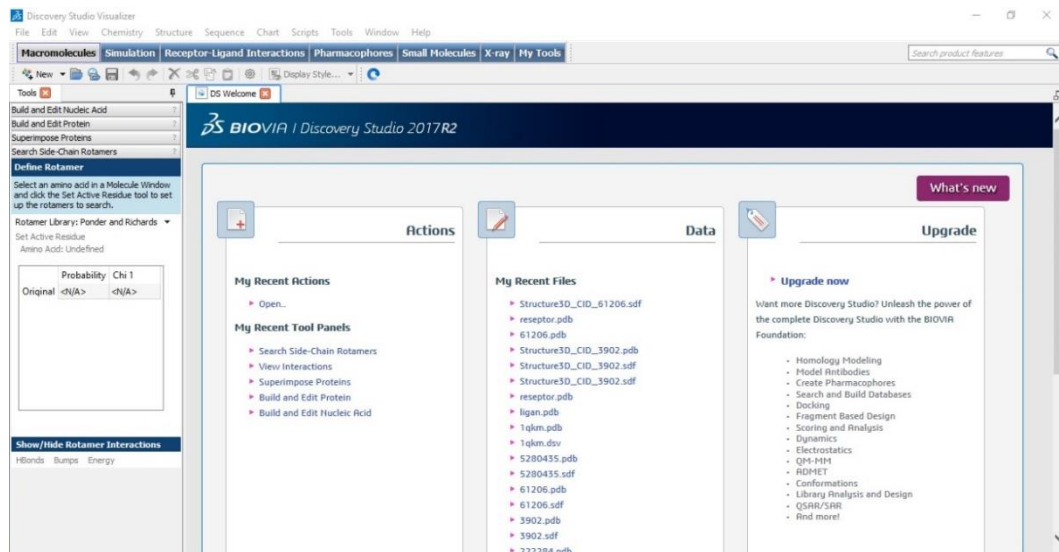


Gambar IV.19 Tampilan utama perangkat lunak Chem3D Pro 12.0



LAMPIRAN 15

PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER

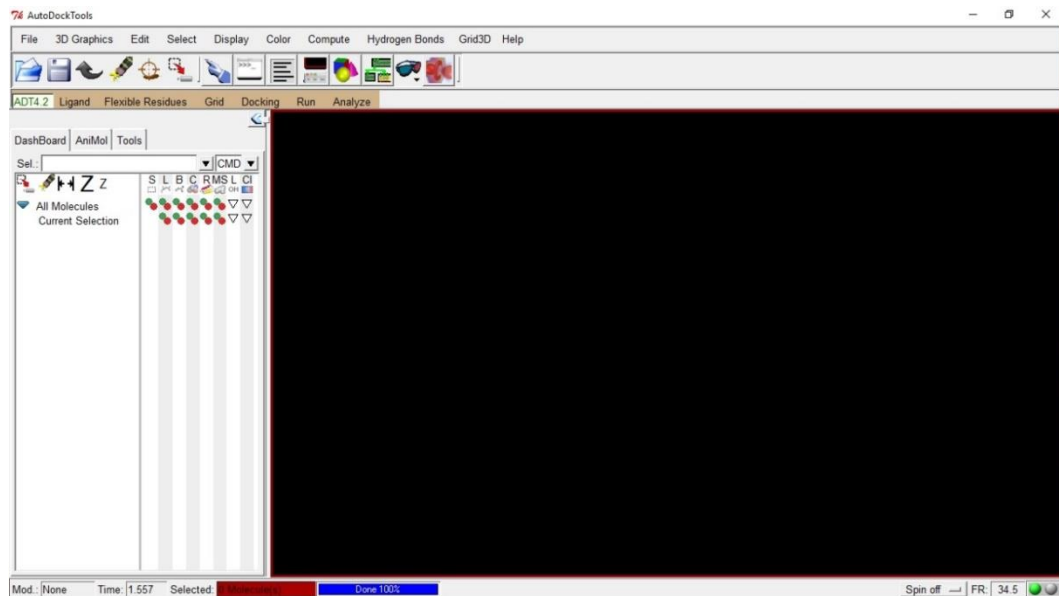


Gambar IV.20 Tampilan utama perangkat lunak Discovery Studio Visualizer



LAMPIRAN 16

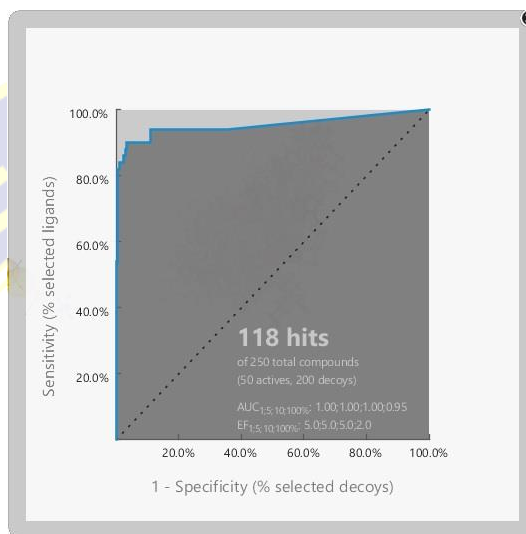
PERANGKAT LUNAK *AUTODOCK TOOLS*



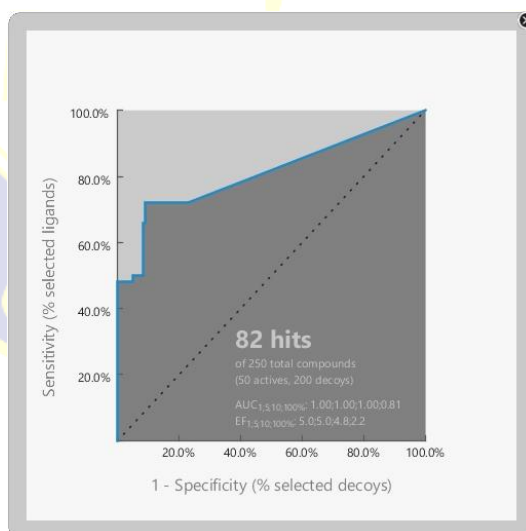
Gambar IV.21 Tampilan perangkat lunak *AutoDock Tools*

UNIGA

LAMPIRAN 17
KURVA VALIDASI *SKRINING* FARMAKOFOR
(KURVA ROC)



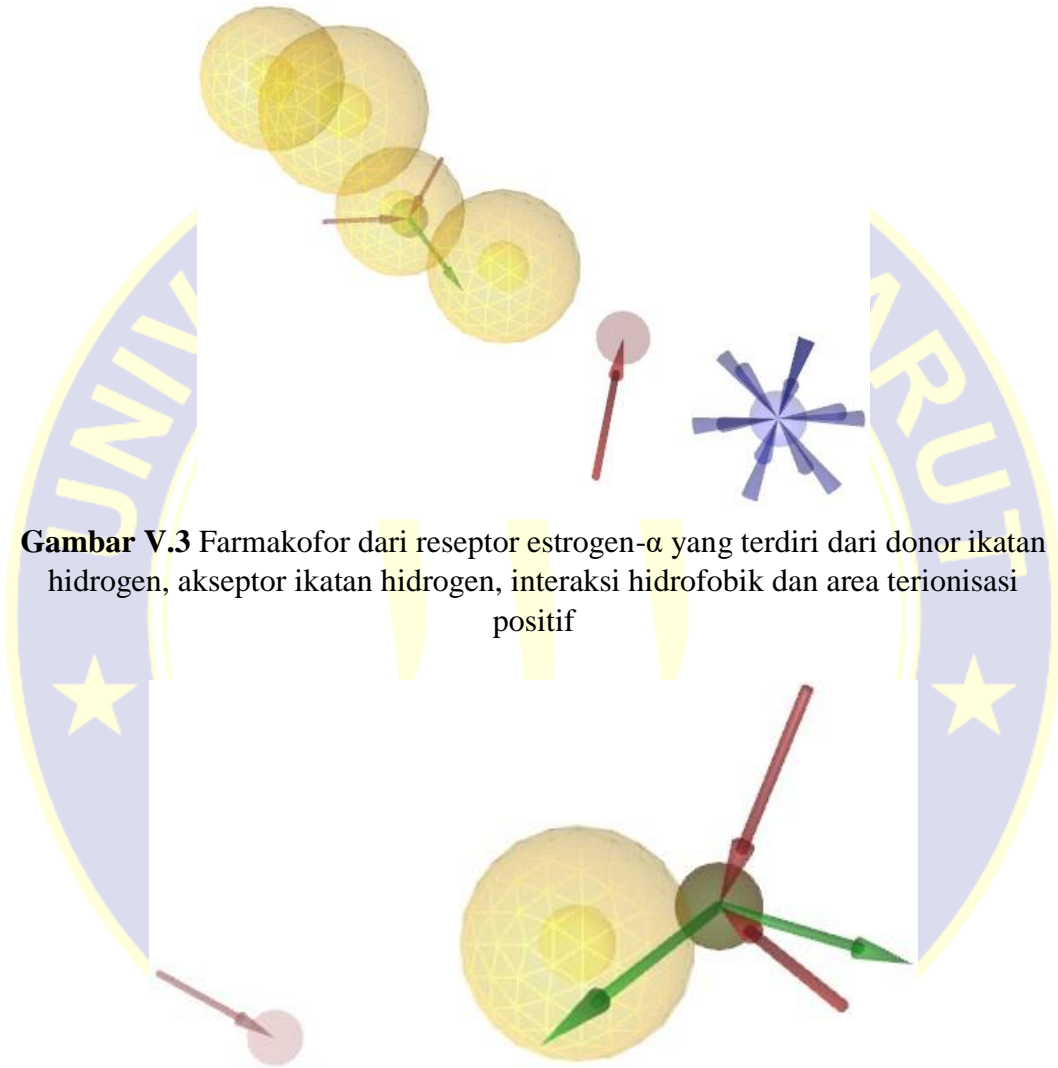
Gambar V.1 Kurva validasi (kurva ROC) ER- α



Gambar V.2 Kurva validasi (kurva ROC) ER- β

LAMPIRAN 18

FARMAKOFOR RESEPTOR

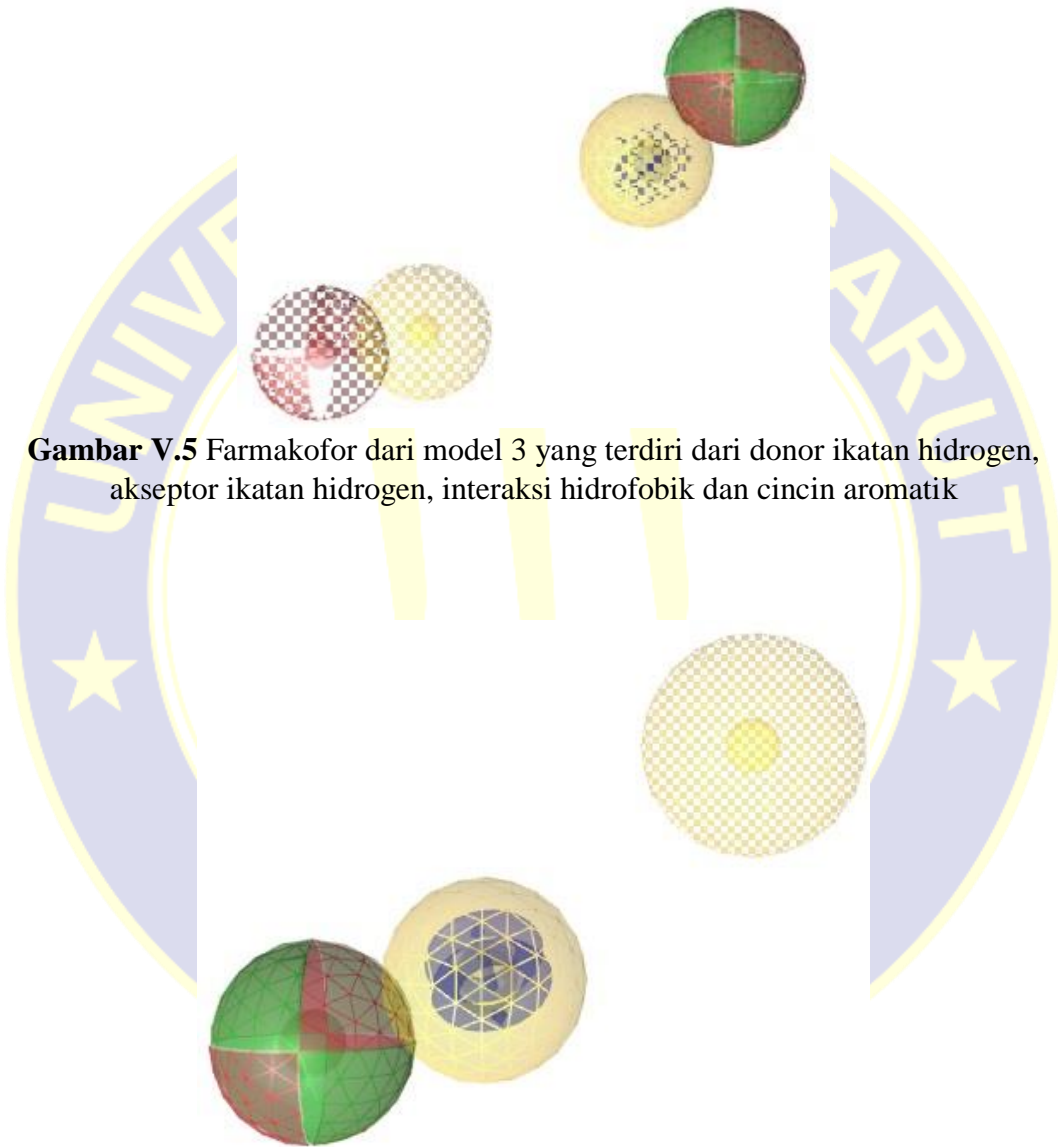


Gambar V.3 Farmakofor dari reseptor estrogen- α yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen, interaksi hidrofobik dan area terionisasi positif

Gambar V.4 Farmakofor dari reseptor estrogen- β yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen dan interaksi hidrofobik

LAMPIRAN 19

MODEL FARMAKOFOR RESEPTOR ESTROGEN ALFA DAN RESEPTOR ESTROGEN BETA (MODEL TERBAIK)

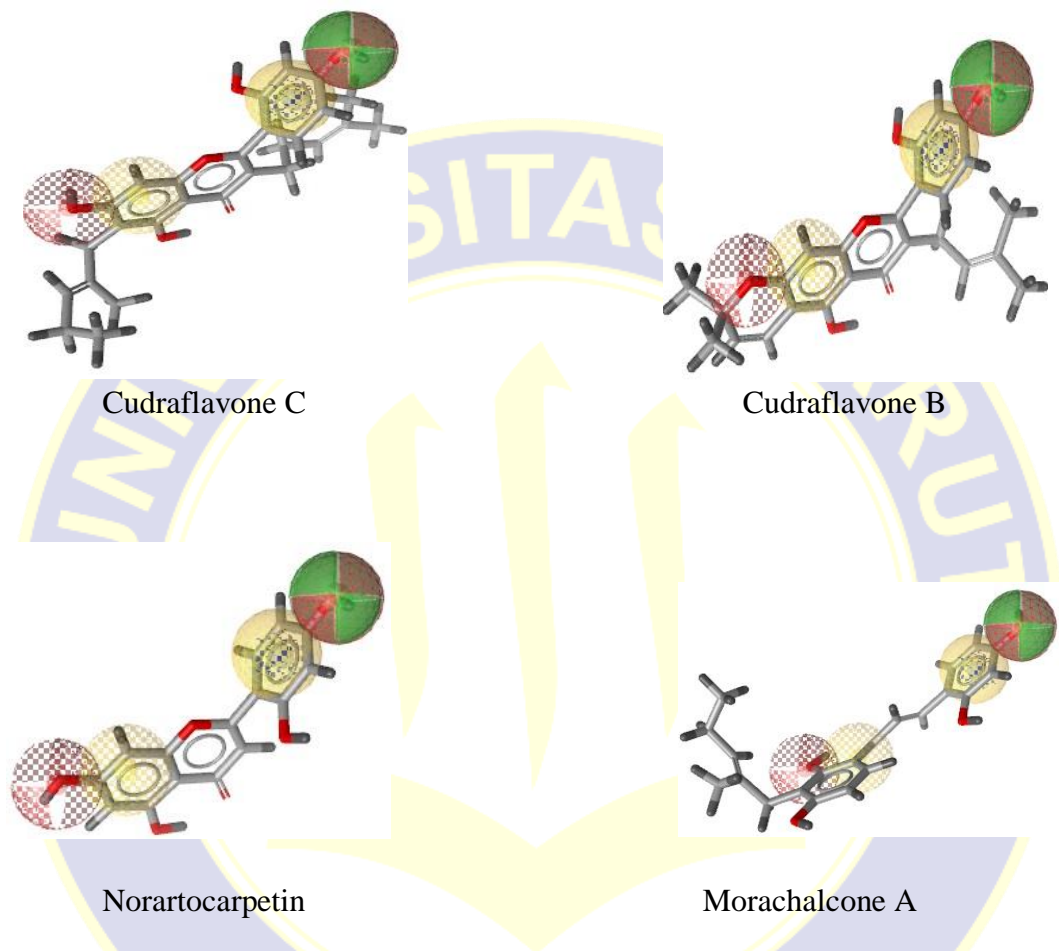


Gambar V.5 Farmakofor dari model 3 yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen, interaksi hidrofobik dan cincin aromatik

Gambar V.6 Farmakofor dari model-1 yang terdiri dari donor ikatan hidrogen, akseptor ikatan hidrogen, interaksi hidrofobik dan cincin aromatik

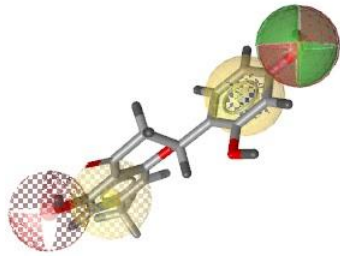
LAMPIRAN 20

HASIL *SKRINING* FARMAKOFOR

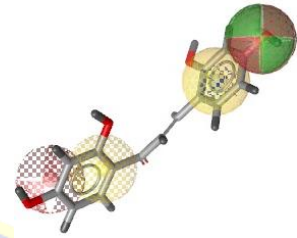


Gambar V.7 Hasil *Skrining* Farmakofor Senyawa Akar Murbei Hitam (*Morus nigra* L.) terhadap 4-Hydroxytamoxifen

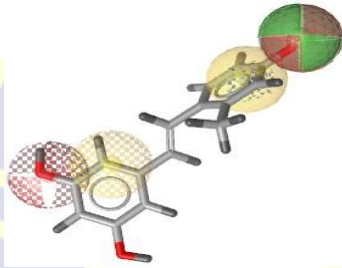
**LAMPIRAN 20
(LANJUTAN)**



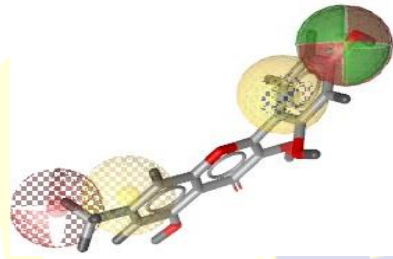
Steppogenin-7-O- β -D-glucoside



2,4,2',4'-tetrahydroxychalcone



Oxyresveratrol-2-O- β -D-glucopyranoside



Morin-7-O- β -D-glucoside

Gambar V.7 Hasil *Skrining* Farmakofor Senyawa Akar Murbei Hitam
(*Morus nigra* L.) terhadap 4-Hydroxytamoxifen

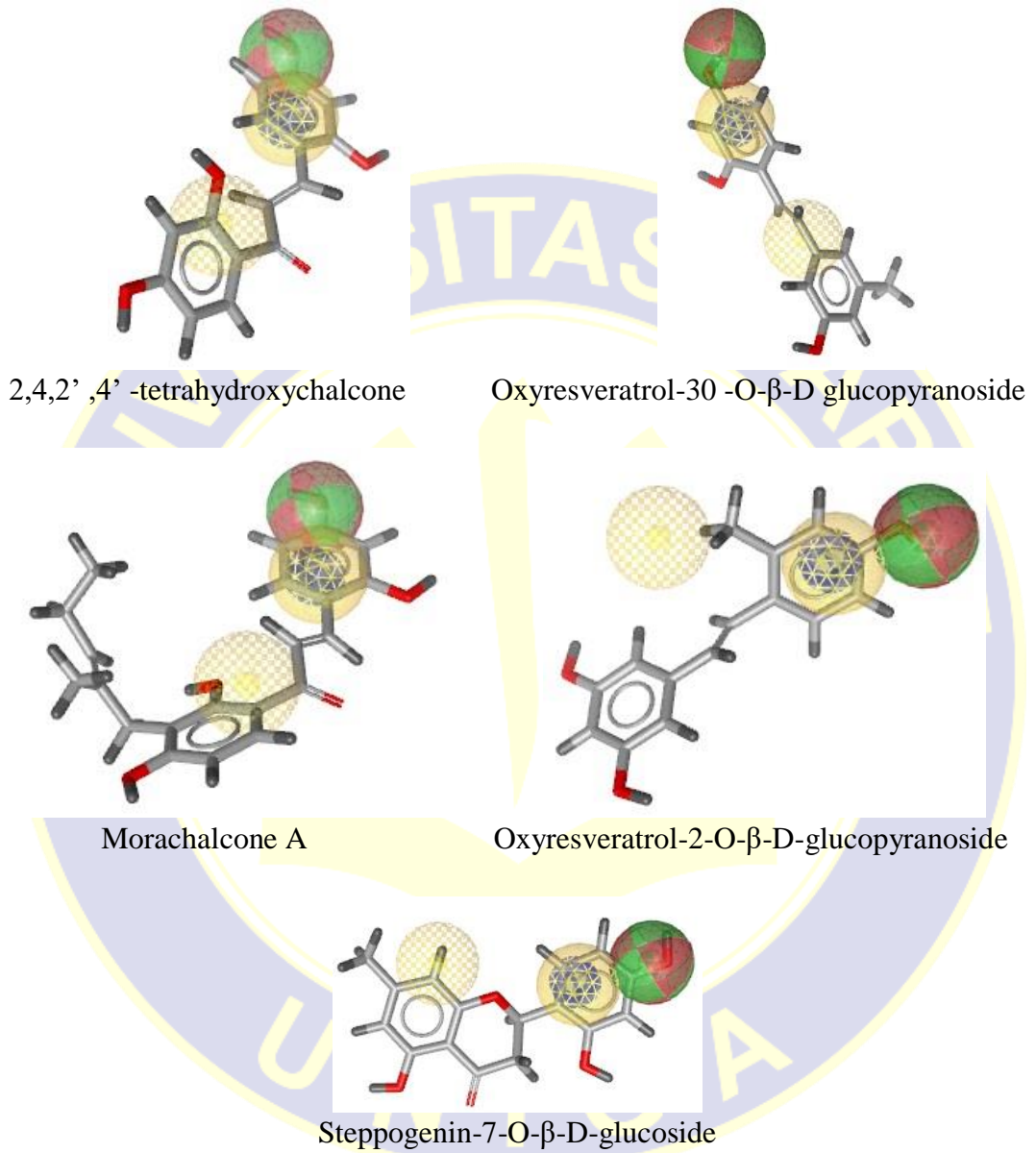
LAMPIRAN 20 (LANJUTAN)

Tabel V.1
Hasil *Skринing* Farmakofor Senyawa Akar Murbei Hitam (*Morus nigra* L.)
terhadap 4-Hydroxytamoxifen

No.	Nama Senyawa	Matching Features	Pharmacophore Fit Score
1	Cudraflavone C		60.84
2	Cudraflavone B		60.76
3	Norartocarpetin		53.74
4	Morachalcone A		53.70
5	Steppogenin-7-O-β-D-glucoside		53.37
6	2,4,2',4' - tetrahydroxychalcone		52.67
7	Oxyresveratrol-2-O-β-D-glucopyranoside		52.43
8	Morin-7-O-β-D-glucoside		51.96

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

LAMPIRAN 20
(LANJUTAN)



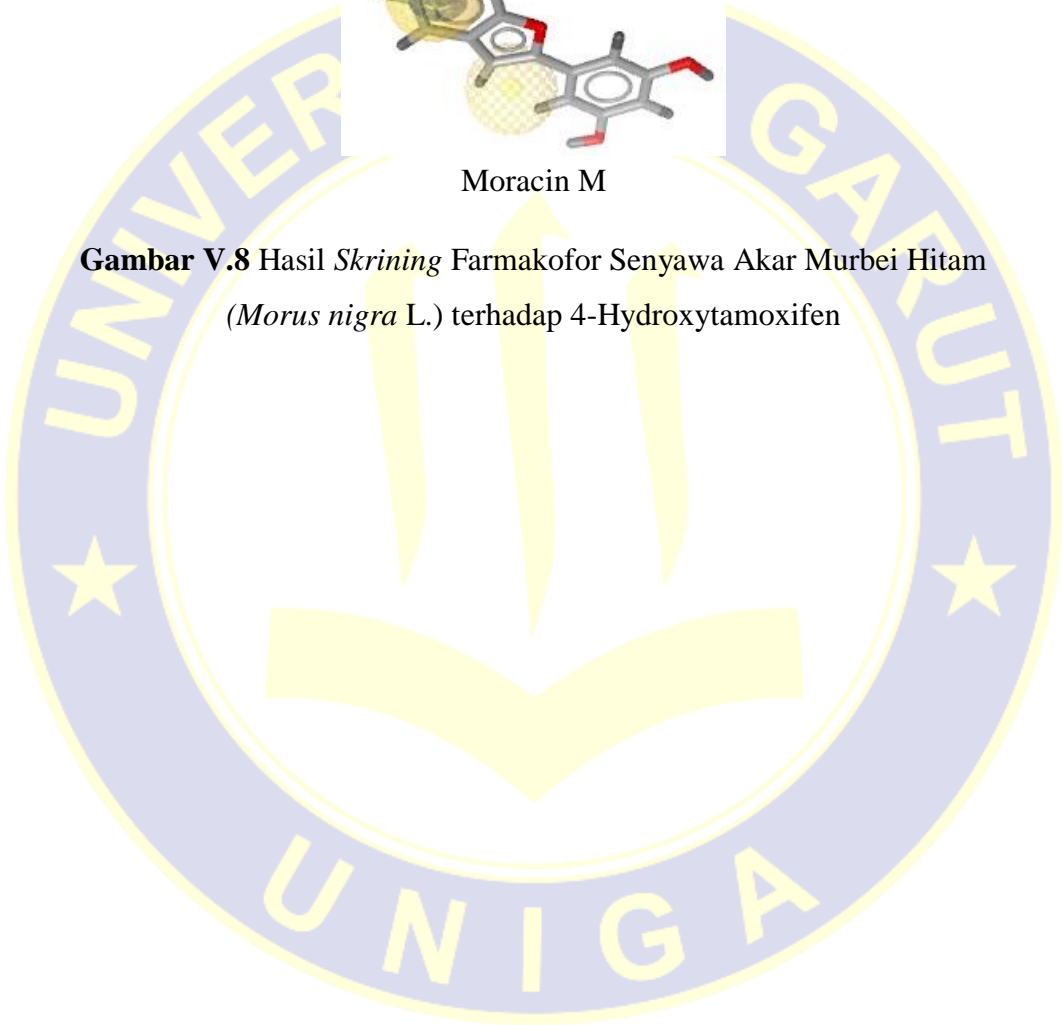
Gambar V.8 Hasil *Skrining* Farmakofor Senyawa Akar Murbei Hitam (*Morus nigra* L.) terhadap 4-Hydroxytamoxifen

LAMPIRAN 20
(LANJUTAN)









Moracin M

Gambar V.8 Hasil *Skrining* Farmakofor Senyawa Akar Murbei Hitam
(*Morus nigra* L.) terhadap 4-Hydroxytamoxifen



LAMPIRAN 20 (LANJUTAN)

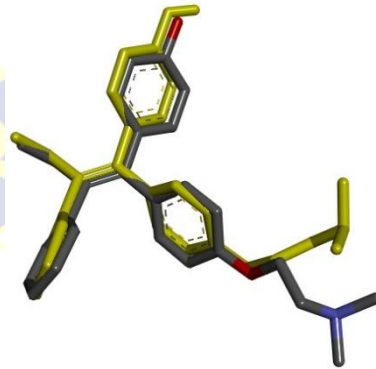
Tabel V.2
Hasil *Skринing* Farmakofor Senyawa Akar Murbei Hitam (*Morus nigra* L.)
terhadap Genistein

No.	Nama Senyawa	Matching Features	Pharmacophore Fit Score
1	2,4,2',4' - tetrahydroxychalcone		67.72
2	Oxyresveratrol-3'-O-β-D-glucopyranoside		67.60
3	Morachalcone A		67.55
4	Oxyresveratrol-2-O-β-D-glucopyranoside		67.51
5	Steppogenin-7-O-β-D-glucoside		67.25
6	Moracin M		51.89

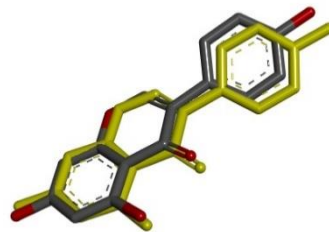
Keterangan: warna kuning = interaksi hidrofobik
 warna merah = akseptor ikatan hidrogen
 warna hijau = donor ikatan hidrogen
 warna biru = cincin aromatik

LAMPIRAN 21

VALIDASI METODE RESEPTOR ESTROGEN α DAN RESEPTOR ESTROGEN β

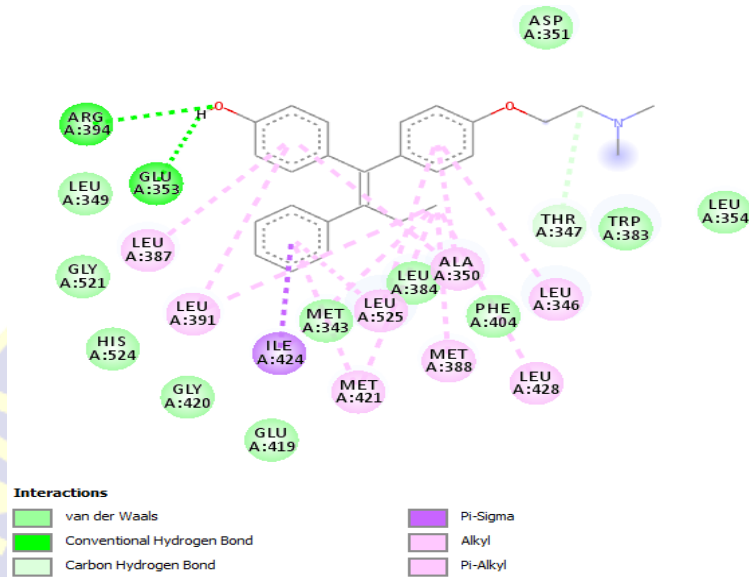


Gambar V.9 Visualisasi tumpang tindih ligan alami 4-Hydroxytamoxifen (warna merah dan abu) dengan ligan hasil *redocking* (warna kuning)

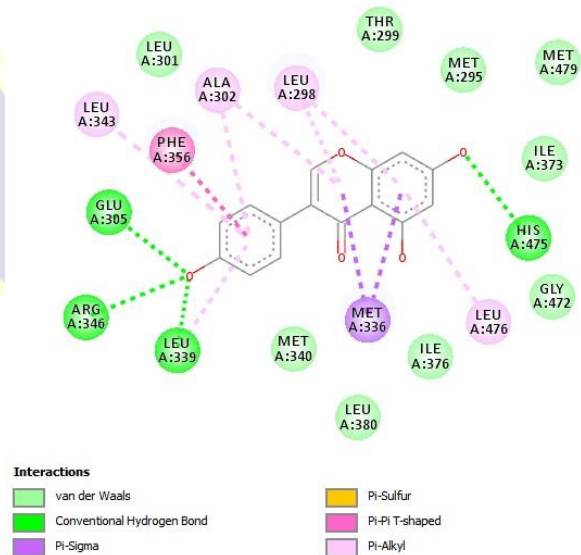


Gambar V.10 Visualisasi tumpang tindih ligan alami Genistein (warna merah dan abu) dengan ligan hasil *redocking* (warna kuning)

LAMPIRAN 21 (LANJUTAN)



Gambar V.11 Visualisasi residu asam amino dengan ikatan hidrogen pada ligan alami 4-Hydroxytamoxifen



Gambar V.12 Visualisasi residu asam amino dengan ikatan hidrogen pada ligan alami Genistein

LAMPIRAN 21 (LANJUTAN)

Tabel V.3

Hasil Validasi Metode dengan *redocking* ligan alaminya didapatkan nilai RMSD < 2 Å yaitu 1.02 Å dan 0,5 Å menunjukkan validasi metode dan reseptor yang sudah valid

Kode PDB	Grid Box	RMSD	Ikatan Energi Bebas	Residu Asam Amino
3ERT	X: 30.010 Y: -1.913 Z: 24.207	1,02 Å	-11,51	ARG394, GLU353
1QKM	X: 22.438 Y: 8.003 Z: 113.539	0,5 Å	-10,25	ARG346, GLU305, LEU339, HIS475

LAMPIRAN 22

HASIL PENAMBATAN MOLEKUL ER- α dan ER- β

Tabel V.4

Hasil Penambatan Molekul ER- α yang diurutkan berdasarkan nilai energi ikatan (ΔG) terendah 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 4-OHT	-11,51	2	ARG394, GLU353	3.64 nM
Senyawa aktif akar murbei hitam (<i>Morus nigra</i> L.)					
1	Cudraflavone C	-9.60	4	GLU353, LEU346, MET343, THR347	92.35 nM
2	Cudraflavone B	-8.99	3	LEU387, MET343, THR347	256.1 7 nM
3	Oxyresveratrol-2-O- β -D-glucopyranoside	-8.82	5	ARG394, GLU353, GLY521, HIS524, THR347	339.8 8 nM
4	Steppogenin-7-O- β -D-glucoside	-8.44	6	ARG394, ASP351, LEU346, LEU384, MET344 THR347	655.0 6 nM

LAMPIRAN 22
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekul ER- α yang diurutkan berdasarkan nilai energi ikatan (ΔG) terendah beserta nilai konstanta inhibisi (KI) dan residu asam aminonya

5	2,4,2',4'- tetrahydroxychalcone	-8.33	5	ARG394, GLU353, GLY521, HIS524, LEU346	789.5 1 nM
6	Morachalcone A	-7.91	2	ASP351, THR347	1.59 μ M
7	Morin-7-O- β -D- glucoside	-7.78	3	GLU353, MET343, THR347	2 μ M
8	Norartocarpetin	-7.38	4	GLU353, GLY521, HIS524, LEU387	3.89 μ M

LAMPIRAN 22 (LANJUTAN)

Tabel V.5

Hasil Penambatan Molekul ER- β yang diurutkan berdasarkan nilai energi ikatan (ΔG) terendah beserta nilai konstanta inhibisi (KI) dan residu asam aminonya

Ligan alami					
Ligan alami Genistein		-10,25	4	ARG346, GLU305, LEU339, HIS475	30.70 nM
Senyawa aktif akar murbei hitam (<i>Morus nigra</i> L.)					
1	Morachalcone A	-11.28	4	GLU305, HIS475, LEU298, GLY472,	5.39 nM
2	Steppogenin-7-O- β - D-glucoside	-9.29	2	GLU305, LEU298	155.5 1 nM
3	2,4,2',4'- tetrahydroxychalcone	-8.91	4	GLU305, ARG346, GLY472, LEU298	296.2 1 nM
4	Oxyresveratrol-2-O- β -D-glucopyranoside	-8.75	4	GLU305, LEU339, HIS475, GLY472	385.0 3 nM
5	Moracin M	-8.64	1	GLU305	464.3 0 nM
6	Oxyresveratrol-3'-O- β -D-glucopyranoside	-8.54	4	GLU305, LEU339, HIS475, GLY472	545.5 2 nM

LAMPIRAN 23

SIFAT FISIKOKIMIA SENYAWA AKAR MURBEI HITAM

BERDASARKAN LIPINSKI'S RULE OF FIVE

Tabel V.6

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	Cudraflavone C	4	6	450	6.14	Memenuhi
2	Cudraflavone B	3	6	420	5.33	Memenuhi
3	Oxyresveratrol-2-O- β -D-glucopyranoside	7	10	408	0.61	Memenuhi
4	Steppogenin-7-O- β -D-glucoside	7	11	450	-0.31	Memenuhi
5	2,4,2',4'-tetrahydroxychalcone	4	5	272	2.4	Memenuhi
6	Morachalcone A	4	5	354	4.3	Memenuhi
7	Morin-7-O- β -D-glucoside	8	12	464	-0.51	Memenuhi
8	Moracin M	3	4	242	3.21	Memenuhi
9	Norartocarpetin	4	6	286	2.12	Memenuhi
10	Oxyresveratrol-3'-O- β -D-glucopyranoside	7	9	406	0.15	Memenuhi

Syarat: 1. BM < 500 mg/mol

2. Log P < 5

3. Donor Hidrogen < 5

4. Akseptor Hidrogen < 10

LAMPIRAN 24

HASIL UJI PREADMET

Tabel V.7
Data Hasil Pengujian PreADME

No	Nama Senyawa	Caco-2 cell (nm ^{sec-1})	HIA (%)	Protein Plasma Binding
1	Cudraflavone C	20.644 ^b	89.999 ^a	99.97 ^a
2	Cudraflavone B	19.35 ^b	92.47 ^a	94.29 ^a
3	Oxyresveratrol-2-O-β-D-glucopyranoside	11.02 ^b	28.29 ^b	96.26 ^a
4	Steppogenin-7-O-β-D-glucoside	9.73 ^b	21.74 ^b	67.34 ^b
5	2,4,2',4'-tetrahydroxychalcone	20.01 ^b	80.61 ^a	100 ^a
6	Morachalcone A	20.57 ^b	86.73 ^a	100 ^a
7	Morin-7-O-β-D-glucoside	9.73 ^b	21.74 ^b	67.34 ^b
8	Moracin M	0.42 ^c	87.26 ^a	96.67 ^a
9	Norartocarpetin	18.57 ^b	79.43 ^a	97.27 ^a
10	Oxyresveratrol-3'-O-β-D-glucopyranoside	10.16 ^b	36.73 ^b	95.24 ^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 25
HASIL UJI TOKSISITAS

Tabel V.8

Data Hasil Pengujian Toksisitas yang dilihat dari potensi mutagen dan karsinogen

No	Nama Senyawa	Mutagenik	Karsinogenik
1	Cudraflavone C	Non-mutagen	Negatif
2	Cudraflavone B	Non-mutagen	Negatif
3	Oxyresveratrol-2-O- β -D-glucopyranoside	Mutagen	Positif
4	Steppogenin-7-O- β -D-glucoside	Non-mutagen	Negatif
5	2,4,2',4'-tetrahydroxychalcone	Mutagen	Positif
6	Morachalcone A	Non-mutagen	Negatif
7	Morin-7-O- β -D-glucoside	Mutagen	Negatif
8	Moracin M	Mutagen	Positif
9	Norartocarpetin	Mutagen	Positif
10	Oxyresveratrol-3'-O- β -D-glucopyranoside	Mutagen	Positif