

DAFTAR PUSTAKA

1. Setia AID, Tjitiaremi A. Aktivitas Antiinflamasi Dari Berbagai Tanaman : Sebuah Review. *Farmaka*. 2016;14(3):77-86.
2. Mahar M. *Farmakologi Dan Terapi*. 4th ed. (Sulistia GG, ed.). Gaya Baru; 2001.
3. Kemenkes RI. Hasil Riset Kesehatan Dasar Tahun 2018. *Kementrian Kesehat RI*. 2018;53(9):1689-1699.
4. Zahra AP, Carolia N. Obat Anti-inflamasi Non-steroid (OAINS) : Gastroprotektif vs Kardiotoksik. *Majority*. 2017;6:153-158.
5. Zullies Ikawati. *Farmakologi Molekular*. UGM PRESS; 2018.
6. Takeuchi K. Pathogenesis of NSAID-induced gastric damage: Importance of cyclooxygenase inhibition and gastric hypermotility. *World J Gastroenterol*. 2012;18(18):2147-2160. doi:10.3748/wjg.v18.i18.2147
7. Ngurah G, Candra H, Adnyana IM, Wijaya P. Molecular Docking Kaempferol sebagai Antiinflamasi pada Aterosklerosis secara In Silico Molecular Docking Kaempferol as Anti-Inflammatory in Atherosclerosis in Silico. 2021;7(1):13-18.
8. Arba M. *Buku Ajar Farmasi Komputasi*. Deepublish; 2019.
9. Endarini LH. *Farmakognosi Dan Fitokimia*. Kementrian Kesehatan RI; 2016.
10. Arifin B, Ibrahim S. Struktur, Bioaktivitas Dan Antioksidan Flavonoid. *J Zarah*. 2018;6(1):21-29. doi:10.31629/zarah.v6i1.313
11. Alfaridz F, Amalia R. Klasifikasi dan Aktivitas Farmakologi dari Senyawa Aktif Flavonoid. *Farmaka*. 2018;16(3):1-9.
12. Astuti S, Pengajar S, Teknologi J, et al. Isoflavon Kedelai Dan Potensinya Sebagai Penangkap Radikal Bebas. 2008;13(2):126-136.
13. Parwata IMO. *Kimia Organik Bahan Alam FLAVONOID*. Universitas Udayana; 2016.
14. Setyawan AD, Darusman LK. Review: Senyawa Biflavonoid pada *Selaginella Pal. Beauv.* dan Pemanfaatannya. *Biodiversitas*. 2008;9:64-81.
15. Chen L, Deng H, Cui H, et al. Inflammatory responses and inflammation-associated diseases in organs. *Oncotarget*. 2018;9(6):7204-7218. doi:10.18632/oncotarget.23208

16. Harvey RA, Champe PC. *Farmakologi: Ulasan Bergambar*. 4th ed. EGC Buku Kedokteran; 2013.
17. Rahayu L, Dewi RS, Ayu G. Uji Efek Anti-Inflamasi dan Analgesik Infusa Daun Senggani (*Melastoma malabathricum L.*) (Anti-Inflammation and Analgesic Test Effect of Senggani Leaves (*Melastoma malabathricum L.*) Infusion. 2016;14(1):93-98.
18. Kumar V, Abbas A, Aster J. *Buku Ajar Patologi Dasar*. 10th ed. (Ham M, Saraswati M, eds.). Elsevier; 2020.
19. Rahmi E, Pahriyani A. *Modul Pembelajaran Patofisiologi Dan Patologi Klinik*. Media Sains Indonesia; 2021.
20. Joyce LK, Evelyn RH. *Farmakologi: Pendekatan Proses Keperawatan*. (Yasmin A, ed.). EGC Buku Kedokteran; 1996.
21. Ernawati T. Penapisan Virtual Senyawa Turunan Metil Sinamat Pada Enzim Siklooksigenase-2 (COX-2). *Pus Penelit Kim*. 2012;14(ISSN 0853-2788):1-9.
22. Muchtaridi, Yanuar Arry, Megantara Sandra P. *Kimia Medisinal Dasar-Dasar Dalam Perancangan Obat*. Prenadamedia Group; 2018.
23. Rollando. *Pengantar Kimia Medisinal*. CV. Seribu Bintang; 2017.
24. Khaerunnisa S, Suhartati, Awaluddin R. *Penelitian in Silico Untuk Pemula*. Airlangga University Press; 2020.
25. Yang SY. Pharmacophore modeling and applications in drug discovery: Challenges and recent advances. *Drug Discov Today*. 2010;15(11-12):444-450. doi:10.1016/j.drudis.2010.03.013
26. Meng X-Y, Zhang H-X, Mezei M, Cui M. *Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery*.
27. Chen X, Li H, Tian L, Li Q, Luo J, Zhang Y. Analysis of the Physicochemical Properties of Acaricides Based on Lipinski's Rule of Five. *J Comput Biol*. 2020;27(9):1397-1406. doi:10.1089/cmb.2019.0323
28. Hamid N, Razak R, Najib A. *Virtual Screening Senyawa Kimia Tumbuhan Terap (Artocarpus Elasticus) Terhadap Reseptor Alpha Estrogen*. PT. Nasya Expanding Management; 2021.
29. Widodo, Miftahhunnafisah. Pengenalan NCBI untuk analisis DNA, protein dan senyawa kimia. Published online 2012:1-22.
30. Kartasmita RE, Anugrah R, Tjahjono DH. Kajian Docking Dan Prediksi Beberapa Aspek Farmakokinetika Desain Molekul Turunan Kuinin Sebagai Upaya Menemukan Kandidat Senyawa Antimalaria Yang Baru. *Kartika J*

Ilm Farm. 2015;3(1):6-13. doi:10.26874/kjif.v3i1.13

31. Pratiwi D, Insanu M, Damayanti S. Studi in Silico Senyawa Antioksidan Alami Golongan Steroid Pada Reseptor Sistem Reproduksi. *Indones Nat Res Pharm J.* 2016;1(1):22-35.
32. Wang Q, He J, Wu D, Wang J, Yan J, Li H. Interaction of α -cyperone with human serum albumin: Determination of the binding site by using Discovery Studio and via spectroscopic methods. *J Lumin.* 2015;164:81-85. doi:10.1016/j.jlumin.2015.03.025
33. Agustina W, Susanti E, Yunita N, Yamtinah S. *Modul Chem Office (Chem Draw & Chem 3D).*; 2018.
34. Mysinger MM, Carchia M, Irwin JJ, Shoichet BK. Directory of useful decoys, enhanced (DUD-E): Better ligands and decoys for better benchmarking. *J Med Chem.* 2012;55(14):6582-6594. doi:10.1021/jm300687e
35. Liu T, Lin Y, Wen X, Jorissen RN, Gilson MK. BindingDB: A web-accessible database of experimentally determined protein-ligand binding affinities. *Nucleic Acids Res.* 2007;35(SUPPL. 1):198-201. doi:10.1093/nar/gkl999
36. Krishna S, Singh DK, Meena S, Datta D, Siddiqi MI, Banerjee D. Pharmacophore-based screening and identification of novel human ligase i inhibitors with potential anticancer activity. *J Chem Inf Model.* 2014;54(3):781-792. doi:10.1021/ci5000032
37. Ferreira LG, Dos Santos RN, Oliva G, Andricopulo AD. *Molecular Docking and Structure-Based Drug Design Strategies.* Vol 20.; 2015. doi:10.3390/molecules200713384
38. Sari IW, Junaidin J, Pratiwi D. STUDI MOLECULAR DOCKING SENYAWA FLAVONOID HERBA KUMIS KUCING (*Orthosiphon stamineus* B.) PADA RESEPTOR α -GLUKOSIDASE SEBAGAI ANTIDIABETES TIPE 2. *J Farmazine.* 2020;7(2):54. doi:10.47653/farm.v7i2.194
39. Lohning AE, Levonis SM, Williams-Noonan B SS. A Practical Guide to Molecular Docking and Homology Modelling for Medicinal Chemists. *Curr Top Med Chem.* 2017;17(18):2023-2040. doi:10.2174/1568026617666170130110827
40. Sharma N, Sharma M, Shakeel E, Jamal QMS, Kamal MA, Sayeed U, Khan MKA, Siddiqui MH, Arif JM AS. Molecular Interaction and Computational Analytical Studies of Pinocembrin for its Antiangiogenic Potential Targeting VEGFR-2: A Persuader of Metastasis. *Med Chem.* 2018;14(6):626-640. doi:10.2174/1573406414666180416125121

41. Schleinkofer K, Wang T, Wade RC. Molecular Docking. *Encycl Ref Genomics Proteomics Mol Med*. 2006;443:1149-1153. doi:10.1007/3-540-29623-9_3820
42. Fakih TM, Jannati FA, Meilani A, Ramadhan DSF, Darusman F. Studi In Silico Aktivitas Analog Senyawa Zizyphine dari Bidara Arab (*Zizyphus spina-christi*) sebagai Antivirus SARS-CoV-2 terhadap Reseptor 3CLpro. *ALCHEMY J Penelit Kim*. 2022;18(1):70-79. doi:10.20961/alchemy.18.1.52188.70-79
43. Nursamsiar, Toding AT, Awaluddin A. Studi In Silico Senyawa Turunan Analog Kalkon Dan Pirimidin Sebagai Antiinflamasi: Prediksi Absorpsi, Distribusi, dan Toksisitas. *Pharmacy*. 2016;13(01):92-100.
44. Suherman M, Prasetiawati R, Ramdani D, et al. Jurnal Ilmiah Farmako Bahari (*Tamarindus indica* L .) ON SELECTIVE INHIBITOR SIKLOOKSIGENASE-2 SKRINING VIRTUAL SENYAWA AKTIF ASAM JAWA (*Tamarindus indica* L .) TERHADAP SELEKTIF INHIBITOR. *J Ilm Farm Bahari*. Published online 2020:125-136.
45. Fakih TM, Putri NWRP, Marillia V, Ramadhan DSF, Darusman F. Identifikasi Aktivitas Biologis, Prediksi Toksisitas, dan Molecular Docking Senyawa Jubanine dari Tanaman Bidara Arab sebagai Kandidat Antivirus SARS-CoV-2. *J Ris Kim*. 2022;13(1):111-121. doi:10.25077/jrk.v13i1.437

LAMPIRAN 1

SENYAWA FLAVONOID DAN SUMBERNYA

Tabel VII.1
Daftar Senyawa Flavonoid dan Sumber Tanamannya

No.	Flavonoid	Sumber Tanaman
Flavon		
1.	Chrysin	<i>Populus</i>
2.	Baicalein	<i>Scutellaria</i>
3.	Apigenin	<i>Petroselinum</i>
4.	Acacetin	<i>Robinia</i>
5.	Scurelarein	<i>Scutellaria</i>
6.	Hispidulin	<i>Ambrosia</i>
7.	Luteolin	<i>Reseda</i>
8.	Chryseoriol	<i>Eriodyction</i>
9.	Diosmetin	<i>Diosma</i>
10.	Tricetin	<i>Lathyrus</i>
11.	Tangeretin	<i>Diosma</i>
12.	Wogonin	<i>Lathyrus</i>
13.	Trisin	Jeruk Nipis
14.	Rhoifoin	<i>Triticum</i>
Flanovol		
15.	Galangin	<i>Alpinia</i>
16.	Fisetin	<i>Rhus</i>
17.	Kaemferol	<i>Delphinium</i>
18.	Kaemferide	<i>Alpinia</i>
19.	Robinetin	<i>Robina</i>
20.	Herbasetin	<i>Gossypium</i>
21.	Quercetin	<i>Quercus</i>
22.	Rhamnetin	<i>Rhamnus</i>

**LAMPIRAN 1
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

No.	Flavonoid	Sumber Tanaman
23.	Isorhamnetin	<i>Cheirhantus</i>
24.	Myricetin	<i>Myrica</i>
25.	Quersetagenin	<i>Tagetes</i>
26.	Gossypetin	<i>Gossypium</i>
27.	Isoquercetin	Apel, anggur merah, asam citrus, bawang, brokoli, cerry, gandum, letus, mangga, teh tomat
28.	Ramnazin	
29.	Rutin	
30.	Morin	
31.	Pachypodol	
Isoflavon		
32.	Daidzein	<i>Pueraria</i>
33.	Formononetin	<i>Ononis</i>
34.	Genistein	<i>Genista</i>
35.	Biokanin A	<i>Cicer</i>
36.	Orobol	<i>Orobus</i>
37.	Tectorigenin	<i>Iris</i>
38.	Baptigenin	<i>Baptisia</i>
Flavanon		
39.	Pinocembrin	<i>Pinus</i>
40.	Liquiririgenin	<i>Glycyrrhiza</i>
41.	Narigenin	<i>Prunus</i>
42.	Sakuranetin	<i>Prunus</i>
43.	Eriodictyol	<i>Eriodictyon</i>
44.	Hesperitin	<i>Prunus</i>
45.	Homoeriodictyol	<i>Citrus maxima</i>

**LAMPIRAN 1
(LANJUTAN)**

**Tabel VII.1
Lanjutan**

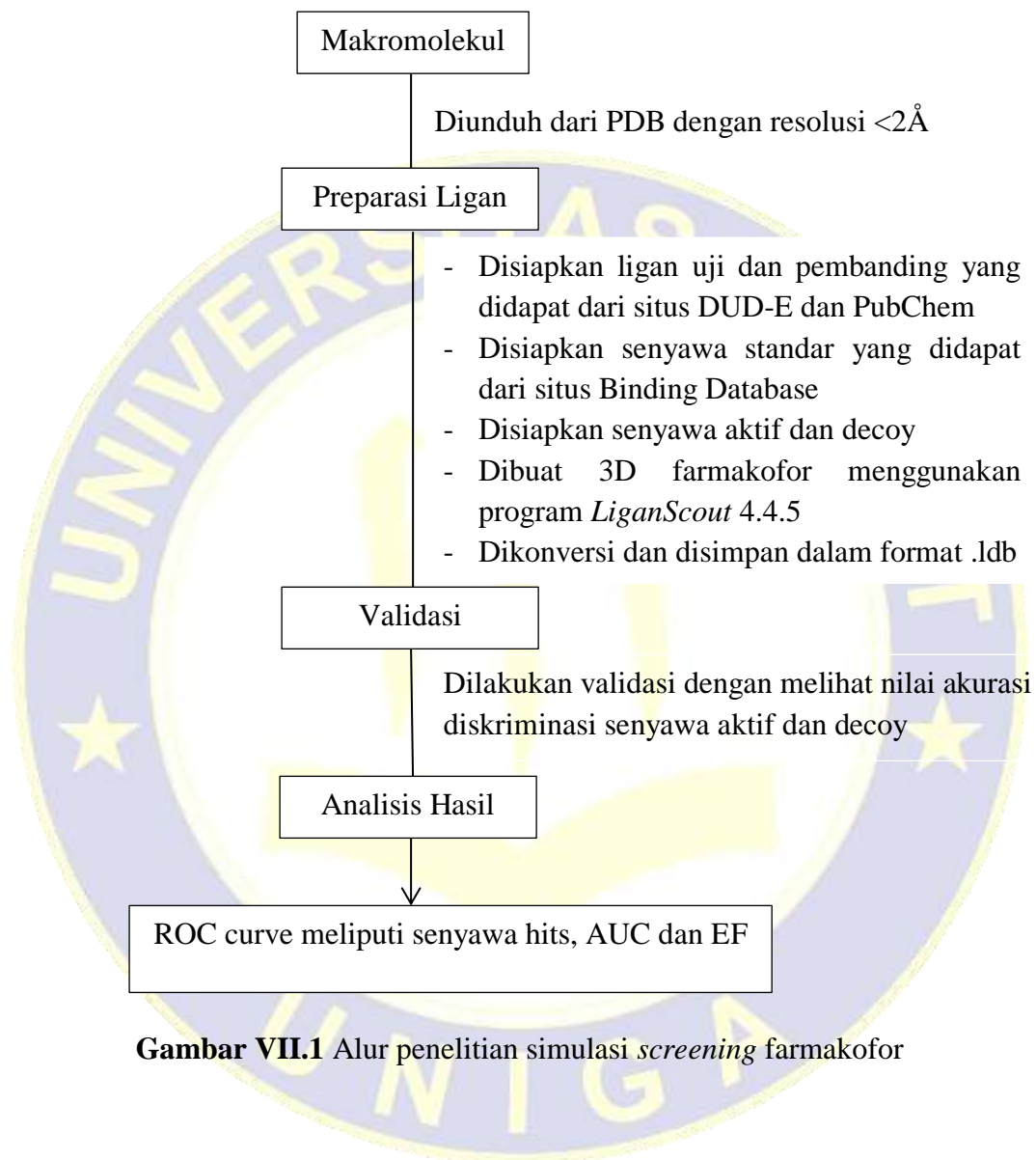
No.	Flavonoid	Sumber Tanaman
46.	Parietin	<i>Citrus maxima</i>
47.	Epigallocatechin	<i>Camellia sinensis</i>
48.	Catechin	<i>Camellia sinensis</i>
49.	Naringin	<i>Citrus maxima</i>
Dehidroflavonol		
50.	Pinobanksin	<i>Pinus</i>
51.	Aromadendron	<i>Eucalyptus</i>
52.	Fustin	<i>Rhus</i>
53.	Taxifolin	<i>Pseudotsuga</i>
Biflavonoid		
54.	Agathisflavone	<i>Agathis</i>
55.	Cupresuflavone	<i>Cupressus</i>
56.	Ginkgetin	<i>Cupressus</i>
57.	Siadopitisin	<i>Ginkgo</i>
58.	Robustaflavone	<i>Ginkgo</i>
59.	Hinokiflavone	<i>Agathis</i>
60.	Ochnaflavone	<i>Cupressus</i>
61.	Amentoflavone	<i>Ochna</i>
Khalkon		
62.	Isoliquiritigenin	<i>Acacia</i>
63.	Khalkonarigenin	<i>Salix</i>
64.	Butein	<i>Acacia</i>
65.	Okanin	<i>Acacia</i>
66.	Phloterin	Strawberry, Tomat
67.	Phlorizin	

**LAMPIRAN 1
(LANJUTAN)**

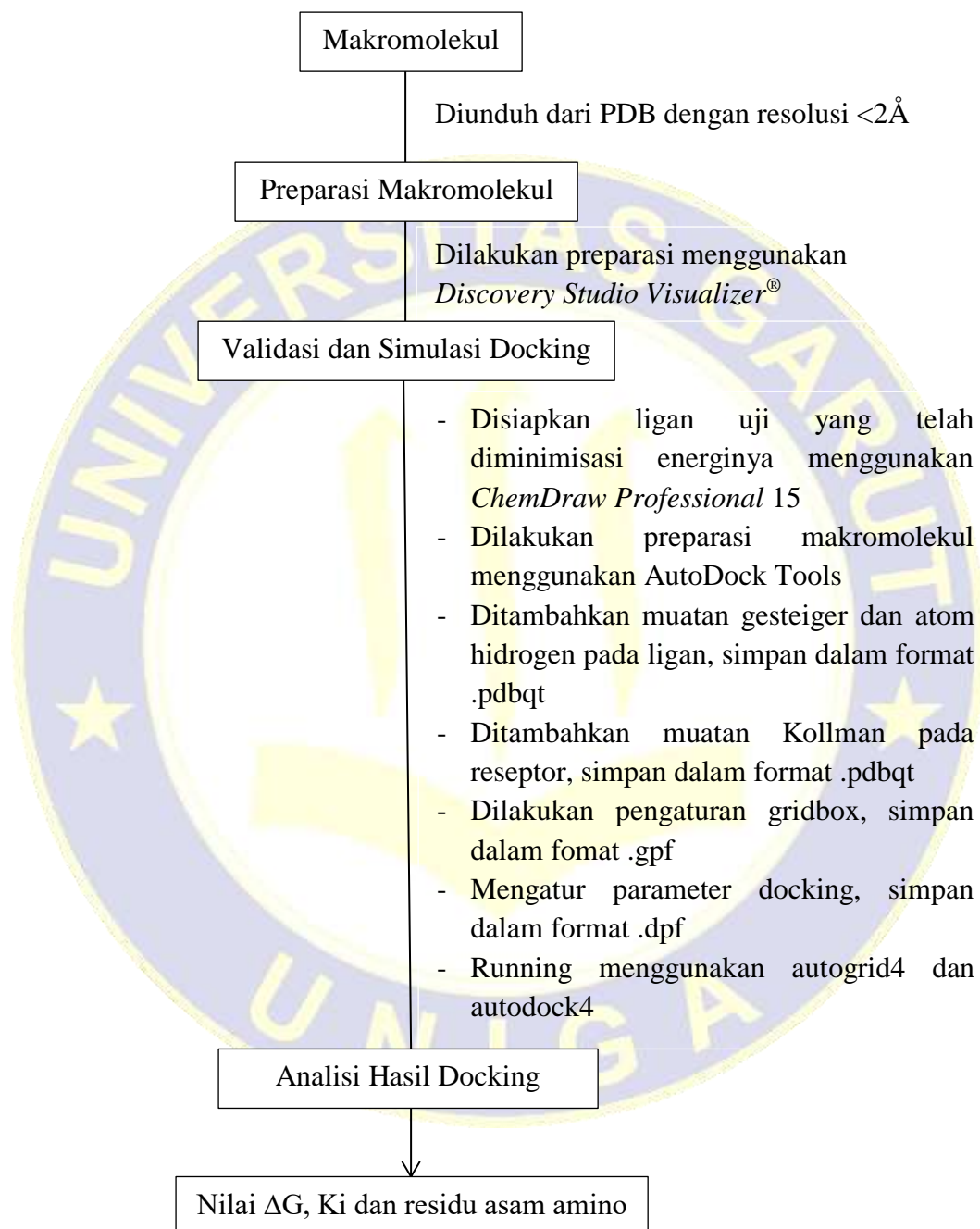
Tabel VII.1
Lanjutan

No.	Flavonoid	Sumber Tanaman
Auron		
68.	Sulfuretin	<i>Bidens</i>
69.	Aureusidin	<i>Antirrhinum</i>
70.	Maritimetin	<i>Bidens</i>
71.	Leptosidin	<i>Coreopsis</i>
Antosianidin		
72.	Apigenidin	<i>Rechsteineria</i>
73.	Luteolinidin	<i>Rechsteineria</i>
74.	Pelargonidin	<i>Pelargonium</i>
75.	Cyanidin	<i>Centaurea</i>
76.	Peonidin	<i>Paeonia</i>
77.	Delpinidin	<i>Delphinium</i>
78.	Petunidin	<i>Petunia</i>
79.	Malvidin	<i>Malva</i>
80.	Rosinidin	Kacang

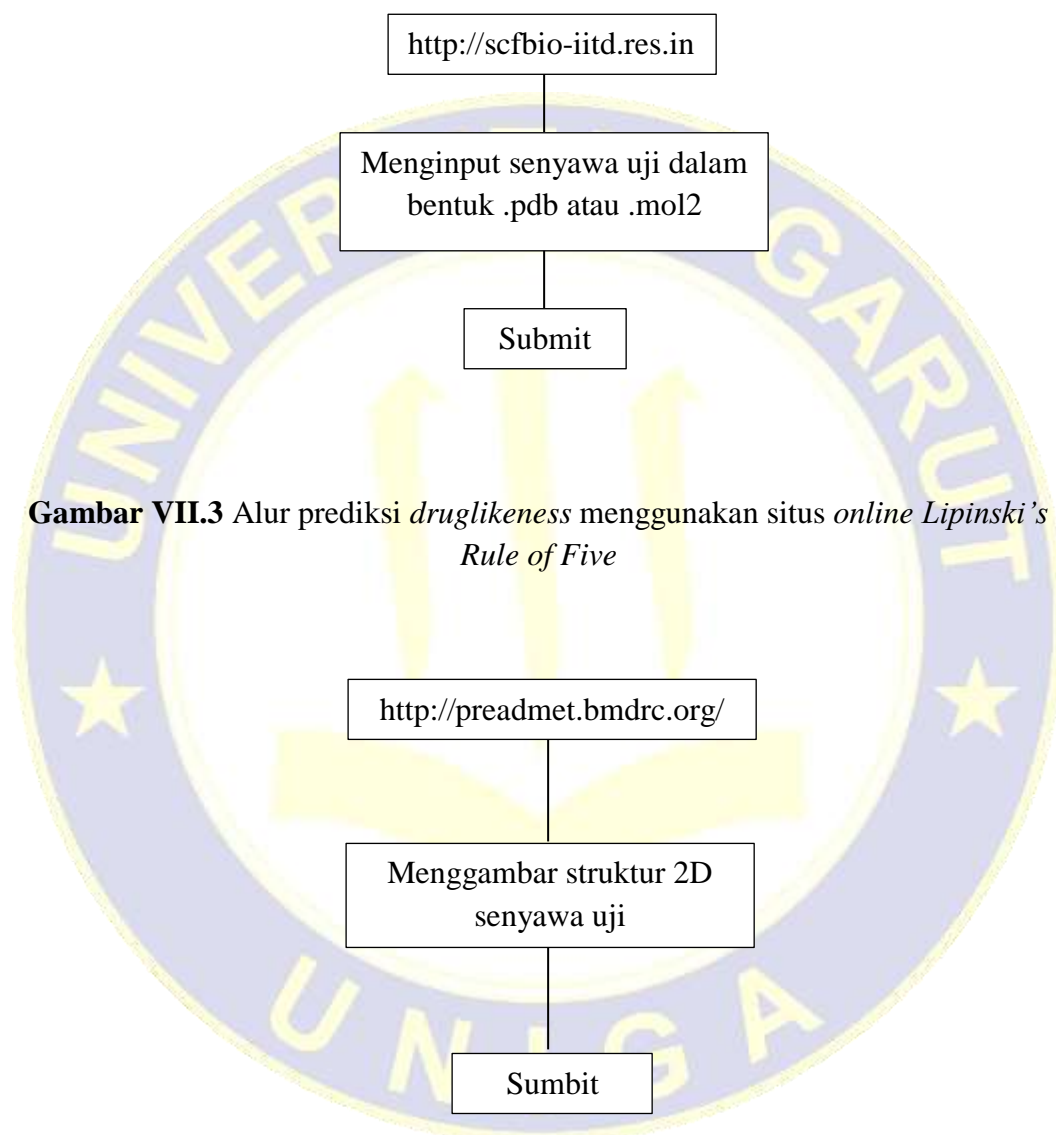
LAMPIRAN 2

ALUR PENELITIAN SIMULASI *SCREENING* FARMAKOFOR**Gambar VII.1** Alur penelitian simulasi *screening* farmakofor

LAMPIRAN 3

ALUR PENELITIAN *MOLECULAR DOCKING*Gambar VII.2 Alur penelitian *molecular docking*

LAMPIRAN 4

ALUR PENELITIAN PREDIKSI *DRUGLIKENESS* dan PREDIKSI FARMAKOKINETIK

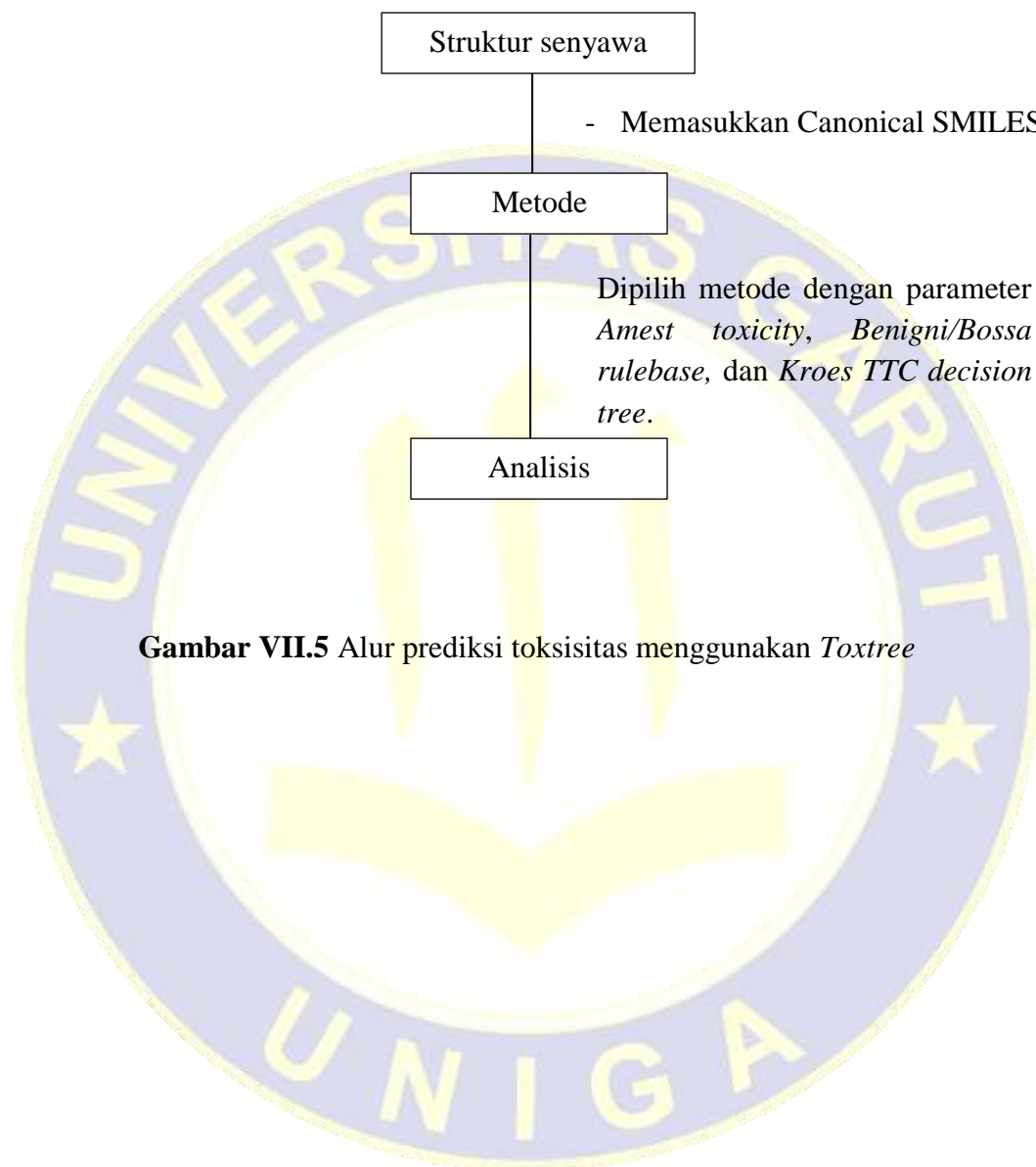
Gambar VII.3 Alur prediksi *druglikeness* menggunakan situs online *Lipinski's Rule of Five*



Gambar VII.4 Alur prediksi farmakokinetik menggunakan situs online *PreADMET*

LAMPIRAN 5

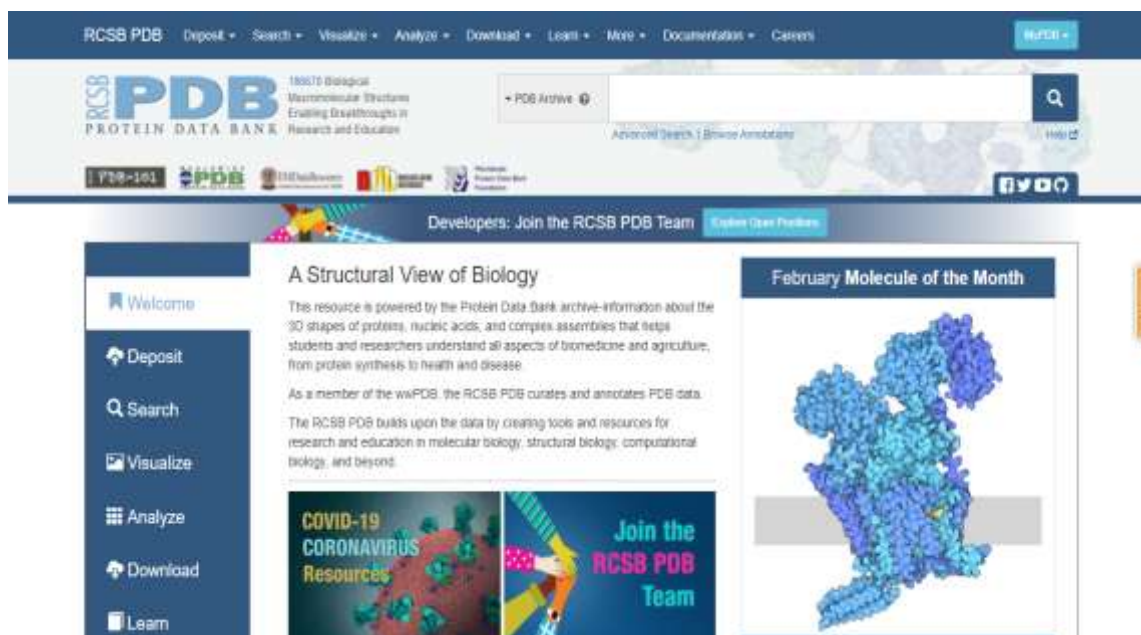
ALUR PENELITIAN PREDIKSI TOKSISITAS



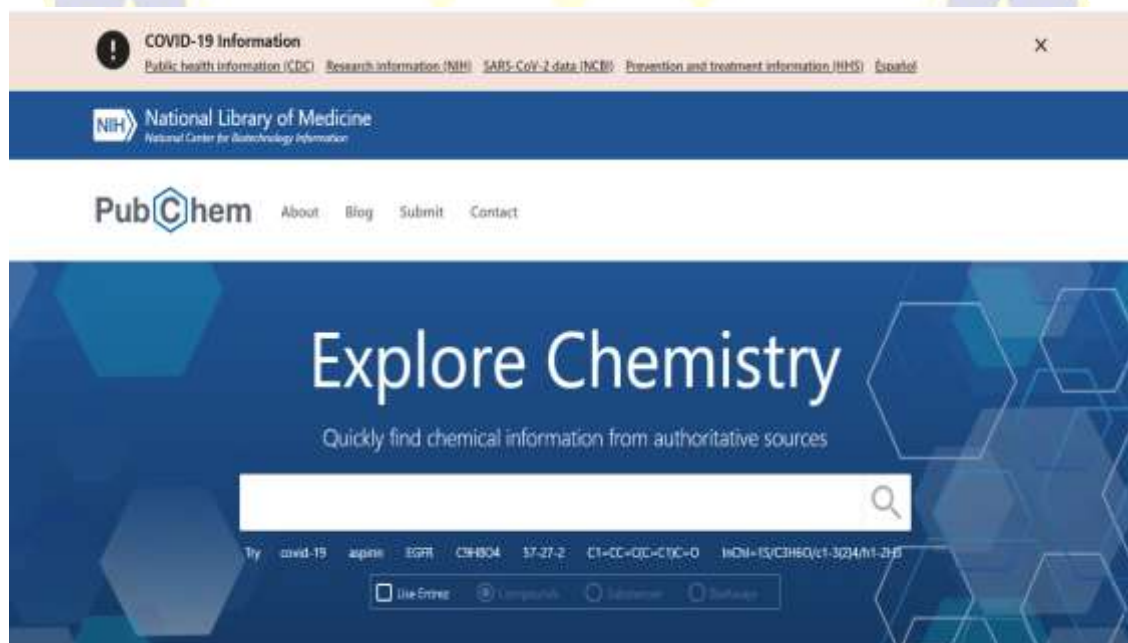
Gambar VII.5 Alur prediksi toksisitas menggunakan *Toxtree*

LAMPIRAN 6

SITUS DAN APLIKASI

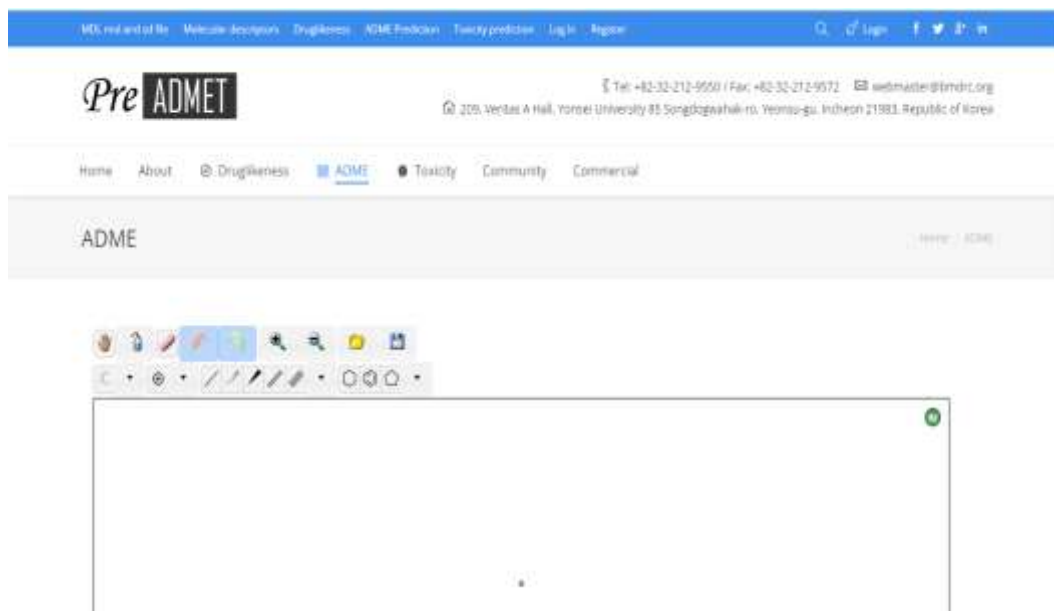


Gambar VII.6 Tampilan situs *Protein Data Bank* (PDB)



Gambar VII.7 Tampilan situs *PubChem*

LAMPIRAN 6 (LANJUTAN)



Gambar VII.8 Tampilan situs *PreADMET*



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

LAMPIRAN 6 (LANJUTAN)

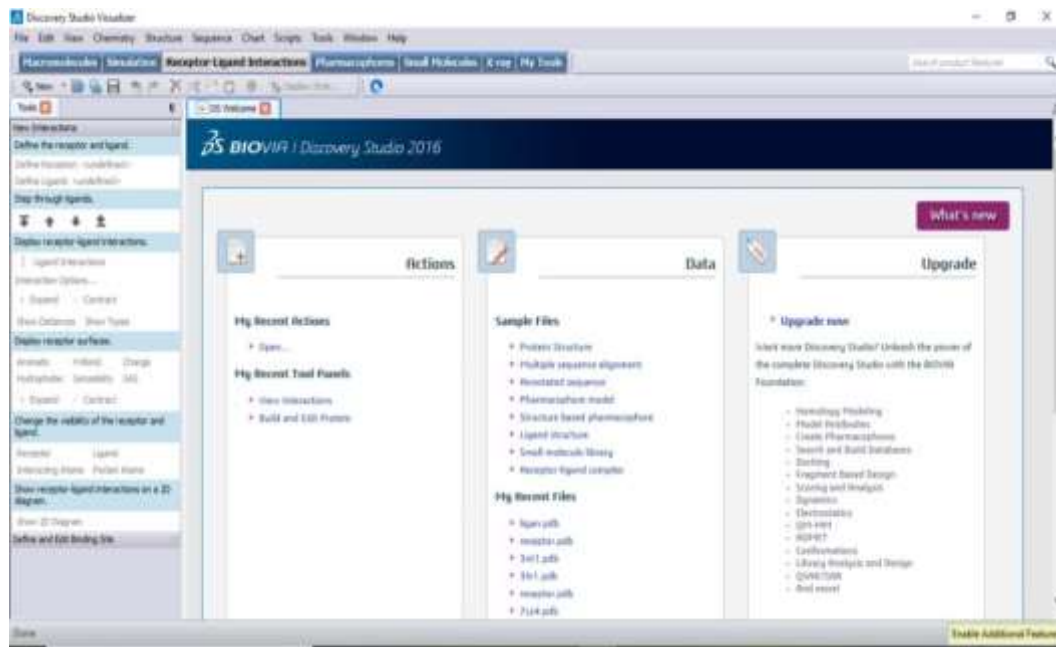


Gambar VII.10 Tampilan situs *DUD-E*

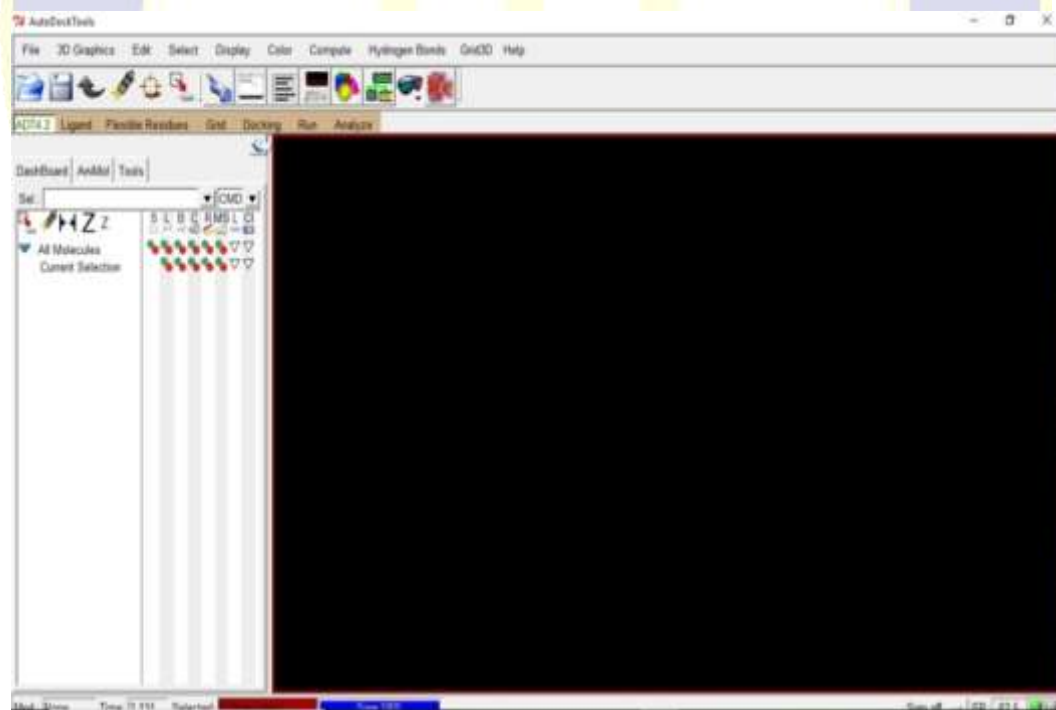


Gambar VII.11 Tampilan situs *Binding Database*

LAMPIRAN 6 (LANJUTAN)

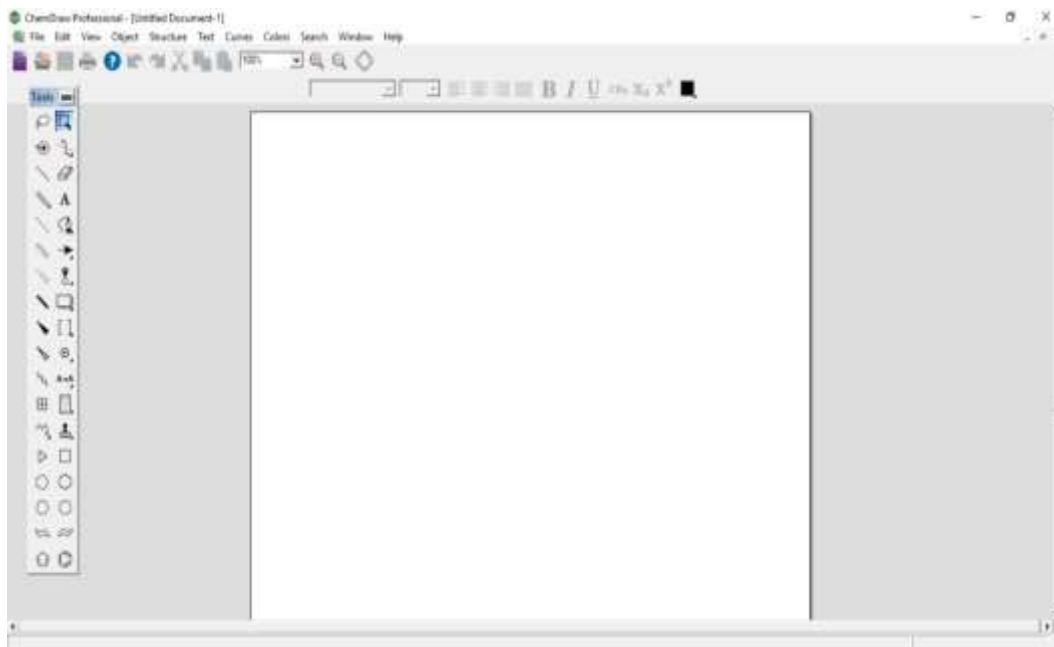


Gambar VII.12 Tampilan aplikasi *Discovery Studio Visualizer 2016*[®]

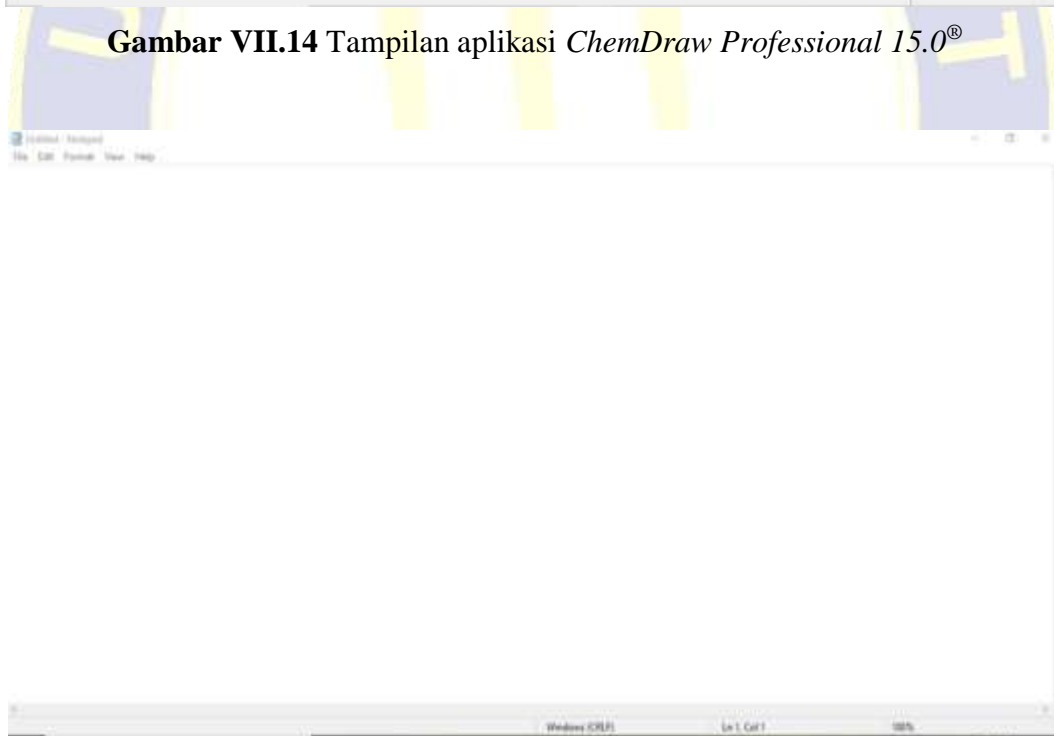


Gambar VII.13 Tampilan aplikasi *AutoDock Tools 1.5.6*[®]

LAMPIRAN 6 (LANJUTAN)



Gambar VII.14 Tampilan aplikasi *ChemDraw Professional 15.0*[®]

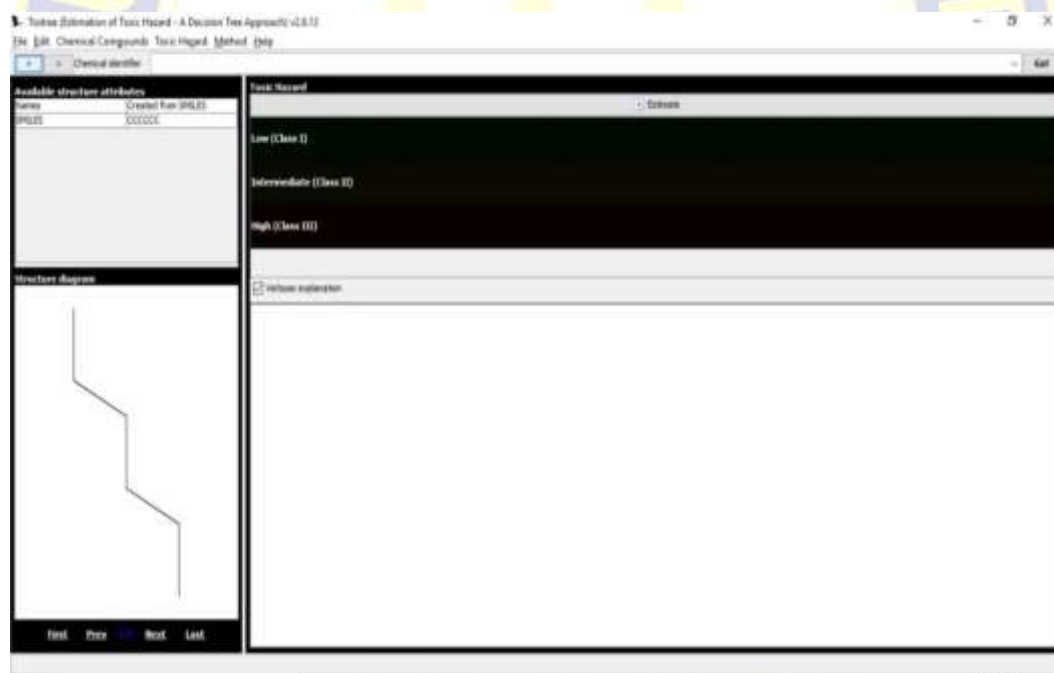


Gambar VII.15 Tampilan aplikasi *Notepad*[®]

LAMPIRAN 6 (LANJUTAN)



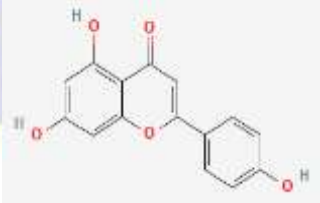
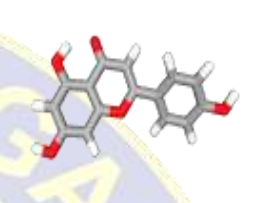
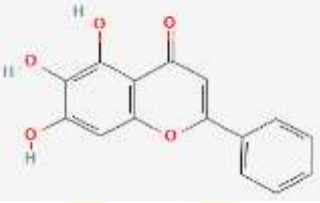
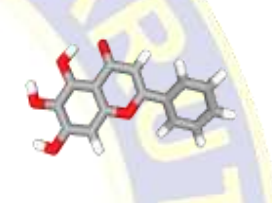
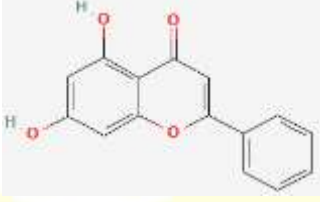
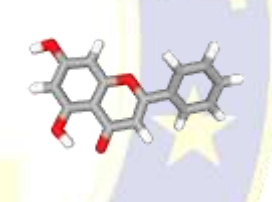
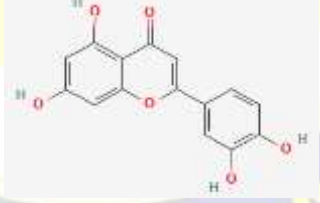
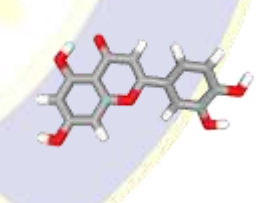
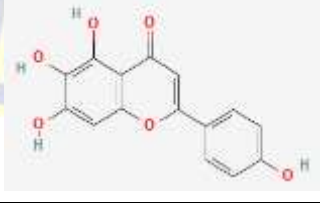
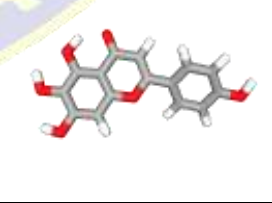
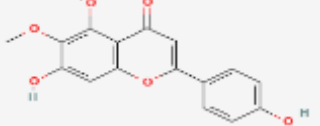
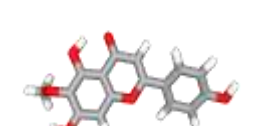
Gambar VII.16 Tampilan aplikasi *LiganScout 4.4.5*[®]



Gambar VII.17 Tampilan aplikasi *Toxtree 2.6.13*[®]

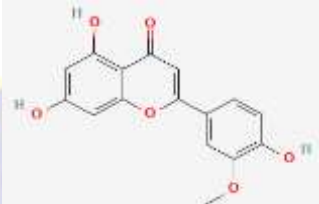
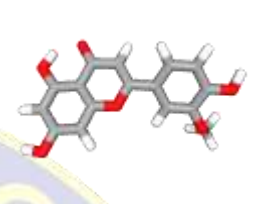
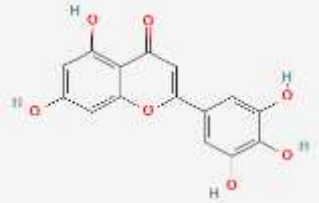
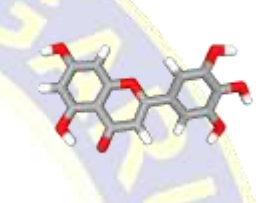
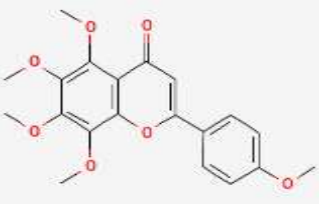
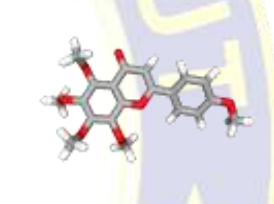
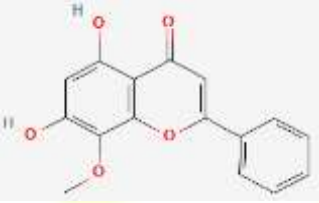

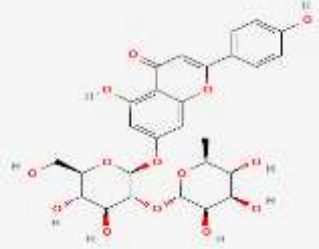

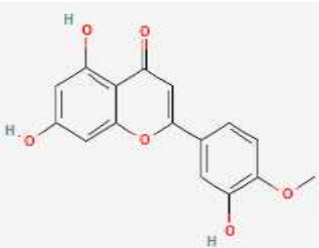
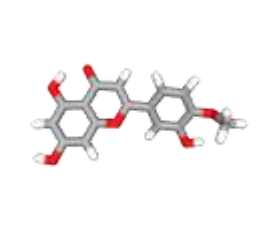
LAMPIRAN 7
STRUKTUR SENYAWA FLAVONOID

Tabel VII.2
Struktur 2D dan 3D Senyawa Flavonoid

No.	Flavonoid	Struktur 2D	Struktur 3D
Flavon			
1.	Apigenin		
2.	Baicalein		
3.	Chrysin		
4.	Luteolin		
5.	Scutelarein		
6.	Hispidulin		

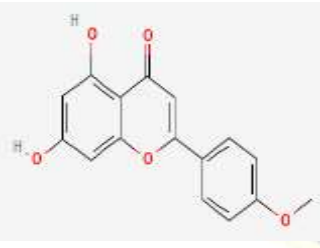
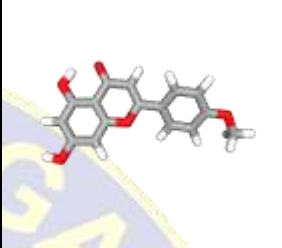
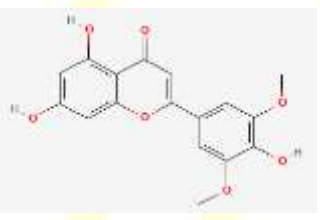
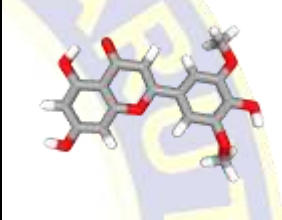
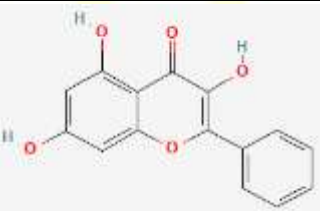
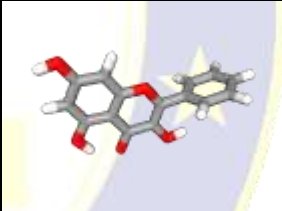
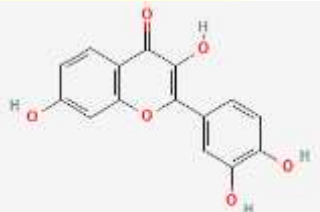
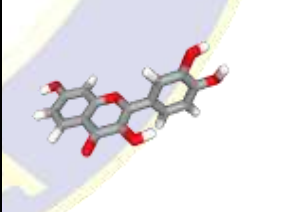
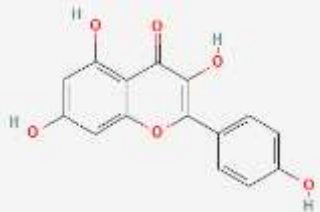
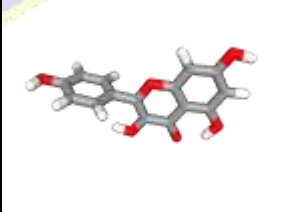
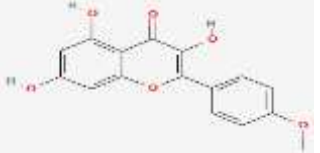
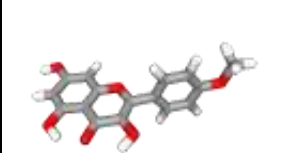
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
7.	Chrysoeriol		
8.	Tricetin		
9.	Tangeretin		
10.	Wogonin		
11.	Rhoifolin		
12.	Diosmetin		

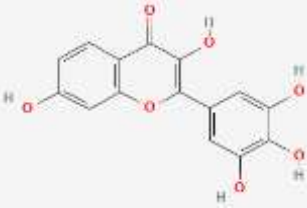
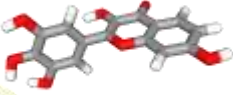
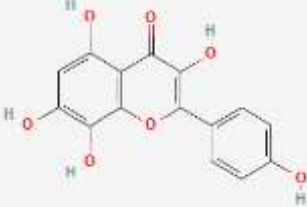
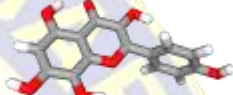
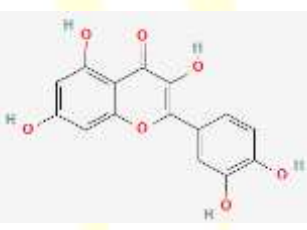
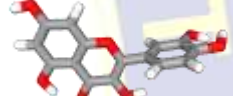
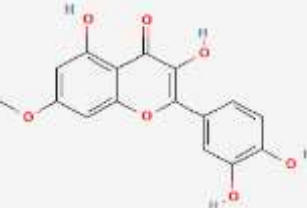
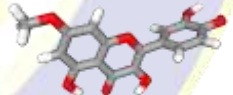
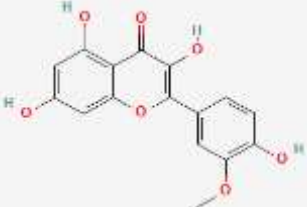
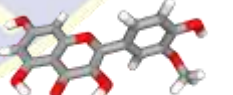
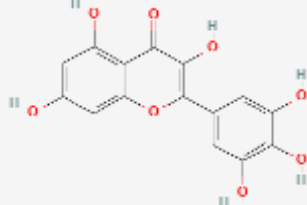
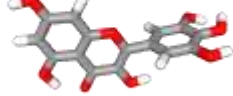
**LAMPIRAN 7
(LANJUTAN)**

Tabel VII.2
Lanjutan

No.	Flavonoid	Struktur 2D	Struktur 3D
13.	Acacetin		
14.	Tricin		
Flavonol			
15.	Galangin		
16.	Fisetin		
17.	Kaempferol		
18.	Kaempferide		

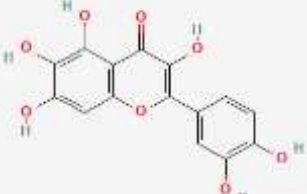
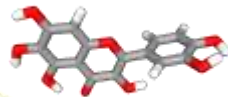
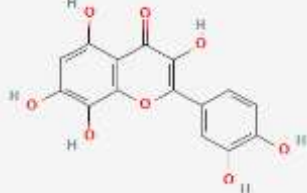
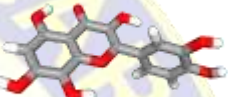
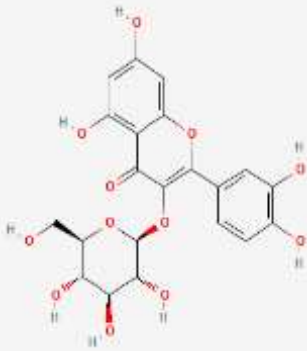
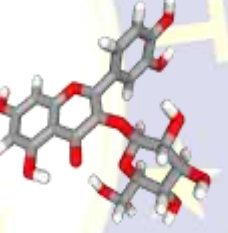
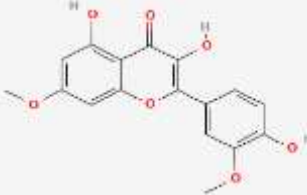
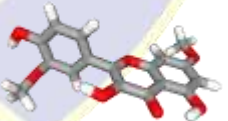

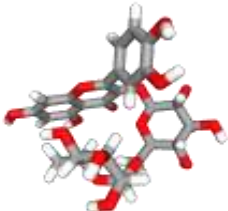
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
19.	Robinetin		
20.	Herbasetin		
21.	Quercetin		
22.	Rhamnetin		
23.	Isorhamnetin		
24.	Myricetin		

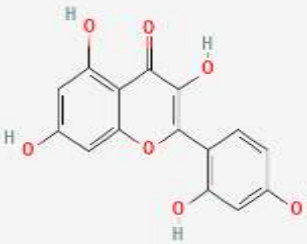
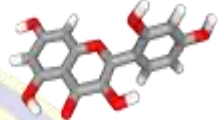
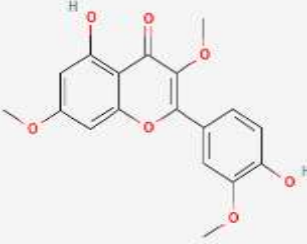
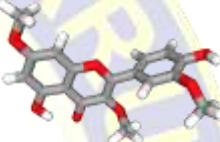
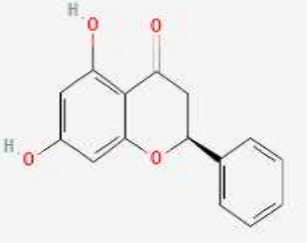
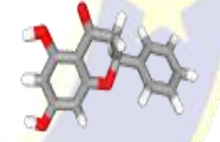
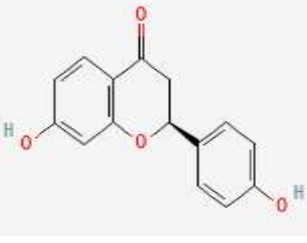
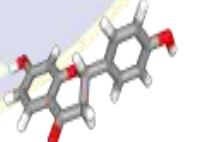
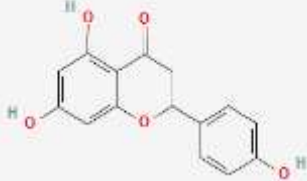
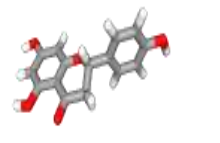
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
25.	Quersetagenin		
26.	Gossypetin		
27.	Isoquercetin		
28.	Ramnazin		
29.	Rutin		

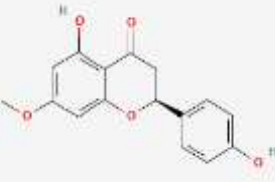
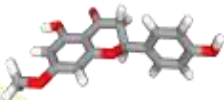
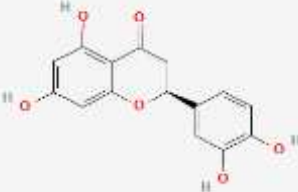
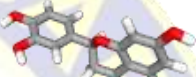
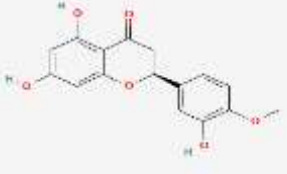
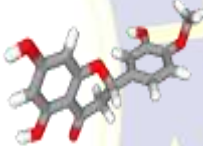
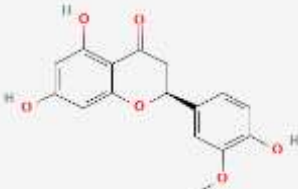
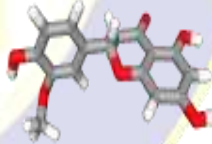
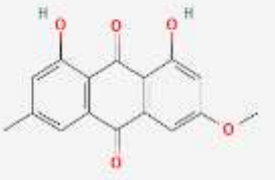
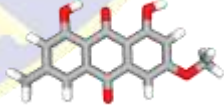
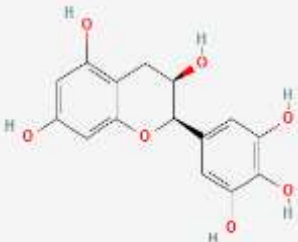
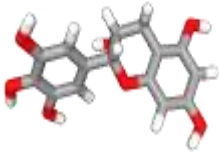
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
30.	Morin		
31.	Pachypodol		
Flavanon			
32.	Pinocembrin		
33.	Liquiritigenin		
34.	Narigenin		

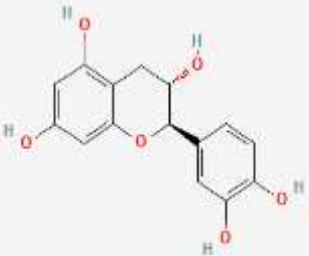
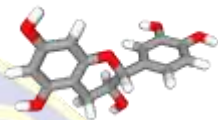
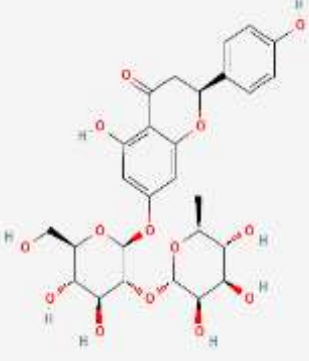
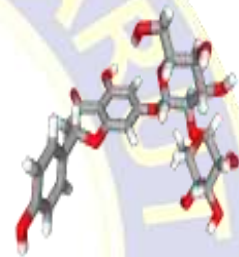
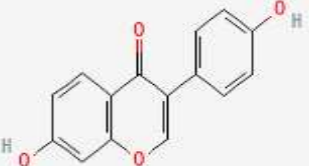
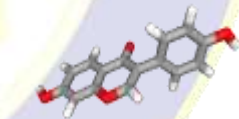
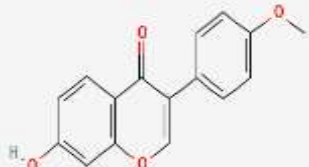
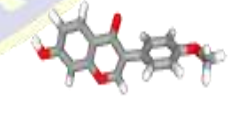
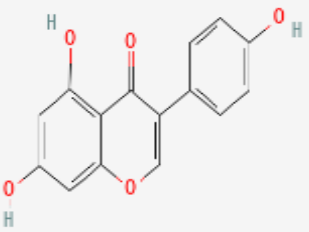
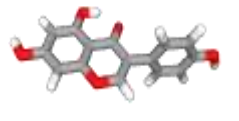
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
35.	Sakuranetin		
36.	Eriodictyol		
37.	Hesperitin		
38.	Homoeriodictyol		
39.	Parietin		
40.	Epigallocatechin		

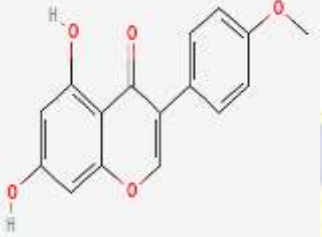
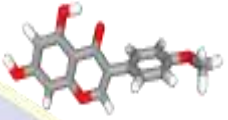
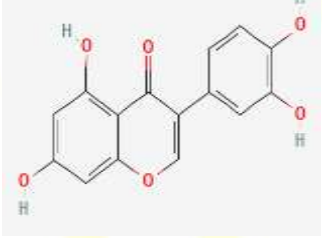
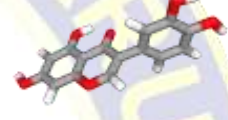
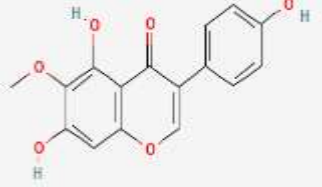
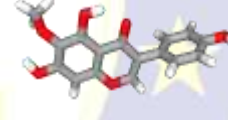
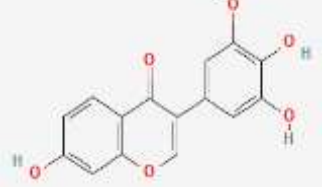

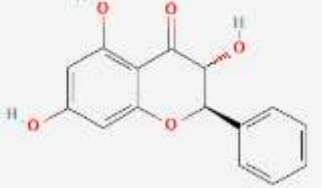
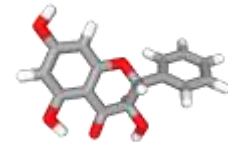
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
41.	Catechin		
42.	Naringin		
Isoflavon			
43.	Daidzein		
44.	Formononetin		
45.	Genistein		

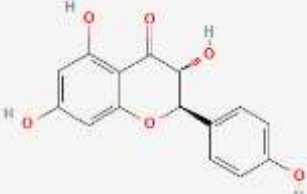
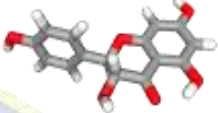
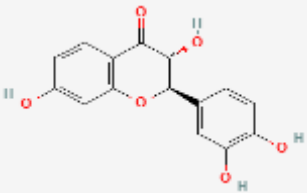
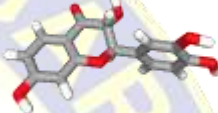
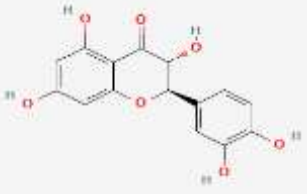
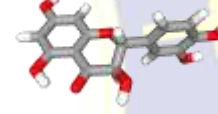
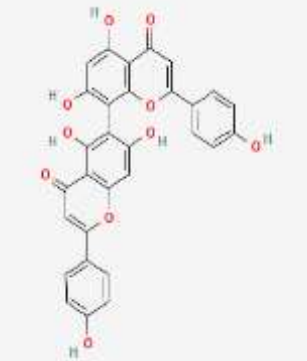
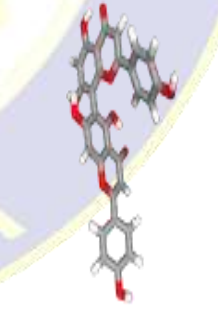

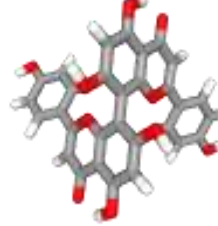
**LAMPIRAN 7
(LANJUTAN)**

**Tabel VII.2
Lanjutan**

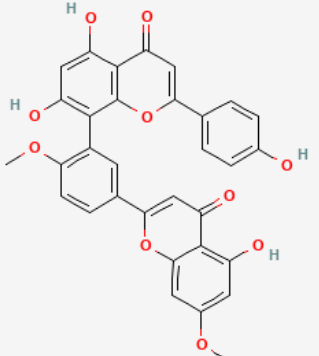
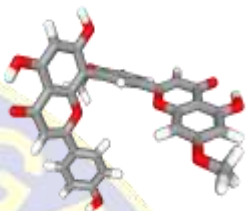
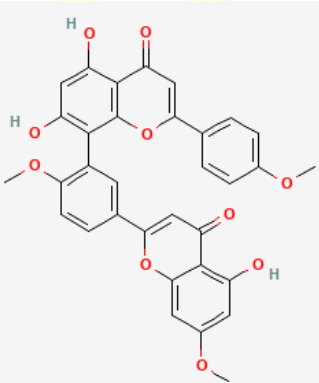
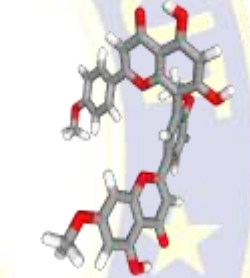
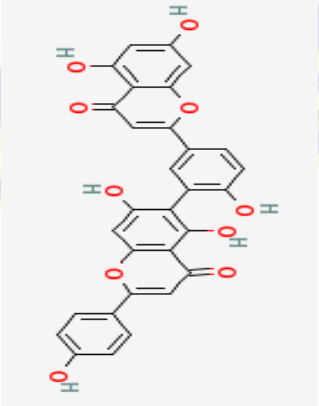
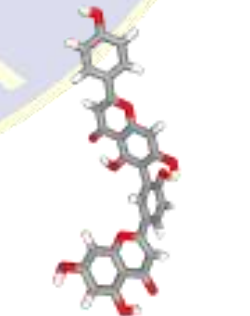
No.	Flavonoid	Struktur 2D	Struktur 3D
46.	Biokanin A		
47.	Orobol		
48.	Tectorigenin		
49.	Baptigenin		
Dehidroflavonol			
50.	Pinobanksin		

**LAMPIRAN 7
(LANJUTAN)**

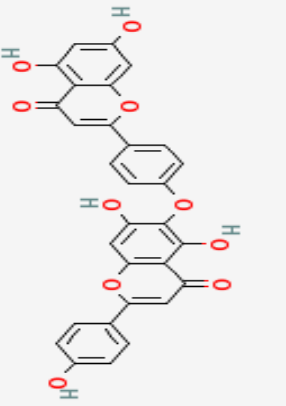

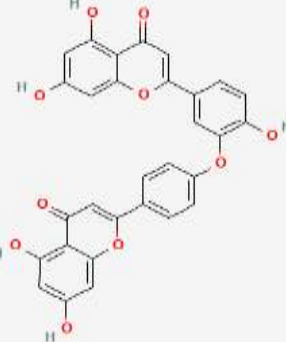
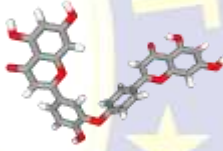
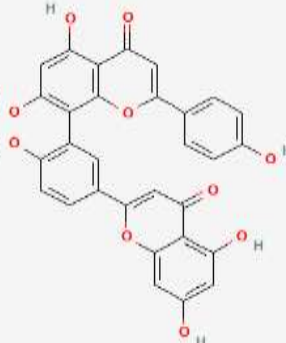
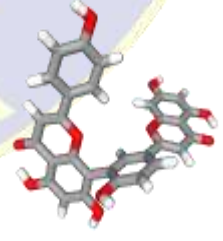
**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
51.	Aromadendrin		
52.	Fustin		
53.	Taksifolin		
BiFlavonoid			
54.	Agathisflavone		
55.	Cupresuflavone		

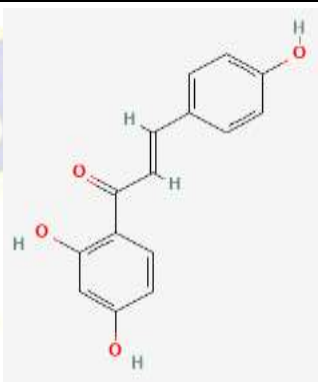
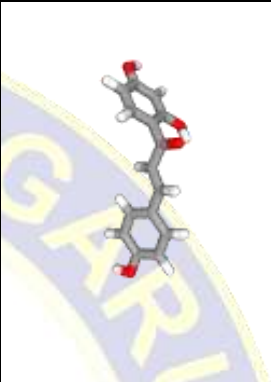
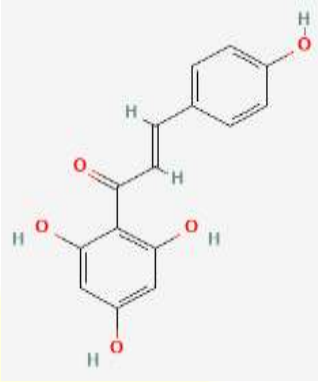
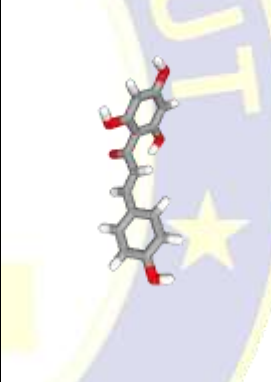
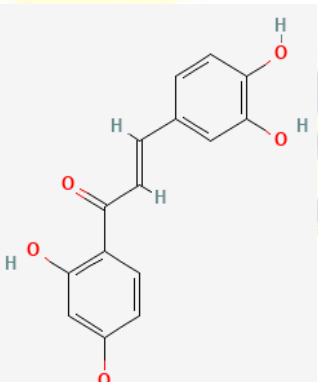
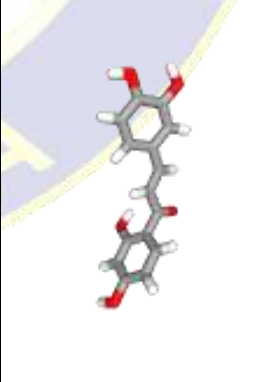
**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
56.	Ginkgetin		
57.	Sciadopitysin		
58.	Robustaflavone		

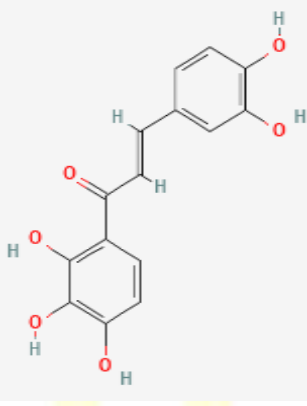

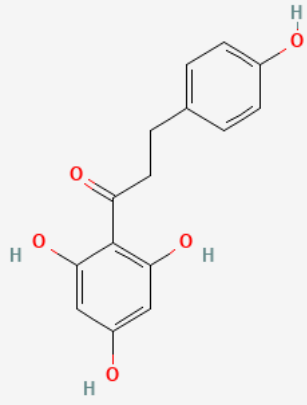

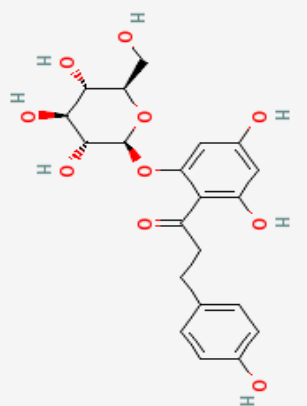

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
59.	Hinokiflavone	 <p>The 2D chemical structure of Hinokiflavone shows a central flavone core. It features a 7-hydroxyflavone skeleton with a 4-hydroxyphenyl group at the 6-position and a 4-hydroxyphenyl group at the 8-position. The structure is drawn with carbon atoms in black, oxygen atoms in red, and hydrogen atoms in white.</p>	 <p>The 3D ball-and-stick model of Hinokiflavone shows the spatial arrangement of the atoms. Carbon atoms are grey, oxygen atoms are red, and hydrogen atoms are white. The model illustrates the planar nature of the flavone core and the orientation of the phenyl rings.</p>
60.	Ochnaflavone	 <p>The 2D chemical structure of Ochnaflavone shows a central flavone core. It features a 7-hydroxyflavone skeleton with a 4-hydroxyphenyl group at the 6-position and a 4-hydroxyphenyl group at the 8-position. The structure is drawn with carbon atoms in black, oxygen atoms in red, and hydrogen atoms in white.</p>	 <p>The 3D ball-and-stick model of Ochnaflavone shows the spatial arrangement of the atoms. Carbon atoms are grey, oxygen atoms are red, and hydrogen atoms are white. The model illustrates the planar nature of the flavone core and the orientation of the phenyl rings.</p>
61.	Amentoflavone	 <p>The 2D chemical structure of Amentoflavone shows a central flavone core. It features a 7-hydroxyflavone skeleton with a 4-hydroxyphenyl group at the 6-position and a 4-hydroxyphenyl group at the 8-position. The structure is drawn with carbon atoms in black, oxygen atoms in red, and hydrogen atoms in white.</p>	 <p>The 3D ball-and-stick model of Amentoflavone shows the spatial arrangement of the atoms. Carbon atoms are grey, oxygen atoms are red, and hydrogen atoms are white. The model illustrates the planar nature of the flavone core and the orientation of the phenyl rings.</p>

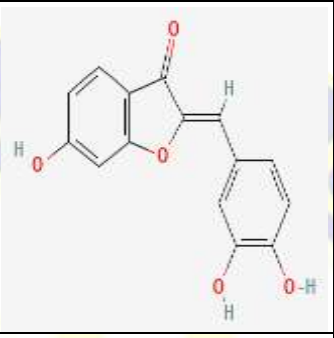
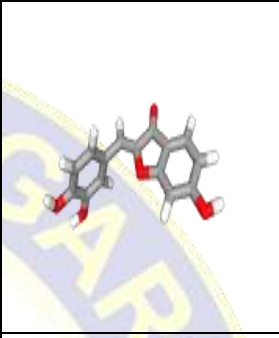
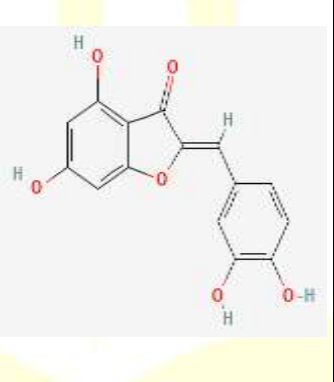
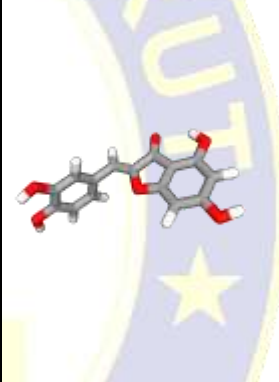
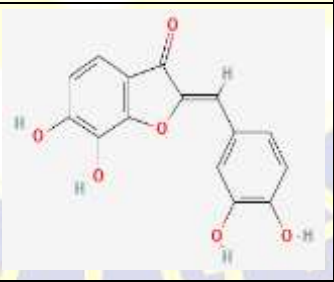
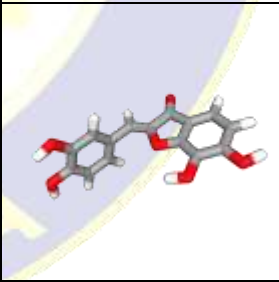
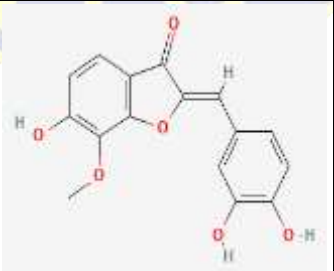
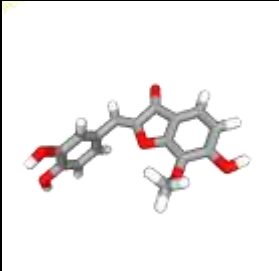
**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
Khalkon			
62.	Isoliquiritigenin		
63.	Khalkonarigenin		
64.	Butein		

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

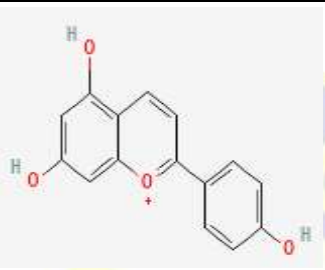
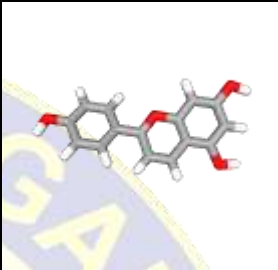
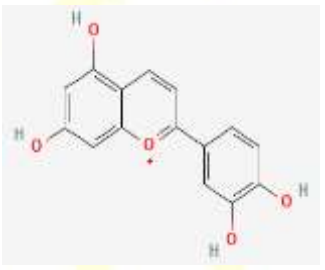
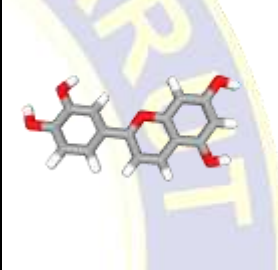
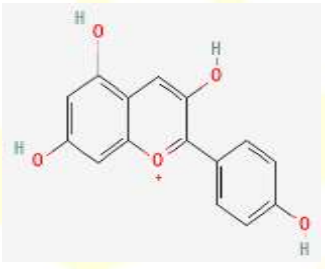

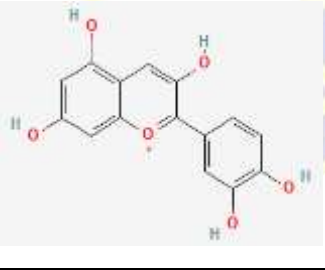
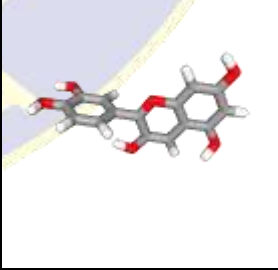
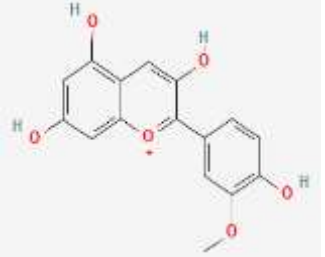
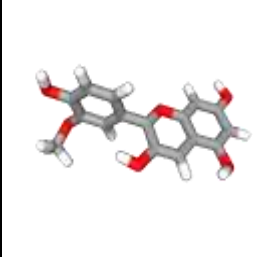
No.	Flavonoid	Struktur 2D	Struktur 3D
65.	Okantin	 <p>The 2D structure of Okantin shows a central benzene ring with three hydroxyl groups at the 2, 4, and 6 positions. A propenyl chain is attached at the 3-position, and a 4-hydroxyphenyl group is attached at the 5-position.</p>	 <p>The 3D ball-and-stick model of Okantin shows the spatial arrangement of the atoms, with carbon in grey, oxygen in red, and hydrogen in white.</p>
66.	Phloretin	 <p>The 2D structure of Phloretin features a central benzene ring with hydroxyl groups at the 2, 4, and 6 positions. A propyl chain is attached at the 3-position, and a 4-hydroxyphenyl group is attached at the 5-position.</p>	 <p>The 3D ball-and-stick model of Phloretin shows the spatial arrangement of the atoms, with carbon in grey, oxygen in red, and hydrogen in white.</p>
67.	Phlorizin	 <p>The 2D structure of Phlorizin is a glycoside consisting of a phloretin aglycone linked to a glucose molecule at the 7-position of the central benzene ring.</p>	 <p>The 3D ball-and-stick model of Phlorizin shows the spatial arrangement of the atoms, with carbon in grey, oxygen in red, and hydrogen in white.</p>

**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

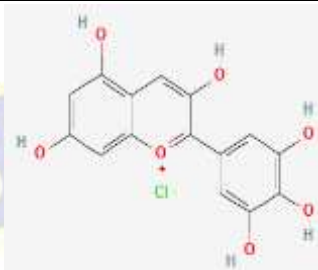
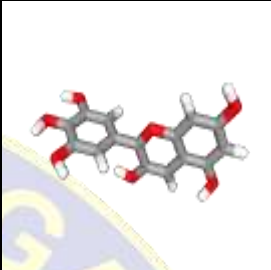
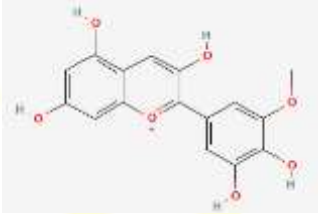
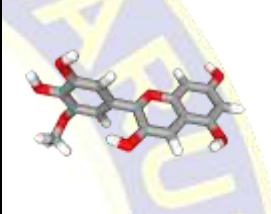
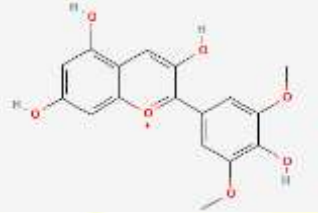
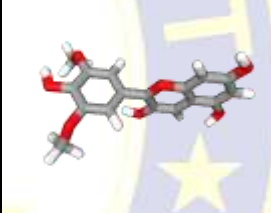
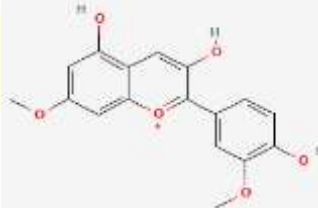
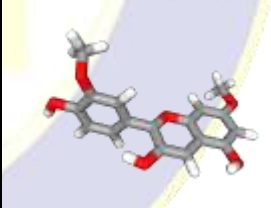
No.	Flavonoid	Struktur 2D	Struktur 3D
Auron			
68.	Sulfuretin		
69.	Aureusidin		
70.	Maritimetin		
71.	Leptosidin		

**LAMPIRAN 7
(LANJUTAN)**

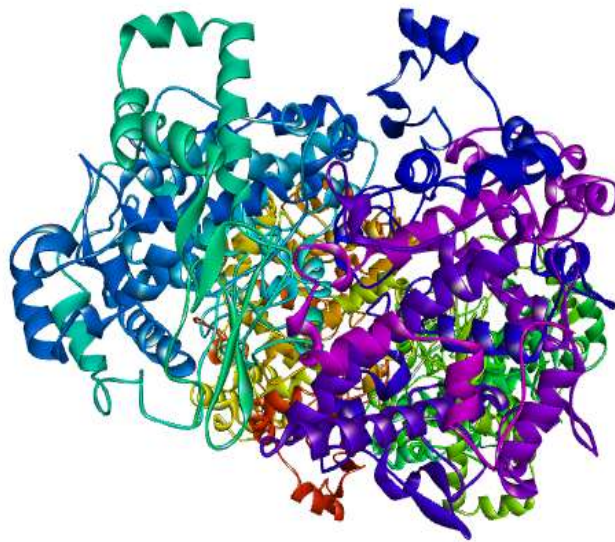
**Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
Antosianidin			
72.	Apigenidin		
73.	Luteolinidin		
74.	Pelargonidin		
75.	Cyanidin		
76.	Peonidin		

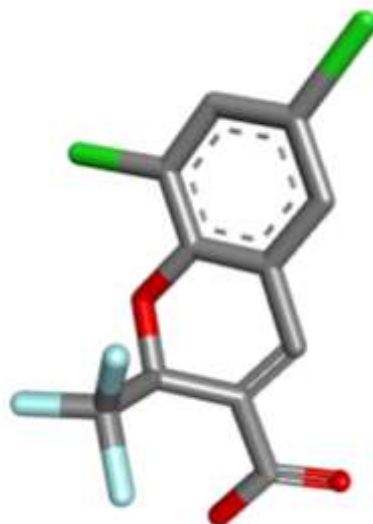
**LAMPIRAN 7
(LANJUTAN)****Tabel VII.2
Lanjutan**

No.	Flavonoid	Struktur 2D	Struktur 3D
77.	Delpinidin		
78.	Petunidin		
79.	Malvidin		
80.	Rosinidin		

LAMPIRAN 8
STRUKTUR 3D MAKROMOLEKUL



Gambar VII.18 Struktur 3D makromolekul reseptor 3LN0



Gambar VII.19 Struktur 3D makromolekul ligan 3LN0

LAMPIRAN 9

HASIL PENELITIAN SKRINING FARMAKOFOR




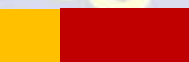














Tabel VII.3

Hasil Penelitian Skrining Farmakofor

No.	Nama Senyawa	Matching Features	Fit-Score
1.	2S-6,8-dichloro-2-(trifluoromethyl)-2H-chromene-3-carboxylic acid (ligan pembeding)		-
2.	Acacetin		36,08
3.	Apigenidin		35,30
4.	Apigenin		44,32
5.	Aromadendrin		36,46
6.	Aureusidin		35,53
7.	Baicalein		35,22
8.	Bichanin A		35,98
9.	Butein		35,25
10.	Catechin		35,25
11.	Chrysin		44,79
12.	Chrysoeriol		36,17
13.	Cupressuflavone		44,78
14.	Cyanidin		35,25
15.	Daidzein		35,99
16.	Diosmetin		35,72
17.	Eriodictyol		35,82


















**LAMPIRAN 9
(LANJUTAN)**

**Tabel VII.3
Lanjutan**

No.	Nama Senyawa	Matching Features	Fit-Score
18.	Fisetin		36,05
19.	Formononetin		35,98
20.	Fustin		45,29
21.	Galangin		36,13
22.	Genistein		35,88
23.	Gossypetin		45,24
24.	Herbacetin		44,94
25.	Hesperetin		35,87
26.	Hinokiflavone		44,83
27.	Hispidulin		35,17
28.	Homoeriodictyol		35,83
29.	Isoliquiritigenin		44,82
30.	Isoquercetin		35,85
31.	Isorhamnetin		35,93
32.	Kaempferid		36,74
33.	Kempferol		36,19
34.	Khalkonarigenin		35,24
35.	Leptosidin		34,98
















**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.3
Lanjutan

No.	Nama Senyawa	Matching Features	Fit-Score
36.	Liquiritigenin		35,89
37.	Luteolin		44,31
38.	Luteolinidin		35,27
39.	Morin		36,13
40.	Narigenin		35,90
41.	Naringin		36,39
42.	Ochnaflavone		36,19
43.	Okanin		44,71
44.	Orobol		35,87
45.	Pachypodol		37,00
46.	Parietin		35,82
47.	Peonidin		35,15
48.	Phloretin		35,24
49.	Phlorizin		35,27
50.	Pinobanksin		36,63
51.	Pinocembrin		44,62
52.	Quercetagenin		36,92

**LAMPIRAN 9
(LANJUTAN)**

Tabel VII.3
Lanjutan

No.	Nama Senyawa	Matching Features	Fit-Score
53.	Quercetin		37,04
54.	Rhamnazin		36,83
55.	Rhamnetin		35,46
56.	Robinetin		36,27
57.	Robustaflavone		44,81
58.	Rosinidin		35,26
59.	Rutin		37,71
60.	Sakuranetin		36,36
61.	Scutellarein		35,23
62.	Sulfuretin		35,25
63.	Taxifolin		36,98
64.	Tectorigenin		34,46
65.	Tricetin		36,13
66.	Tricin		36,14
67.	Wogonin		36,59

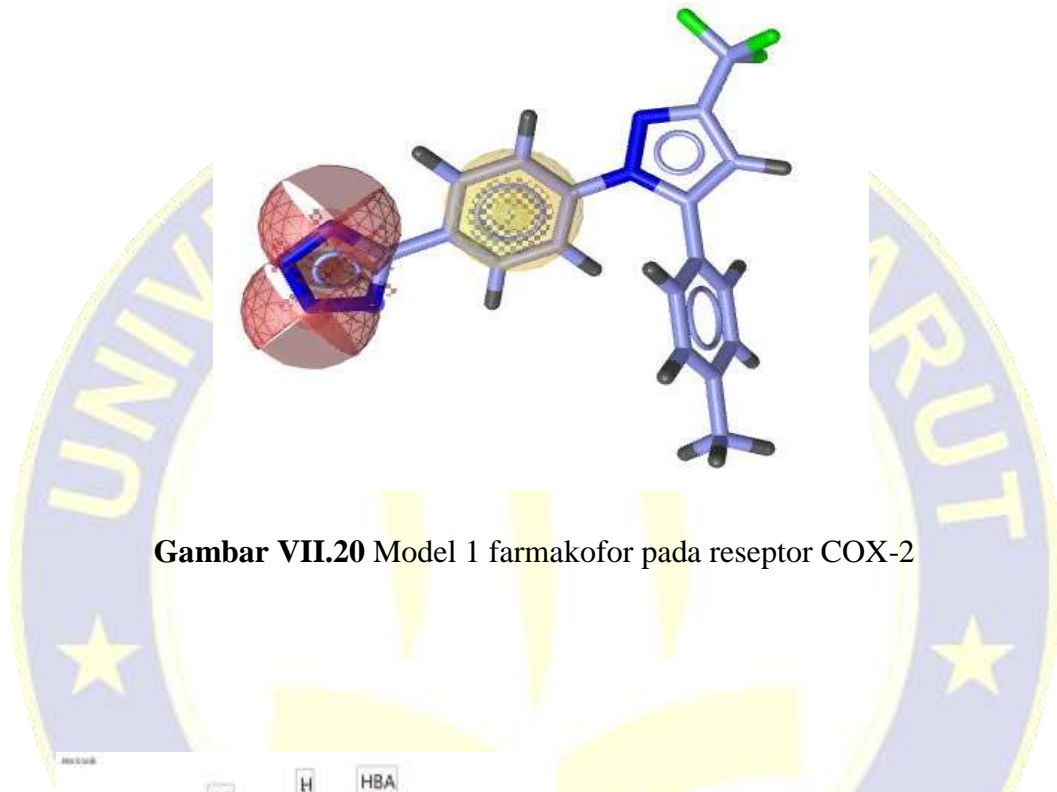
Keterangan :

Warna biru : Cincin aromatik

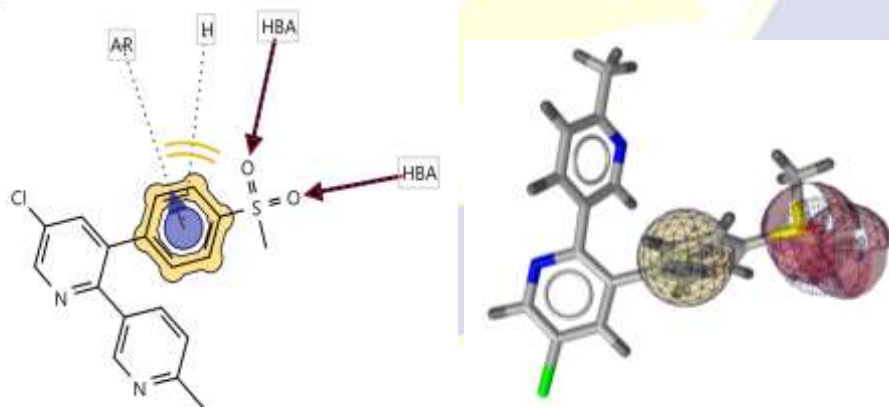
Warna kuning : Interaksi hidrofobik

Warna merah : Akseptor ikatan hidrogen

LAMPIRAN 10
VISUALISASI SKRINING FARMAKOFOR

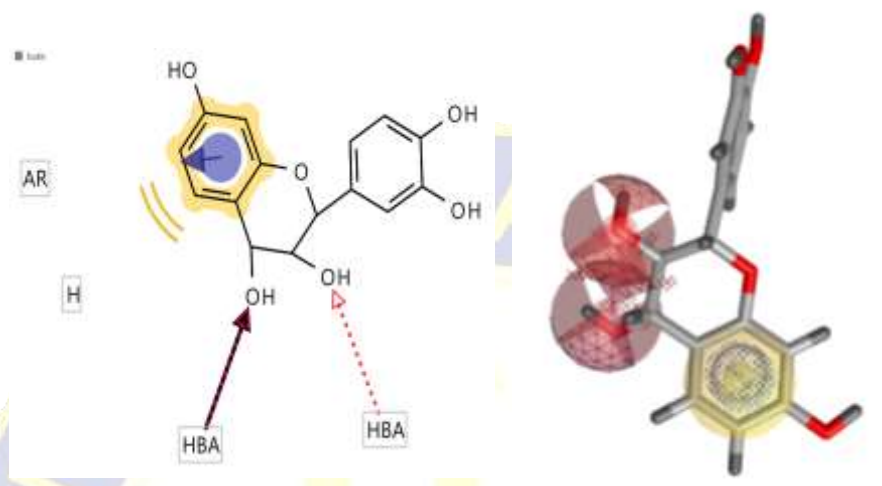


Gambar VII.20 Model 1 farmakofor pada reseptor COX-2

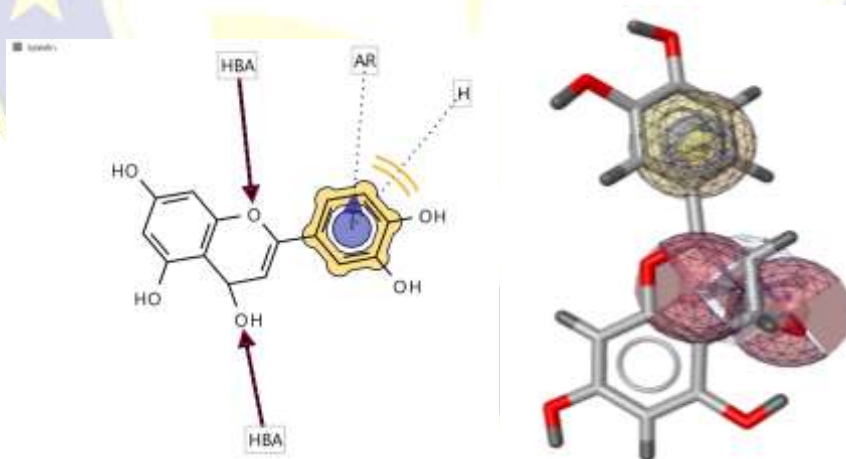


Gambar VII.21 Visualisasi 2D dan 3D farmakofor ligan pembanding Etoricoxib terhadap reseptor COX-2

**LAMPIRAN 10
(LANJUTAN)**



Gambar VII.22 Visualisasi 2D dan 3D farmakofor senyawa Fustin terhadap reseptor COX-2



Gambar VII.23 Visualisasi 2D dan 3D farmakofor senyawa Luteolin terhadap reseptor COX-2

LAMPIRAN 11

HASIL PENELITIAN SIMULASI MOLECULAR DOCKING

Tabel VII.4

Hasil Penambatan Senyawa Flavonoid pada Reseptor COX-2 ID PDB 3LN0

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
1.	2S-6,8-dichloro-2-(trifluoromethyl)-2H-chromene-3-carboxylic acid (<i>native</i> ligan)	-7,18	$5,47 \times 10^3$	Ser516, Tyr371, Tyr 341, Val509, dan Gly512	Phe504, Ala513, Leu338, Trp373, Val335, dan Met508
2.	Etoricoxib (ligan pembanding)	-10,19	34,15	Ser516, Tyr371, Tyr341, dan Arg106	Val509, Ser339, Leu338, Leu517, Ala513, Val102, His75, Val335, Ala502, Tyr341, Trp373 dan Tyr 334
3.	Chrysin	-7,80	$1,92 \times 10^3$	Met508	Val509, Leu338, dan Trp373
4.	Baicalein	-8,00	$1,37 \times 10^3$	Tyr341, His75, Ser339, Gln178, dan Leu338	Val509
5.	Apigenin	-7,92	$1,57 \times 10^3$	Met508, His75, Ser339	Val509, Leu338, Trp373
6.	Acacetin	-8,19	993,62	Tyr371, Tyr341, Leu338, dan Gln178	Ser516, Val509, Val335, dan Ala513
7.	Scutellarein	-8,23	934,89	Tyr341, Ser339, His75, Gln178, Leu338, dan Tyr371	Val509 dan Val335

LAMPIRAN 11
(LANJUTAN)

Tabel VII.4
Lanjutan

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
8.	Hispidulin	-8,02	$1,32 \times 10^3$	Tyr341, Ser516, Ser339, Gln178, dan Leu338	Val509 dan Val335
9.	Luteolin	-8,26	$1,08 \times 10^3$	Tyr341, Tyr371, Ser516, dan Met508	Val335, Leu517, dan Ala513
10.	Chrysoeriol	-7,91	$1,59 \times 10^3$	Met508, Ser339, His75, Tyr371 dan Gln178	Val509, Trp373, Leu338, dan Val335
11.	Diosmetin	-7,37	$3,99 \times 10^3$	Ser516, Tyr371, Met508, Tyr341, dan Arg106	Ala513, Val335, dan Leu517
12.	Tricetin	-8,28	855,44	Met508, Leu338, Gln178, Ser339, dan His75	Val509 dan Trp371
13.	Tricin	-7,37	$3,99 \times 10^3$	Tyr341 dan Ser516	Val335, Leu517, Gly512, Ala513, Val102, dan Leu345
14.	Tangeretin	-7,55	$2,94 \times 10^3$	Leu338, Ser516, dan Tyr371	Val335, Val509, dan Ala513

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
15.	Rhoifolin	-7,77	$2,00 \times 10^3$	Tyr341, Ser339, Leu338, Met508, Ser516, Tyr371, dan Gly512	Gln178, Trp373, Val509, Ala513
16.	Wogonin	-7,53	$3,01 \times 10^3$	Leu338 dan Tyr341	Val509, Met508, Trp373, Gly512, Leu370, Val335, dan Ala513
17.	Galangin	-7,96	$1,46 \times 10^3$	Ser339, Val335, dan Met508	Val509, Trp375, dan Leu338
18.	Fisetin	-8,55	544,52	Val335, Ser339, dan Met508	Val509, Leu338, dan Trp373
19.	Kaempferol	-8,05	$1,27 \times 10^3$	Val335, Ser339, dan Met508	Val509, Leu338, dan Trp373
20.	Kaempferide	-7,96	$1,45 \times 10^3$	Tyr341, Tyr371, Leu338, dan Gln178	Ser516, Val509, Ala513, dan Val335
21.	Robinetin	-8,94	280,16	Ser516, Leu338, Met508, dan Tyr371	Gly512, Val335, Val509, dan Trp373
22.	Herbacetin	-7,83	$1,83 \times 10^3$	Tyr371, Val335, Ser339, His75, dan Met508	Val509, Leu338, dan Trp373

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
23.	Quercetin	-8,40	696,24	Val335, Ser339, dan Met508	Val509, Leu338, dan Trp373
24.	Rhamnetin	-8,24	913	Met508, Leu338, Gln178, Gly512, Tyr371, dan Ser516	Val509, Trp373, dan Val335
25.	Isorhamnetin	-8,13	$1,10 \times 10^3$	Met508, Tyr371, Val335, Ser339, His75, dan Gln178	Val509, Trp373, dan Leu338
26.	Myricetin	-8,49	598,56	Gln178, Ser339, Leu338, Met508, dan Val335	Val509 dan Trp373
27.	Quercetagenin	-8,11	$1,13 \times 10^3$	Val335, Leu338, Gln178, Ser339, dan Met508	Val509, Trp373
28.	Gossypetin	-8,49	599,92	Ser339, His75, Gln178, Leu338, Val335, dan Met508	Val509 dan Trp373
29.	Isoquercetin	-7,70	$2,29 \times 10^3$	Met508, Ser516, Tyr341, Arg106, Tyr371, dan Gly512	Ala513, Val335, Val509, Ser339, dan Leu517

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
30.	Rhamnazin	-8,57	526,93	Met508, Ser339, Gly512, Tyr371, dan Gln178	Val509, Trp373, Val335, dan Leu338
31.	Rutin	-4,05	$1,08 \times 10^6$	Tyr341, Tyr371, dan Ser516	Val509, Ser339, Phe367, Phe195, Phe191, Leu517, Ala513, dan Val335
32.	Morin	-6,62	$14,09 \times 10^3$	Met508, Tyr341, Tyr371, dan Ser516	Gly512, Val335, Ala513, dan Leu517
33.	Pachypodol	-7,82	$1,86 \times 10^3$	Tyr371, dan Tyr341	Ser516, Val509, Ala513, Val335, dan Leu338
34.	Daidzein	-7,86	$1,72 \times 10^3$	Tyr371, Ser339, His75, dan Val509	Val335, Leu338, dan Ser339
35.	Formononetin	-8,17	$1,03 \times 10^3$	Tyr371, Gln178, Val509, dan Leu338	Val509, Trp373, dan Val335
36.	Genistein	-7,69	$2,31 \times 10^3$	His75, Ser339, Met508, dan Val509	Trp373, Val335, dan Leu338

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
37.	Biokanin A	-8,33	786,49	Tyr371, Tyr341, dan Ser339	Val509, Leu338, Trp373, dan Val335
38.	Orobol	-8,09	$1,17 \times 10^3$	Ser339, His75, Met508, dan Val509	Trp373, Leu338, dan Val335
39.	Tectorigenin	-7,91	$1,60 \times 10^3$	His75, Ser339, Ser516, Tyr371, dan Leu338	Val509, dan Val335
40.	Baptigenin	-8,47	619,23	Gln178, Leu338, Ser339, His75, dan Gly512	Val509, dan Trp373
41.	Pinocembrin	-8,02	$1,32 \times 10^3$	Met508	Arg499, Val509, Trp373, Ala502, dan Leu338
42.	Liquiritigenin	-8,06	$1,23 \times 10^3$	Ser516, Tyr341, dan Met508	Ala513, Leu517, dan Val335
43.	Narigenin	-7,74	$2,11 \times 10^3$	Tyr341, Ser516, Tyr371, dan Leu338	Val509, dan Val335
44.	Sakuranetin	-7,94	$1,51 \times 10^3$	Tyr341, Ser516, dan Tyr371	Gln178, Val509, Val335, dan Leu338
45.	Eriodictyol	-8,39	707,96	His75, Ser339, dan Met508	Val509, Leu338, dan Trp373

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
46.	Hesperetin	-8,08	$1,20 \times 10^3$	Tyr371, Tyr341, dan Ser339	Val509, Leu338, Trp373, dan Val335
47.	Homoeriodictyol	-8,23	923,24	Met508, Ser339, His75, Gln178, dan Tyr371	Val509, dan Trp373
48.	Parietin	-7,97	$1,43 \times 10^3$	Tyr341, Ser339, dan Ala513	Val509, Val335, dan Leu338
49.	Epigallocatechin	-7,85	$1,73 \times 10^3$	Ser339, His75, Gln178, dan Leu338	Val509, dan Met508
50.	Catechin	-7,79	$1,94 \times 10^3$	Ser516, Val335, Ser339, His75, dan Gly512	Val509, Trp373, dan Leu338
51.	Naringin	-8,61	489,92	Met508, Tyr341, Leu338, dan His75	Gly512, Tyr371, Ser516, Arg106, Trp373, Val509, Val330, Leu520, Leu517, dan Val335
52.	Pinobanksin	-7,70	$2,27 \times 10^3$	Met508, Ser339, dan Val335	Val509

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
53.	Aromadendrin	-7,50	$3,16 \times 10^3$	Tyr371, Ser339, Gln178, Ser339, dan Tyr341	Val509, dan Val335
54.	Fustin	-8,31	$6,29 \times 10^3$	Tyr341, Tyr371, Leu338, dan Gln178	Val335, dan Val509
55.	Taxifolin	-7,85	$1,76 \times 10^3$	Val335, Ser339, His75, dan Met508	Val509, Leu338, dan Trp373
56.	Agathisflavone	29,54	-	Val509	Ala513, Val335, Arg106, Tyr371, Ser516, Tyr341, His75, Arg499, Phe504, dan Leu338
57.	Cupressuflavone	-4,20	830,61	Ser516	Tyr371, Val509, Ala513, Val335, Ser339, Gly512, Phe504, Leu517, dan Val330

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
58.	Ginkgetin	1,59	-		Val335, Tyr341, Leu517, Leu345, Ala513, Val509, His75, Met99, Leu338, dan Ile331
59.	Sciadopitysin	3,86	-	Arg499, His75, Gln178, Met508, dan Tyr341	Ile503, Val509, Ser339, Ala513, Val335, Leu517, Leu338, Gly512, dan Leu345
60.	Robustaflavone	27,94	-	Ser516, Phe504, dan Ser339	Val335, Phe195, Tyr371, His75, Val509, Leu338, Ala513, Tyr341, dan Ala502

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
61.	Hinokiflavone	78,46	-		Phe367, Phe195, Leu338, Arg499, His75, Val509, Tyr341, Glu510, Ser516, Tyr371, Trp373, Phe191, dan Val335
62.	Ochnaflavone	0,54	-	Tyr371	Ser516, Tyr341, Ser339, Arg106, Val509, Leu338, Tyr334, Leu345, Val102, Leu517, Val335, dan Ala513
63.	Amentoflavone	-2,32	$19,84 \times 10^6$	Leu338, Ser516, dan Tyr341	Arg106, Val335, Leu517, Leu345, Ala513, Val509, dan Met99
64.	Isoliquiritigenin	-7,31	$4,37 \times 10^3$	Tyr371, Ser516, Tyr341, dan Met508	Ala513, Leu517, dan Val335

**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
65.	Khalkonarigenin	-7,32	$4,28 \times 10^3$	Ser516, Tyr371, Tyr341, Val509, dan Met508	Ala513, Leu517, dan Val335
66.	Butein	-7,62	$2,60 \times 10^3$	Ser516, Tyr371, Ser339, His75, Gly512, dan Val509	Val335, Leu338, dan Trp373
67.	Okanin	-7,16	$5,19 \times 10^3$	Ser516, Met508, dan Tyr341	Arg106, Gly512, Ala513, Leu517, dan Val335
68.	Phloretin	-7,01	$7,23 \times 10^3$	Met508, Tyr341, His75, dan Ser339	Val509, Gly512, dan Ala513
69.	Phlorizin	-6,39	$20,83 \times 10^3$	Tyr341, Gly512, Tyr341, dan Ser339	Val509, Leu517, Val102, Ala513, Val335, Leu345, dan Leu338
70.	Sulfuretin	-8,05	$1,26 \times 10^3$	Leu338, Ser516, dan Ser339	Tyr371, Trp371, Val509, dan Val335
71.	Aureusidin	-7,88	$1,67 \times 10^3$	Tyr371, Ser339, His75, dan Met508	Val509, Trp375, dan Leu338

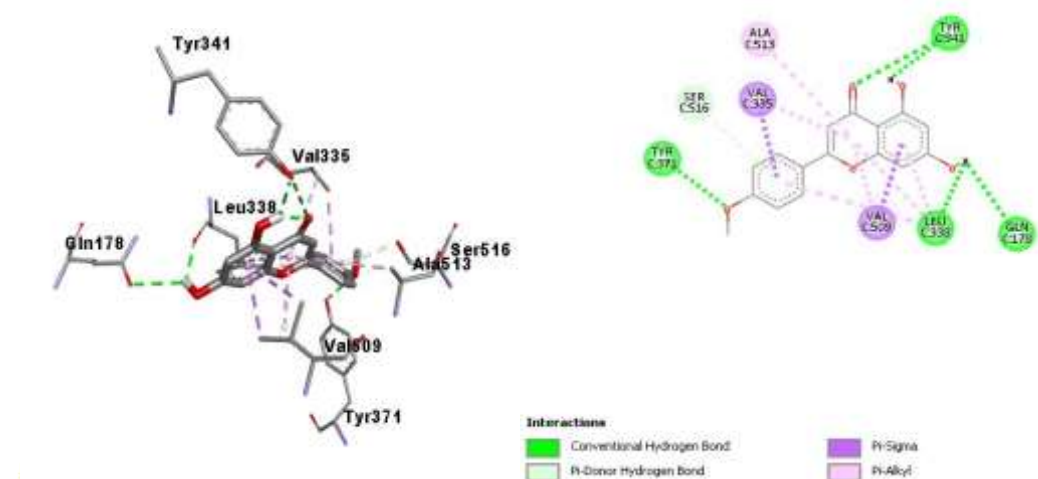
**LAMPIRAN 11
(LANJUTAN)**

**Tabel VII.4
Lanjutan**

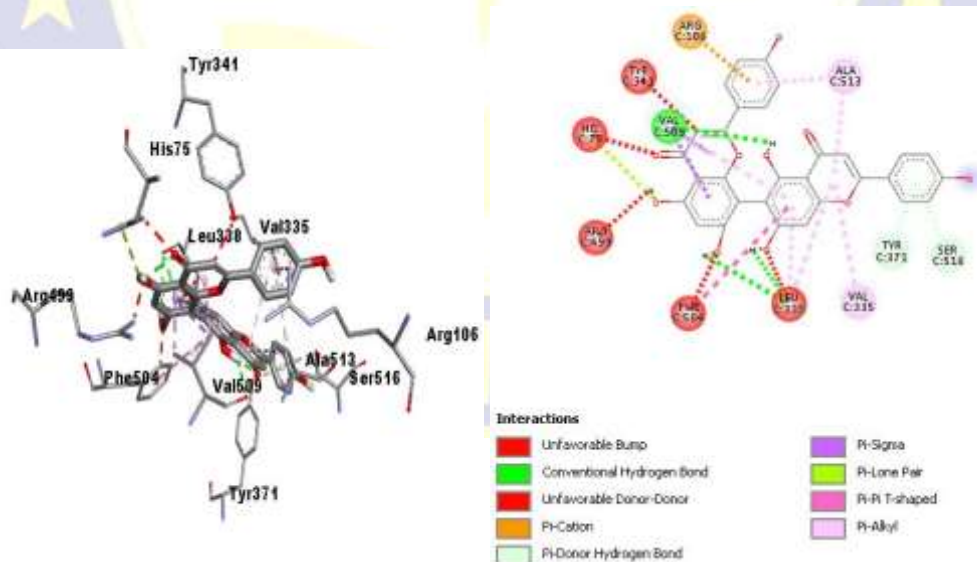
No.	Ligan	ΔG (kkal/ mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
72.	Maritimetin	-8,13	$1,10 \times 10^3$	Met508, Ala513, Arg106, Tyr341, dan Ser516	Leu517, dan Val335
73.	Leptosidin	-8,17	$1,03 \times 10^3$	Ser516, Leu338, dan Gln178	Val509, Tyr371, dan Trp373
74.	Apigenidin	-7,85	$1,76 \times 10^3$	His75, Ser339, dan Met508	Val509, Leu338, dan Trp373
75.	Luteolinidin	-8,22	947,24	Met508, Ser339, dan His75	Val509, Trp373, dan Leu338
76.	Pelargonidin	-7,79	$1,95 \times 10^3$	Ser516, Val335, Ser339, Gly512 dan His75	Val509, Leu338, dan Trp373
77.	Cyanidin	-8,12	$1,11 \times 10^3$	Val335, Ser339, dan Met508	Val509, Leu338, dan Trp373
78.	Peonidin	-8,13	$1,10 \times 10^3$	Val335, Ser339, His75, Tyr371, Met508, dan Gln178	Val509, Leu338, dan Trp373

LAMPIRAN 12

VISUALISASI RESIDU ASAM AMINO LIGAN UJI

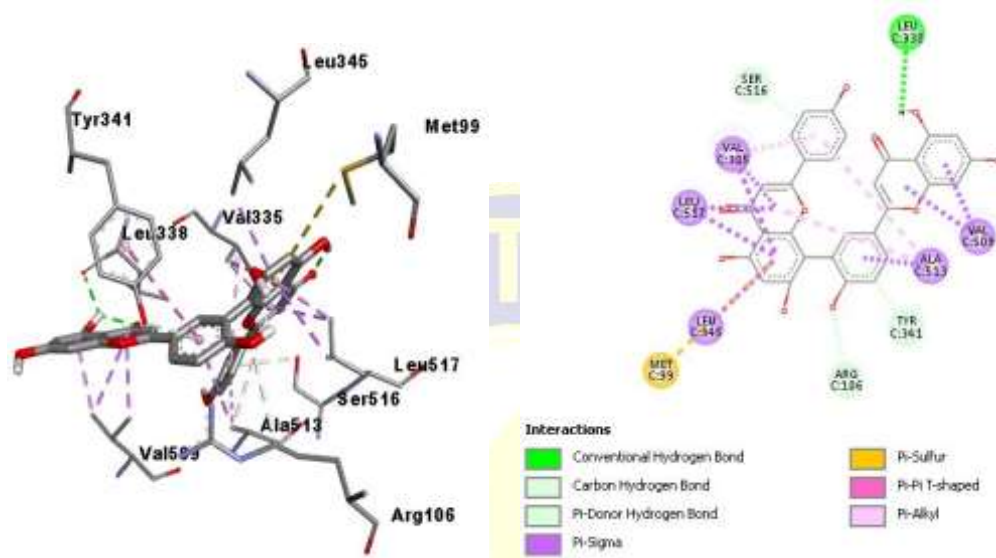


Gambar VII.24 Visualisasi 2D dan 3D senyawa Acacetin terhadap reseptor COX-2 ID PDB 3LN0

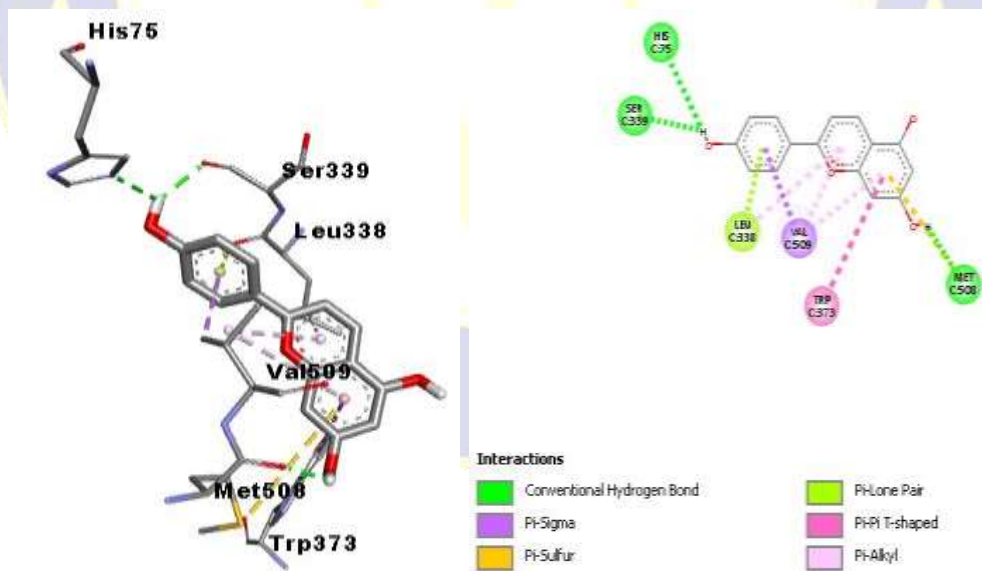


Gambar VII.25 Visualisasi 2D dan 3D senyawa Agathisflavone terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

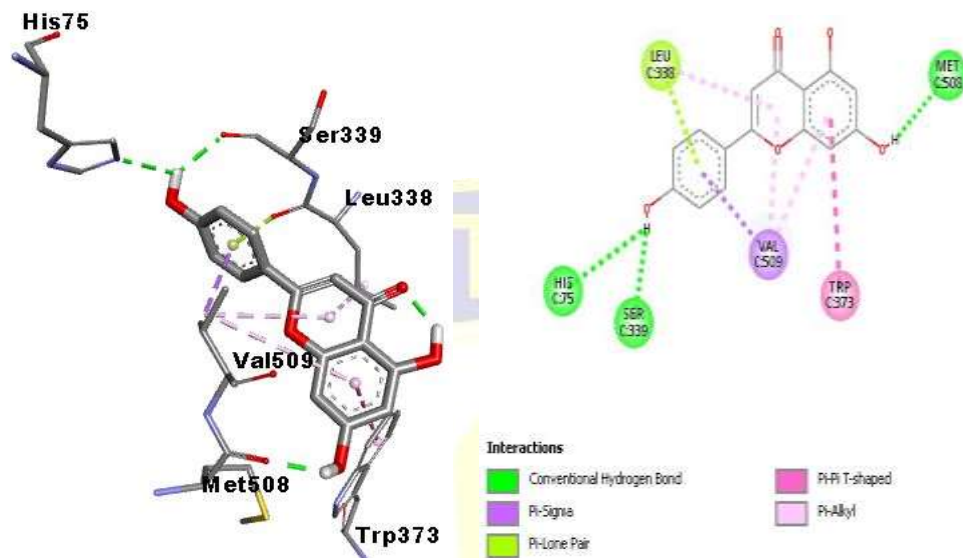


Gambar VII.26 Visualisasi 2D dan 3D senyawa Amentoflavone terhadap reseptor COX-2 ID PDB 3LN0

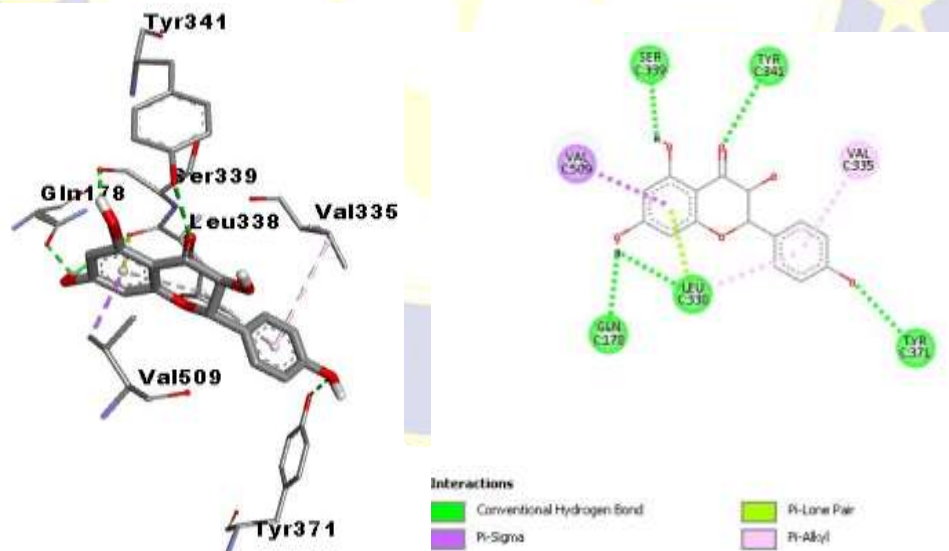


Gambar VII.27 Visualisasi 2D dan 3D senyawa Apigenidin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

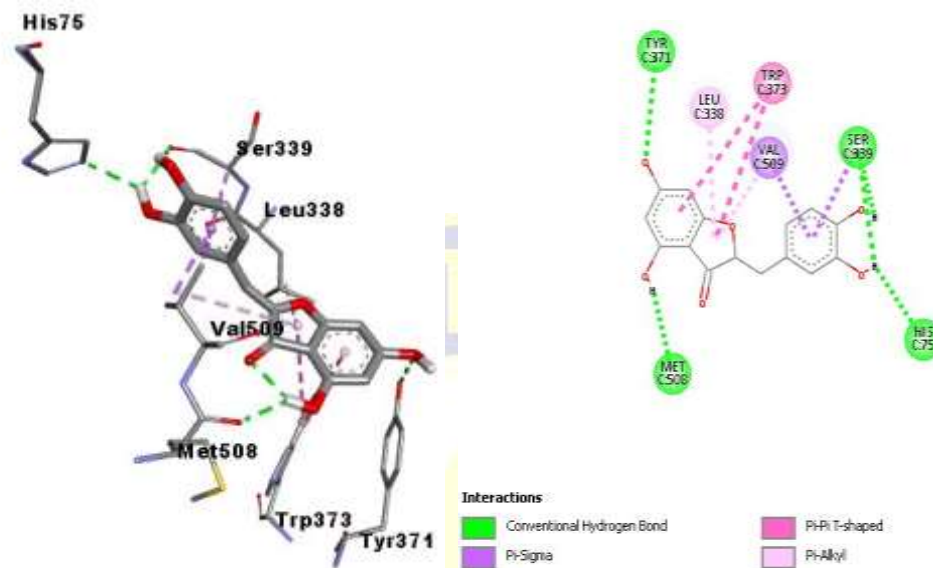


Gambar VII.28 Visualisasi 2D dan 3D senyawa Apigenin terhadap reseptor COX-2 ID PDB 3LN0

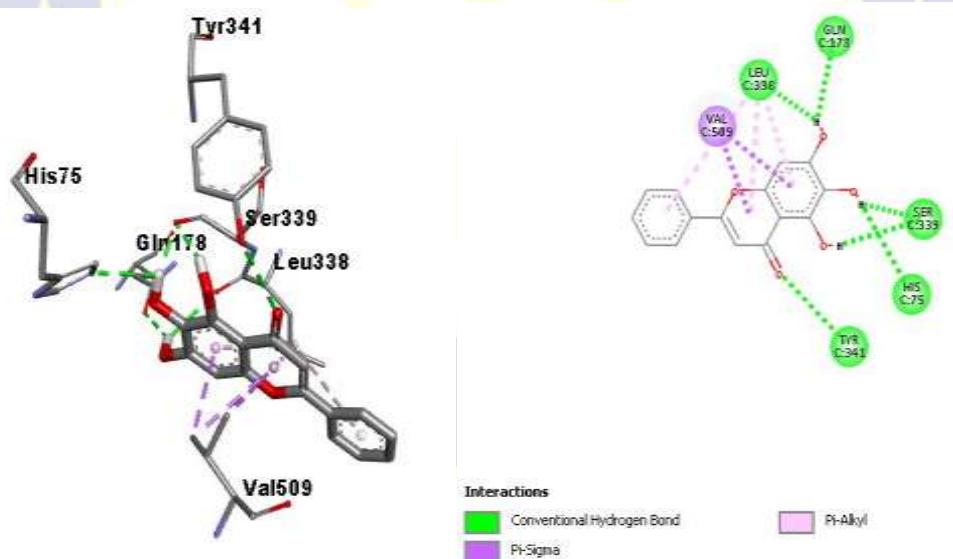


Gambar VII.29 Visualisasi 2D dan 3D senyawa Aromadendrin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

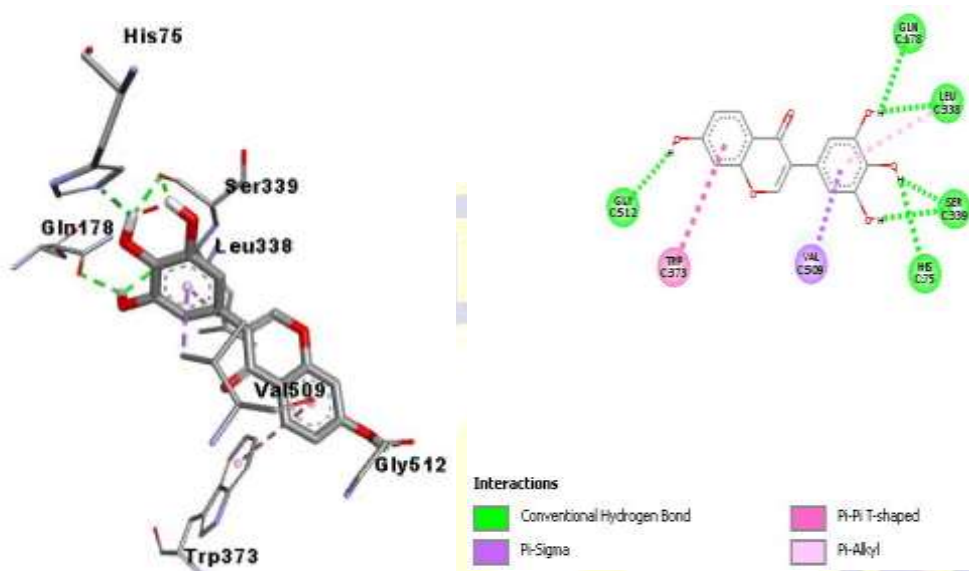


Gambar VII.30 Visualisasi 2D dan 3D senyawa Aureusidin terhadap reseptor COX-2 ID PDB 3LN0

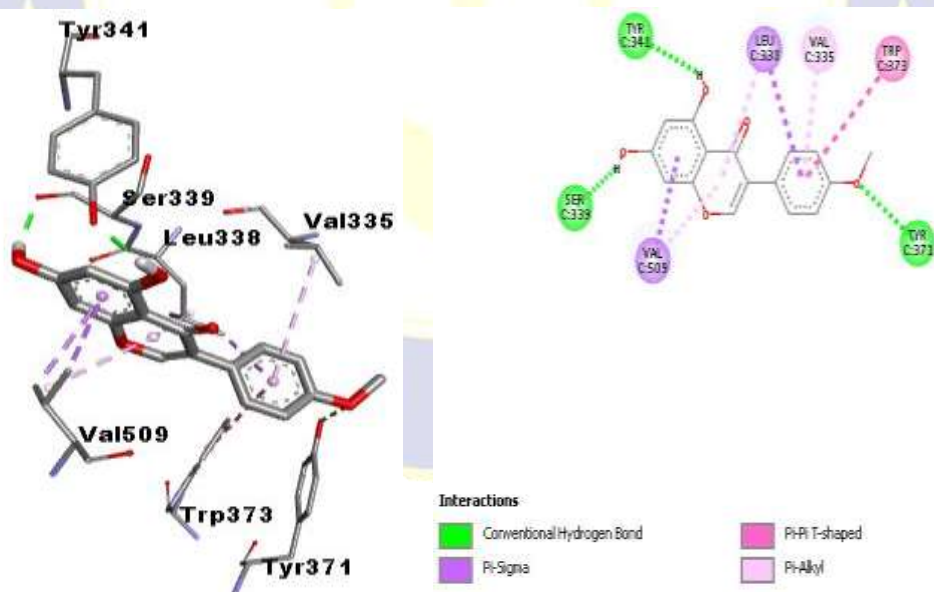


Gambar VII.31 Visualisasi 2D dan 3D senyawa Baicalein terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

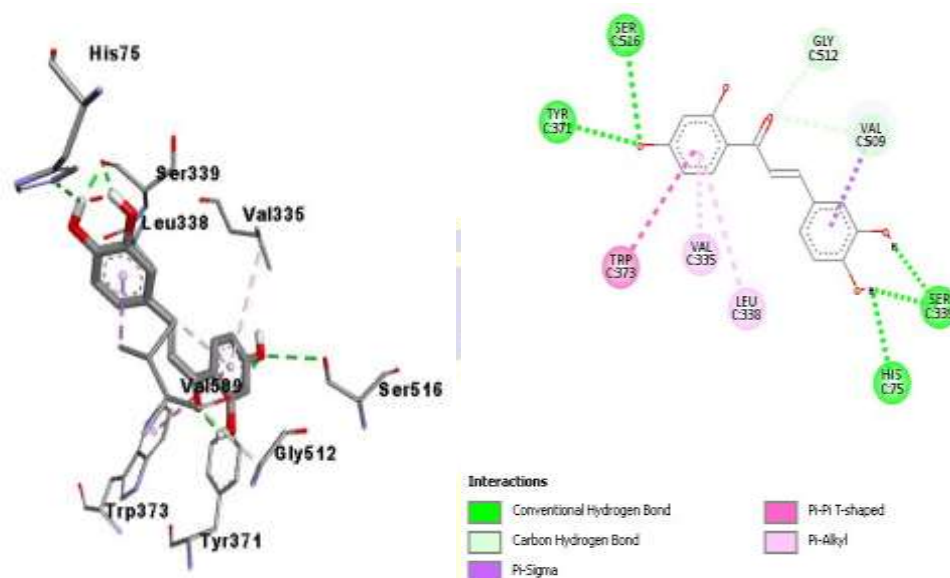


Gambar VII.32 Visualisasi 2D dan 3D senyawa Baptigenin terhadap reseptor COX-2 ID PDB 3LN0

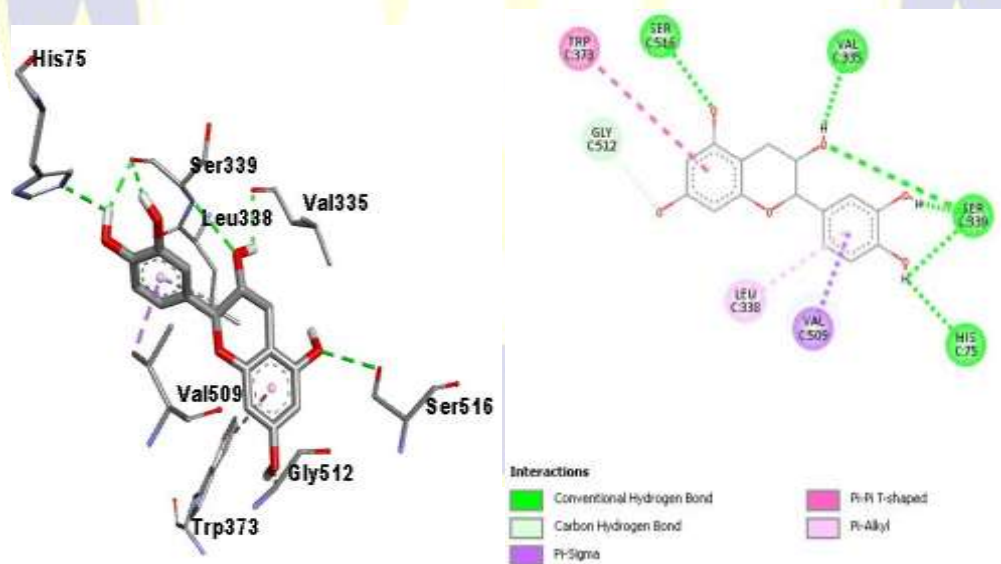


Gambar VII.33 Visualisasi 2D dan 3D senyawa Biochanin A terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

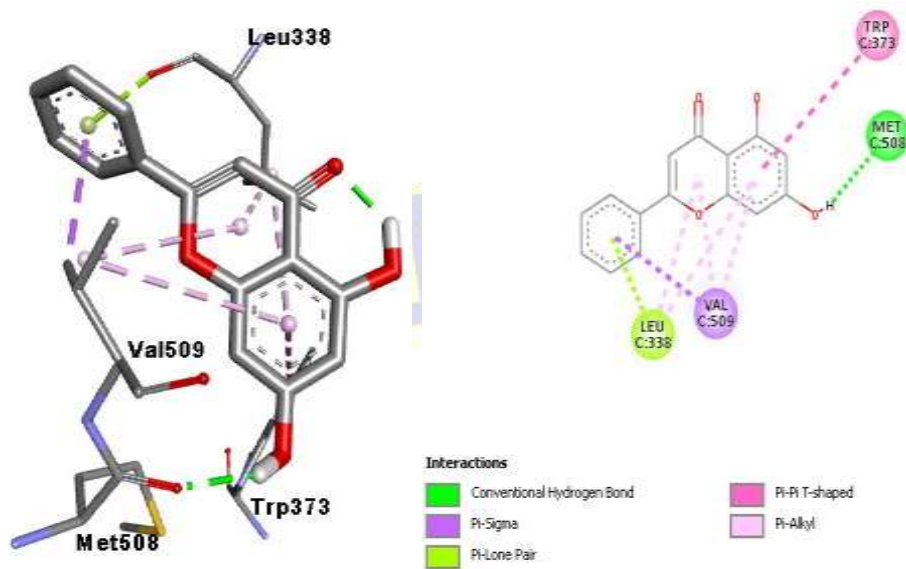


Gambar VII.34 Visualisasi 2D dan 3D senyawa Butein terhadap reseptor COX-2 ID PDB 3LN0

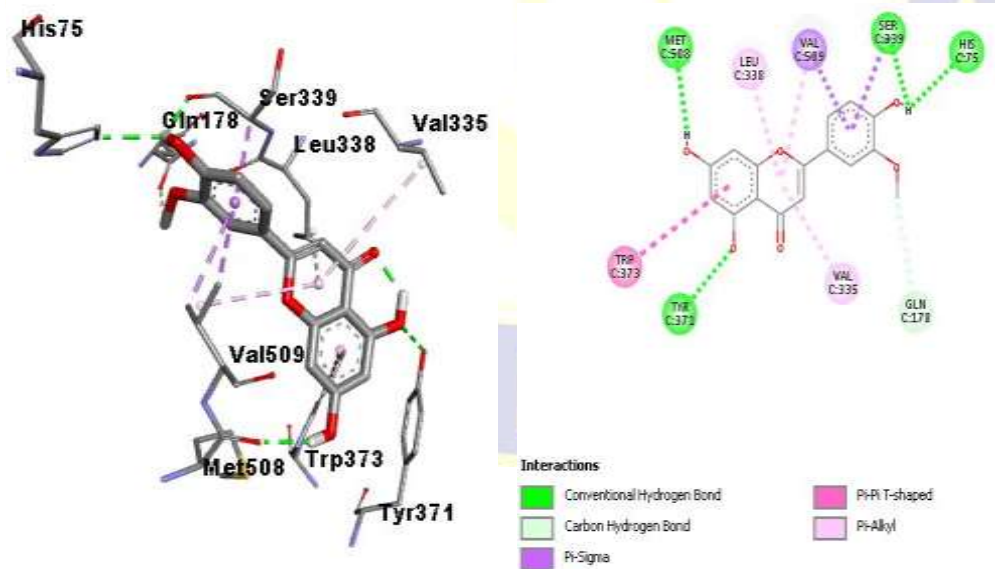


Gambar VII.35 Visualisasi 2D dan 3D senyawa Catechin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

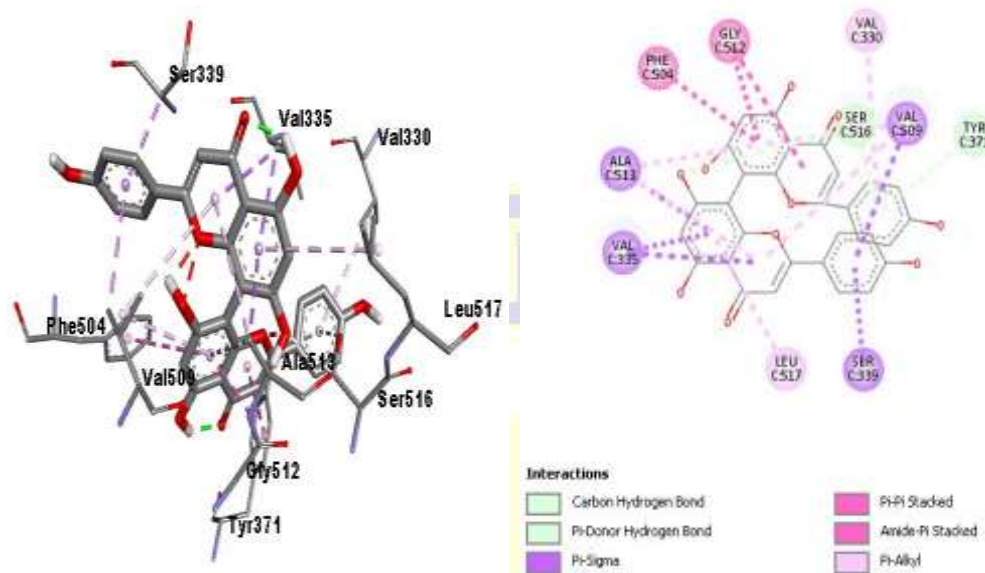


Gambar VII.36 Visualisasi 2D dan 3D senyawa Chrysin terhadap reseptor COX-2 ID PDB 3LN0

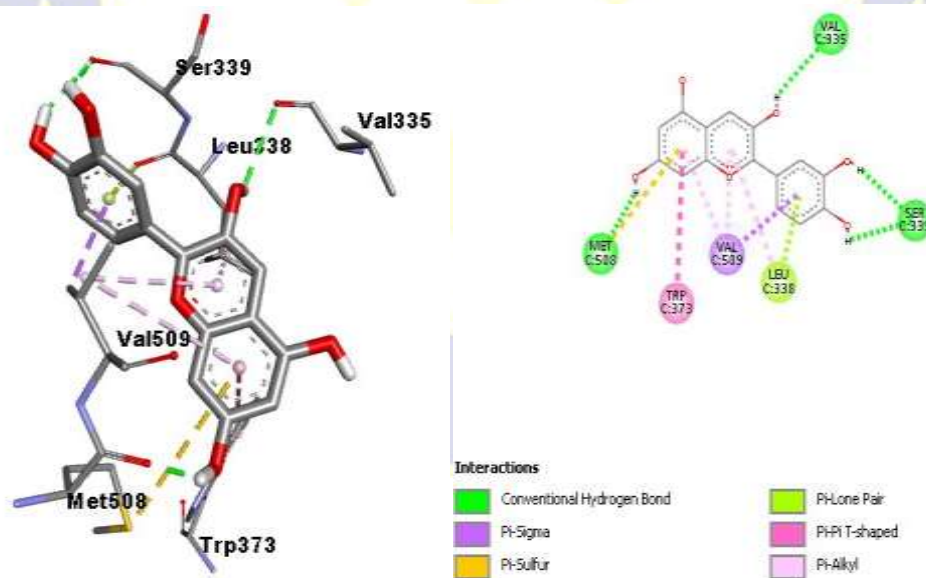


Gambar VII.37 Visualisasi 2D dan 3D senyawa Chrysoeriol terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

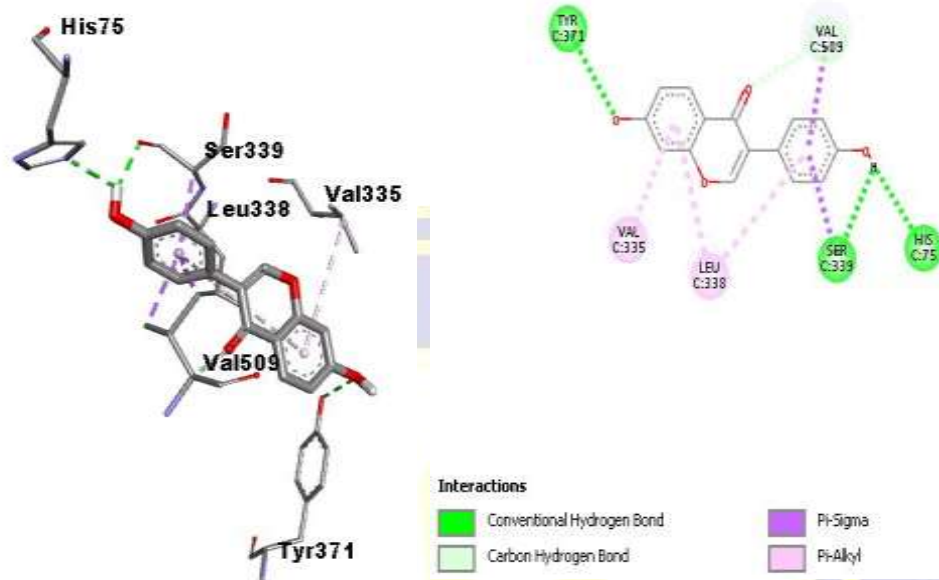


Gambar VII.38 Visualisasi 2D dan 3D senyawa Cupressuflavone terhadap reseptor COX-2 ID PDB 3LN0

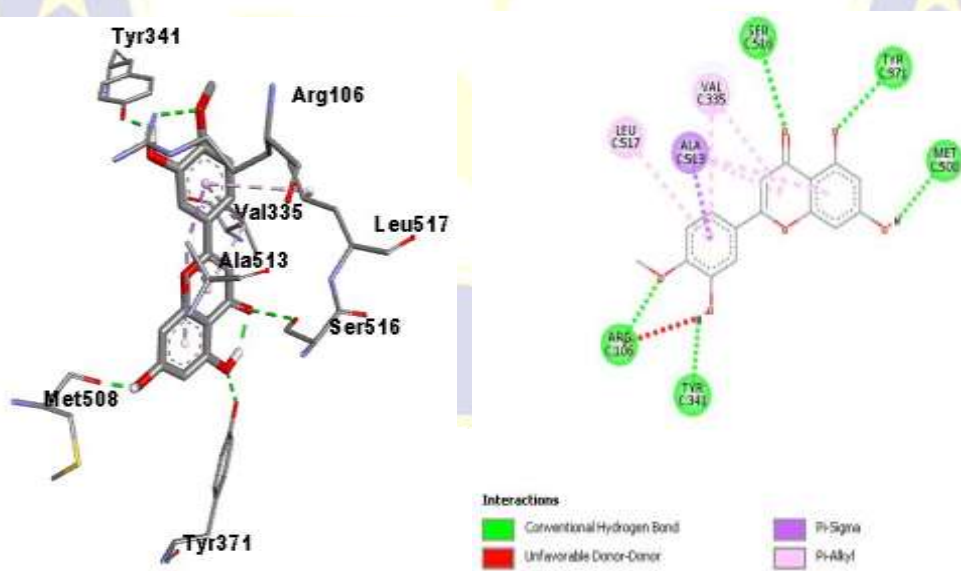


Gambar VII.39 Visualisasi 2D dan 3D senyawa Cyanidin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

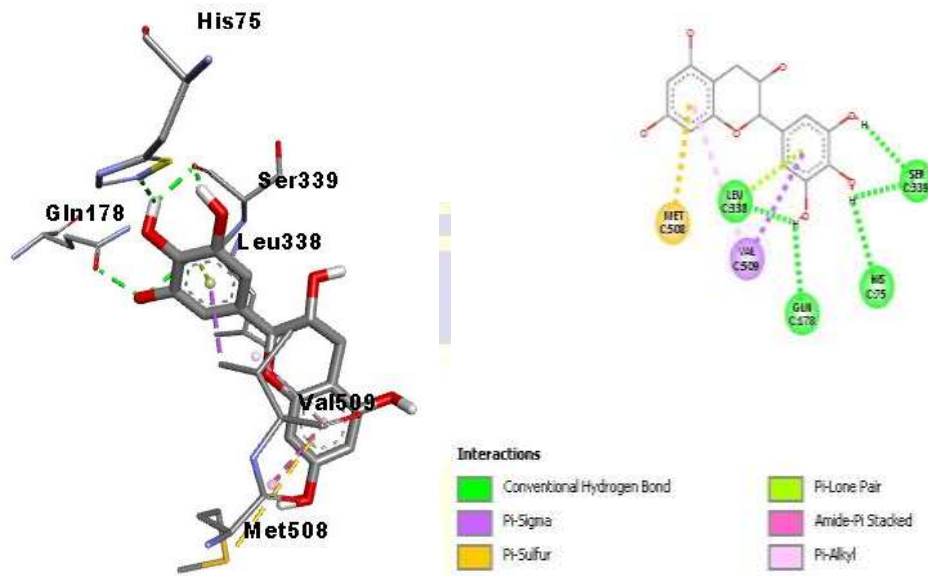


Gambar VII.40 Visualisasi 2D dan 3D senyawa Daidzein terhadap reseptor COX-2 ID PDB 3LN0

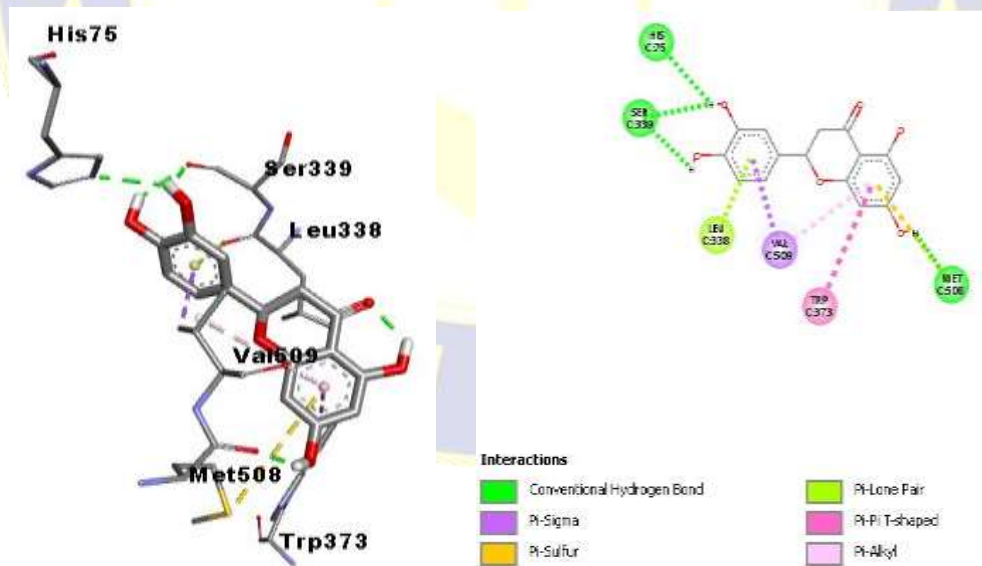


Gambar VII.41 Visualisasi 2D dan 3D senyawa Diosmetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

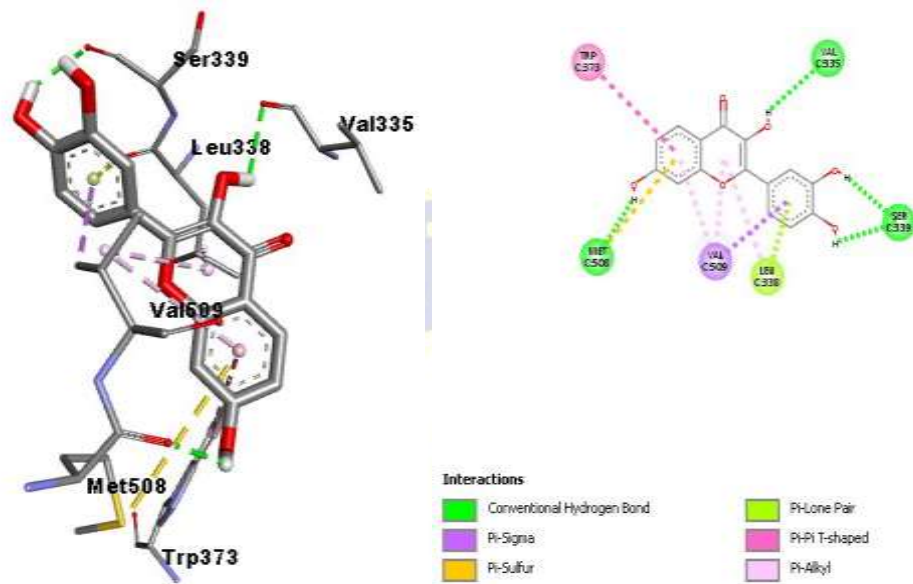


Gambar VII.42 Visualisasi 2D dan 3D senyawa Epigallocatechin terhadap reseptor COX-2 ID PDB 3LN0

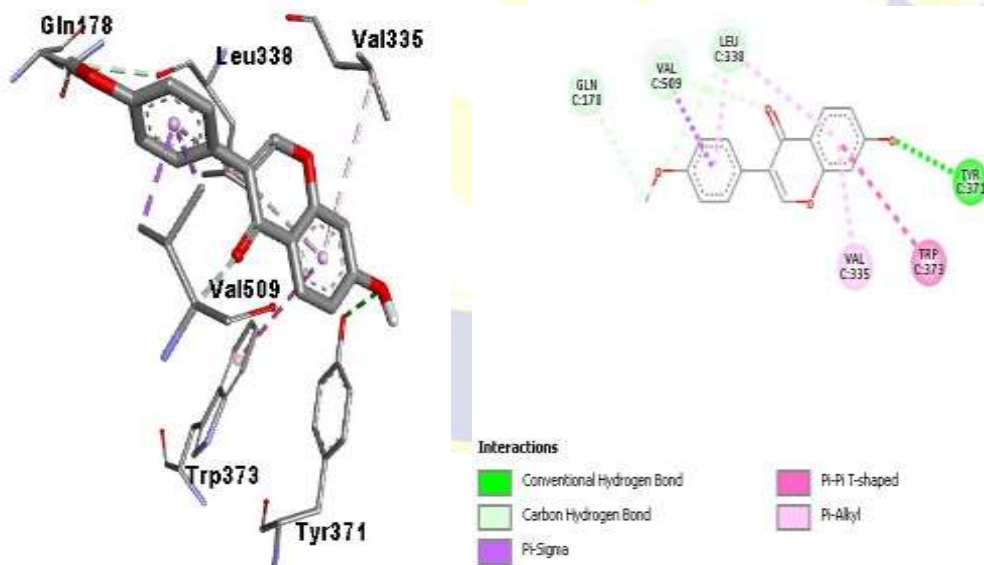


Gambar VII.43 Visualisasi 2D dan 3D senyawa Eriodictyol terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

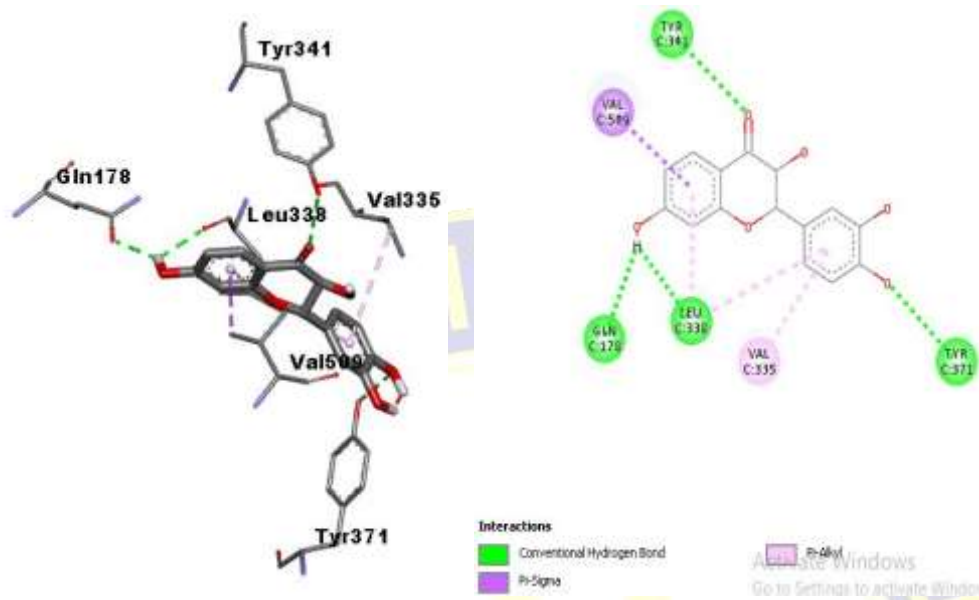


Gambar VII.44 Visualisasi 2D dan 3D senyawa Fisetin terhadap reseptor COX-2 ID PDB 3LN0

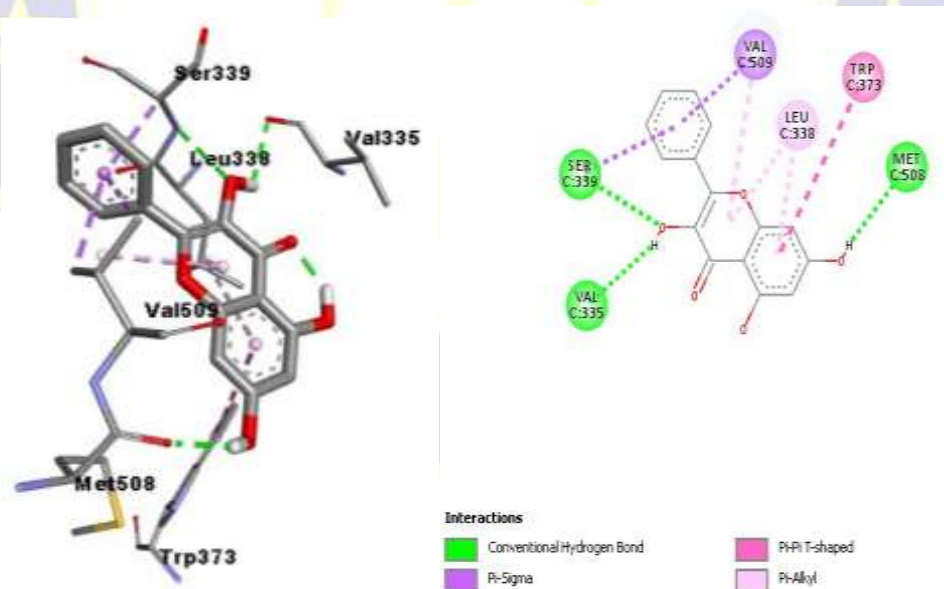


Gambar VII.45 Visualisasi 2D dan 3D senyawa Formononetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

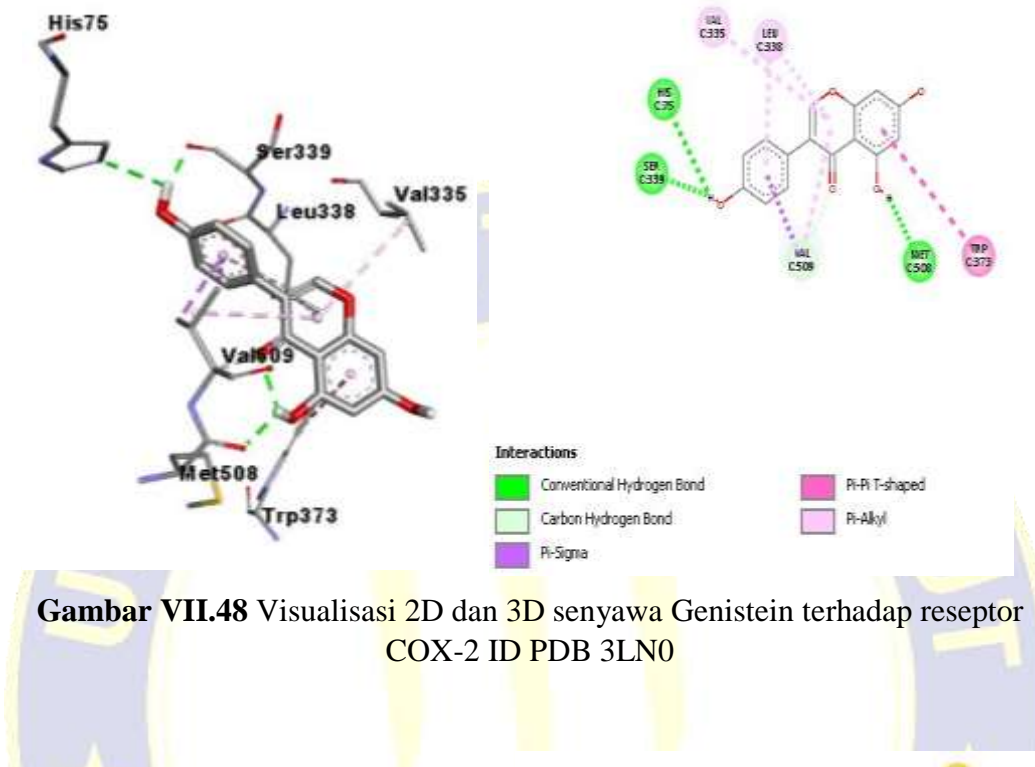


Gambar VII.46 Visualisasi 2D dan 3D senyawa Fustin terhadap reseptor COX-2 ID PDB 3LN0

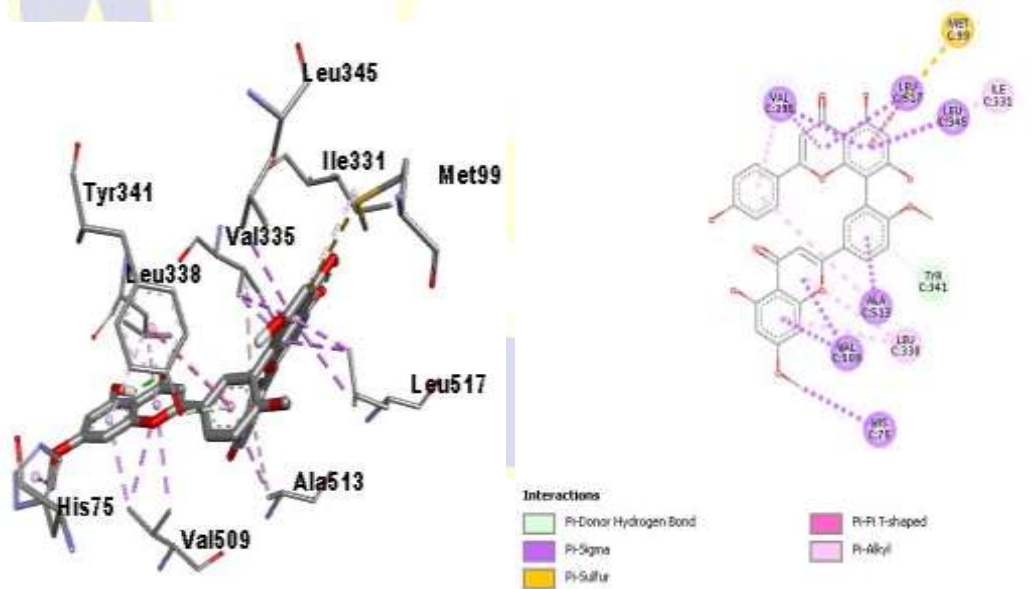


Gambar VII.47 Visualisasi 2D dan 3D senyawa Galangin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

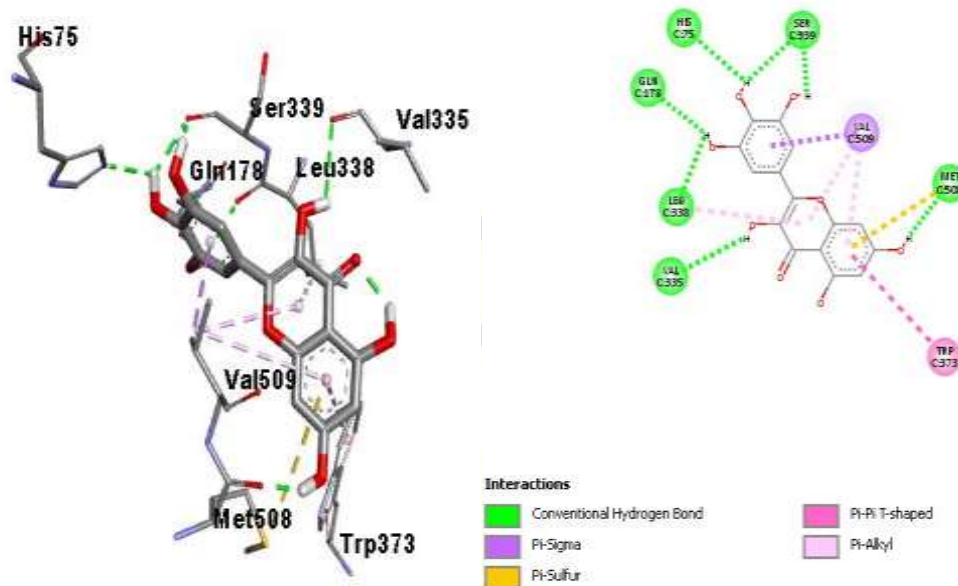


Gambar VII.48 Visualisasi 2D dan 3D senyawa Genistein terhadap reseptor COX-2 ID PDB 3LN0

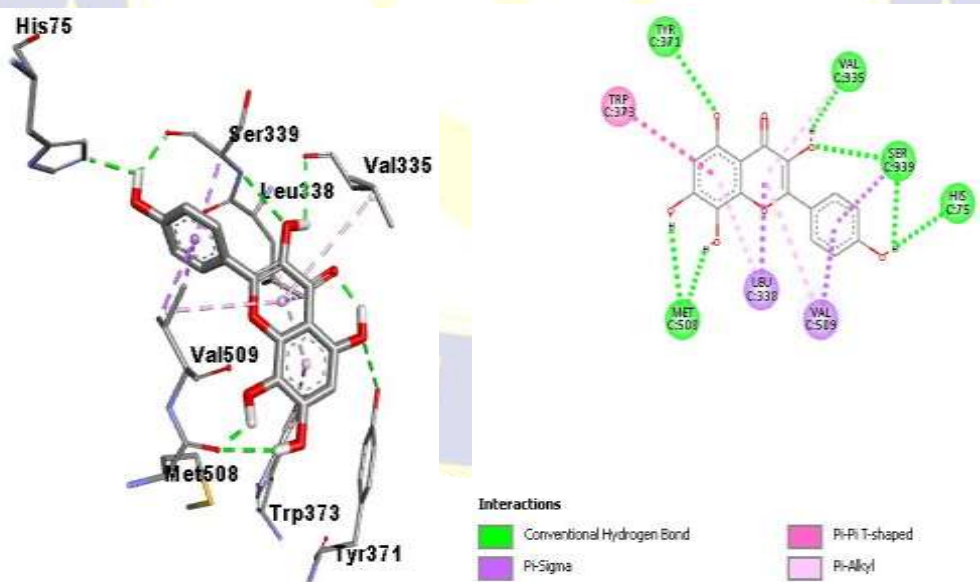


Gambar VII.49 Visualisasi 2D dan 3D senyawa Ginkgetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

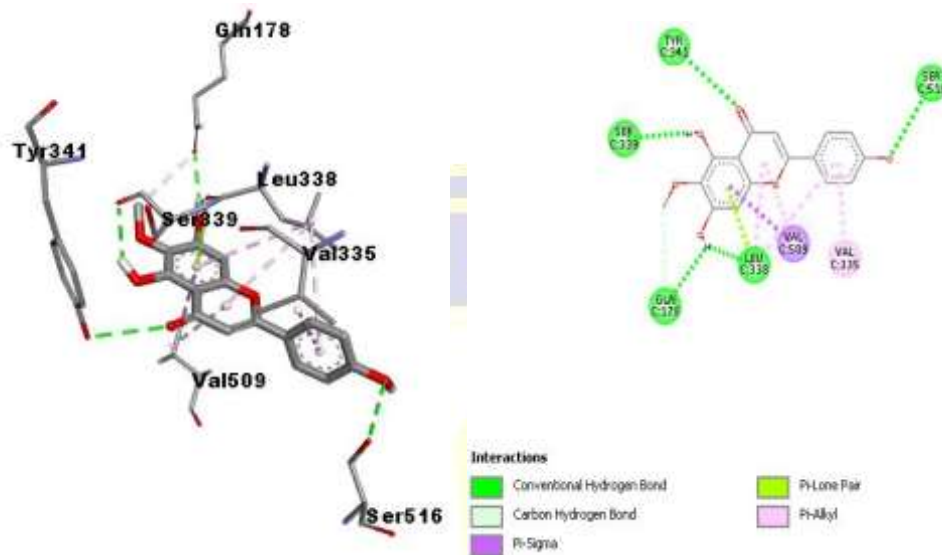


Gambar VII.50 Visualisasi 2D dan 3D senyawa Gossypetin terhadap reseptor COX-2 ID PDB 3LN0

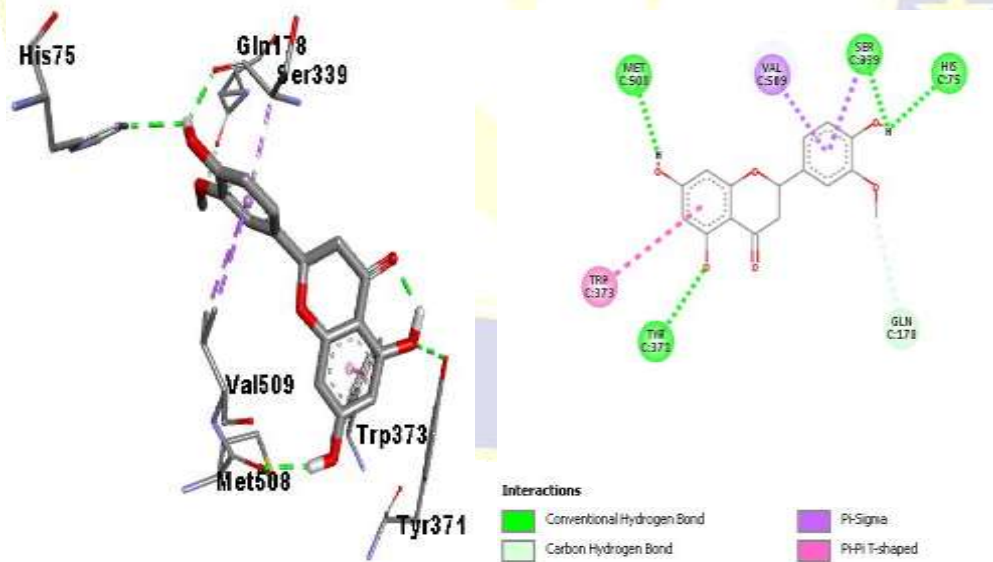


Gambar VII.51 Visualisasi 2D dan 3D senyawa Herbacetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

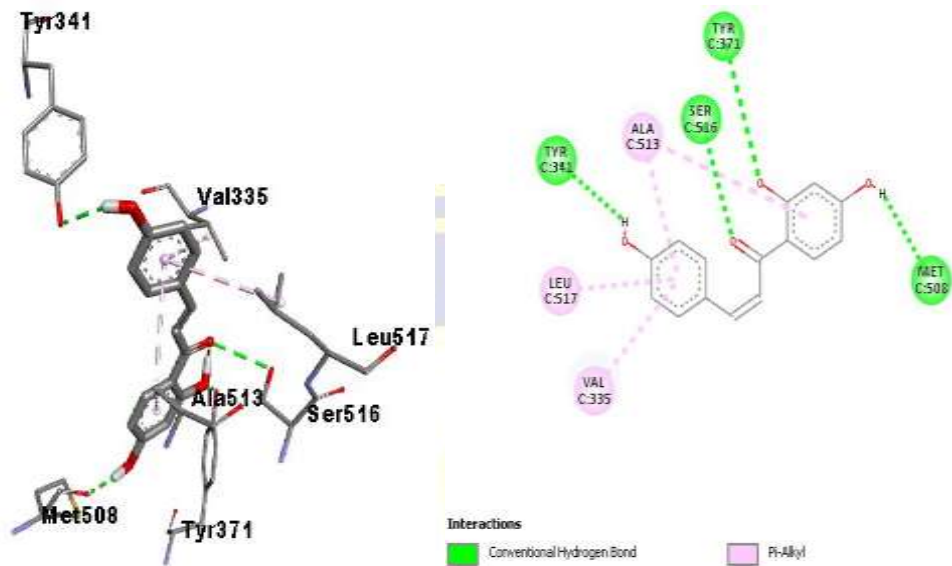


Gambar VII.54 Visualisasi 2D dan 3D senyawa Hispidulin terhadap reseptor COX-2 ID PDB 3LN0

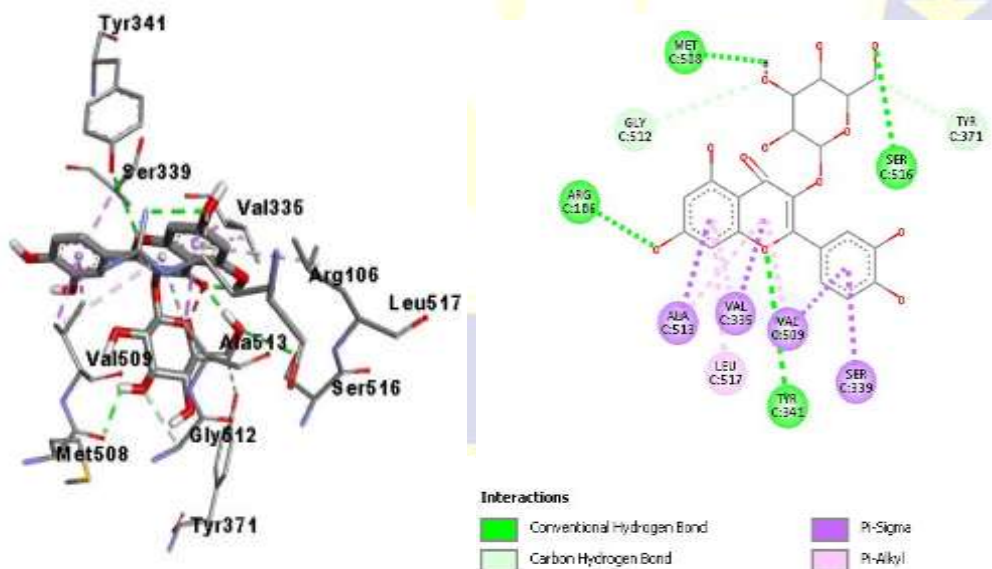


Gambar VII.55 Visualisasi 2D dan 3D senyawa Homoeriodictyol terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

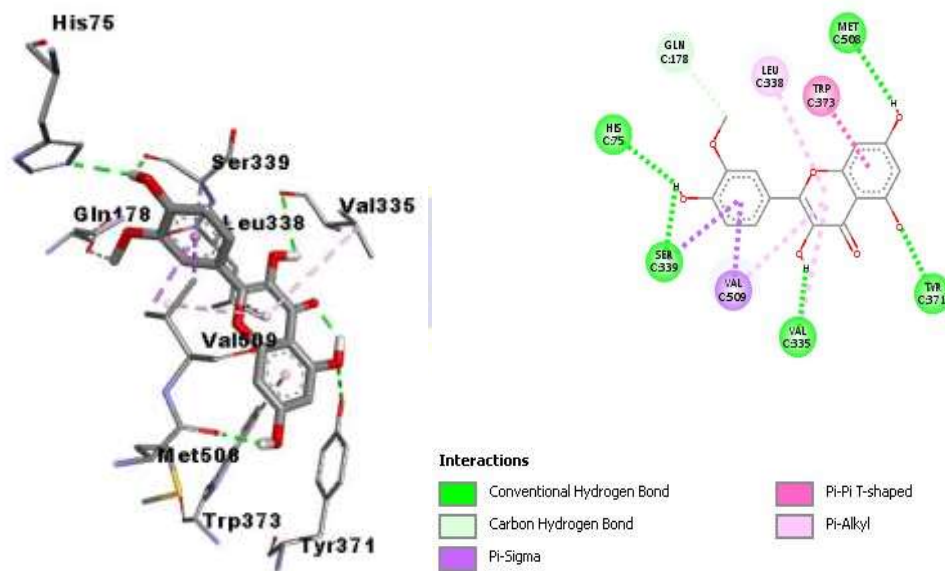


Gambar VII.56 Visualisasi 2D dan 3D senyawa Isoliquiritigenin terhadap reseptor COX-2 ID PDB 3LN0

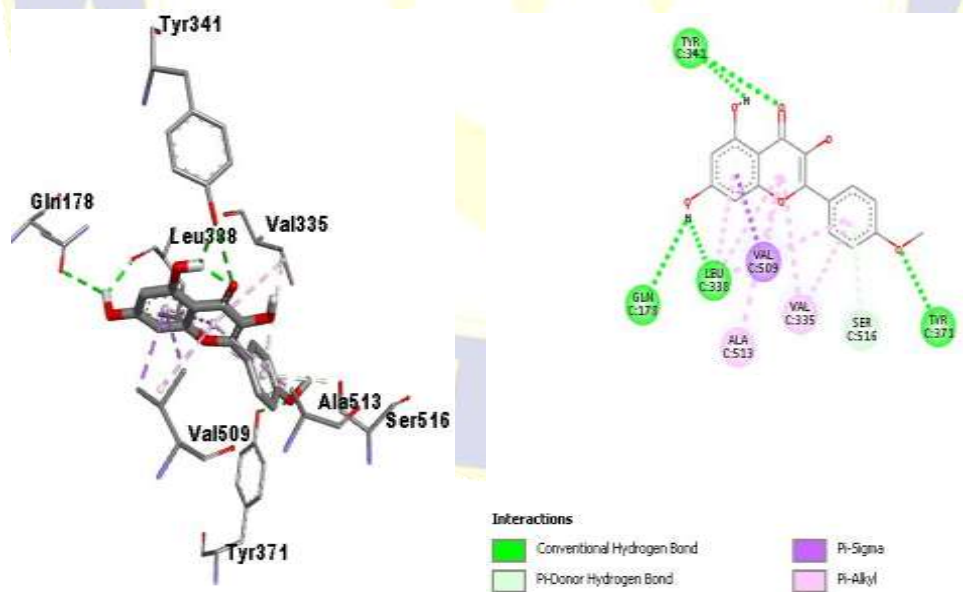


Gambar VII.57 Visualisasi 2D dan 3D senyawa Isoquercetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

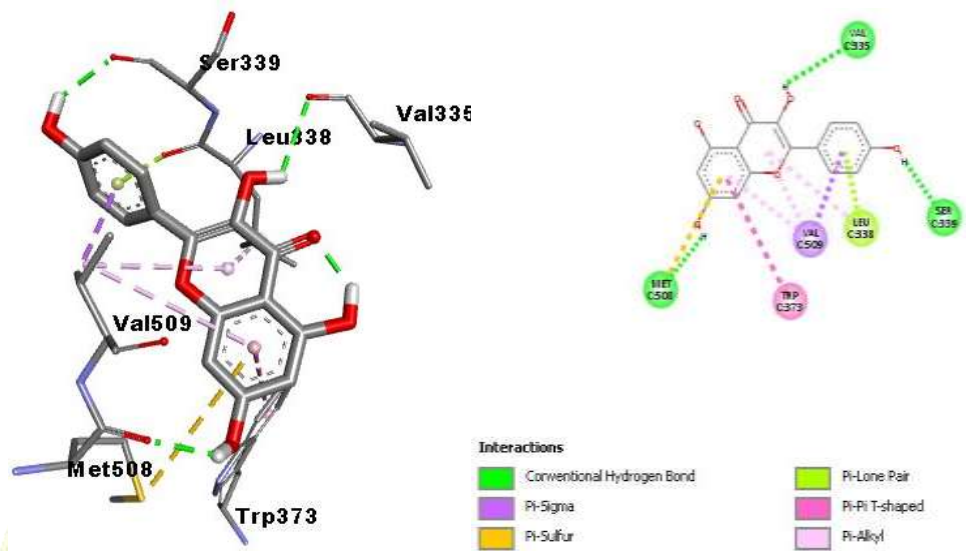


Gambar VII.58 Visualisasi 2D dan 3D senyawa Isorhamnetin terhadap reseptor COX-2 ID PDB 3LN0

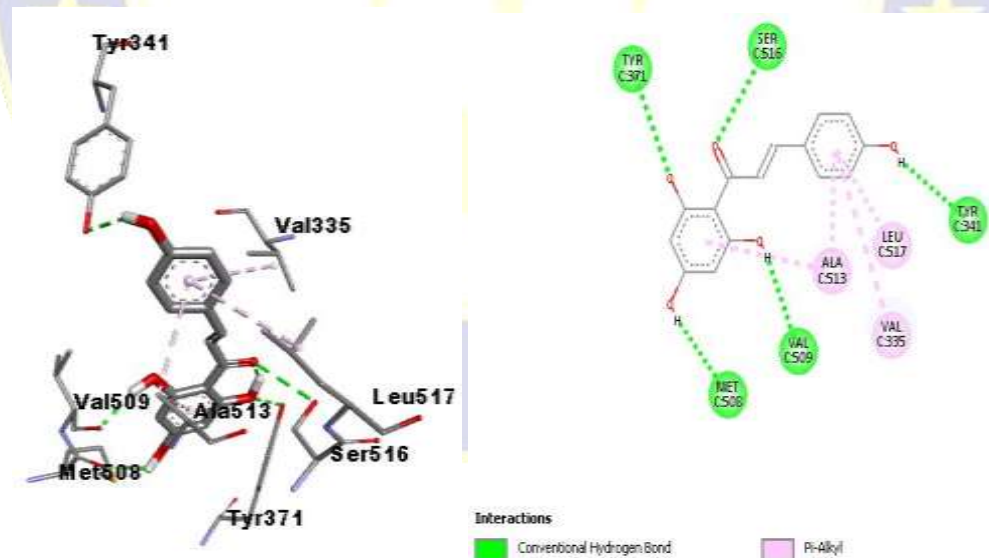


Gambar VII.59 Visualisasi 2D dan 3D senyawa Kaempferide terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

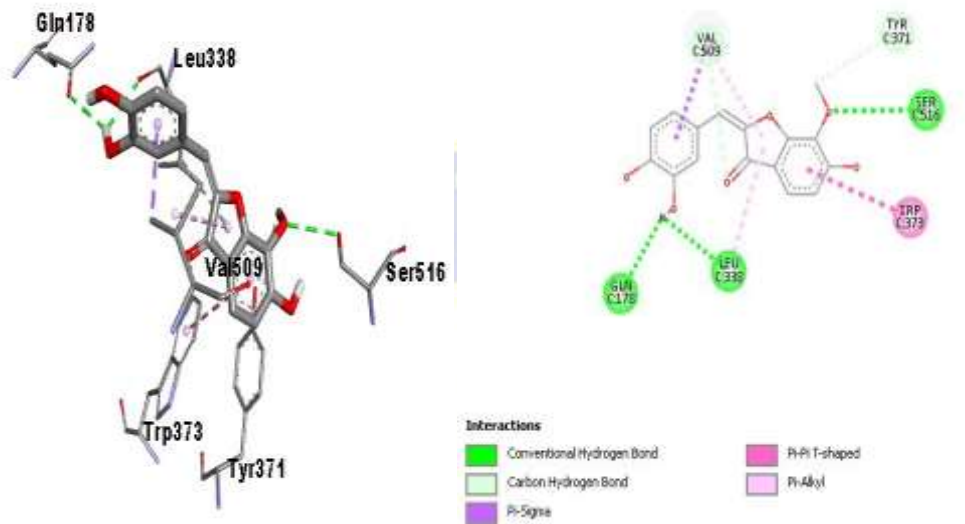


Gambar VII.60 Visualisasi 2D dan 3D senyawa Kaempferol terhadap reseptor COX-2 ID PDB 3LN0

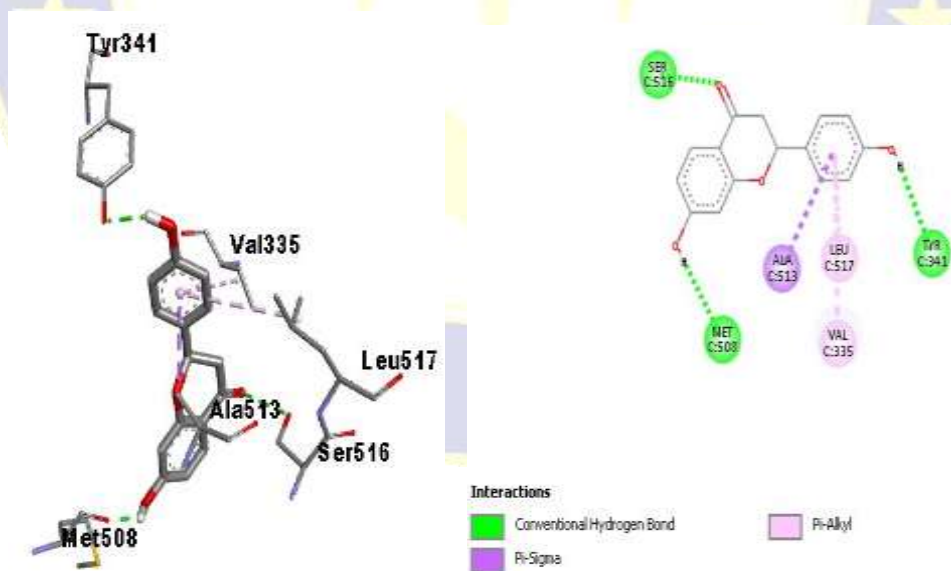


Gambar VII.61 Visualisasi 2D dan 3D senyawa Khalkonarigenin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

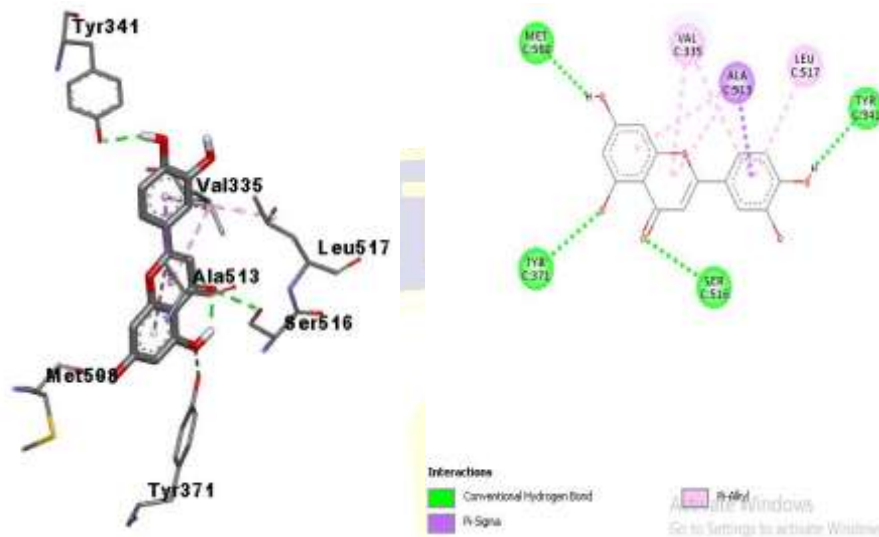


Gambar VII.62 Visualisasi 2D dan 3D senyawa Leptosidin terhadap reseptor COX-2 ID PDB 3LN0

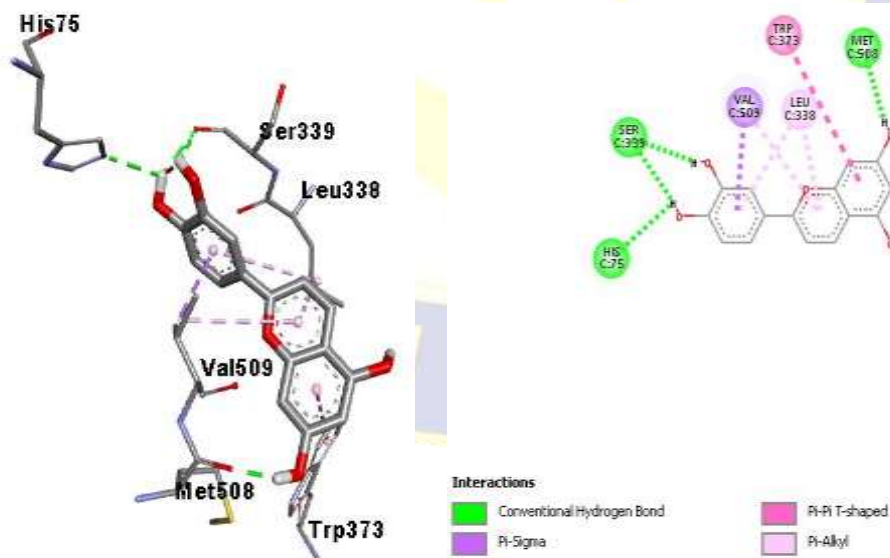


Gambar VII.63 Visualisasi 2D dan 3D senyawa Liquiritigenin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

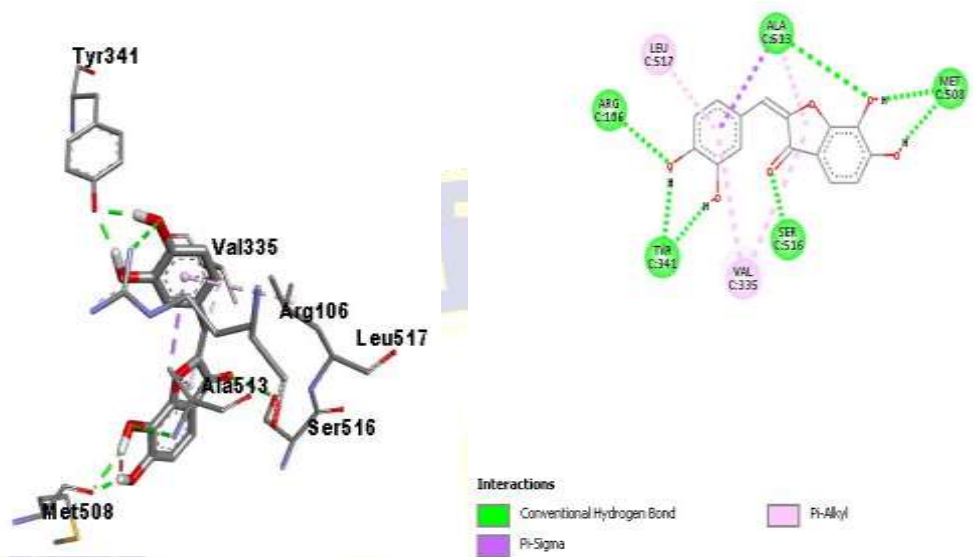


Gambar VII.64 Visualisasi 2D dan 3D senyawa Luteolin terhadap reseptor COX-2 ID PDB 3LN0

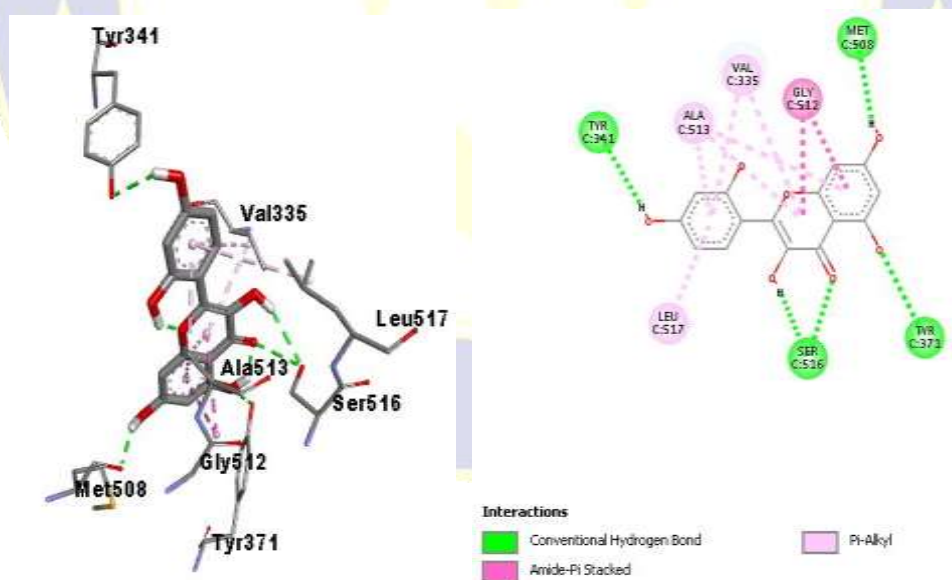


Gambar VII.65 Visualisasi 2D dan 3D senyawa Luteolinidin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

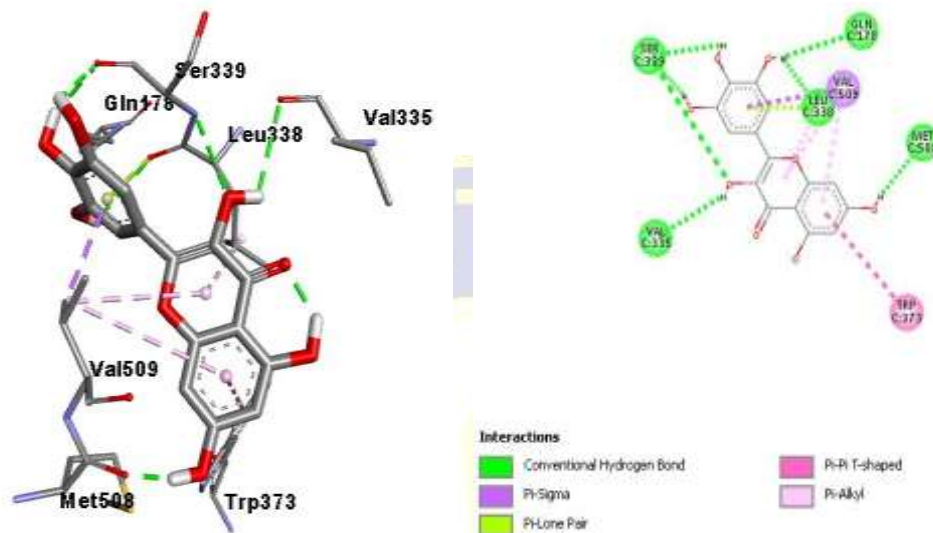


Gambar VII.66 Visualisasi 2D dan 3D senyawa Maritimetin terhadap reseptor COX-2 ID PDB 3LN0

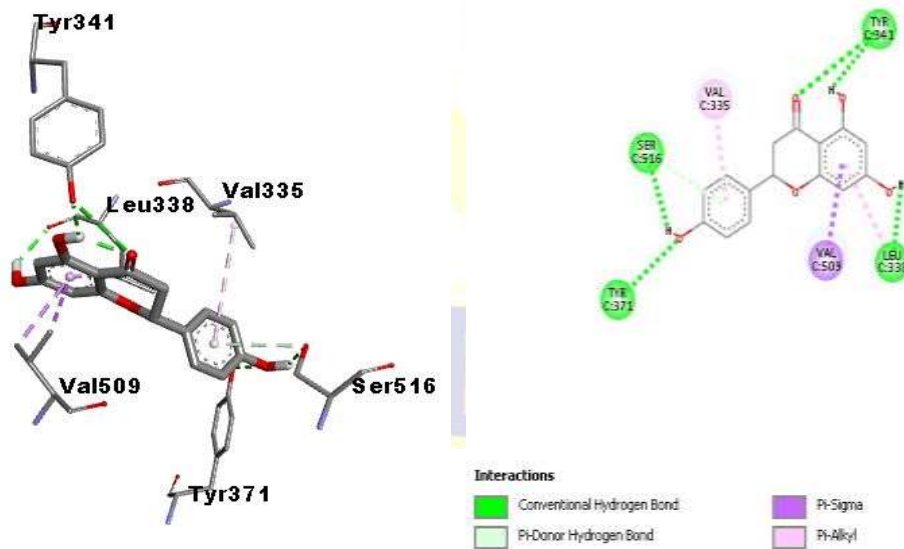


Gambar VII.67 Visualisasi 2D dan 3D senyawa Morin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

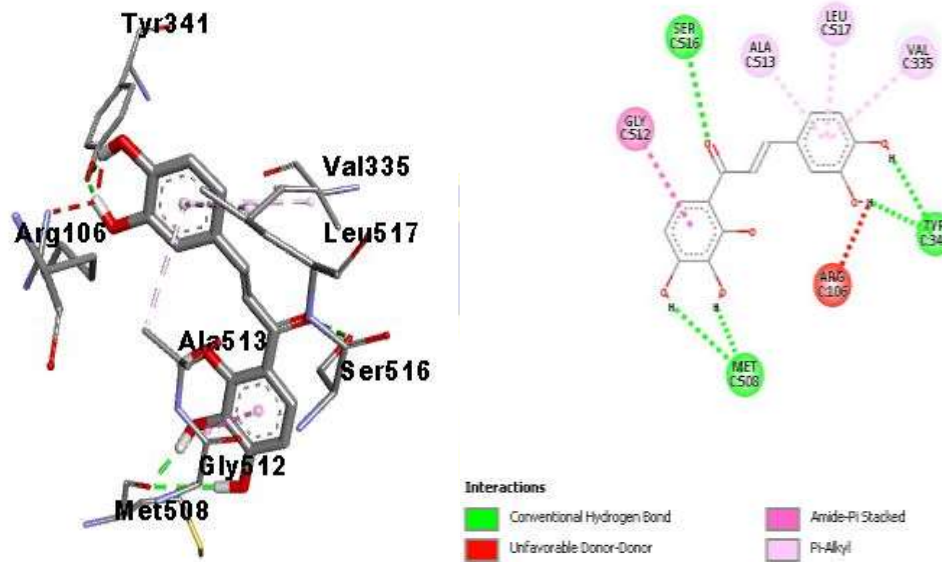


Gambar VII.68 Visualisasi 2D dan 3D senyawa Myricetin terhadap reseptor COX-2 ID PDB 3LN0

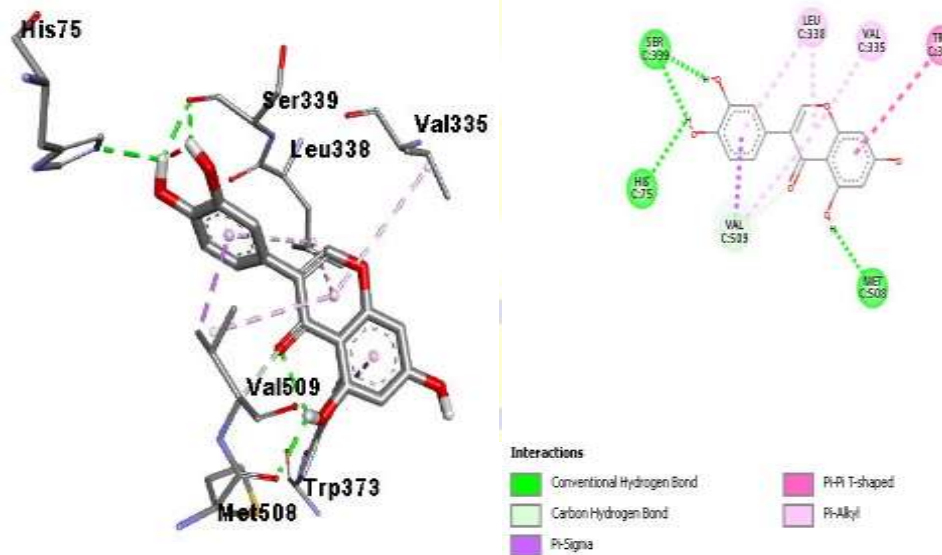


Gambar VII.69 Visualisasi 2D dan 3D senyawa Narigenin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

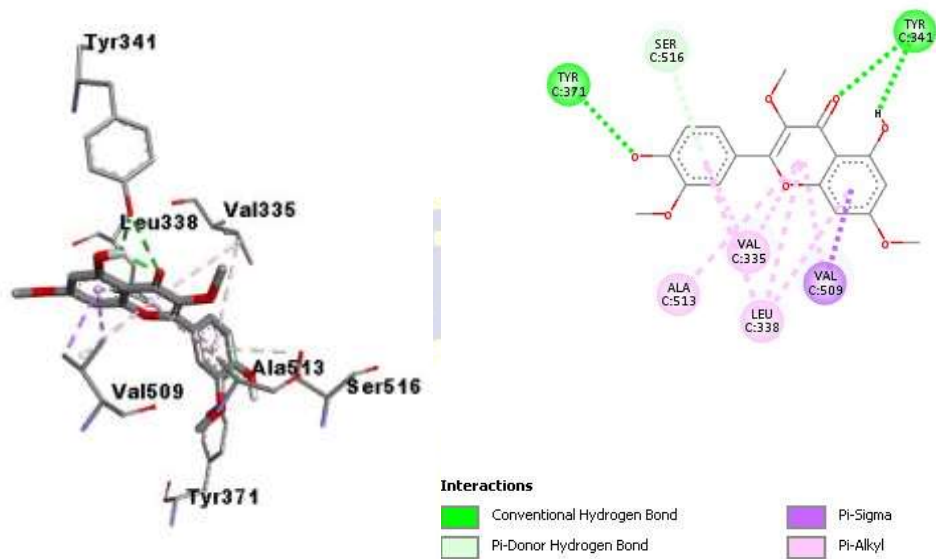


Gambar VII.72 Visualisasi 2D dan 3D senyawa Okanin terhadap reseptor COX-2 ID PDB 3LN0

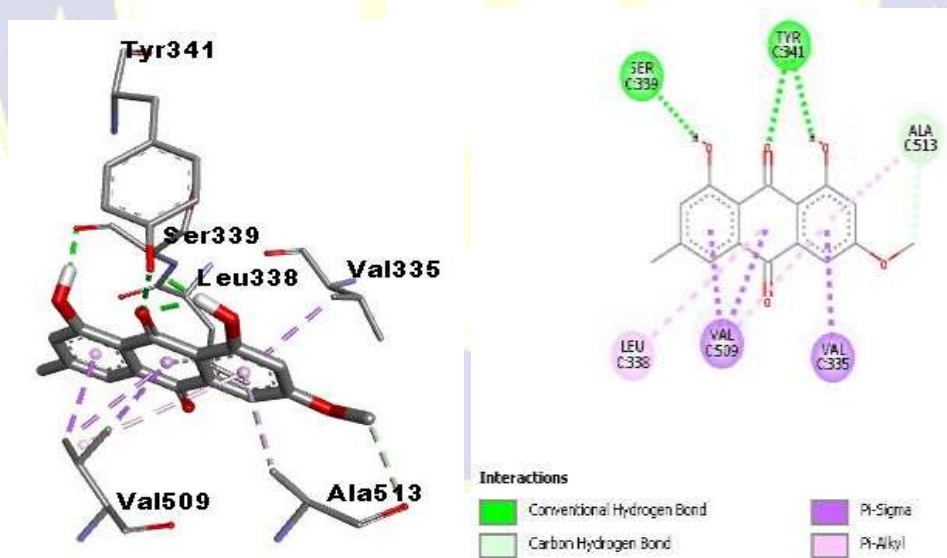


Gambar VII.73 Visualisasi 2D dan 3D senyawa Orobol terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

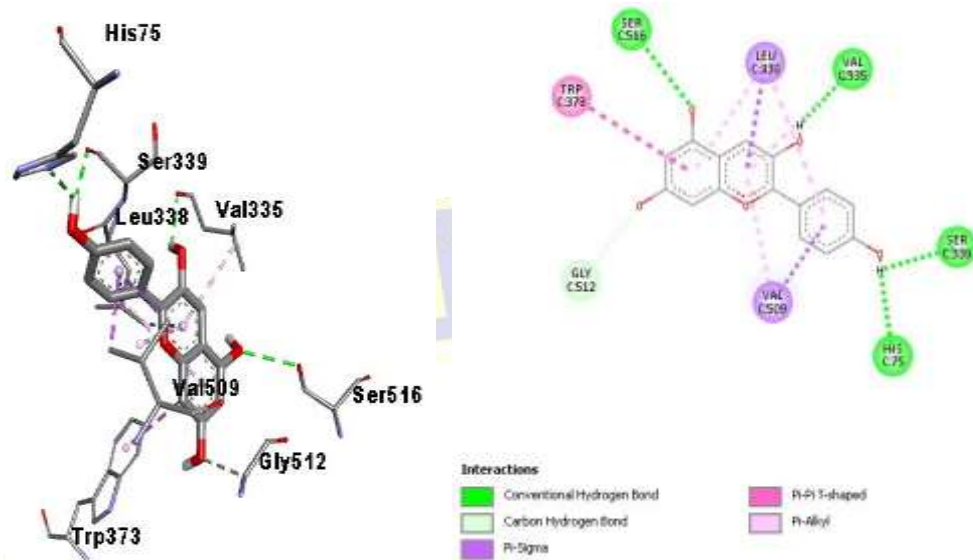


Gambar VII.74 Visualisasi 2D dan 3D senyawa Pachypodol terhadap reseptor COX-2 ID PDB 3LN0

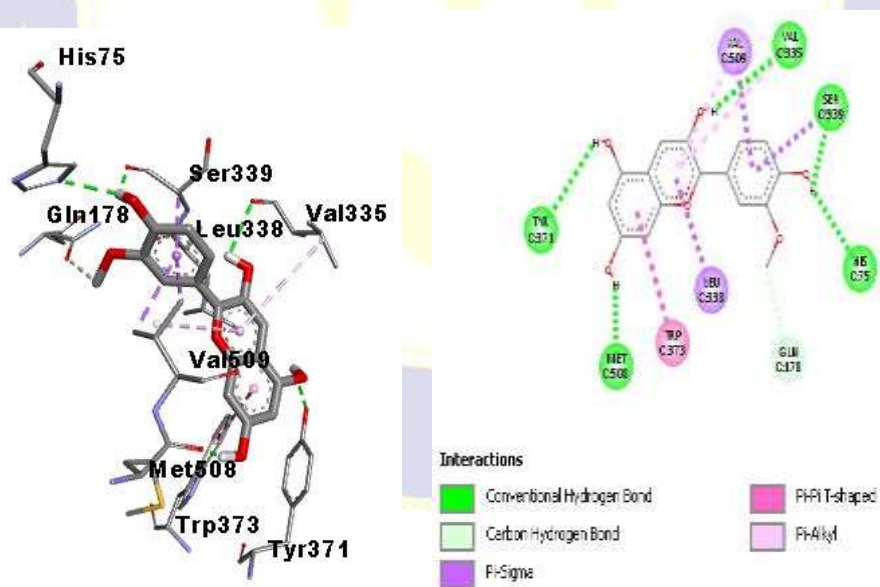


Gambar VII.75 Visualisasi 2D dan 3D senyawa Parietin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

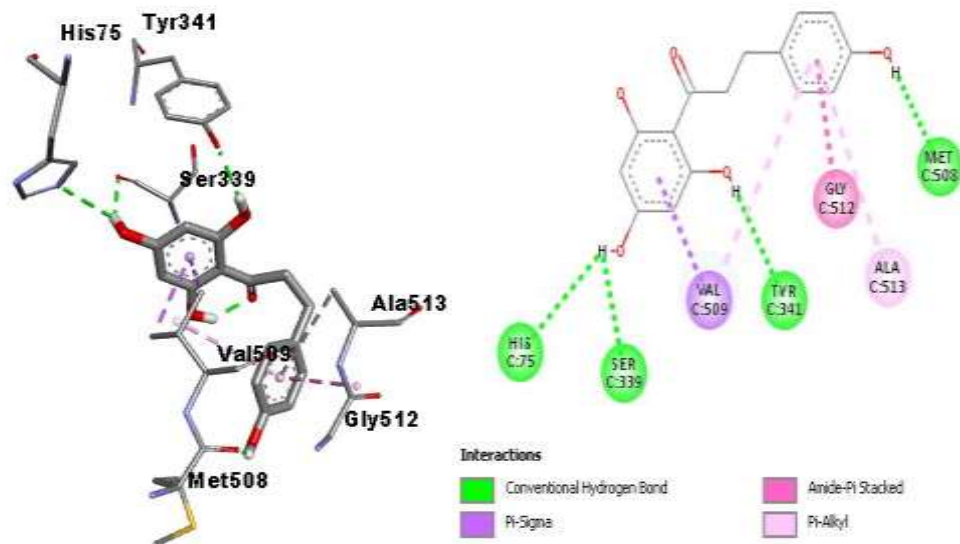


Gambar VII.76 Visualisasi 2D dan 3D senyawa Pelargonidin terhadap reseptor COX-2 ID PDB 3LN0

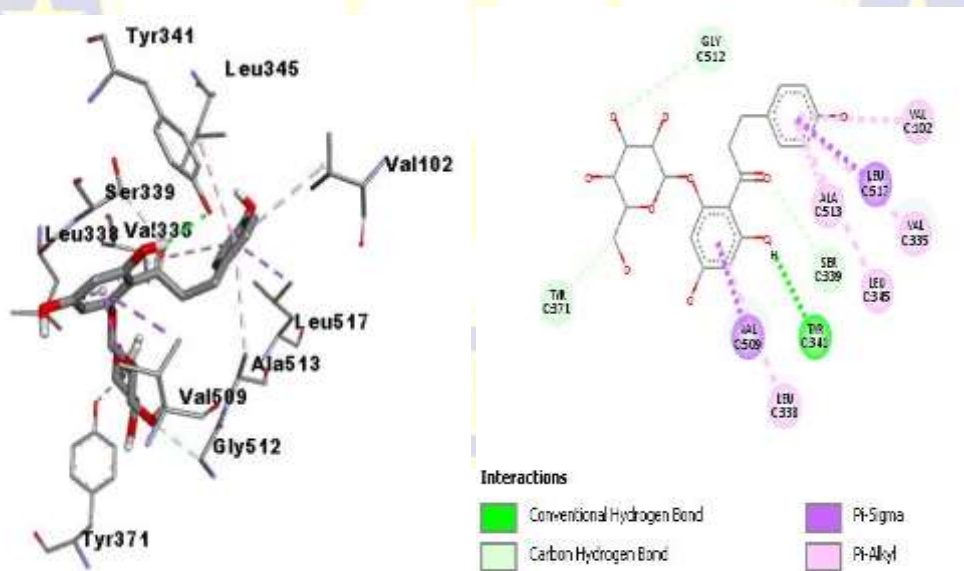


Gambar VII.77 Visualisasi 2D dan 3D senyawa Peonidin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

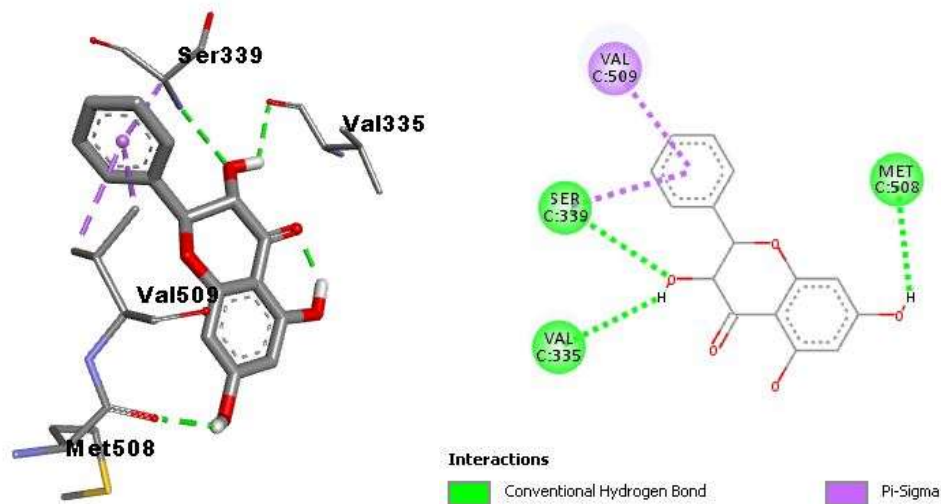


Gambar VII.78 Visualisasi 2D dan 3D senyawa Phloretin terhadap reseptor COX-2 ID PDB 3LN0

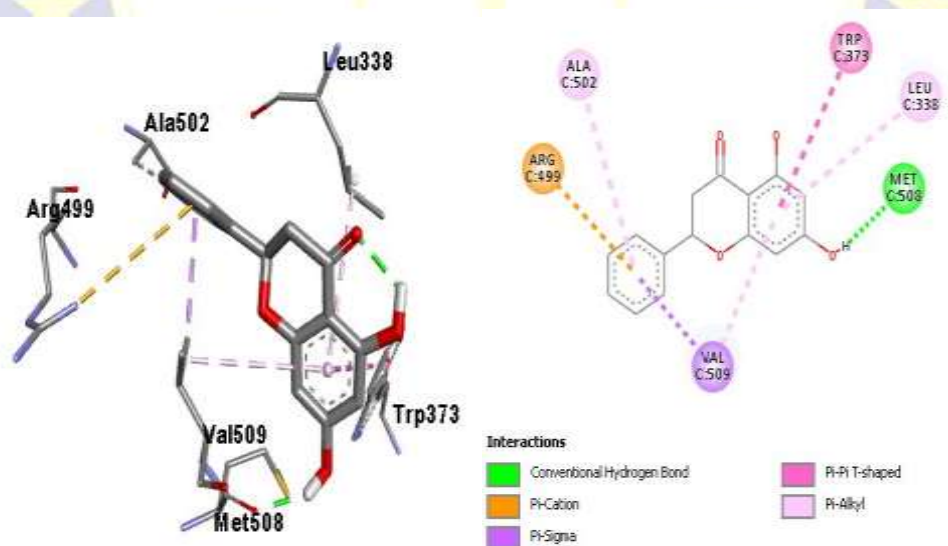


Gambar VII.79 Visualisasi 2D dan 3D senyawa Phlorizin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

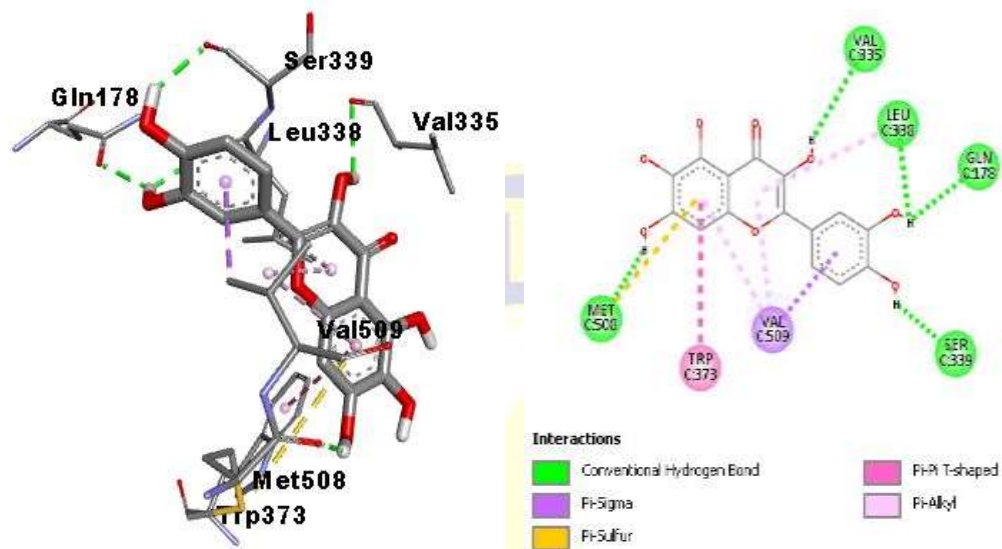


Gambar VII.80 Visualisasi 2D dan 3D senyawa Pinobanksin terhadap reseptor COX-2 ID PDB 3LN0

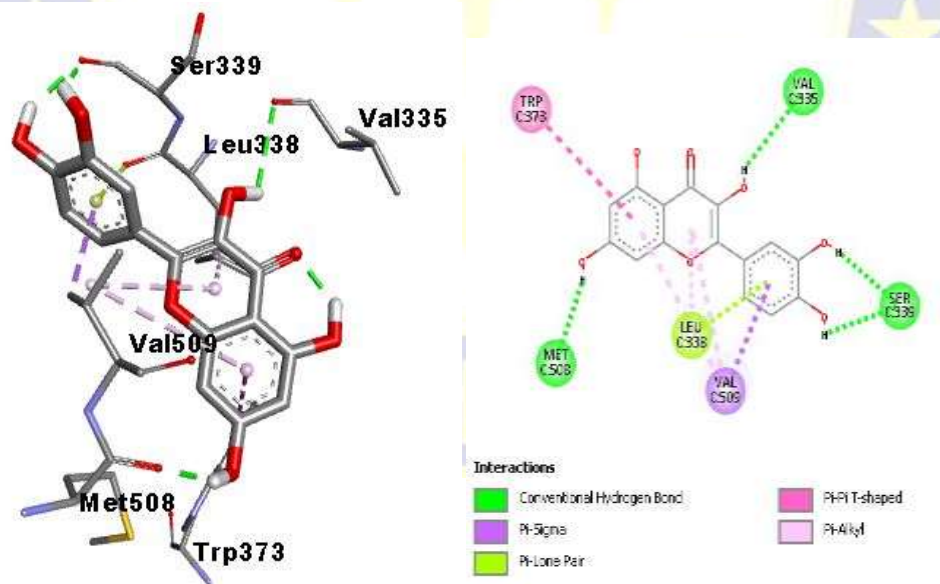


Gambar VII.81 Visualisasi 2D dan 3D senyawa Pinocembrin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

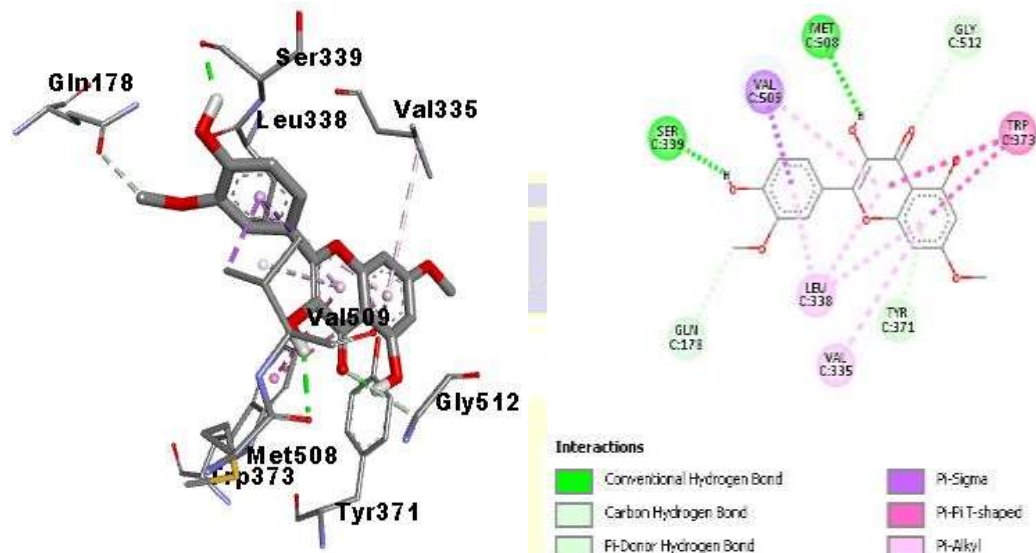


Gambar VII.82 Visualisasi 2D dan 3D senyawa Quercetagenin terhadap reseptor COX-2 ID PDB 3LN0

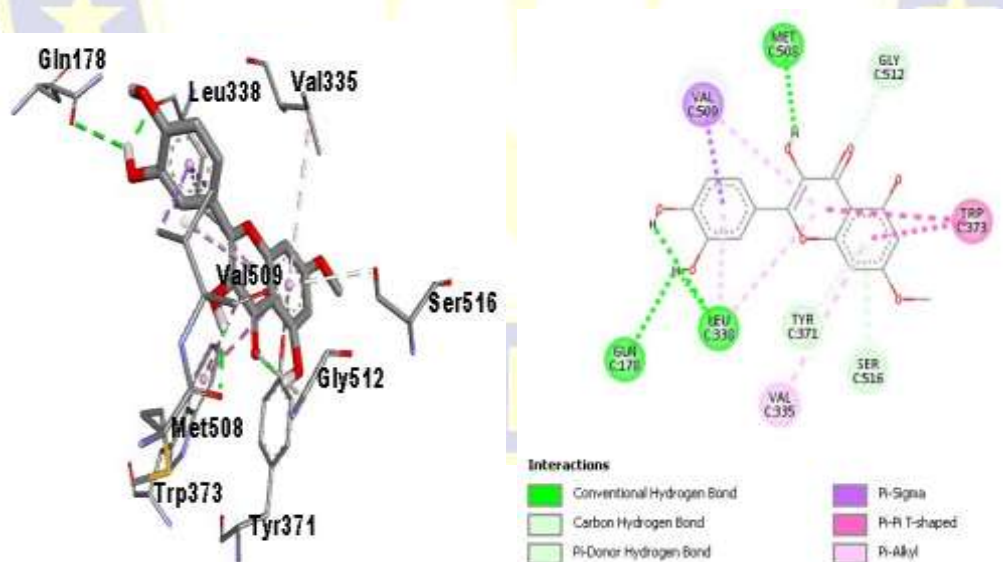


Gambar VII.83 Visualisasi 2D dan 3D senyawa Quercetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

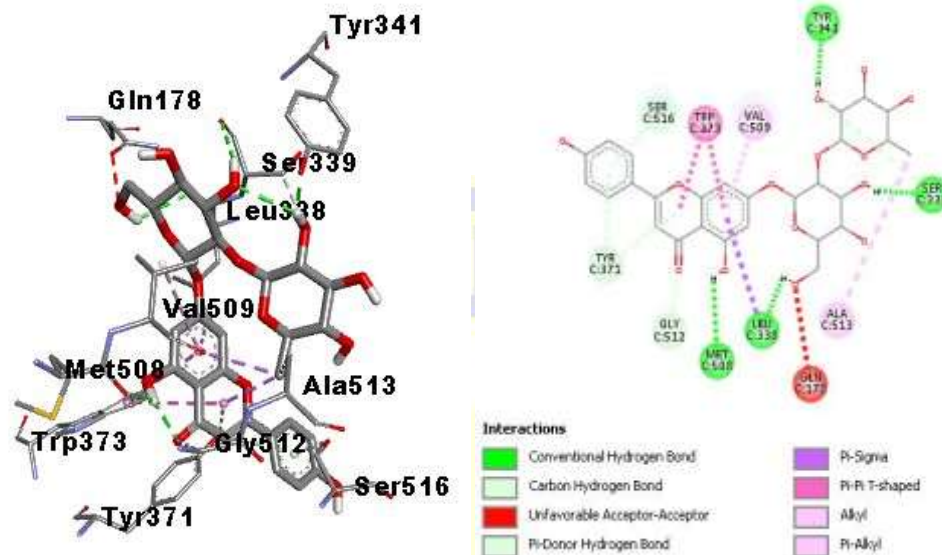


Gambar VII.84 Visualisasi 2D dan 3D senyawa Rhamnazin terhadap reseptor COX-2 ID PDB 3LN0

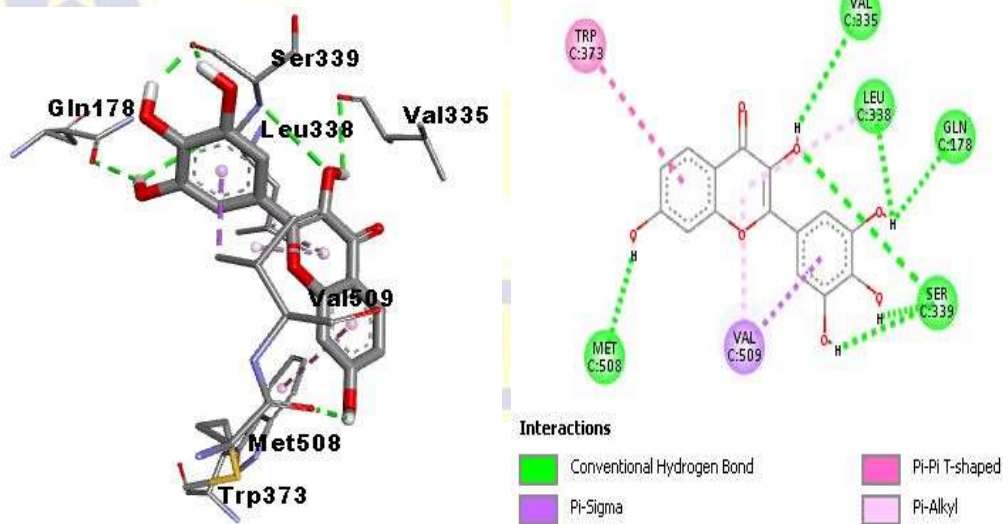


Gambar VII.85 Visualisasi 2D dan 3D senyawa Rhamnetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

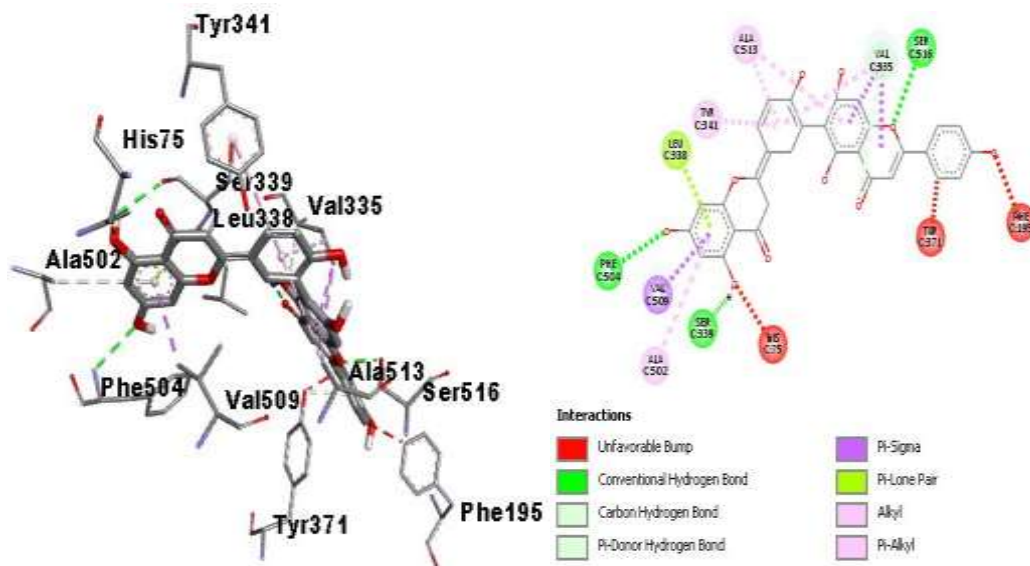


Gambar VII.86 Visualisasi 2D dan 3D senyawa Rhoifolin terhadap reseptor COX-2 ID PDB 3LN0

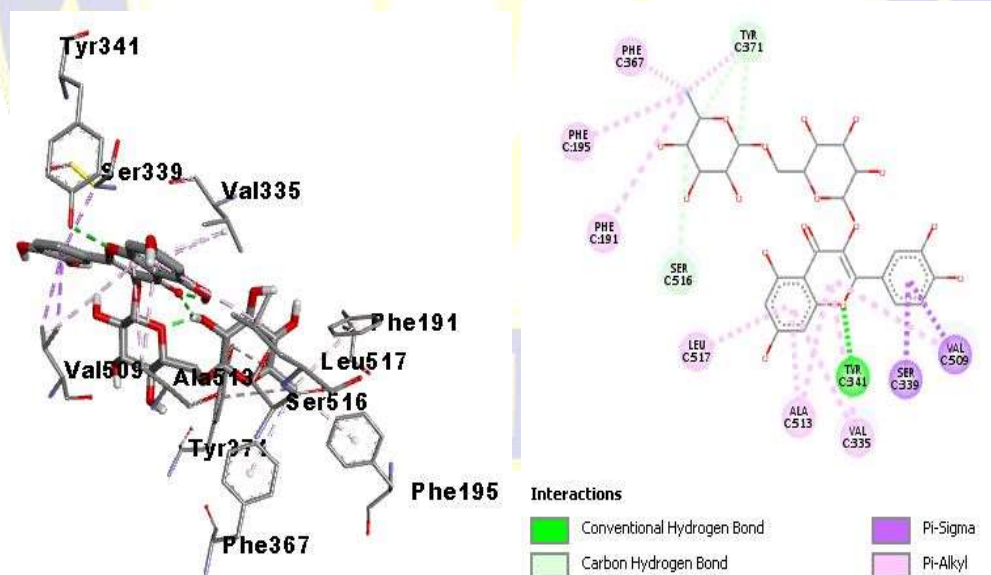


Gambar VII.87 Visualisasi 2D dan 3D senyawa Robinetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

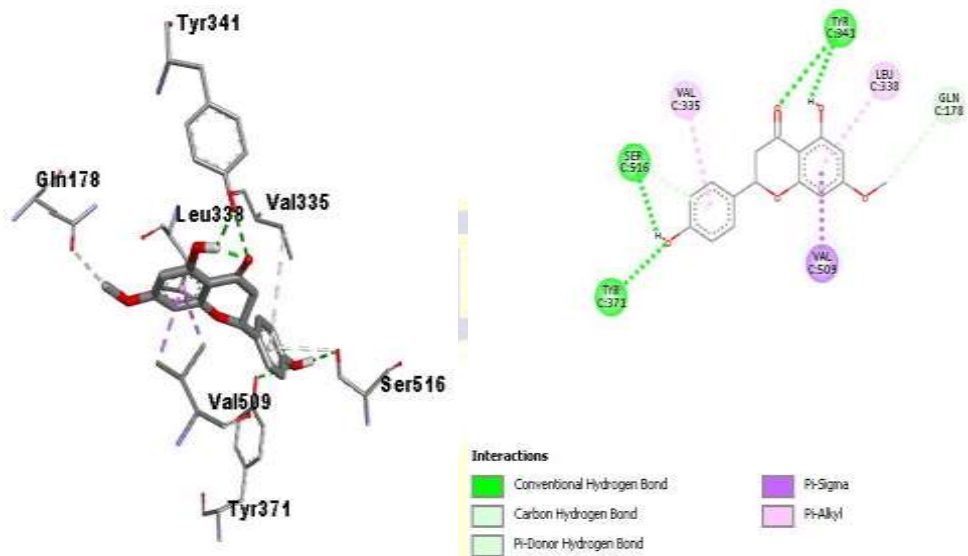


Gambar VII.88 Visualisasi 2D dan 3D senyawa Robustaflavone terhadap reseptor COX-2 ID PDB 3LN0

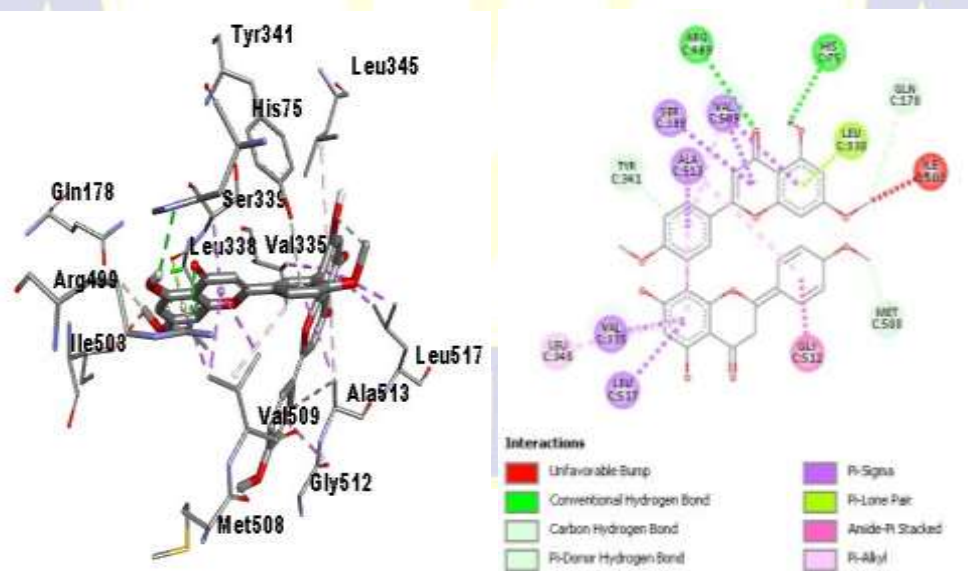


Gambar VII.89 Visualisasi 2D dan 3D senyawa Rutin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

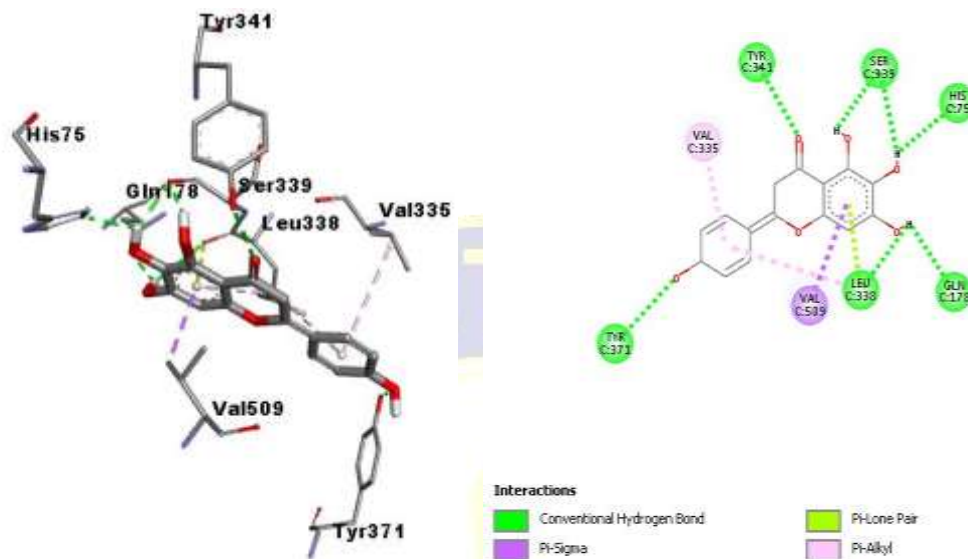


Gambar VII.90 Visualisasi 2D dan 3D senyawa Sakuranetin terhadap reseptor COX-2 ID PDB 3LN0

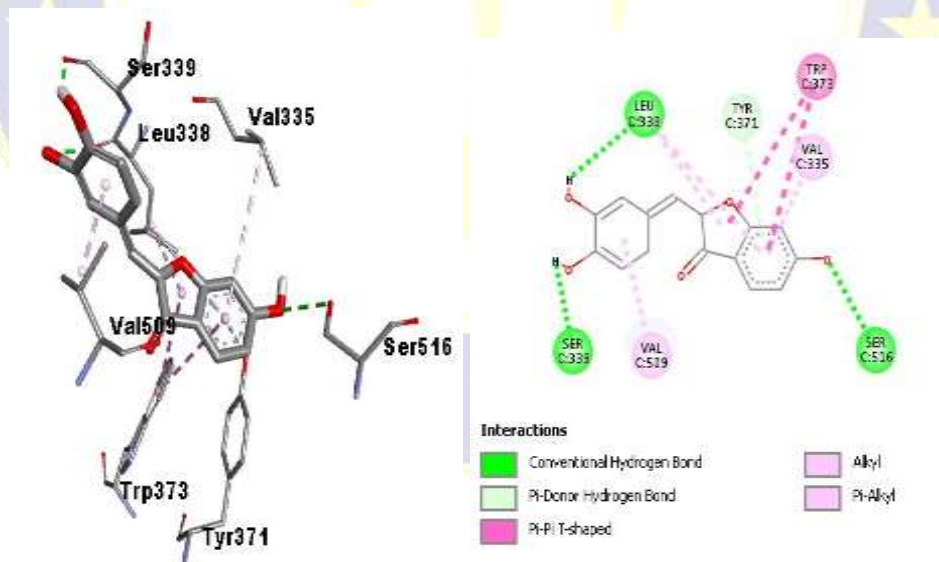


Gambar VII.91 Visualisasi 2D dan 3D senyawa Sciadopitysin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

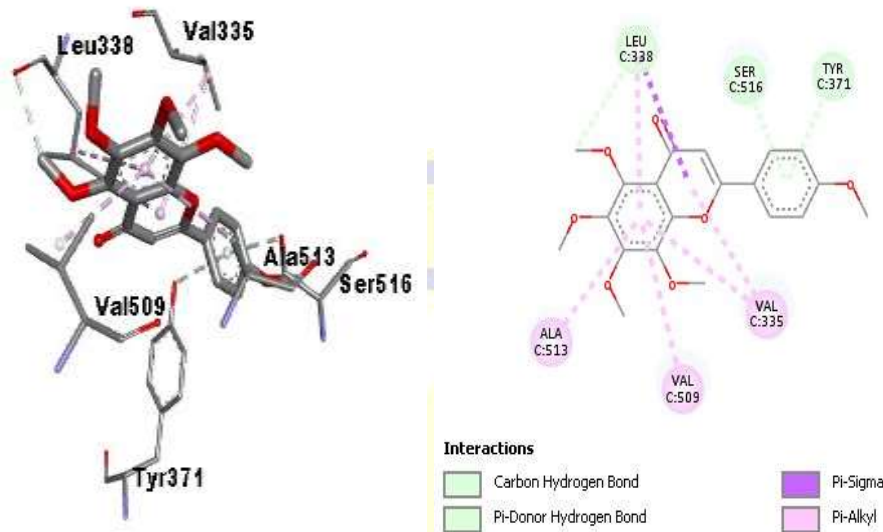


Gambar VII.92 Visualisasi 2D dan 3D senyawa Scutellarein terhadap reseptor COX-2 ID PDB 3LN0

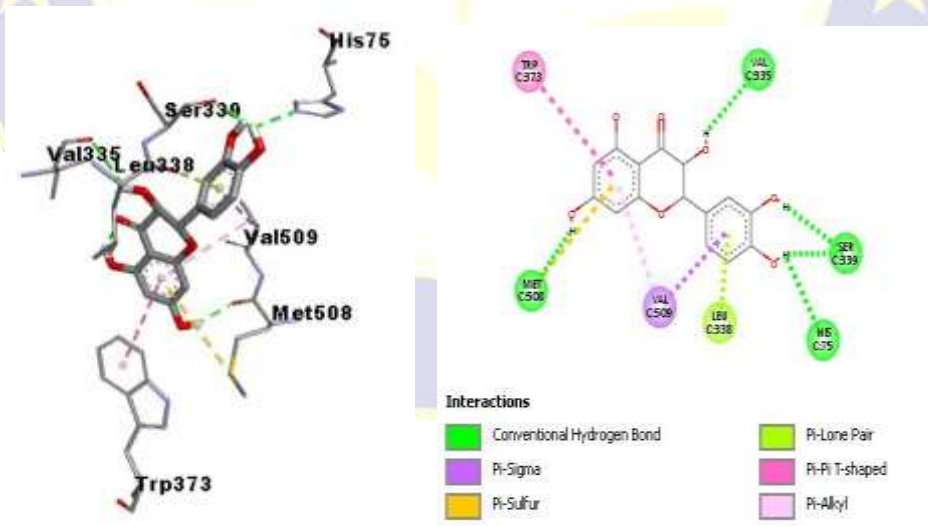


Gambar VII.93 Visualisasi 2D dan 3D senyawa Sulfuretin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

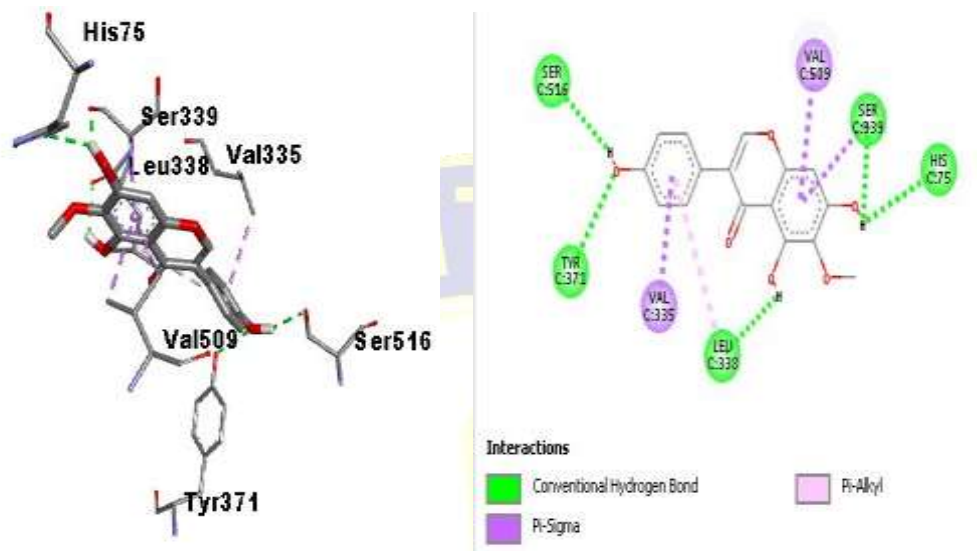


Gambar VII.94 Visualisasi 2D dan 3D senyawa Tangeretin terhadap reseptor COX-2 ID PDB 3LN0

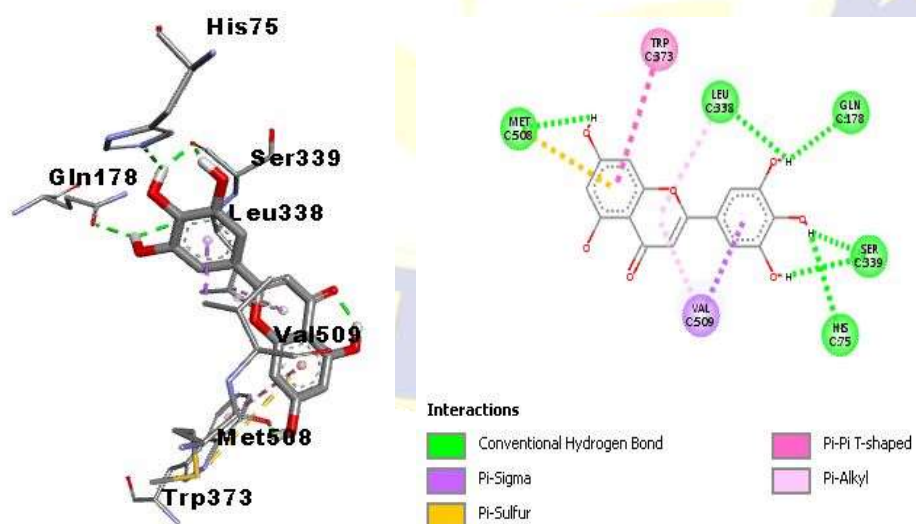


Gambar VII.95 Visualisasi 2D dan 3D senyawa Taxifolin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)

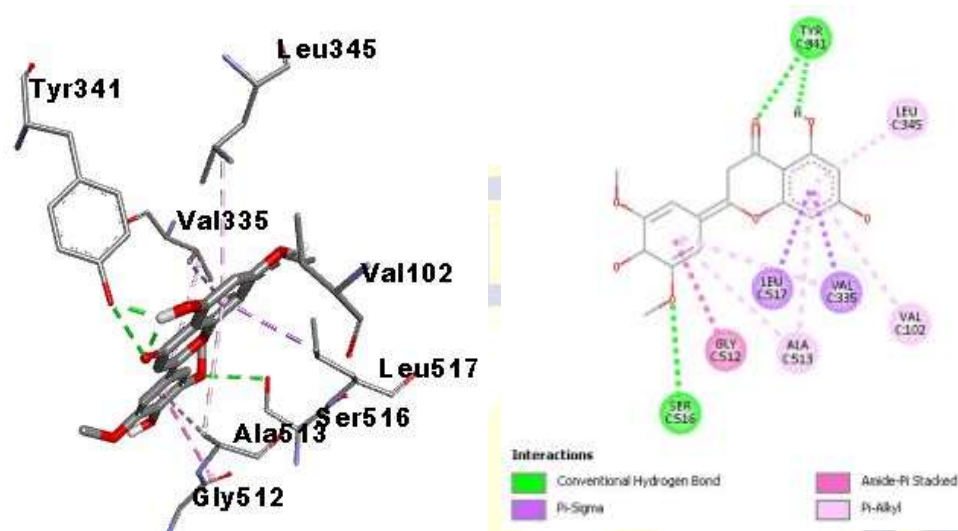


Gambar VII.96 Visualisasi 2D dan 3D senyawa Tectorigenin terhadap reseptor COX-2 ID PDB 3LN0

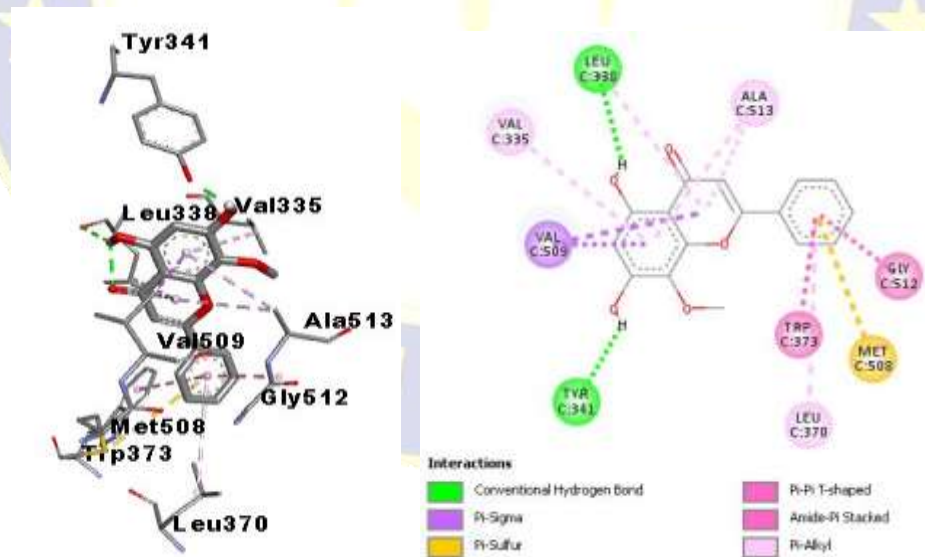


Gambar VII.97 Visualisasi 2D dan 3D senyawa Tricetin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 12 (LANJUTAN)



Gambar VII.98 Visualisasi 2D dan 3D senyawa Tricin terhadap reseptor COX-2 ID PDB 3LN0



Gambar VII.99 Visualisasi 2D dan 3D senyawa Wogonin terhadap reseptor COX-2 ID PDB 3LN0

LAMPIRAN 13

HASIL PENELITIAN PREDIKSI *DRUGLIKENESS*

Tabel VII.5

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

No	Ligan	BM (Da)	Akseptor Ikatan H	Donor Ikatan H	LogP	Ket.
1	Chrysin	254	4	2	2,71	Memenuhi
2	Baicalein	270	5	2	2,42	Memenuhi
3	Apigenin	270	5	3	2,42	Memenuhi
4	Acacetin	284	5	2	2,71	Memenuhi
5	Scutelarein	286	6	4	2,13	Memenuhi
6	Hispidulin	300	6	3	2,43	Memenuhi
7	Luteolin	286	6	4	2,13	Memenuhi
8	Chrysoeriol	300	6	3	2,43	Memenuhi
9	Diosmetin	300	6	3	2,43	Memenuhi
10	Tricetin	302	7	5	1,83	Memenuhi
11	Tricin	330	7	3	2,44	Memenuhi
12	Tangeretin	372	7	0	3,35	Memenuhi
13	Rhoifolin	578	14	8	-1,26	Tidak Memenuhi
14	Wogonin	284	5	2	2,72	Memenuhi
15	Galangin	270	5	3	2,6	Memenuhi
16	Fisetin	286	6	4	2,31	Memenuhi
17	Kaempferol	286	6	4	2,31	Memenuhi
18	Kaempferide	300	6	4	2,61	Memenuhi
19	Robinetin	302	7	5	2,01	Memenuhi
20	Herbacetin	302	7	5	2,01	Memenuhi
21	Quercetin	302	7	5	2,01	Memenuhi
22	Rhamnetin	316	7	4	2,31	Memenuhi
23	Isorhamnetin	316	7	4	2,31	Memenuhi

**LAMPIRAN 13
(LANJUTAN)**

**Tabel VII.5
Lanjutan**

No	Ligan	BM (Da)	Akseptor Ikatan H	Donor Ikatan H	LogP	Ket.
24	Myricetin	318	8	6	1,72	Tidak Memenuhi
25	Quercetagenin	318	8	6	1,72	Tidak Memenuhi
26	Gossypetin	318	8	6	1,72	Tidak Memenuhi
27	Isoquercetin	464	12	8	-0,73	Tidak Memenuhi
28	Rhamnazin	330	7	3	2,62	Memenuhi
29	Rutin	610	16	10	-1,88	Tidak Memenuhi
30	Morin	302	7	5	2,01	Memenuhi
31	Pachypodol	344	7	2	2,71	Memenuhi
32	Daidzein	254	4	2	2,71	Memenuhi
33	Formononetin	268	4	1	3,02	Memenuhi
34	Genistein	270	5	3	2,42	Memenuhi
35	Biokanin A	284	5	2	2,72	Memenuhi
36	Orobol	286	6	4	2,12	Memenuhi
37	Tectorigenin	300	6	3	2,43	Memenuhi
38	Baptigenin	286	6	4	2,13	Memenuhi
39	Pinocembrin	256	4	2	2,8	Memenuhi
40	Liquiritigenin	256	4	2	2,8	Memenuhi
41	Narigenin	272	5	3	2,51	Memenuhi
42	Sakuranetin	286	5	2	2,81	Memenuhi
43	Eriodictyol	288	6	4	2,22	Memenuhi
44	Hesperitin	302	6	3	2,52	Memenuhi
45	Homeriodictyol	302	6	3	2,52	Memenuhi

**LAMPIRAN 13
(LANJUTAN)**

**Tabel VII.5
Lanjutan**

No	Ligan	BM (Da)	Akseptor Ikatan H	Donor Ikatan H	LogP	Ket.
46	Parietin	284	5	2	2.19	Memenuhi
47	Epigallocatechin	306	7	6	1,25	Tidak Memenuhi
48	Catehcin	290	6	5	1,55	Memenuhi
49	Naringin	580	14	8	-1,16	Tidak Memenuhi
50	Pinobanksin	272	5	3	1,77	Memenuhi
51	Aromadendrin	288	6	4	1,48	Memenuhi
52	Fustin	288	6	4	1,48	Memenuhi
53	Taxifolin	304	7	5	1,18	Memenuhi
54	Agathisfalvone	538	10	6	4,82	Tidak Memenuhi
55	Cupressuflavone	538	10	6	3,88	Tidak Memenuhi
56	Ginkgetin	566	10	4	5,42	Tidak Memenuhi
57	Sciadopitisin	580	10	3	5,72	Tidak Memenuhi
58	Robustaflavone	538	10	6	4,81	Tidak Memenuhi
59	Hinokiflavone	538	10	5	5,23	Tidak Memenuhi
60	Ochnaflavone	538	10	5	5,23	Tidak Memenuhi
61	Amentoflavone	538	10	6	4,81	Tidak Memenuhi

LAMPIRAN 13
(LANJUTAN)

Tabel VII.5
Lanjutan

No	Ligan	BM (Da)	Akseptor Ikatan H	Donor Ikatan H	LogP	Ket.
62	Isoliquiritigenin	256	4	3	2,7	Memenuhi
63	Khalkonarigenin	272	5	4	2,41	Memenuhi
64	Butein	272	5	4	2,41	Memenuhi
65	Okanin	288	6	5	2,11	Memenuhi
66	Phloretin	274	5	4	2,32	Memenuhi
67	Phlorizin	436	10	7	-0,2	Tidak Memenuhi
68	Sulfuretin	270	5	3	2,42	Memenuhi
69	Aureusidin	286	6	4	2,13	Memenuhi
70	Maritimetin	286	6	4	2,13	Memenuhi
71	Leptosidin	300	6	3	2,43	Memenuhi
72	Apigenidin	290	4	3	2,68	Memenuhi
73	Luteolinidin	271	5	4	3,01	Memenuhi
74	Pelargonidin	271	5	4	3,01	Memenuhi
75	Cyanidin	287	6	5	2,71	Memenuhi
76	Peonidin	301	6	4	3,02	Memenuhi
77	Delpinidin	338	7	6	2,42	Tidak Memenuhi
78	Petunidin	317	7	5	2,73	Memenuhi
79	Malvinidin	366	7	4	3,03	Memenuhi
80	Rosinidin	315	6	3	3,32	Memenuhi

Keterangan :

BM (Berat Molekul) : <500 Dalton
 Akseptor ikatan hidrogen : <10
 Donor ikatan hidrogen : <5
 LogP : <5

LAMPIRAN 14

HASIL PENELITIAN PREDIKSI FARMAKOKINETIKA

Tabel VII.6

Hasil Prediksi Farmakokinetika Menggunakan Situs *Online Pre-ADMET*

No.	Ligan	Absrobsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
1	Chrysin	92,64 ^a	2,48 ^c	95,09 ^a
2	Baicalein	88,11 ^a	1,28 ^c	98,98 ^a
3	Apigenin	88,12 ^a	10,54 ^b	97,25 ^a
4	Acacetin	93,04 ^a	12,79 ^b	90,92 ^a
5	Scutellarein	79,41 ^a	4,53 ^b	100 ^a
6	Hispidulin	88,18 ^a	5,46 ^b	91,55 ^a
7	Luteolin	79,43 ^a	4,54 ^b	99,72 ^a
8	Chrysoeriol	88,18 ^a	5,18 ^b	90,87 ^a
9	Diosmetin	88,18 ^a	7,02 ^b	90,16 ^a
10	Tricetin	63,47 ^b	1,48 ^c	100 ^a
11	Tricin	87,82 ^a	3 ^c	87,07 ^b
12	Tangeretin	98,88 ^a	53,60 ^b	87,17 ^b
13	Rhoifolin	20,15 ^b	9,91 ^b	68,62 ^b
14	Wogonin	93,04 ^a	4,28 ^b	90,45 ^a
15	Galangin	88,12 ^a	3,71 ^c	88,12 ^b
16	Fisetin	79,43 ^a	9,57 ^b	88,73 ^b
17	Kaempferol	79,44 ^a	9,58 ^b	89,61 ^b
18	Kaempferide	88,19 ^a	9,33 ^b	83,99 ^b
19	Robinetin	63,47 ^b	3,41 ^c	92,64 ^a
20	Herbacetin	63,48 ^b	5,32 ^b	93,07 ^a

**LAMPIRAN 14
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Ligan	Absrobsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
21	Quercetin	63,49 ^b	3,41 ^a	93,24 ^a
22	Rhamnetin	78,34 ^a	4,94 ^b	85,35 ^b
23	Isorhamnetin	78,35 ^a	4,94 ^b	83,55 ^b
24	Myricetin	40,96 ^b	0,99 ^c	96,78 ^a
25	Quercetagenin	40,95 ^b	0,99 ^c	96,78 ^a
26	Gossypetin	40,96 ^b	5,20 ^b	96,48 ^a
27	Isoquercetin	11,78 ^c	9,44 ^b	59,16 ^b
28	Rhamnazin	87,83 ^a	5,09 ^b	81,22 ^b
29	Rutin	2,86 ^c	7,91 ^b	43,89 ^b
30	Morin	63,49 ^b	17,10 ^b	91,63 ^a
31	Pachypodol	93,45 ^a	4,38 ^b	79,88 ^b
32	Daidzein	92,65 ^a	7,72 ^b	88,70 ^b
33	Formononetin	95,55 ^a	7,60 ^b	85,08 ^b
34	Genistein	88,12 ^a	5,75 ^b	89,74 ^b
35	Biokanin A	93,04 ^a	3,41 ^c	85,01 ^b
36	Orobol	79,43 ^a	11,29 ^b	90,31 ^a
37	Tectorigenin	88,18 ^a	5,59 ^b	87,63 ^b
38	Baptigenin	79,42 ^a	1,56 ^c	90,36 ^a
39	Pinocembrin	92,35 ^a	2,47 ^c	98,45 ^a
40	Liquiritigenin	92,35 ^a	17,65 ^b	97,99 ^a
41	Narigenin	87,32 ^a	10,52 ^b	100 ^a
42	Sakuranetin	92,75 ^a	12,82 ^b	95,21 ^a
43	Eriodictyol	77,43 ^a	4,53 ^b	100 ^a

**LAMPIRAN 14
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Ligan	Absrobsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
44	Hesperitin	87,19 ^a	7,00 ^b	96,79 ^a
45	Homoeriodictyol	87,19 ^a	5,16 ^b	98,06 ^a
46	Parietin	94,04 ^a	20,74 ^b	95,22 ^a
47	Epigallocatechin	45,95 ^b	0,38 ^c	100 ^a
48	Catechin	66,71 ^b	0,65 ^c	100 ^a
49	Naringin	11,74 ^c	7,89 ^b	51,06 ^b
50	Pinobanksin	87,61 ^a	3,69 ^c	86,64 ^b
51	Aromadendrin	77,83 ^a	9,56 ^b	89,67 ^b
52	Fustin	77,82 ^a	9,56 ^b	88,03 ^b
53	Taksifolin	60,16 ^b	3,42 ^c	95,16 ^a
54	Agathisflavone	81,19 ^a	11,09 ^b	100 ^a
55	Cupressuflavone	81,19 ^a	11,68 ^b	100 ^a
56	Ginkgetin	91,41 ^a	11,98 ^b	95,55 ^a
57	Sciadopitysin	94,05 ^a	13,68 ^b	90,51 ^a
58	Robustaflavone	81,19 ^a	12,04 ^b	100 ^a
59	Hinokiflavone	86,95 ^a	4,34 ^b	100 ^a
60	Ochnaflavone	86,95 ^a	6,77 ^b	100 ^a
61	Amentoflavone	81,19 ^a	12,87 ^b	100 ^a
62	Isoliquiritigenin	88,30 ^a	20,16 ^b	98,25 ^a
63	Khalkonarigenin	80,61 ^a	18,10 ^b	100 ^a
64	Butein	80,60 ^a	18,10 ^b	99,72 ^a
65	Okanin	66,57 ^b	14,31 ^b	100 ^a
66	Phloretin	78,98 ^a	18,10 ^b	100 ^a

**LAMPIRAN 14
(LANJUTAN)**

**Tabel VII.6
Lanjutan**

No.	Ligan	Absrobsi		Distribusi
		HIA (%)	CaCo-2 Cell (nm sec)	Plasma Protein Binding (%)
67	Phlorizin	26,79 ^b	9,51 ^b	75,47 ^b
68	Sulfuretin	89,54 ^a	13,36 ^b	100 ^a
69	Aureusidin	82,57 ^a	8,15 ^b	100 ^a
70	Maritimetin	82,56 ^a	8,15 ^b	100 ^a
71	Leptosidin	89,74 ^a	9,81 ^b	98,09 ^a
72	Apigenidin	89,72 ^a	1,01 ^c	100 ^a
73	Luteolinidin	83,57 ^a	0,68 ^c	100 ^a
74	Pelargonidin	83,58 ^a	1,29 ^c	100 ^a
75	Cyanidin	72,5 ^a	0,65 ^c	100 ^a
76	Peonidin	83,43 ^a	1,65 ^c	100 ^a
77	Petunidin	71,32 ^a	0,97 ^c	100 ^a
78	Rosinidin	90,13 ^a	2,12 ^c	87,78 ^a

Keterangan :

% Human Intestinal Absorption (% HIA) : (a) 70-100% terserap baik
(b) 20-70% terserap cukup
(c) 0-20% kurang terserap

In Vitro Caco-2 cell permeability (nm sec-1): (a) >70 permeabilitas tinggi
(b) 4-70 permeabilitas sedang
(c) <4 permeabilitas rendah

Plasma protein binding (%) : (a) >90 terikat kuat
(b) <90 terikat lemah

LAMPIRAN 15

HASIL PENELITIAN PREDIKSI TOKSISITAS

Tabel VII.7

Hasil Prediksi Toksisitas Menggunakan Aplikasi *Toxtree*

No	Senyawa Uji	Mutagen (Amest Tes)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
1	Chrysin	(-)	(-)	(-)	Tidak Beresiko
2	Baicalein	(-)	(-)	(-)	Tidak Beresiko
3	Apigenin	(-)	(-)	(-)	Tidak Beresiko
4	Acacetin	(-)	(-)	(-)	Tidak Beresiko
5	Scutellarein	(-)	(-)	(-)	Tidak Beresiko
6	Hispidulin	(-)	(-)	(-)	Tidak Beresiko
7	Luteolin	(-)	(-)	(-)	Tidak Beresiko
8	Chrysoeriol	(-)	(-)	(-)	Tidak Beresiko
9	Diosmetin	(-)	(-)	(-)	Tidak Beresiko
10	Tricetin	(-)	(-)	(-)	Tidak Beresiko
11	Tricin	(-)	(-)	(-)	Tidak Beresiko
12	Tangeretin	(-)	(-)	(-)	Tidak Beresiko
13	Rhoifolin	(-)	(-)	(-)	Tidak Beresiko
14	Wogonin	(-)	(-)	(-)	Tidak Beresiko
15	Galangin	(-)	(-)	(-)	Tidak Beresiko

**LAMPIRAN 15
(LANJUTAN)**

**Tabel VII.7
Lanjutan**

No	Senyawa Uji	Mutagen (Amest Tes)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
16	Fisetin	(-)	(-)	(-)	Tidak Beresiko
17	Kaempferol	(-)	(-)	(-)	Tidak Beresiko
18	Kaempferide	(-)	(-)	(-)	Tidak Beresiko
19	Robinetin	(-)	(-)	(-)	Tidak Beresiko
20	Herbacetin	(-)	(-)	(-)	Tidak Beresiko
21	Quercetin	(-)	(-)	(+)	Tidak Beresiko
22	Rhamnetin	(+)	(-)	(+)	Tidak Beresiko
23	Isorhamnetin	(+)	(-)	(+)	Tidak Beresiko
24	Myricetin	(+)	(-)	(+)	Tidak Beresiko
25	Quercetagenin	(+)	(-)	(+)	Tidak Beresiko
26	Gossypetin	(+)	(-)	(+)	Tidak Beresiko
27	Isoquercetin	(+)	(-)	(+)	Tidak Beresiko
28	Rhamnazin	(+)	(-)	(+)	Tidak Beresiko
29	Rutin	(+)	(-)	(+)	Tidak Beresiko
30	Morin	(-)	(-)	(-)	Tidak Beresiko
31	Pachypodol	(+)	(-)	(+)	Tidak Beresiko
32	Daidzein	(+)	(+)	(-)	Resiko Rendah

**LAMPIRAN 15
(LANJUTAN)**

**Tabel VII.7
Lanjutan**

No	Senyawa Uji	Mutagen (Amest Tes)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
33	Formononetin	(+)	(+)	(-)	Resiko Rendah
34	Genistein	(+)	(+)	(-)	Resiko Rendah
35	Biochanin A	(+)	(+)	(-)	Resiko Rendah
36	Orobol	(+)	(+)	(-)	Resiko Rendah
37	Tectorigenin	(+)	(+)	(-)	Resiko Rendah
38	Baptigenin	(+)	(+)	(-)	Resiko Rendah
39	Pinocembrin	(-)	(-)	(-)	Tidak Beresiko
40	Liquiritigenin	(-)	(-)	(-)	Tidak Beresiko
41	Narigenin	(-)	(-)	(-)	Tidak Beresiko
42	Sakuranetin	(-)	(-)	(-)	Tidak Beresiko
43	Eriodictyol	(-)	(-)	(-)	Tidak Beresiko
44	Hesperitin	(-)	(-)	(-)	Tidak Beresiko
45	Homoeriodictyol	(-)	(-)	(-)	Tidak Beresiko
46	Parietin	(+)	(+)	(-)	Resiko Rendah
47	Epigallocatechin	(-)	(-)	(-)	Tidak Beresiko
48	Catechin	(-)	(-)	(-)	Tidak Beresiko
49	Naringin	(-)	(-)	(-)	Tidak Beresiko

**LAMPIRAN 15
(LANJUTAN)**

**Tabel VII.7
Lanjutan**

No	Senyawa Uji	Mutagen (Amest Tes)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
50	Pinobanksin	(-)	(-)	(-)	Tidak Beresiko
51	Aromadendrin	(-)	(-)	(-)	Tidak Beresiko
52	Fustin	(-)	(-)	(-)	Tidak Beresiko
53	Taxifolin	(-)	(-)	(-)	Tidak Beresiko
54	Agathisflavone	(-)	(-)	(+)	Tidak Beresiko
55	Cupressuflavone	(-)	(-)	(+)	Tidak Beresiko
56	Ginkgetin	(-)	(-)	(+)	Tidak Beresiko
57	Sciadopytisin	(-)	(-)	(+)	Tidak Beresiko
58	Robustaflavone	(-)	(-)	(+)	Tidak Beresiko
59	Hinokiflavone	(-)	(-)	(-)	Tidak Beresiko
60	Ochnaflavone	(-)	(-)	(-)	Tidak Beresiko
61	Amentoflavone	(-)	(-)	(+)	Tidak Beresiko
62	Isoliquiritigenin	(+)	(+)	(-)	Resiko Rendah
63	Khalkonarigenin	(+)	(+)	(-)	Resiko Rendah
64	Butein	(+)	(+)	(-)	Resiko Rendah
65	Okanin	(+)	(+)	(-)	Resiko Rendah
66	Phloretin	(-)	(-)	(-)	Tidak Beresiko

**LAMPIRAN 15
(LANJUTAN)**

**Tabel VII.7
Lanjutan**

No	Senyawa Uji	Mutagen (Amest Tes)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
67	Phlorizin	(-)	(-)	(-)	Tidak Beresiko
68	Sulfuretin	(-)	(-)	(-)	Tidak Beresiko
69	Aureusidin	(-)	(-)	(-)	Tidak Beresiko
70	Maritimetin	(-)	(-)	(-)	Tidak Beresiko
71	Leptosidin	(-)	(-)	(-)	Tidak Beresiko
72	Apigenidin	(-)	(-)	(-)	Tidak Beresiko
73	Luteolinidin	(-)	(-)	(-)	Tidak Beresiko
74	Pelargonidin	(-)	(-)	(-)	Tidak Beresiko
75	Cyanidin	(-)	(-)	(-)	Tidak Beresiko
76	Peonidin	(-)	(-)	(-)	Tidak Beresiko
77	Delpinidin	(-)	(-)	(-)	Tidak Beresiko
78	Petunidin	(-)	(-)	(-)	Tidak Beresiko
79	Malvinidin	(-)	(-)	(-)	Tidak Beresiko
80	Rosinidin	(-)	(-)	(-)	Tidak Beresiko

DAFTAR RIWAYAT HIDUP**DATA PRIBADI**

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PENDIDIKAN**Formal**

Jenjang Pendidikan	Nama Sekolah/Perguruan Tinggi	Tahun Masuk	Tahun Lulus
SD	SDN 1 Pamalayan	2006	2012
SMP	MTsN 3 Garut	2012	2015
SMA	SMK Plus Sukaraja	2015	2018
Perguruan Tinggi	Universitas Garut	2018	2022

Non Formal

Praktek Kerja Lapangan	Tahun
RSUD dr. Slamet	2017
Puskesmas Wanaraja	2017
RSU Nurhayati	2022