

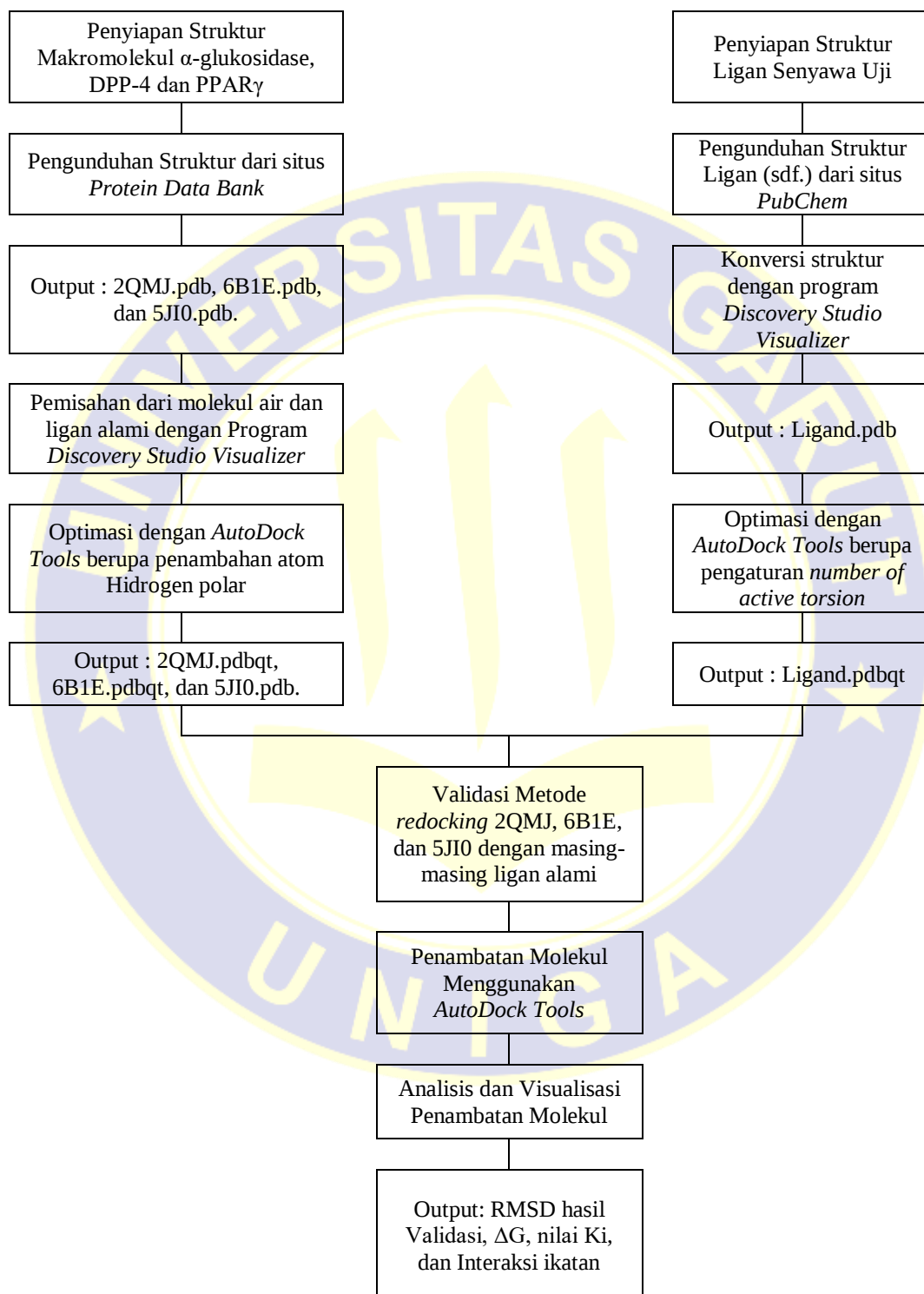
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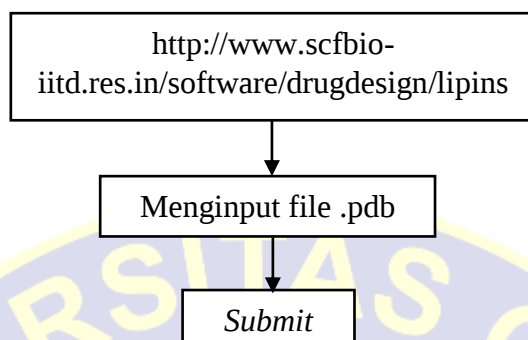
LAMPIRAN 1

ALUR PENELITIAN

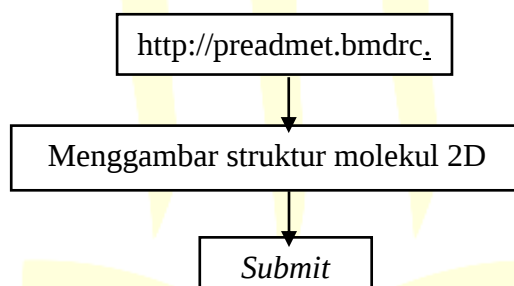


Gambar IV.1 Alur penelitian penambatan molekul

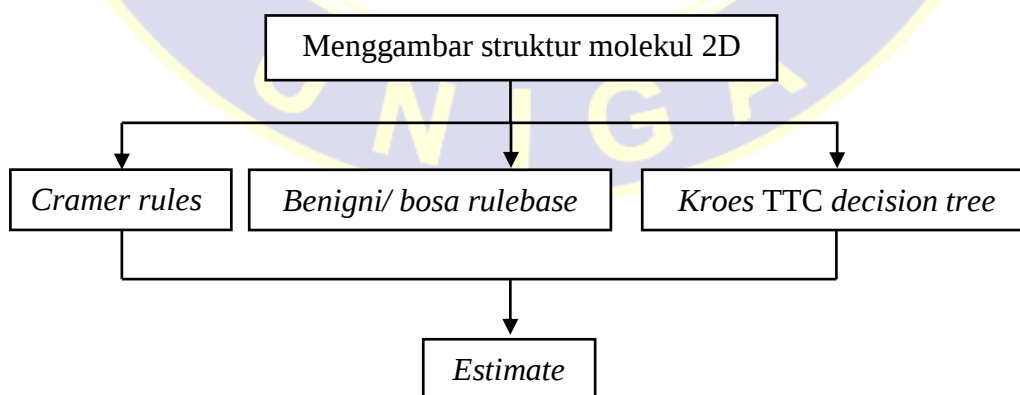
**LAMPIRAN 1
(LANJUTAN)**



Gambar IV.2 Analisis *Lipinski Rule of Five*



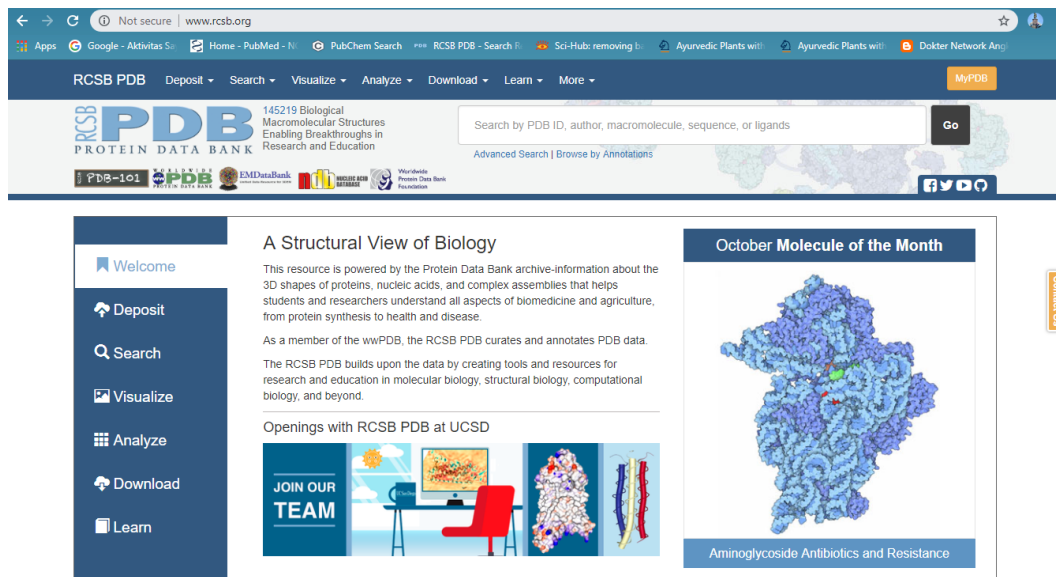
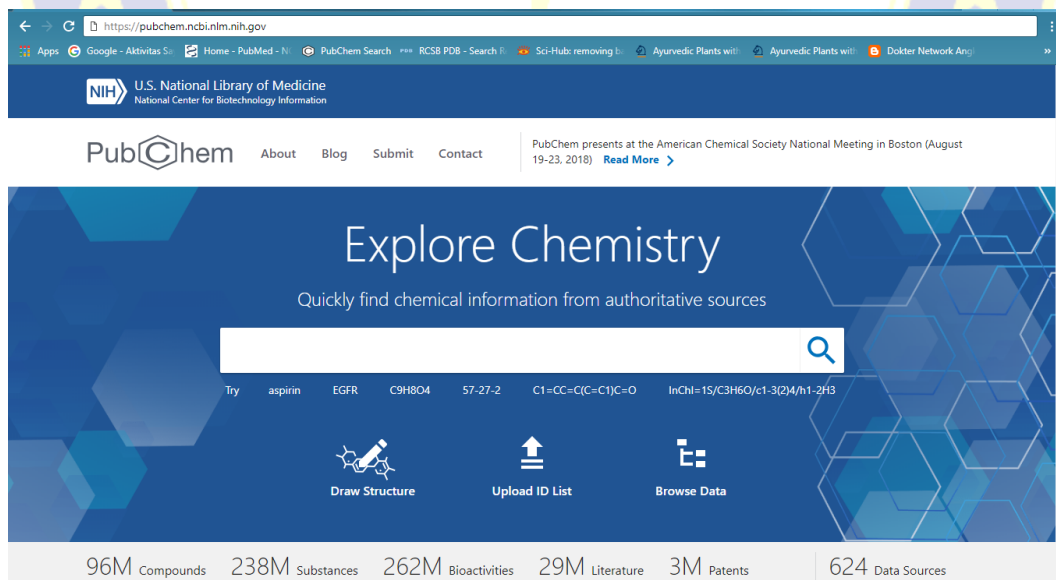
Gambar IV.3 Analisis Pre-ADME



Gambar IV.4 Analisis Toksisitas

LAMPIRAN 2

SITUS

Gambar IV.5 Tampilan situs *Protein Data Bank*Gambar IV.6 Tampilan situs *Pubchem*

LAMPIRAN 2 (LANJUTAN)

www.scfbio-iitd.res.in

Apps Google - Aktivitas S Home - PubMed - N PubChem Search RCSB PDB - Search Sci-Hub: removing Ayurvedic Plants with Ayurvedic Plants with Dokter Network Ang

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 format *.ndb, *.mol, *.mol2, *.xyz, *.sdf, *.xml

Gambar IV.7 Tampilan situs *Lipinski Rule of Five*

https://preadmet.bmdrc.kr

Apps Google - Aktivitas S Home - PubMed - N PubChem Search RCSB PDB - Search Sci-Hub: removing Ayurvedic Plants with Ayurvedic Plants with Dokter Network Ang

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

PreADMET

+82 2 393 9550~1 webmaster@bmdrc.kr

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

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's 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

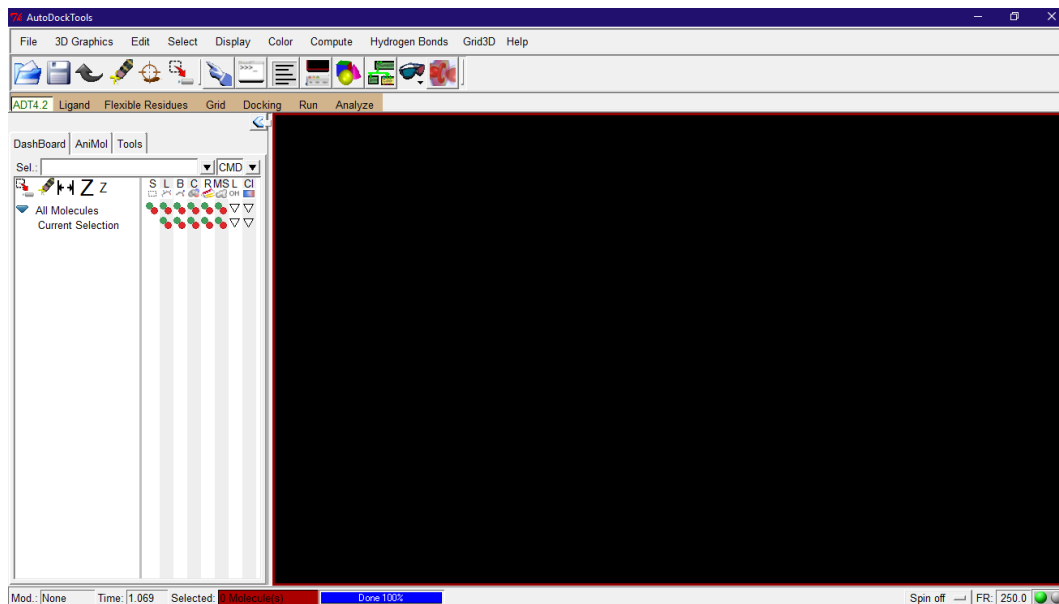
Lastest News

- 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

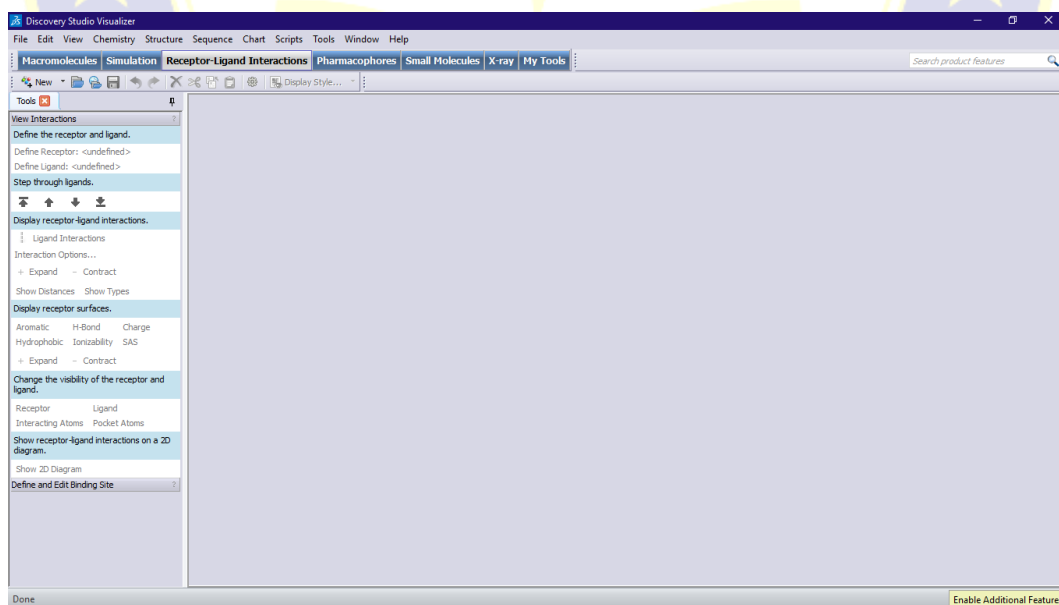
Gambar IV.8 Tampilan situs Pre-ADME

LAMPIRAN 3

SOFTWARE

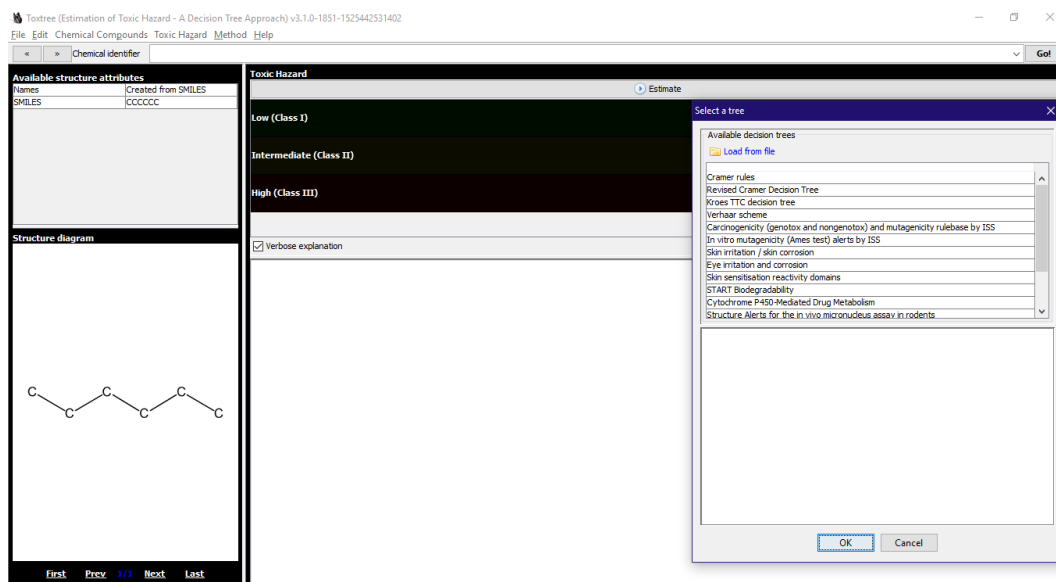


Gambar IV.9 Tampilan aplikasi *AutoDock Tools*[®]

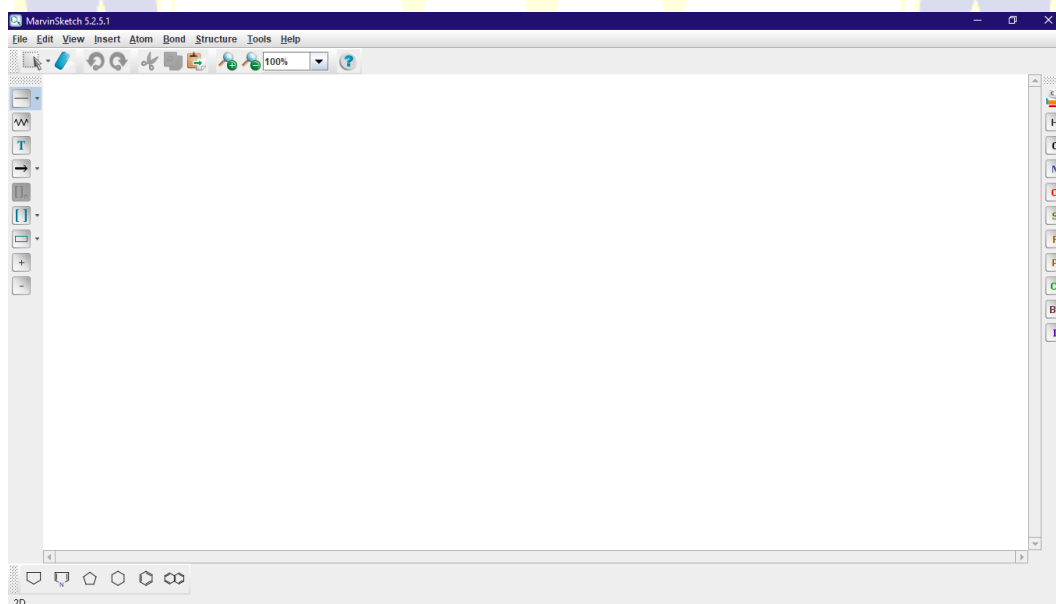


Gambar IV.10 Tampilan aplikasi *Discovery Studio Visualizer*[®]

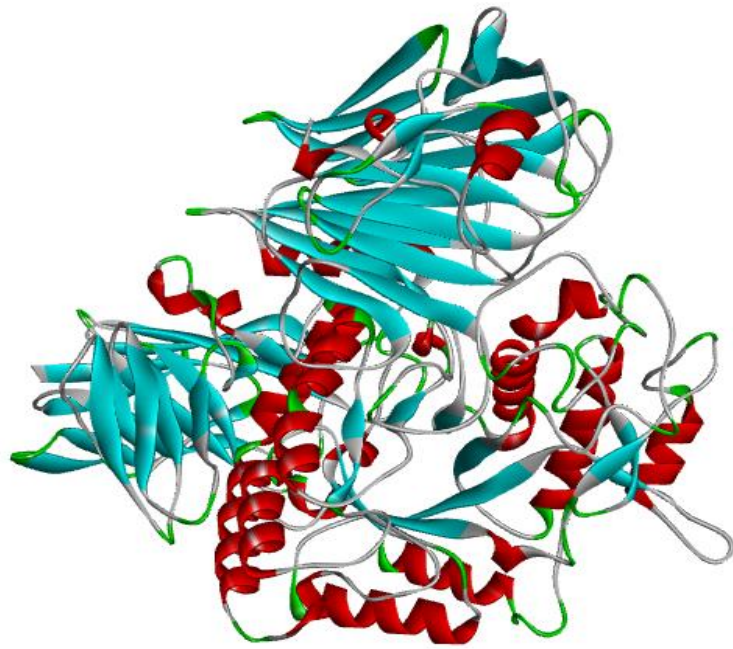
LAMPIRAN 3 (LANJUTAN)



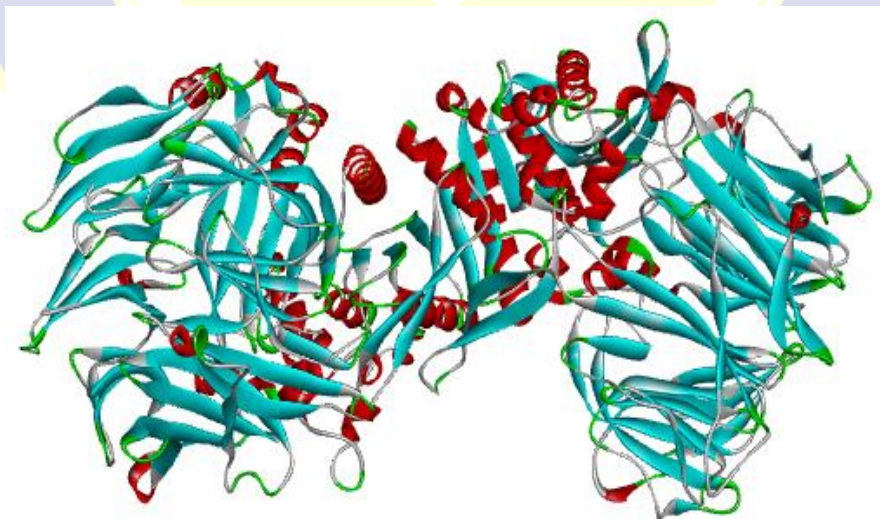
Gambar IV.11 Tampilan aplikasi *Toxtree*[®]



Gambar IV.12 Tampilan aplikasi *Marvin Sketch*[®]

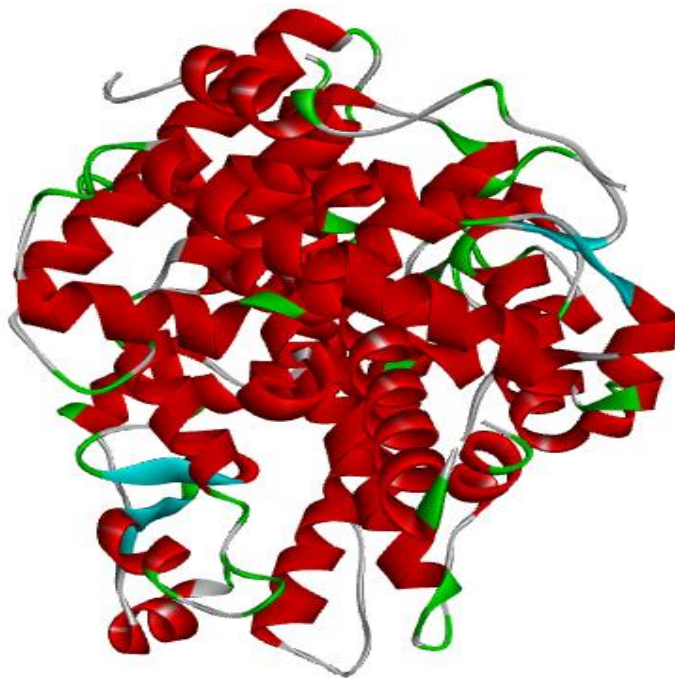
LAMPIRAN 4**STRUKTUR 3D MAKROMOLEKUL PROTEIN**

Gambar V.1 Reseptor α -Glukosidase dengan PDB ID 2QMJ



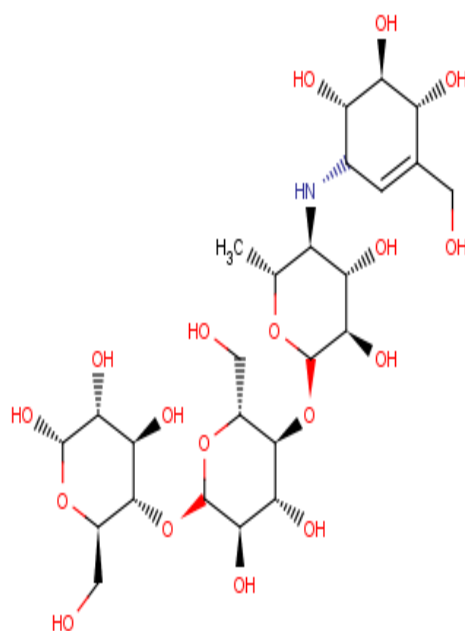
Gambar V.2 Reseptor DPP-4 dengan PDB ID 6B1E

**LAMPIRAN 4
(LANJUTAN)**

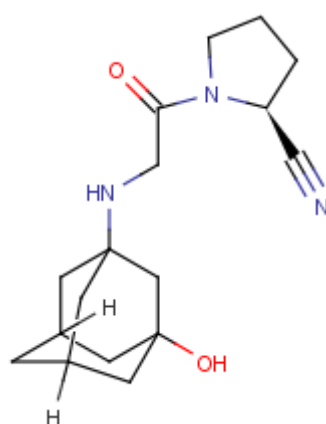


Gambar V.3 Reseptor PPAR γ dengan PDB ID 5JI0

LAMPIRAN 5
STRUKTUR 2D LIGAN ALAMI

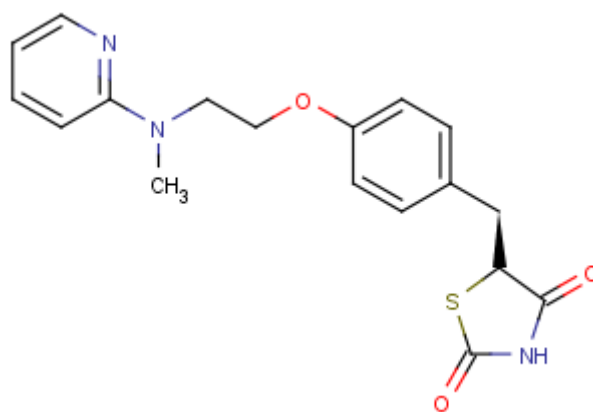


Gambar V.4 α-Glukosidase (Acarbose)



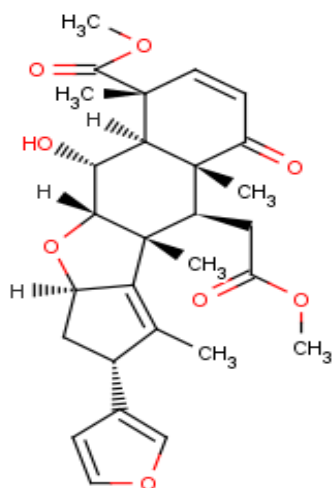
Gambar V.5 DPP-4 (Vildagliptin)

**LAMPIRAN 5
(LANJUTAN)**

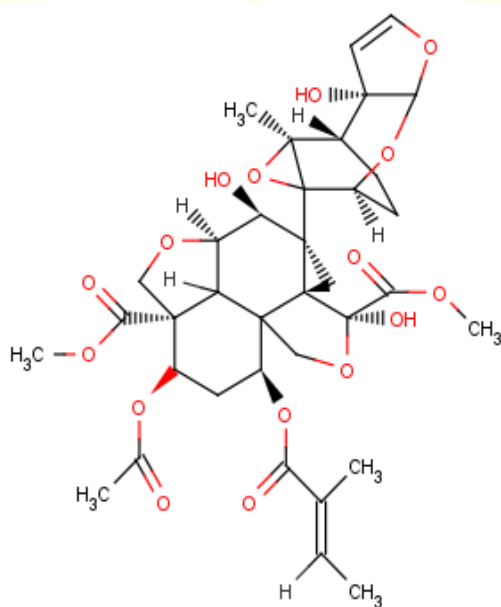


Gambar V.6 PPAR γ (Rosiglitazone)

LAMPIRAN 6
STRUKTUR 2D SENYAWA UJI

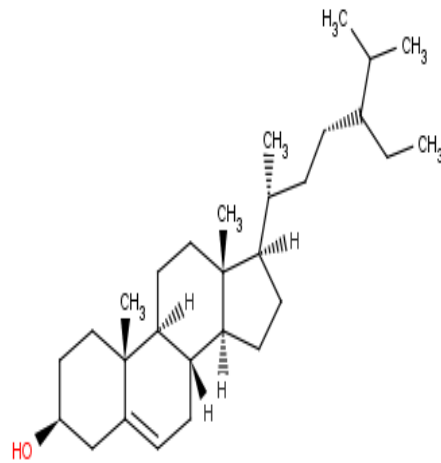


Gambar V.7 6-Deacetylnimbin

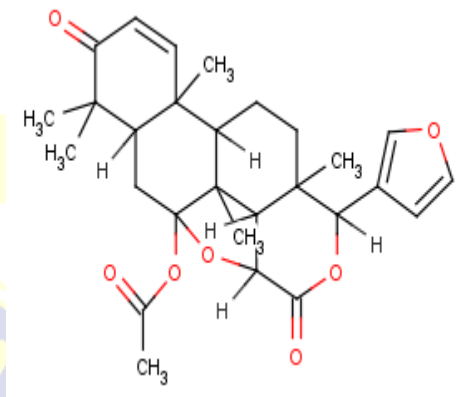


Gambar V.8 Azadirachtin

**LAMPIRAN 6
(LANJUTAN)**

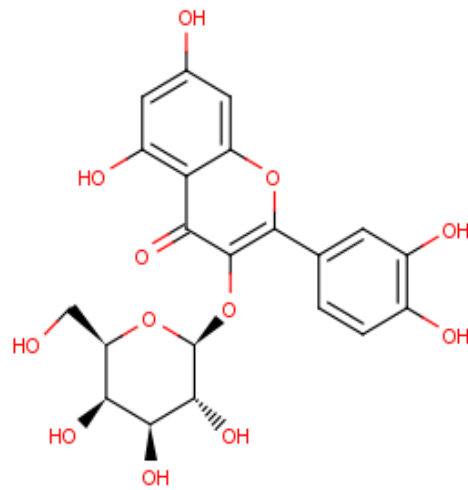


Gambar V.9 Beta Sitosterol

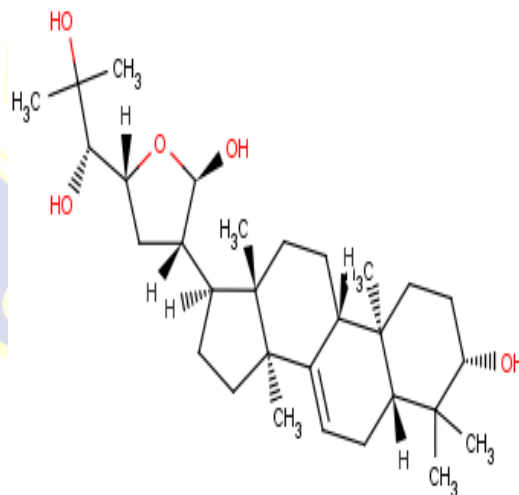


Gambar V.10 Gedunin

**LAMPIRAN 6
(LANJUTAN)**

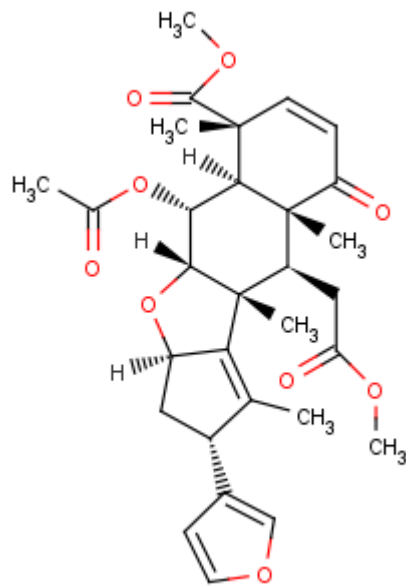


Gambar V.11 Hyperoside

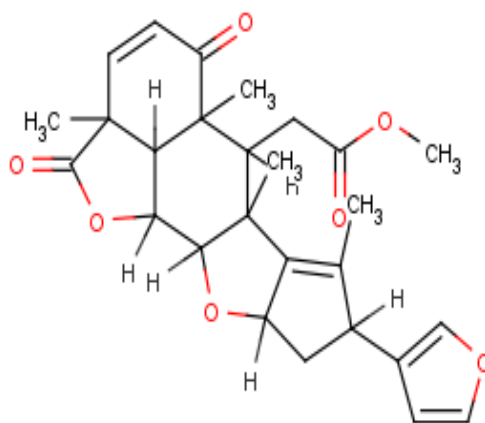


Gambar V.12 Meliantriol

**LAMPIRAN 6
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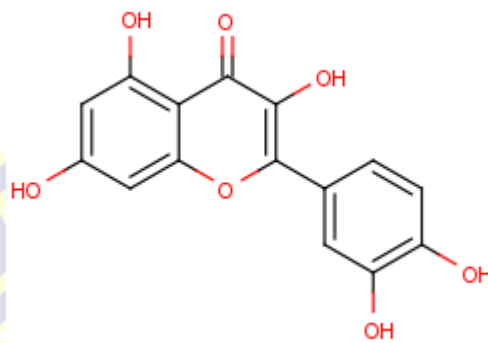


Gambar V.13 Nimbin

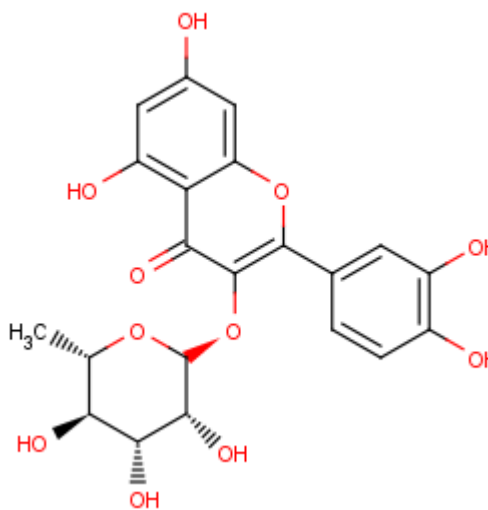


Gambar V.14 Nimbolida

**LAMPIRAN 6
(LANJUTAN)**

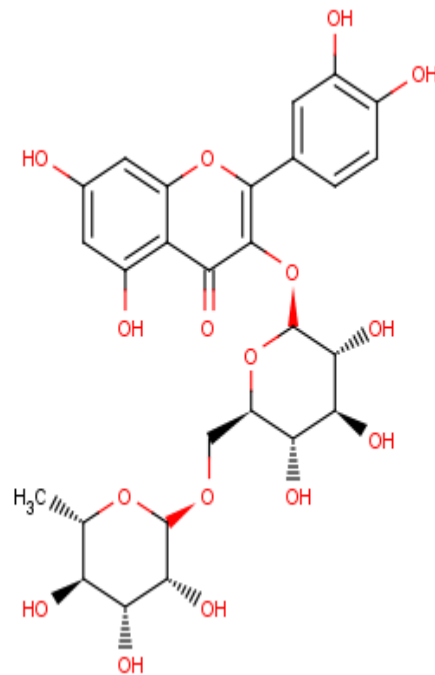


Gambar V.15 Quercetin

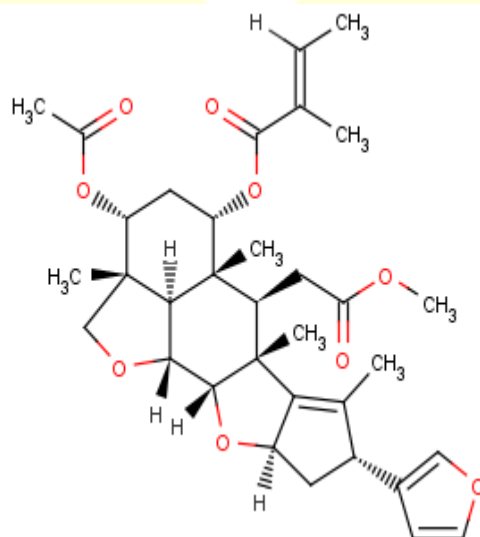


Gambar V.16 Quercitrin

**LAMPIRAN 6
(LANJUTAN)**



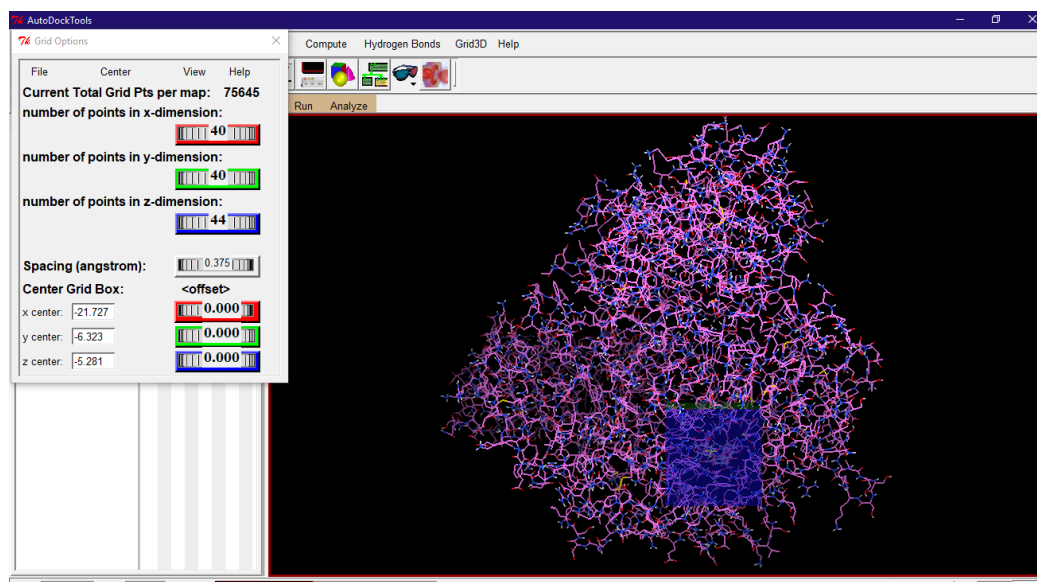
Gambar V.17 Rutin



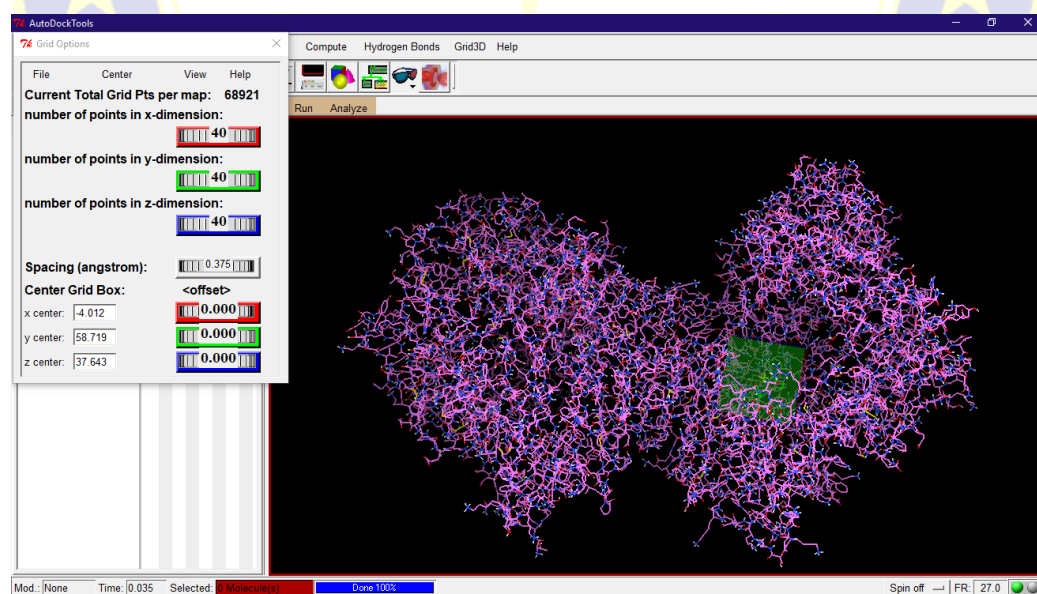
Gambar V.18 Salannin

LAMPIRAN 7

PARAMETER *GRIDBOX*

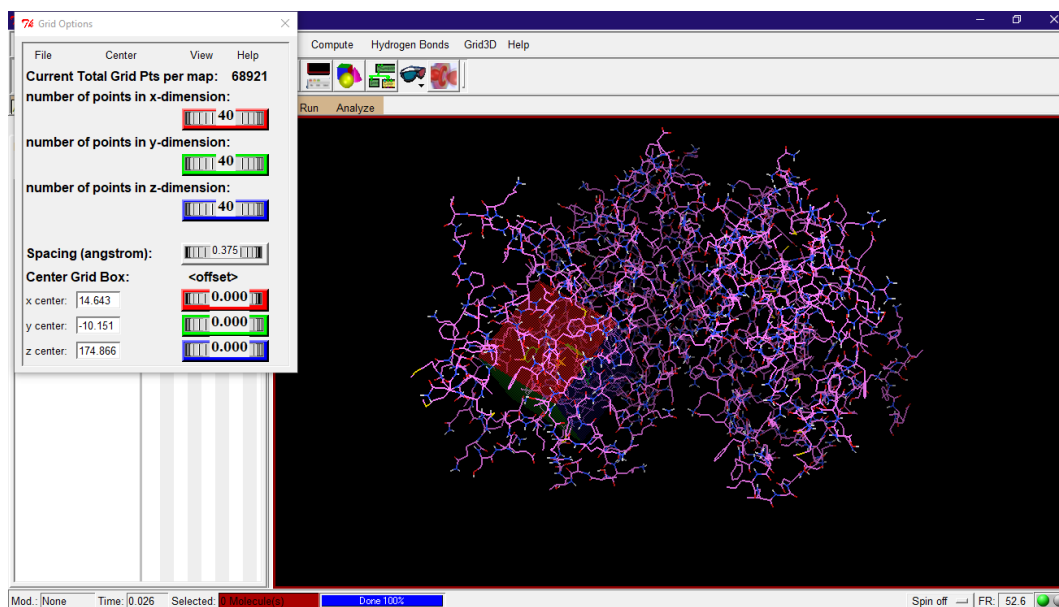


Gambar V.19 Tampilan parameter *gridbox* reseptor α -Glukosidase



Gambar V.20 Tampilan parameter *gridbox* reseptor DPP-4

LAMPIRAN 7 (LANJUTAN)



Gambar V.21 Tampilan parameter *gridbox* reseptor PPAR γ

LAMPIRAN 8

HASIL VALIDASI METODE

10470	CLUSTERING HISTOGRAM						
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10474	Clus	Lowest	Run	Mean	Num	Histogram	
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10476	Rank	Energy		Energy	Clus	5	10
10477						15	20
10478						25	30
10479	1	-7.75	56	-7.75	100	#####	#####
10480							
10481							
10482							
10483	Number of multi-member conformational clusters found = 1, out of 100 runs.						
10484							
10485	RMSD TABLE						
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10489	Rank	Sub-	Run	Binding	Cluster	Reference	Grep
10490		Rank		Energy	RMSD	RMSD	Pattern
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10492							
10493	1	1	56	-7.75	0.00	0.71	RANKING
10494	1	2	22	-7.75	0.01	0.71	RANKING
10495	1	3	30	-7.75	0.01	0.71	RANKING
10496	1	4	2	-7.75	0.00	0.71	RANKING
10497	1	5	11	-7.75	0.00	0.71	RANKING
10498	1	6	98	-7.75	0.00	0.71	RANKING
10499	1	7	6	-7.75	0.01	0.71	RANKING
10500	1	8	80	-7.75	0.00	0.72	RANKING
10501	1	9	64	-7.75	0.00	0.71	RANKING
10502	1	10	59	-7.75	0.01	0.71	RANKING
10503	1	11	67	-7.75	0.01	0.71	RANKING
10504	1	12	31	-7.75	0.02	0.70	RANKING
10505	1	13	100	-7.75	0.01	0.71	RANKING
10506	1	14	12	-7.75	0.01	0.71	RANKING
10507	1	15	96	-7.75	0.01	0.71	RANKING
10508	1	16	97	-7.75	0.02	0.71	RANKING
10509	1	17	86	-7.75	0.01	0.71	RANKING

Gambar V.22 Hasil validasi metode *redocking* α -Glukosidase 2QMJ

LAMPIRAN 8 (LANJUTAN)

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9266	Clus	Lowest	Run	Mean	Num	Histogram		
9267	-ter	Binding		Binding	in			
9268	Rank	Energy		Energy	Clus	5	10	15
9269						20	25	30
9270	1	-8.27	38	-8.27	100	#####	#####	#####
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9274	Number of multi-member conformational clusters found = 1, out of 100 runs.							
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9276	RMSD TABLE							
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9279								
9280	Rank	Sub-	Run	Binding	Cluster	Reference	Grep	
9281		Rank		Energy	RMSD	RMSD	Pattern	
9282								
9283	1	1	38	-8.27	0.00	1.86	RANKING	
9284	1	2	21	-8.27	0.02	1.86	RANKING	
9285	1	3	69	-8.27	0.01	1.86	RANKING	
9286	1	4	13	-8.27	0.00	1.86	RANKING	
9287	1	5	98	-8.27	0.01	1.85	RANKING	
9288	1	6	22	-8.27	0.01	1.86	RANKING	
9289	1	7	73	-8.27	0.01	1.86	RANKING	
9290	1	8	80	-8.27	0.00	1.86	RANKING	
9291	1	9	11	-8.27	0.00	1.86	RANKING	
9292	1	10	42	-8.27	0.01	1.86	RANKING	
9293	1	11	32	-8.27	0.00	1.86	RANKING	
9294	1	12	9	-8.27	0.01	1.86	RANKING	
9295	1	13	74	-8.27	0.01	1.86	RANKING	
9296	1	14	16	-8.27	0.01	1.86	RANKING	
9297	1	15	4	-8.27	0.01	1.86	RANKING	
9298	1	16	66	-8.27	0.01	1.86	RANKING	
9299	1	17	60	-8.27	0.02	1.85	RANKING	
9300								

Gambar V.23 Hasil validasi metode *redocking* DPP-4 6B1E

LAMPIRAN 8 (LANJUTAN)

8353 CLUSTERING HISTOGRAM

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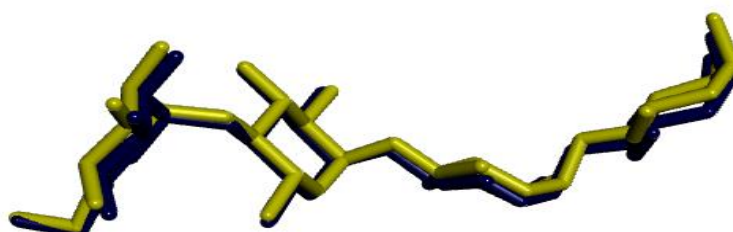
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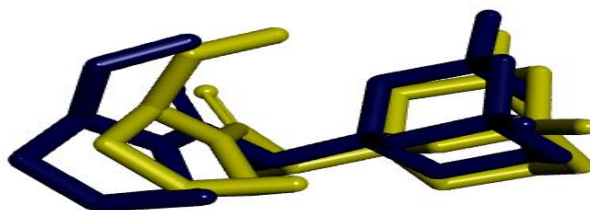
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Gambar V.24 Hasil validasi metode *redocking* PPAR γ 5JI0

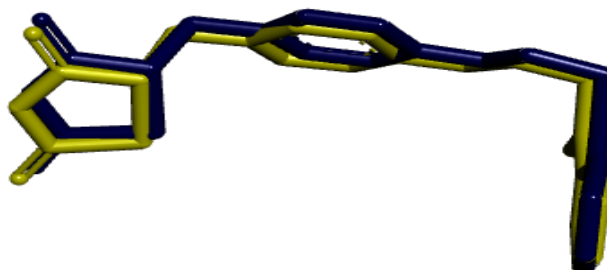
LAMPIRAN 9
VISUALISASI *REDOCKING*



Gambar V.25 Hasil visualisasi tumpang tindih ligan alami dari reseptor α -Glukosidase dari hasil kristalografi sinar-X (Biru) dengan ligan hasil *redocking* (kuning)



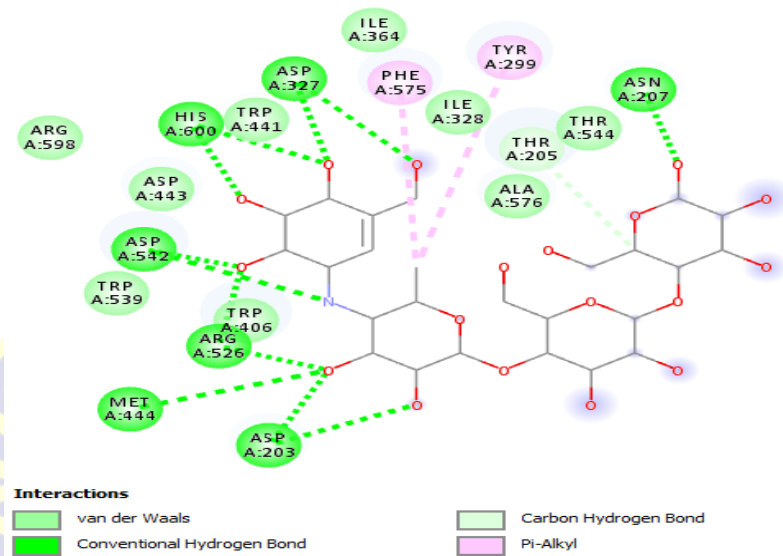
Gambar V.26 Hasil visualisasi tumpang tindih ligan alami dari reseptor DPP-4 dari hasil kristalografi sinar-X (biru) dengan ligan hasil *redocking* (kuning)



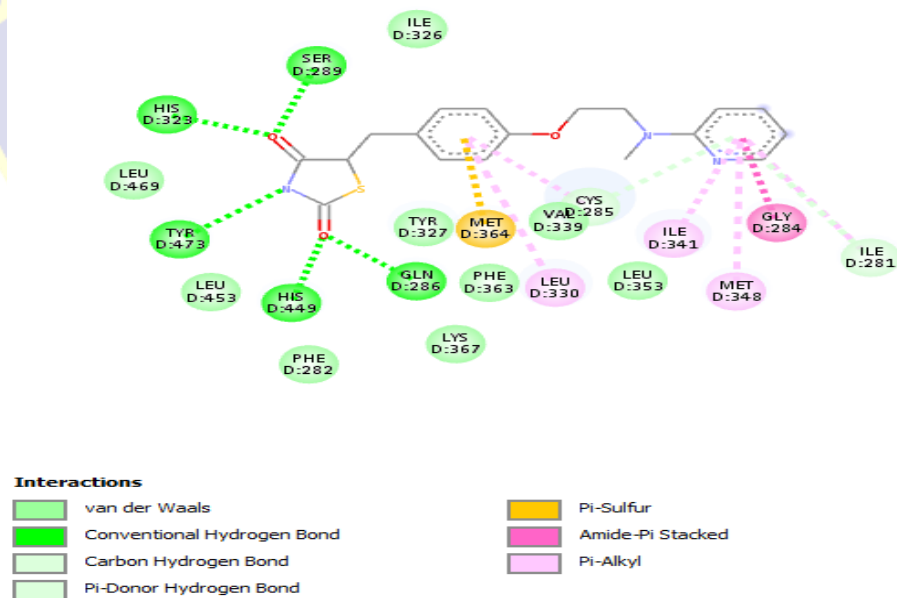
Gambar V.27 Hasil visualisasi tumpang tindih ligan alami dari reseptor PPAR γ dari hasil kristalografi sinar-X (biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 10

VISUALISASI INTERAKSI IKATAN KIMIA

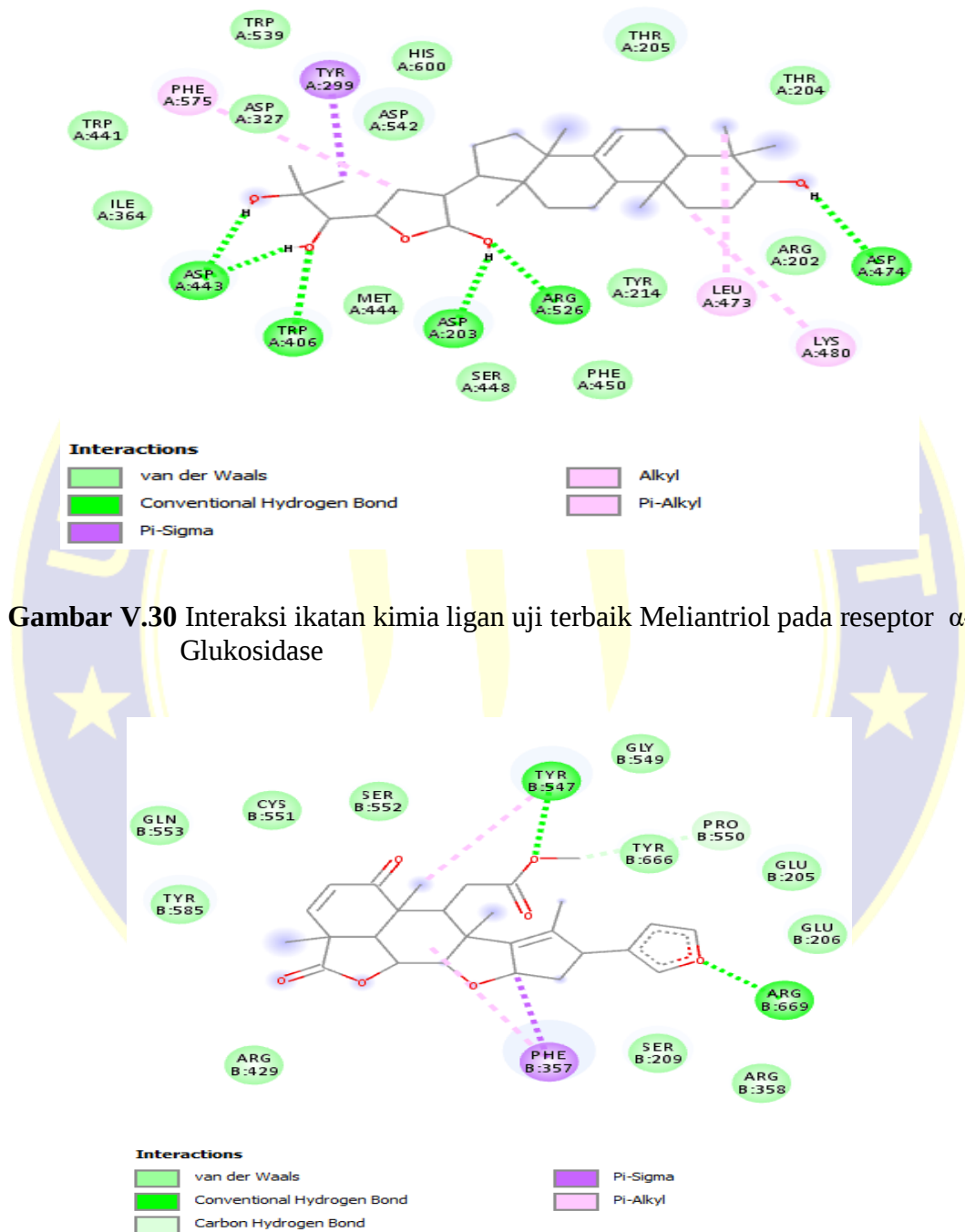


Gambar V.28 Interaksi ikatan kimia ligan alami pada reseptor α -Glukosidase

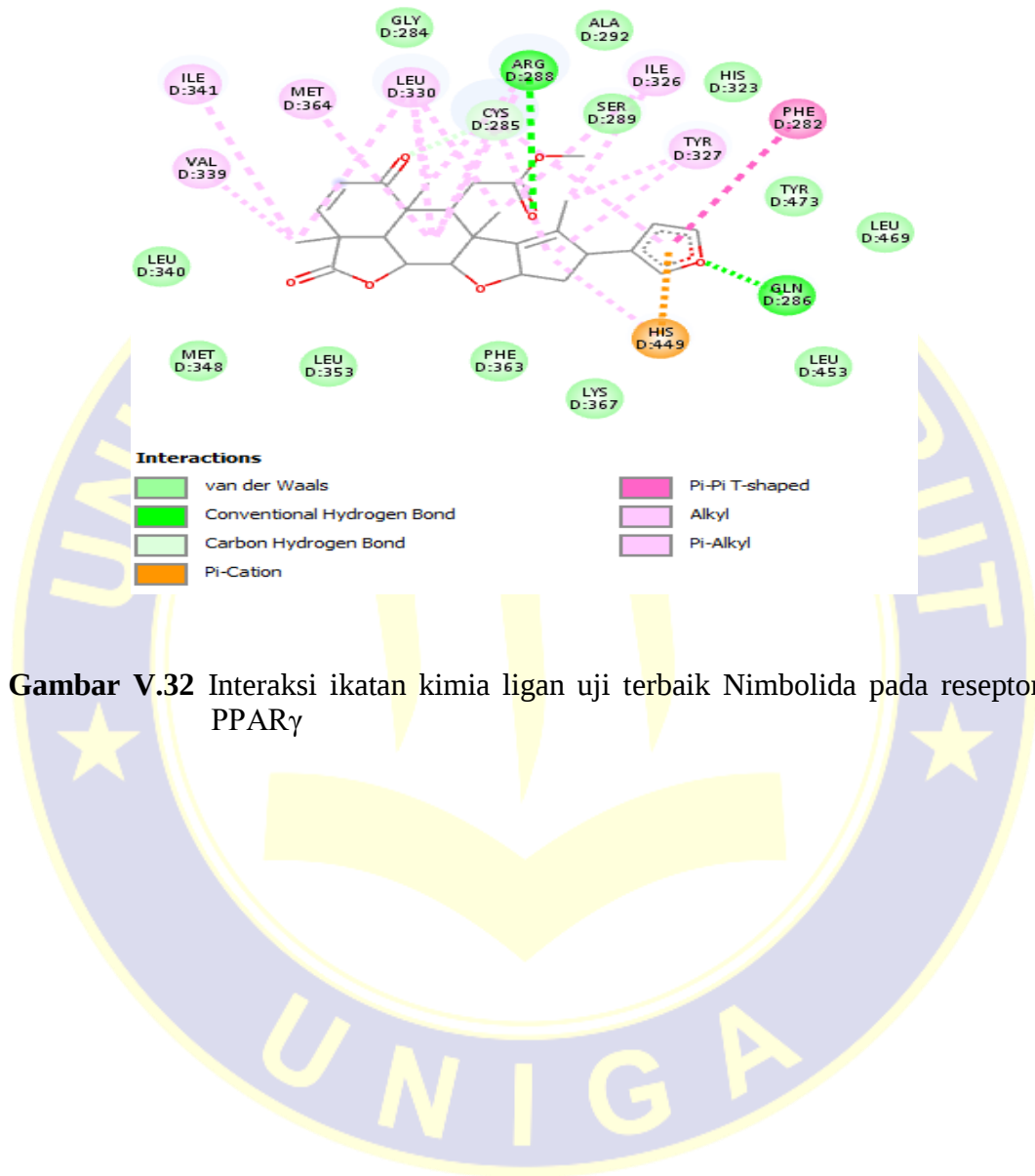


Gambar V.29 Interaksi ikatan kimia ligan alami pada reseptor PPAR γ

LAMPIRAN 10 (LANJUTAN)



LAMPIRAN 10 (LANJUTAN)



Gambar V.32 Interaksi ikatan kimia ligan uji terbaik Nimbolida pada reseptor PPAR γ