

DAFTAR PUSTAKA

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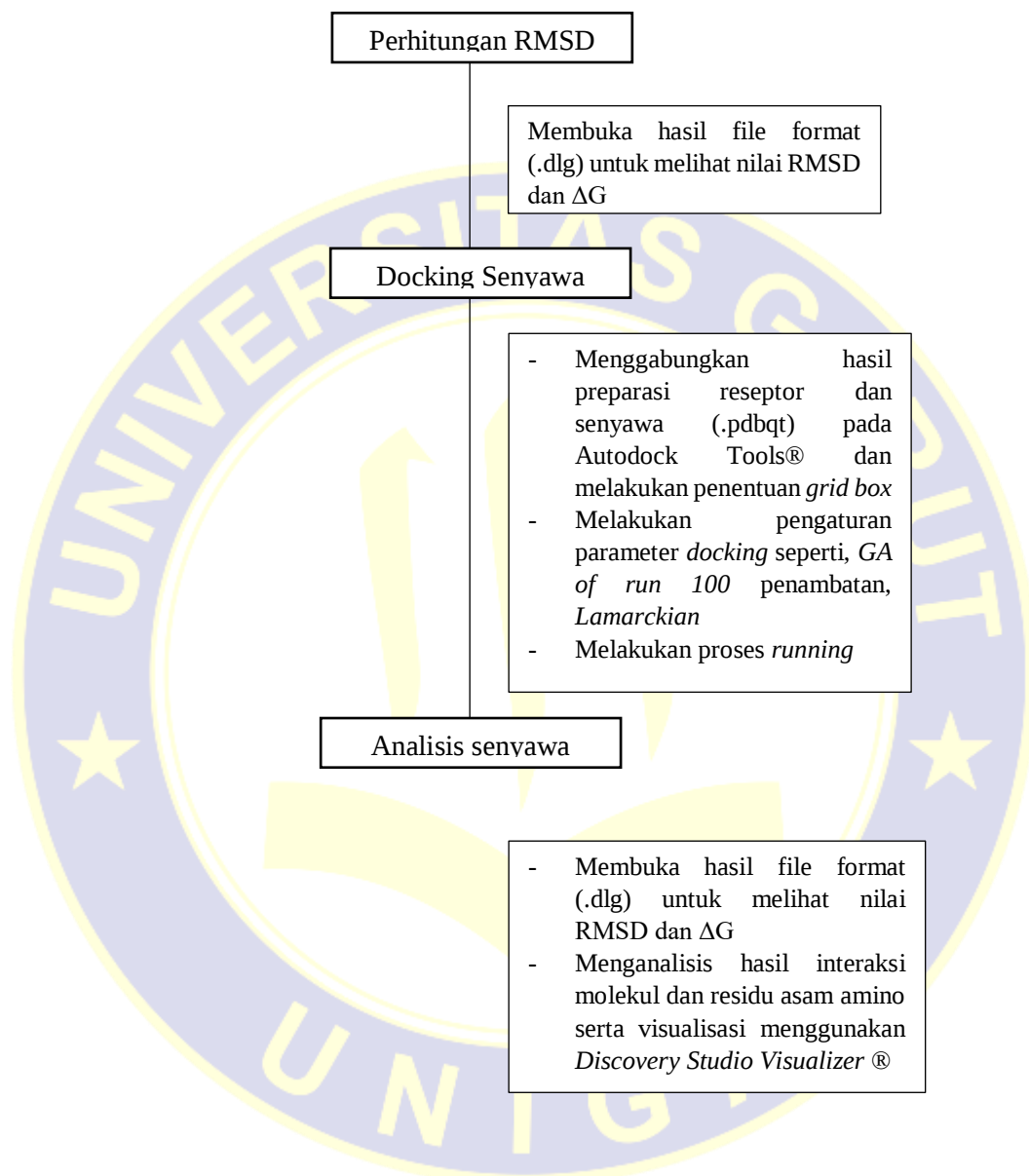
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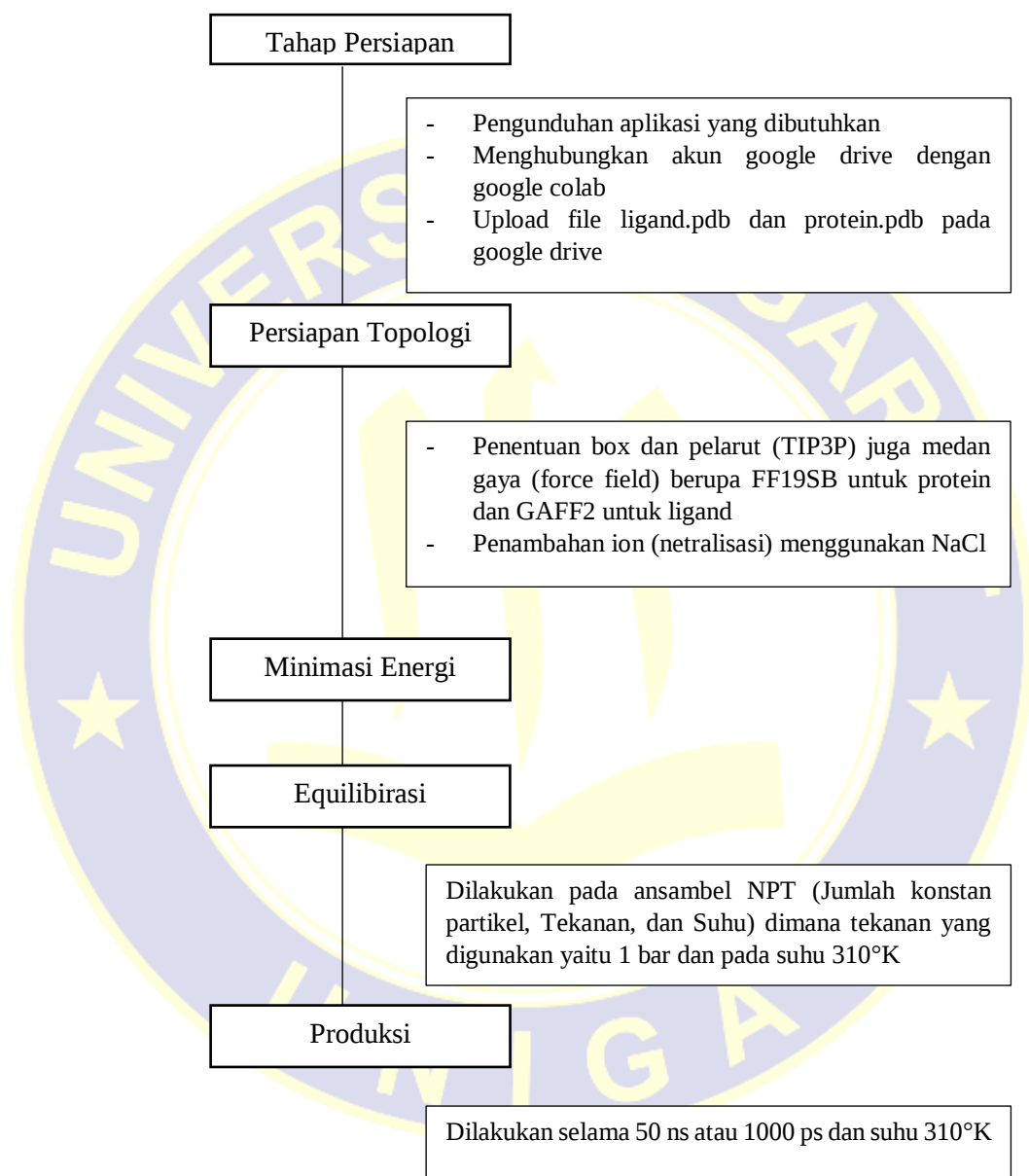
LAMPIRAN 1 (LANJUTAN)



Gambar VII.1 Lanjutan

LAMPIRAN 2

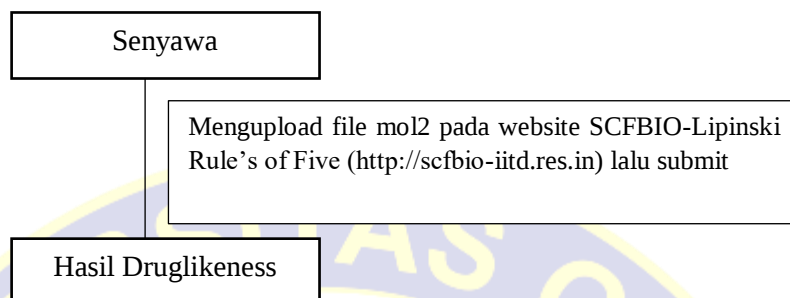
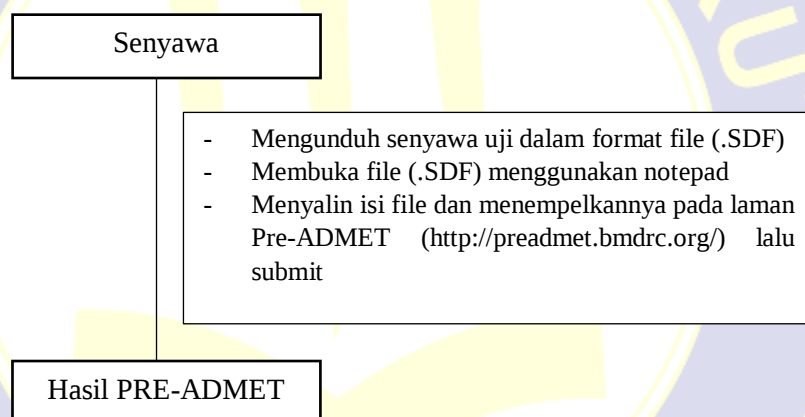
ALUR PENELITIAN SIMULASI DINAMIKA MOLEKULER



Gambar VII. 2 Alur penelitian simulasi dinamika molekuler

LAMPIRAN 3

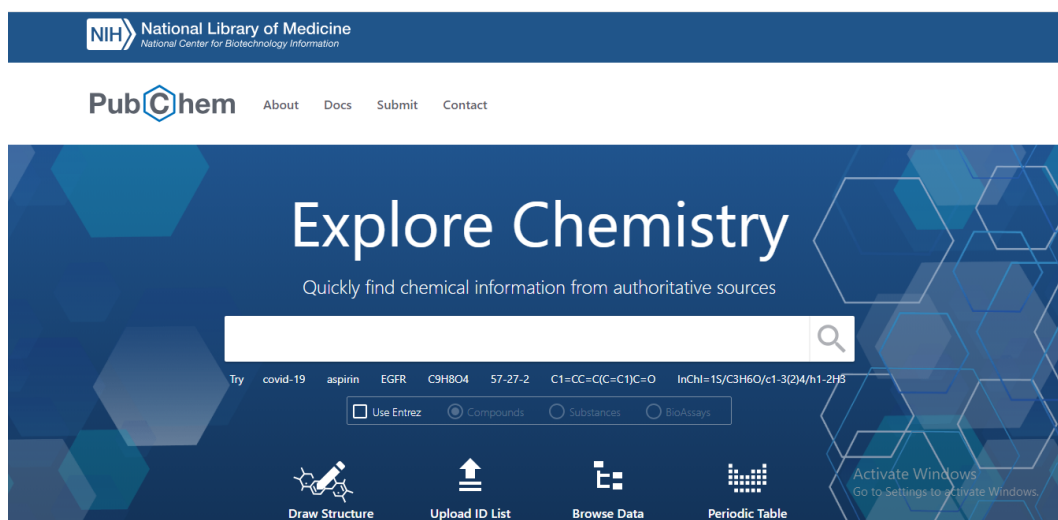
ALUR PREDIKSI DRUGLIKENESS, PREDIKSI ADMET

Gambar VII.3 Alur penelitian prediksi *druglikenes*

Gambar VII.4 Alur penelitian prediksi ADMET

LAMPIRAN 4

SITUS DAN APLIKASI



Gambar VII.5 Tampilan situs *Pubchem*



Gambar VII.6 Tampilan situs *Protein Data Bank*

LAMPIRAN 4 (LANJUTAN)

Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi

Lipinski Rule of Five

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

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.

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, *.xyz, *.sdf, *.smi]

Activate Windows
Go to Settings to activate Windows.

Pre ADMET

Tel: +82-32-212-9550 / Fax: +82-32-212-9572 | webmaster@bmdrc.org
209, Veritas A Hall, Yonsei University 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, Republic of Korea

Gambar VII.7 Tampilan situs *Lipinski's Rule of Five*

Pre ADMET

Home About Druglikeness ADME Toxicity Community Commercial

Welcome to the PreADMET

PreADMET is a web-based application for predicting ADME data and building drug-like library using in silico method. PreADMET ver 2.0 is also commercially available in the four editions: Descriptors, Endpoint, Standard and Professional.

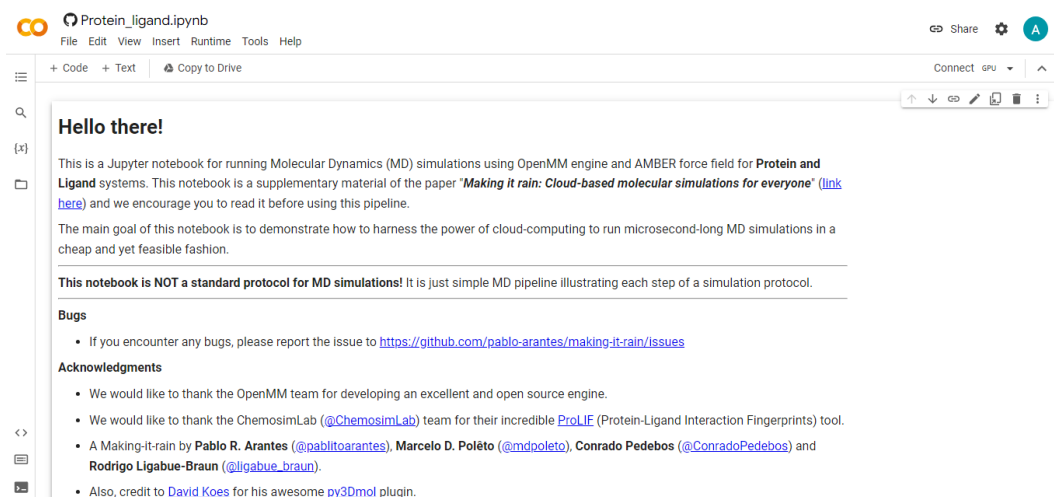
- Drug-Likeness Prediction**
Lipinski rule, lead-like rule, Drug DB like rule
- ADME Prediction**
caco-2, MDCK, BBB, HIA, plasma protein binding and skin permeability data
- Toxicity Prediction**
Ames test and rodent carcinogenicity assay

Latest News

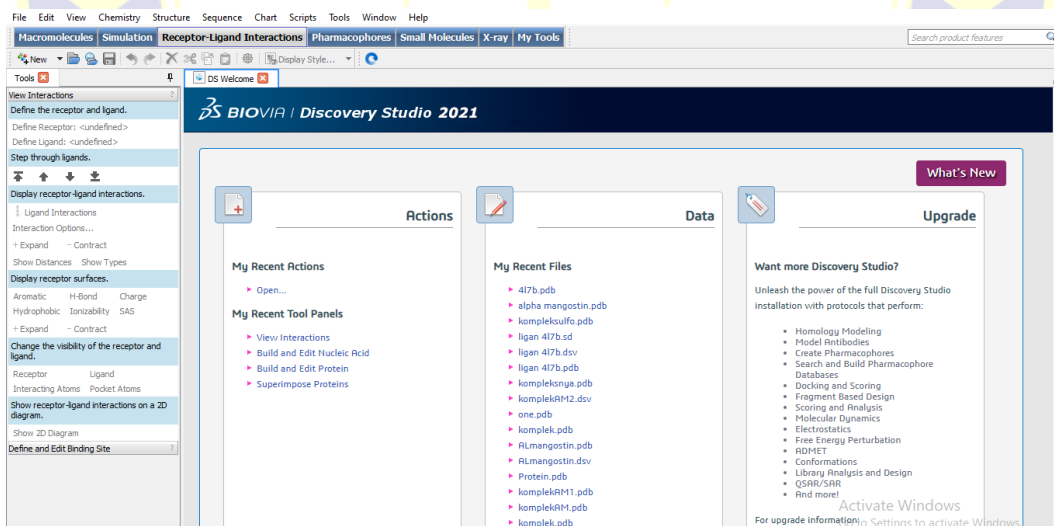
- G-SFED and Human Nephrotoxicity models will be added in Aug 2017
January 24, 2017
- PreADMET Ver 2.1 is coming soon in this month.
January 9, 2015
- [2008/11] PreADME is one of the most popular sites by Cheminformatics.org.
November 27, 2008
- [2008/10] New release of PreADMET v2.0 windows version to activate Windows.
October 27, 2008

Gambar VII.8 Tampilan situs *PreADMET*

LAMPIRAN 4 (LANJUTAN)

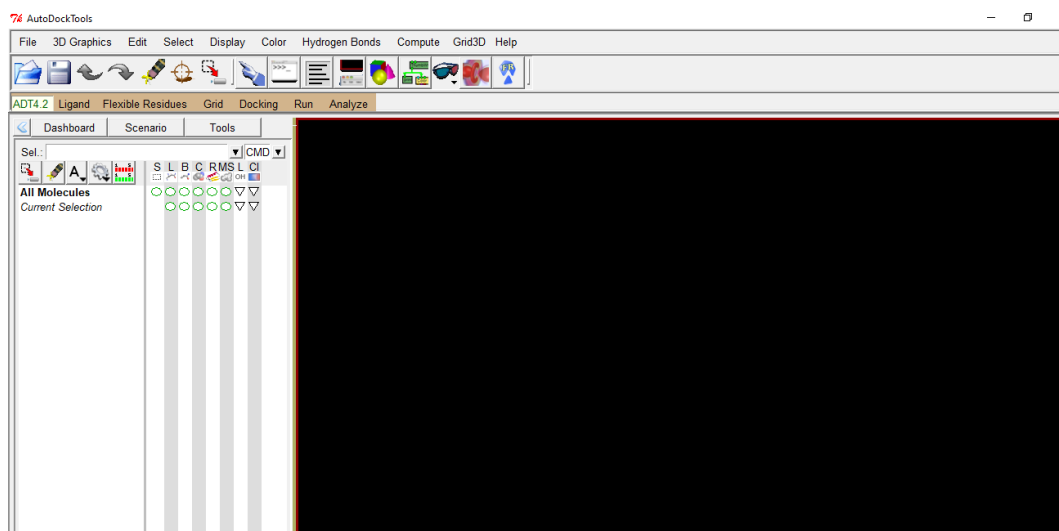


Gambar VII.5 Tampilan situs *Google Colab*

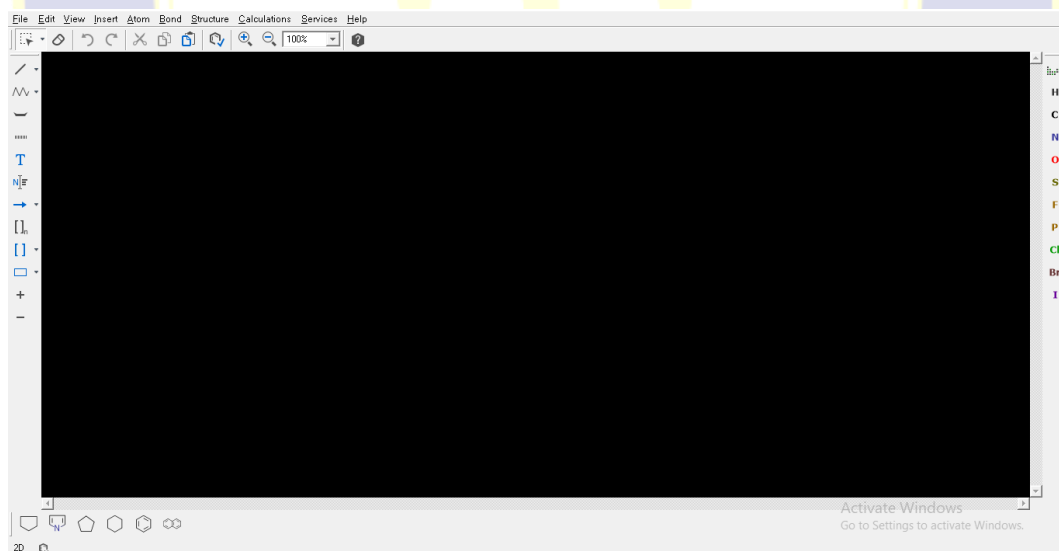


Gambar VII.6 Tampilan *software Discovery Studio Visualizer*

LAMPIRAN 4 (LANJUTAN)



Gambar VII.11 Tampilan *software Autodock Tools*

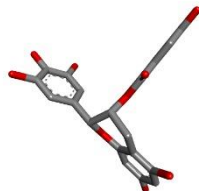


Gambar VII.12 Tampilan *software MarvinSketch*

LAMPIRAN 5
STRUKTUR 3D SENYAWA UJI

Tabel VII. 1

Struktur 2D Senyawa Uji

Senyawa Uji	Rumus Molekul	Struktur Senyawa
EGCG	C ₂₂ H ₁₈ O ₁₁	

LAMPIRAN 6
STRUKTUR 3D RESEPTOR

Tabel VII. 2

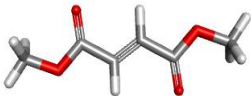
Struktur 3D Reseptor Nrf2-Keap1

ID PDB	STRUKTUR KOMPLEKS
4L7B	

LAMPIRAN 7
STRUKTUR 3D LIGAN PEMBANDING

Tabel VII. 3

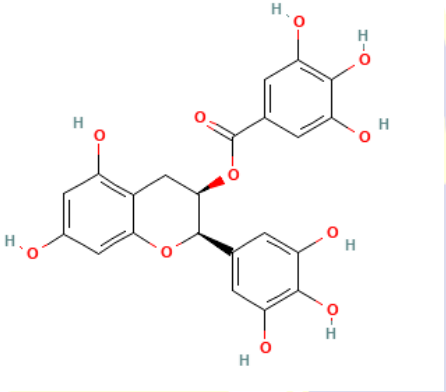
Struktur 3D Ligan Pembanding

NAMA LIGAN PEMBANDING	STRUKTUR SENYAWA
Dimethyl Fumarate	 <chem>COC(=O)/C=C/C(=O)OC</chem>

LAMPIRAN 8
STRUKTUR 2D SENYAWA UJI

Tabel VII. 4

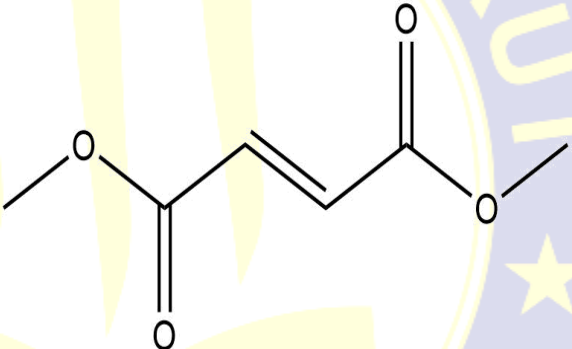
Struktur 2D Senyawa Uji

SenyawaUji	Rumus Molekul	Struktur Senyawa
EGCG	C ₂₄ H ₂₂ O ₆	

LAMPIRAN 9
STRUKTUR 2D LIGAND PEMBANDING

Tabel VII. 5

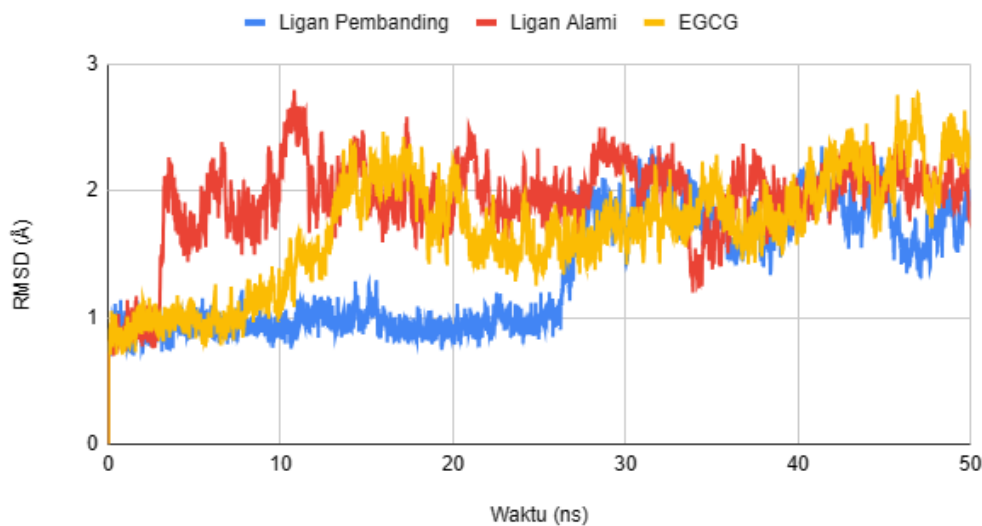
Struktur 2D Ligand Pembanding

Ligand Pembanding	Struktur Senyawa
Dimethyl Fumarate	 The chemical structure of Dimethyl Fumarate is shown. It consists of a central trans-alkene (C=C) with two carboxylate groups attached to the double-bonded carbons. Each carboxylate group is represented as a carbonyl group (C=O) bonded to a methoxy group (-OCH₃). The structure is drawn in a skeletal format with explicit oxygen atoms and double bonds. <chem>COC(=O)/C=C/C(=O)OC</chem>

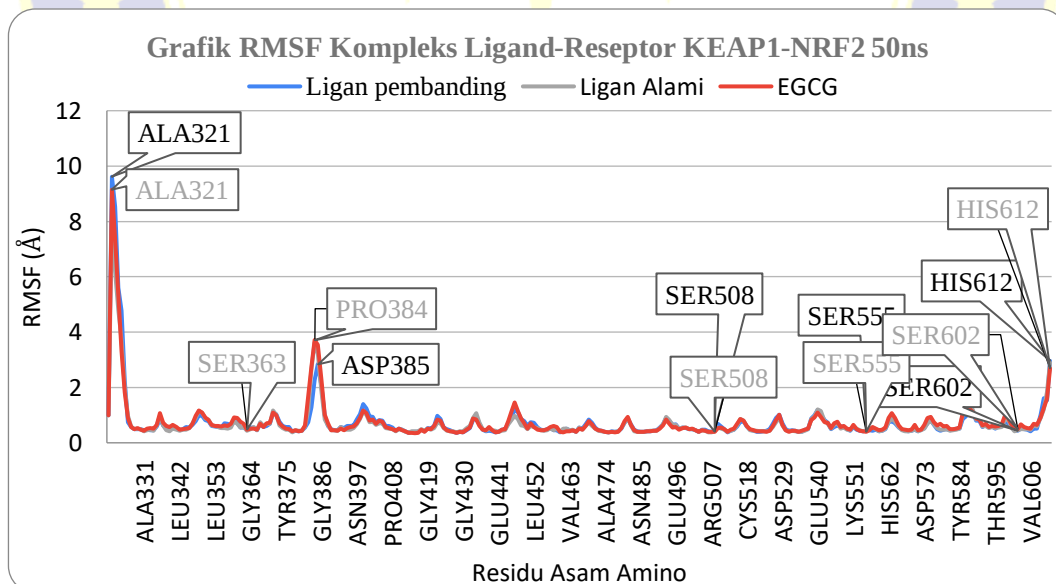
LAMPIRAN 10

GRAFIK SIMULASI DINAMIK KOMPLEKS LIGAN DENGAN RESEPTOR

Grafik RMSD Kompleks Ligand-Reseptor KEAP1-NRF2 50ns



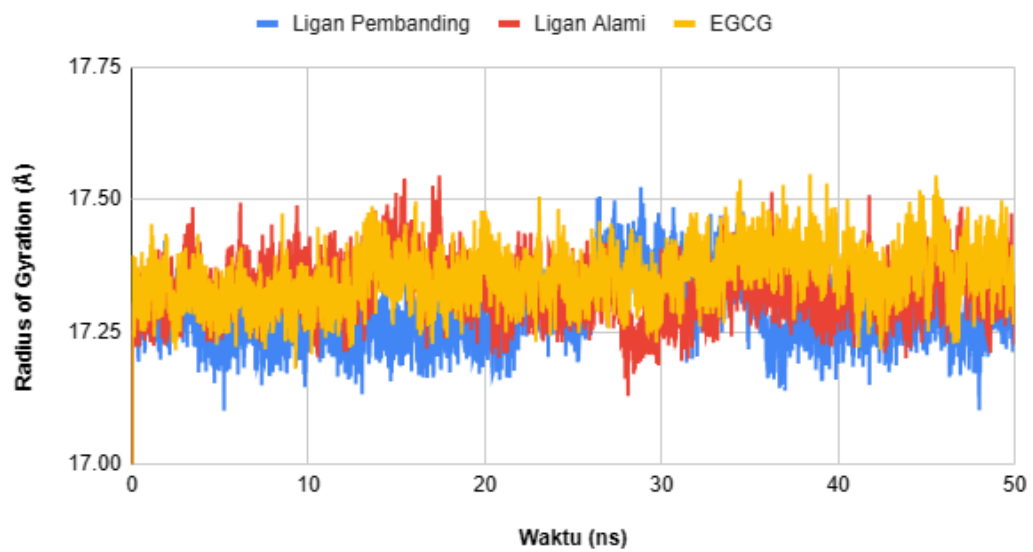
Gambar VII.7 Grafik RMSD



Gambar VII.8 Grafik RMSF

LAMPIRAN 10 (LANJUTAN)

Grafik RG Kompleks Ligand-Reseptor KEAP1-NRF2 50ns



Gambar VII.9 Grafik *Radius Of gyration*

DAFTAR RIWAYAT HIDUP

I. IDENTITAS DIRI

Nama : Adilla Nurul Aliefah
 Tempat, Tanggal Lahir : Garut, 18 September 2001
 Jenis kelamin : Perempuan
 Agama : Islam
 Kewarganegaraan : Indonesia
 Status : Mahasiswa
 Alamat : Kp. Sukasirna RT 04 RW 07
 Ds. Karangmulya Kec. Kadungora
 Kab. Garut, Jawa Barat 44153
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 Email : adillanurul.9e@gmail.com



II. RIWAYAT PENDIDIKAN

Jenjang Pendidikan	Nama Sekolah/Perguruan Tinggi	Tahun Masuk	Tahun Lulus
SD/MI	SDN 4 Karangmulya	2007	2013
SMP/MTs	SMPN 1 Kadungora	2013	2016
SMA/MA/SMK	SMAN 2 Garut	2016	2019
Perguruan Tinggi	Universitas Garut	2019	2023

III. PENGALAMAN ORGANISASI DAN KEPANITIAAN

1. Panitia PUBDEKDOK FMIPA CUP (2019)
2. Anggota Komisi Pengawasan HMF MPM KEMA FMIPA UNIGA (2021-2022)
3. Anggota Event Organizer Sobot Paper (2021-2022)