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LAMPIRAN 1
TANAMAN KUMIS KUCING

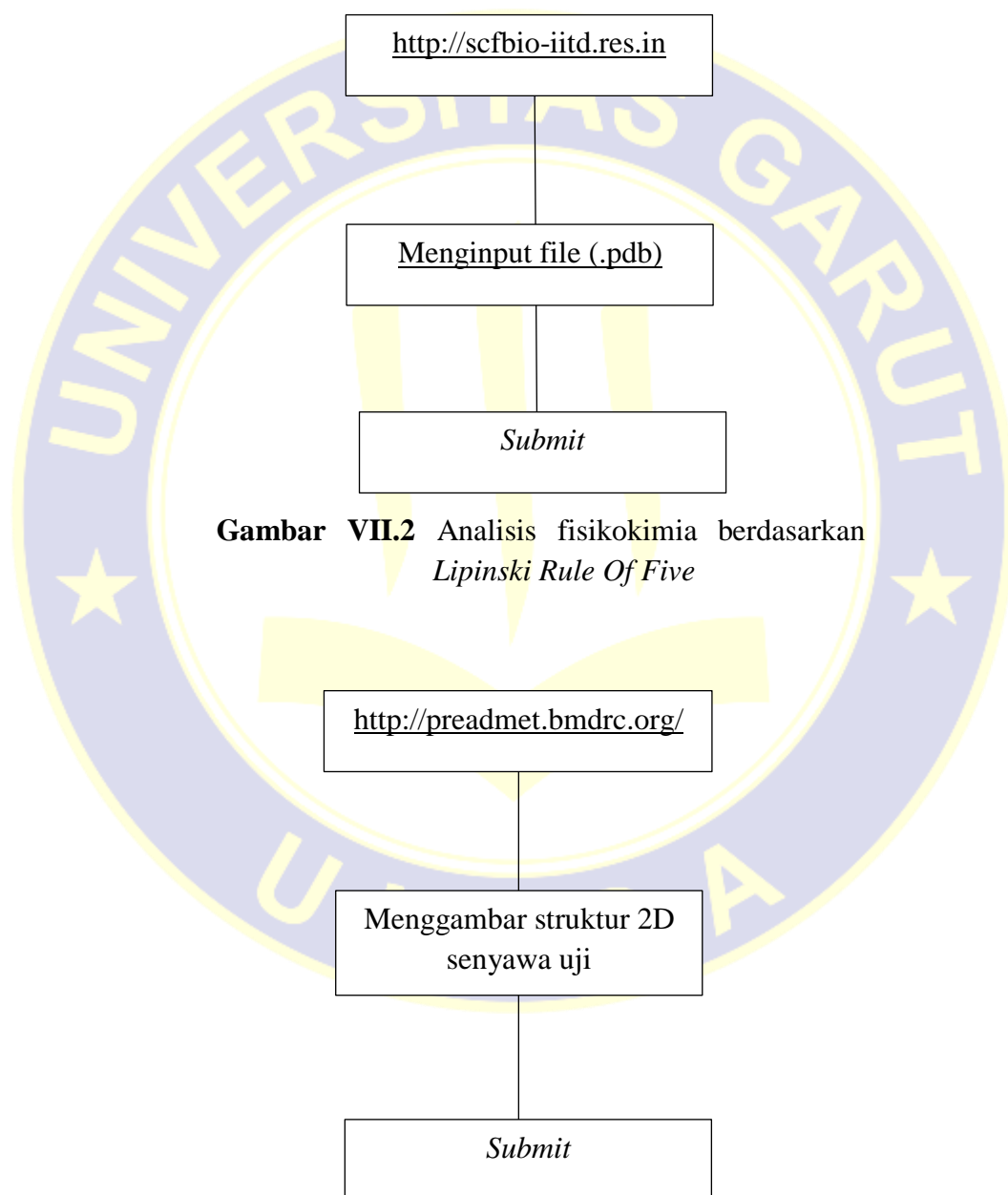


Gambar VII.1 Tanaman Kumis Kucing (*Orthosiphon stamineus* Benth)

LAMPIRAN 2

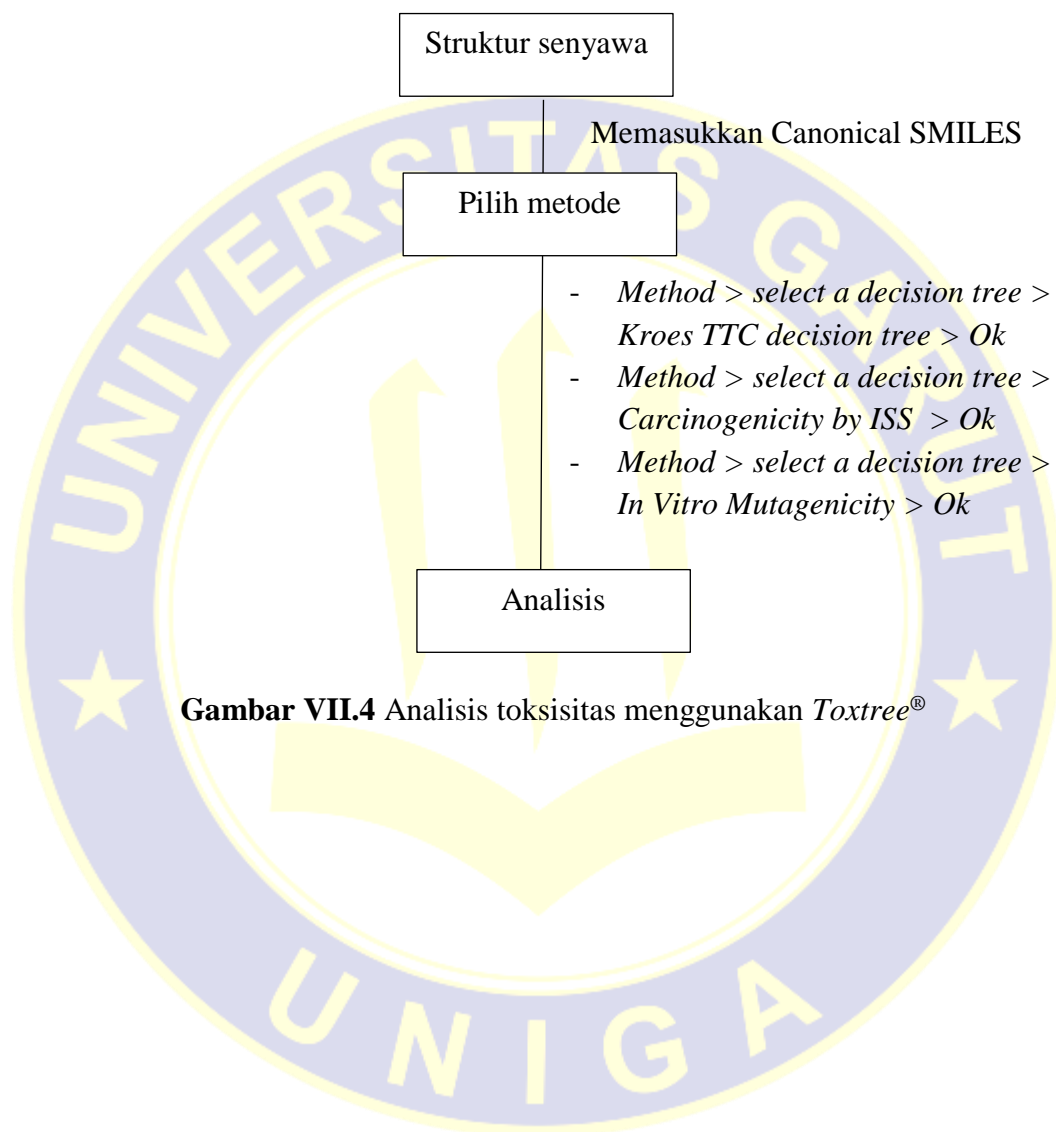
ALUR PENELITIAN ANALISIS SIFAT FISIKOKIMIA DAN

FARMAKOKINETIK



Gambar VII.2 Analisis fisikokimia berdasarkan *Lipinski Rule Of Five*

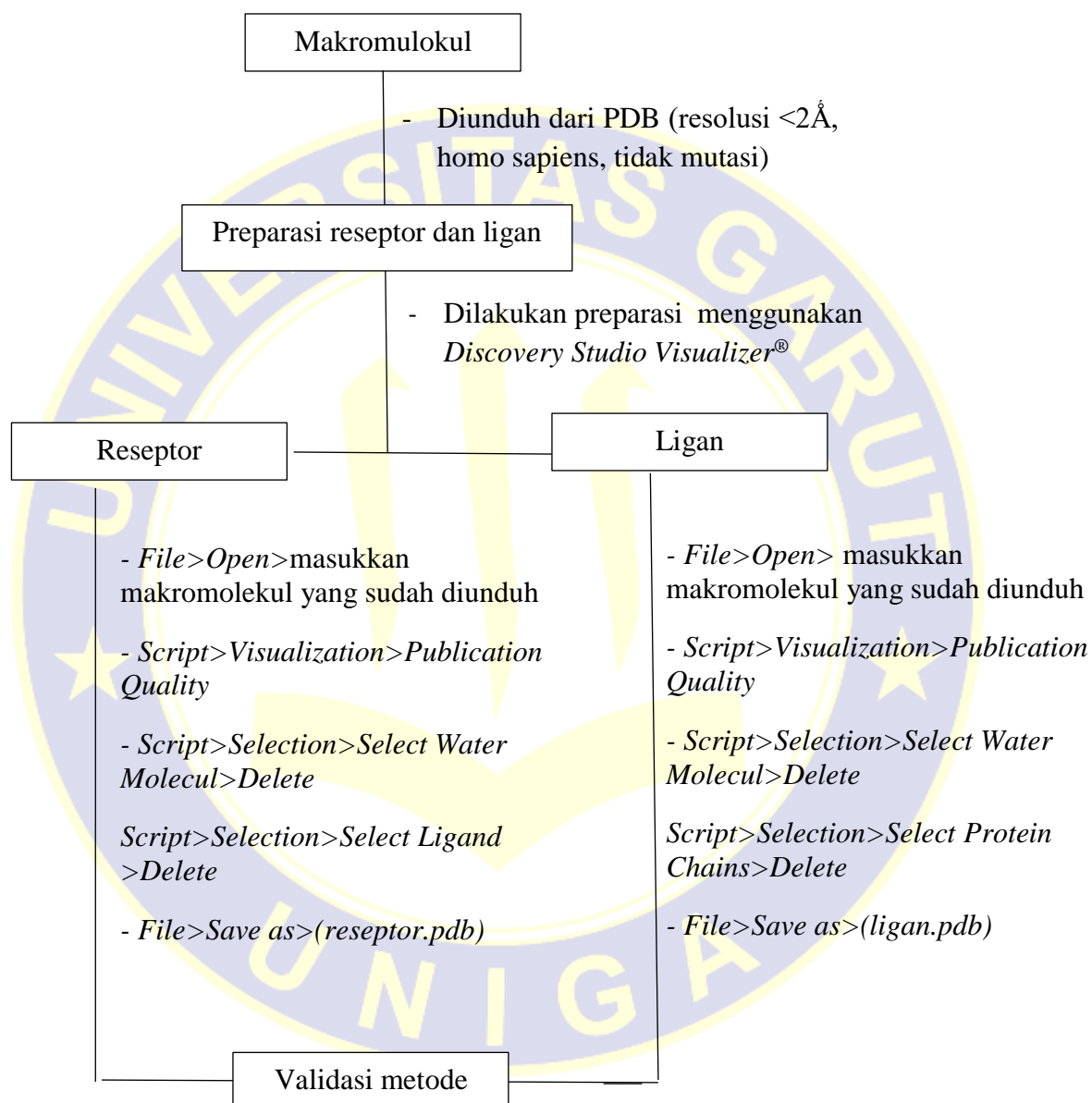
Gambar VII.3 Analisis farmakokinetik PreADMET

LAMPIRAN 2**(LANJUTAN)**

Gambar VII.4 Analisis toksisitas menggunakan *Toxtree*[®]

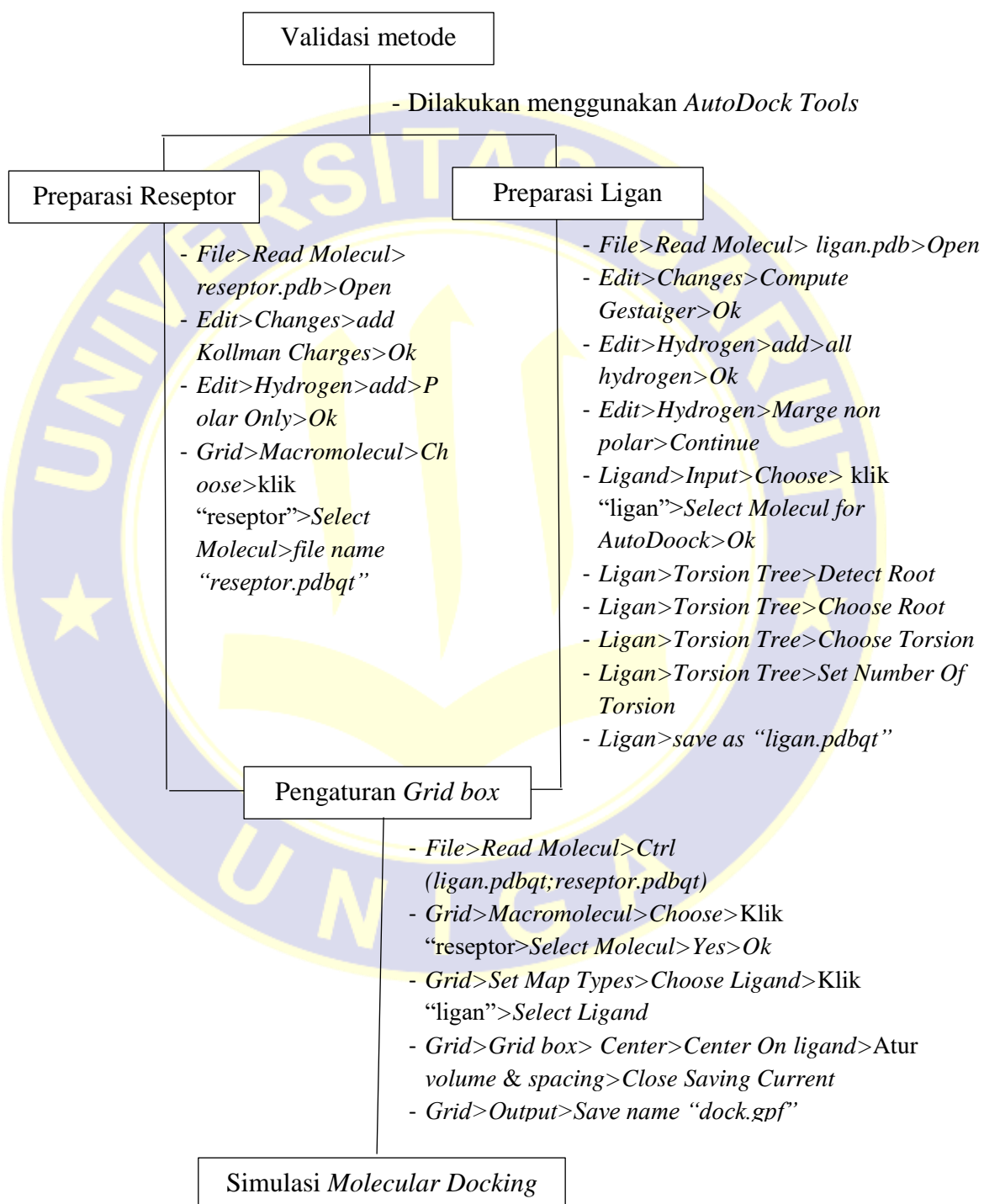
LAMPIRAN 3

ALUR PENELITIAN SIMULASI *MOLECULAR DOCKING*



LAMPIRAN 3

(LANJUTAN)



LAMPIRAN 3

(LANJUTAN)

Optimasi ligan

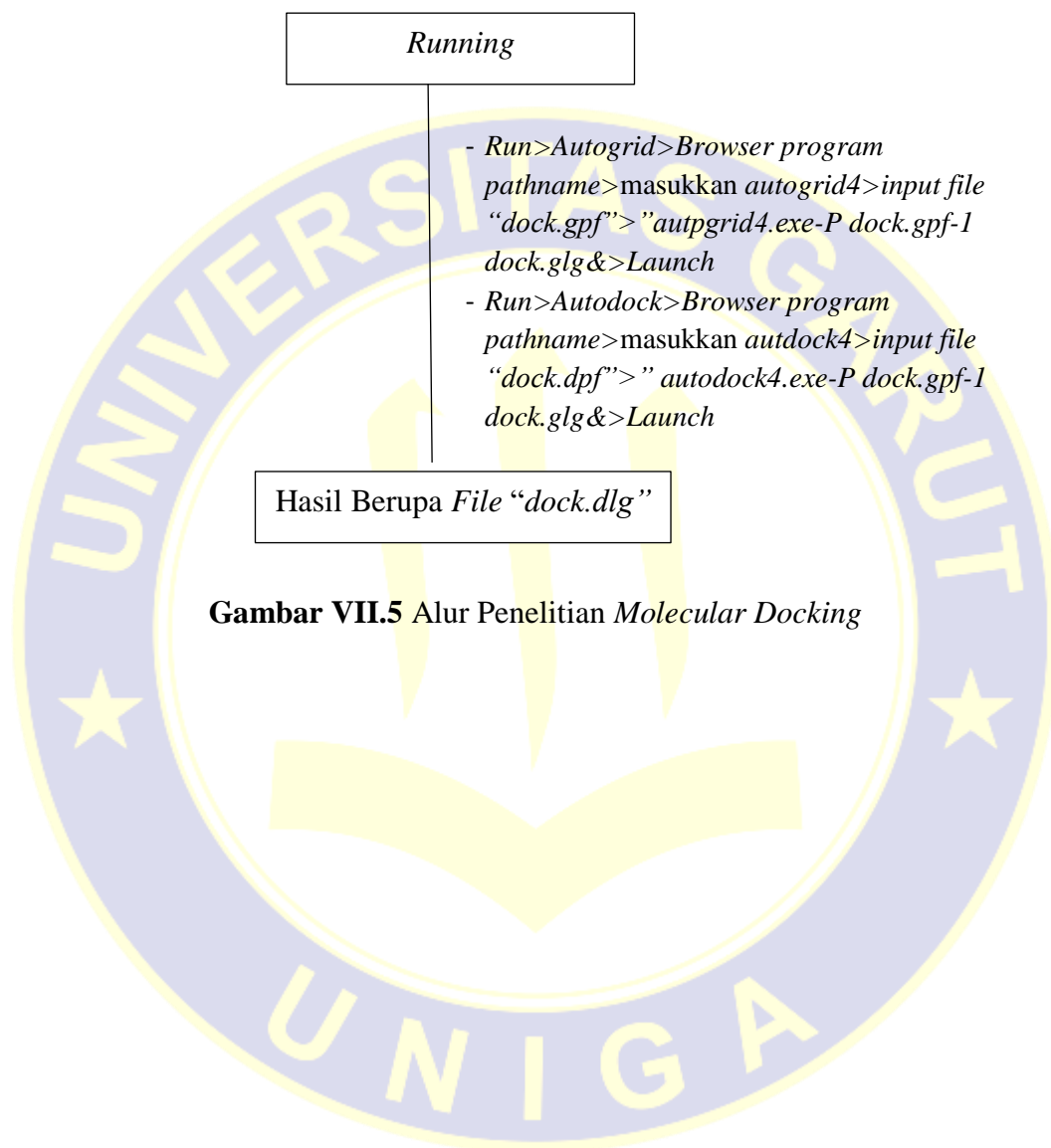
- Dilakukan menggunakan *ChemDraw Professional 15.0*[®]
- *File>Open>Gambar Struktur>Edit>Get 3D Model>Edit Chem 3D xml Object*
- *Calculation>MM2>Minimize Energy>Run>Save Copy As "ligan.pdb"*

Simulasi *Molecular Docking*

- *File>Preference>Set>Copy Paste alamat penyimpanan ke Startup directory>Set>Dismiss*
- *Docking>Macromolecul>Set Rigid File name"reseptor.pdbqt"*
- *Docking>Ligand>Choose>Klik "ligan">Select Ligan>Accept*

Pengatur Parameter *Docking* Metode *Lamarckian GA*

- *Docking>Search Parameter>Genetic Algorithm>Number Of GA Runs (100)>Accept*
- *Docking>Docking Parameter>Use Default>Accept*
- *Docking>Output>Lamarckian GA (4.2)> Save as "dock.dpf"*

LAMPIRAN 3**(LANJUTAN)****Gambar VII.5** Alur Penelitian *Molecular Docking*

LAMPIRAN 4

SITUS DAN APLIKASI

Not secure | scfbio-iitd.res.in/software/drugdesign/lipinski.jsp

Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi

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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)
- The input file name should not contain whitespace(s).

Gambar VII.6 Tampilan Situs *Lipinski Rule of Five*

preadmet.bmdrc.kr

MDL mol and sdf file | Molecular descriptors | Druglikeness | ADME Prediction | Toxicity prediction | Log In | Register

PreADMET

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B138A, YONSEI ENGINEERING RESEARCH COMPLEX, YONSEI UNIVERSITY, SEOUL, REPUBLIC OF KOREA.

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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

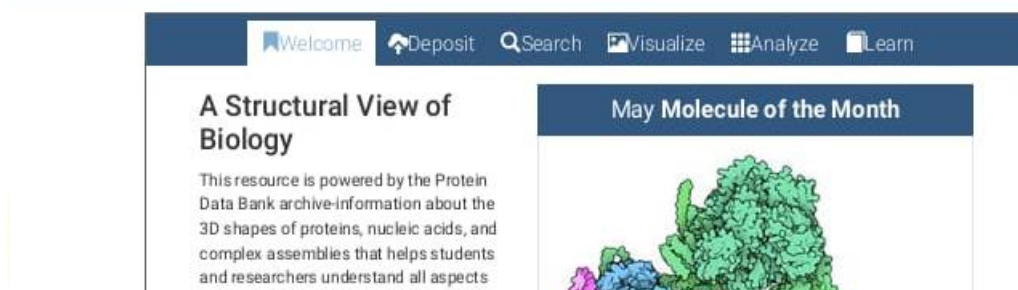
Lastest News

- 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
October 27, 2008

Gambar VII.7 Tampilan Situs PreADMET

LAMPIRAN 4

(LANJUTAN)



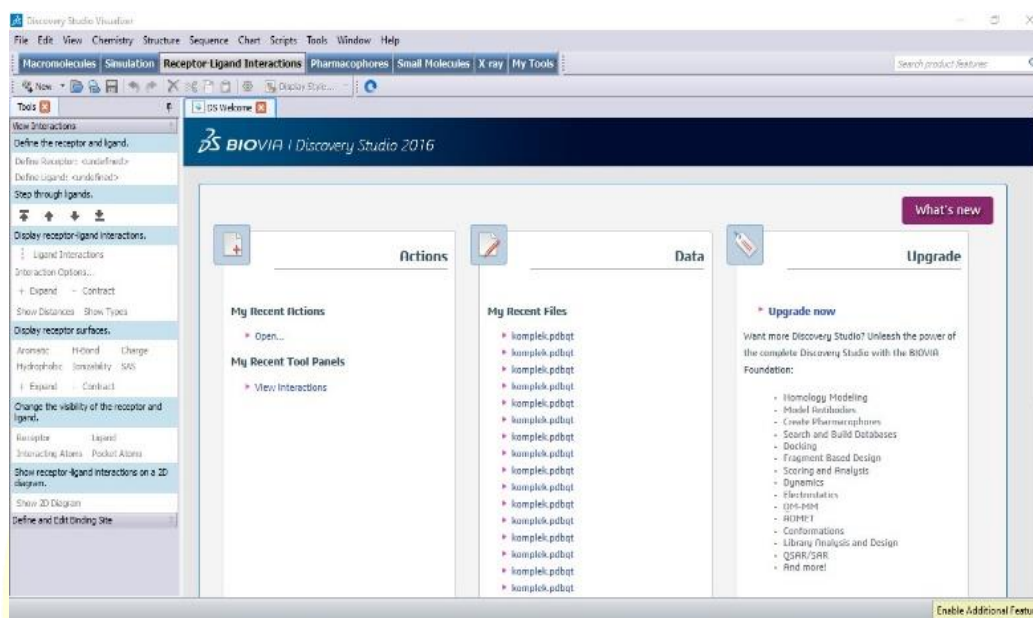
Gambar VII.8 Tampilan Situs *Protein Data Bank* (PDB)



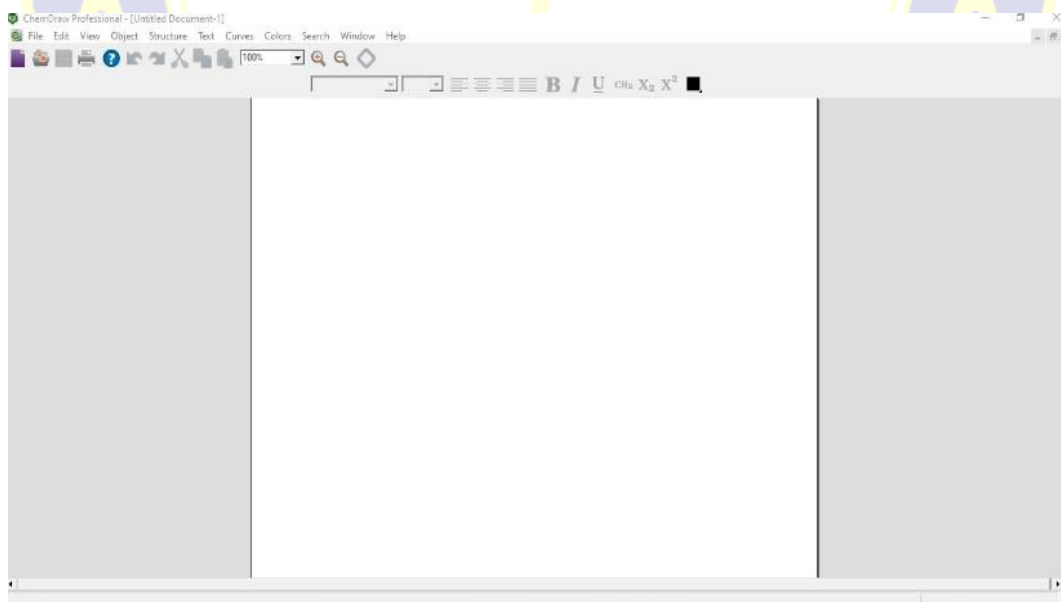
Gambar VII.9 Tampilan Situs *PubChem*

LAMPIRAN 4

(LANJUTAN)



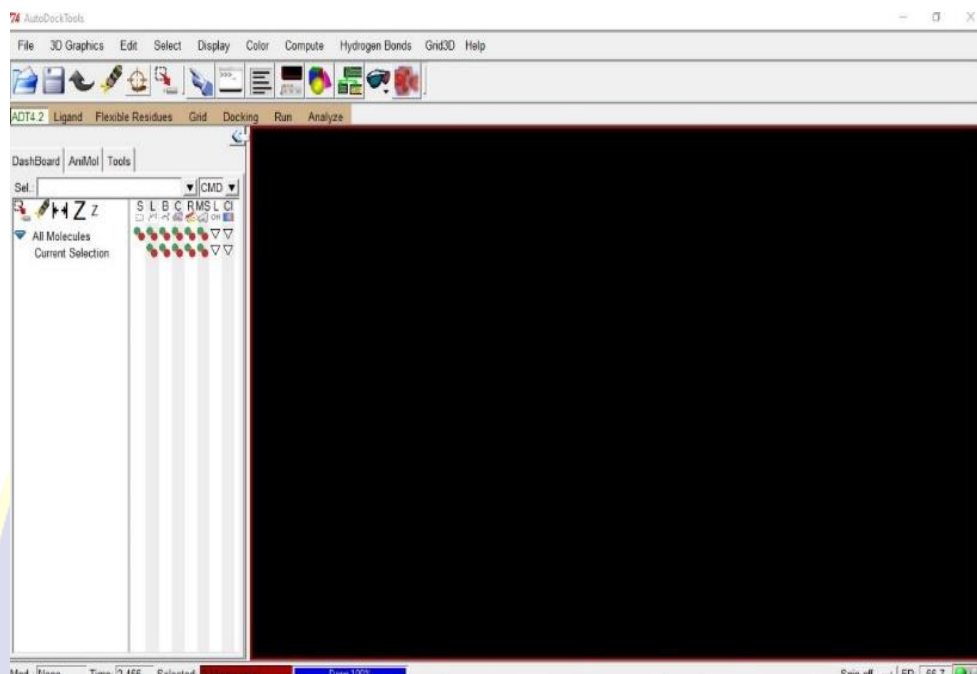
Gambar VII.10 Tampilan Aplikasi *Discovery Studio Visualizer*[®]



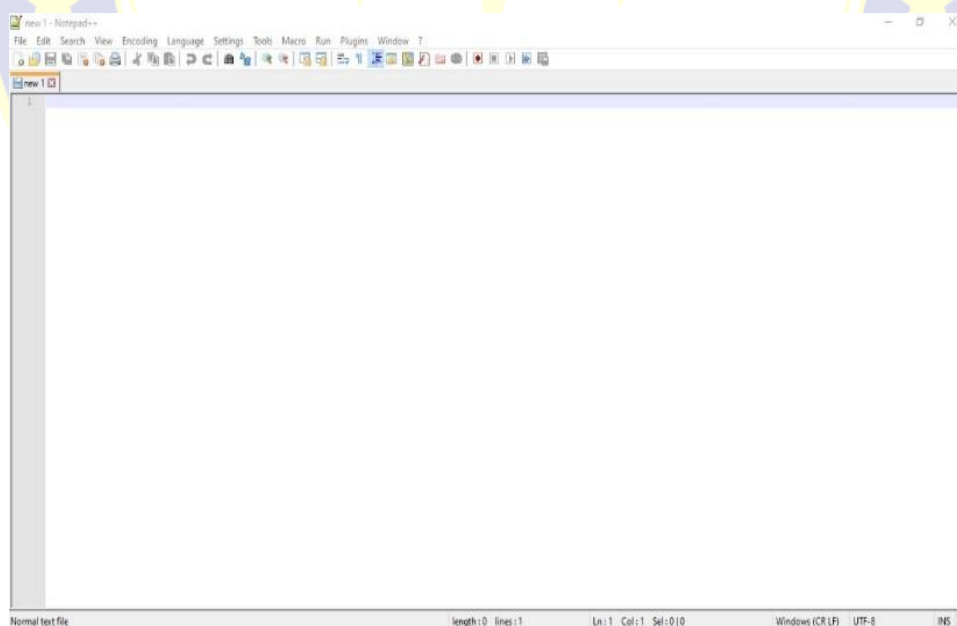
Gambar VII.11 Tampilan Aplikasi *ChemDraw Professional 15.0*[®]

LAMPIRAN 4

(LANJUTAN)



Gambar VII.12 Tampilan Aplikasi *AutoDock Tools*[®]



Gambar VII.13 Tampilan Aplikasi *Notepad*^{++®}

LAMPIRAN 5

RESIDU ASAM AMINO

Tabel VII.1

Residu asam amino simulasi *molecular docking* senyawa turunan flavonoid tanaman kumis kucing (*Orthosiphon stamineus* Benth.) terhadap reseptor ID 2F70

No.	Senyawa	Residu Asam Amino
1	Cirsimaritin	ARG A:221, ASP A:48, PHE A:182, CYS A:215, ALA A:217, TYR A:46, VAL A:49, ASP A:181
2	Eupatorin	ASP A:48, ALA A:217, ILE A:219, TYR A:46, VAL A:49
3	Ladanein	ARG A:221, ALA A:217, TYR A:46, GLY A:220, ASP A:48, CYS A:215, ALA A:217, TYR A:46, PHE A:182, ASP A:181
4	Luteolin	ARG A:221, SER A:216, VAL A:49, TYR A:46, ALA A:217, ASP A:181
5	Quersetin	ASP A:48, ALA A:217, PHE A:182, CYS A:215, ALA A:217, ILE A:219, VAL A:49, ASP A:181, ARG A:221
6	Salvigenin	ASP A:48, ARG A:221, SER A:216, ALA A:217, ILE A:219, TYR A:46, VAL A:49, ASP A:181, ARG A:221
7	Sinensetin	ASP A:48, GLY A:220, VAL A:49, TYR A:46, PHE A:182
8	<i>4'-hydroxy-5,6,7-trimethoxyflavone</i>	ARG A:221, ALA A:217, CYS A:215, CYS A:215, TYR A:46, ALA A:217, VAL A:49, ASP A:181
9	<i>4', 5,6,7-tetramethoxyflavone</i>	ARG A:221, ASP A:48, ALA A:217, ILE A:219, VAL A:49
10	<i>5-hydroxy-6,7,3,4'-tetramethoxyflavone</i>	ASP A:181, ASP A:48, SER A:216, GLY A:220, TYR A:46, PHE A:182, ALA A:217, TYR A:46, VAL A:49
11	<i>6-hydroxy-5,7,4'-trimethoxyflavone</i>	ASP A:181, ASP A:48, SER A:216, GLY A:220, TYR A:46, ALA A:217, ILE A:219, VAL A:49, ARG A:221

LAMPIRAN 5

(LANJUTAN)

Tabel VII.2

Residu asam amino simulasi *molecular docking* senyawa turunan flavonoid tanaman kumis kucing (*Orthosiphon stamineus* Benth.) terhadap reseptor ID 4YVP

No.	Senyawa	Residu Asam Amino
1	Cirsimaritin	TYR B:55, TYR B:216, HIS B:117, TYR B:24, TRP B:227, TRP B:86, LEU B:54, LEU B:308, PHE B:118
2	Eupatorin	GLU B:224, ASN A:167, TRP B:227, TYR B:24, TRP B:227, LEU B:54, LEU B:308, HIS B:117, HIS B:117
3	Ladanein	LEU B:54, TYR B:55, TRP B:227, TYR B:24, LEU B:54, VAL B:128
4	Luteolin	HIS B:117, GLU B:224, LEU B:54, TRP B:86, PHE B:118, LEU B:308, TRP B:227, PHE B:118, TYR B:24
5	Quersetin	HIS B:117, GLU B:224, LEU B:54, TRP B:86, PHE B:118, LEU B:308, TRP B:227
6	Salvigenin	LYS B:31, TRP B:227, TYR B:24, LEU B:54
7	Sinensetin	GLU B:224, LEU B:54, ALA B:25, TRP B:227, LEU B:54, HIS B:222
8	<i>4'-hydroxy-5,6,7-trimethoxyflavone</i>	LYS B:31, HIS B:222, TRP B:227, TYR B:24, LEU B:54
9	<i>4', 5,6,7-tetramethoxyflavone</i>	LYS B:31, ASN B:56, TYR B:24, LEU B:54
10	<i>5-hydroxy-6,7,3,4'-tetramethoxyflavone</i>	HIS B:222, ALA B:25, TRP B:227, TYR B:24, LEU B:54
11	<i>6-hydroxy-5,7,4'-trimethoxyflavone</i>	LYS B:31, TRP B:227, TYR B:24, LEU B:54

LAMPIRAN 5

(LANJUTAN)

Tabel VII.3

Residu asam amino simulasi *molecular docking* senyawa turunan flavonoid tanaman kumis kucing (*Orthosiphon stamineus* Benth.) terhadap reseptor ID 4YVX

No.	Senyawa	Residu Asam Amino
1	Cirsimaritin	GLU B:192, SER B:221, TYR B:23, PHE B:306, TRP B:227, TYR B:24
2	Eupatorin	LEU B:54, LYS B:207, ASP B:204, SER B:32, SER B:208, LEU B:63
3	Ladanein	LEU B:54, LYS B:207, SER B:32, ASP B:204
4	Luteolin	ASN B:167, HIS B:117, TYR B:55, LEU B:54, TYR B:216, PHE B:306, TRP B:227, LEU B:54B
5	Quersetin	LEU A:35, LYS B:207, SER A:32, LYS B:207, SER B:208, GLU A:59
6	Salvigenin	LEU A:35, LYS B:207, ASP B:204, GLU A:59, LEU A:63
7	Sinensetin	HIS B:117, LEU B:54, TRP B:227, TRP B:55
8	<i>4'-hydroxy-5,6,7-trimethoxyflavone</i>	LYS A:105, GLN A:60, ASP B:204, LEU A:35, GLU A:59, LYS B:207, ASP B:204
9	<i>4', 5,6,7-tetramethoxyflavone</i>	LYS A:105, GLU A:59, LYS B:207, ASP B:204
10	<i>5-hydroxy-6,7,3,4'-tetramethoxyflavone</i>	LYS A:105, LEU A:63, LEU A:35, LYS B:207, SER A:32, SER B:208, LYS B:207
11	<i>6-hydroxy-5,7,4'-trimethoxyflavone</i>	LEU A:35, LYS B:207

DAFTAR RIWAYAT HIDUP

DATA PRIBADI

Nama : Febia Citraeni Rusdaita
Tempat/Tanggal Lahir : Cilacap, 24 Februari 1998
Jenis Kelamin : Perempuan
Agama : Islam
Warga Negara : Indonesia
Status : Mahasiswa
Alamat : Jl. Banteng Loreng Km.11 RT 03 RW 01 Desa
Ujungbarang, Kec. Majenang, Kab. Cilacap, Jawa Tengah
No telp : 082288160024
Email : cfobia198@gmail.com

PENDIDIKAN

Formal

SD Negeri Ujungbarang 02 (2004-2010)
SMP Negeri 01 Salem (2010-2013)
SMK Negeri 01 Purwokerto (2013-2016)
S1 Farmasi Universitas Garut (2016-2020)

Non Formal

Latihan Kepemimpinan 1 Ismafarsi Priangan 2016
Priangan Pharmacist Leadership Forum 2016

Pelatihan Bela Negara Yonif 303 Cibuluh 2018

Pondok Pesantren Hudan Al-Islami (2016-sekarng)

Pengalaman Kerja

Student Intern, PT. Bio Farma (Persero) (Februari 2020-July 2020)

Student Intern, Apotek Farrel Farma 2015

Student Intern, Apotek Arca Mandiri 2015

Organisasi

Departemen Humas, BEM KEMA FMIPA UNIGA (2017-2018)

SA Keuangan dan Bisnis Ismafarsi Priangan (2018-2020)

Komunitas Berdaya Care (2017-2018)

