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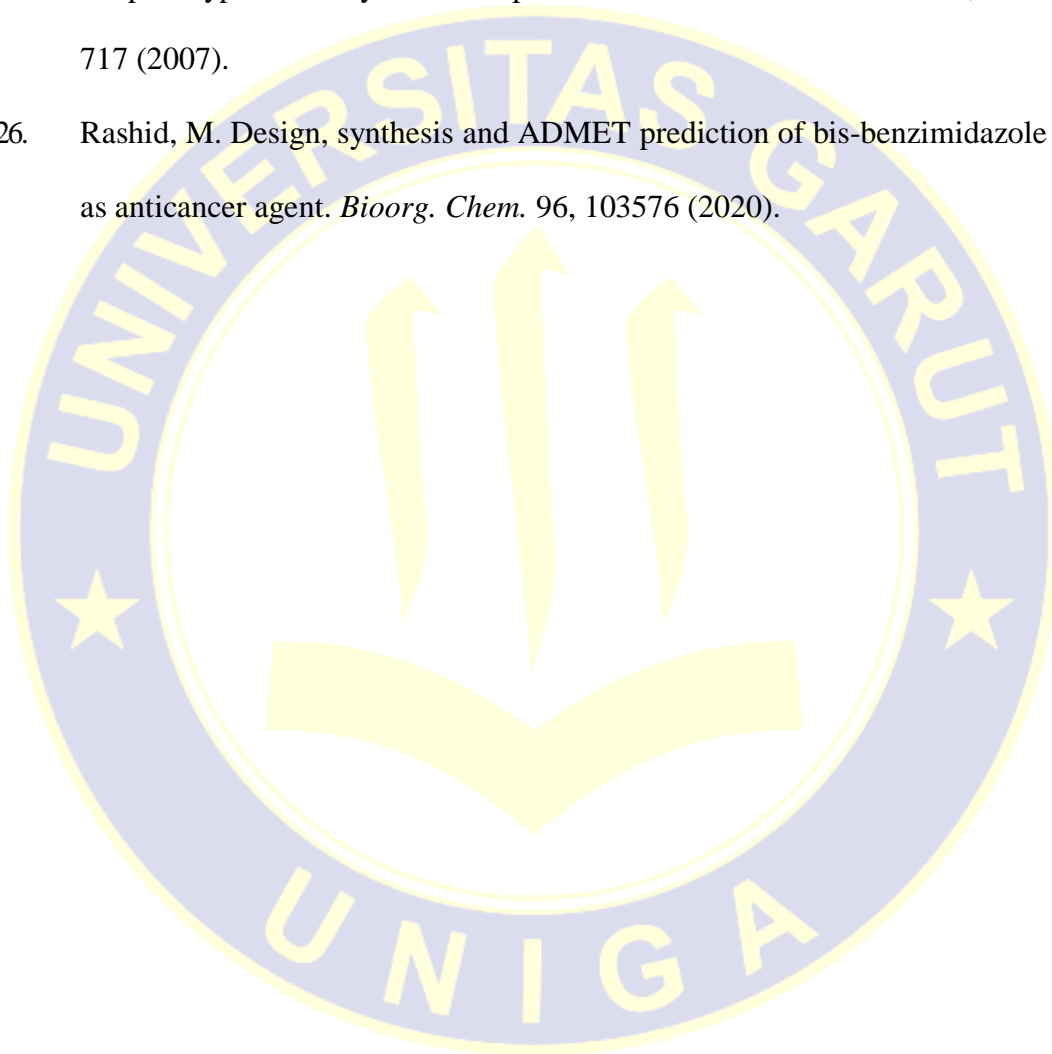
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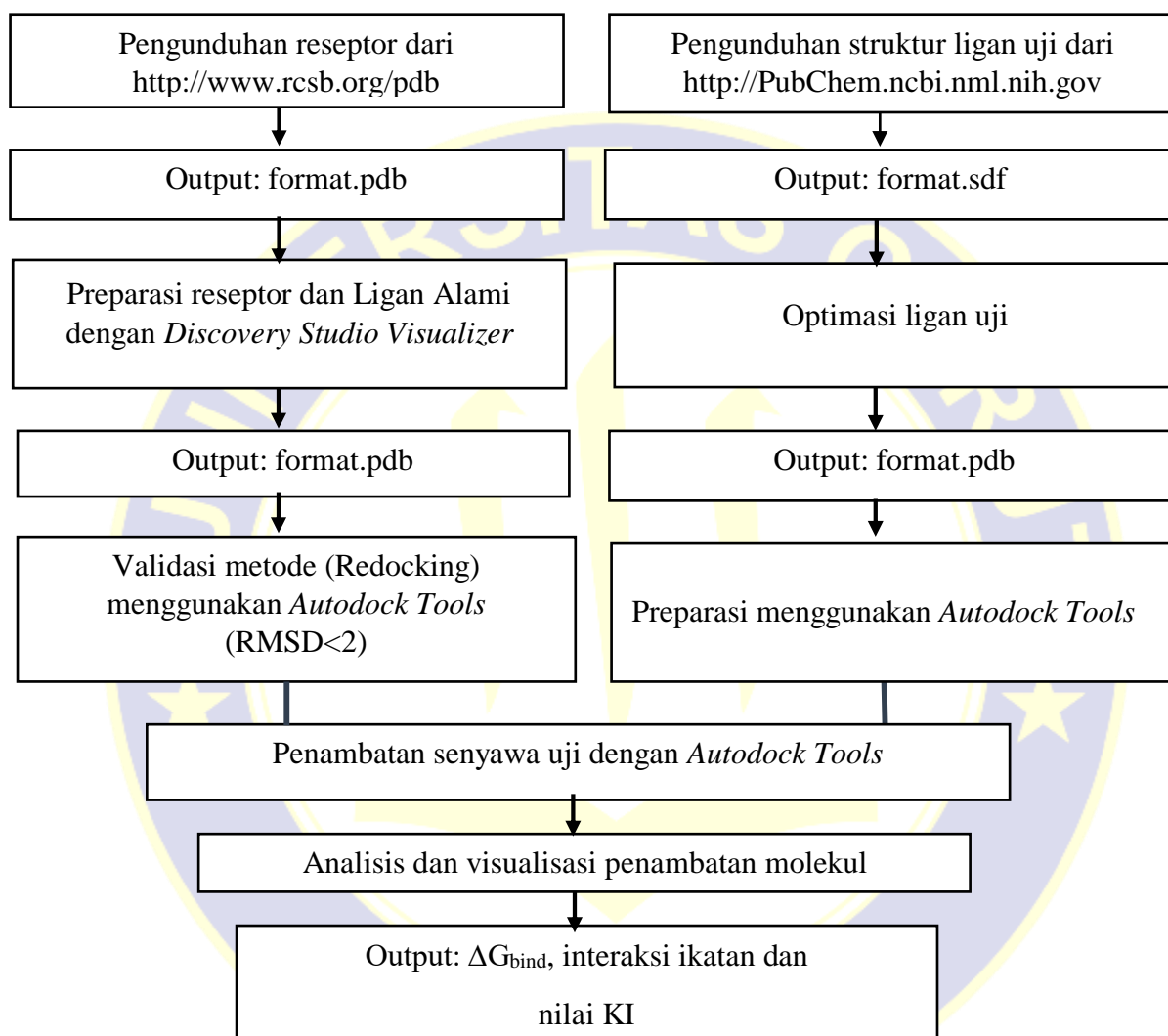
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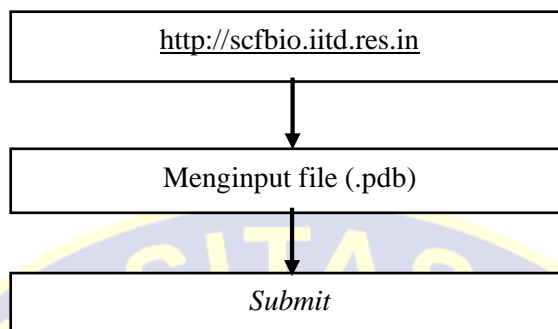
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SKEMA KERJA

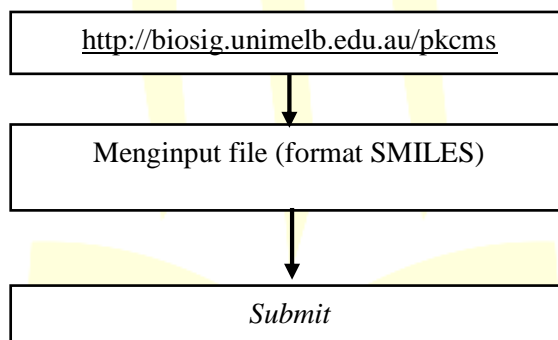


Gambar III 1. Alur penelitian

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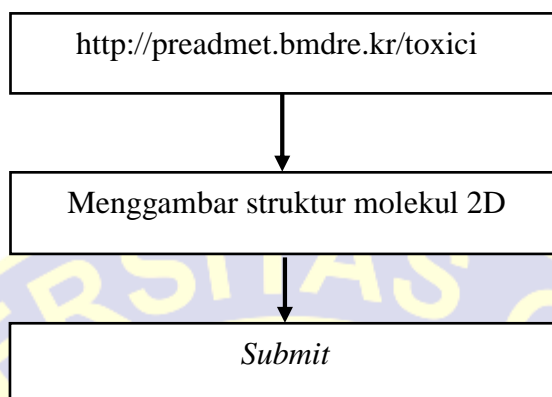


Gambar III 2. Analisis lipinski's rule of five

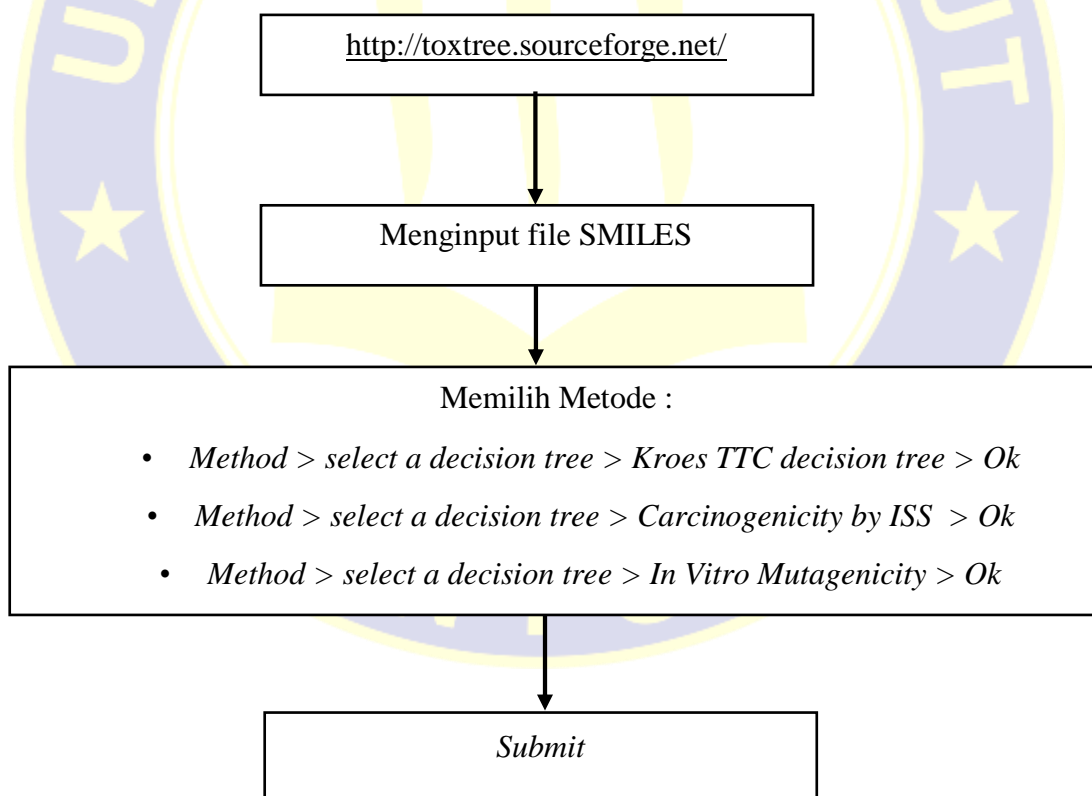


Gambar III 3. Analisis Toksisitas berdasarkan pkcms

LAMPIRAN 1 (LANJUTAN)



Gambar III 4. Analisis pre-ADME



Gambar III.3 Analisis toksisitas menggunakan *Toxtree 3.1.0*[®]

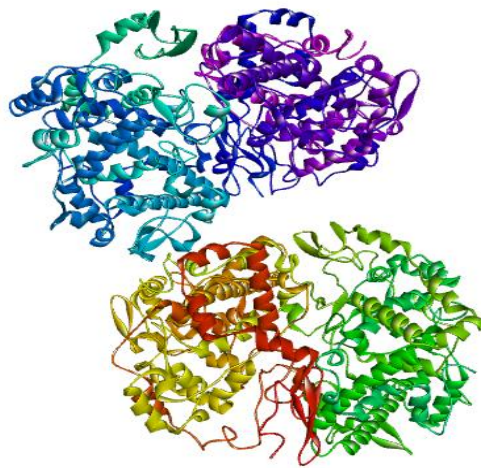
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DAUN PEPAYA GUNUNG



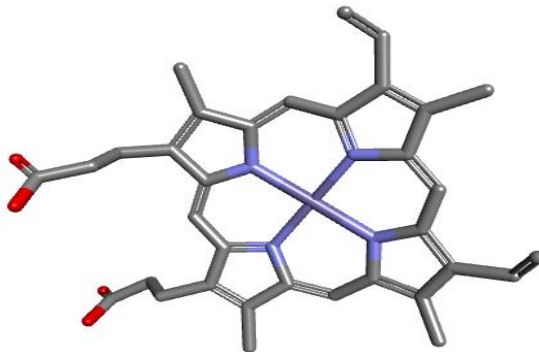
Gambar IV 1. Tanaman daun pepaya gunung



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STRUKTUR 3D MAKROMOLEKUL



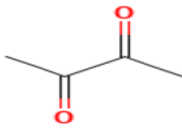
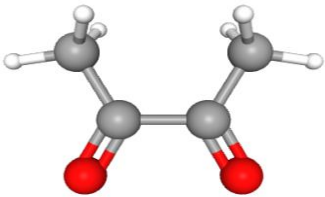
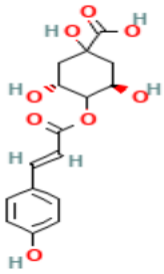
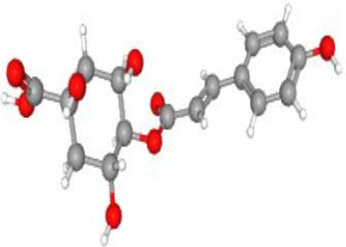
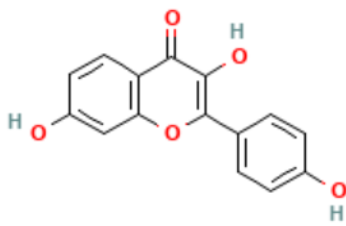
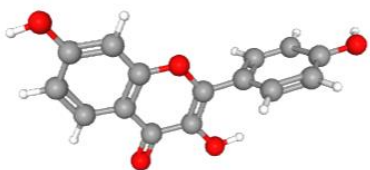
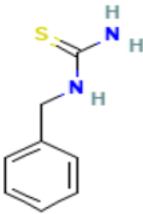
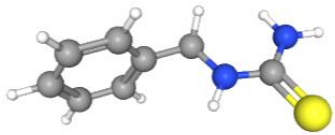
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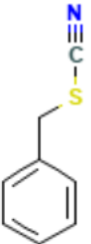
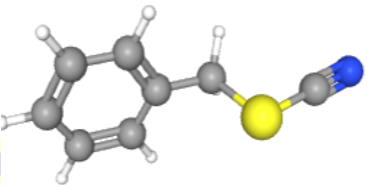
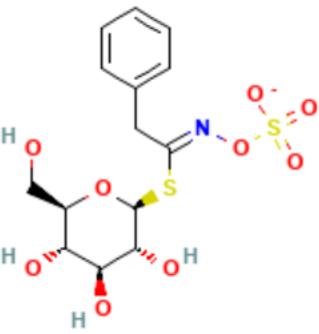
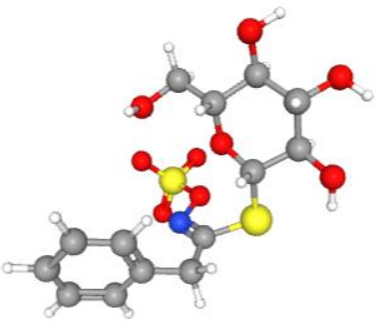
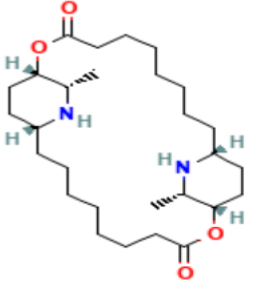
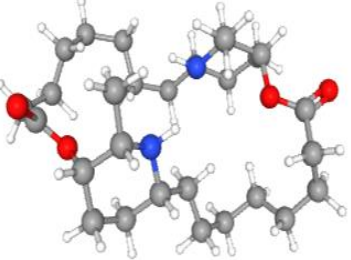
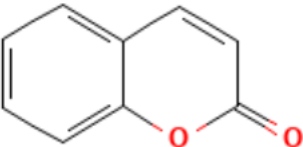
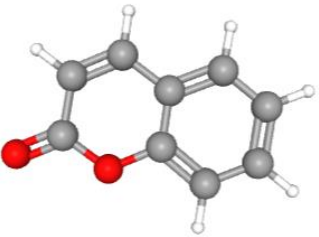
Gambar V 2. Ligan alami reseptor COX-2 (PROTOPORPHYRIN IX CONTAINING FE)

LAMPIRAN 4

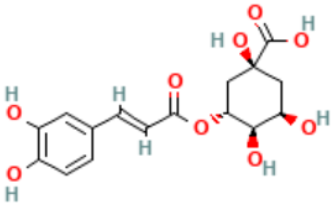
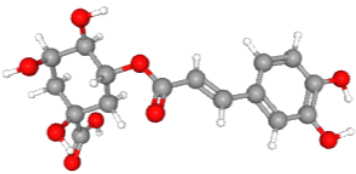
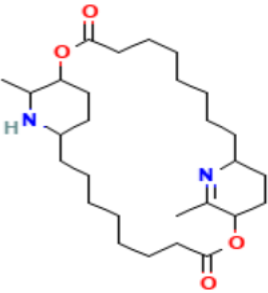
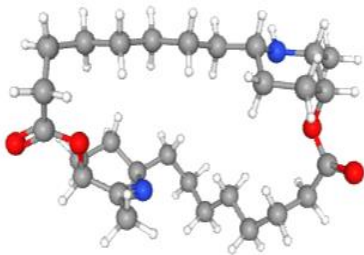
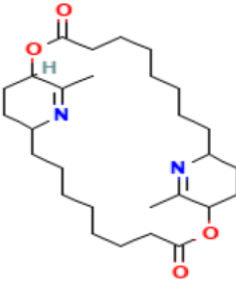
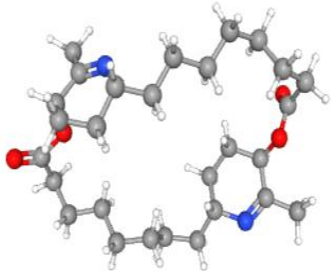
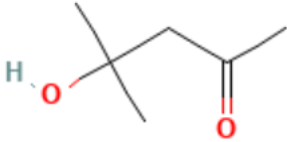
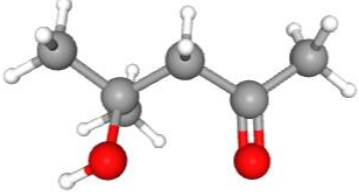
STRUKTUR 2D DAN 3D SENYAWA UJI

No	Nama	Struktur 2D	Struktur 3D
1.	2,3 butanedione		
2.	4p Coumaroylquinic acid		
3.	5 Deoxykaempferol		
4.	Benzyl thiourea		

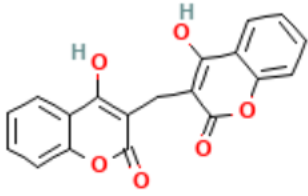

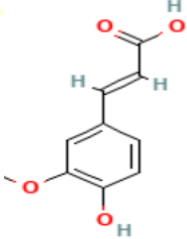
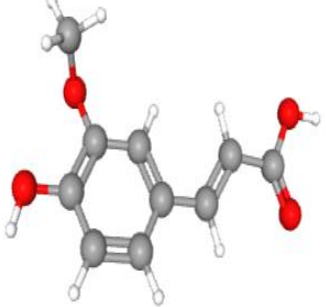
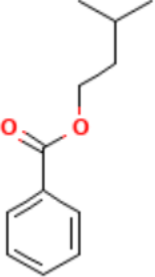
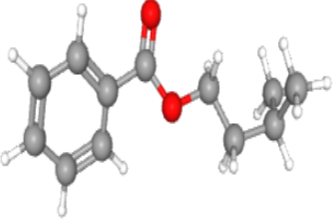
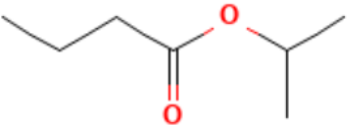
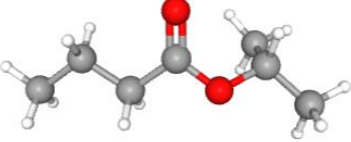
**LAMPIRAN 4
(LANJUTAN)**

No	Nama	Struktur 2D	Struktur 3D
5.	Benzyl thiocyanate	 <p>The 2D structure shows a benzene ring attached to a methylene group (-CH₂-), which is further attached to a thiocyanate group (-N=C=S). The nitrogen atom is blue, carbon is black, and sulfur is yellow.</p>	 <p>The 3D model shows the spatial arrangement of atoms in benzyl thiocyanate. The benzene ring is represented by grey spheres (carbon) and white spheres (hydrogen). The thiocyanate group consists of a yellow sphere (sulfur), a black sphere (carbon), and a blue sphere (nitrogen).</p>
6.	Benzyl glucosinolate	 <p>The 2D structure shows a glucose molecule in its cyclic form, with a benzyl group attached to the C-6 position via a sulfur atom. The sulfur atom is bonded to a nitrogen atom, which is in turn bonded to a sulfonate group (-SO₃⁻). The sulfur is yellow, nitrogen is blue, and oxygen is red.</p>	 <p>The 3D model shows the complex spatial arrangement of the benzyl glucosinolate molecule, highlighting the interaction between the glucose ring and the benzyl-sulfonate side chain.</p>
7.	Carpaine	 <p>The 2D structure of carpaine is a complex polycyclic alkaloid. It features a long chain with multiple nitrogen atoms (blue) and carbonyl groups (C=O, red oxygen).</p>	 <p>The 3D model illustrates the intricate three-dimensional structure of carpaine, showing the spatial orientation of its various rings and functional groups.</p>
8.	Coumarin	 <p>The 2D structure of coumarin consists of a benzene ring fused to a pyrone ring. The oxygen atom in the pyrone ring is red, and the carbonyl oxygen is also red.</p>	 <p>The 3D model shows the spatial arrangement of the coumarin molecule, highlighting the planar nature of the fused ring system.</p>

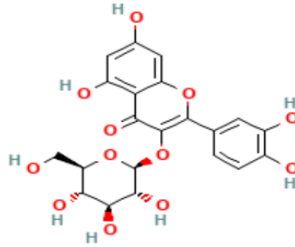
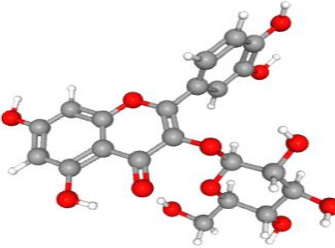
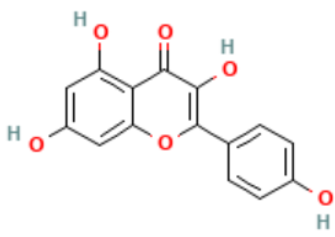
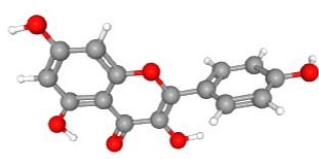
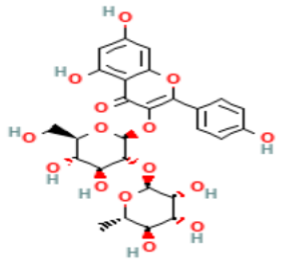
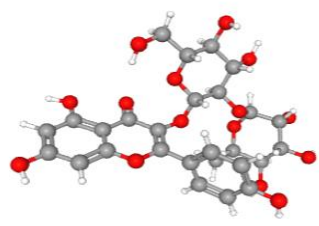
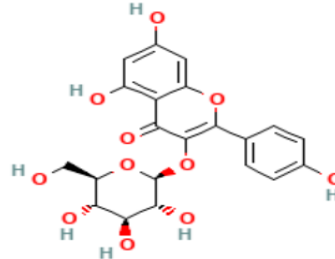
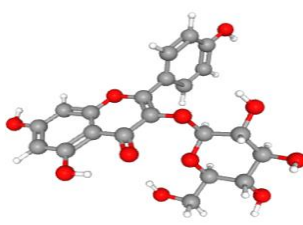
LAMPIRAN 4
(LANJUTAN)

No	Nama	Struktur 2D	Struktur 3D
9.	Chlorogenic acid	 <p>The 2D structure of chlorogenic acid shows a central pyrogallate moiety (a benzene ring with three hydroxyl groups) linked via an ester bond to a quinic acid moiety (a cyclohexane ring with four hydroxyl groups and a carboxylic acid group).</p>	 <p>The 3D ball-and-stick model of chlorogenic acid shows the spatial arrangement of atoms, with carbon in grey, oxygen in red, and hydrogen in white.</p>
10.	Dehydrocarpaine I	 <p>The 2D structure of Dehydrocarpaine I is a large macrocyclic compound featuring a long chain with two nitrogen atoms, a carbonyl group, and a methyl group.</p>	 <p>The 3D ball-and-stick model of Dehydrocarpaine I shows the complex, elongated ring structure of the macrocycle.</p>
11.	Dehydrocarpaine II	 <p>The 2D structure of Dehydrocarpaine II is a macrocyclic compound similar to Dehydrocarpaine I, but with a different ring size and substitution pattern.</p>	 <p>The 3D ball-and-stick model of Dehydrocarpaine II shows the spatial arrangement of the macrocyclic ring.</p>
12.	Diacetone alcohol	 <p>The 2D structure of diacetone alcohol is a branched molecule with a central carbon atom bonded to a methyl group, a hydroxyl group, and a 2-acetylpropyl group.</p>	 <p>The 3D ball-and-stick model of diacetone alcohol shows the branched structure of the molecule.</p>

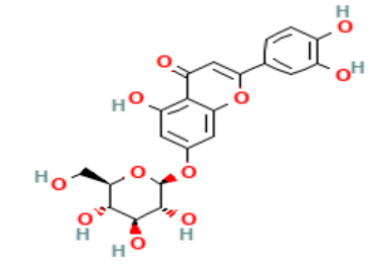
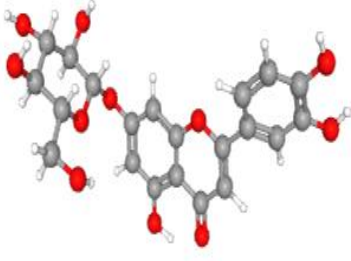
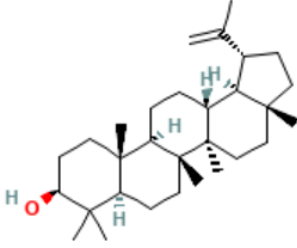
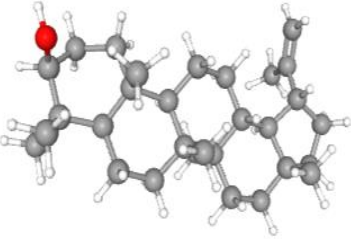
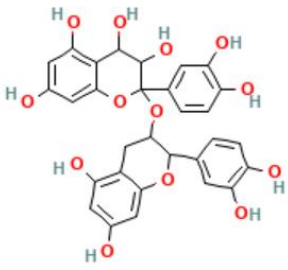
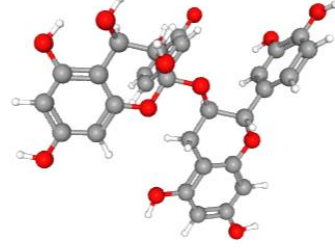
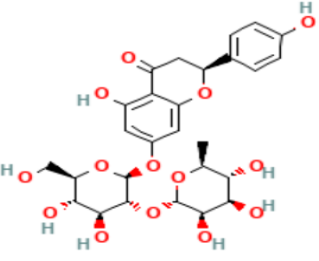
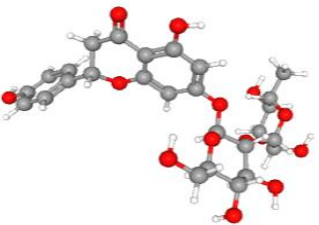
LAMPIRAN 4
(LANJUTAN)

No	Nama	Struktur 2D	Struktur 3D
13.	Dicoumarol	 <p>The 2D structure of Dicoumarol shows two coumarin rings connected by a methylene bridge (-CH₂-) at the 3-position of each ring. Each coumarin ring has a hydroxyl group (-OH) at the 7-position and a carbonyl group (=O) at the 2-position.</p>	 <p>The 3D ball-and-stick model of Dicoumarol shows the spatial arrangement of the two coumarin units, with carbon atoms in grey, oxygen atoms in red, and hydrogen atoms in white.</p>
14.	Ferulic acid	 <p>The 2D structure of Ferulic acid consists of a benzene ring with a methoxy group (-OCH₃) at the 3-position and a hydroxyl group (-OH) at the 4-position. A propenoic acid side chain (-CH=CH-COOH) is attached to the 1-position of the ring.</p>	 <p>The 3D ball-and-stick model of Ferulic acid shows the spatial arrangement of the benzene ring, the methoxy group, the hydroxyl group, and the propenoic acid side chain.</p>
15.	Isopentyl benzoate	 <p>The 2D structure of Isopentyl benzoate shows a benzene ring attached to a carbonyl group (-C(=O)-), which is further connected to an oxygen atom (-O-). This oxygen atom is bonded to an isopentyl group, represented as a four-carbon chain with a methyl branch on the second carbon.</p>	 <p>The 3D ball-and-stick model of Isopentyl benzoate shows the spatial arrangement of the benzene ring, the carbonyl group, the ester oxygen, and the isopentyl group.</p>
16.	Isopropyl butyrate	 <p>The 2D structure of Isopropyl butyrate shows a four-carbon butyrate chain (CH₃-CH₂-CH₂-C(=O)-) attached to an oxygen atom (-O-), which is further bonded to an isopropyl group (a three-carbon chain with a methyl branch on the second carbon).</p>	 <p>The 3D ball-and-stick model of Isopropyl butyrate shows the spatial arrangement of the butyrate chain, the ester oxygen, and the isopropyl group.</p>

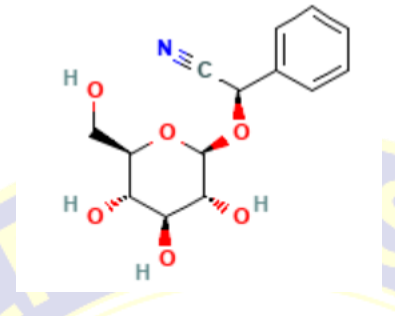
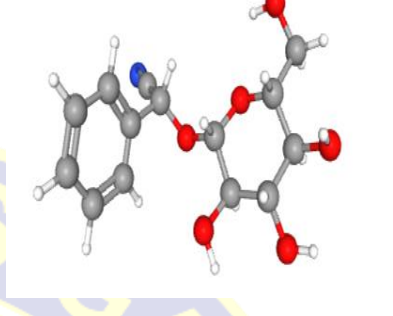
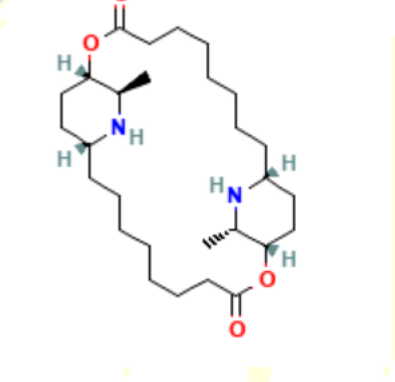
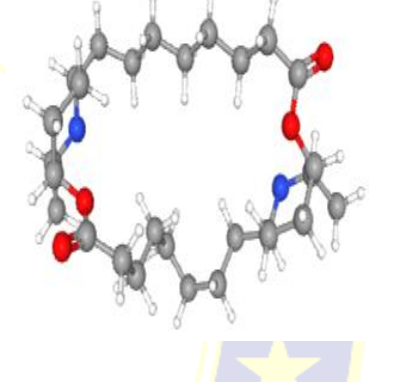
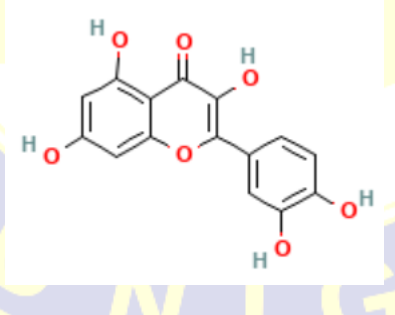
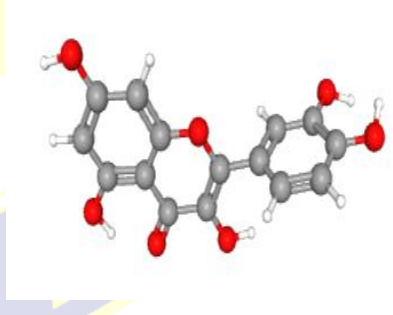
LAMPIRAN 4
(LANJUTAN)

No	Nama	Struktur 2D	Struktur 3D
17.	Isoquercitrin	 <p>The 2D chemical structure of Isoquercitrin shows a flavan-3-ol core (quercetin) with a rhamnoside sugar moiety attached to the 3-position of the flavan ring. The quercetin part has hydroxyl groups at positions 5, 7, and 3', and a 4'-hydroxyphenyl group at position 2'.</p>	 <p>The 3D ball-and-stick model of Isoquercitrin illustrates the spatial arrangement of the atoms, showing the rhamnoside sugar moiety attached to the 3-position of the flavan ring.</p>
18.	Kaempferol	 <p>The 2D chemical structure of Kaempferol shows a flavan-3-ol core with hydroxyl groups at positions 5, 7, and 3', and a 4'-hydroxyphenyl group at position 2'.</p>	 <p>The 3D ball-and-stick model of Kaempferol illustrates the spatial arrangement of the atoms, showing the 4'-hydroxyphenyl group at position 2'.</p>
19.	Kaempferol 3 rhamnoside	 <p>The 2D chemical structure of Kaempferol 3 rhamnoside shows a flavan-3-ol core with hydroxyl groups at positions 5, 7, and 3', and a 4'-hydroxyphenyl group at position 2'. A rhamnoside sugar moiety is attached to the 3-position of the flavan ring.</p>	 <p>The 3D ball-and-stick model of Kaempferol 3 rhamnoside illustrates the spatial arrangement of the atoms, showing the rhamnoside sugar moiety attached to the 3-position of the flavan ring.</p>
20.	Kaempferol 3 OD glukosida	 <p>The 2D chemical structure of Kaempferol 3 OD glukosida shows a flavan-3-ol core with hydroxyl groups at positions 5, 7, and 3', and a 4'-hydroxyphenyl group at position 2'. A glucose sugar moiety is attached to the 3-position of the flavan ring.</p>	 <p>The 3D ball-and-stick model of Kaempferol 3 OD glukosida illustrates the spatial arrangement of the atoms, showing the glucose sugar moiety attached to the 3-position of the flavan ring.</p>

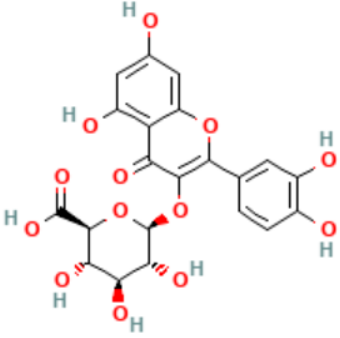
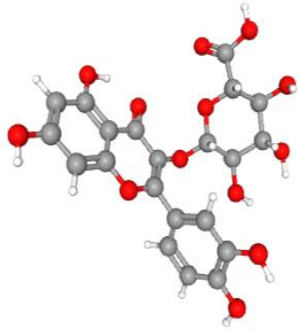

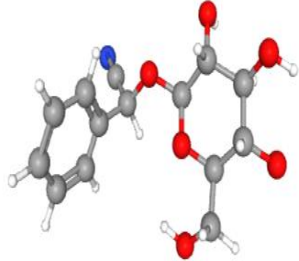
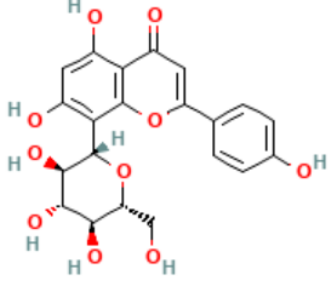
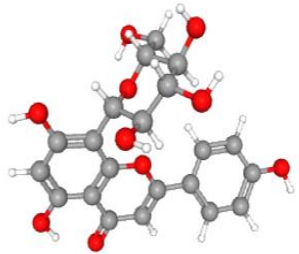
LAMPIRAN 4
(LANJUTAN)

No	Nama	Struktur 2D	Struktur 3D
21.	Luteolin 7 glukosida	 <p>The 2D structure shows a luteolin aglycone (a flavone with hydroxyl groups at positions 5, 7, and 3', 4') linked to a glucose molecule at the 7-position via an O-glycosidic bond. The glucose is shown in its cyclic pyranose form with hydroxyl groups at positions 2, 3, and 6.</p>	 <p>The 3D model illustrates the spatial arrangement of the luteolin aglycone and the glucose moiety, showing the relative orientations of the rings and the glycosidic bond.</p>
22.	Lupeol	 <p>The 2D structure depicts Lupeol, a pentacyclic triterpene. It features a complex ring system with multiple methyl groups and a hydroxyl group, characteristic of the lupane skeleton.</p>	 <p>The 3D model shows the bulky, non-planar structure of Lupeol, highlighting the spatial arrangement of its five fused rings and various substituents.</p>
23.	Procyanidin	 <p>The 2D structure shows Procyanidin, a dimeric flavan-3-ol. It consists of two catechin units linked together at their C4 and C8 positions via a C-C bond, with multiple hydroxyl groups on the aromatic rings.</p>	 <p>The 3D model illustrates the dimeric structure of Procyanidin, showing the relative orientation of the two catechin units and their respective hydroxyl groups.</p>
24.	Naringin	 <p>The 2D structure shows Naringin, a flavanone glycoside. It features a naringenin aglycone (a flavanone with hydroxyl groups at positions 5, 7, and 3', 4') linked to a glucose molecule at the 7-position via an O-glycosidic bond. The glucose is shown in its cyclic pyranose form.</p>	 <p>The 3D model illustrates the spatial arrangement of the naringenin aglycone and the glucose moiety, showing the relative orientations of the rings and the glycosidic bond.</p>

LAMPIRAN 4
(LANJUTAN)

No	Nama	Struktur 2D	Struktur 3D
25.	Prunasin	 <p>The 2D structure of Prunasin shows a pyranose ring with hydroxyl groups at C2, C3, and C6. A cyanide group (-C≡N) is attached to C4, and a benzyl group (-CH2-C6H5) is attached to C5.</p>	 <p>The 3D ball-and-stick model of Prunasin shows the spatial arrangement of atoms, with carbon in grey, oxygen in red, hydrogen in white, nitrogen in blue, and cyanide in grey and blue.</p>
26.	Pseudocarpaine	 <p>The 2D structure of Pseudocarpaine is a large macrocyclic molecule with a long chain of carbon atoms, two secondary amine groups (-NH-), and two amide groups (-C(=O)-) at the ends of the chain.</p>	 <p>The 3D ball-and-stick model of Pseudocarpaine shows the complex, ring-like structure of the macrocycle with carbon in grey, oxygen in red, and nitrogen in blue.</p>
27.	Quercetin	 <p>The 2D structure of Quercetin is a flavonoid with a central chromone ring system and two phenolic rings, each substituted with three hydroxyl groups.</p>	 <p>The 3D ball-and-stick model of Quercetin shows the spatial arrangement of the flavonoid structure, with carbon in grey, oxygen in red, and hydrogen in white.</p>

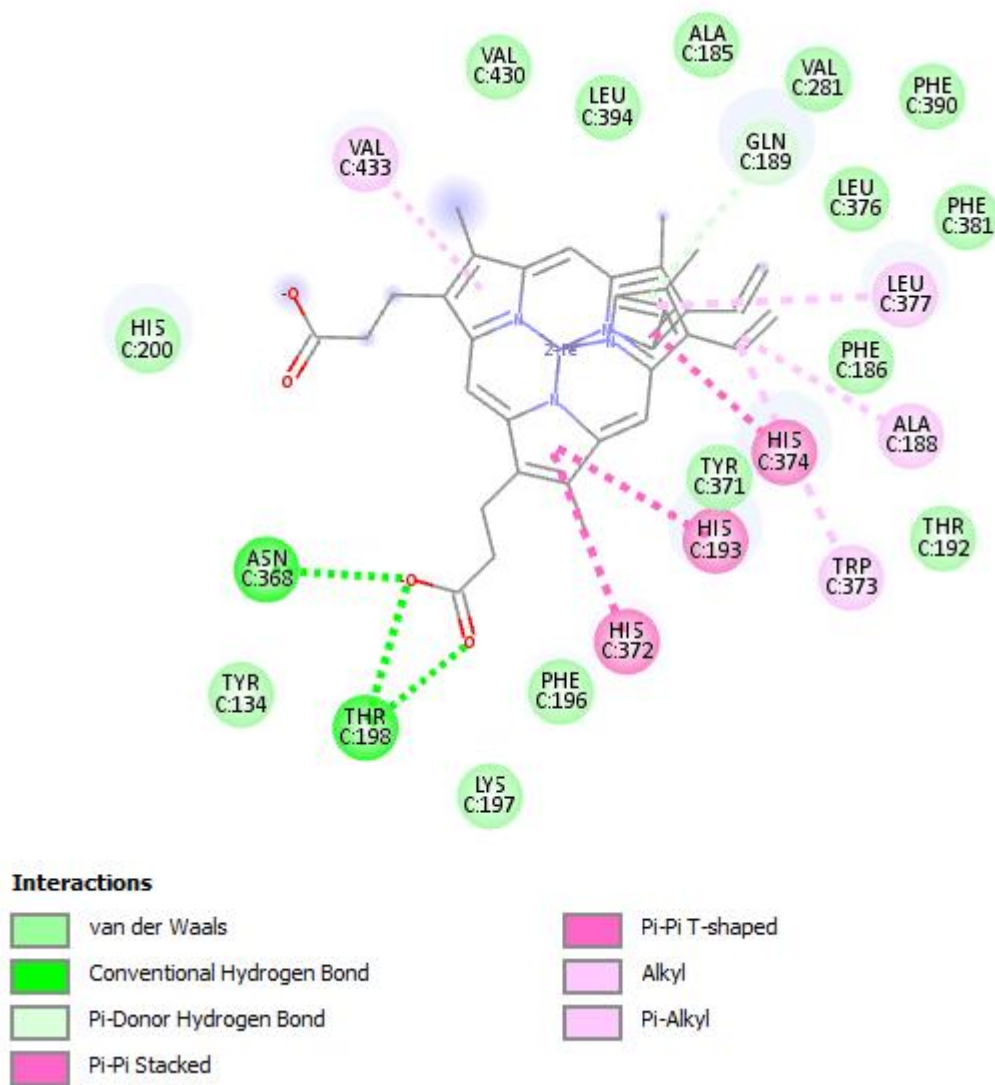
**LAMPIRAN 4
(LANJUTAN)**

No	Nama	Struktur 2D	Struktur 3D
28.	Quercituron	 The 2D chemical structure of Quercituron shows a central flavanone core. It features a 3,4,5-trihydroxyphenyl group at the 2-position and a 3,4-dihydroxyphenyl group at the 3-position. The C-4 position is substituted with a D-glucopyranosyl moiety. The glucose ring is shown in its chair conformation with hydroxyl groups at C-2, C-3, and C-6.	 The 3D ball-and-stick model of Quercituron illustrates the spatial arrangement of the atoms. Carbon atoms are shown in grey, oxygen in red, and hydrogen in white. The structure highlights the three-dimensional orientation of the phenolic rings and the glucose moiety.
29.	Sambunigrin	 The 2D chemical structure of Sambunigrin consists of a D-glucopyranose molecule with a cyanide group (-C≡N) attached to the C-2 position via an oxygen atom. The glucose ring is shown in its chair conformation.	 The 3D ball-and-stick model of Sambunigrin shows the spatial arrangement of the cyanide group and the glucose moiety. The cyanide group is represented by a blue nitrogen atom and a grey carbon atom triple-bonded to another grey carbon atom.
30.	Vitexin	 The 2D chemical structure of Vitexin features a flavanone core with a 3,4,5-trihydroxyphenyl group at the 2-position and a 4-hydroxyphenyl group at the 3-position. The C-4 position is substituted with a D-glucopyranosyl moiety. The glucose ring is shown in its chair conformation.	 The 3D ball-and-stick model of Vitexin illustrates the spatial arrangement of the atoms, showing the relative positions of the phenolic rings and the glucose moiety.

Gambar VI 1. Struktur 2D dan 3D Senyawa uji tanaman daun pepaya gunung

LAMPIRAN 5

VALIDASI METODE



Gambar VII 1. Hasil visualisasi interaksi ligan alami dengan reseptor COX-2

LAMPIRAN 6

HASIL PENAMBATAN MOLEKUL

Tabel V.2

Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor COX-2

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	PROTOPORPHYRIN IX CONTAINING FE (Ligan alami)	-11.74	10	ASN C:368 THR C:198 GLN C:189 HIS C:372 HIS C:193 HIS C:374 VAL C:433 LEU C:377 ALA C:188 TRP C:373	85.47
2	Celecoxib (pembanding)	-8.66	6	GLU A:506 GLU A:466 ARG A:453 LYS A:459 TYR A:461 LYS A:497	452.04
3	2,3 butanedione	-4.04	2	TRP C:373	1.10
4	4p Coumaroylquinic acid	-8.55	7	TRP C:373 HIS C:200 THR C:198 HIS C:374 HIS C:372 TYR C:371 HIS C:193	536.15
5	5 Deoxykaempferol	-9.76	8	THR C:192 ASN C:368 HIS C:374 TRP C:373 HIS C:193 HIS C:372 ALA C:188 LEU C:376	70.27
6	Benzyl thiourea	-5.50	2	TYR C:371 TRP C:373	93.72

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
7	Benzyl thiocyanate	-5.85	8	THR C:192 HIS C:193 TRP C:373 HIS C:374 ALA C:188 ALA C:185 14LEU C:15376 LEU1 C:377	51.52
8	Benzyl glucosinolate	-8.59	8	THR C:198 PHE C:196 GLN C:189 TRP C:373 HIS C:193 HIS C:372 HIS C:374	508.36
9	Carpaine	-7.94	1	THR C:198	1.52
10	Coumarin	-6.64	6	THR C:192 TRP C:373 TYR C:371 HIS C:193 HIS C:374 ALA C:188	13.51
11	Chlorogenic acid	-8.92	10	TRP C:373 ALA C:188 THR C:192 ASN C:368 TYR C:134 THR C:198 HIS C:374 TYR C:371 HIS C:193 HIS C:372	291.37
12	Dehydrocarpaine I	-7.15	3	GLU C:466 LYS C:471 TYR C:461	5.72

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
13	Dehydrocarpaine II	-11.00	5	THR C:198 HIS C:374 HIS C:200 LEU C:376 LEU C:377	8.67
14	Diacetone alcohol	-4.94	3	THR C:192 TYR C:371 TRP C:373	240.21
15	Dicoumarol	-10.17	10	TRP C:373 THR C:192 HIS C:193 HIS C:374 GLN C:189 HIS C:372 ALA C:185 ALA C:188 LEU C:376 LEU C:377	35.13
16	Ferulic acid	-6.60	7	THR C:192 HIS C:193 GLN C:189 TRP C:373 ALA C:188 PHE C:196 TYR C:371	14.45
17	Isopentyl benzoate	-7.17	7	THR C:192 TRP C:373 HIS C:193 HIS C:372 ALA C:185 LEU C:376 LEU C:377	5.56
18	Isopropyl butyrate	-4.98	2	THR C:192 TRP C:373	221.90

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
19	Isoquercitrin	-9.97	7	HIS C:193 LEU C:280 GLN C:189 TRP C:373 HIS C:374 LEU C:377 VAL C:281	49.02
20	Kaempferol	-9.32	6	THR C:192 THR C:198 ASN C:368 HIS C:374 HIS C:193 HIS C:372	142.28
21	Kaemferol 3 rhamnoside	-9.98	8	HIS C:193 HIS C:374 TYR C:371 TRP C:373 HIS C:372 GLN C:189 VAL C:281 LEU C:377	48.15
22	Kaemferol 3 OD glukosida	-10.91	8	LEU C:280 VAL C:277 HIS C:193 GLN C:189 TRP C:373 HIS C:374 LEU C:377 VAL C:281	10.01
23	Luteolin 7 glukosida	-10.27	5	THR C:192 PHE C:196 THR C:198 HIS C:193 LEU C:377	29.75
24	Lupeol	-8.54	2	HIS C:193 HIS C:372	553.99

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
25	Naringin	-10.79	12	TRP C:373 TYR C:371 PHE C:196 TYR C:134 ASN C:368 THR C:198 GLN C:189 HIS C:193 HIS C:372 HIS C:374 LEU C:377 VAL C:281 PHE C:381	12.39
26	Procyanidin	-11.89	12	LEU C:284 HIS C:193 VAL C:277 THR C:198 TYR C:134 ASN C:368 THR C:192 HIS C:374 LEU C:377 VAL C:281 HIS C:372 GLN C:189	1.92
27	Prunasin	-8.11	9	THR C:192 HIS C:374 ASN C:368 TYR C:371 ALA C:185 LEU C:376 LEU C:377 TRP C:373	1.14
28	Pseudocarpaine	-9.80	-	-	65.93

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa/Ligan	Energi Ikatan (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
29	Quercetin	-9.27	7	THR C:192 THR C:198 ASN C:368 HIS C:374 HIS C:193 HIS C:372 PHE C:196	161.41
30	Quercituron	-9.51	6	HIS C:193 GLN C:189 VAL C:277 LEU C:377 HIS C:374 VAL C:281	106.72
31	Sambunigrin	-8.29	6	THR C:192 ASN C:368 HIS C: 374 HIS C:372 ALA C:185 LEU C:376	842.66
32	Vitexin	-9.72	7	GLN C:189 HIS C:374 TYR C:371 TRP C:373 HIS C:193 LEU C:377 VAL C:281	74.88

LANJUTAN 6 (LANJUTAN)

Tabel V.3

Sifat Fisiko kimia Senyawa yang Terkandung Didalam Daun Pepaya Gunung
Berdasarkan Aturan Lipinski's Rule of Five

No	Senyawa Uji	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul (Dalton)	LogP	Memenuhi Syarat/Tidak
1.	2,3 butanedione	0	2	86,09	0,1644	Memenuhi Syarat
2.	4p Coumaroylquinic acid	5	7	338.312	-0,3515	Memenuhi Syarat
3.	5 Deoxykaempferol	3	5	270,24	2.5768	Memenuhi Syarat
4.	Benzyl thiourea	2	1	166.429	1.0198	Memenuhi Syarat
5.	Benzyl thiocyanate	0	2	149.218	2.40088	Memenuhi Syarat
6.	Benzyl glucosinolate	4	11	408.43	-1.4475	Tidak memenuhi
7.	Carpaine	2	6	478.718	5.566	Memenuhi Syarat
8.	Coumarin	0	2	146.145	1.793	Memenuhi Syarat
9.	Chlorogenic acid	6	8	354.311	-0.6459	Memenuhi Syarat
10.	Dehydrocarpaine I	1	6	476.702	6.0488	Tidak memenuhi
11.	Dehydrocarpaine II	0	6	474.686	6.5316	Tidak memenuhi
12.	Diacetone alcohol	1	2	116.16	0.7364	Memenuhi Syarat
13.	Dicoumarol	2	6	336.299	2.9014	Memenuhi Syarat
14.	Ferulic acid	2	3	194.186	1.4986	Memenuhi Syarat
15.	Isopentyl benzoate	0	2	192.258	2.8895	Memenuhi Syarat

**LAMPIRAN 6
(LANJUTAN)**

No	Senyawa Uji	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul (Dalton)	LogP	Memenuhi Syarat/Tidak
16.	Isopropyl butyrate	0	2	130.187	1.7381	Memenuhi Syarat
17.	Isoquercitrin	8	12	464.379	0.5389	Tidak memenuhi
18.	Kaempferol	4	6	286.239	2.2824	Memenuhi Syarat
19.	Kaemferol 3 rhamnoside	6	10	432.381	0.7831	Memenuhi Syarat
20.	Kaemferol 3 OD glukosida	7	11	448.38	-0.2445	Tidak memenuhi
21.	Luteolin 7 glukosida	7	11	448.38	-0.2445	Tidak memenuhi
22.	Lupeol	1	1	426.729	8.0248	Tidak memenuhi
23.	Naringin	8	14	580.539	-1.1652	Tidak memenuhi
24.	Procyanidin	5	10	394.525	2.7327	Memenuhi Syarat
25.	Prunasin	4	7	295.291	-0.9322	Memenuhi Syarat
26.	Pseudocarpaine	2	5	476.718	5.566	Tidak Memenuhi
27.	Quercetin	5	7	302.238	1.988	Memenuhi Syarat
28.	Quercituron	8	12	478.362	-0.4466	Tidak memenuhi
29.	Sambunigrin	4	7	295.291	-0.9322	Memenuhi Syarat
30.	Vitexin	7	10	432.381	0.0917	Tidak memenuhi

LAMPIRAN 7

HASIL PENGUJIAN PreADME

Tabel V.4
Uji PreADME

No	Senyawa/Ligan	Absorpsi		Distribusi
		Caco-2 cell (nm sec-1)	HIA (%)	Protein Plasma Binding (%)
1	2,3 butanedione	3.35	100	77.75
2	4p Coumaroylquinic acid	20.38	27.577	34.39
3	5 Deoxykaempferol	16.63	92.943	85.33
4	Benzyl thiourea	21	90.163	39.93
5	Benzyl thiocyanate	41.78	93.425	81.22
6	Benzyl glucosinolate	0.36	13.031	61.11
7	Carpaine	40.74	91.891	88.29
8	Coumarin	3.67	97.344	-
9	Chlorogenic acid	18.73	36.377	29.89
10	Dehydrocarpaine I	49.69	92.193	88.29
11	Dehydrocarpaine II	51.42	94.006	91.60
12	Diacetone alcohol	21.49	94.195	86.47
13	Dicoumarol	14.45	93.074	93.57
14	Ferulic acid	21.12	93.685	38.58
15	Isopentyl benzoate	44.27	95.156	94.78
16	Isopropyl butyrate	45.13	96.712	100
17	Isoquercitrin	9.43	47.999	59.15
18	Kaempferol	9.57	74.29	89.6
19	Kaemferol 3 rhamnoside	8.19	60.006	65.99
20	Kaemferol 3 OD glukosida	11.13	48.052	44.57
21	Luteolin 7 glukosida	4.86	37.556	44.37
22	Lupeol	47.17	95.782	100
23	Procyanidin	8.63	55.527	100
24	Naringin	7.8	25.796	51.06
25	Prunasin	3.17	47.261	38.34
26	Pseudocarpaine	48.33	91.891	80
27	Quercetin	3.41	77.207	93.23
28	Quercituron	11.50	25.112	62.01
29	Sambunigrin	3.17	47.261	38.34
30	Vitexin	5.48	46.695	40.99

LAMPIRAN 7 (LANJUTAN)

Keterangan: HIA (*Human Intestinal Absorpsi*) = 70-100% *well absorbed*

20-70 *moderately absorbed*

0-20% *poorly absorbed*

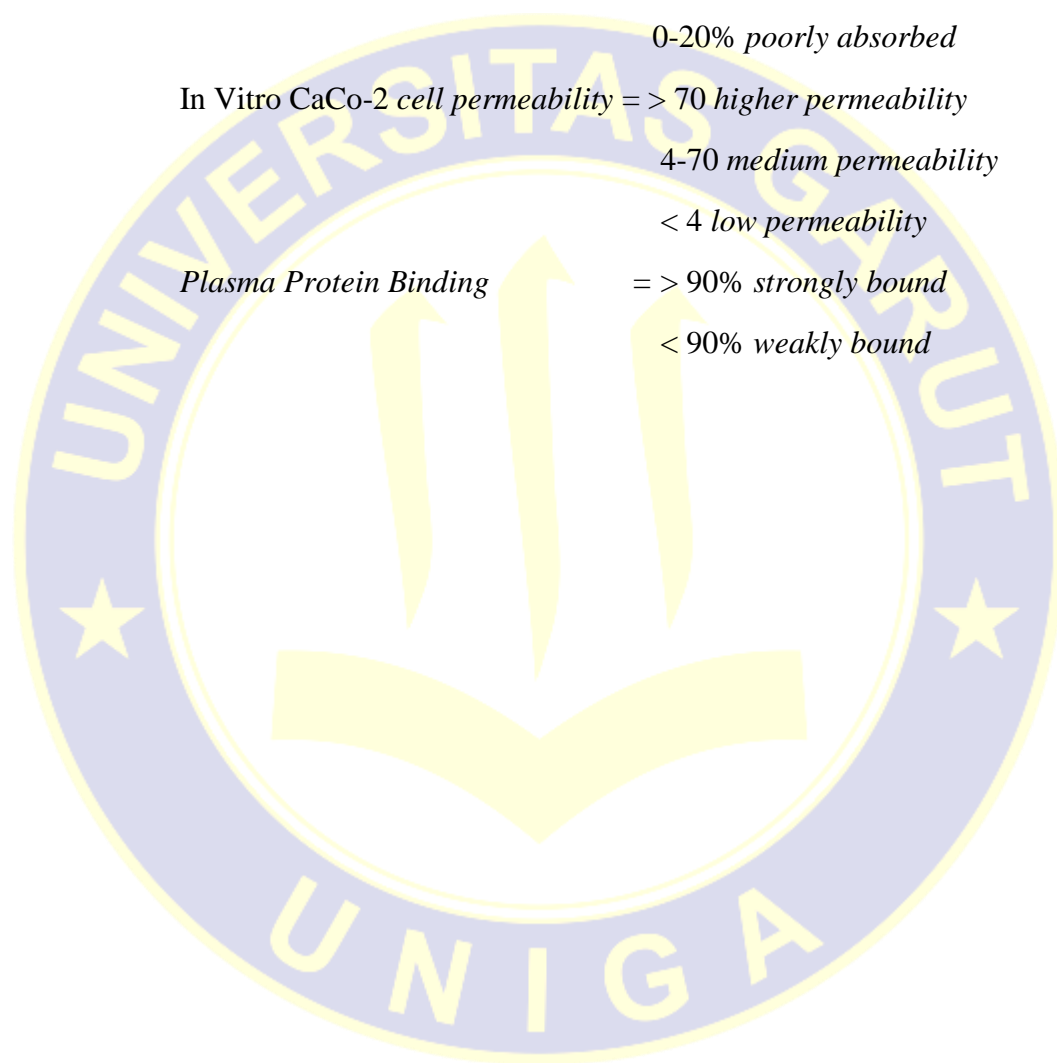
In Vitro CaCo-2 *cell permeability* = > 70 *higher permeability*

4-70 *medium permeability*

< 4 *low permeability*

Plasma Protein Binding = > 90% *strongly bound*

< 90% *weakly bound*



LAMPIRAN 8
UJI TOKSISITAS

Tabel V.5
Uji Toksisitas

No	Senyawa/Ligan	Ames Test	Karsinogenik	Hepatotoxicity	Skin Sensitisation
		Mutagen / Non-Mutagen	(-) / (+)		
1	2,3 butanedione	Non-Mutagen	(-)	No	Yes
2	4p Coumaroylquinic acid	Non-Mutagen	(-)	No	No
3	5 Deoxykaempferol	Non-Mutagen	(-)	No	No
4	Benzyl thiourea	Non-Mutagen	(-)	No	Yes
5	Benzyl thiocyanate	Non-Mutagen	(-)	No	Yes
6	Benzyl glucosinolate	Non-Mutagen	(-)	Yes	No
7	Carpaine	Non-Mutagen	(-)	No	No
8	Coumarin	Non-Mutagen	(+)	No	No
9	Chlorogenic acid	Non-Mutagen	(-)	No	No
10	Dehydrocarpaine I	Non-Mutagen	(-)	Yes	No
11	Dehydrocarpaine II	Non-Mutagen	(-)	No	No
12	Diacetone alcohol	Non-Mutagen	(-)	No	Yes
13	Dicoumarol	Mutagen	(+)	Yes	No
14	Ferulic acid	Non-Mutagen	(-)	No	No
15	Isopentyl benzoate	Non-Mutagen	(-)	No	Yes
16	Isopropyl butyrate	Non-Mutagen	(-)	No	Yes
17	Isoquercitrin	Non-Mutagen	(-)	No	No
18	Kaempferol	Non-Mutagen	(-)	No	No
19	Kaemferol 3 rhamnoside	Non-Mutagen	(-)	No	No
20	Kaemferol 3 OD glukosida	Non-Mutagen	(-)	No	No
21	Luteolin 7 glukosida	Non-Mutagen	(-)	No	No

**LAMPIRAN 8
(LANJUTAN)**

No	Senyawa/Ligan	Ames Test	Karsinogenik	Hepatotoxicity	Skin Sensitisation
22	Lupeol	Non-Mutagen	(-)	No	No
23	Naringin	Non-Mutagen	(-)	No	No
24	Procyanidin	Non-Mutagen	(-)	No	No
25	Prunasin	Non-Mutagen	(-)	No	No
26	Pseudocarpaine	Non-Mutagen	(-)	No	No
27	Quercetin	Non-Mutagen	(-)	No	No
28	Quercituron	Non-Mutagen	(-)	No	No
29	Sambunigrin	Non-Mutagen	(-)	No	No
30	Vitexin	Non-Mutagen	(-)	No	No

