

DAFTAR PUSTAKA

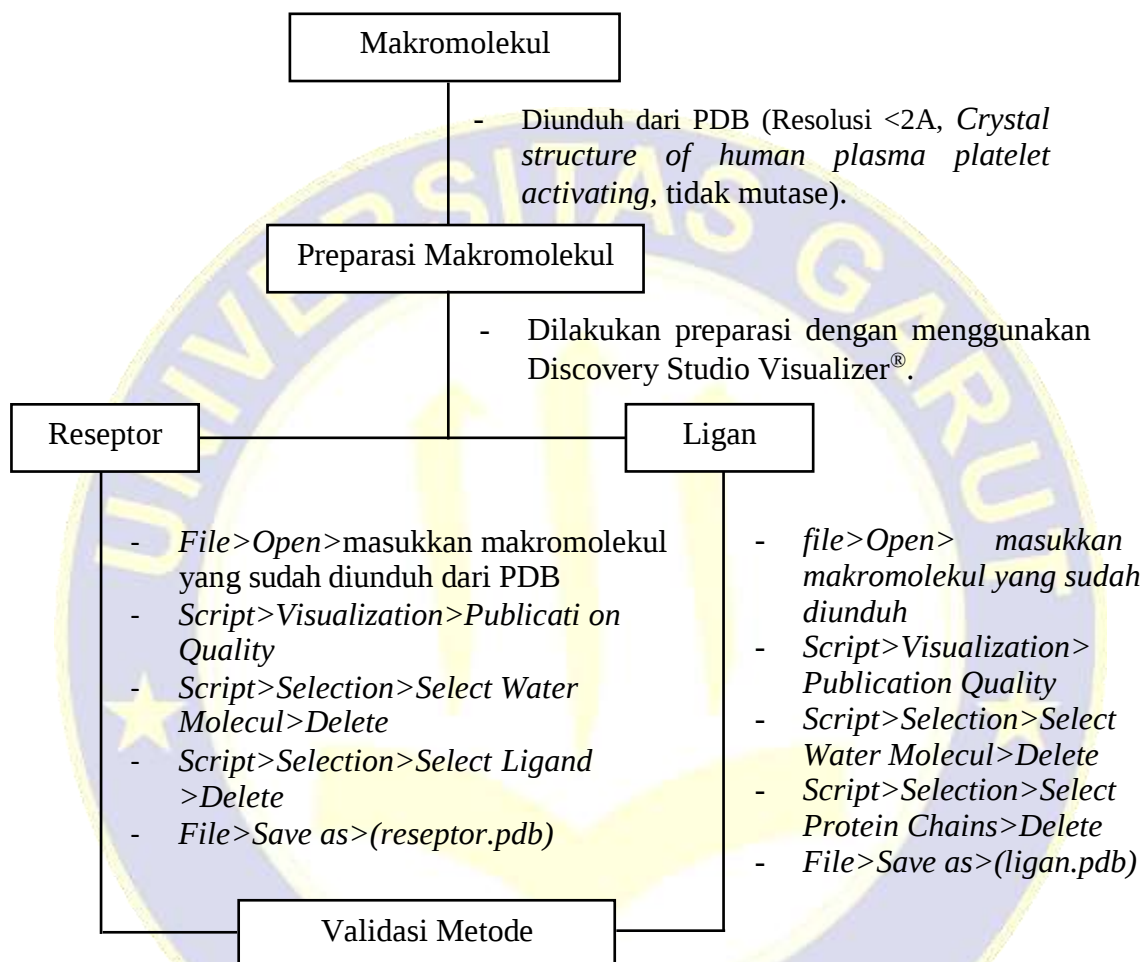
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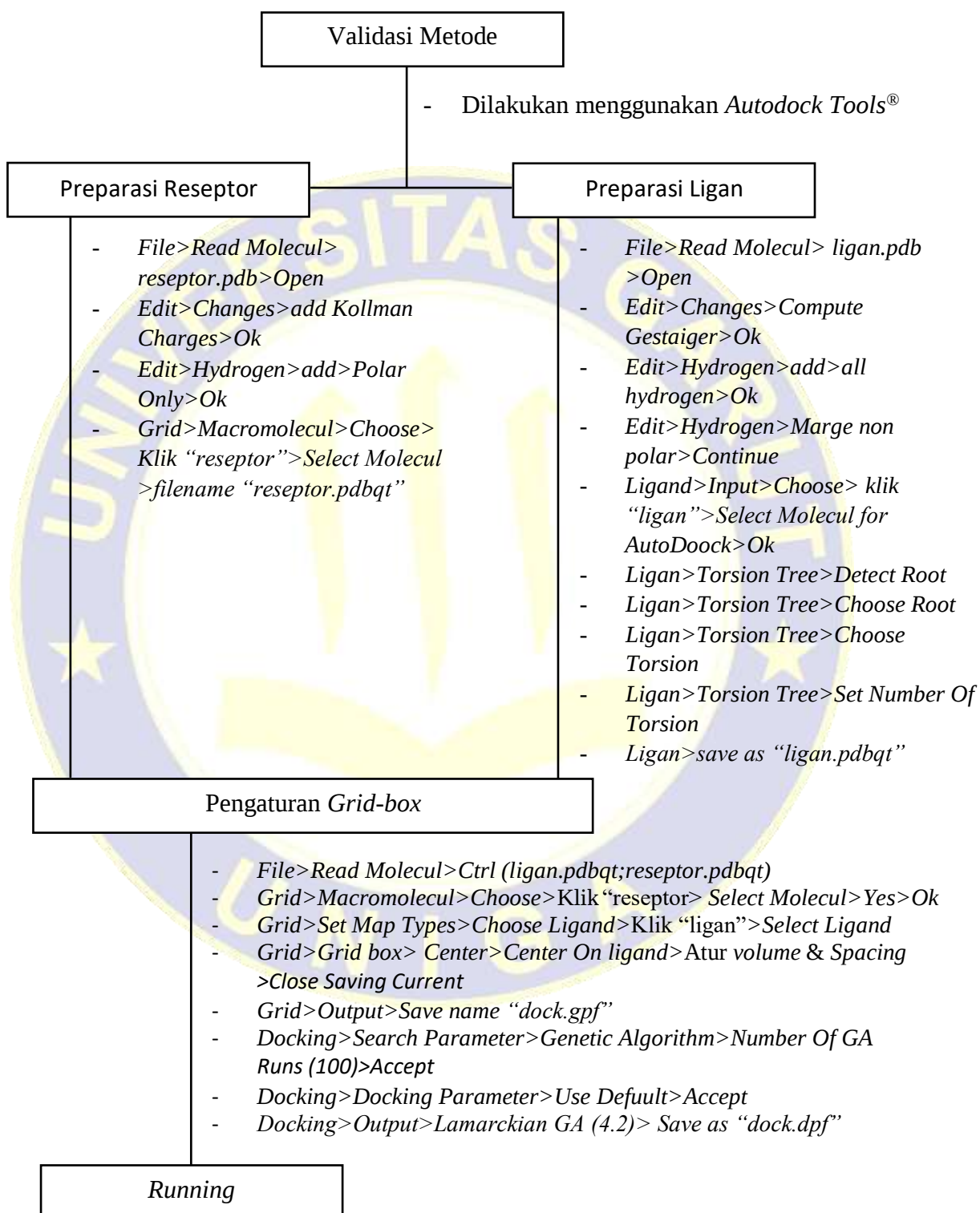
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LAMPIRAN 1

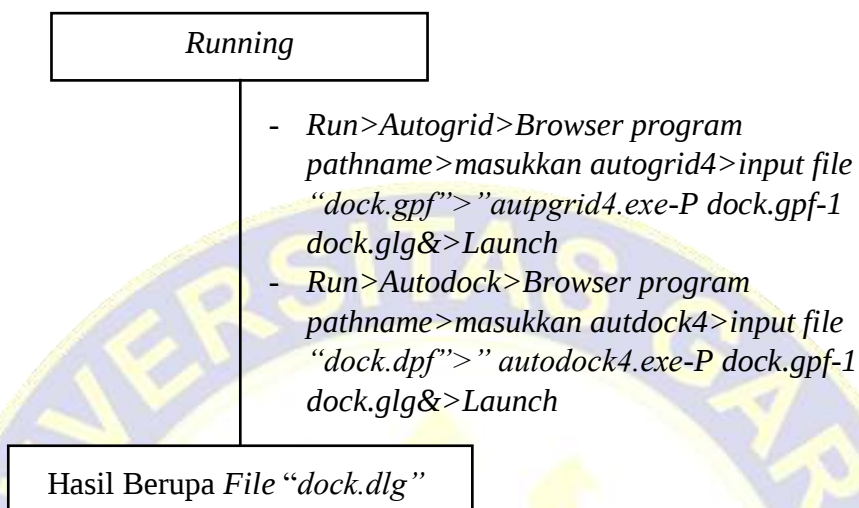
**ALUR PENELITIAN VALIDASI METODE MOLECULAR DOCKING
DAN PREDIKSI DRUGLIKENESS**



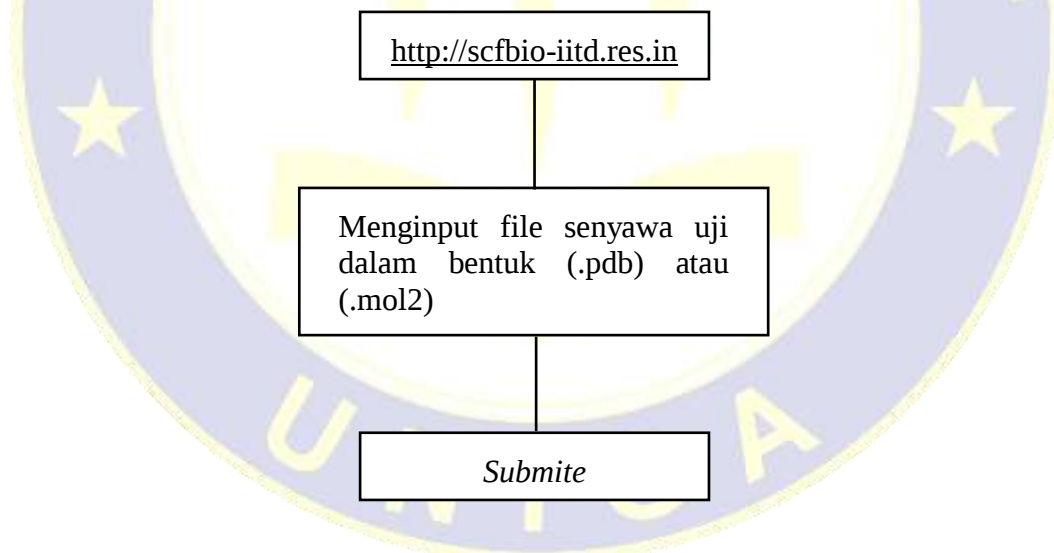
LAMPIRAN 1 (LANJUTAN)



LAMPIRAN 1 (LANJUTAN)



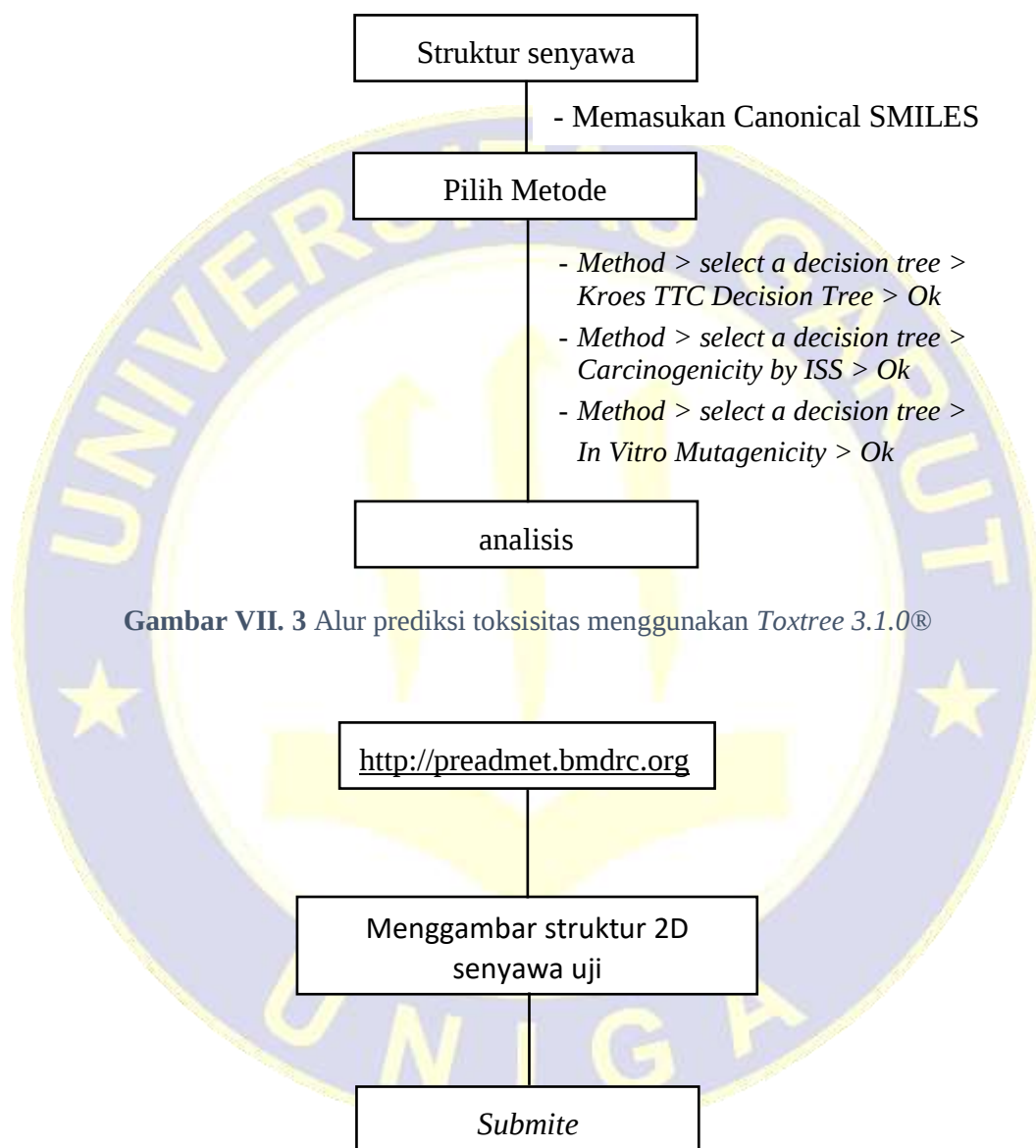
Gambar VII. 1 Alur penelitian validasi metode *molecular docking*



Gambar VII. 2 Alur prediksi *druglikeness* menggunakan situs online *lipinski rule's of five*

LAMPIRAN 2

ALUR PENELITIAN PREDIKSI TOKSISITAS DAN PREDIKSI
FARMAKOKINETIK



Gambar VII. 3 Alur prediksi toksisitas menggunakan Toxtree 3.1.0®

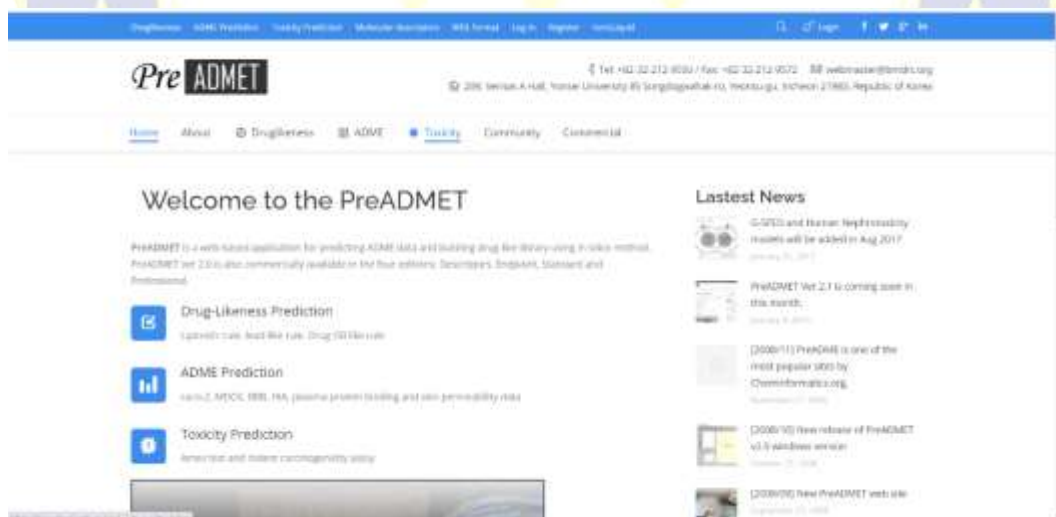
Gambar VII. 4 Alur prediksi farmakokinetik menggunakan situs online Pre-ADMET

LAMPIRAN 3

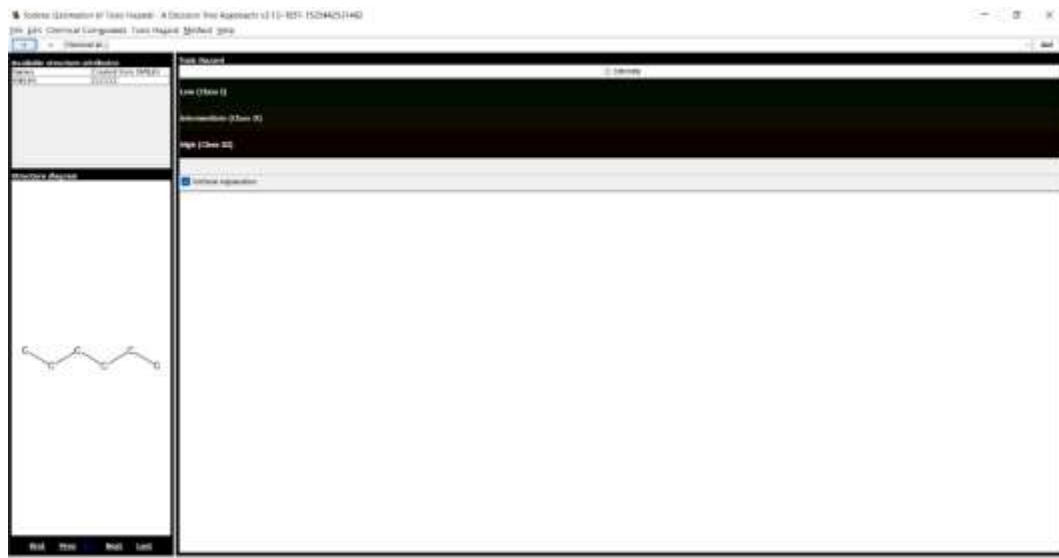
SITUS DAN APLIKASI



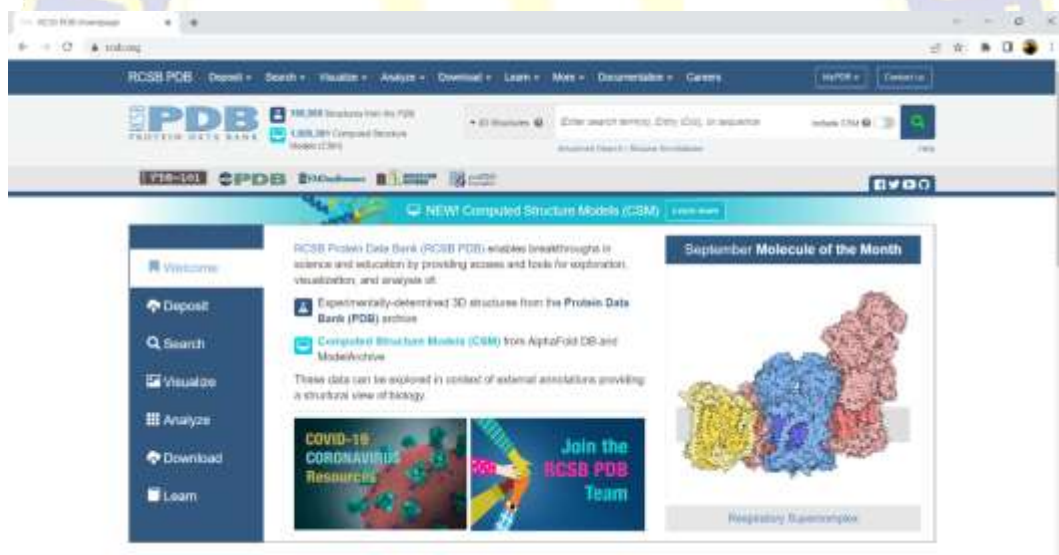
Gambar VII. 5 Tampilan *lipinski rule's of five*



Gambar VII. 6 Tampilan situs *Pre-ADMET*

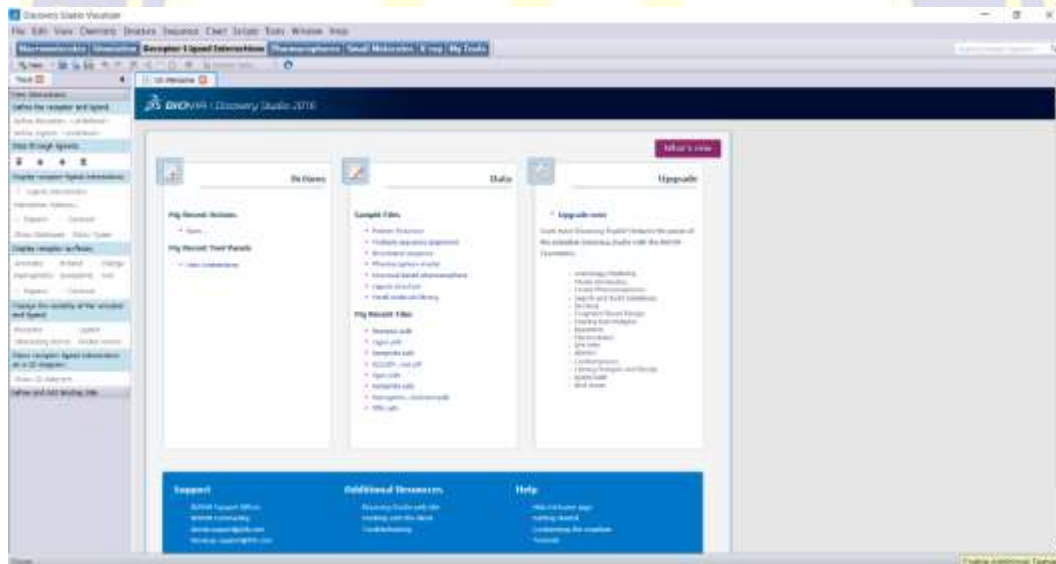


Gambar VII. 7 Tampilan aplikasi ToxTree®

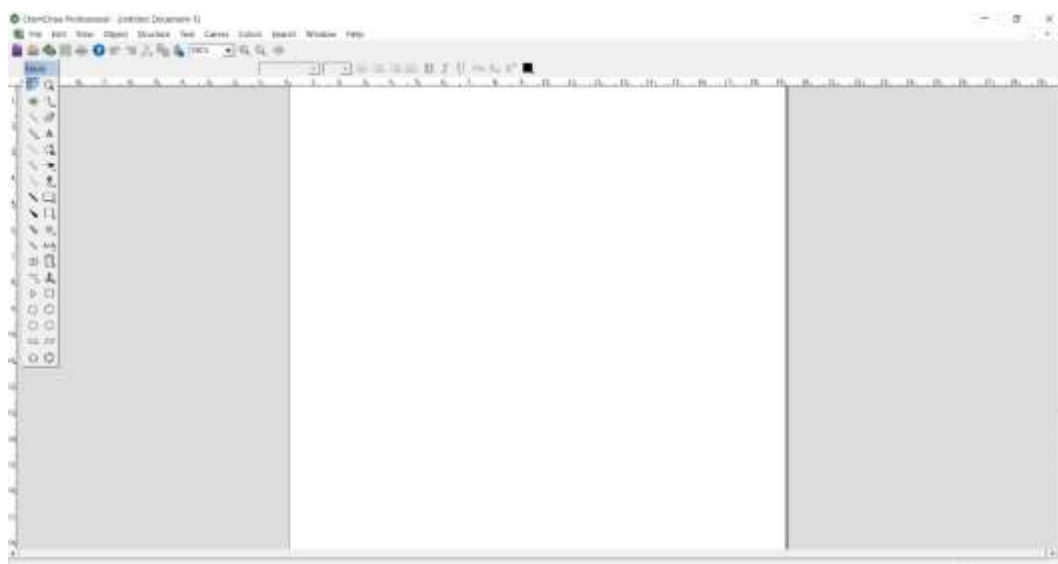


Gambar VII. 8 Tampilan situs protein data bank (PDB)

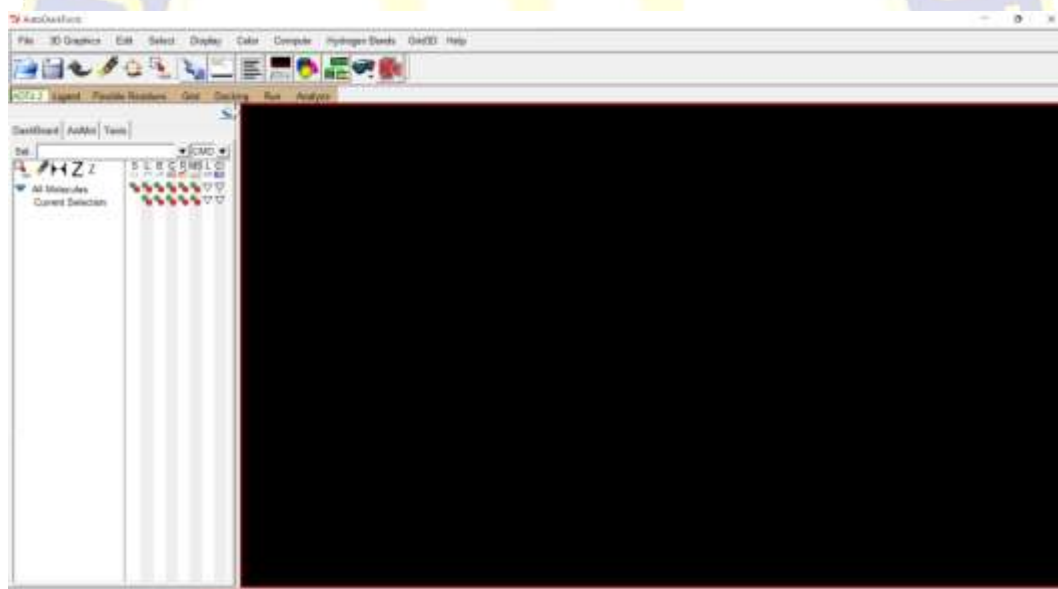
Gambar VII. 9 Tampilan situs *PubChem*



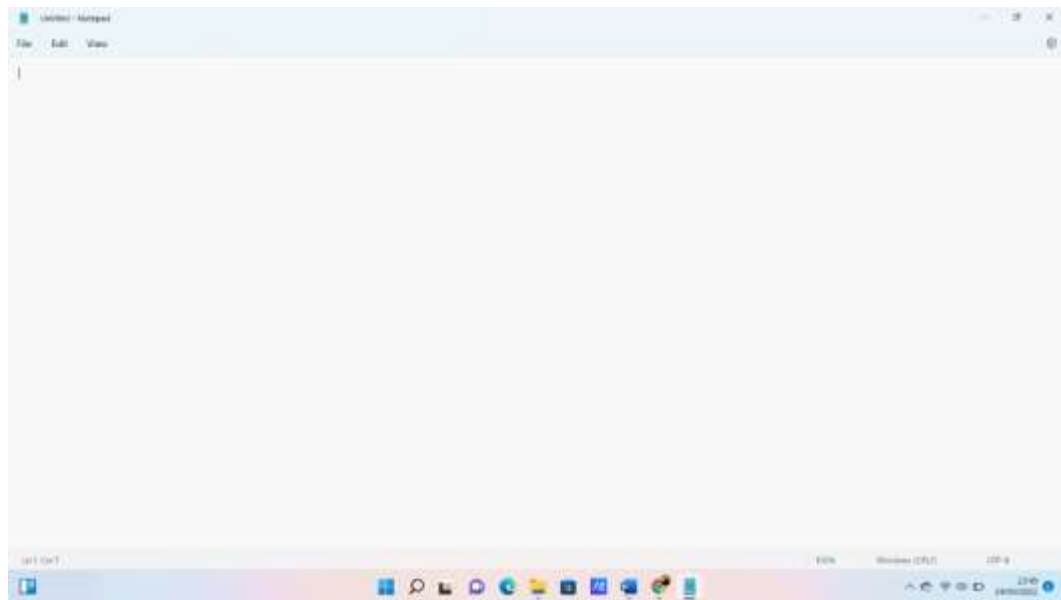
Gambar VII. 10 Tampilan aplikasi *Discovery Studio Visualizer*[®]



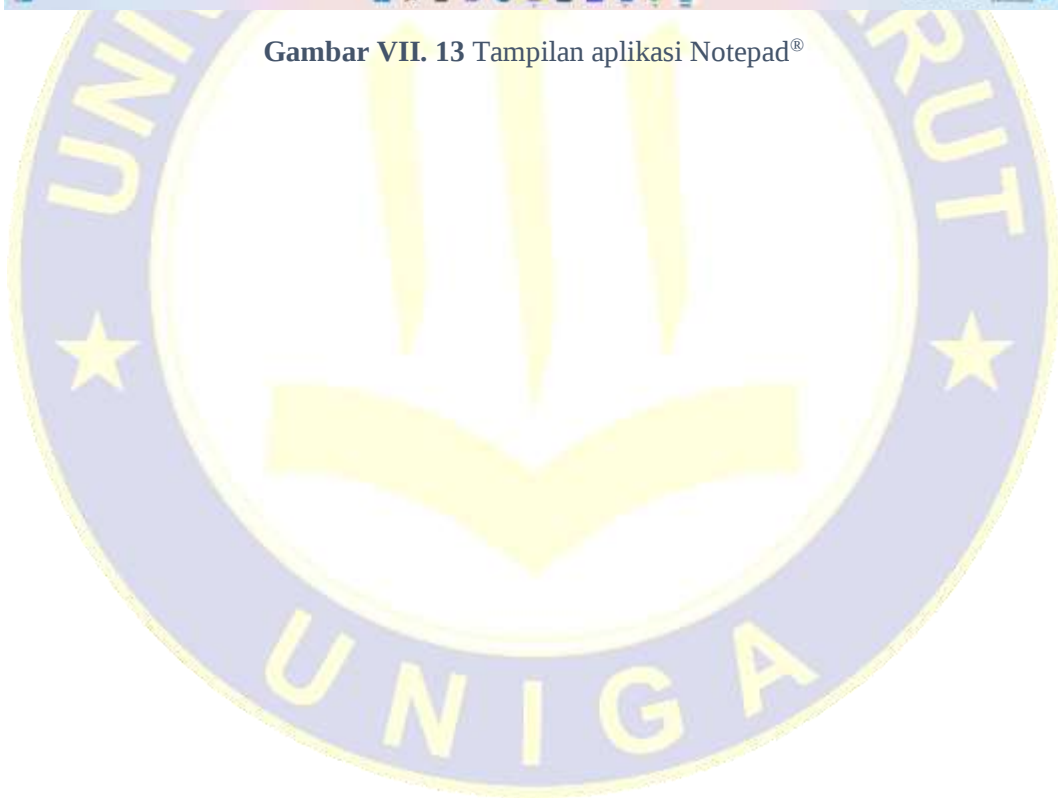
Gambar VII. 11 Tampilan aplikasi *ChemDraw Professional 16.0*[®]



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



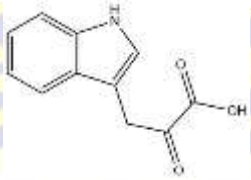
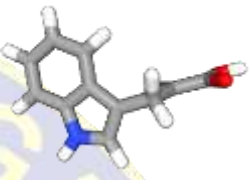
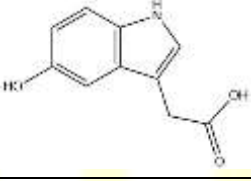
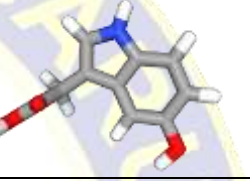
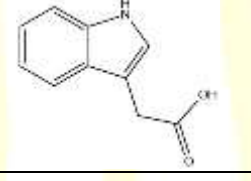
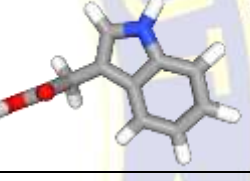
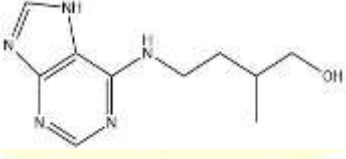
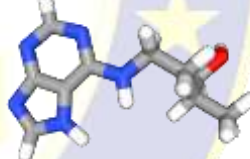
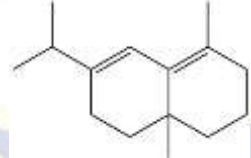
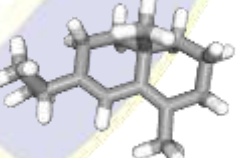
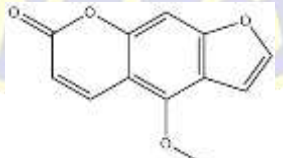
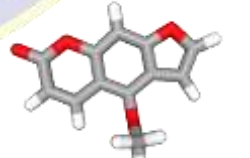
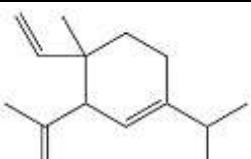
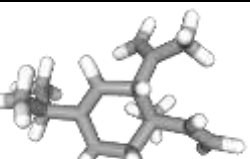
Gambar VII. 13 Tampilan aplikasi Notepad®



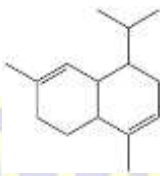
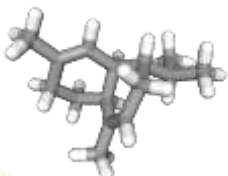
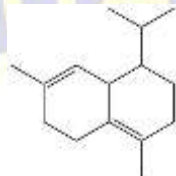
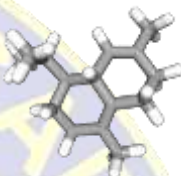
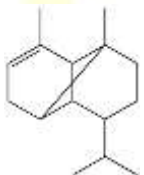
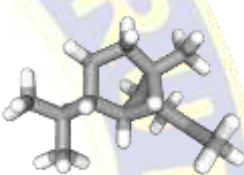
LAMPIRAN 4
STRUKTUR SENYAWA TOMAT

Tabel VII. 1

Struktur 2D dan 3D 10 senyawa terbaik tomat

NO	SENYAWA	STRUKTUR 2D	STRUKTUR 3D
1	Indolepyruvate		
2	5-Hydroxyindole-3-acetic acid		
3	Indoleacetic acid		
4	Dihydrozeatin		
5	Delta-Selinene		
6	Bergapten		
7	Delta-Elemene		

**LAMPIRAN 4
(LANJUTAN)****Tabel VII.1**
Lanjutan

8	Alpha-Muurolene		
9	Delta-Cadinene		
10	Copaene		

LAMPIRAN 5

HASIL PENELITIAN PREDIKSI MOLECULAR DOCKING

Tabel VII. 2 Hasil penelitian prediksi *Molecular Docking* 168 senyawa tomat

NO	METABOLITE	ΔG	Ki
1	Gibberellin A4	+6,46	-
2	Gibberellin A29	+5,83	-
3	Gibberellin A34	+3,54	-
4	Gibberellin A51	+16,42	-
5	Gibberellin A53	+31,11	-
6	Gibberellin A81	+5,12	-
7	trans-Zeatin	-2,34	1,04
8	N6-Benzyladenine	-4,30	120,76
9	Dihydrozeatin	-6,64	13,55
10	N6-(delta2-Isopentenyl)adenine	-5,07	193,20
11	9-Ribosyl-trans-zeatin	+6,47	-
12	Indoleacetic acid	-6,82	10,01
13	Methyl indole-3-acetate	-5,57	82,97
14	5-Hydroxyindole-3-acetic acid	-7,00	7,44
15	Indole-3-acetonitrile	-5,22	149,92
16	Indole-3-acetyl-L-aspartic acid	-5,60	78,50
17	N-Malonyltryptophan	-4,59	134,90
18	Absciscic acid	-5,04	200,56
19	Gibberellin A97	+95,58	-
20	(2E)-2-Hexanal	+3,2	-
21	(Z)-3-Hexenal	-3,82	1,57
22	cis-3-Hexen-1-ol	-3,69	1,96
23	Hexanal	-3,20	1,84
24	Bergaptan	-6,03	37,79
25	Caffeic acid	-4,73	339,39
26	(+)-alpha-Pinene	-4,43	569,90
27	(-)-beta-Pinene	-4,52	483,16
28	beta-Pinene	-4,52	410,91
29	alpha-Terpinolene	-4,62	410,91
30	Phytoene	+363,57	-
31	Prolycopene	+2,55	-
32	Lycopene	+2,58	-
33	gamma-Carotene	+2,62	-
34	Naringenin 7-O-beta-D-glucoside	+9,60	-
35	Maltose	+0,11	-

36	Sucrose	-1,48	82,87
37	Trehalose	+0,05	-
38	Erythritol	-3,45	2,94
39	Inositol	-2,83	8,44
40	3-Methylbutyric acid	-5,34	121,78
41	Dodecane	-3,60	2,28
42	Hentriacontane	+45,92	-
43	Falcarindiol	-3,67	4,17
44	Glycine	-3,09	5,41
45	L-Phenylalanine	-5,42	106,66
46	Dopamine	-3,62	2,21
47	Putrescine	-0,81	253,24
48	5-Hydroxytryptamine	-4,73	340,21
49	Spermidine	-0,56	386,23
50	Tryptamine	-3,29	1,34
51	Tyramine	-3,86	1,49
52	Trigonelline	-5,62	76,24
53	Chaconine	+1,20	-
54	alpha-Solanine	+8,88	-
55	Solasodine	+2,89	-
56	Tomatidine	+3,93	-
57	Tomatine	+1,61	-
58	3-O-Caffeoylquinic acid	+9,62	-
59	alpha-Phellandrene	-4,63	402,94
60	alpha-Terpinene	-4,79	308,83
61	beta-Caryophyllene	-5,30	131,01
62	Copaene	-5,72	63,78
63	alpha-Caryophyllene (obsol.)	-4,83	287,02
64	Nerolidol	-4,75	327,90
65	Cholesterol	+3,17	-
66	beta-Amyrin	+2,52	-
67	alpha-Carotene	+2,63	-
68	Lycoxanthin	+2,68	-
69	Mutatochrome	+2,57	-
70	Kaempferol	+190,64	-
71	Quercitrin	+2,15	-
72	Rutin	+2,78	-
73	Petanin	+3,52	-
74	Naringenin chalcone	+96,41	-
75	(S)-2,3-Epoxy-squalene	+57,42	-
76	24-Episteasterone	+7,74	-
77	24-Epityphasterol	+7,44	-

78	Obtusifoliol	+6,57	-
79	Sucrose 6-phosphate	+0,02	-
80	beta-Elemene	-4,97	227,33
81	Benzeneacetaldehyde	-4,60	424,81
82	Indolepiruvate	-7,35	4,10
83	delta-Selinene	-6,46	18,53
84	delta-Cadinene	-5,73	63,09
85	beta-Phellendrene	-4,34	343,09
86	Germacrene D	-5,32	125,05
87	delta-Elemene	-5,86	50,66
88	gamma-Elemene	-5,02	210,33
89	Aristolene	-5,01	211,76
90	D-Galactose	-4,13	932,83
91	alpha-Gurjunene	-5,42	106,62
92	(+)-Aromadendrene	-4,41	589,43
93	(E,E)-4,8,12-Trimethyl-1,3,7,11-tridecate	+3,90	-
94	psi,psi-Carotene-16,16'-diol	+2,80	-
95	1',2'-Epoxy-1',2'-dihydro-beta,psi-carote	+1,29	-
96	1',2'-Epoxy-1',2'-dihydro-epsilon,psi-car	+2,30	-
97	Lycopene 1,2-epoxide	+2,65	-
98	1,2-Epoxy-1,2,7,7',8,8'-hexahydro-psi,p	+2,75	-
99	Phytoene 1,2-epoxide	+494	-
100	6'-Apo-psi,psi-carotenal	+1,49	-
101	Apo-8'-lycopenal	+1,15	-
102	Soladulcidine	+3,93	-
103	Lycoperodine 1	-4,59	431,98
104	N,N'-Bis(4-hydroxy-3-methoxycinnamoy	+1,18	-
105	gamma-Tomatine	+1,32	-
106	23R-Acetoxytomatine	+5,90	-
107	Lycoperoside B	+6,18	-
108	Lycoperoside C	+1,15	-
109	Tomatidenol	-2,78	64,93
110	(E)-beta-Ocimene	-4,44	557,34
111	2-Carene	-4,46	540,94
112	Cryptochlorogenic acid	+2,33	-
113	alpha-Muurolene	-5,76	59,85
114	Decanal	-4,35	642,37
115	Esculeoside A	+84,13	-
116	Esculeoside B	+79,86	-
117	Esculeoside C	+5,17	-
118	Esculeoside D	+2,37	-
119	Lycoperoside G	+61,54	-

120	Methyl salicylate	-4,88	265,35
121	Neochlorogenic acid	+8,85	-
122	Nonanal	-4,28	728,99
123	Octanal	-4,10	979,66
124	Isoesculeogenin A	+3,21	-
125	Lycoperoside F	+3,64	-
126	Fructose	-3,53	2,59
127	Quinic acid	-4,93	242,86
128	Ribose	-3,11	5,22
129	Benzaldehyde	-4,11	977,03
130	Progesterone	+262,71	-
131	2-Pentylfuran	-4,53	474,38
132	Nonane	-3,41	3,17
133	Fucose	-3,69	1,97
134	3-Octanol	-4,06	1,05
135	1,3-Dimethylbenzene	-3,84	1,54
136	1,5-Heptadien-3-yne	-3,42	3,11
137	1-Pentanol	-3,22	4,36
138	pent-1-en-3-one	-3,61	2,25
139	3-Methyl-1-pentanol	-3,55	2,49
140	6-Methyl-1-heptene	-3,62	2,21
141	n-Butanol	-2,87	7,89
142	Limonene oxide	-5,04	203,50
143	Cyclohexylmethane	-3,80	1,64
144	Octane	-3,28	3,96
145	n-Tetradecane	-3,50	2,71
146	trans-2,4-hexadienal	-3,93	1,32
147	6-Deoxo-28-nortyphasterol	+3,93	-
148	Deoxy phytoprostane J1	+4,49	-
149	Isoledene	-5,71	64,93
150	trans-2-Phenylcyclopropane-1-carboxyli	+3,90	-
151	25-Hydroxyvitamin D3	+2,98	-
152	Vitamin D3	+3,39	-
153	Lycoperoside H	+1,60	-
154	Decane	-3,57	2,41
155	3-Hexenal	-3,82	1,58
156	22-Hydroxycholesterol	+2,58	-
157	22,26-Dihydroxycholesterol	+1,11	-
158	Furostanol-26-aldehyde	+1,10	-
159	26-Amino-furostanol	+9,83	-
160	Tomatidine galactoside	+60,89	-
161	beta1-Tomatine	+5,13	-

162	alpha-Tomatine	+8,17	-
163	5-Methoxytryptamine	-4,87	237,88
164	Melatonin	-4,92	249,22
165	Dehydrotomatine	+1,90	-
166	Hydroxytomatine	-2,76	89,44
167	beta2-Tomatine	+3,12	-
168	delta-Tomatine	+5,71	-



LAMPIRAN 6

10 SENYAWA TERBAIK TOMAT

Tabel VII. 3 10 Senyawa terbaik tomat dari hasil penelitian prediksi *Molecular Docking*

NO	LIGAN	ΔG (kcal/mol)	Ki (μM)	RESIDU ASAM AMINO
1	Indolepyruvate	-7,35	4,10	PHE B:274, LEU B:153, SER B:273, ALA B:155, dan GLN B:352.
2	5-Hydroxyindole-3-acetic acid	-7,00	7,44	PHE B:274, LEU B:153, SER B:273, PHE B:110 dan HIS B:351.
3	Indoleacetic acid	-6,82	10,01	PHE B:274, LEU B:153, SER B:273, dan HIS B:351.
4	Dihydrozeatin	-6,64	13,55	PHE B:274, LEU B:153, SER B:273, TRP B:298, ALA B:155, GLN B:325, TYR B:160
5	Delta-Selinene	-6,46	18,53	PHE B:110, LEU B:153, TRP B:298, ALA B:155, HIS B:351, HIS B:272
6	Bergaptan	-6,03	37,79	PHE B:322, PHE B:274, LEU B:153, SER B:273, ALA B:155, GLN B:352, HIS B:351
7	Delta-Elemene	-5,86	50,66	PHE B:274, PHE B:110, LEU B:153, HIS B:272, HIS B:351, ALA B:155, TRP B:298
8	Alpha-Murolene	-5,76	59,85	PHE B:322, PHE B:110, LEU B:153, TRP B:298, HIS B:331, HIS B:272
9	Delta-Cadinene	-5,73	63,09	PHE B:110, LEU B:153, HIS B:272, HIS B:351, ALA B:155.
10	Copaene	-5,72	63,78	PHE B:110, LEU B:153, HIS B:272, HIS B:351, TRP B:298

LAMPIRAN 7

HASIL PENELITIAN PREDIKSI LIPINSKI RULE'S OF FIVE

Tabel VII. 4 Hasil prediksi *lipinski rule's of five*

NO	LIGAN	BM(g/mol)	Log P	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Ket
1	Indolepyruvate	203	1,36	2	3	Terpenuhi
2	5-Hydroxyindole-3-acetic acid	191	1,50	3	3	Terpenuhi
3	Indoleacetic acid	175	1,79	2	2	Terpenuhi
4	Dihydrozeatin	221	0,78	3	5	Terpenuhi
5	Delta-Selinene	204	4,86	0	0	Terpenuhi
6	Bergaptan	216	2,37	0	4	Terpenuhi
7	Delta-Elemene	204	4,74	0	0	Terpenuhi
8	Alpha-Murolene	204	4,58	0	0	Terpenuhi
9	Delta-Cadinene	204	4,72	0	0	Terpenuhi
10	Copaene	204	4,27	0	0	Terpenuhi

*Ket :

- Massa Molekul kurang dari 500 Dalton
- Log P kurang dari 5
- Ikatan Hidrogen kurang dari 5
- Ikatan Akseptor kurang dari 10

LAMPIRAN 8

HASIL PENELITIAN PREDIKSI TOKSISITAS

Tabel VII. 5 Hasil prediksi toksisitas

NO	LIGAN	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genetoxic	Non Genetoxic	
1	Indolepyruvate	(-)	(-)	(-)	Tidak beresiko
2	5-Hydroxyindole- 3-acetic acid	(-)	(-)	(-)	Tidak beresiko
3	Indoleacetic acid	(-)	(-)	(-)	Tidak beresiko
4	Dihydrozeatin	(-)	(-)	(+)	Beresiko rendah
5	Delta-Selinene	(-)	(-)	(-)	Tidak beresiko
6	Bergaptan	(+)	(+)	(-)	Tidak beresiko
7	Delta-Elemene	(-)	(-)	(-)	Tidak beresiko
8	Alpha-Muurolene	(-)	(-)	(-)	Tidak beresiko
9	Delta-Cadinene	(-)	(-)	(-)	Tidak beresiko
10	Copaene	(-)	(-)	(-)	Tidak beresiko

LAMPIRAN 9

HASIL PENELITIAN PREDIKSI FARMAKOKINETIK

Tabel VII. 6 Hasil prediksi *Pre-ADMET*

NO	LIGAN	Caco2	HIA	PPB
1	Indolepyruvate	0.31***	89.31*	85.07**
2	5-Hydroxyindole-3-acetic acid	19.63**	82.24*	17.22**
3	Indoleacetic acid	20.62**	88.97*	75.92**
4	Dihydrozeatin	10.17**	73.69*	36.37**
5	Delta-Selinene	23.47**	100.00*	100.00*
6	Bergaptan	43.47**	98.16*	91.65*
7	Delta-Elemene	23.64**	100.00*	100.00*
8	Alpha-Muurolene	23.63**	100.00*	100.00*
9	Delta-Cadinene	23.63**	100.00*	100.00*
10	Copaene	23.63**	100.00*	100.00*

*Ket :

HIA (%) :

- * : 70-100 Terserap baik
- ** : 20-70 Terserap cukup
- *** : <20 Kurang Terserap

CaCo-2 :

- * : >70 Permeabilitas Tinggi
- ** : 4-70 Permeabilitas Sedang
- *** : <4 Permeabilitas rendah

PPB (%) :

- * : >90 Terikat Kuat
- ** : <90 Terikat lemah

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