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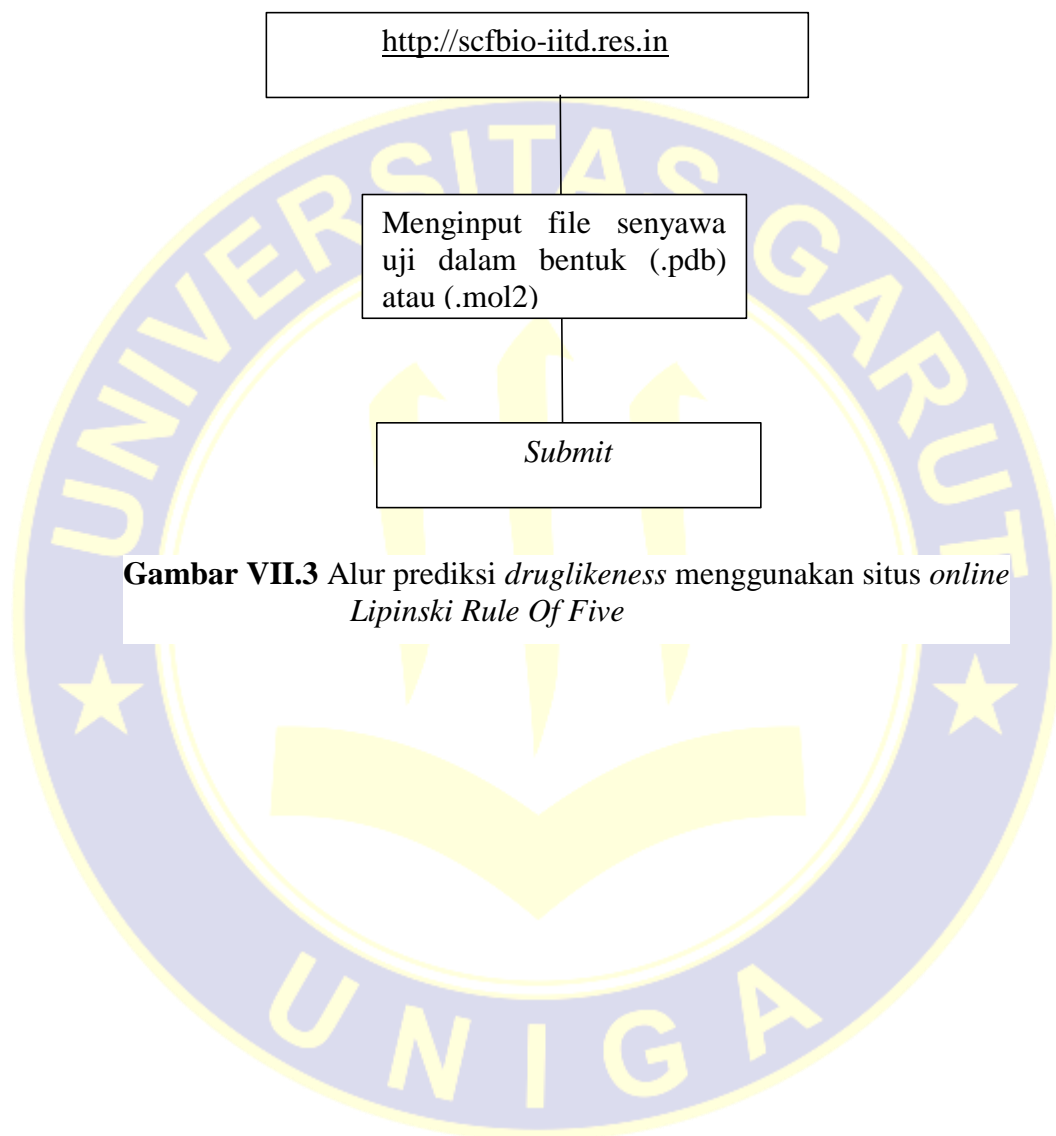
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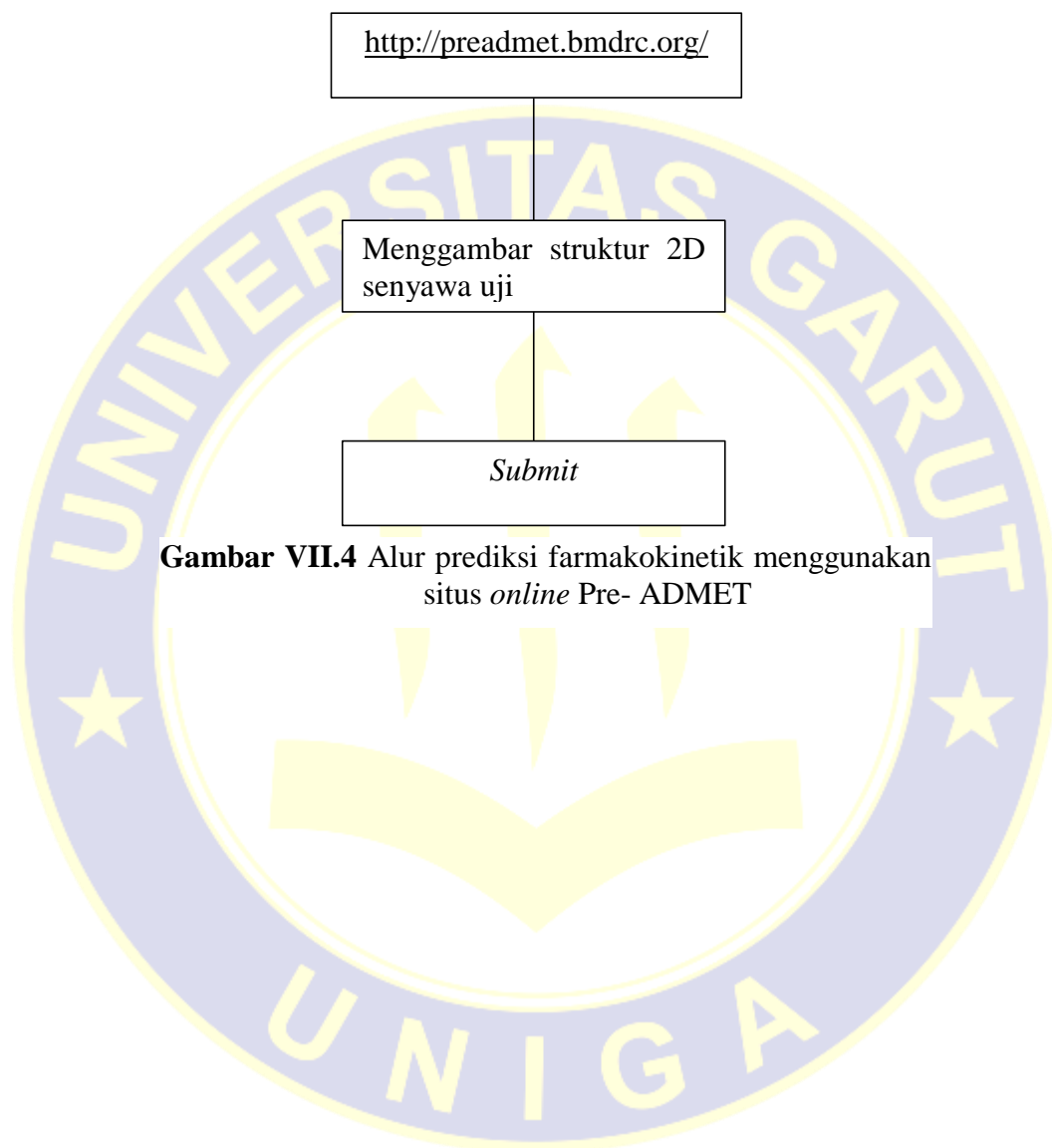
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LAMPIRAN 1**TANAMAN *Lantana camara* dan *Lantana involucrata*****Gambar VII.1** Tanaman *Lantana camara***Gambar VII.2** Tanaman *Lantana involucrata*

LAMPIRAN 2

ALUR PENELITIAN PREDIKSI *DRUGLIKENESS*

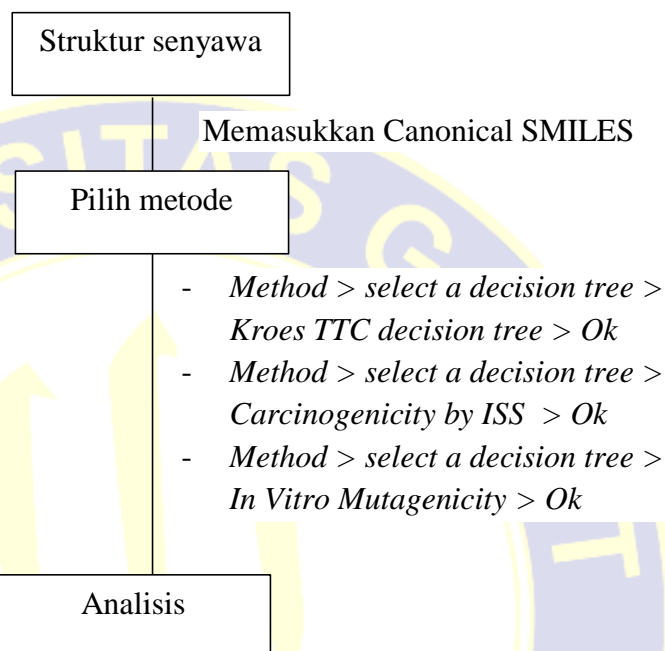
Gambar VII.3 Alur prediksi *druglikeness* menggunakan situs *online Lipinski Rule Of Five*

LAMPIRAN 3**ALUR PENELITIAN PREDIKSI FARMAKONINETIKA**

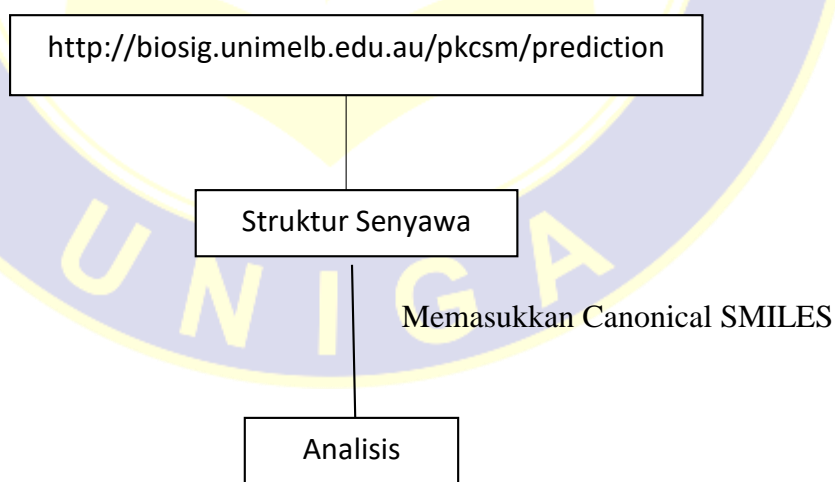
Gambar VII.4 Alur prediksi farmakokinetik menggunakan situs *online* Pre- ADMET

LAMPIRAN 4

ALUR PENELITIAN PREDIKSI TOKSISITAS



Gambar VII.5 Alur prediksi toksisitas menggunakan *Toxtree 3.1.0*[®]

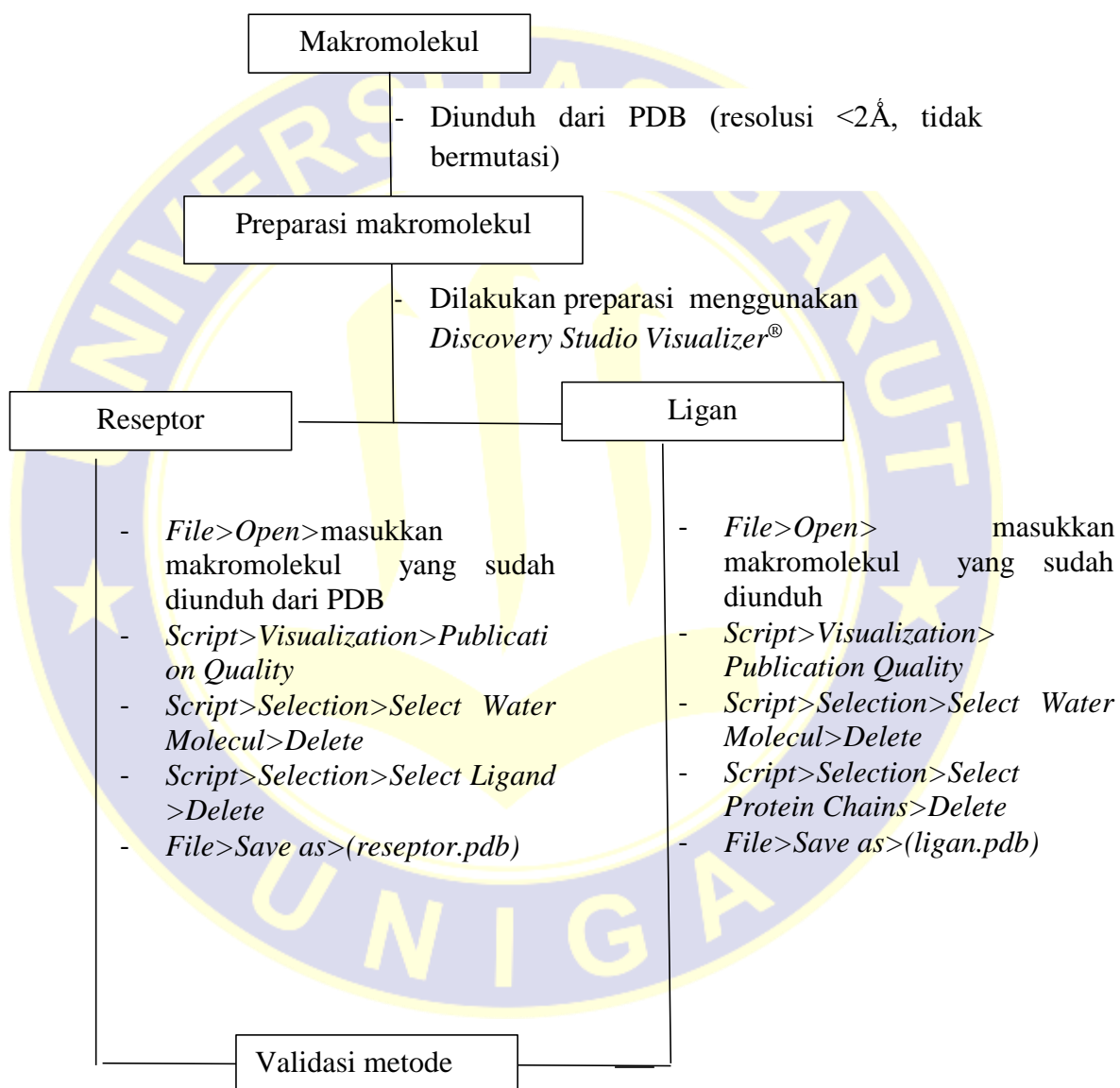


Gambar VII.6 Alur prediksi toksisitas menggunakan *PKCSM*

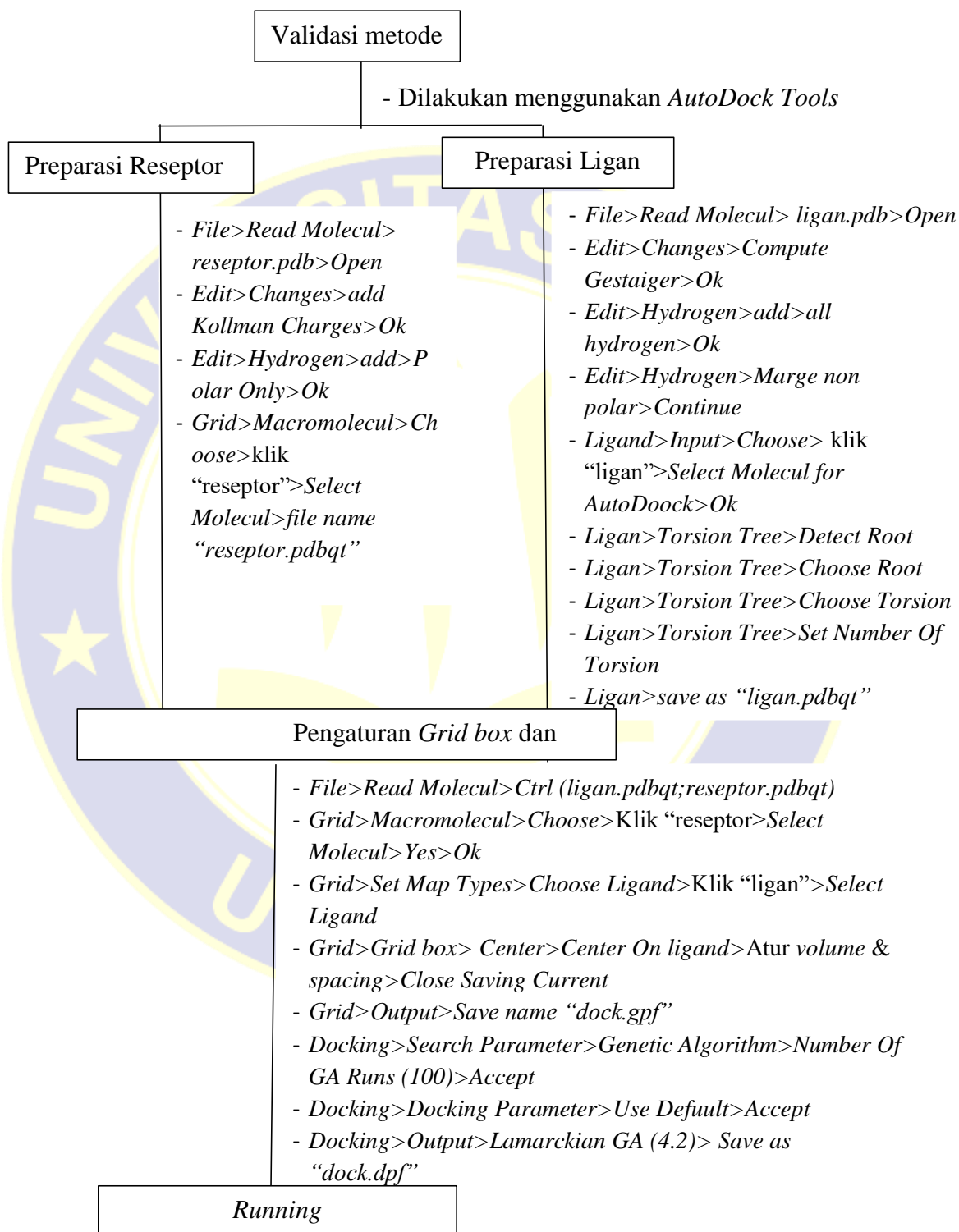
LAMPIRAN 5

ALUR PENELITIAN VALIDASI METODE MOLECULAR

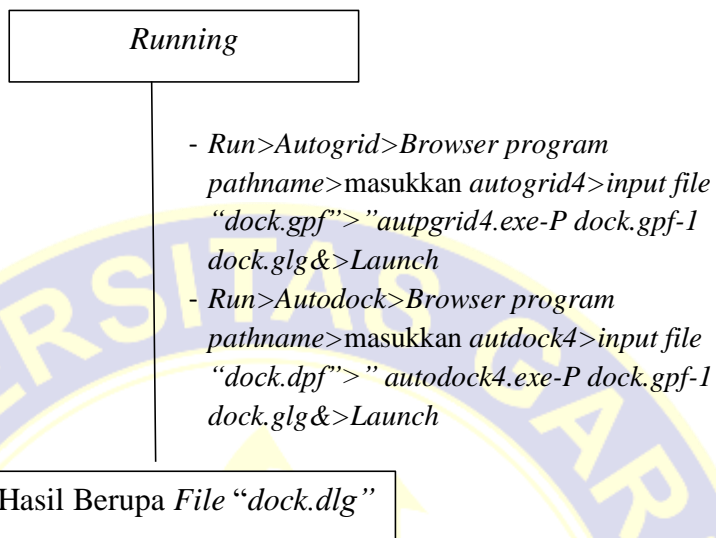
DOCKING



LAMPIRAN 5 (LANJUTAN)



LAMPIRAN 5 (LANJUTAN)



Gambar VII.7 Alur penelitian validasi metode *molecular docking*

LAMPIRAN 6

SITUS DAN APLIKASI

scfbio-iitd.res.in/software/drugdesign/lipinski.jsp

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](#)]
- The input file name should not contain whitespaces.

Gambar VII.9 Tampilan situs *Lipinski Rule of Five*

← → ↻ 🔒 preadmet.bmdrcr

MDL mol and sdf file Molecular descriptors Druglikeness ADME Prediction Toxicity prediction Log In Register 🔍 🔗 Login f 🐦 ⌘ in

Pre ADMET Tel: +82-32-212-9550 / Fax: +82-32-212-9572 ✉ webmaster@bmdrcr

🏠 209, Veritas A Hall, Yonsei University 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, 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'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



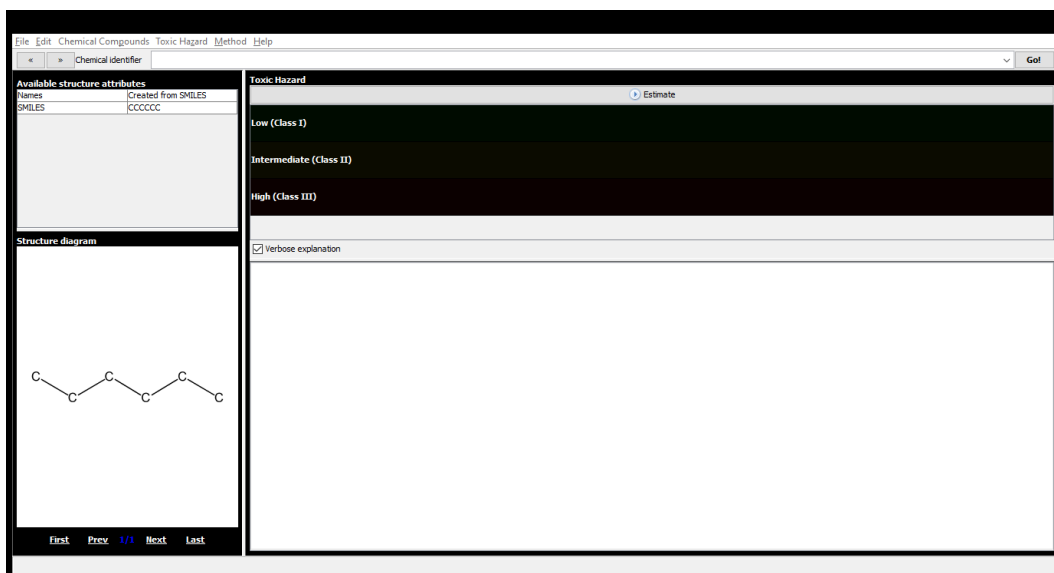
[2008/11] PreADME is one of the most popular sites by Cheminformatics.org.
November 27, 2008



[2008/10] New release of PreADMET v2.0 windows version
October 27, 2008

Gambar VII.10 Tampilan situs *PreADMET*

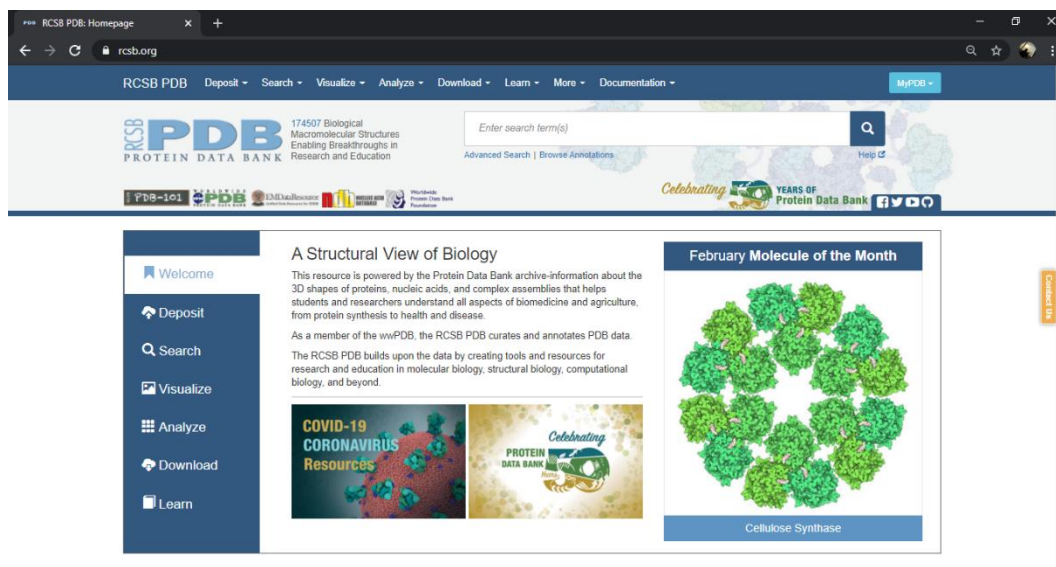
LAMPIRAN 6 (LANJUTAN)



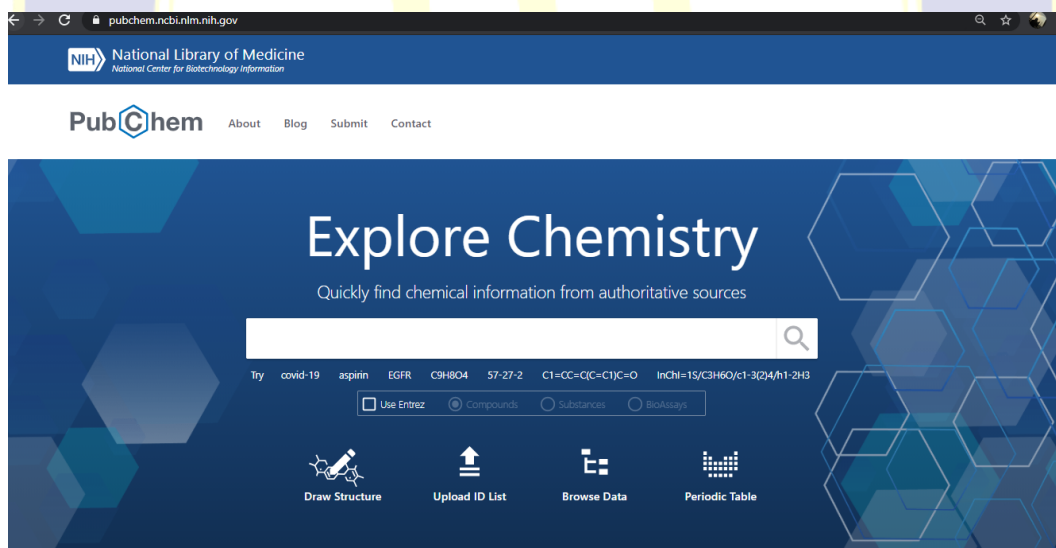
Gambar VII.11 Tampilan aplikasi *Toxtree*[®]

Gambar VII.12 Tampilan situs *PKCSM*

LAMPIRAN 6 (LANJUTAN)

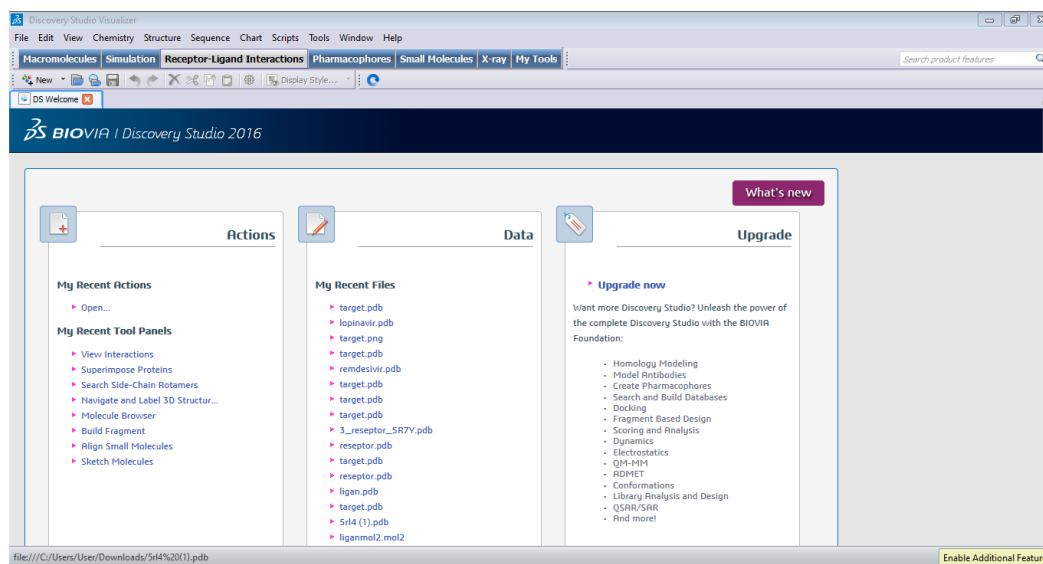


Gambar VII.13 Tampilan situs Protein Data Bank (PDB)

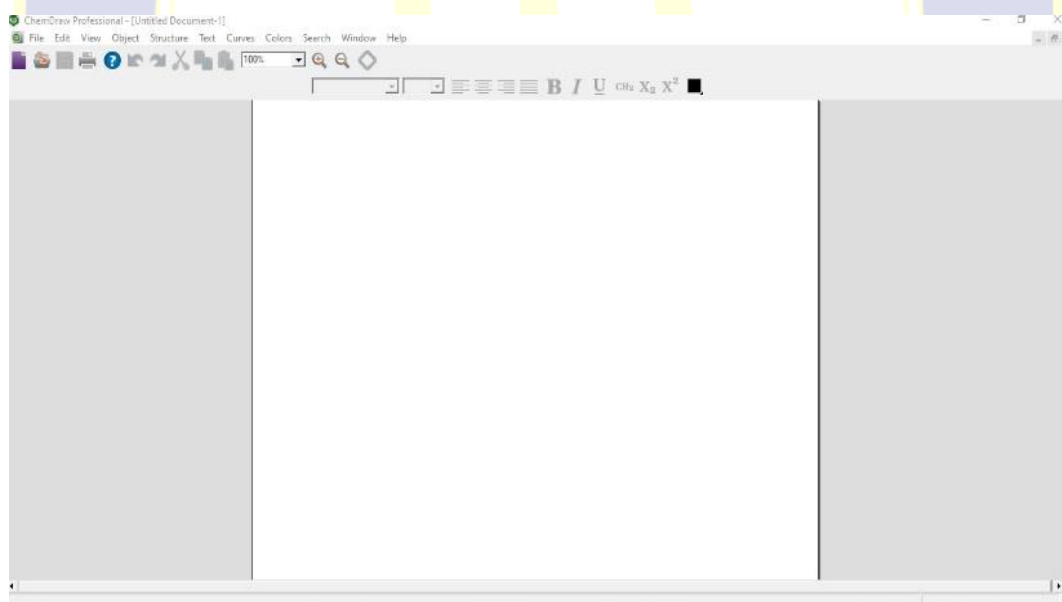


Gambar VII.14 Tampilan situs *PubChem*

LAMPIRAN 6 (LANJUTAN)

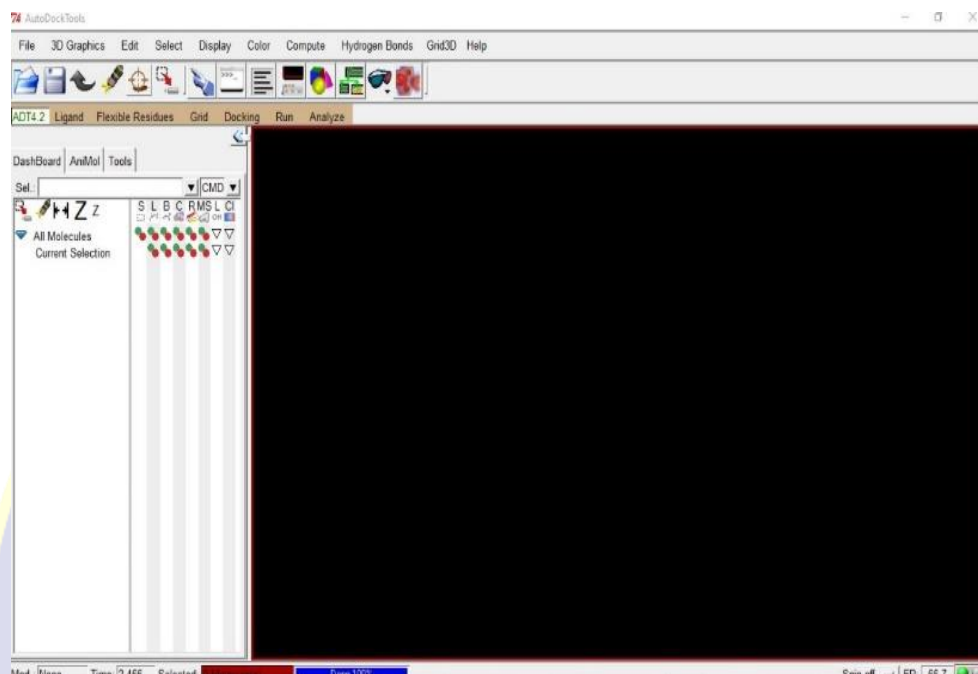


Gambar VII.15 Tampilan aplikasi *Discovery Studio Visualizer*[®]

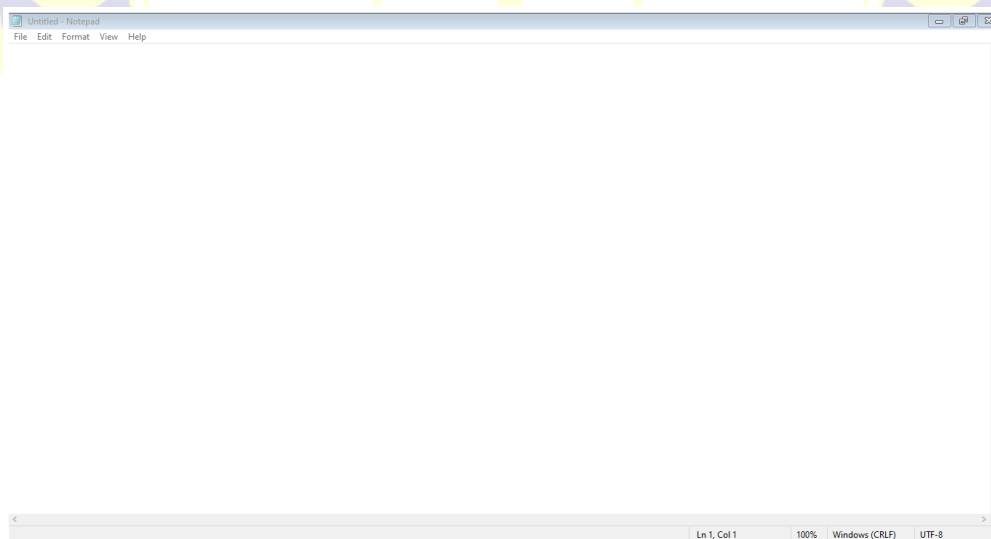


Gambar VII.16 Tampilan aplikasi *ChemDraw Professional 15.0*[®]

LAMPIRAN 6 (LANJUTAN)



Gambar VII.17 Tampilan aplikasi *AutoDock Tools*[®]



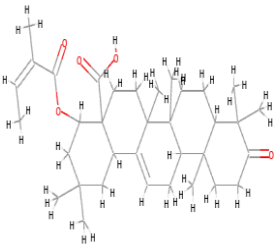
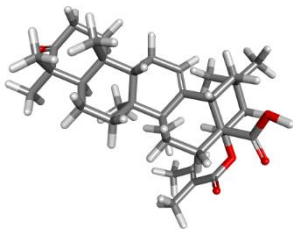
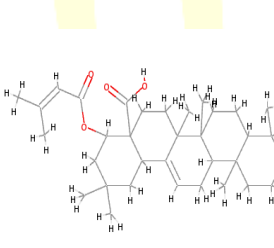
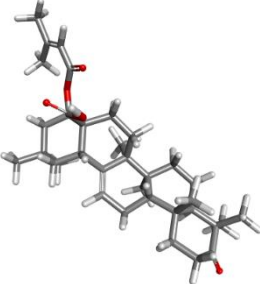
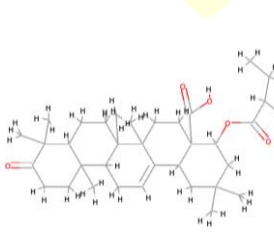
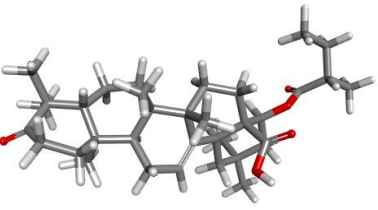
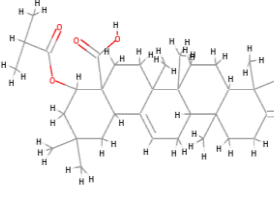
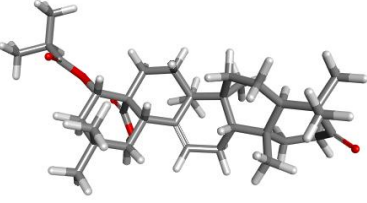
Gambar VII.18 Tampilan aplikasi *Notepad*[®]

LAMPIRAN 7

STRUKTUR SENYAWA AKTIF *Lantana Camara* DAN *Lantana involucrata*

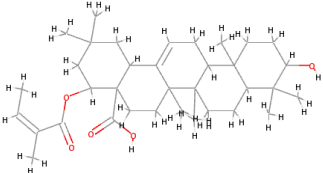
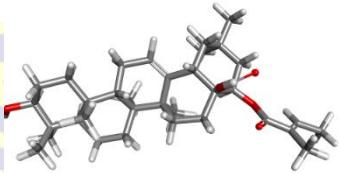
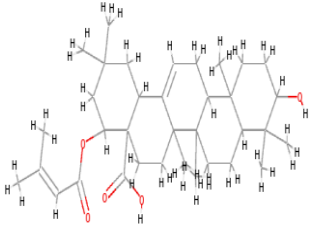
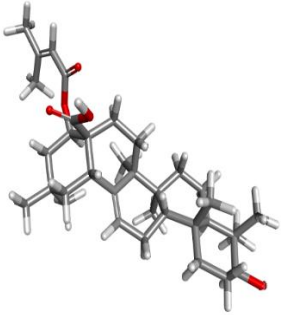
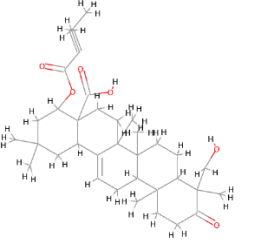
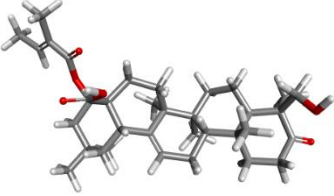
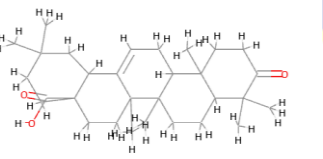
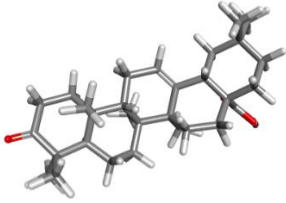
Tabel VII. 1

Struktur 2D dan 3D Senyawa Aktif *Lantana Camara* dan *Lantana involucrata*

No	Senyawa	2D	3D
1	Lantadene A		
2	Lantadene B		
3	Lantadene C		
4	Lantadene D		

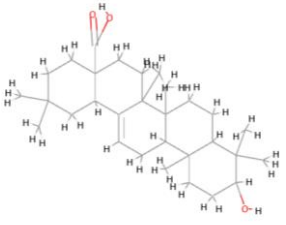
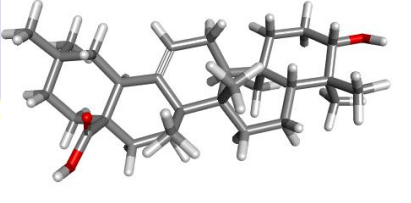
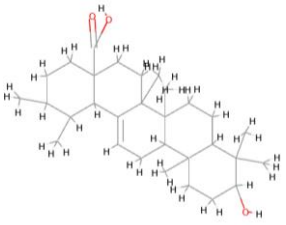
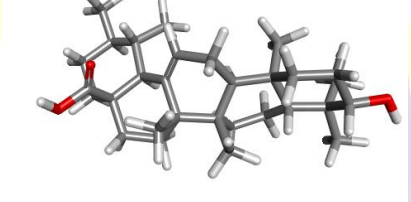
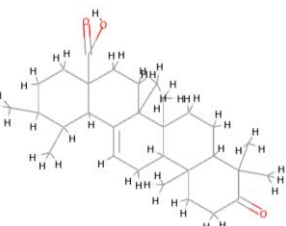
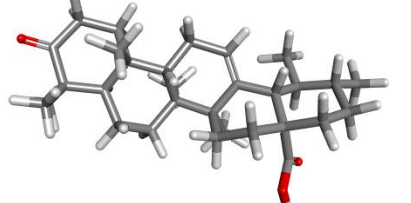
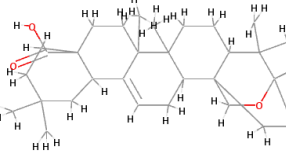
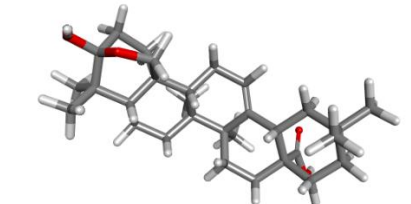
LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

No	Senyawa	2D	3D
5	Reduced lantadene A		
6	Reduced lantadene B		
7	Icterogenin		
8	Oleanonic acid (3-oxoolean-12-en-28-oic acid)		

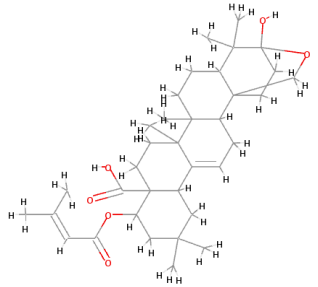
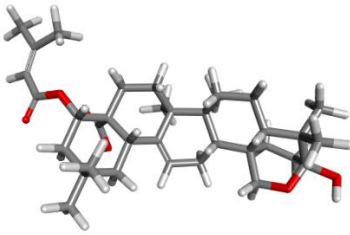
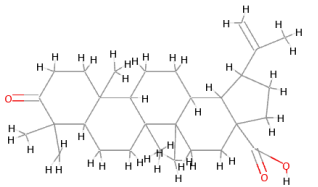
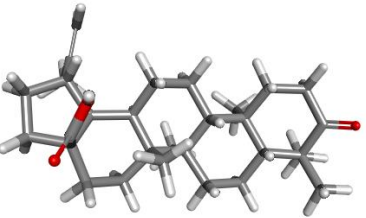
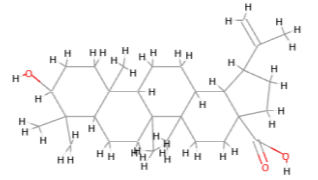
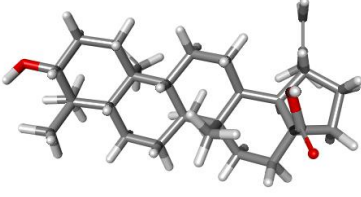
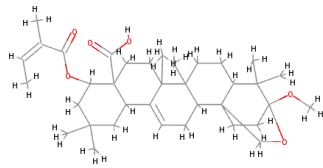
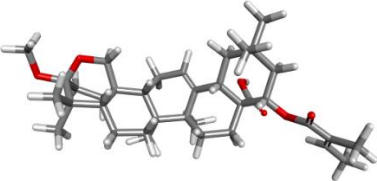
LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

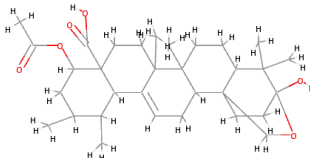
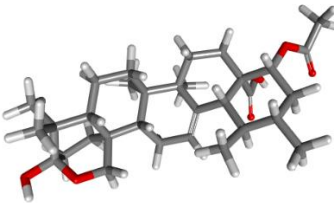
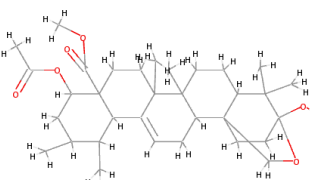
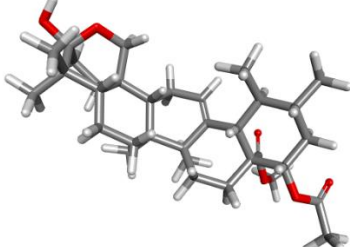
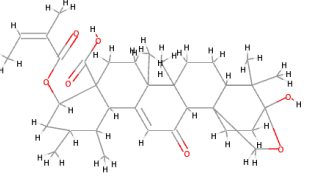
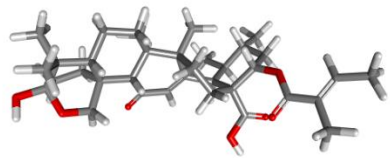
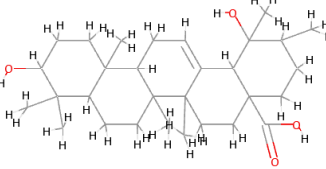
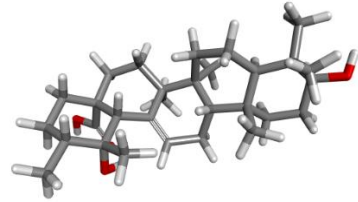
No	Senyawa	2D	3D
9	Oleanolic acid (3β -hydroxyolean-12-en-28-oic acid)		
10	Ursolic acid (3β -hydroxyurs-12-en-28-oic acid)		
11	Ursonic acid (3-oxours-12-en-28-oic acid)		
12	Lantanolic acid		

LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

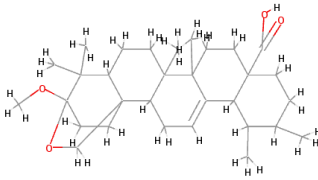
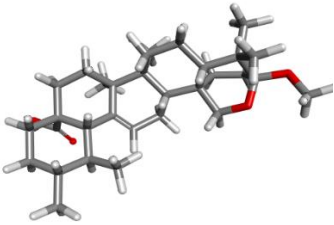
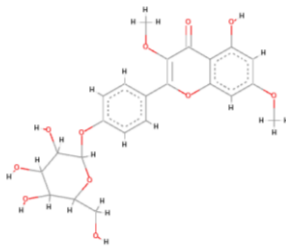
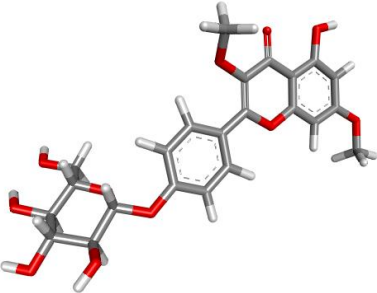
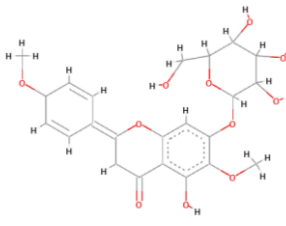
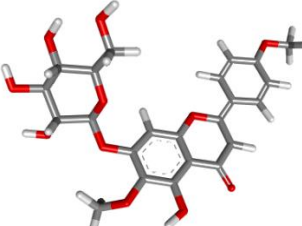
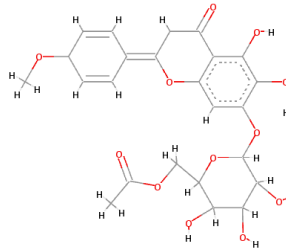
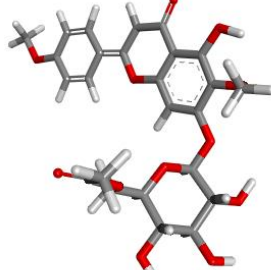
No	Senyawa	2D	3D
13	Lantanilic acid		
14	Betulonic acid (3-oxolup-20(29)-en-28-oic acid)		
15	Betulinic acid (3β-hydroxylup-20(29)-en-28-oic acid)		
16	Camarilic acid		

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.1
Lanjutan**

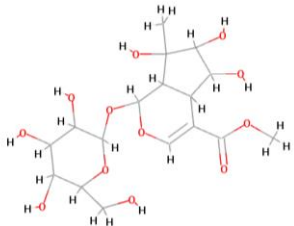
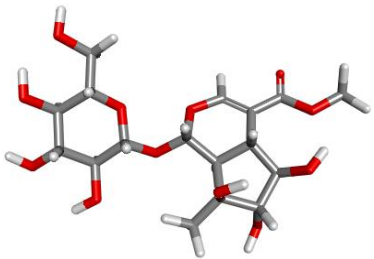
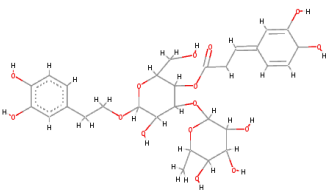
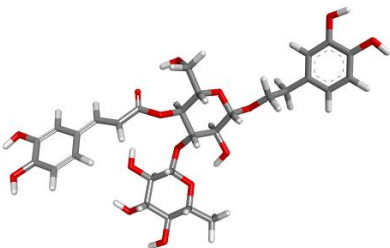
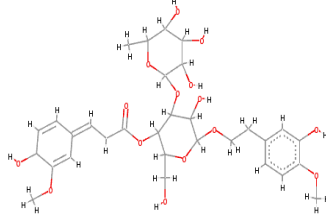
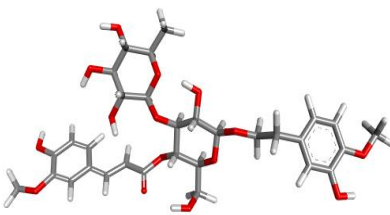
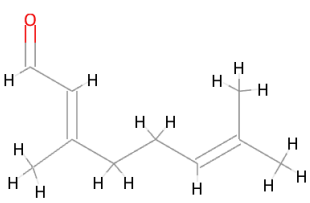
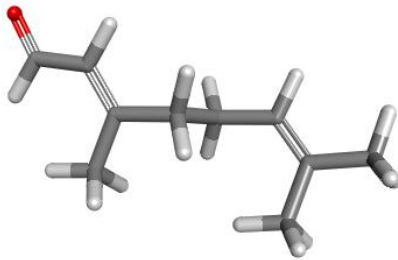
No	Senyawa	2D	3D
17	Camarinic acid	 The 2D chemical structure of Camarinic acid shows a long, branched carbon chain with several methyl groups and two hydroxyl groups. The chain is drawn in a zig-zag pattern, with the hydroxyl groups attached to the second and third carbons from the left end.	 The 3D ball-and-stick model of Camarinic acid shows the spatial arrangement of the atoms. Carbon atoms are represented by grey spheres, hydrogen atoms by white spheres, and oxygen atoms by red spheres. The structure is shown in a perspective view, highlighting the three-dimensional nature of the molecule.
18	Methyl camaralate	 The 2D chemical structure of Methyl camaralate is similar to Camarinic acid, but with a methyl ester group instead of a hydroxyl group at the end of the chain. The structure is drawn in a zig-zag pattern, with the methyl ester group attached to the second carbon from the left end.	 The 3D ball-and-stick model of Methyl camaralate shows the spatial arrangement of the atoms. Carbon atoms are represented by grey spheres, hydrogen atoms by white spheres, and oxygen atoms by red spheres. The structure is shown in a perspective view, highlighting the three-dimensional nature of the molecule.
19	Camangeloyl acid	 The 2D chemical structure of Camangeloyl acid shows a long, branched carbon chain with several methyl groups and two hydroxyl groups. The chain is drawn in a zig-zag pattern, with the hydroxyl groups attached to the second and third carbons from the left end.	 The 3D ball-and-stick model of Camangeloyl acid shows the spatial arrangement of the atoms. Carbon atoms are represented by grey spheres, hydrogen atoms by white spheres, and oxygen atoms by red spheres. The structure is shown in a perspective view, highlighting the three-dimensional nature of the molecule.
20	Pomolic acid	 The 2D chemical structure of Pomolic acid shows a long, branched carbon chain with several methyl groups and two hydroxyl groups. The chain is drawn in a zig-zag pattern, with the hydroxyl groups attached to the second and third carbons from the left end.	 The 3D ball-and-stick model of Pomolic acid shows the spatial arrangement of the atoms. Carbon atoms are represented by grey spheres, hydrogen atoms by white spheres, and oxygen atoms by red spheres. The structure is shown in a perspective view, highlighting the three-dimensional nature of the molecule.

LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

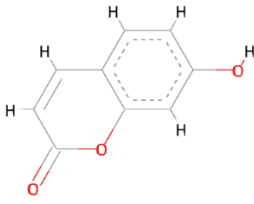
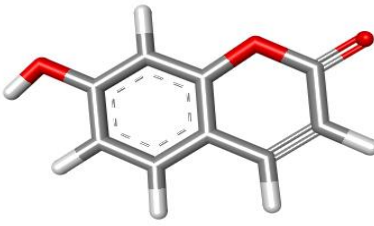
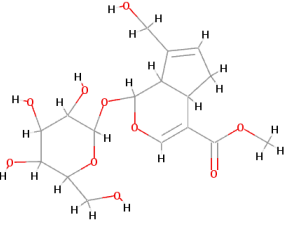
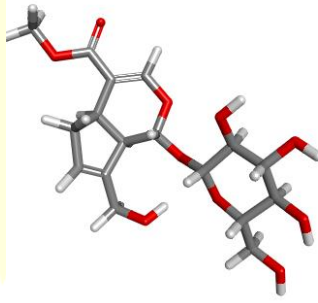
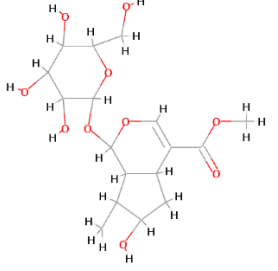
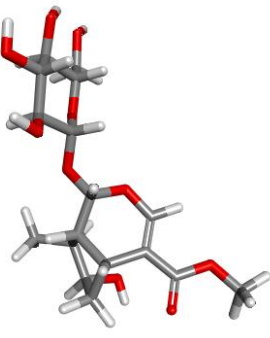
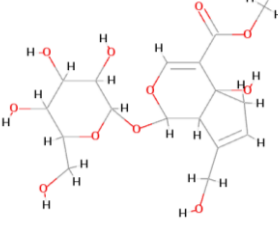
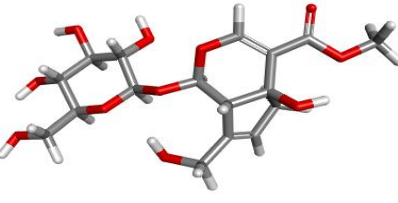
No	Senyawa	2D	3D
21	Ursoxy acid	 <p>The 2D structure shows a pentacyclic triterpene skeleton with four hydroxyl groups and a methyl group at the C-13 position.</p>	 <p>The 3D model illustrates the spatial arrangement of atoms in Ursolic acid, showing its complex, rigid tricyclic core.</p>
22	Camaroside	 <p>The 2D structure depicts Camaroside as a flavonoid glycoside, consisting of a flavone aglycone linked to a glucose moiety via an ether bridge.</p>	 <p>The 3D model shows the conformation of Camaroside, highlighting the orientation of the glucose ring relative to the flavone core.</p>
23	Linaroside	 <p>The 2D structure shows Linaroside as a flavonoid glycoside, similar to Camaroside, with a flavone aglycone and a glucose moiety.</p>	 <p>The 3D model illustrates the spatial structure of Linaroside, showing the glycosidic linkage between the aglycone and the sugar.</p>
24	Lantoside	 <p>The 2D structure shows Lantoside as a flavonoid glycoside, featuring a flavone aglycone and a glucose moiety.</p>	 <p>The 3D model displays the three-dimensional structure of Lantoside, including the glycosidic bond.</p>

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.1
Lanjutan**

No	Senyawa	2D	3D
25	Lamiridoside		
26	Verbascoside		
27	Martynoside		
28	Citral		

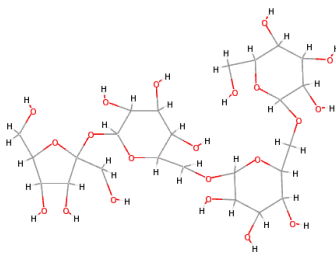
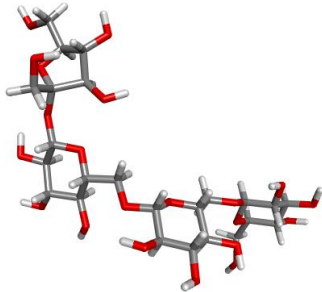
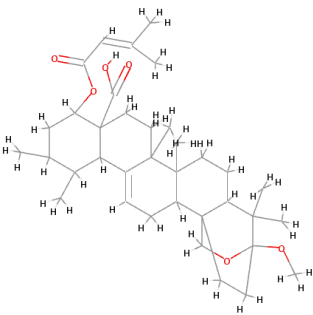
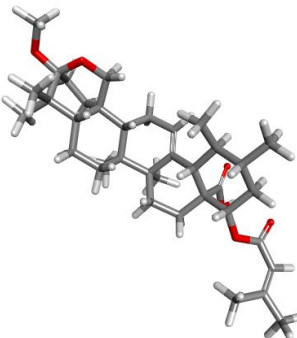
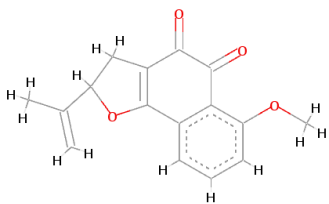
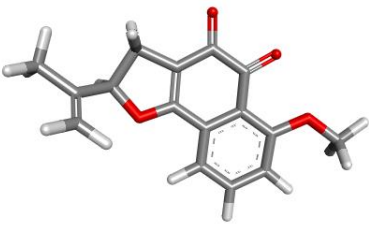
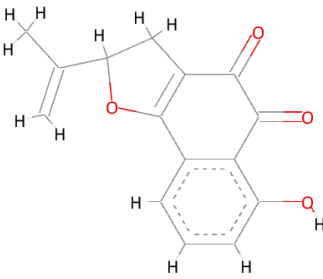
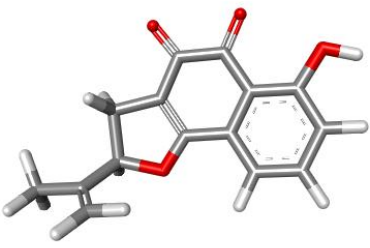
LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

No	Senyawa	2D	3D
29	Umbelliferone		
30	Geniposide		
31	8-Epigallicin		
32	Theviridoside		

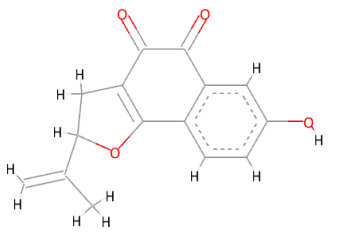
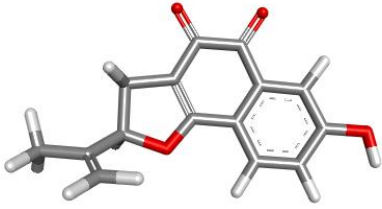
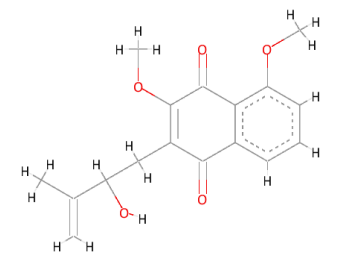
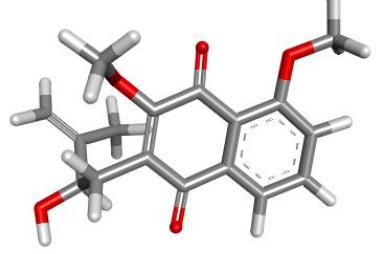
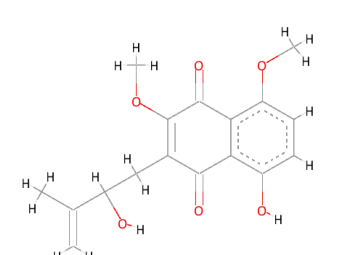

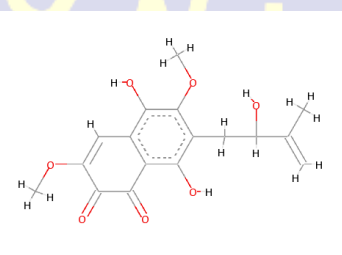
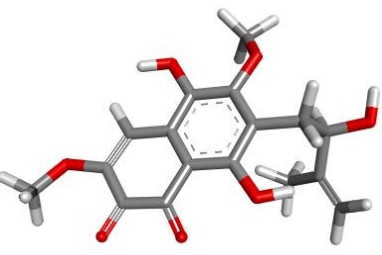
LAMPIRAN 7 (LANJUTAN)

Tabel VII.1
Lanjutan

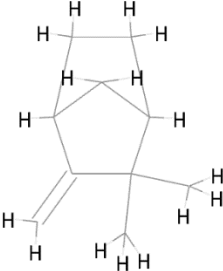
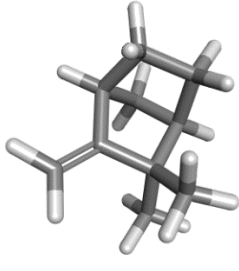
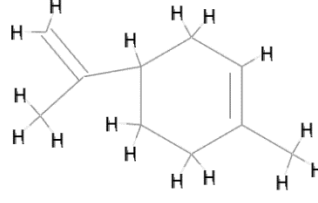
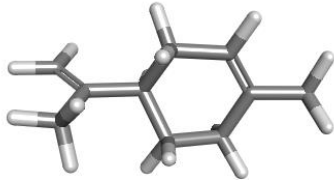
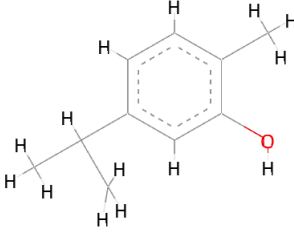
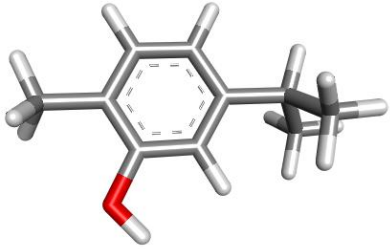
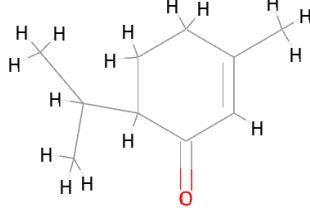
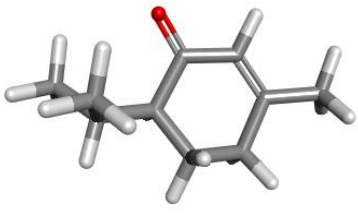
No	Senyawa	2D	3D
33	Stachyose		
34	Camaryolic acid		
35	lantalucre tins A		
36	lantalucre tins B		

LAMPIRAN 7 (LANJUTAN)

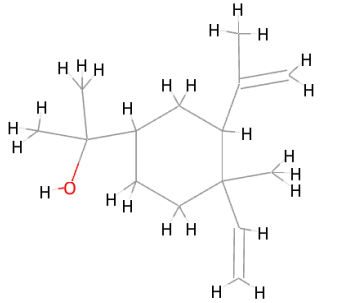
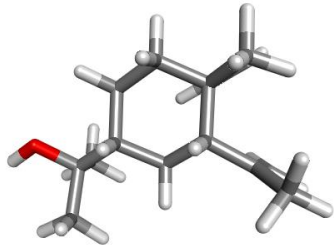
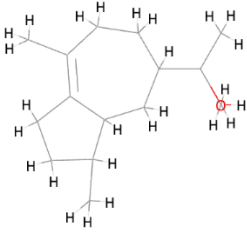
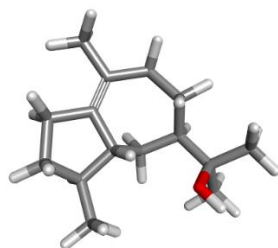
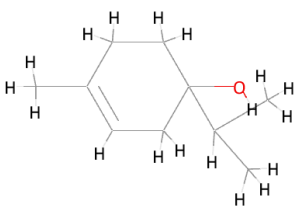
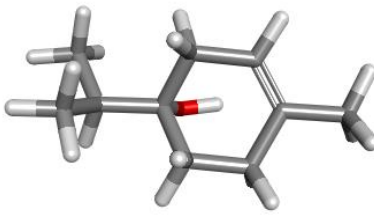
Tabel VII.1
Lanjutan

No	Senyawa	2D	3D
37	lantalu- cra- tins C	 <p>The 2D structure shows a central benzene ring with two carbonyl groups (C=O) at the 1 and 4 positions. A furan ring is fused to the benzene ring at the 2 and 3 positions. A propenyl group is attached to the furan ring at the 5-position. A hydroxyl group (-OH) is attached to the benzene ring at the 6-position.</p>	 <p>The 3D model shows the spatial arrangement of the atoms in lantalucratins C, with carbon atoms in grey, oxygen in red, and hydrogen in white.</p>
38	lantalu- cra- tins D	 <p>The 2D structure is similar to lantalucratins C, but the propenyl group is attached to the benzene ring at the 6-position instead of the furan ring.</p>	 <p>The 3D model shows the spatial arrangement of the atoms in lantalucratins D.</p>
39	lantalu- cra- tins E	 <p>The 2D structure is similar to lantalucratins D, but it has an additional hydroxyl group (-OH) attached to the benzene ring at the 3-position.</p>	 <p>The 3D model shows the spatial arrangement of the atoms in lantalucratins E.</p>
40	lantalu- cra- tins F	 <p>The 2D structure is similar to lantalucratins E, but the propenyl group is attached to the benzene ring at the 5-position.</p>	 <p>The 3D model shows the spatial arrangement of the atoms in lantalucratins F.</p>

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.1
Lanjutan**

No	Senyawa	2D	3D
41	Camphene		
42	Limonene		
43	Carvacrol		
44	Piperiton		

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.1
Lanjutan**

No	Senyawa	2D	3D
45	Elemol		
46	bulnesol		
47	terpinen-4-ol		

LAMPIRAN 8

HASIL PENELITIAN PREDIKSI *DRUGLIKENESS*

Tabel VII. 2

Hasil Prediksi *Druglikeness* Menggunakan Situs *Online Lipinski's Rule of Five*

No.	Ligan	BM (g/mol)	Log P	Donor Ikatan H	Akseptor Ikatan H	Ket.
1	Lantadene A	552	7,93	1	5	tidak memenuhi
2	Lantadene B	552	7,93	1	5	tidak memenuhi
3	Lantadene C	554	8,01	1	5	tidak memenuhi
4	Lantadene D	540	7,62	1	5	tidak memenuhi
5	Reduced lantadene A	554	7,72	2	5	tidak memenuhi
6	Reduced lantadene B	554	7,72	2	5	tidak memenuhi
7	Icterogenin	568	6,9	2	5	tidak memenuhi
8	Oleanonic acid (3-oxoolean- 12-en-28-oic acid)	454	7,44	1	3	tidak memenuhi
9	Oleanolic acid (3 β - hydroxyolean- 12-en-28-oic acid)	456	7,23	2	3	tidak memenuhi
10	Ursolic acid (3 β -hydroxyurs- 12-en-28-oic acid)	312	-0,05	5	6	memenuhi

LAMPIRAN 8 (LANJUTAN)

Tabel VII.2
Lanjutan

No.	Ligan	BM (g/mol)	Log P	Donor Ikatan H	Akseptor Ikatan H	Ket.
11	Uronic acid (3-oxours-12- en-28-oic acid)	454	7,29	1	3	tidak memenuhi
12	Lantanolic acid	470	6,57	2	4	tidak memenuhi
13	Lantanilic acid	568	7,06	2	6	tidak memenuhi
14	Betulonic acid (3-oxolup- 20(29)-en-28- oic acid)	454	7,3	1	3	tidak memenuhi
15	Betulic acid (3 β - hydroxylup- 20(29)-en-28- oic acid)	456	7,1	2	3	tidak memenuhi
16	Camarilic acid	582	7,71	1	6	tidak memenuhi
17	Camarinic acid	528	5,97	2	6	tidak memenuhi
18	Methyl camaralate	542	6,06	1	6	tidak memenuhi
19	Camangeloyl acid	582	6,09	2	7	tidak memenuhi
20	Pomolic acid	472	6,2	3	4	tidak memenuhi

LAMPIRAN 8 (LANJUTAN)

Tabel VII.2
Lanjutan

No.	Ligan	BM (g/mol)	Log P	Donor Ikatan H	Akseptor Ikatan H	Ket.
21	Ursoxy acid	484	7,08	1	4	tidak memenuhi
22	Camaroside	476	0,17	5	11	tidak memenuhi
23	Linaroside	476	0,2	5	11	tidak memenuhi
24	Lantanoside	518	0,77	4	12	tidak memenuhi
25	Lamiridoside	422	-4,06	7	12	tidak memenuhi
26	Verbascoside	624	-1,02	9	15	tidak memenuhi
27	Martynoside	652	-0,41	7	15	tidak memenuhi
28	Citral	152	2,88	0	1	memenuhi
29	Umbelliferone	162	1,32	1	3	memenuhi
30	Geniposide	388	-2,23	5	10	memenuhi
31	8-Epiloganin	390	-2,15	5	10	memenuhi
32	Theviridoside	404	-3,11	6	11	tidak memenuhi
33	Stachyose	666	-9,75	14	21	tidak memenuhi
34	Camaryolic acid	582	7,57	1	6	tidak memenuhi
35	lantalucratins A	270	2,54	0	4	memenuhi
36	lantalucratins B	256	2,24	1	4	memenuhi
37	lantalucratins C	256	2,24	1	4	memenuhi

LAMPIRAN 8 (LANJUTAN)

Tabel VII.2
Lanjutan

No.	Ligan	BM (g/mol)	Log P	Donor Ikatan H	Akseptor Ikatan H	Ket.
38	lantalucreatins D	302	2,3	1	5	memenuhi
39	lantalucreatins E	318	2,01	2	6	memenuhi
40	lantalucreatins F	334	1,34	3	7	memenuhi
41	Camphene	136	2,99	0	0	memenuhi
42	Limonene	136	3,31	0	0	memenuhi
43	Carvacrol	150	2,82	1	1	memenuhi
44	Piperiton	152	2,57	0	1	memenuhi
45	Elemol	222	3,94	1	1	memenuhi
46	Bulnesol	222	3,92	1	1	memenuhi
47	terpinen-4-ol	154	2,5	1	1	memenuhi

LAMPIRAN 9

HASIL PENELITIAN PREDIKSI FARMAKOKINETIKA

Tabel VII. 3

Hasil Prediksi Farmakokinetika Menggunakan Situs *Online Pre-ADMET*

No.	Ligan	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
1	Lantadene A	89,966*	21,815**	100*
2	Lantadene B	89,966*	21,801**	100*
3	Lantadene C	89,966*	21,815**	100*
4	Lantadene D	89,498*	21,668**	100*
5	Reduced lantadene A	89,966*	21,815**	100*
6	Reduced lantadene B	89,966*	21,801**	100*
7	Icterogenin	84,606*	21,134**	100*
8	Oleanonic acid (3-oxoolean-12-en-28-oic acid)	91,816*	21,623**	100*
9	Oleanolic acid (3 β -hydroxyolean-12-en-28-oic acid)	91,816*	21,623**	100*
10	Ursolic acid (3 β -hydroxyurs-12-en-28-oic acid)	91,815*	21,603**	100*
11	Ursolic acid (3-oxours-12-en-28-oic acid)	91,815*	21,603**	100*
12	Lantanolic acid	91,586*	22,004**	100*
13	Lantanilic acid	89,385*	21,899**	99,627*

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.3
Lanjutan

No.	Ligan	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
14	Betulonic acid (3-oxolup-20(29)-en-28-oic acid)	91,815*	21,829**	100*
15	Betulinic acid (3 β -hydroxylup-20(29)-en-28-oic acid)	91,815*	21,603**	100*
16	Camarilic acid	92,893*	25,205**	97,732*
17	Camarinic acid	87,723*	21,342**	94,432*
18	Methyl camaralate	92*	24**	92*
19	Camangeloyl acid	83,253*	21,098**	93,382*
20	Pomolic acid	88,044*	21,252**	100*
21	Ursoxy acid	94,303*	26,366**	100*
22	camaroside	21,203**	3,012***	33,041**
23	Linaroside	21,203**	10,111**	33,307**
24	Lantanoside	20,114**	10,551**	33,207**
25	Lamiridoside	3,414***	12,367**	11,073**
26	Verbascoside	1,992***	11,541**	30,183**
27	Martynoside	6,675***	9,337**	33,922**
28	Citral	100*	9,066**	100*

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.3
Lanjutan

No.	Ligan	Absorbsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
29	Umbelliferone	85,432*	19,587**	26,251**
30	Geniposide	14,434***	17,035**	29,524**
31	8-Epiloganin	14,433***	16,739**	28,693**
32	Theviridoside	7,005***	14,623**	18,337**
33	Stachyose	0***	1,969***	3,558**
34	Camaryolic acid	92,894*	25,157**	94,224*
35	lantaluclratins A	90,116*	15,137**	85,275**
36	lantaluclratins B	82,165*	5,75**	93,944*
37	lantaluclratins C	82,165*	14,036**	85,387**
38	lantaluclratins D	82,623*	22,234**	63,847**
39	lantaluclratins E	66,867**	19,872**	43,622**
40	lantaluclratins F	43,752**	17,599**	36,863**
41	camphene	100*	22,303**	100*
42	Limonene	100*	22,302**	100*
43	carvacrol	100*	39,49	63,442

LAMPIRAN 9 (LANJUTAN)

Tabel VII.3
Lanjutan

No.	Ligan	Absorpsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
44	Piperiton	100*	39,49**	100*
45	Elemol	100*	55,35**	100*
46	Bulnesol	100*	55,465**	100*
47	terpinen-4-ol	100*	50,971**	100*

HIA (%) :

* : 70-100 terserap baik

** : 20-70 terserap cukup

*** : <20 kurang terserap

CaCo-2 (nm sec) :

* : >70 permeabilitas tinggi

** : 4-70 permeabilitas sedang

*** : <4 permeabilitas rendah

PPB (%) :

* : >90 terikat kuat

** : <90 terikat lemah

LAMPIRAN 10

HASIL PENELITIAN PREDIKSI TOKSISITAS

Tabel VII. 4

Hasil Prediksi Toksisitas Menggunakan Aplikasi *Toxtree*[®]

No.	Ligan	Mutagen (<i>Amest Test</i>)	Karsinogenik		<i>Kroes TTC</i>
			<i>Genotoxic</i>	<i>Non Genotoxic</i>	
1	Lantadene A	(-)	(-)	(-)	Tidak Beresiko
2	Lantadene B	(-)	(-)	(-)	Tidak Beresiko
3	Lantadene C	(-)	(-)	(+)	Tidak Beresiko
4	Lantadene D	(-)	(-)	(-)	Tidak Beresiko
5	Reduced lantadene A	(-)	(-)	(-)	Tidak Beresiko
6	Reduced lantadene B	(-)	(-)	(-)	Tidak Beresiko
7	Icterogenin	(-)	(-)	(-)	Tidak Beresiko
8	Oleanonic acid (3-oxoolean-12-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko
9	Oleanolic acid (3 β -hydroxyolean-12-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko
10	Ursolic acid (3 β -hydroxyurs-12-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko

LAMPIRAN 10
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Ligan	Mutagen (<i>Amest Test</i>)	Karsinogenik		<i>Kroes TTC</i>
			<i>Genotoxic</i>	<i>Non Genotoxic</i>	
11	Ursonic acid (3-oxours-12-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko
12	Lantanolic acid	(-)	(-)	(-)	Tidak Beresiko
13	Lantanilic acid	(-)	(-)	(-)	Tidak Beresiko
14	Betulonic acid (3-oxolup-20(29)-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko
15	Betulic acid (3 β -hydroxylup-20(29)-en-28-oic acid)	(-)	(-)	(-)	Tidak Beresiko
16	Camarilic acid	(-)	(-)	(-)	Tidak Beresiko
17	Camarinic acid	(-)	(-)	(-)	Tidak Beresiko
18	Methyl camaralate	(-)	(-)	(-)	Tidak Beresiko
19	Camangeloyl acid	(+)	(+)	(-)	Beresiko Rendah
20	Pomolic acid	(-)	(-)	(-)	Tidak Beresiko

**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
21	Ursoxy acid	(-)	(-)	(-)	Tidak Beresiko
22	camaroside	(-)	(-)	(-)	Tidak Beresiko
23	Linaroside	(-)	(-)	(-)	Tidak Beresiko
24	Lantoside	(-)	(-)	(-)	Tidak Beresiko
25	Lamiridoside	(-)	(-)	(-)	Tidak Beresiko
26	Verbascoside	(-)	(-)	(-)	Tidak Beresiko
27	Martynoside	(-)	(-)	(-)	Tidak Beresiko
28	Citral	(-)	(-)	(-)	Tidak Beresiko
29	Umbelliferone	(+)	(+)	(-)	Beresiko Rendah
30	Geniposide	(-)	(-)	(-)	Tidak Beresiko
31	8-Epiloganin	(-)	(-)	(-)	Tidak Beresiko
32	Theviridoside	(-)	(-)	(-)	Tidak Beresiko
33	Stachyose	(-)	(-)	(-)	Tidak Beresiko
34	Camaryolic acid	(-)	(-)	(-)	Tidak Beresiko
35	lantalucratins A	(+)	(+)	(-)	Beresiko Rendah
36	lantalucratins B	(+)	(+)	(-)	Beresiko Rendah

**LAMPIRAN 10
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
37	lantalucrains C	(+)	(+)	(-)	Beresiko Rendah
38	lantalucrains D	(+)	(+)	(-)	Beresiko Rendah
39	lantalucrains E	(+)	(+)	(-)	Beresiko Rendah
40	lantalucrains F	(+)	(+)	(-)	Beresiko Rendah
41	camphene	(-)	(-)	(-)	Tidak Beresiko
42	Limonene	(-)	(-)	(-)	Tidak Beresiko
43	carvacrol	(-)	(-)	(-)	Tidak Beresiko
44	Piperiton	(+)	(+)	(-)	Beresiko Rendah
45	Elemol	(-)	(-)	(-)	Tidak Beresiko
46	bulnesol	(-)	(-)	(-)	Tidak Beresiko
47	terpinen-4-ol	(-)	(-)	(-)	Tidak Beresiko

LAMPIRAN 10

Tabel VII.5

Hasil Prediksi Toksisitas Menggunakan Aplikasi *PKCSM*

No.	Ligan	LD ₅₀ (mol/kg)	Hepatotoksik
1	Lantadene A	2,406	Tidak Toksik
2	Lantadene B	2,406	Tidak Toksik
3	Lantadene C	2,398	Tidak Toksik
4	Lantadene D	2,38	Tidak Toksik
5	Reduced lantadene A	2,419	Tidak Toksik
6	Reduced lantadene B	2,419	Tidak Toksik
7	Icteroenin	2,59	Tidak Toksik
8	Oleanonic acid (3-oxoolean-12-en-28-oic acid)	2,259	Tidak Toksik
9	Oleanolic acid (3 β -hydroxyolean-12-en-28-oic acid)	2,349	Toksik
10	Ursolic acid (3 β -hydroxyurs-12-en-28-oic acid)	2,346	Toksik
11	Ursonic acid (3-oxours-12-en-28-oic acid)	2,256	Tidak Toksik
12	Lantanolic acid	2,443	Toksik
13	Lantanilic acid	2,534	Tidak Toksik
14	Betulonic acid (3-oxolup-20(29)-en-28-oic acid)	2,215	Tidak Toksik

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.5
Lanjutan

No.	Ligan	LD₅₀ (mol/kg)	Hepatotoksik
15	Betulinic acid (3 β -hydroxylup-20(29)-en-28-oic acid)	2,256	Toksik
16	Camarilic acid	2,52	Tidak Toksik
17	Camarinic acid	2,578	Tidak Toksik
18	Methyl camaralate	2,488	Tidak Toksik
19	Camangeloyl acid	2,614	Tidak Toksik
20	Pomolic acid	2,317	Toksik
21	Ursoxy acid	2,341	Tidak Toksik
22	camaroside	2,755	Tidak Toksik
23	Linaroside	2,635	Tidak Toksik
24	Lantoside	2,591	Tidak Toksik
25	Lamiridoside	2,24	Tidak Toksik
26	Verbascoside	2,527	Tidak Toksik
27	Martynoside	2,607	Tidak Toksik

**LAMPIRAN 10
(LANJUTAN)**

Tabel VII.5
Lanjutan

No.	Ligan	LD₅₀ (mol/kg)	Hepatotoksik
28	Citral	1,815	Tidak Toksik
29	Umbelliferone	2,047	Toksik
30	Geniposide	2,188	Tidak Toksik
31	8-epiloganin	2,214	Tidak Toksik
32	Theviridoside	2,449	Tidak Toksik
33	Stachyose	2,51	Tidak Toksik
34	Camaryolic acid	2,565	Tidak Toksik
35	Lantalucratins A	1,954	Toksik
36	Lantalucratins B	1,844	Toksik
37	Lantalucratins C	1,844	Toksik
38	Lantalucratins D	1,947	Tidak Toksik
39	Lantalucratins E	1,922	Tidak Toksik
40	Lantalucratins F	1,605	Tidak Toksik

**LAMPIRAN 10
(LANJUTAN)****Tabel VII.5**
Lanjutan

No.	Ligan	LD₅₀ (mol/kg)	Hepatotoksik
41	Camphene	1,554	Tidak Toksik
42	Limonene	1,88	Tidak Toksik
43	Carvacrol	2,074	Toksik
44	Piperiton	1,777	Tidak Toksik
45	Elemol	1,686	Tidak Toksik
46	Bulnesol	1,702	Tidak Toksik
47	Terpinen-4-ol	1,811	Tidak Toksik

LAMPIRAN 11

HASIL PENELITIAN SIMULASI MOLECULAR DOCKING

Tabel VII. 6

Hasil Penambatan Senyawa Aktif *Lantana camara* Dan *Lantana involucrata*

Pada Reseptor MAP3K7/TAK1 ID PDB 5V5N

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
1.	N~1~-(1-propyl-1,3-dihydro-2H benzimidazol-2-ylidene)benzene-1,3-dicarboxamide	-7,97	1,44 uM (micromolar)	VAL A:50, VAL A:42, VAL A:90, ALA A:61, MET A:104, CYS A:174, LYS A:63, ASP A:175, LEU A:163, ALA A:107, GLY A:110
2.	Takinib (ligan pembanding)	-7,42	3.62 uM (micromolar)	SER A:111, ASN A:114, VAL A:42, LEU A:163, ALA A:107
3.	Lantadene A	-7,15	5,78 uM (micromolar)	PRO A:160, VAL A:50, VAL A:42, TYR A:106, ALA A:61, ALA A:107, LEU A:163, ARG A:44
4.	Lantadene B	-7,16	5,62 uM (micromolar)	VAL A:50, VAL A:42, TYR A:106, ALA A:61, ALA A:107, LEU A:163, ARG A:44
5.	Lantadene C	-7,16	5,66 uM (micromolar)	VAL A:50, VAL A:42, TYR A:106, ALA A:61, ALA A:107, LEU A:163, CYS A:174, MET A:104, VAL A:90, ASN A:114

LAMPIRAN 11
(LANJUTAN)

Tabel VII.6
Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
6	Lantadene D	-6,84	9,69 uM (micromolar)	LEU A:163, CYS A:174, LYS A:63, ASP A:175, VAL A:50, SER A:111, VAL A:42, ASN A:114
7	Reduced lantadene A	-6,98	7,71 uM (micromolar)	VAL A:50, CYS A:174, MET A:104, VAL A:90, ALA A:61, ALA A:107, LEU A:163, VAL A:42, ARG A:44
8	Reduced lantadene B	-7,11	6,17 uM (micromolar)	PRO A:160, VAL A:50, VAL A:42, ALA A:107, LEU A:163, TYR A:106, ALA A:61, GLY A:43
9	Icterogenin	-6,55	15,69 uM (micromolar)	ARG A:44, ALA A:61, MET A:104, ALA A:107, VAL A:50, LEU A:163
10	Oleanonic acid (3-oxoolean-12-en-28-oic acid)	-8,76	381,63 nM (nanomolar)	PRO A:160, LEU A:163, VAL A:50, CYS A:174, ALA A:61, MET A:104, ALA A:107, VAL A:42
11	Oleanolic acid (3 β -hydroxyolean-12-en-28-oic acid)	-9,27	159,91 nM (nanomolar)	VAL A:42, ALA A:107, CYS A:174, MET A:104, VAL A:90, ALA A:61, LEU A:163, VAL A:50

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
12	Ursolic acid (3 β -hydroxyurs-12-en-28-oic acid)	-8,52	571,17 nM (nanomolar)	SER A:111, VAL A:50, VAL A:42, ALA A:61, TYR A:106, ALA A:107, CYS A:174, LEU A:163, PRO A:160
13	Ursonic acid (3-oxours-12-en-28-oic acid)	-9,28	156,92 nM (nanomolar)	VAL A:42, ALA A:107, ALA A:61, MET A:104, LEU A:163, VAL A:50
14	Lantanolic acid	-9,57	95,86 nM (nanomolar)	ALA A: 107, VAL A:42, PRO A:160, ARG A:44, LEU A:163, VAL A:50, ALA A:61, MET A:104, CYS A:174
15	Lantanilic acid	-6,49	17,60 μ M (micromolar)	ARG A:44, CYS A:174, LYS A:63, MET A:104, VAL A:50, ALA A:61, LEU A:163, ALA A:107, SER A:111
16	Betulonic acid (3-oxolup-20(29)-en-28-oic acid)	-8,77	373,06 nM (nanomolar)	LEU A:163, MET A:104, CYS A:174, VAL A:50, ALA A:61, VAL A:42, ALA A:107
17	Betulinic acid (3 β -hydroxylup-20(29)-en-28-oic acid)	-8,4	692,96 nM (nanomolar)	MET A:104, CYS A:174, ALA A:61, LEU A:163, VAL A:50, ALA A:107, VAL A:42

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
18	Camarilic acid	-6,79	10,54 uM (micromolar)	ALA A:61, MET A:104, VAL A:42, LYS A:63, TYR A:106, LEU A:163, ALA A:107, VAL A:50
19	Camarinic acid	-7,27	4,67 uM (micromolar)	ALA A:107, VAL A:42, LEU A:163, ALA A:61, VAL A:50, MET A:104, LYS A:63, CYS A:174
20	Methyl camaralate	-7,73	2,17 uM (micromolar)	LYS A:63, VAL A:50, MET A:104, ALA A:107, LEU A:163, TYR A:106, ALA A:61, VAL A:42
21	Camangeloyl acid	-8,6	498,32 nM (nanomolar)	ALA A:46, PRO A:160, ASN A:114, SER A:111, LEU A:163, CYS A:174, VAL A:42, VAL A:50, ALA A:61, TYR A:106, GLY A:110
22	Pomolic acid	-8,29	840,50 nM (nanomolar)	SER A:111, VAL A:50, VAL A:42, TYR A:106, ALA A:61, ALA A:107, CYS A:174, LEU A:163, PRO A:160
23	Ursoxy acid	-8,7	422,03 nM (nanomolar)	ALA A:107, VAL A:50, LEU A:163, MET A:104, ALA A:61, GLU A:105, VAL A:42, TYR A:106
24	camaroside	-7,71	2.22 uM (micromolar)	ASN A:114, VAL A:42, VAL A:50, GLY A:45, ASP A:175, LYS A:63, GLU A:77, GLU A:105

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
25	Linaroside	-8.45	642.52 nM (nanomolar)	VAL A: 42, ASN A:114, SER A:111, GLU A:105, CYS A:174, MET A:104, VAL A:50, PRO A:160
26	Lantoside	-8.21	959.61 nM (nanomolar)	GLU A:77, TYR A:106, GLY A:110, VAL A:42, ALA A:107, LEU A:163, VAL A:50, CYS A:174, MET A:104, LYS A:63
27	Lamiridoside	-5.44	102.27 uM (micromolar)	ARG A:44, VAL A:50, LYS A:63, MET A:104, ALA A:107, GLU A:105
28	Verbascoside	-4.53	475.60 uM (micromolar)	ARG A:44, GLY A:43, VAL A:42, VAL A:90, LEU A:163, ALA A:107, MET A:104, ALA A:61, GLU A:105
29	Martynoside	-4.94	237.49 uM (micromolar)	VAL A:42, ARG A:44, VAL A:50, PRO A:160
30	Citral	-4.91	253.67 uM (micromolar)	ALA A:107, ALA A:61, LEU A:163, TYR A:106, MET A:104, CIS A:174, VAL A:90, ASP A:175, LYS A:63
31	Umbelliferone	-5.81	55.57 uM (micromolar)	ALA A:107, DLU A:105, ASP A:175, LYS A:63, ALA A:61, VAL A:50, MET A:104, CIS A:174, LEU A:163

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
32	Geniposide	-5.49	94.66 uM (micromolar)	ALA A:107, GLU A:108, ALA A:46, ASP A:175, LYS A:63, GLY A:110, ARG A:44, TYR A:106, LEU A:163, VAL A:42
33	8-epiloganin	-6.20	28.60 uM (micromolar)	GLU A:108, VAL A:42, VAL A:50, TYR A:106, PRO A:160
34	Theviridoside	-5.92	45.66 uM (micromolar)	ALA A:107, ARG A:44, GLU A:105, VAL A:42, PRO A:160
35	Stachyose	-2,38	18,03 mM (millimolar)	ALA A:107, ARG A:44, ASN A:114, GLY A:110, PRO A:160, VAL A:42, SER A:111, UNK 1
36	Camaryolic acid	-7,51	3,10 uM (micromolar)	ALA A:61,LYS A:63, MET A:104, VAL A:42, VAL A:50, TYR A:106
37	Lantalucratins A	-7,07	6,62 uM (micromolar)	ALA A:61, CIS A:174, MET A:104, LEU A:163, VAL A:90, VAL A:42, GLU A:105, ALA A:107, VAL A:50, TYR A:106
38	Lantalucratins B	-6,94	8,16 uM (micromolar)	ALA A:107, ALA A:62, CIS A:174, MET A:104, LEU A:163, VAL A:42, VAL A:50, GLU A:105, TYR A:106

**LAMPIRAN 11
(LANJUTAN)**

Tabel VII.6
Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
39	Lantalucratins C	-7,19	5,41 μ M (micromolar)	ALA A:61, ALA A:107, CIS A:174, VAL A:42, VAL A:50, LEU A:163, ASP A:175, LYS A:63, MET A:104, GLU A:105
40	Lantalucratins D	-6,79	10,53 μ M (micromolar)	ALA A:61, ALA A:107, CIS A:174, VAL A:42, VAL A:50, LEU A:163, ASP A:175, VAL A:90, MET A:104
41	Lantalucratins E	-6,74	11,38 μ M (micromolar)	ALA A:61, ALA A:107, VAL A:42, VAL A:50, LEU A:163, ASP A:175, MET A:104, TYR A:106
42	Lantalucratins F	-6,33	22,75 μ M (micromolar)	ALA A:61, ALA A:107, ARG A:44, VAL A:42, VAL A:50, LEU A:163, GLU A:105, TYR A:106, SER A:111
43	Camphene	-5,03	204,66 μ M (micromolar)	ALA A:61, CIS A:174, LEU A:163, LYS A:63, VAL A:50, VAL A:90
44	Limonene	-4,58	436,03 μ M (micromolar)	ALA A:61, ALA A:107, CIS A:164, LEU A:163, LYS A:63, MET A:104, VAL A:50
45	Carvacrol	-5,1	182,87 μ M (micromolar)	ALA A:61, ALA A:107, CIS A:164, LEU A:163, LYS A:63, MET A:104, VAL A:50, VAL A:90, TYR A:106

**LAMPIRAN 11
(LANJUTAN)**

Tabel VII.6
Lanjutan

No.	Senyawa	ΔG (kcal/mol)	KI (nM)	Residu asam amino yang berikatan
46	Piperiton	-5,27	136,66 uM (micromolar)	ALA A:61, ALA A:107, LEU A:163, MET A:104, VAL A:50, VAL A:90
47	Elemol	-6,8	10,44 uM (micromolar)	ALA A:107, CIS A:174, LEU A:163, VAL A:42, VAL A:50
48	bulnesol	-6,98	7,70 uM (micromolar)	ALA A:61, ALA A:107, CIS A:174, LEU A:163, MET A: 104, VAL A:50, VAL A:90
49	terpinen- 4-ol	-5,24	145,14 uM (micromolar)	ALA A:61, ALA A: 107, LEU A:163, VAL A:42, VAL A:50, TYR A:106

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