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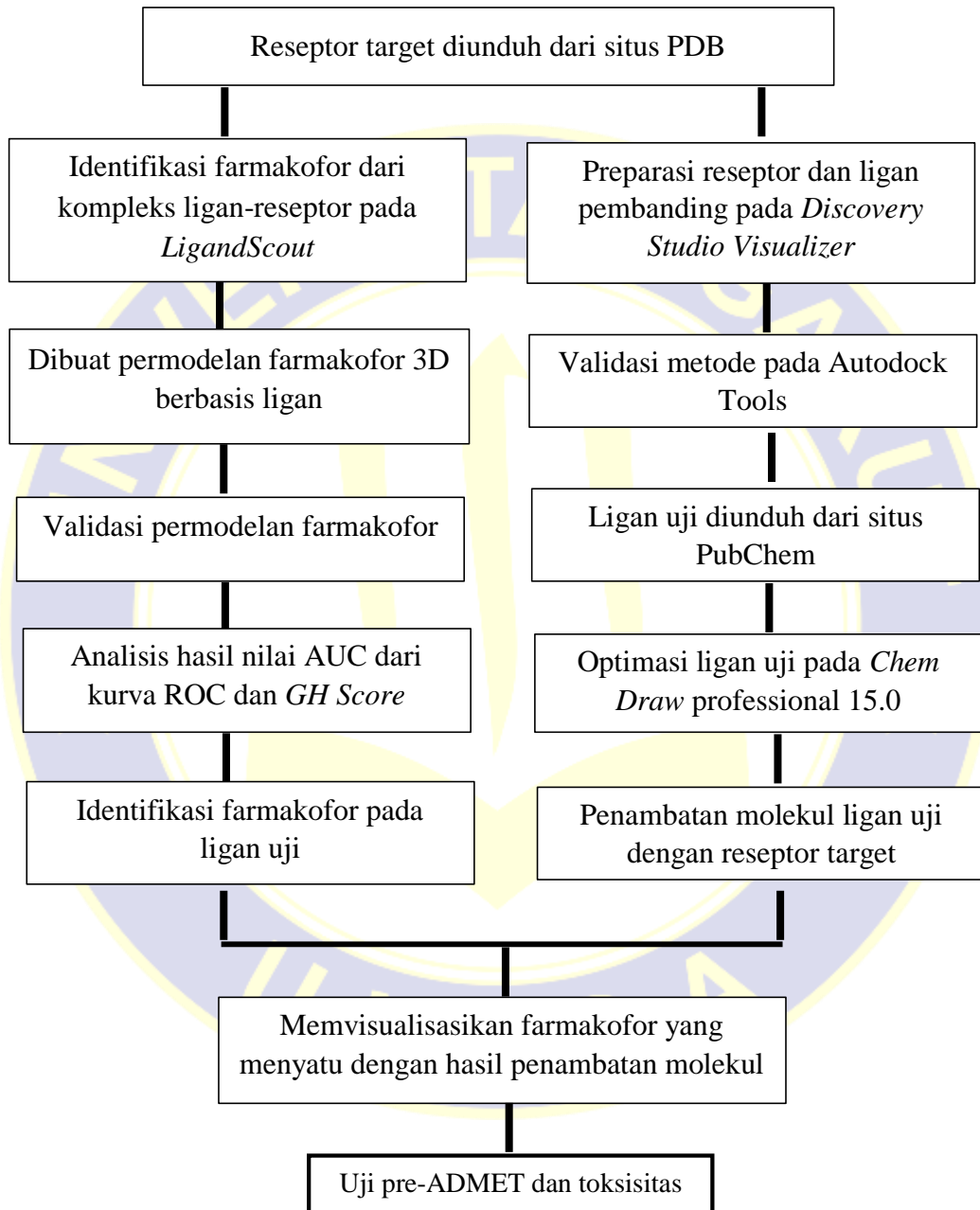
LAMPIRAN 1
TANAMAN MANGGIS



Gambar II.1 Tanaman manggis

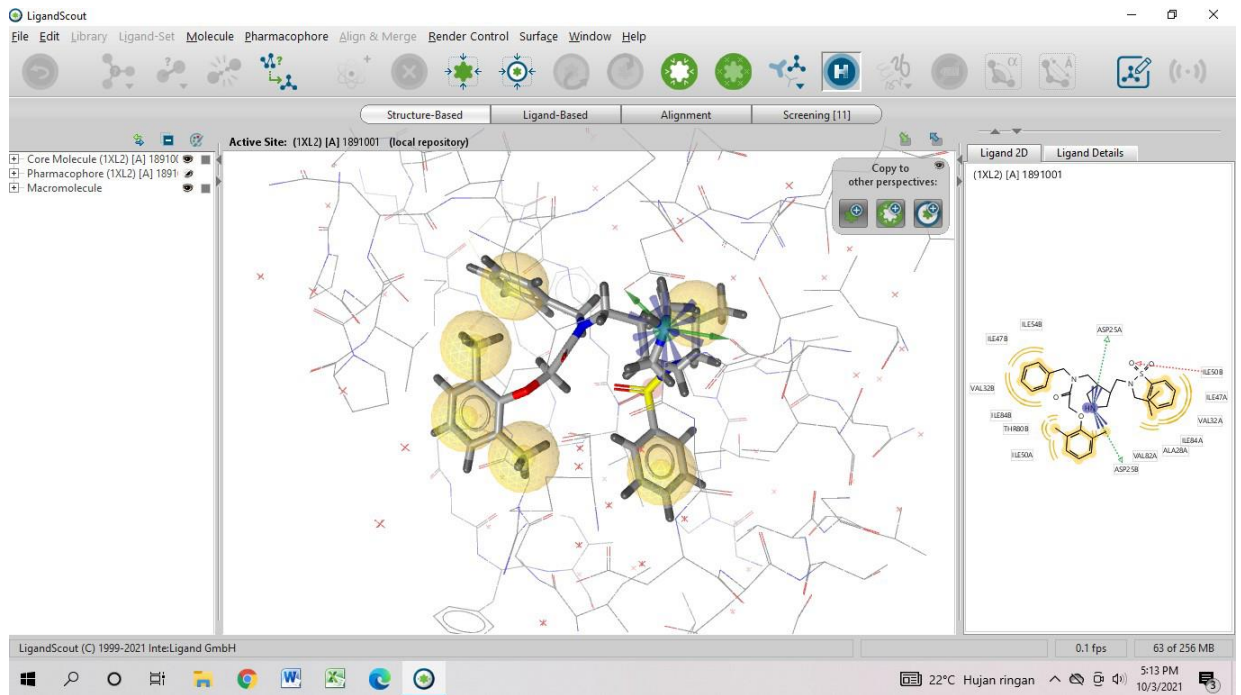
LAMPIRAN 2

ALUR PENELITIAN FARMAKOFOR MODELING DAN MOLECULAR DOCKING

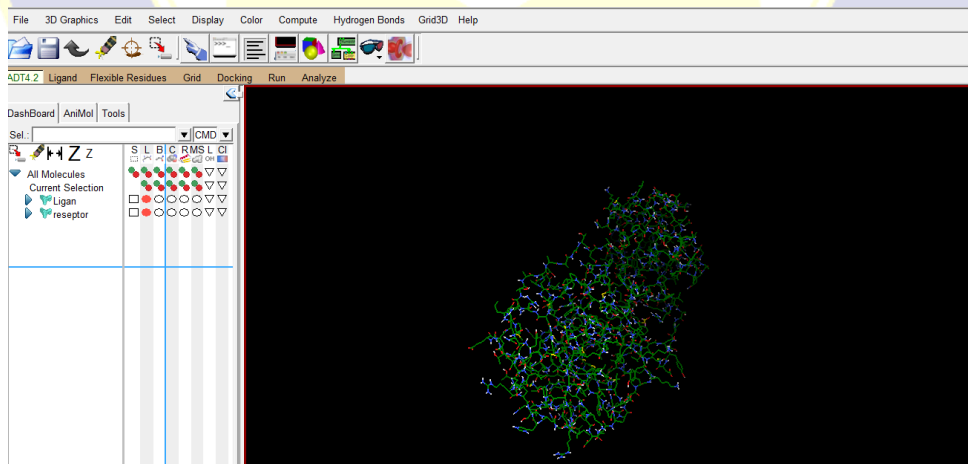


LAMPIRAN 3

APLIKASI DAN SITUS

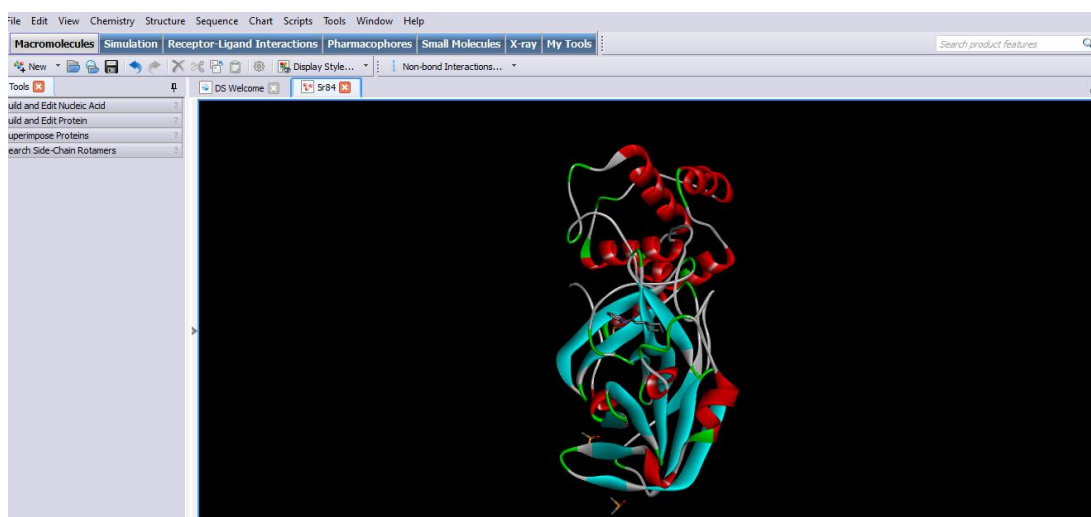


Gambar IV.1 Tampilan *LigandScout*[®]

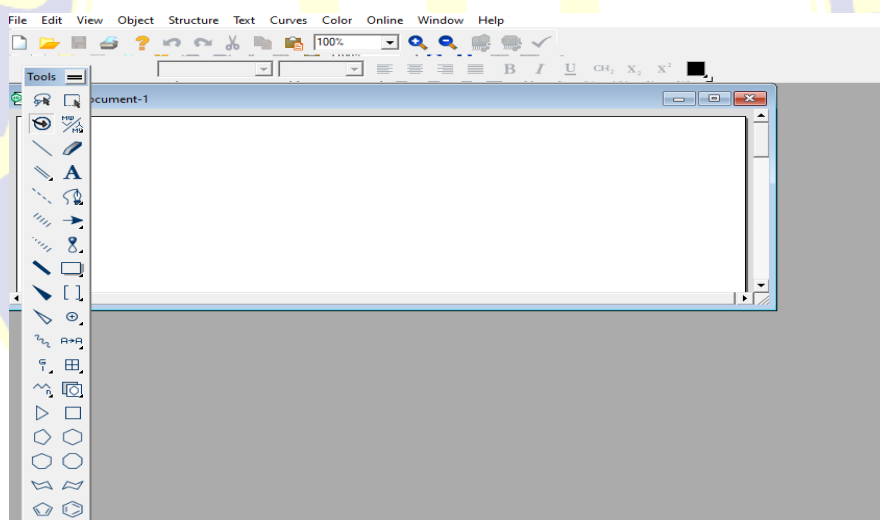


Gambar IV.2 Tampilan *Autodock Tools*[®]

LAMPIRAN 3 (LANJUTAN)



Gambar IV.3 Tampilan *Discovery Studio Visualizer*[®]



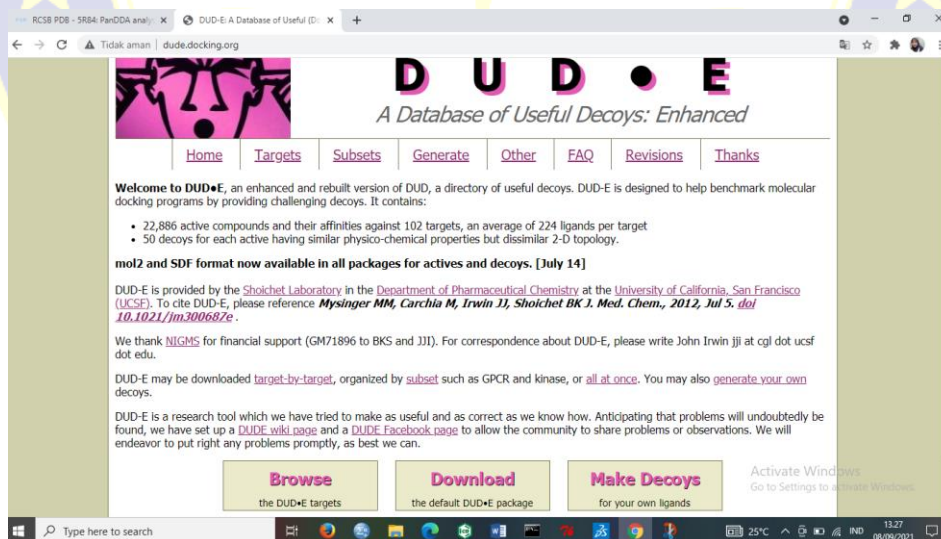
Gambar IV.4 Tampilan *ChemDraw 12.0*[®]

LAMPIRAN 2 (LANJUTAN)



The screenshot displays the RCSB PDB website interface. At the top, there is a navigation bar with options like 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', 'More', 'Documentation', and 'Careers'. Below this is the PDB logo and a search bar. The main content area shows the entry for 5R84, titled 'PanDDA analysis group deposition -- Crystal Structure of COVID-19 main protease in complex with Z31792168'. It includes a 3D ribbon diagram of the protein structure, classification as a 'HYDROLASE/HYDROLASE INHIBITOR', and deposition details from 2020-03-03. The interface also features tabs for 'Structure Summary', '3D View', 'Annotations', 'Experiment', 'Sequence', 'Genome', 'Ligands', and 'Versions'.

Gambar IV.5 Tampilan situs *Protein Data Bank*



The screenshot shows the DUD-E website, titled 'A Database of Useful Decoys: Enhanced'. The page features a navigation menu with links for 'Home', 'Targets', 'Subsets', 'Generate', 'Other', 'FAQ', 'Revisions', and 'Thanks'. A welcome message describes the database as an enhanced and rebuilt version of DUD, containing 22,886 active compounds and 50 decoys per target. It also mentions that 'mol2 and SDF format now available in all packages for actives and decoys. [July 14]'. At the bottom, there are three buttons: 'Browse the DUD-E targets', 'Download the default DUD-E package', and 'Make Decoys for your own ligands'.

Gambar IV.6 Tampilan situs DUD-E

LAMPIRAN 2 (LANJUTAN)

The Binding Database

Search by KI (Enzyme Inhibition Constant)

Affinity Unit: nM uM

Search

<input type="checkbox"/> α -Carbonic anhydrase (α CA) [37]	<input type="checkbox"/> Integrin α 4 β 1 (VLA-4) [44]
<input type="checkbox"/> α -galactosidase [8]	<input type="checkbox"/> Integrin β 3-Vitronectin receptor α [220]
<input type="checkbox"/> α -glucosidase [25]	<input type="checkbox"/> Integrin β 5-Vitronectin receptor α [4]
<input type="checkbox"/> β -1,4-Galactosyltransferase I (β 4GalT) [12]	<input type="checkbox"/> Interferon-induced, double-stranded RNA-activated protein kinase [13]
<input type="checkbox"/> β -Carbonic anhydrase (β CA) [37]	<input type="checkbox"/> Interferon-inducible RNA-dependent protein kinase [13]
<input type="checkbox"/> β -Carbonic anhydrase (CA) [69]	<input type="checkbox"/> Interleukin [1]
<input type="checkbox"/> β -Carbonic anhydrase (CA1) [14]	<input type="checkbox"/> Interleukin 1-Alpha [1]
<input type="checkbox"/> β -Carbonic anhydrase 1 (CA 1) [166]	<input type="checkbox"/> Interleukin 1-beta [1]
<input type="checkbox"/> β -Carbonic anhydrase 2 (CA 2) [66]	<input type="checkbox"/> Interleukin 8 precursor [14]
<input type="checkbox"/> β -Carbonic anhydrase 3 (CA 3) [22]	<input type="checkbox"/> Interleukin-1 α [1]
<input type="checkbox"/> β -galactosidase [25]	<input type="checkbox"/> Interleukin-1 β [1]
<input type="checkbox"/> β -glucuronidase [10]	<input type="checkbox"/> Interleukin-1 β convertase [362]
<input type="checkbox"/> β -ketoacyl-ACP synthase I (C171Q KasA) [1]	<input type="checkbox"/> Interleukin-1 β converting enzyme [362]
<input type="checkbox"/> β -ketoacyl-ACP synthase I (KasA) [22]	<input type="checkbox"/> Interleukin-1 receptor-associated kinase [2]
<input type="checkbox"/> β -lactamase (Bla2) [3]	<input type="checkbox"/> Interleukin-1 receptor-associated kinase 1 (IRAK-1) [2]
<input type="checkbox"/> κ opioid receptor (KOR D138A) [4]	<input type="checkbox"/> Interleukin-1 receptor-associated kinase 4 [36]
<input type="checkbox"/> κ opioid receptor (KOR D138N) [4]	<input type="checkbox"/> Interleukin-1 receptor-associated kinase 4 (IRAK-4) [36]
<input type="checkbox"/> κ opioid receptor (KOR E297A) [4]	<input type="checkbox"/> Interleukin-1 receptor-associated kinase 4 (IRAK4) [36]
<input type="checkbox"/> κ opioid receptor (KOR H291A) [4]	<input type="checkbox"/> Interleukin-18 [1]

Gambar IV.7 Tampilan situs *Binding Database*

PubChem

Explore Chemistry

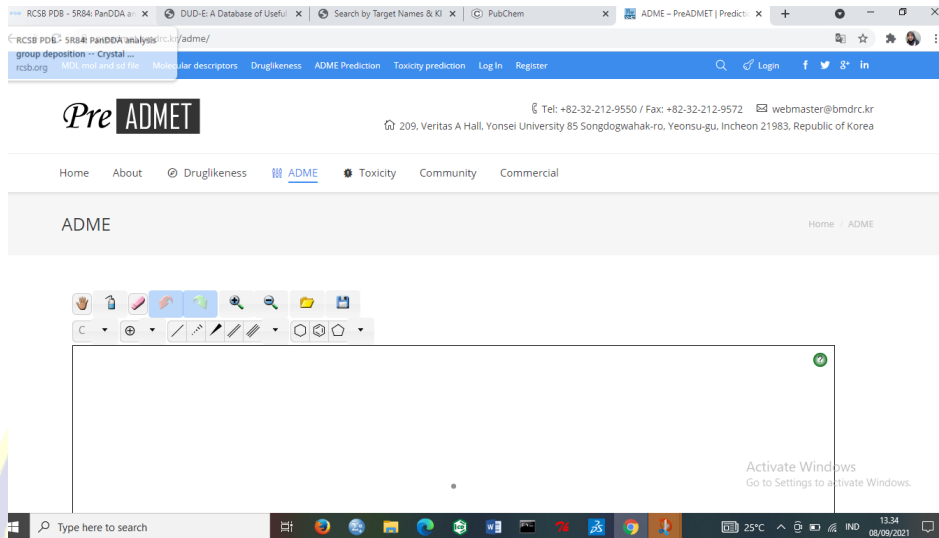
Quickly find chemical information from authoritative sources

alpha mangostin

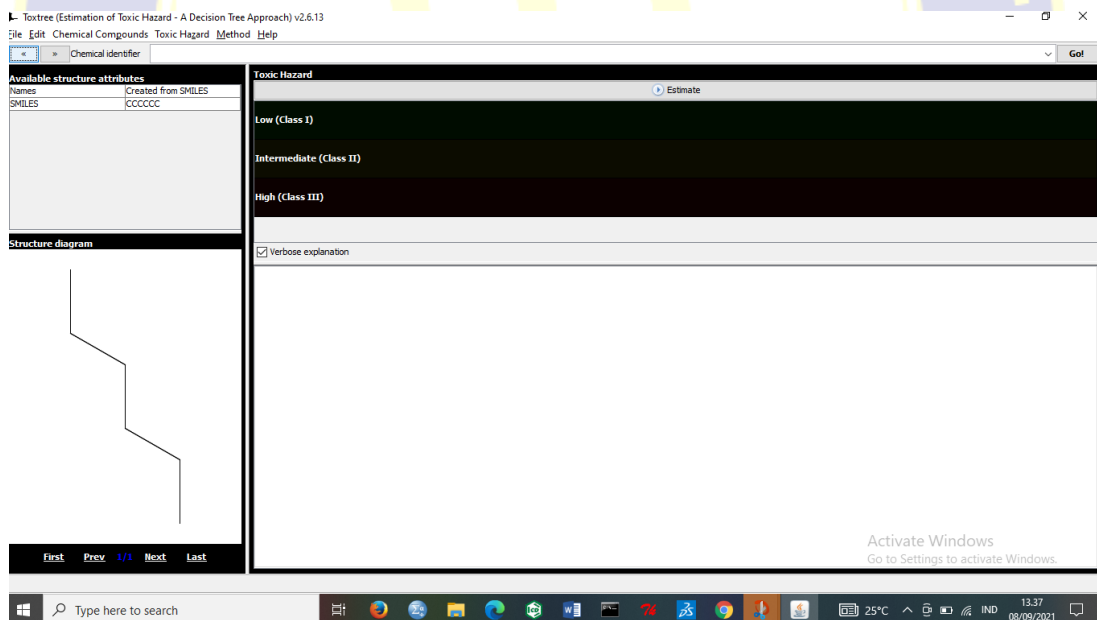
Compound	Gene
alpha-Mangostin	laminin, alpha 1
di-O-acetylmangostin	laminin, alpha 2
di-O-methylmangostin	laminin, alpha 3
gamma-Mangostin	laminin, alpha 4
beta-Mangostin	laminin subunit alpha 1
Mangostin	laminin subunit alpha 2
3-isomangostin	laminin subunit alpha 3
1-isomangostin	laminin subunit alpha 4

Gambar IV.8 Tampilan situs *PubChem*

LAMPIRAN 3 (LANJUTAN)

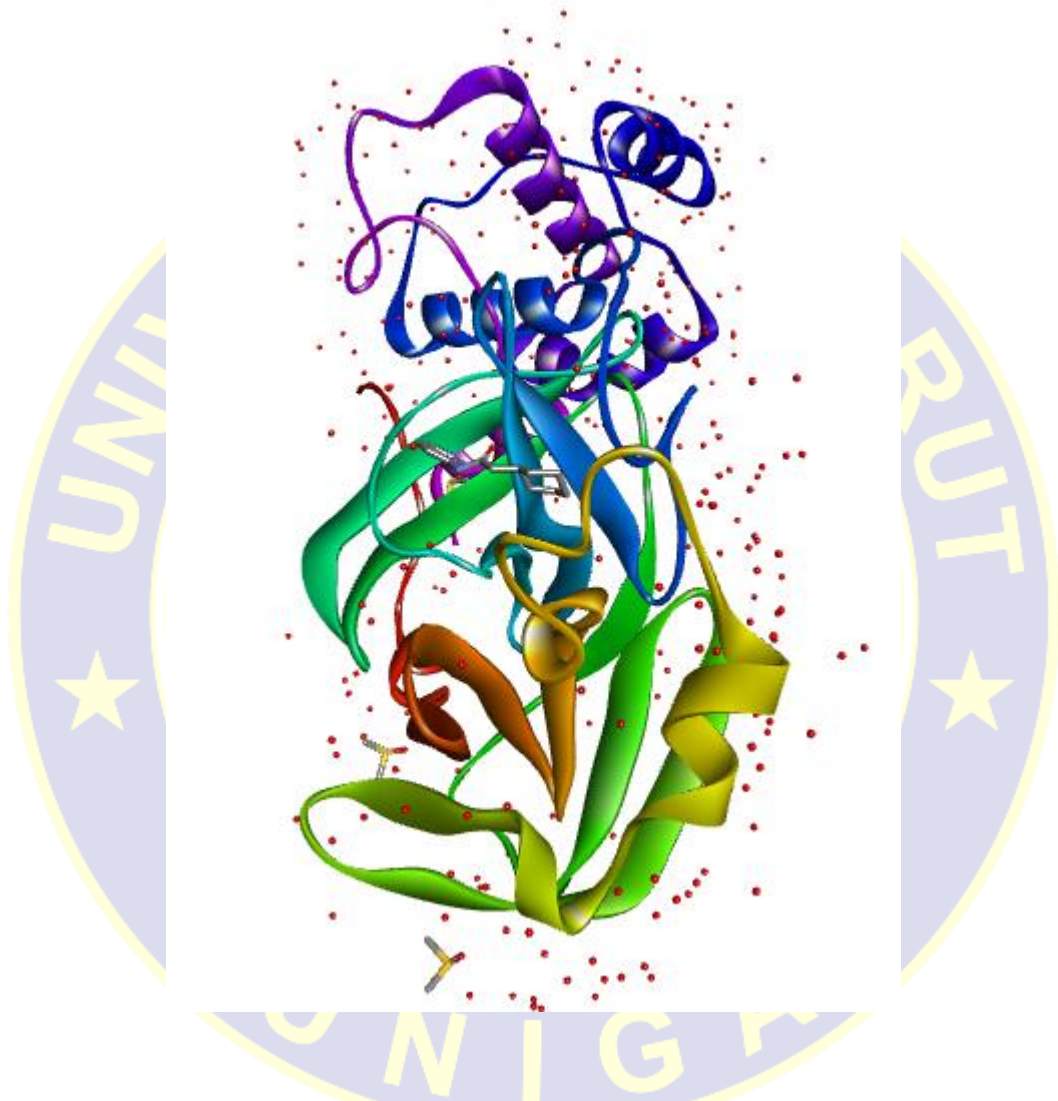


Gambar IV.9 Tampilan situs PreADMET



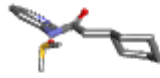
Gambar IV.10 Tampilan situs aplikasi *Toxtree*

LAMPIRAN 4
STRUKTUR 3 DIMENSI RESEPTOR MAIN PROTEASE DAN LIGAN
ALAMI

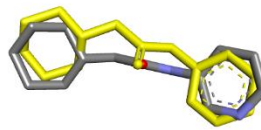


Gambar V.1 *Main Protease 5R84*

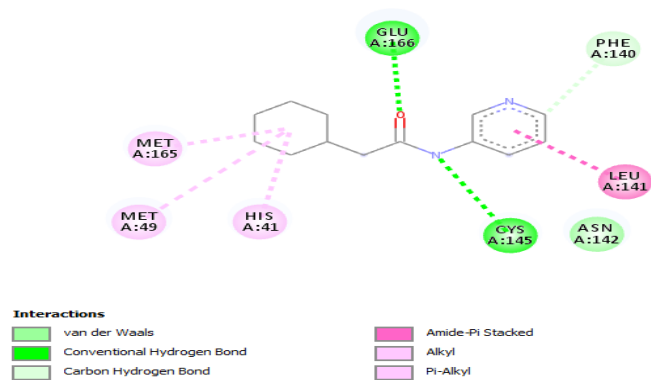
LAMPIRAN 4
(LANJUTAN)



Gambar V.2 Ligan alami



Gambar V.3 Visualisasi tumpang tindih ligan alami 5R84 (merah-abu-biru) dengan hasil *redocking* (kuning)



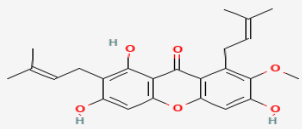
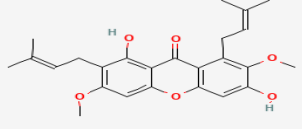
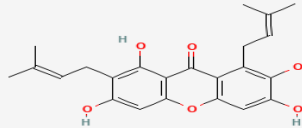
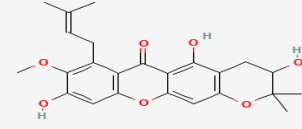
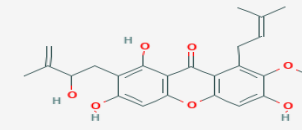
Gambar V.4 Residu asam amino

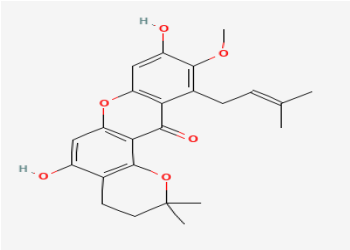
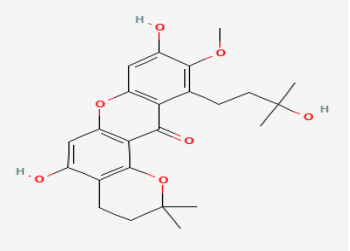
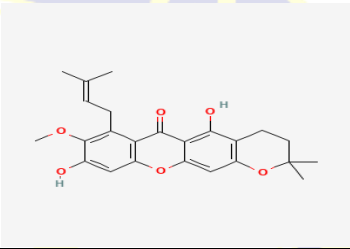
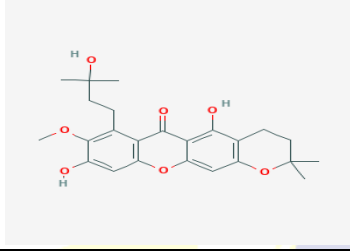
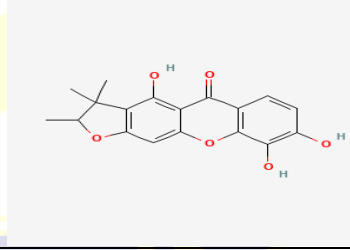
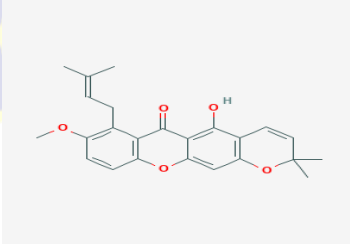
LAMPIRAN 5

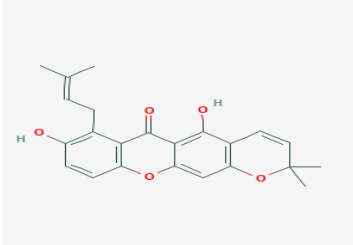
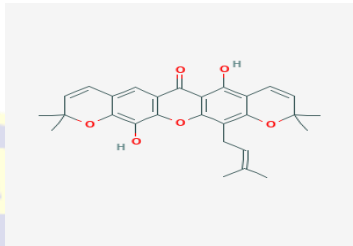
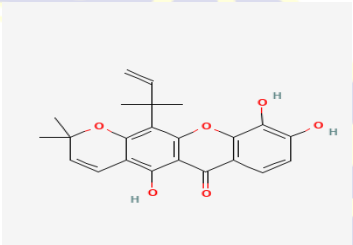
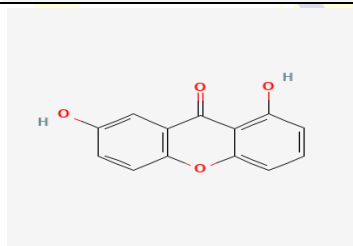
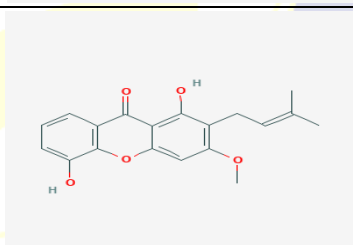
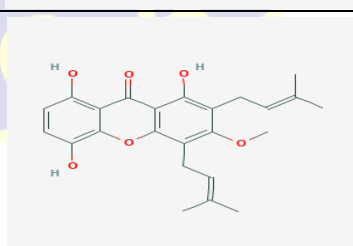
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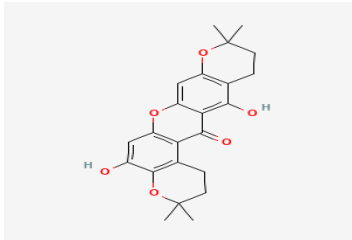
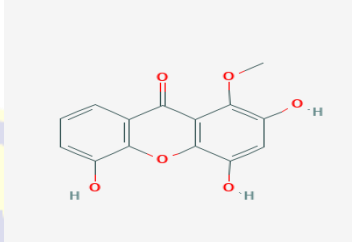
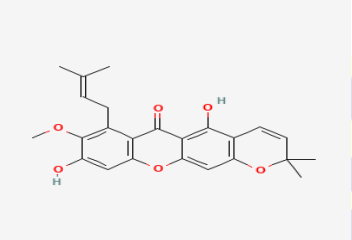
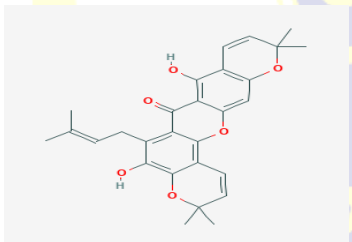
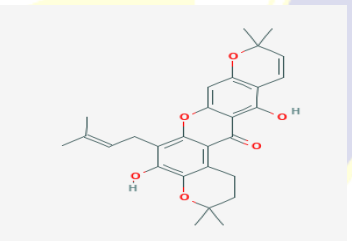
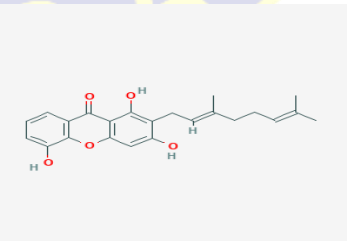
Tabel V.1

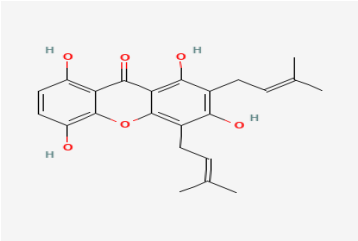
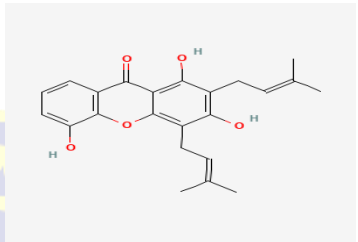
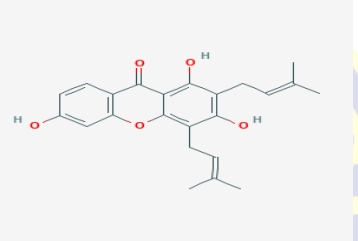
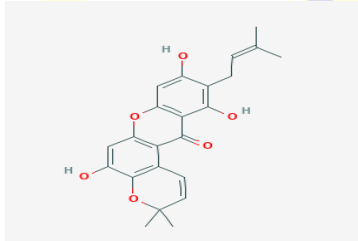
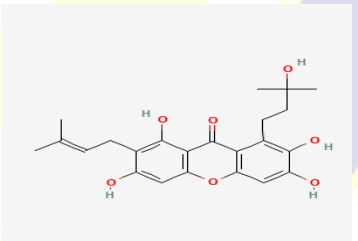
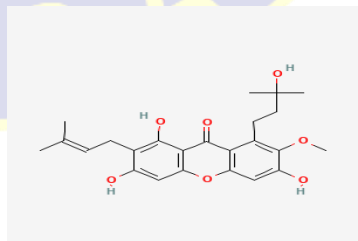
Senyawa yang Terdapat di Dalam Manggis (*Garcinia mangostana* L.)

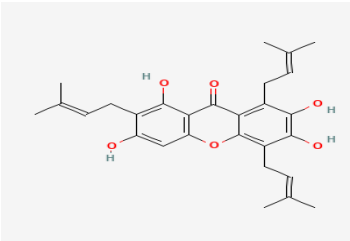
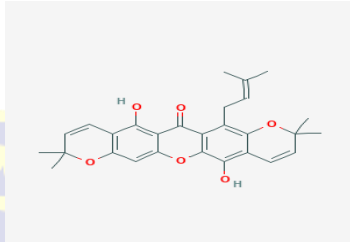
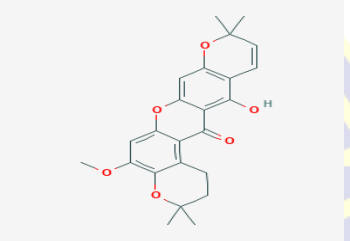
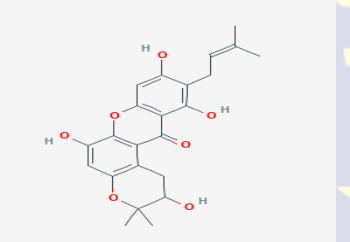
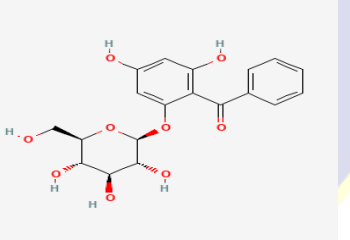
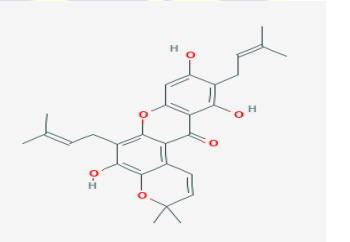
Nama Senyawa	Gambar Struktur
α-Mangostin	 <p>The chemical structure of α-Mangostin is a xanthone derivative. It features a central xanthone core with two phenyl rings. The left phenyl ring has a prenyl group at the 2-position and hydroxyl groups at the 3 and 4 positions. The right phenyl ring has a methoxy group at the 2-position, a prenyl group at the 3-position, and hydroxyl groups at the 4 and 5 positions.</p>
β-Mangostin	 <p>The chemical structure of β-Mangostin is a xanthone derivative. It features a central xanthone core with two phenyl rings. The left phenyl ring has a prenyl group at the 2-position, a methoxy group at the 3-position, and hydroxyl groups at the 4 and 5 positions. The right phenyl ring has a prenyl group at the 2-position, a methoxy group at the 3-position, and hydroxyl groups at the 4 and 5 positions.</p>
γ-Mangostin	 <p>The chemical structure of γ-Mangostin is a xanthone derivative. It features a central xanthone core with two phenyl rings. The left phenyl ring has a prenyl group at the 2-position and hydroxyl groups at the 3 and 4 positions. The right phenyl ring has a prenyl group at the 2-position, a hydroxyl group at the 3-position, and hydroxyl groups at the 4 and 5 positions.</p>
Mangostanol	 <p>The chemical structure of Mangostanol is a xanthone derivative. It features a central xanthone core with two phenyl rings. The left phenyl ring has a prenyl group at the 2-position, a methoxy group at the 3-position, and hydroxyl groups at the 4 and 5 positions. The right phenyl ring has a prenyl group at the 2-position, a hydroxyl group at the 3-position, and hydroxyl groups at the 4 and 5 positions.</p>
Mangostenol	 <p>The chemical structure of Mangostenol is a xanthone derivative. It features a central xanthone core with two phenyl rings. The left phenyl ring has a prenyl group at the 2-position, a hydroxyl group at the 3-position, and hydroxyl groups at the 4 and 5 positions. The right phenyl ring has a prenyl group at the 2-position, a hydroxyl group at the 3-position, and hydroxyl groups at the 4 and 5 positions.</p>

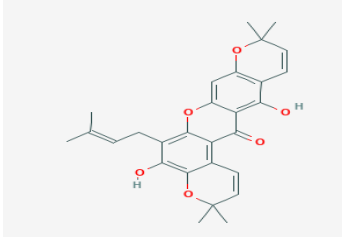
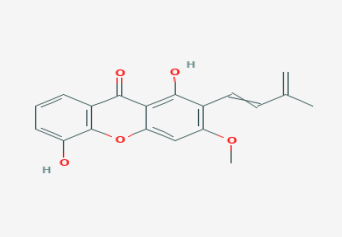
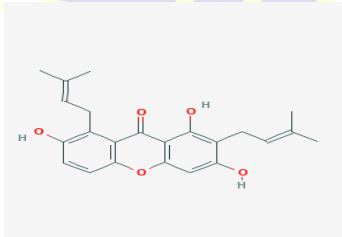
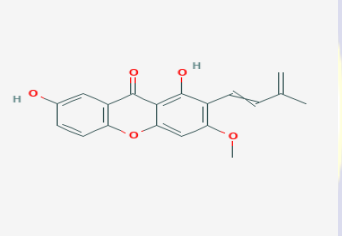
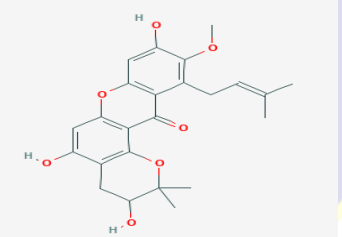

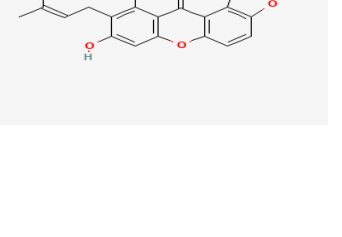
1-Isomangostin	
1-Isomangostin hydrate	
3-Isomangostin	
3-Isomangostin hydrate	
Toxyloxanthone	
Calabaxanthone	

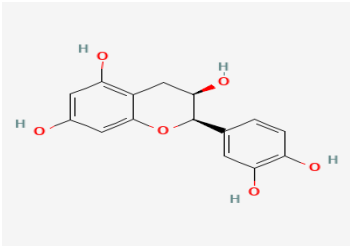
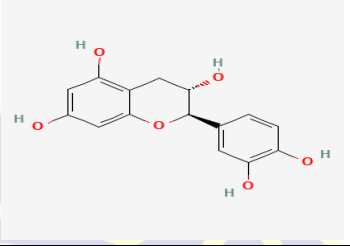
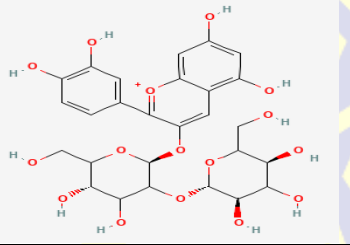
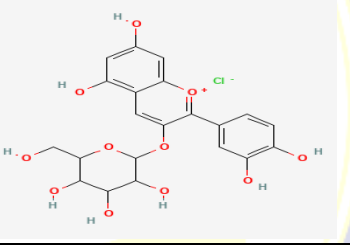
Demethylcalabaxanthone	
Caloxanthone	
Macluraxanthone	
1,7-dihydroxyxanthone (euxanthone)	
Cudraxanthone	
8-Hydroxycudraxanthone	

BR-xanthone A	
BR-xanthone B	
Mangostanin	
Mangostenone A	
Mangostenone B	
Mangostinone	

Gartanin	
8-Desoxygartanin	
Garcinone A	
Garcinone B	
Garcinone C	
Garcinone D	

Garcinone E	
Garcimangosone A	
Garcimangosone B	
Garcimangosone C	
Garcimangosone D	
Tovophyllin A	

Tovophyllin B	
1,5-dihydroxy-2-isoprenyl-3-methoxyxanthone	
6-Deoxy-gamma-mangostin	
1,7-Dihydroxy-2-isoprenyl-3-methoxyxanthone	
11-hydroxy-1-isomangostin	
1,2-dihydro-1,8,10-trihydroxy-2-(2-hydroxypropan-2-yl)-9-(3-methylbut-2-enyl)furo[3,2-a]xanthen-11-one	
Norathyriol	

Epicatechin	 <p>The structure shows a flavan-3-ol core consisting of a chromane ring system. The C-2 position is substituted with a catechol group (a benzene ring with hydroxyl groups at the 3 and 4 positions). The C-3 position has a hydroxyl group, and the C-4 position is substituted with another catechol group. Stereochemistry is indicated with a wedge bond for the C-3 hydroxyl group and a dashed bond for the C-4 catechol group.</p>
Catechin	 <p>The structure is identical to Epicatechin, but the stereochemistry is reversed: the C-3 hydroxyl group is on a dashed bond and the C-4 catechol group is on a wedge bond.</p>
Cyanidin 3-sophoroside	 <p>The structure shows a cyanidin cation (a flavylium ion) where the C-3 position is substituted with a sophoroside group. The sophoroside group is a disaccharide composed of a glucose unit and a sucrose unit. The glucose unit is linked to the C-3 position of the cyanidin core via an oxygen atom. The sucrose unit is attached to the glucose unit. The structure is highly complex with multiple hydroxyl groups and a positive charge on the oxygen atom at the C-4 position of the cyanidin core.</p>
Cyanidin 3-glucoside	 <p>The structure shows a cyanidin cation where the C-3 position is substituted with a glucose unit. The glucose unit is linked to the C-3 position of the cyanidin core via an oxygen atom. The structure is highly complex with multiple hydroxyl groups and a positive charge on the oxygen atom at the C-4 position of the cyanidin core. A chloride ion (Cl⁻) is shown as a counterion to the cyanidin cation.</p>

LAMPIRAN 6

PREDIKSI *DRUG LIKENESS* BERDASARKAN ATURAN *LIPINSKI'S*

RULE OF FIVE

Tabel V.4

Hasil Prediksi Sifat Fisika Kimia dari Senyawa Uji

Nama Senyawa	BM (g/mol)	Ikatan Hidrogen		Log P	Keterangan
		Donor	Akseptor		
α -Mangostin	410.05	3	6	6.3	Tidak Memenuhi Syarat
β -Mangostin	424.05	2	6	6.6	Tidak Memenuhi Syarat
γ -Mangostin	396.04	4	6	5.9	Tidak Memenuhi Syarat
Mangostanol	426.05	3	7	4.7	Memenuhi Syarat
Mangostenol	426.05	4	7	5.2	Tidak Memenuhi Syarat
1-Isomangostin	410.05	2	6	5.1	Tidak Memenuhi Syarat
1-Isomangostin hydrate	428.05	3	7	3.8	Memenuhi Syarat
3-Isomangostin	410.05	2	6	5.7	Tidak Memenuhi Syarat
3-Isomangostin hydrate	428.05	3	7	4.3	Memenuhi Syarat
Toxyloxanthone	328.03	3	6	3.8	Memenuhi Syarat

Calabaxanthone	392.04	1	5	6	Tidak Memenuhi Syarat
Demethylcalabaxanthone	378.04	2	5	5.7	Tidak Memenuhi Syarat
Caloxanthone	460.05	2	6	6.6	Tidak Memenuhi Syarat
Macluraxanthone	394.04	3	6	5.3	Tidak Memenuhi Syarat
1,7-dihydroxyxanthone (euxanthone)	228.20	2	4	2.8	Memenuhi Syarat
Cudraxanthone	326.03	2	5	4.7	Memenuhi Syarat
8-Hydroxycudraxanthone	410.05	3	6	6.3	Tidak Memenuhi Syarat
BR-xanthone A	396.04	2	6	4.8	Memenuhi Syarat
BR-xanthone B	274.22	3	6	1.9	Memenuhi Syarat
Mangostanin	408.04	2	6	5.6	Tidak Memenuhi Syarat
Mangostenone A	460.05	2	6	6.6	Tidak Memenuhi Syarat
Mangostenone B	462.05	2	6	6.6	Tidak Memenuhi Syarat
Mangostinone	380.04	3	5	6.2	Tidak Memenuhi Syarat

Gartanin	396.04	4	6	5.9	Tidak Memenuhi Syarat
8-Desoxygartanin	380.04	3	5	6.3	Tidak Memenuhi Syarat
Garcinone A	380.04	3	5	6.3	Tidak Memenuhi Syarat
Garcinone B	394.04	3	6	5.3	Tidak Memenuhi Syarat
Garcinone C	414.04	5	7	4.6	Memenuhi Syarat
Garcinone D	428.05	4	7	4.9	Memenuhi Syarat
Garcinone E	464.05	4	6	7.9	Tidak Memenuhi Syarat
Garcimangosone A	460.05	2	6	6.6	Tidak Memenuhi Syarat
Garcimangosone B	408.04	1	5	5	Memenuhi Syarat
Garcimangosone C	412.04	4	7	4.4	Memenuhi Syarat
Garcimangosone D	392.04	6	9	0.7	Memenuhi Syarat
Tovophyllin A	462.05	3	6	7.2	Tidak Memenuhi Syarat
Tovophyllin B	460.05	2	6	6.6	Tidak Memenuhi Syarat

1,5-dihydroxy-2-isoprenyl-3-methoxyxanthone	324.03	2	5	4.8	Memenuhi Syarat
6-Deoxy-gamma-mangostin	380.04	3	5	6.3	Tidak Memenuhi Syarat
1,7-Dihydroxy-2-isoprenyl-3-methoxyxanthone	324.03	2	5	4.8	Memenuhi Syarat
11-hydroxy-1-isomangostin	426.05	3	7	4.2	Memenuhi Syarat
1,2-dihydro-1,8,10-trihydroxy-2-(2-hydroxypropan-2-yl)-9-(3-methylbut-2-enyl)furo[3,2-a]xanthen-11-one	412.04	4	7	4.2	Memenuhi Syarat
Norathyriol	260.20	4	6	2.1	Memenuhi Syarat
Epicatechin	290.27	5	6	0,5	Memenuhi Syarat
Catechin	290.27	5	6	0.5	Memenuhi Syarat
Cyanidin 3-sophoroside	611.05	11	15	0	Tidak Memenuhi Syarat
Cyanidin 3-glucoside	484.8	8	11	0	Tidak Memenuhi Syarat

Keterangan: BM (Berat molekul) <500 Dalton, Log P <5, Donor ikatan hidrogen <5 dan Akseptor ikatan hidrogen <10.

