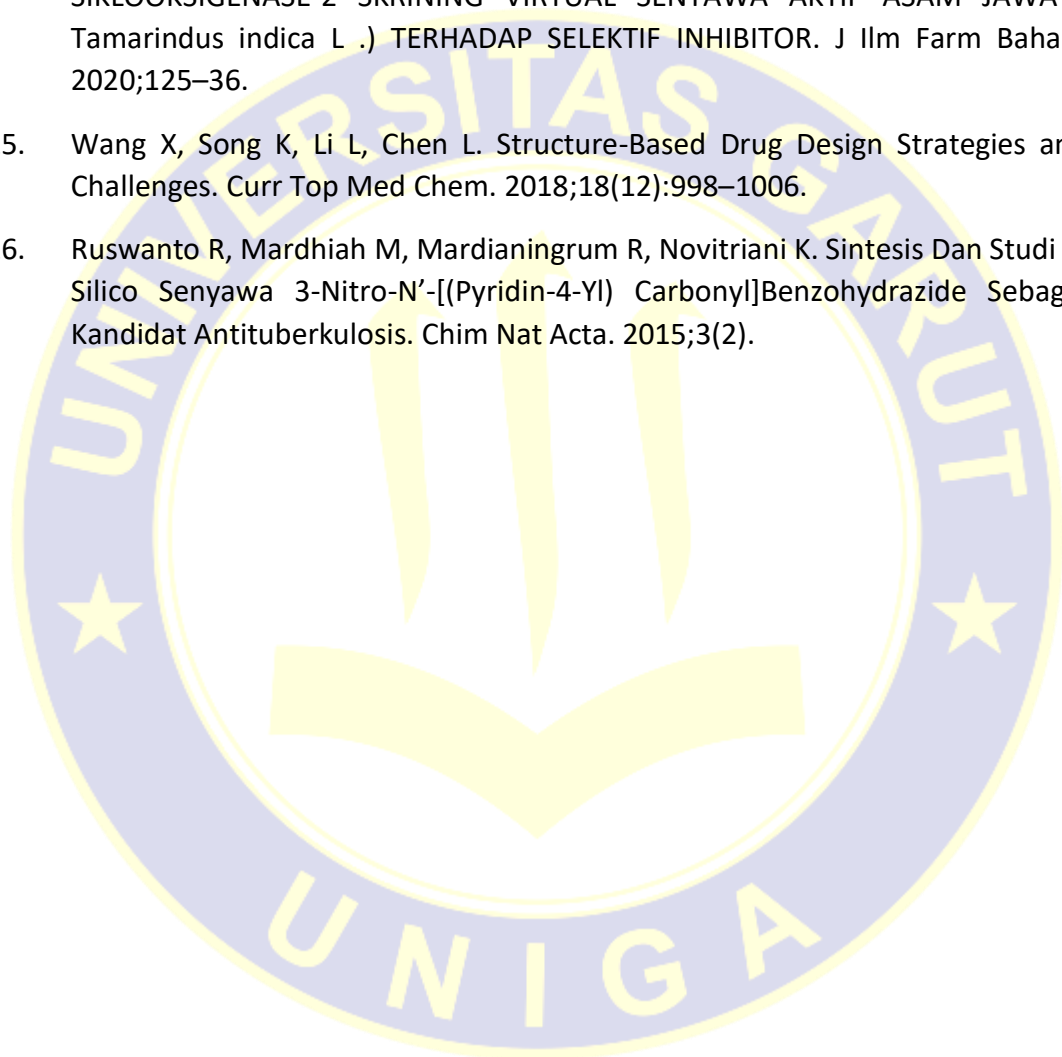


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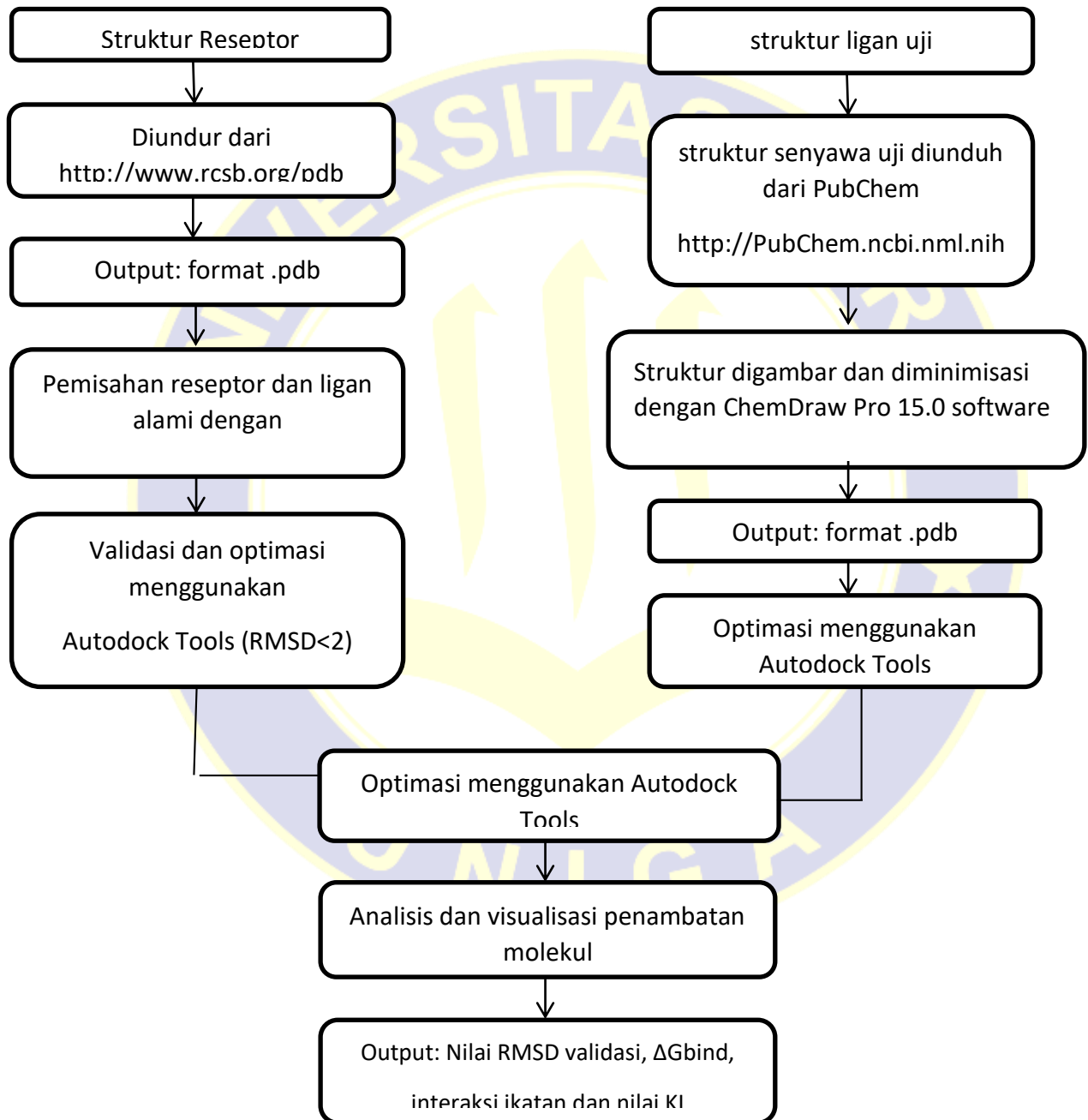
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LAMPIRAN 1

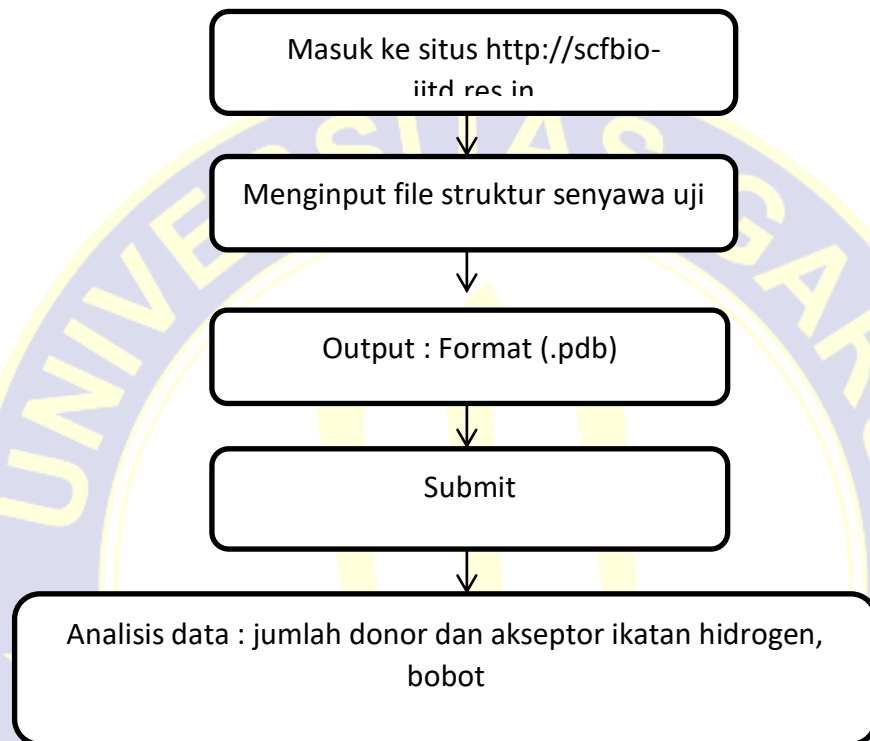
ALUR PENELITIAN SIMULASI MOLEKULER DOCKING



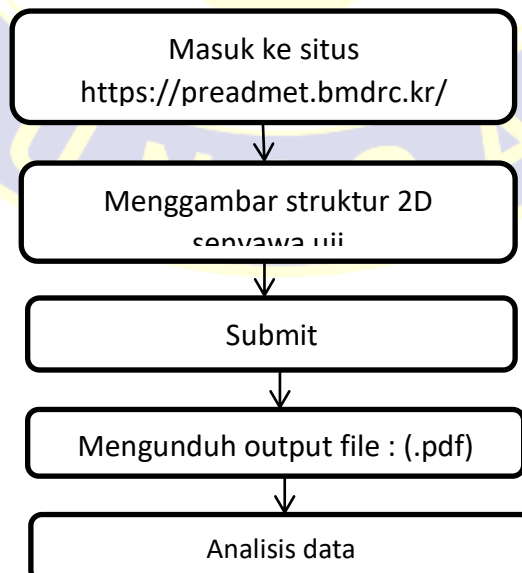
Gambar IV.1 Alur penelitian simulasi molecular docking

LAMPIRAN 1

ALUR PENELITIAN ANALISIS FISIKO KIMIA, ANALISIS FARMAKOKINETIKA, SERTA ANALISIS TOKSISITAS

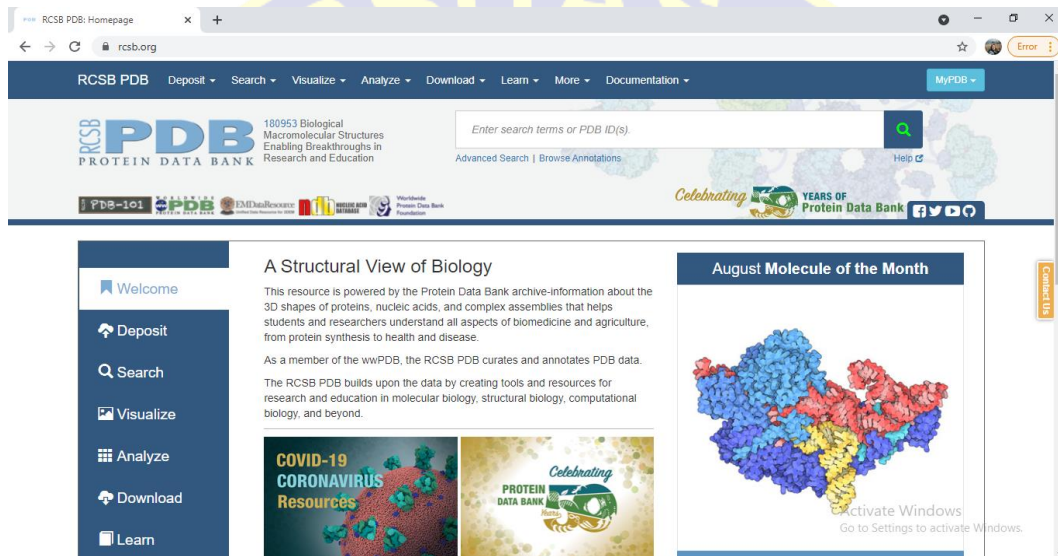


Gambar IV.2 Analisis fisikokimia berdasarkan lipinski rule of five

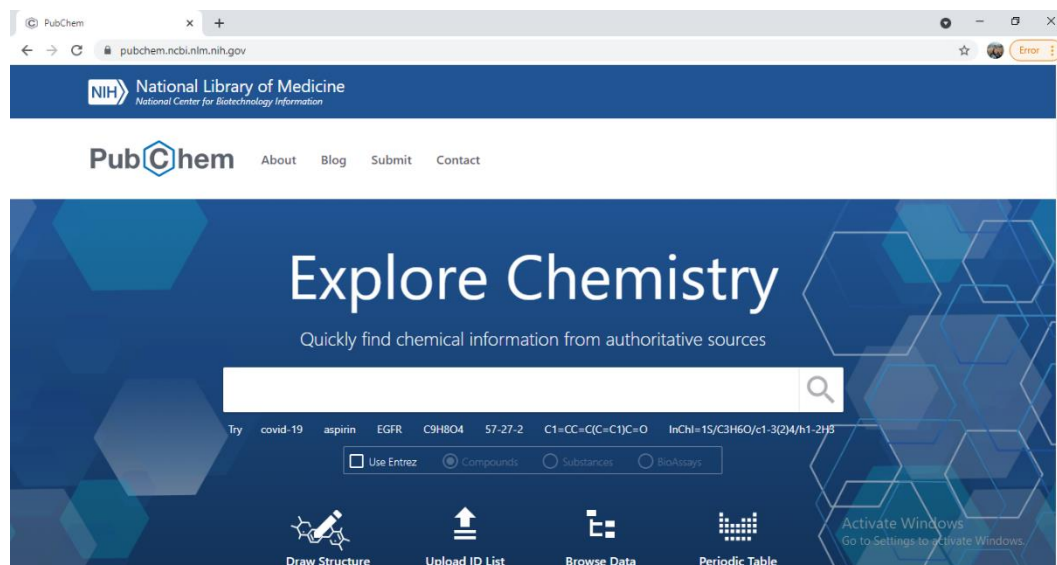


Gambar IV.3 Analisis pre-adme dan toksisitas LAMPIRAN 2

SITUS DAN APLIKASI



Gambar IV.4 Tampilan situs *protein data bank*

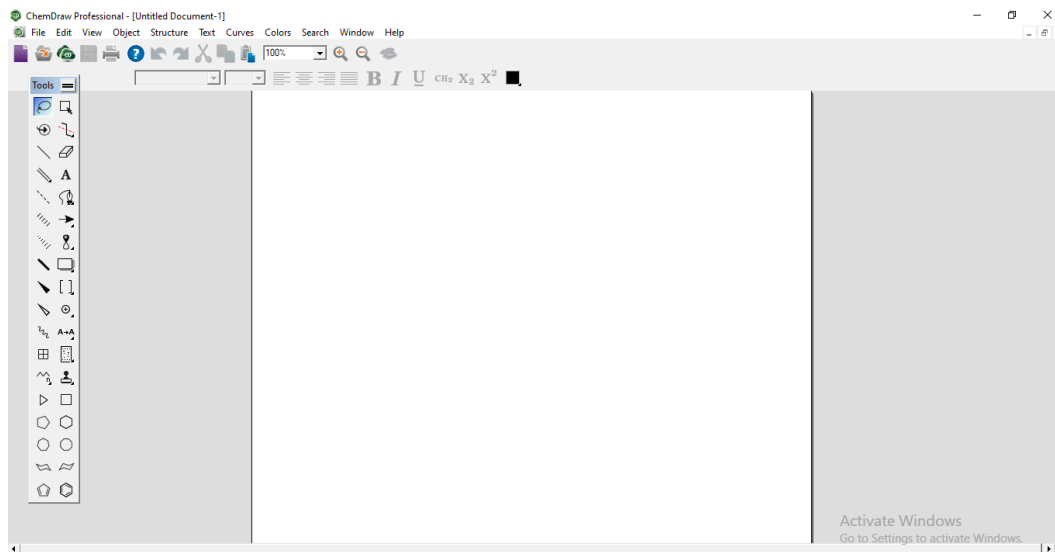


Gambar IV.5 Tampilan situs *pubChem*

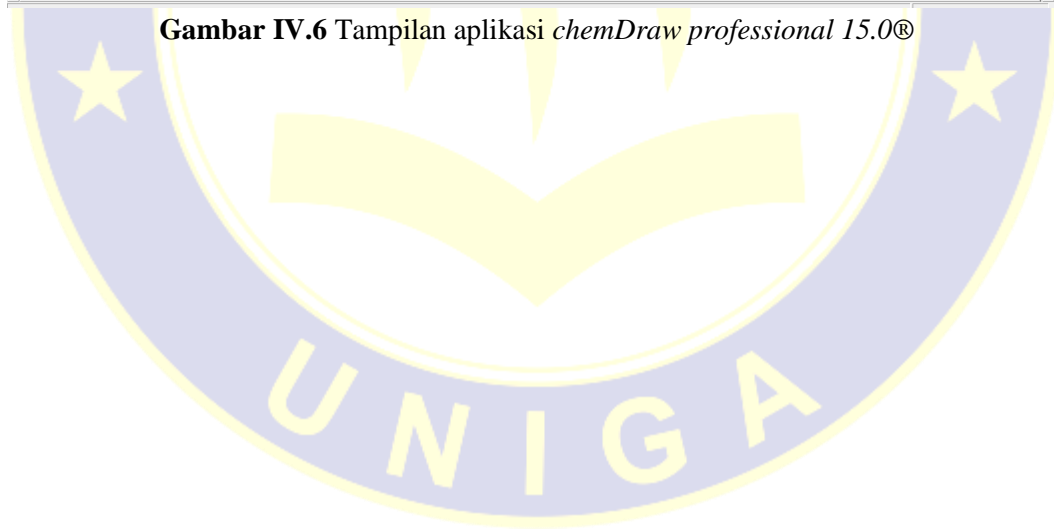


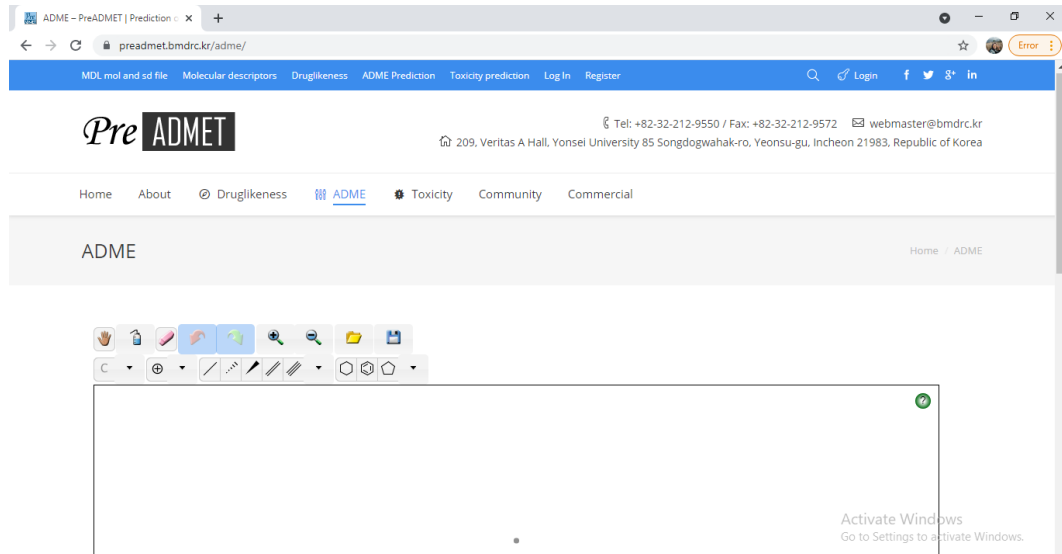
**LAMPIRAN 2
(LANJUTAN)**

SITUS DAN APLIKASI



Gambar IV.6 Tampilan aplikasi *chemDraw professional 15.0®*



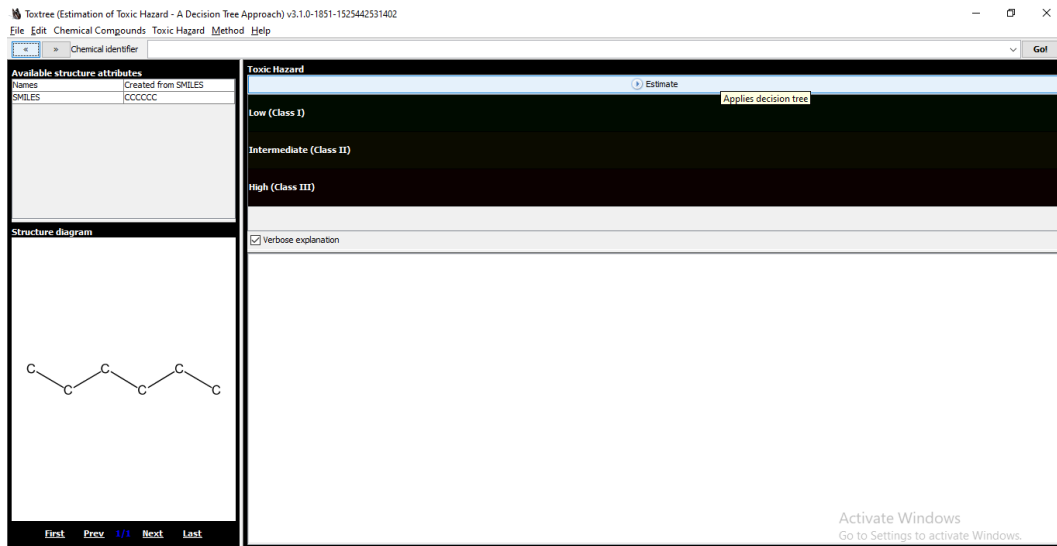


Gambar IV.7 Tampilan situs *pre-admet*

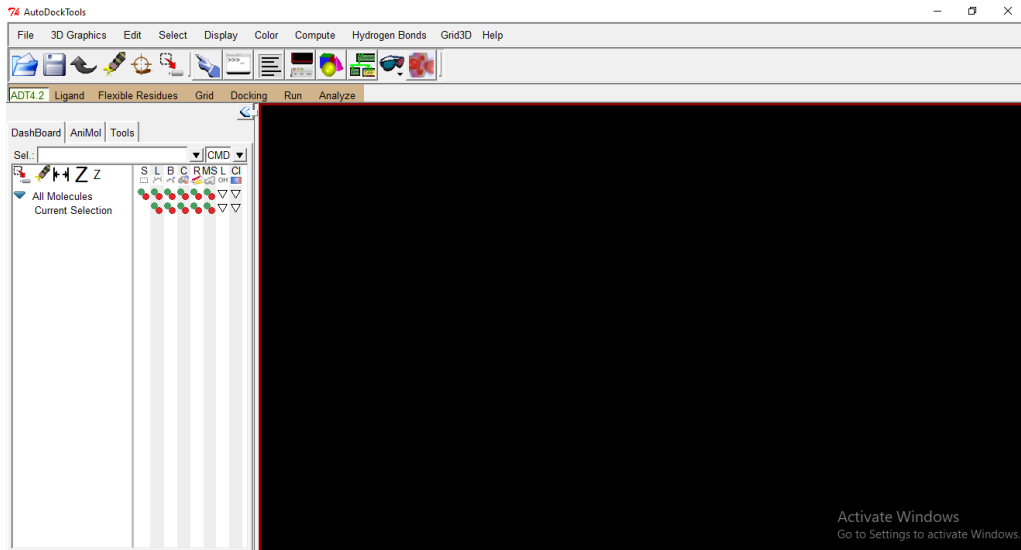


**LAMPIRAN 2
(LANJUTAN)**

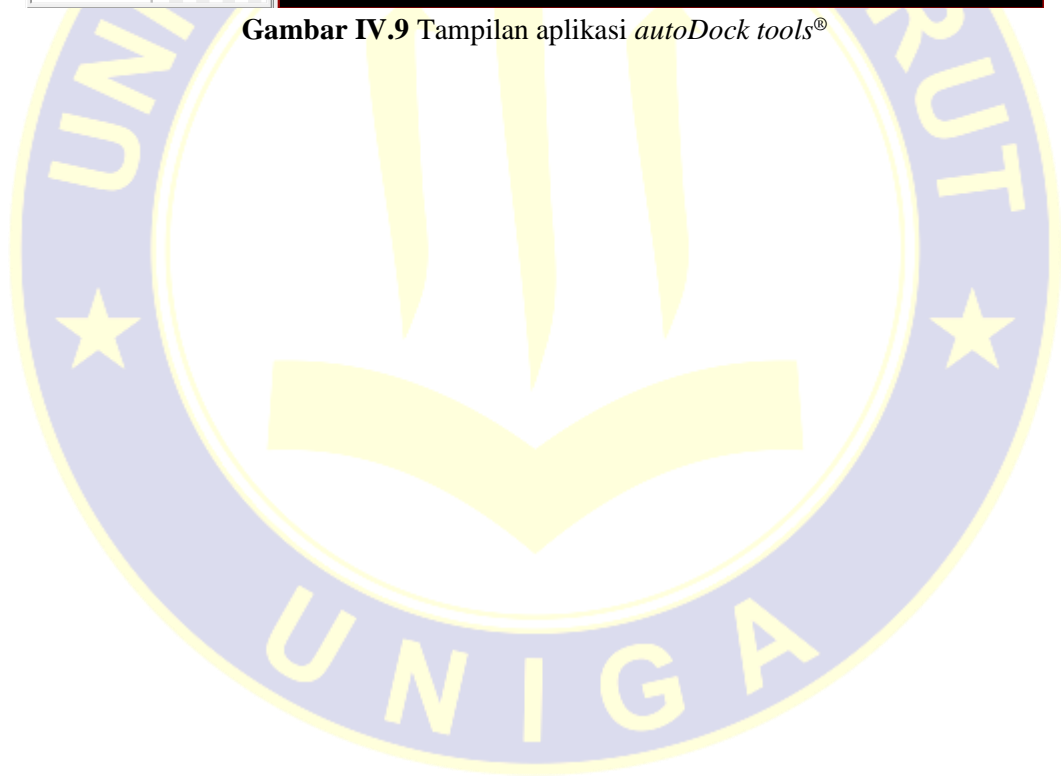
SITUS DAN APLIKASI



Gambar IV.8 Tampilan aplikasi *toxtree*[®]



Gambar IV.9 Tampilan aplikasi *autoDock tools*[®]



LAMPIRAN 3

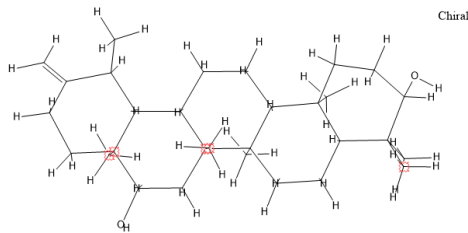
TANAMAN DANIELION



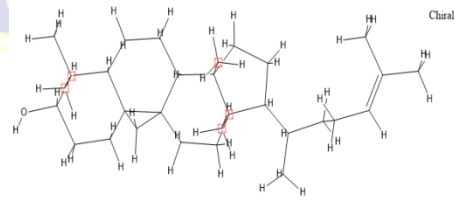
Gambar II.1 Tanaman danielion

LAMPIRAN 4

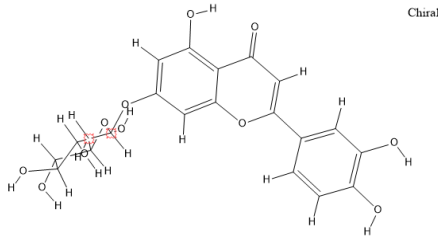
STRUKTUR SENYAWA



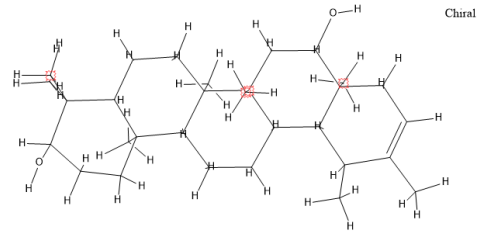
ARNIDIOL



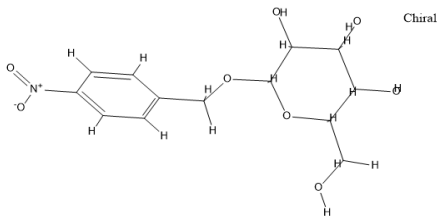
CYCLOARTENOL



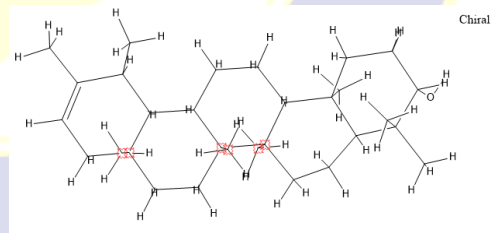
CYNAROSIDE



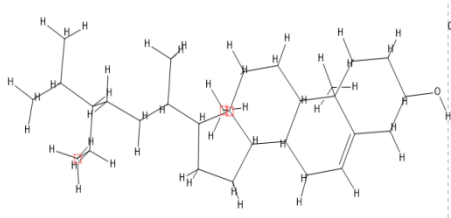
FARADIOL



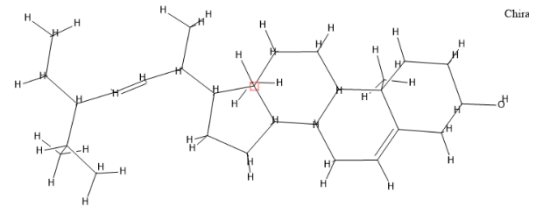
BETA-DGLUCOPYRANOSID



PSI-TARAXASTEROL



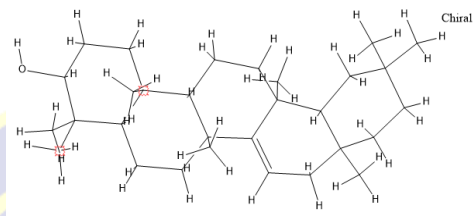
SITOSTEROL



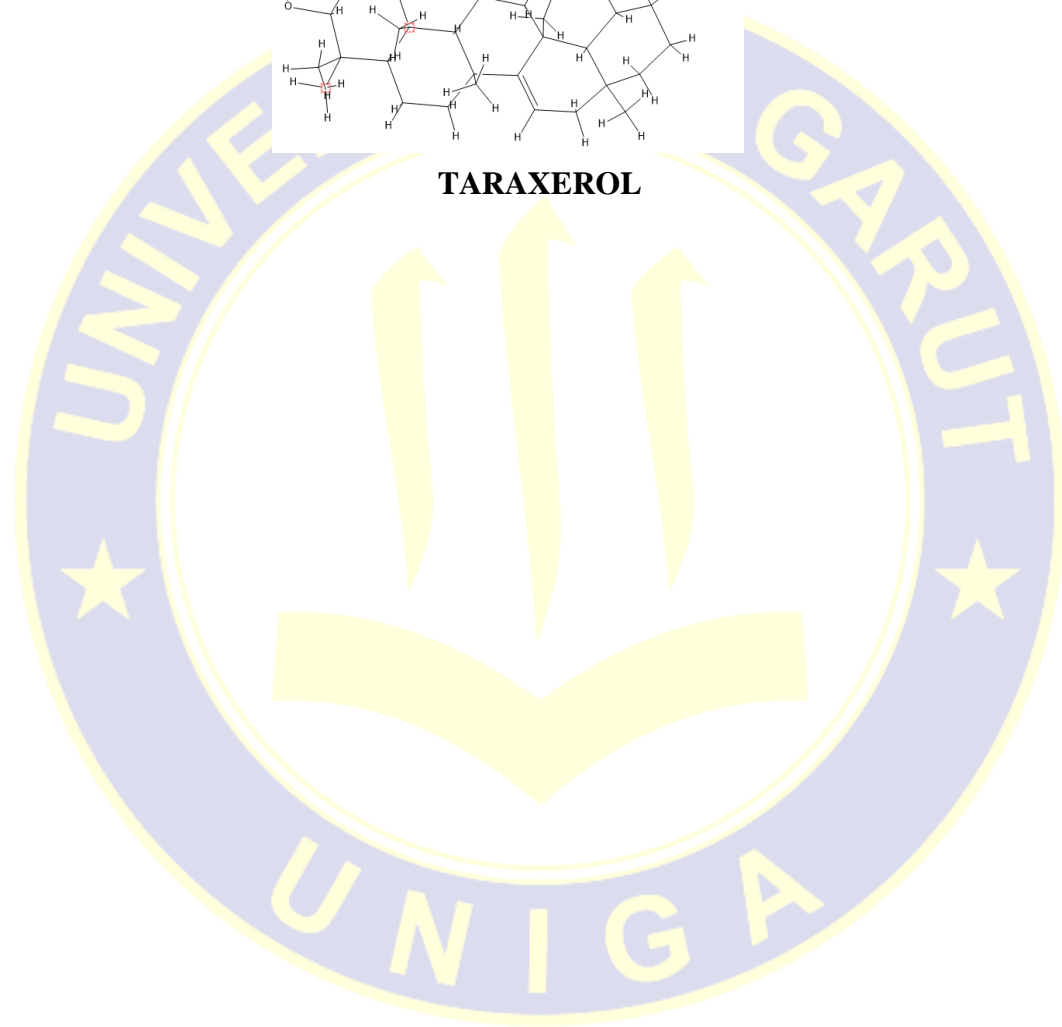
TARAXASTEROL



**LAMPIRAN 4
(LANJUTAN)**

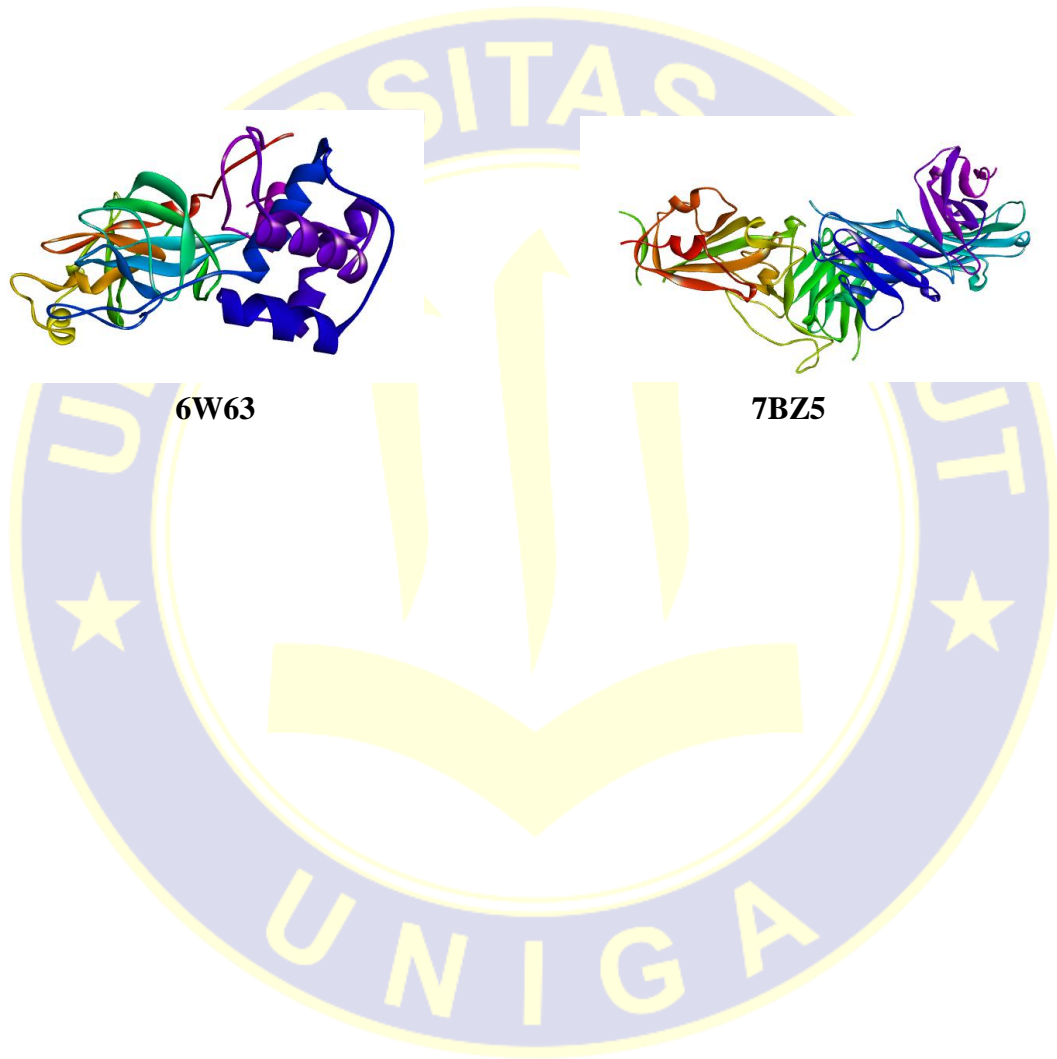


TARAXEROL

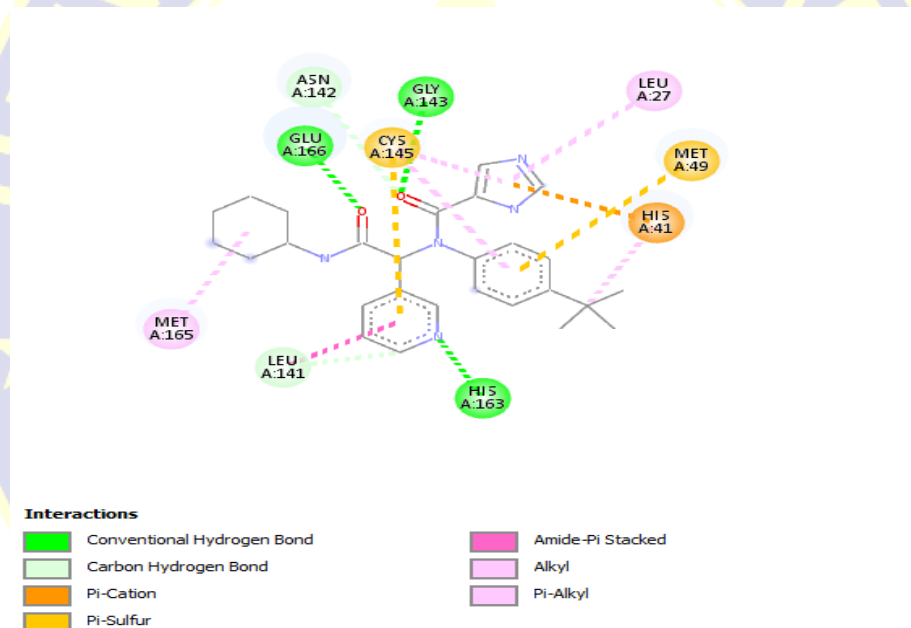


LAMPIRAN 5

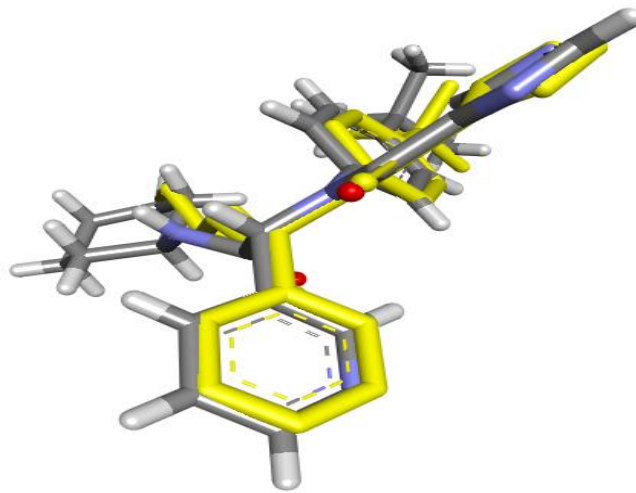
RESEPTOR



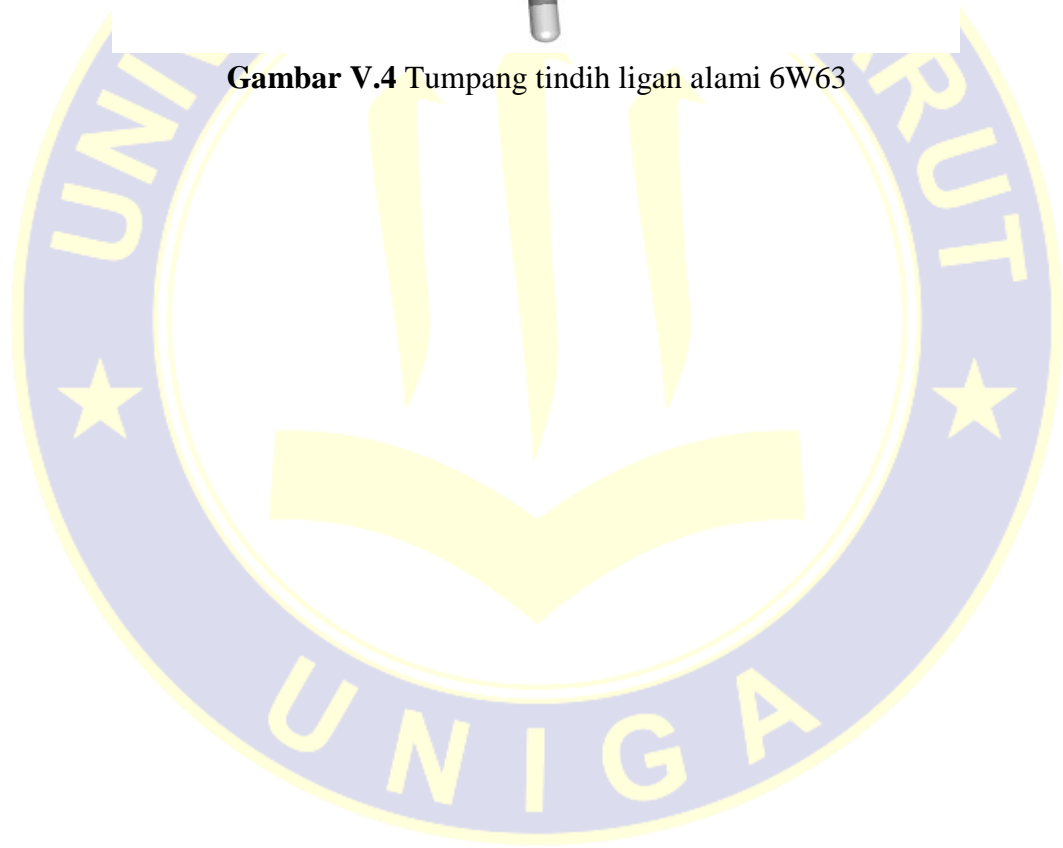
LAMPIRAN 6
VALIDASI METODE



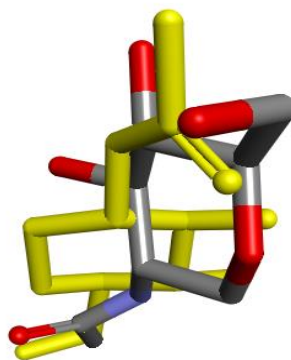
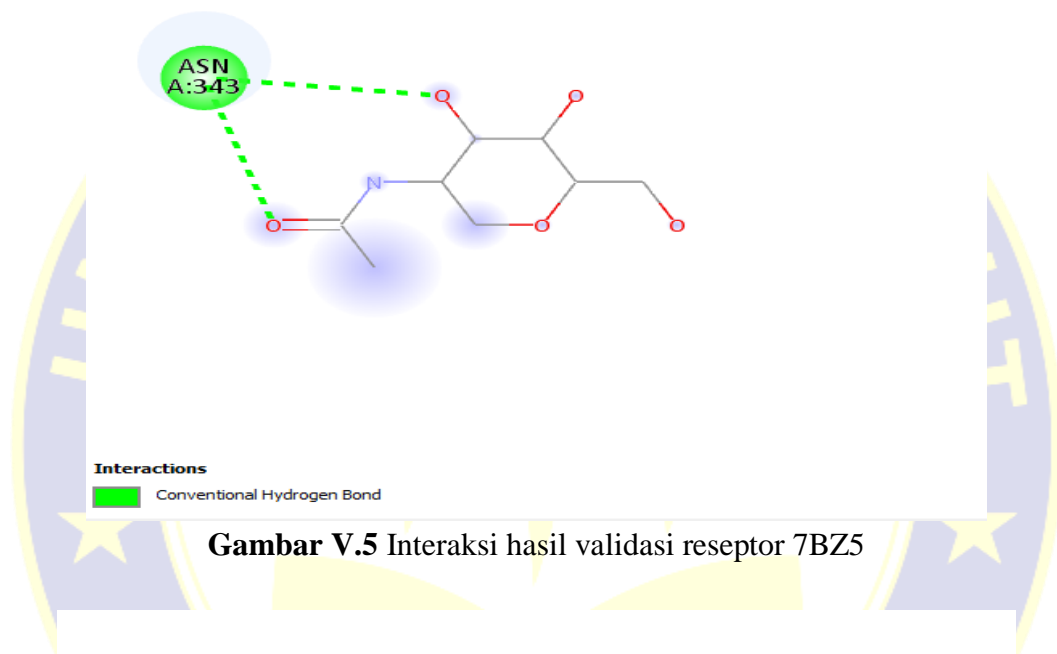
Gambar V.3 Interaksi hasil validasi reseptor 6W63



Gambar V.4 Tumpang tindih ligan alami 6W63



LAMPIRAN 6 (LANJUTAN)



Gambar V.6 Tumpang tindih alami 7BZ5

LAMPIRAN 7

HASIL PENAMBATAN MOLEKUL SENYAWA UJI

TABEL V.I

HASIL PENAMBATAN PADA RESTOR 6W63

No	SENYAWA	ΔG (kcal/Mol)	k_i (μ molar)	ASAM AMINO
1.	arniadol	-0,10	841,24	ASN;228
2.	beta-dglucopyranosid	+1,25	-	-
3.	cycloartenol	+0,36	-	ASN;228
4.	cynaroside	+0,90	-	ASN;228
5.	faradiol	-0,42	488,99	ASN;228
6.	Psi-taraxasterol	-2,10	28,68	MET;235, LYS; 236
7.	sitosterol	+0,92	-	ASN;228
8.	stigmasterol	+0,62	-	ASN;228
9.	taraxasterol	-0,34	559,98	ASN;228
10.	taraxerol	-0,69	313,91	ASN;228
11.	favipiravir	-0,91	213,73	ASN;228, LEU;232
12.	N-(4-tert-butylpheny)-N- [(1R)-2-(cyclohexylamino)-	-9,63	86,90	ASN;142, GLY;143, CYS;145, GLU;166,

2-oxo-1-(pyridine-3-yl)ethyl]-1H-imidazole-4-carboxamide			LEU;27,LEU;141,ME ET;49,MET;165,HI S;41,HIS;163
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**LAMPIRAN 7
(LANJUTAN)**

**TABEL V.2
HASIL PENAMBATAN PADA RESEPTOR 7BZ5**

No	SENYAWA	ΔG (kcal/Mol)	ki (μmolar)	ASAM AMINO
1.	arniadol	-4,70	356.52	LYS;131,SER;130,SER;132,SER;134
2.	beta- dglucopyranosid	-4,84	281.21	LYS;131, SER;130,SER;132,SER;134,SER;188, THR;133
3.	cycloartenol	-2,65	11.34	LYS;131, SER;130,SER;132,SER;134,SER;188, THR;133
4.	cynaroside	-4,09	1,00	LYS;131, SER;130,SER;132,SER;134
5.	faradiol	-4.08	1,03	LYS;131, SER;130,SER;132,SER;134
6.	Psi-taraxasterol	-5,22	150.22	ASN;143,LYS;150,SER;204,SER;209, THR;207,PRO;205,VAL;206,WAA;19 2
7.	sitosterol	-2,07	30.23	LYS;131,SER;132,SER;134
8.	stigmasterol	-2.90	7,50	LYS;131,SER;132,SER;134,THR;133
9.	taraxasterol	-3.53	2,59	LYS;131,SER;132,SER;134,THR;133
10.	taraxerol	-3.26	4,05	LYS;131,SER;132,SER;134,THR;133
11.	favipiravir	-2,15	26.63	LYS; 131, SER;132
12.	2-acetamido- 2deoxy-beta-D- glucopyranose	-2,02	32,81	ASN;343

LAMPIRAN 8

TABEL V.3

HASIL PREDIKSI DRUG *LIKENESS* BERDASARKAN ATURAN *LIPINSKI*
RULE OF FIVE

NO	SENYAWA	BM	Log P	IKATAN HIDROGEN		keterangan
				Donor	Akseptor	
1.	arniadol	442	6,995	2	2	Tidak memenuhi syarat
2.	beta-dglucopyranosid	616	1,102	5	11	Tidak memenuhi syarat
3.	cycloartenol	426	8,168	1	1	Tidak memenuhi syarat
4.	cynaroside	448	-0,401	7	11	Tidak memenuhi syarat
5.	faradiol	442	6,995	2	2	Tidak memenuhi syarat
6.	Psi-taraxasterol	425	8,356	0	1	Tidak memenuhi syarat
7.	sitosterol	414	8,024	1	1	Tidak memenuhi syarat
8.	stigmasterol	412	7,800	1	1	Tidak memenuhi syarat
9.	taraxasterol	426	8,024	1	1	Tidak memenuhi syarat
10.	taraxerol	426	8,168	1	1	Tidak memenuhi syarat

LAMPIRAN 9

TABEL V.4
HASIL PREDIKSI TOKSISITAS LIGAN PEMBANDING DAN SENYAWA
AKTIF TANAMAN DANDELION
(*Taraxacum officinale* WEBB)

NO	SENYAWA	Crame Ruls	Kross TTC	Benigni
1.	arniadol	1	1	8,9
2.	beta-dglucopyranosid	3	2	1,9
3.	cycloartenol	3	1	8,9
4.	cynaroside	3	1	8,9
5.	faradiol	1	1	8,9
6.	Psi-taraxasterol	1	1	8,9
7.	sitosterol	3	1	8,9
8.	stigmasterol	3	1	8,9
9.	taraxasterol	1	1	8,9
10.	taraxerol	1	1	8,9

**LAMPIRAN 9
(LANJUTAN)**

**TABEL V.5
LANJUTAN (KETERANGAN TABEL)**

Keterangan :

- Cramer rules* = (1) *Substances with simple chemical structures and fix which efficient modes of meabolism exist, suggesting a low order of oral toxicity.*
- (2) *Substances which possess structures that are less innocuous than class I Substances, but do not contain structural features suggestive of toxicity like those substances in class III.*
- (3) *Substances with chemical structures that permit no strong unitial presumption of safety or may even suggest significant toxicity it have reactive functional groups.*
- Benigni/Bossa* = (1) *Structural Alert for genotoxic carcinogenicity.*
- Rulebase* (2) *Structural Alert for nongenotoxic carcinogenicity*

(3) *Negative for genotoxic carcinogenicity.*

(4) *Negative for nongenotoxic carcinogenicity.*

Kroes TTC

(1) *Substance would not be expected to be a safety concern.*

(2) *Negligible risk (low probability of life-time cancer risk greater than 1 in 10⁶)*



LAMPIRAN 10

TABEL V.6

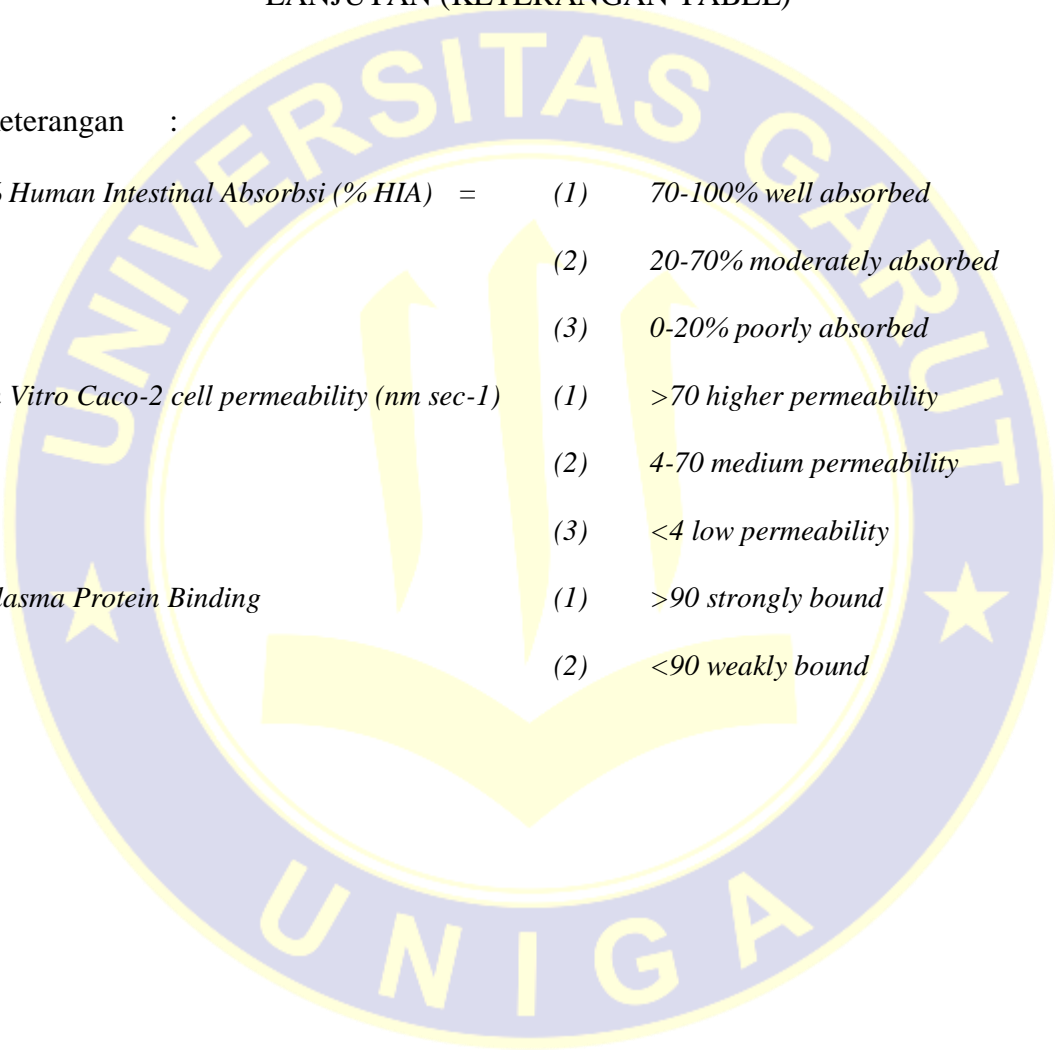
HASIL PREDIKSI PROPIL ABSORPSI DAN DISTRIBUSI LIGAN
PEMBANDING DAN SENYAWA AKTIF TANAMAN DANDELION
(*Taraxacum officinale* WEBB)

NO	SENYAWA	HIA	Caco-2	Protein plasma binding
1.	arniadol	94,404	31,124	100,00
2.	beta-dglucopyranosid	25,292	2938	36,086
3.	cycloartenol	100,00	50,025	100,00
4.	cynaroside	25,165	4,872	73,279
5.	faradiol	94,404	31,124	100,00
6.	Psi-taraxasterol	100,00	47,174	100,00
7.	sitosterol	100,00	52,373	100,00
8.	stigmasterol	100,00	52,337	100,00
9.	taraxasterol	100,00	47,174	100,00
10.	taraxerol	100,00	46,732	100,00

**LAMPIRAN 10
(LANJUTAN)**

**TABEL V.6
LANJUTAN (KETERANGAN TABEL)**

Keterangan :



<i>% Human Intestinal Absorpsi (% HIA)</i>	(1)	<i>70-100% well absorbed</i>
	(2)	<i>20-70% moderately absorbed</i>
	(3)	<i>0-20% poorly absorbed</i>
<i>In Vitro Caco-2 cell permeability (nm sec-1)</i>	(1)	<i>>70 higher permeability</i>
	(2)	<i>4-70 medium permeability</i>
	(3)	<i><4 low permeability</i>
<i>Plasma Protein Binding</i>	(1)	<i>>90 strongly bound</i>
	(2)	<i><90 weakly bound</i>