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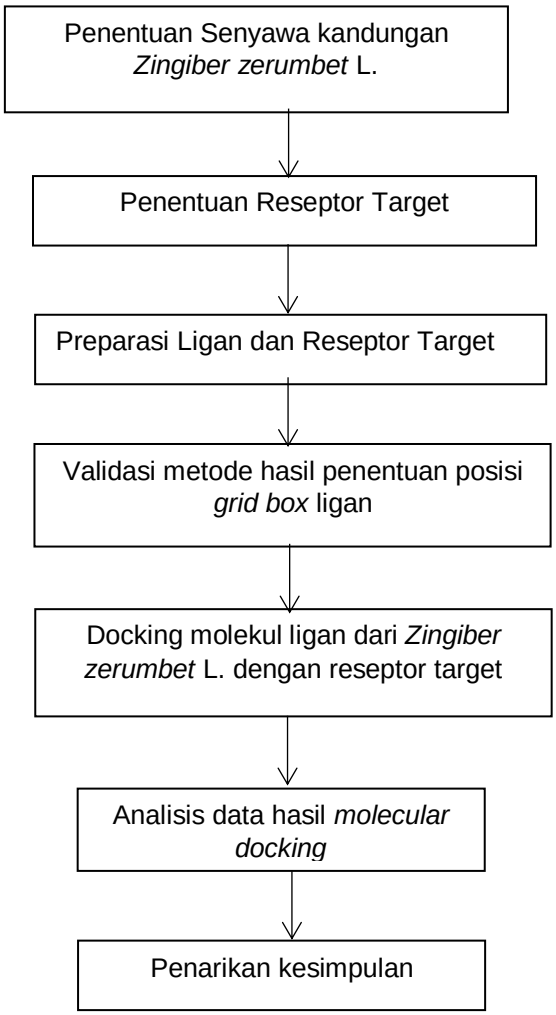
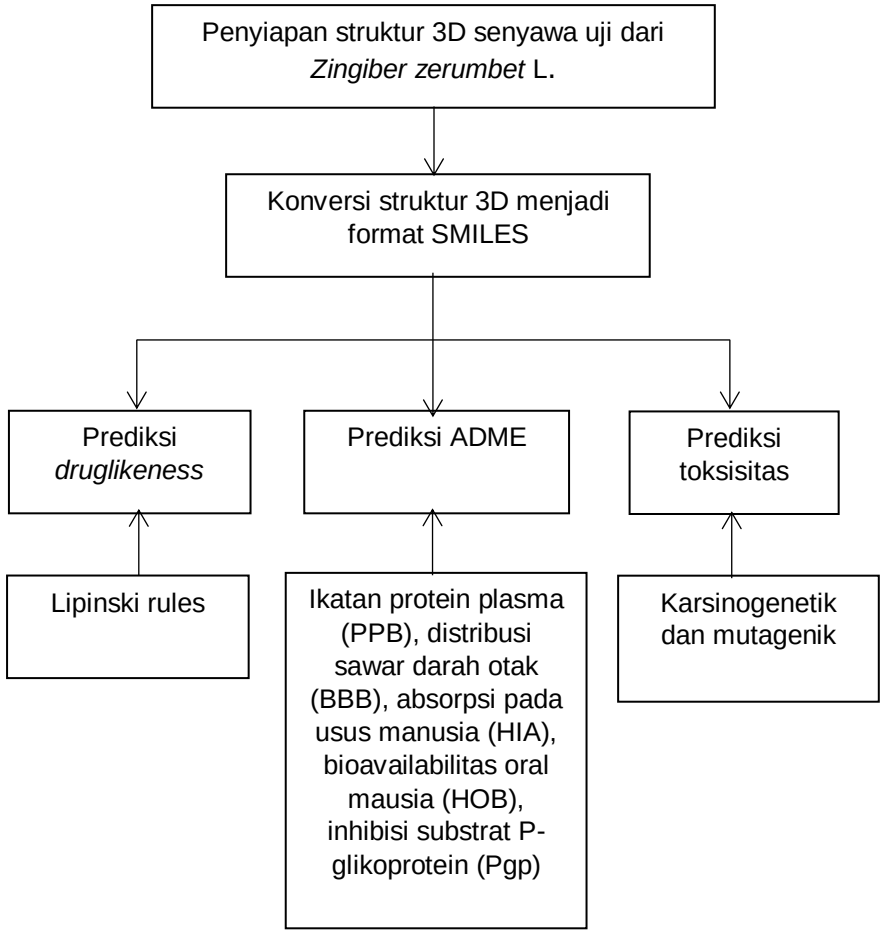
LAMPIRAN

Lampiran 1. Skema Kerja

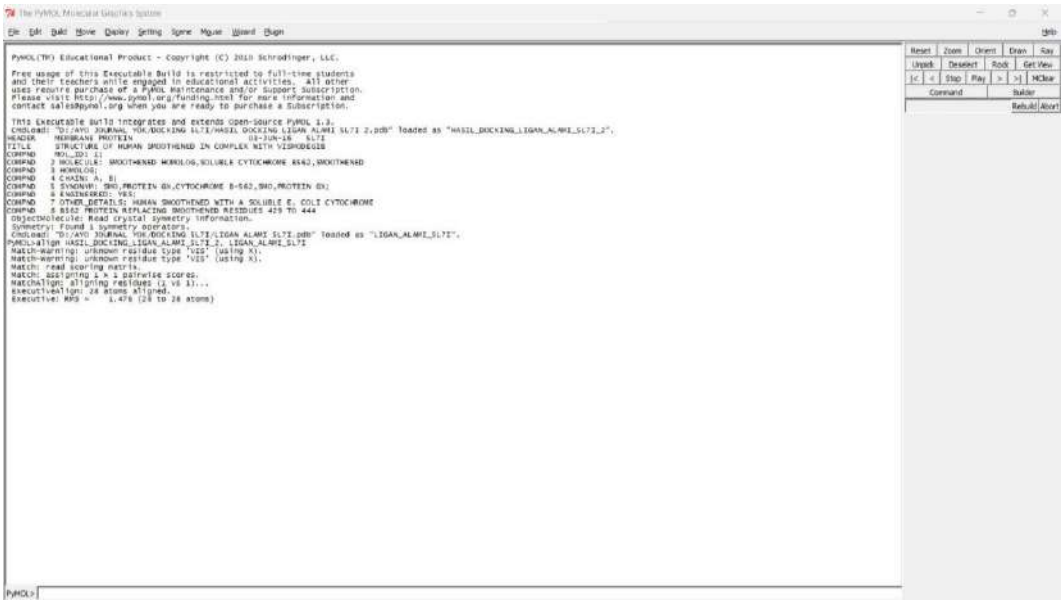
1.1 ***Molecular Docking***



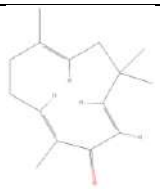
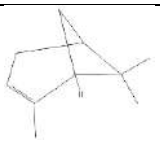
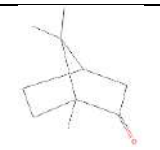
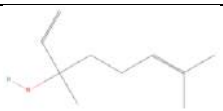
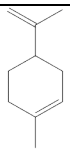
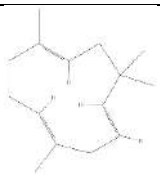
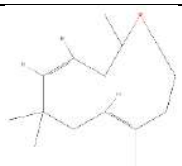
1.2 Profil Farmakokinetik dan Toksisitas

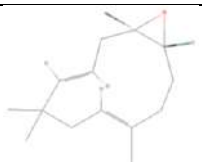
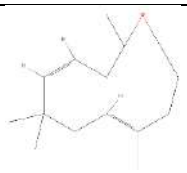
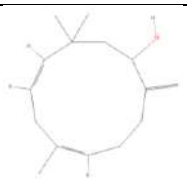
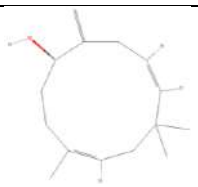
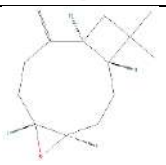
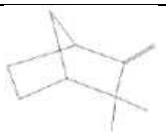
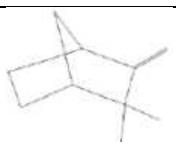
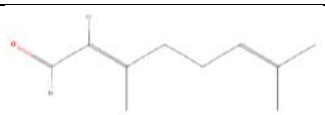
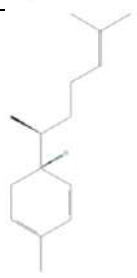


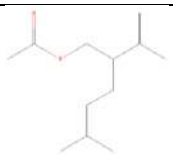
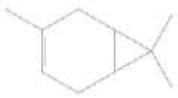
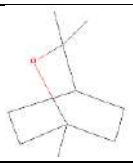
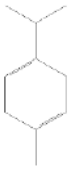
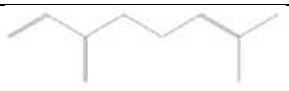
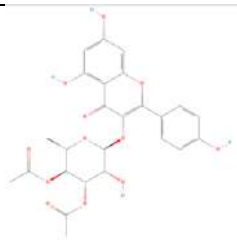
Lampiran 2. Hasil RMSD *native ligand* terhadap reseptor Smo

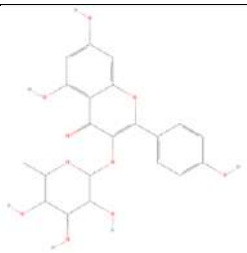
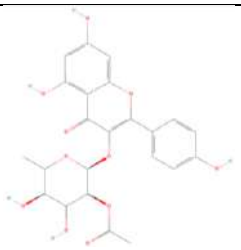
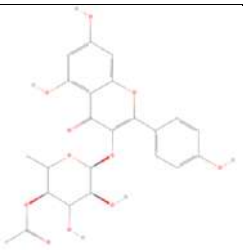
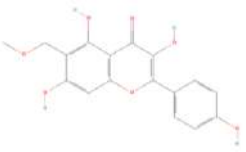
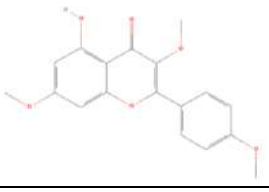


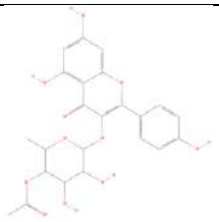
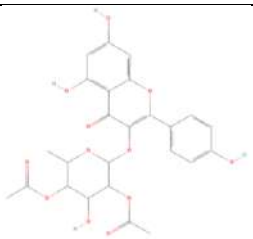
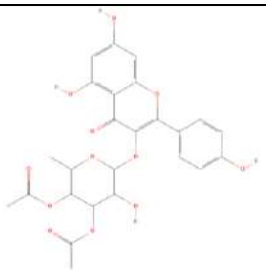
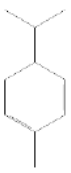
Lampiran 3. Gambar Struktur Senyawa *Zingiber zerumbet* L. (Koga *et al.*, 2016; Tian *et al.*, 2020)

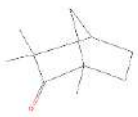
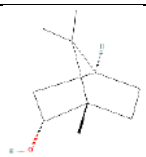
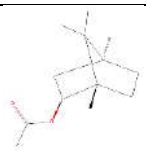
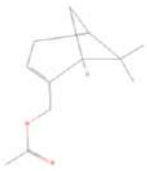
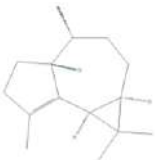
No.	Ligan	Rumus Struktur	Kelas
1	Zerumbone		Terpen
2	Borneol		
3	α-Pinene		
4	Camphor		
5	Linalool		
6	Limonene		
7	α-Humulene		
8	β-Caryophyllene		
			

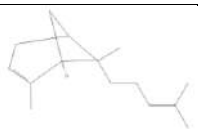
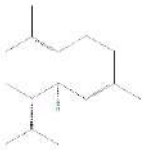
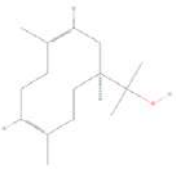
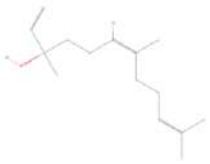
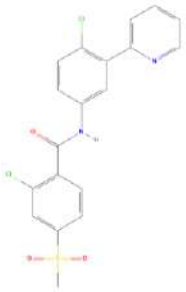
10	Humulene Epoksida II		Terpen
11	Humulene Epoksida III		
12	Humulenol I		
13	Humulenol II		
14	Caryophyllene Oxide		
15	Camphene		
16	Sabinene		
17	Citral		
			

19	Lavandulyl Acetate		Terpen
20	3-Carene		
21	4-Terpineol		
22	Eucalyptol		
23	γ-Terpinene		
24	β- Phellandrene		
25	β-Myrcene		
26	3-methyl kaempferol, kaempferol-3- O-(2,4-di-O-acetyl-α-l-rhamnopyranoside)		Flavonoid
	3-O- etyl-α- noside)		

28	Kaempferol-3-O-rhamnoside		Flavonoid
29	Kaempferol 3-(2''-acetylrhamnoside)		
30	Kaempferol 3-(3''-acetylrhamnoside)		
31	Kaempferol 3-(4''-acetylrhamnoside)		
32	Kaempferol-3,4’ -O-dimethylether		
33	Kaempferol-3-O-methylether		
	3,4’ ,7-ther		

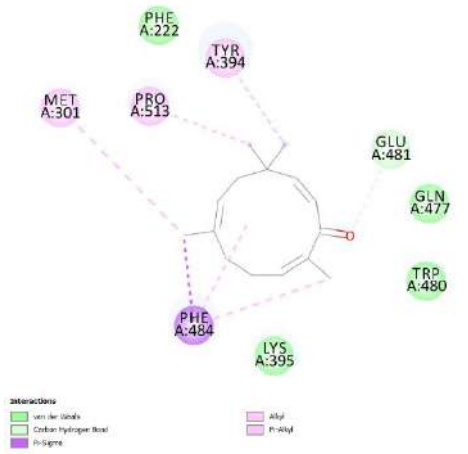
35	4”-O-Acetylafzelin		Flavomoid
36	2",4"-Diacetylafzelin		
37	3",4"-Diacetylafzelin		
38	Tricyclene		Terpen
39	α-Terpineol		
40	β-Pinene		
41	α-Phellandrene		
			

43	p-Cymene		Terpen
44	Fenchone		
45	l-Borneol		
46	Verbenone		
47	l-Bornyl acetate		
48	Isobornyl acetate		
49	Myrtenyl acetate		
50	α-Copaene		
51	β-Elemene		
			

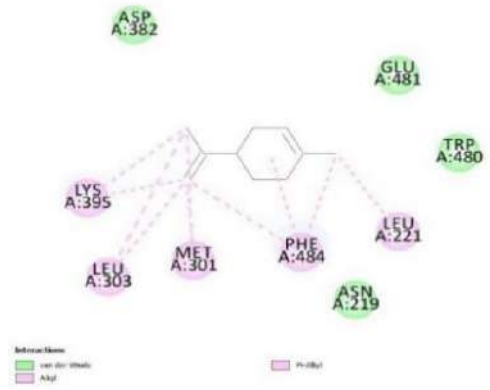
53	α-Bergamotene		Terpen
54	δ-Cadinene		
55	Hedycaryol		
56	d-Nerolidol		
57	Allo-Aromadendrene epoxide		
58	β-Eudesmol		
59	Vismodegib		

Lampiran 4. Visualisasi Interaksi Senyawa Uji dengan Reseptor Smo

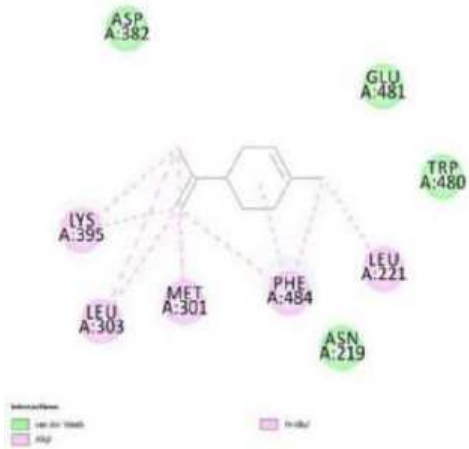
1. Zaerumbone



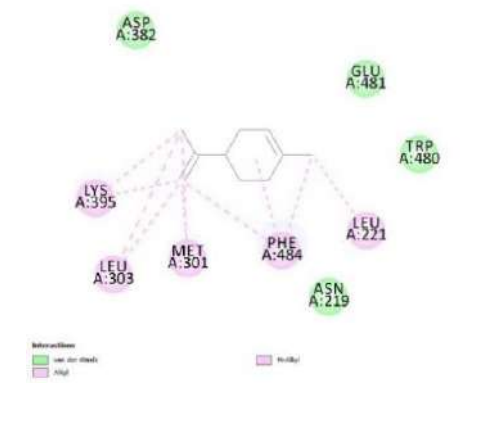
2. Borneol



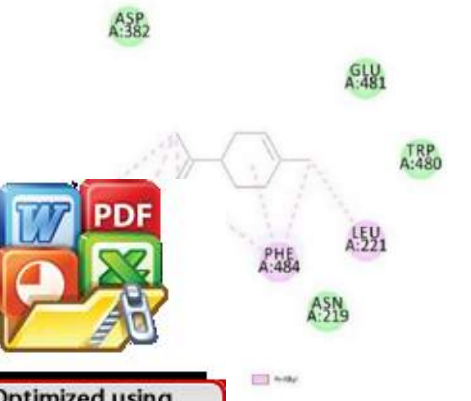
3. α-Pinene



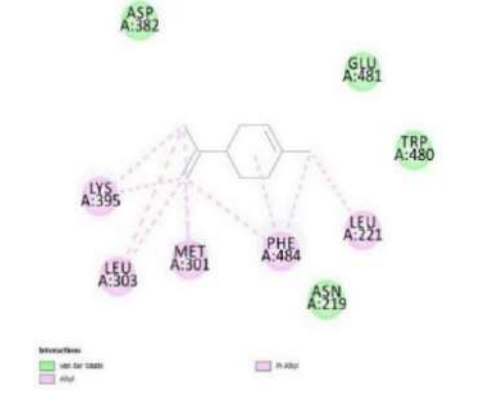
4. Camphor

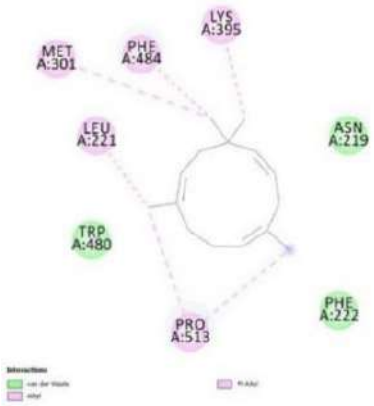
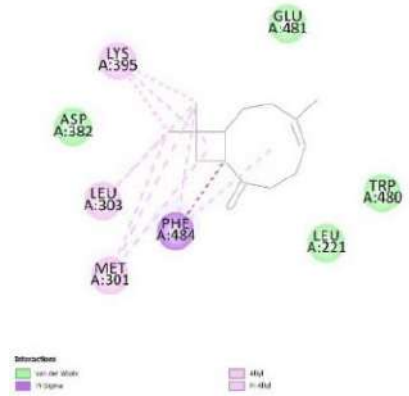
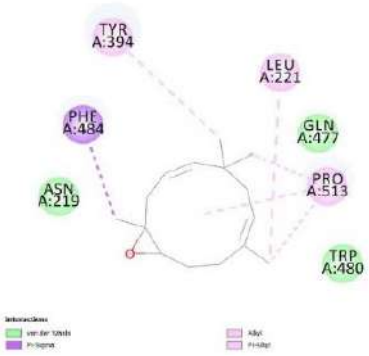
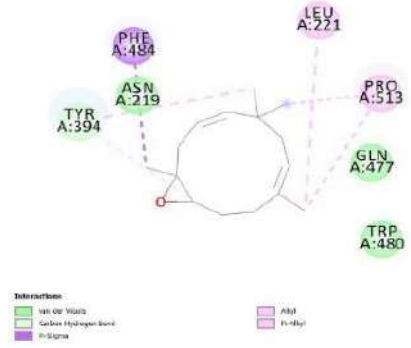
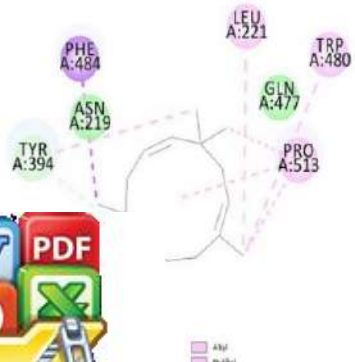
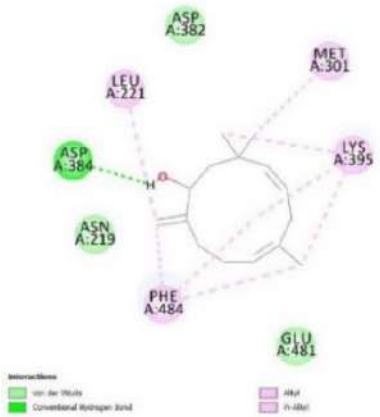


5. Linalool

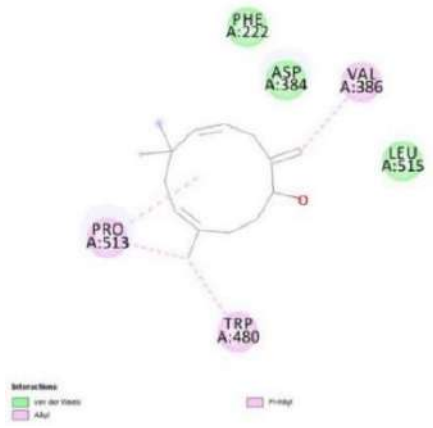


6. Limonene

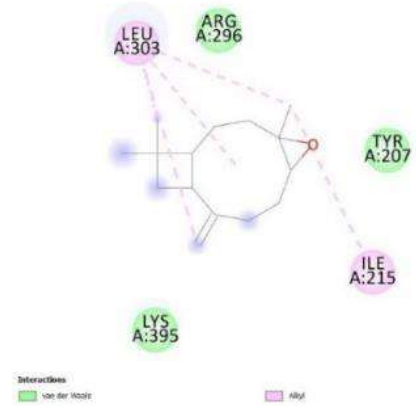


7. α-Humulene 	8. β-Caryophyllene 
9. Humulene Epoksida I 	10. Humulene Epoksida II 
11. Humulene Epoksida III 	12. Humulenol I 

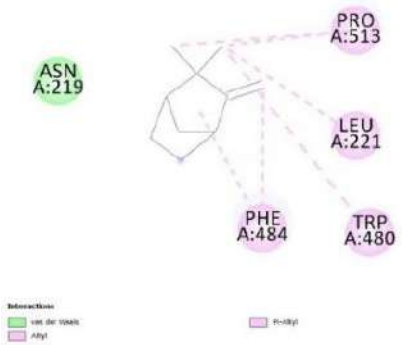
13. Humulenol II



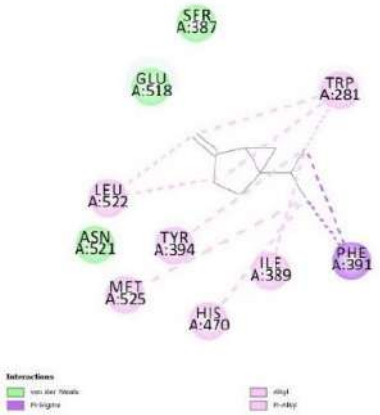
14. Caryophyllene Oxide



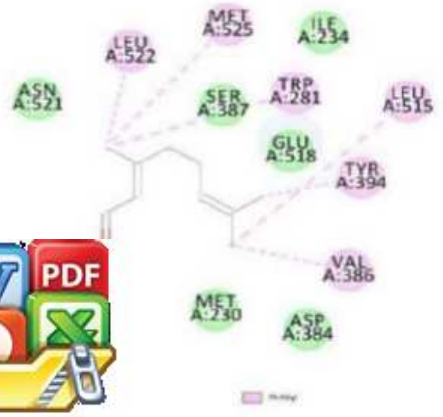
15. Camphene



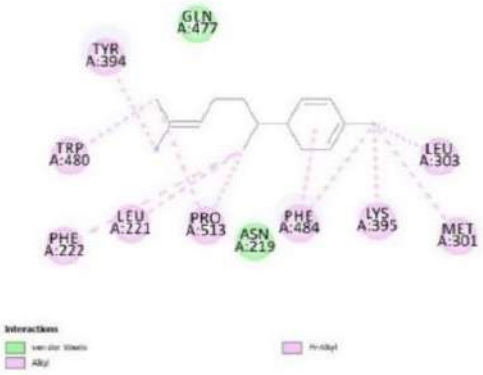
16. Sabinene



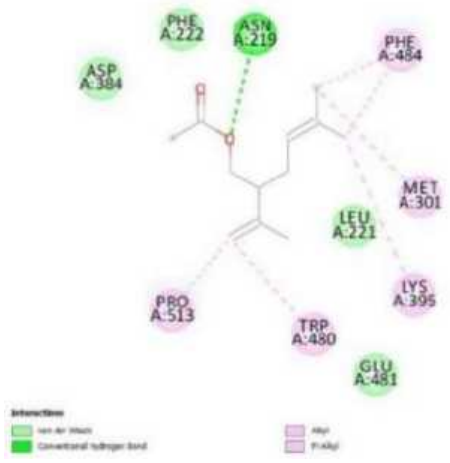
17. Citral



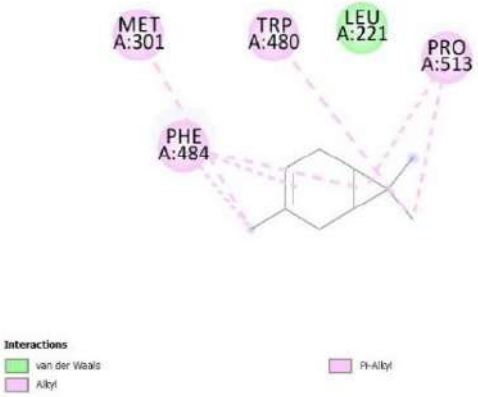
18. Zingiberene



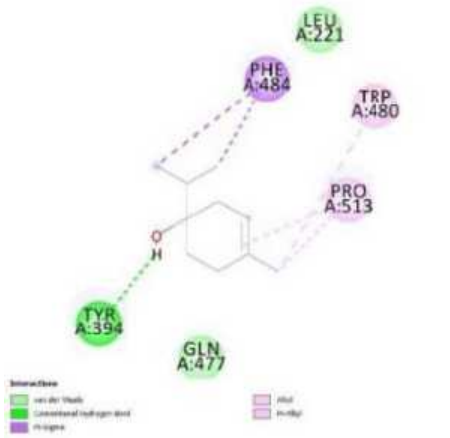
19. Lavandulyl Acetate



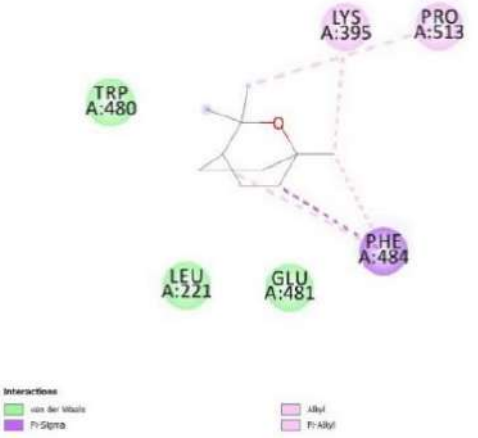
20. 3-Carene



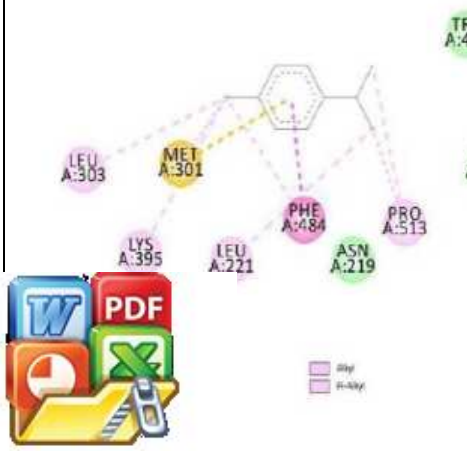
21. 4-Terpineol



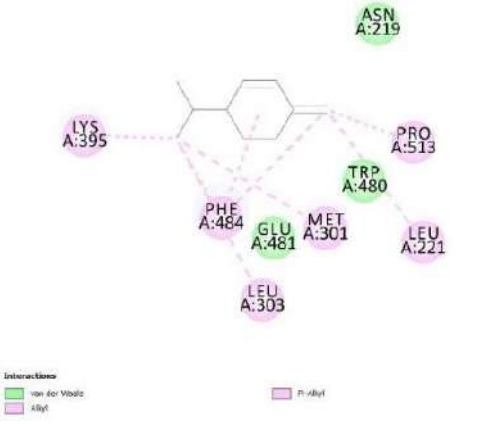
22. Eucalyptol



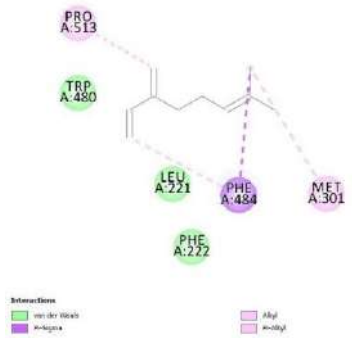
23. γ-Terpinene



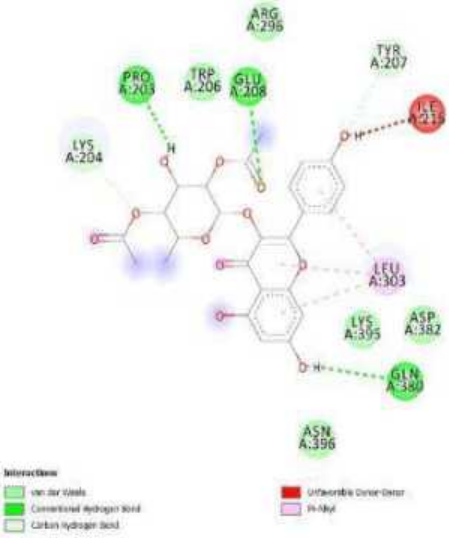
24. β- Phellandrene



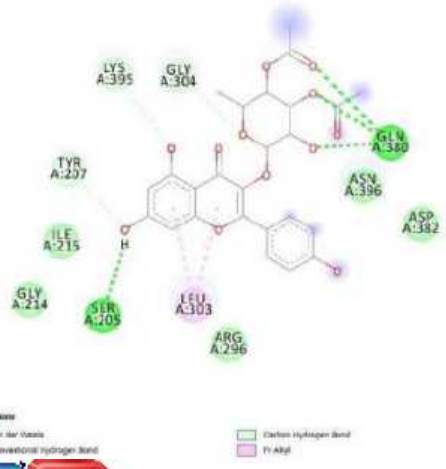
25. β-Myrcene



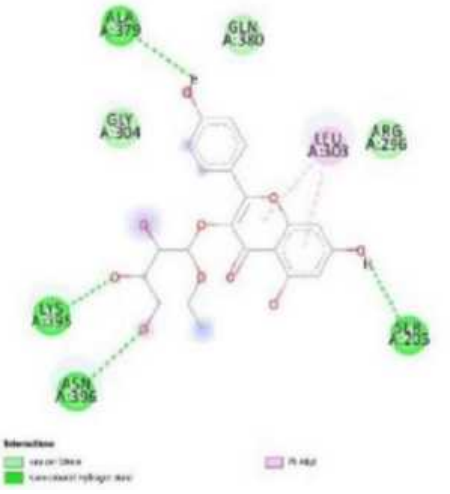
26. 3-methyl kaempferol, kaempferol-3-O-(2,4-di-O-acetyl-α-l-rhamnopyranoside)



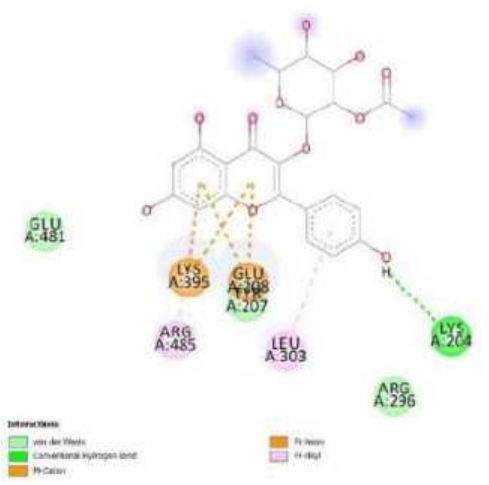
27. Kaempferol-3-O-(3,4-di-O-acetyl-α-l-rhamnopyranoside)



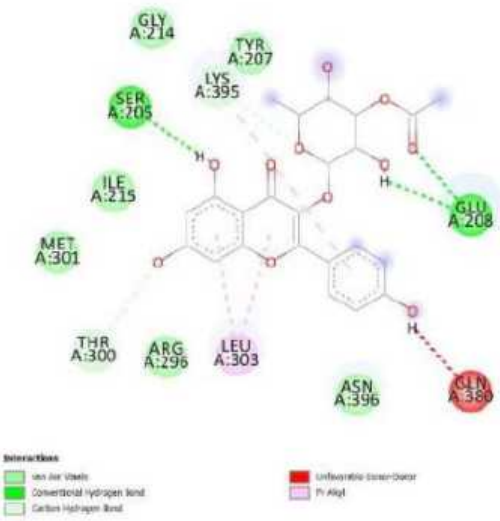
28. Kaempferol-3-O-rhamnoside



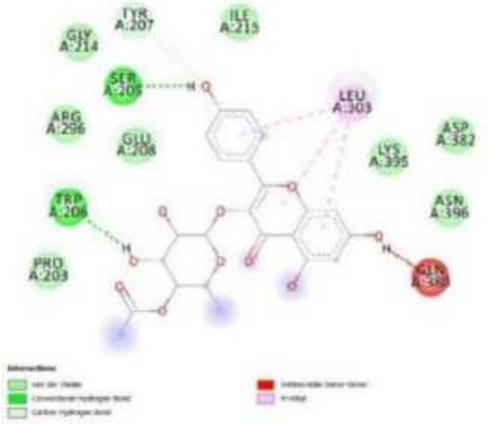
29. Kaempferol 3-(2''-acetylrhamnoside)



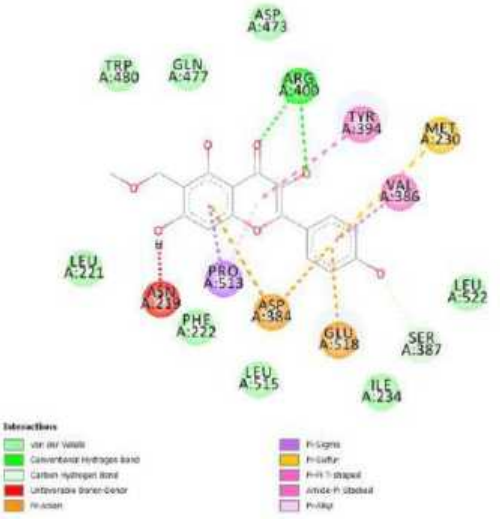
30. Kaempferol 3-(3''-acetylrhamnoside)

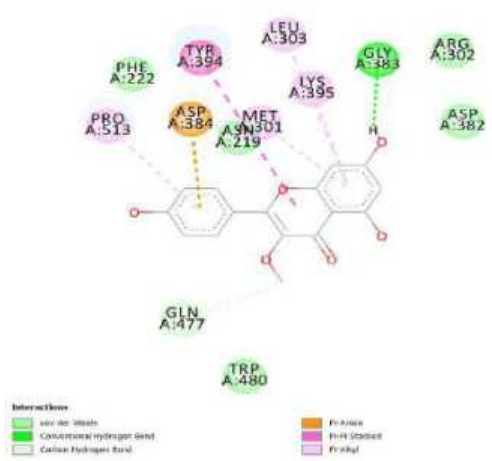
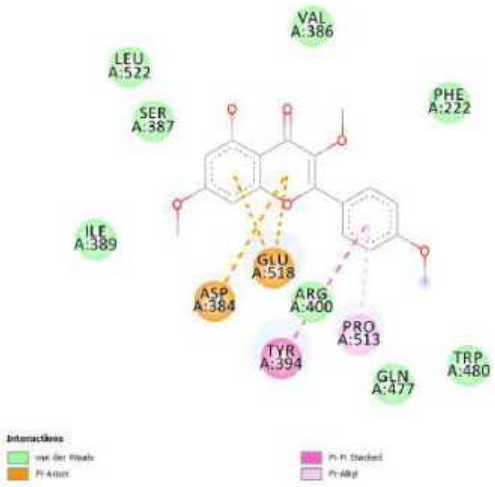
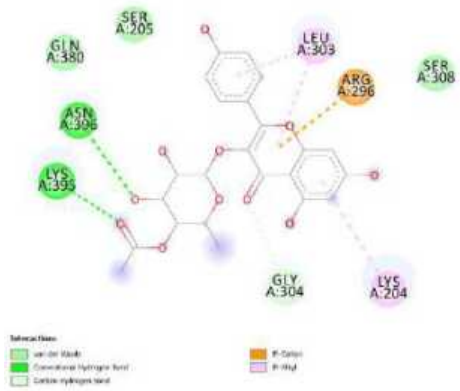
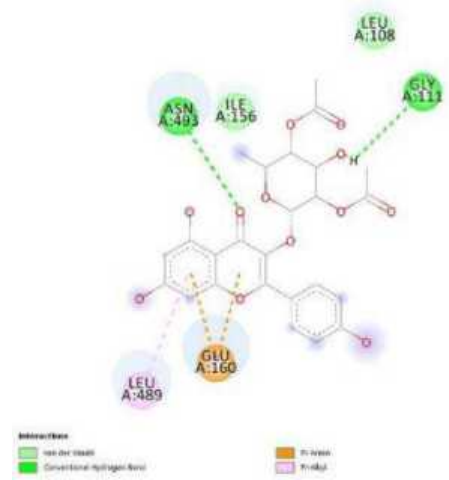


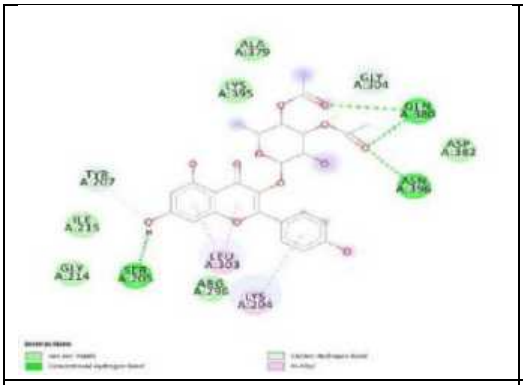
31. Kaempferol 3-(4''-acetylrhamnoside)

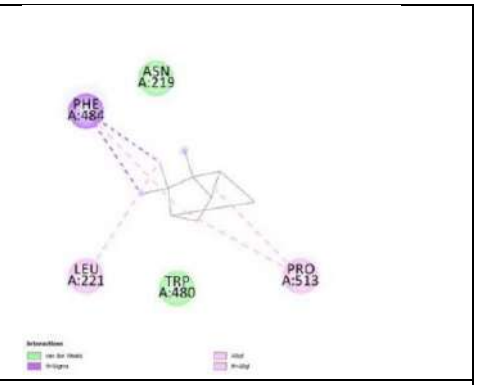


32. Kaempferol-3,4’ -O-dimethylether



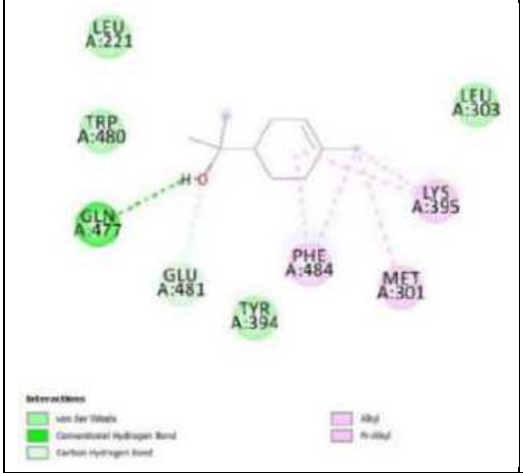
33. Kaempferol-3-O-methylether	34. Kaempferol-3,4’ ,7-O-trimethylether
	
35. 4”-O-Acetylafzelin	36. 2'',4''-Diacetylafzelin
	
37. 3'',4''-Diacetylafzelin	38. Tricyclene

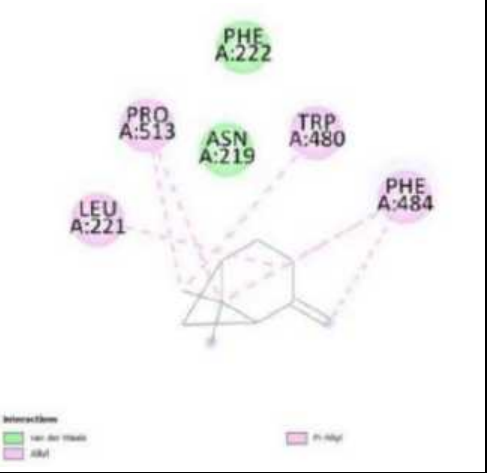




39. α-Terpineol

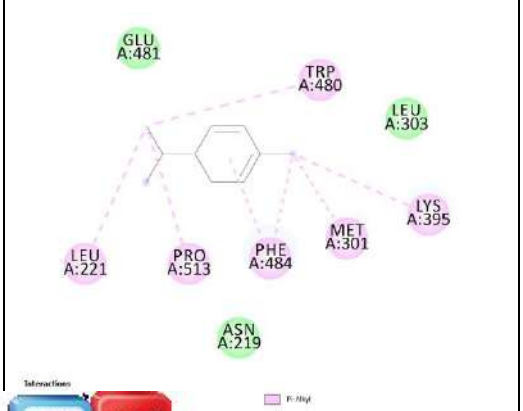
40. β-Pinene

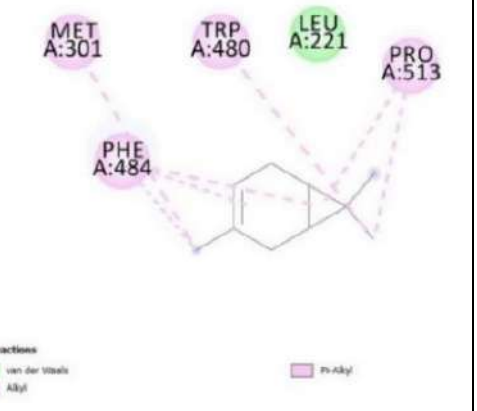




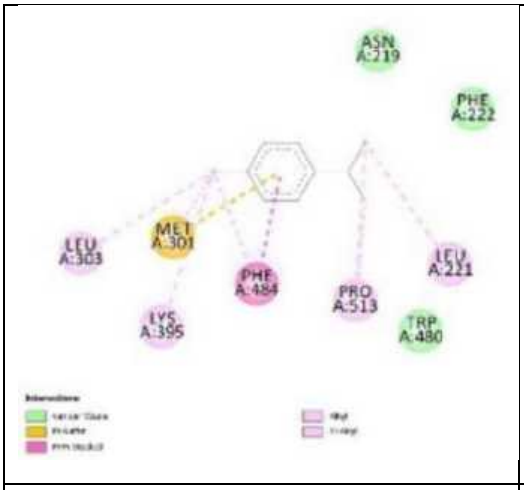
41. α-Phellandrene

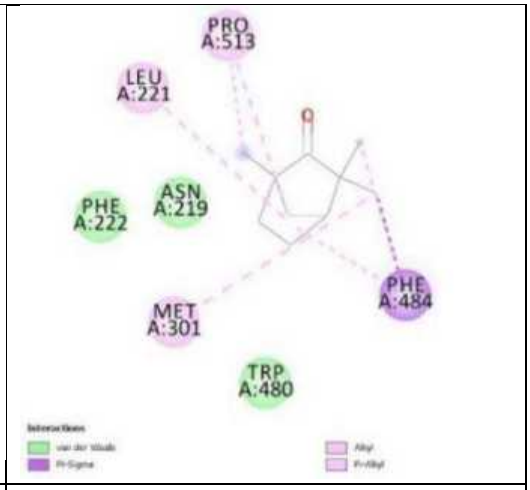
42. δ-3-Carene





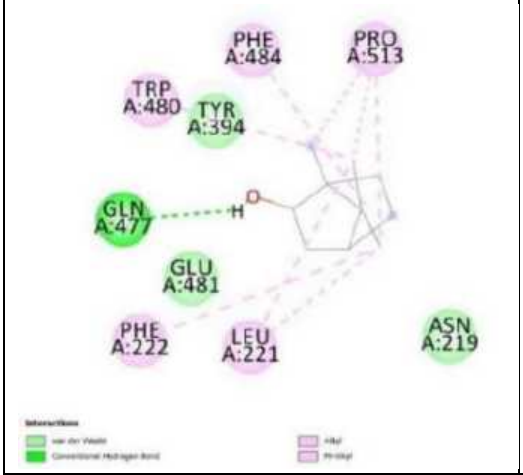
44. Fenchone

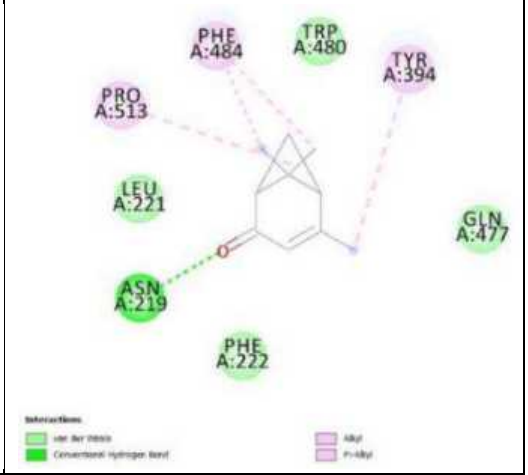




45. l-Borneol

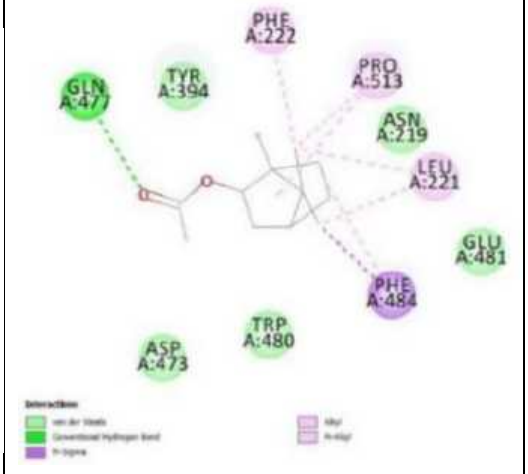
46. Verbenone



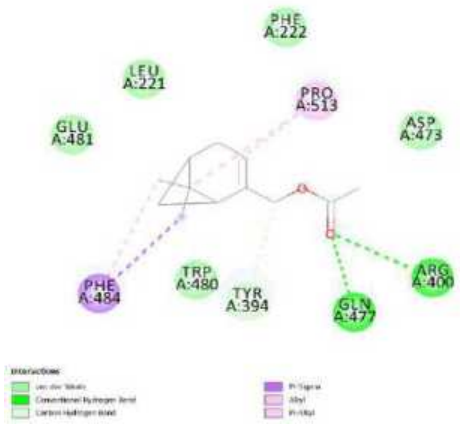


47. l-Bornyl acetate

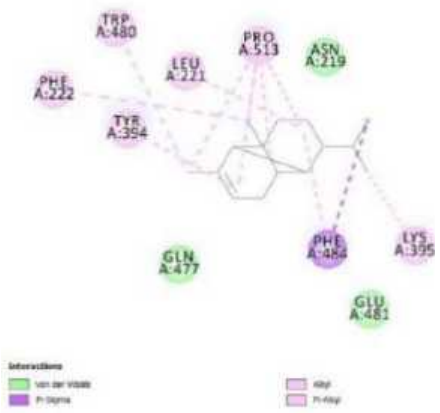
48. Isobornyl acetate



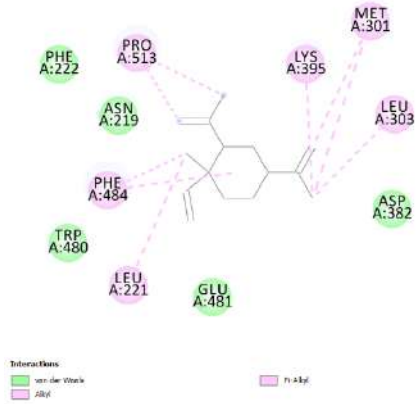
49. Myrtenyl acetate



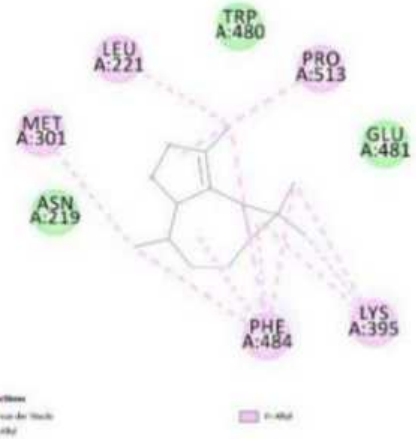
50. α-Copaene



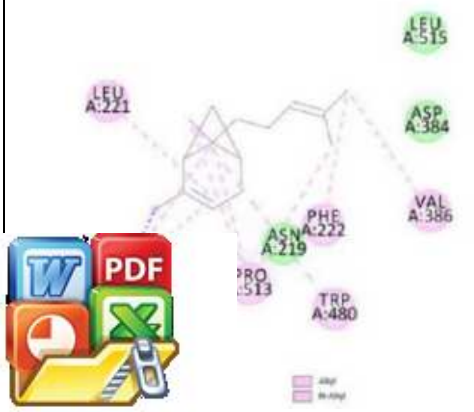
51. β-Elemene



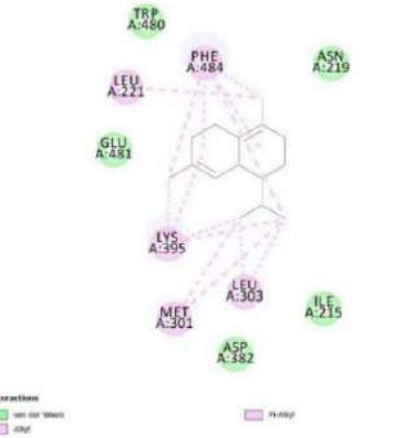
52. α-Gurjunene

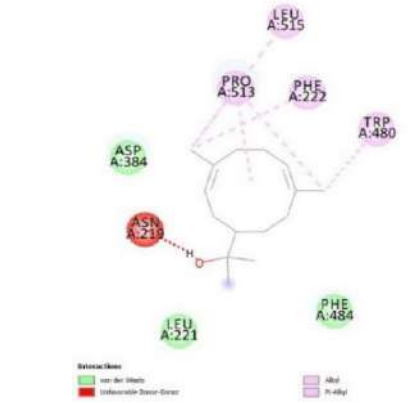
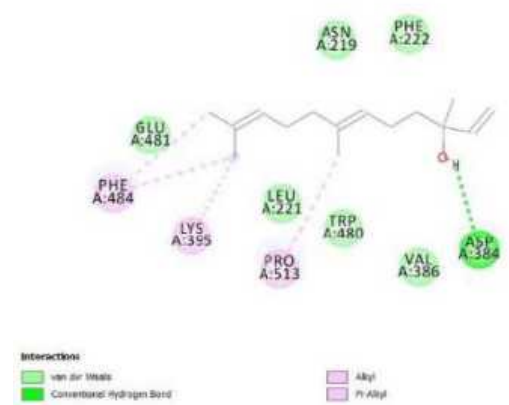
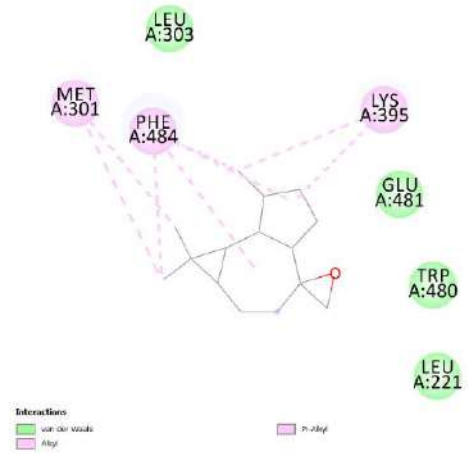
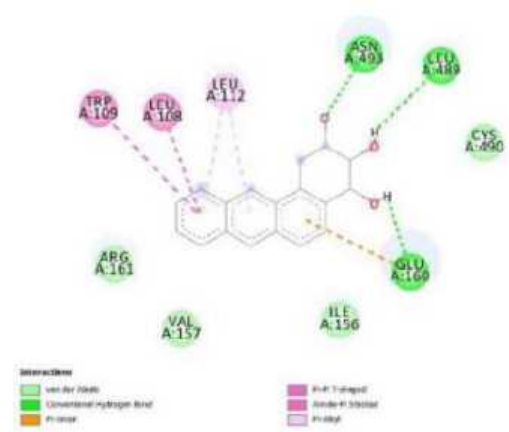


53. α-Bergamotene



54. δ-Cadinene



55. Hedycaryol	56. d-Nerolidol
	
57. Allo-Aromadendrene epoxide	58. β-Eudesmol
	

Lampiran 5. Visualisasi Boiled Egg senyawa uji