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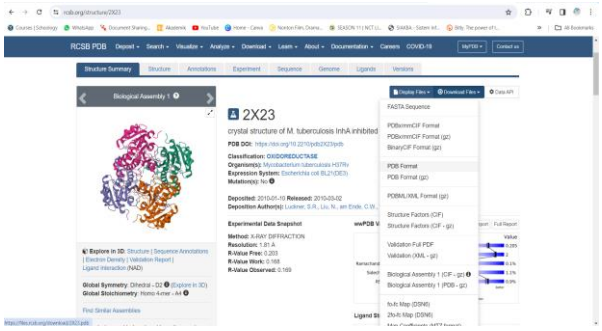
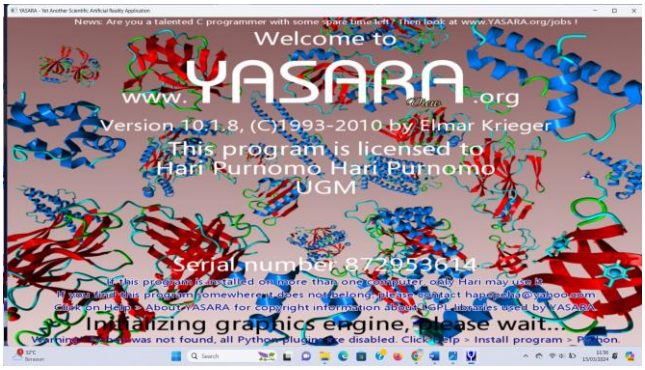
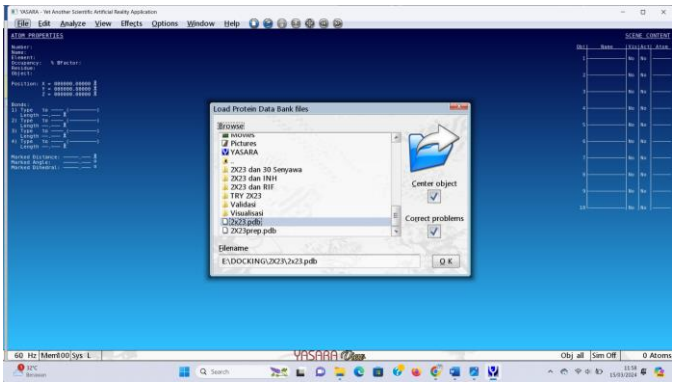
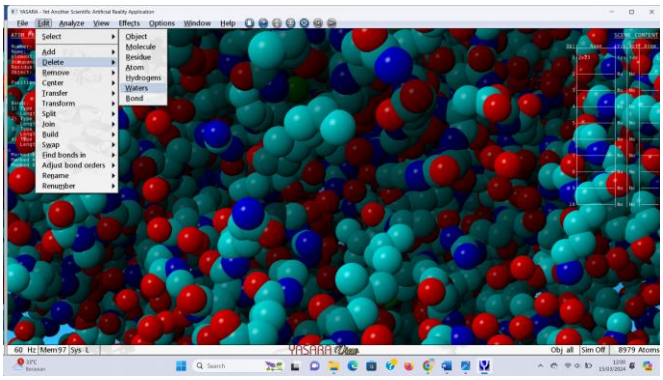
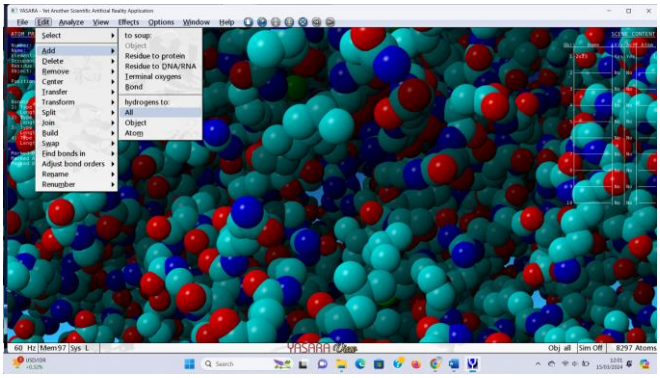
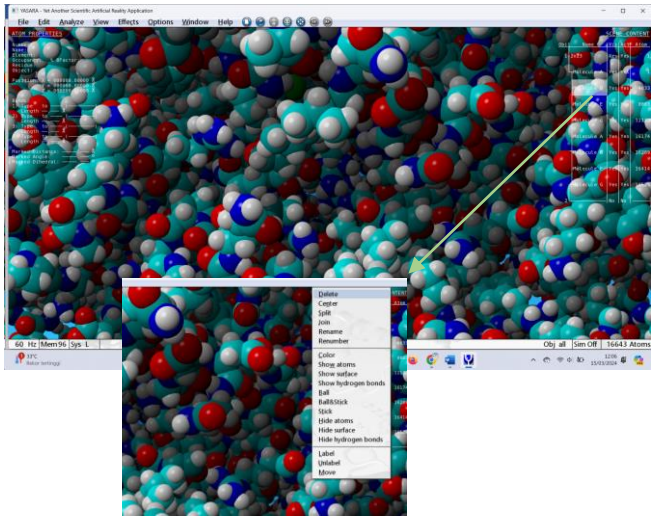
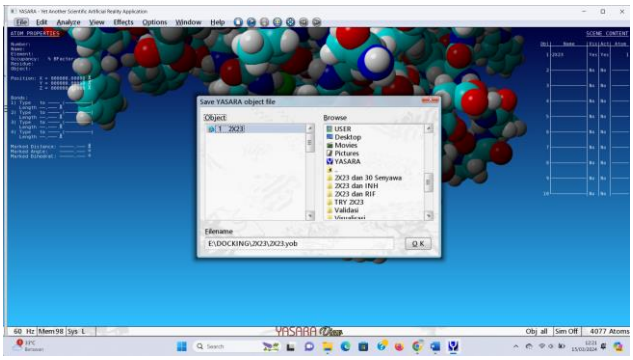
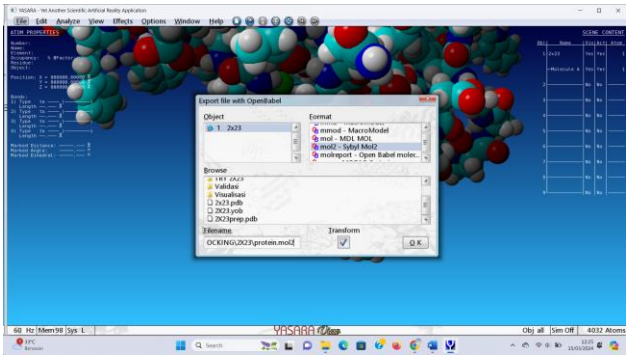
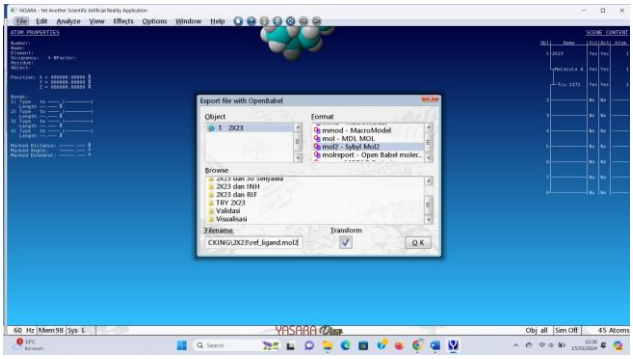
LAMPIRAN

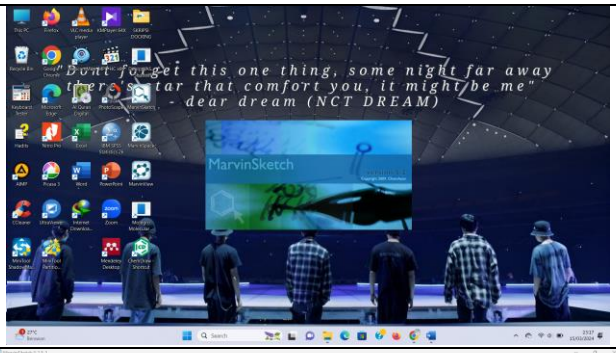
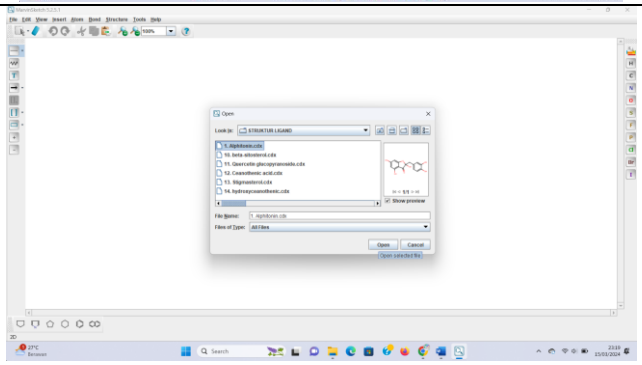
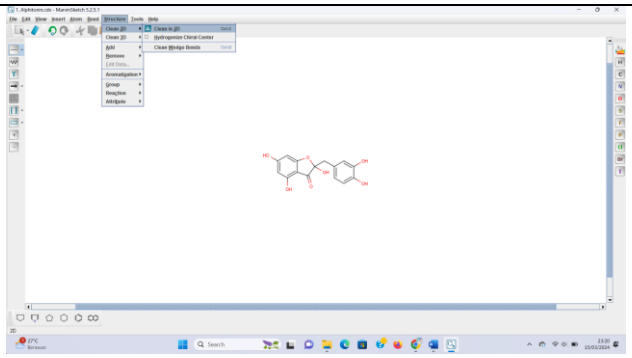
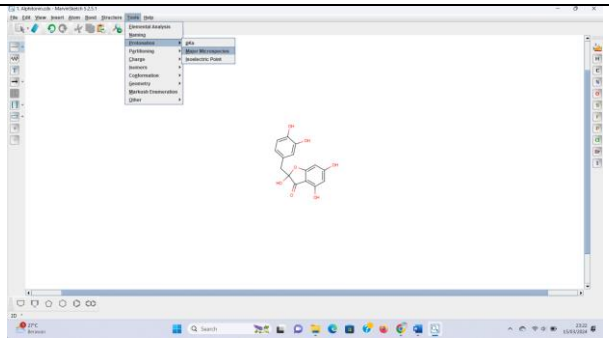
Lampiran 1. Tahapan Preparasi Protein dan *Native Ligand*

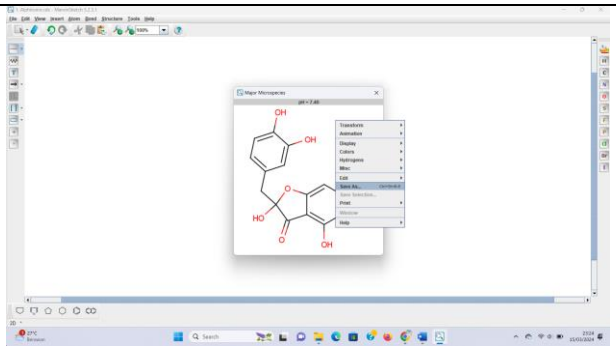
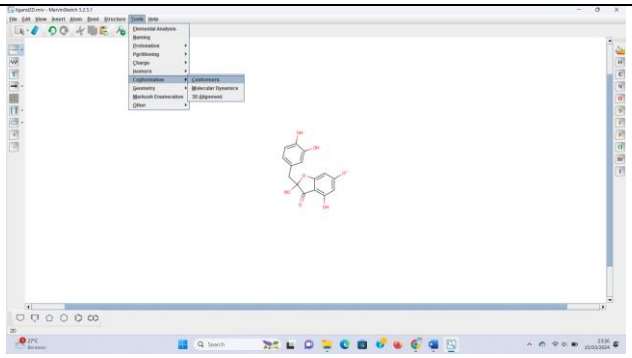
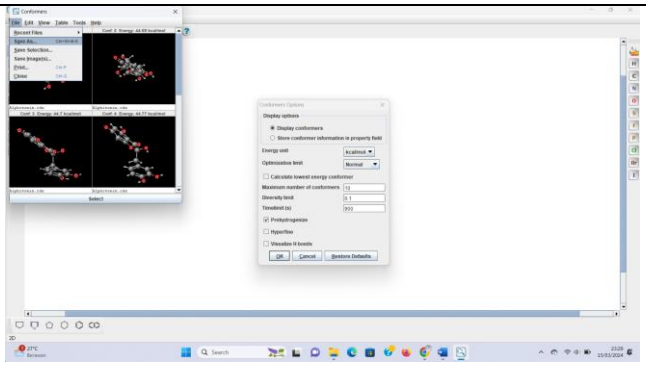
No	Tahapan	Dokumentasi
1.	*Download* protein di PDB *(Protein Data Bank)* melalui *website :* https://rcsb.org/ Dengan file format .pdb	
2.	Preparasi protein menggunakan aplikasi YASARA,	
3.	Input file pdb dengan cara : File → Load → Pdb File → Pilih protein → Ok	

4.	Hapus molekul air dengan cara : Edit → Delete → Water	
5.	Tambahkan molekul hidrogen dengan cara : Edit → Add → hydrogen to : All	
6.	Hapus rantai yang tidak digunakan, sisakan protein dan *native ligand* yang digunakan dengan cara : Dibagian ujung kanan terdapat protein → klik → tampak berbagai molekul → hapus dengan klik kanan di bagian molekul.	

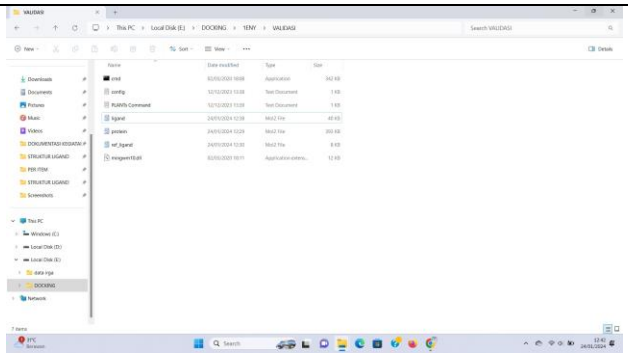
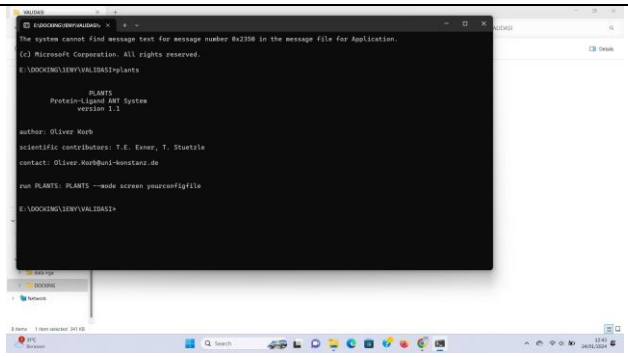
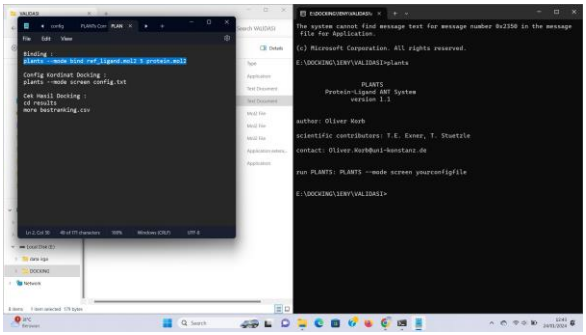
7.	Simpan hasil preparasi dengan format .yob (contoh : 2X23.yob) File → Save as → Yasara Object	
8.	Pemisahan protein dan *native ligand* dengan cara: File → Load → Yasara Object → hapus *native ligand* → save as → other file format → mol2 (contoh : protein.mol2) File → Load → Yasara Object → hapus protein→ save as → other file format → mol2 (contoh : ref_ligand.mol2)	 

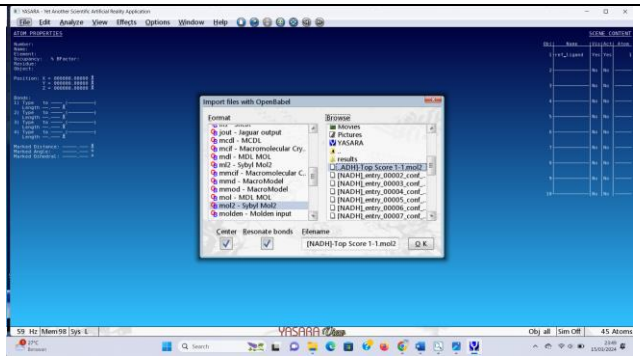
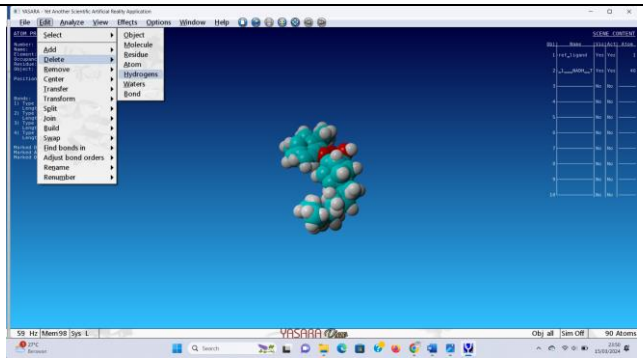
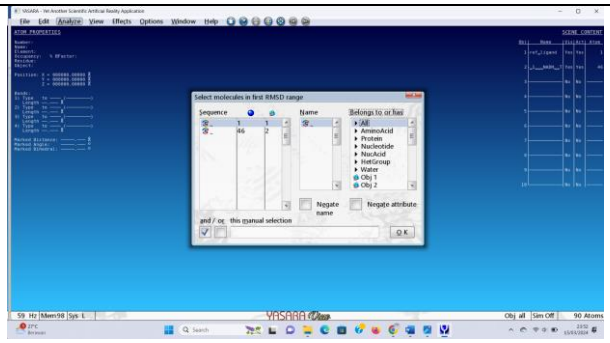
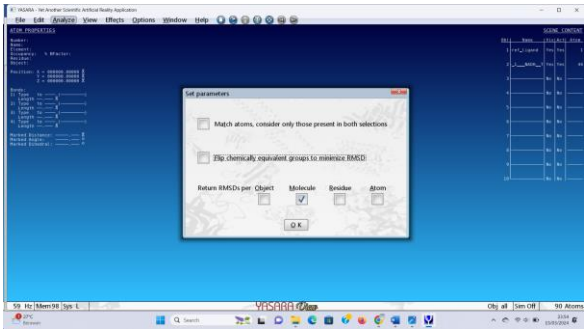
Lampiran 2. Tahapan Preparasi *Native Ligand*, Obat Pembanding dan Senyawa Uji

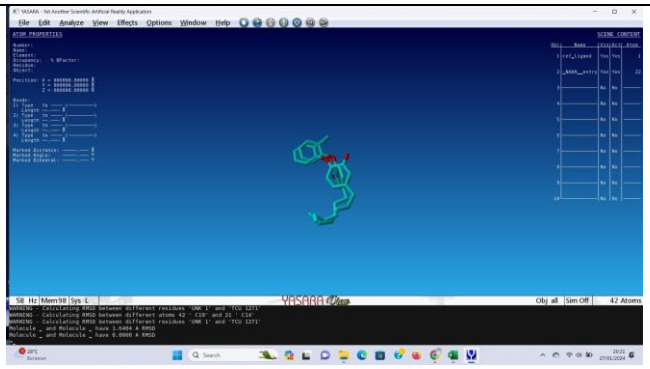
No	Tahapan	Dokumentasi
1.	Preparasi senyawa menggunakan aplikasi Marvin Sketch.	
2.	Input file senyawa (*native ligand*, obat pembanding atau senyawa uji) dengan cara : File → Open → pilih file	
3.	Ubah bentuk 2D dengan cara : Structure → Clean 2D → Clean in 2D	
4.	Stabilkan dengan cara protanation pH yakni : Tools → Protonation → Major Microspecies → Ok PH 7,4	

5.	Simpan file dengan cara : Klik kanan → Save As (rename : ligand2D.mrv)	
6.	Konformasi senyawa dengan cara : Input file ligand2D.mrv → Tools → Conformation → Conformer → OK	
7.	Simpan file konformasi File → Save as (rename : ligand.mol2	

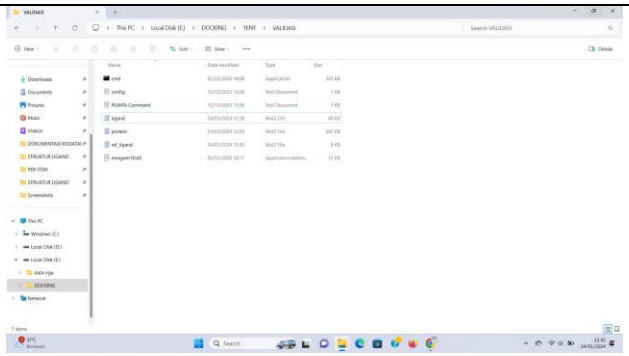
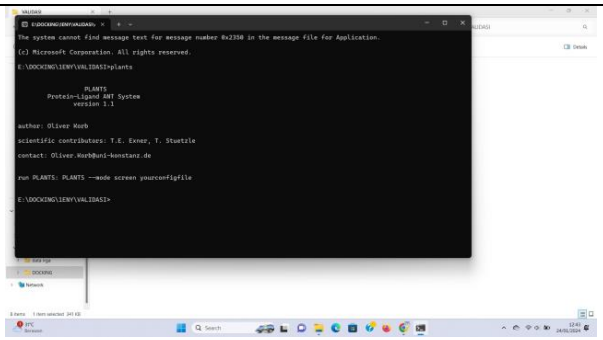
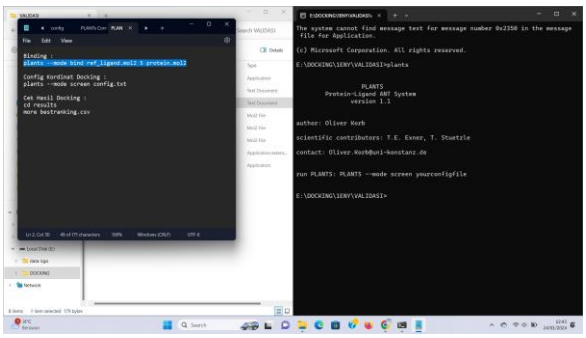
Lampiran 3. Tahapan Validasi Protein dan Penetapan RMSD

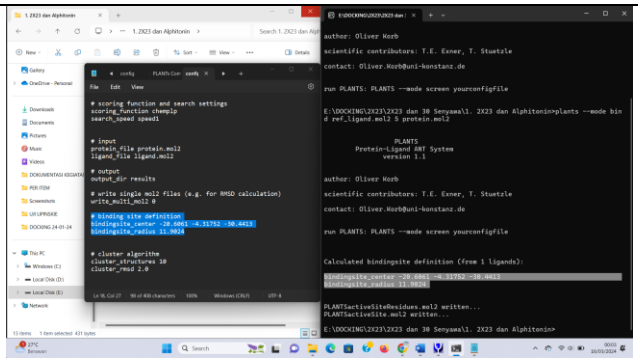
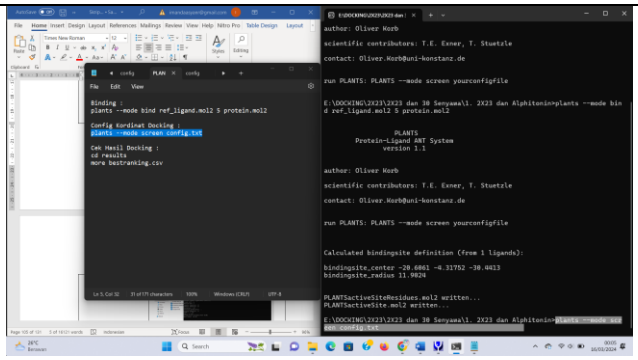
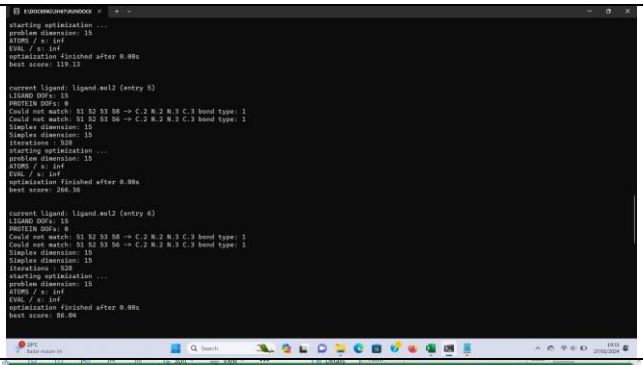
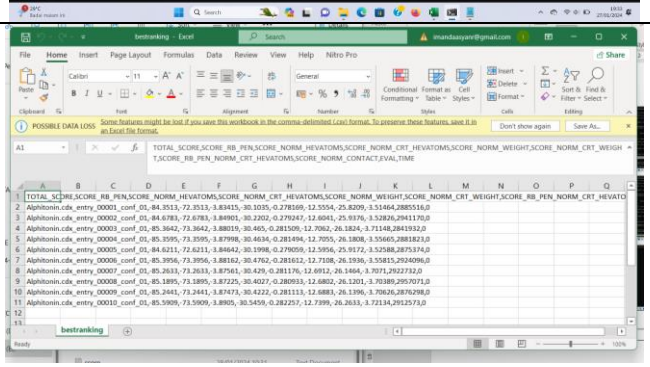
No	Tahapan	Dokumentasi
1.	Siapkan folder yang berisi : - File CMD - File config. - File Plants Command - File mingwm10.dll - File protein.mol2 - File ref_ligand.mol2 - File ligand.mol2 (conformer) Keterangan : : Sudah dipreparasi	
2.	Docking Senyawa *Native Ligand* Menggunakan PLANTs dengan cara : Klik file cmd → ketik plants → masukkan kode binding di file Plants Command → copy → enter → tunggu	 

3.	Buka YASARA input ref_ligand dan hasil docking (konformasi 1-10) dengan cara : File → Load → other file format → ref_ligand.mol2 dan konformer	
4.	Hapus Hidrogen dengan cara : Edit → Delete → Hydrogens	
5.	Analisis nilai RMSD dengan cara : Analyze → RMSD of → molecules → sesuaikan parameter	 

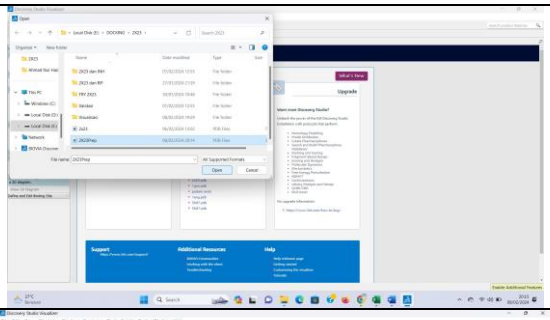
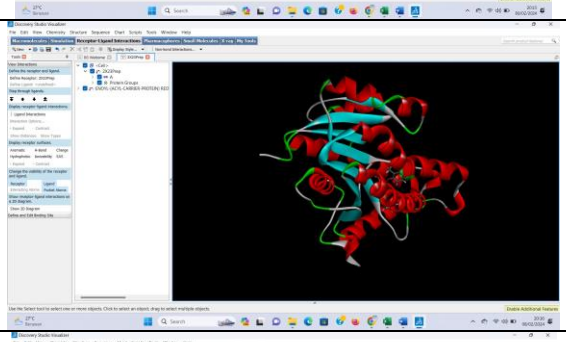
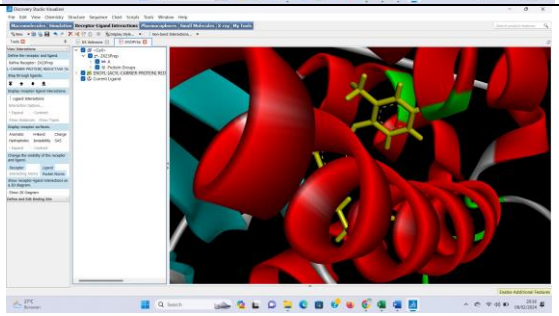
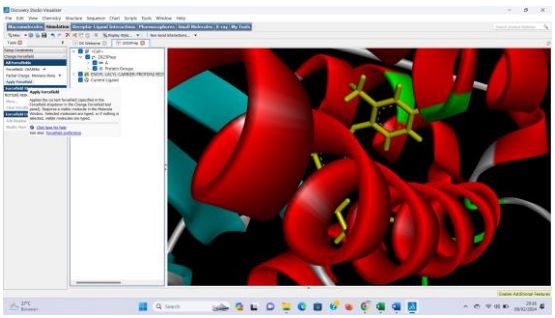
6.	Lihat nilai hasil RMSD	

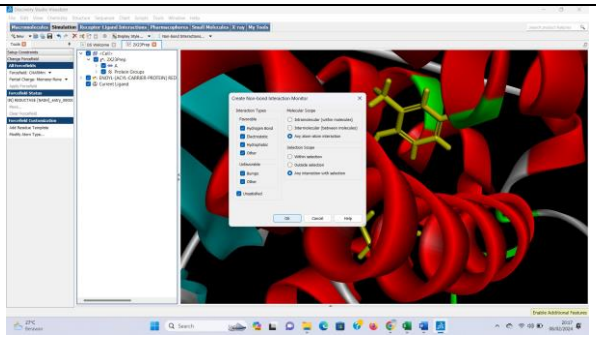
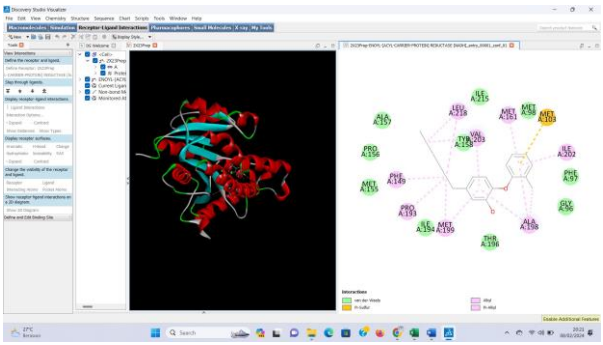
Lampiran 4. Tahapan Docking Protein dengan Obat Pembanding dan Senyawa Uji

No	Tahapan	Dokumentasi
1.	Siapkan folder yang berisi : - File CMD - File config. - File Plants Command - File mingwm10.dll - File protein.mol2 - File ref_ligand.mol2 - File ligand.mol2 (conformer) Keterangan : : Sudah dipreparasi	
2.	Docking Protein dan Senyawa Uji Menggunakan PLANTs dengan cara : Klik file cmd → ketik plants → masukkan kode **binding "plants --mode bind ref_ligand.mol2 5 protein.mol2"** → copy → enter	 

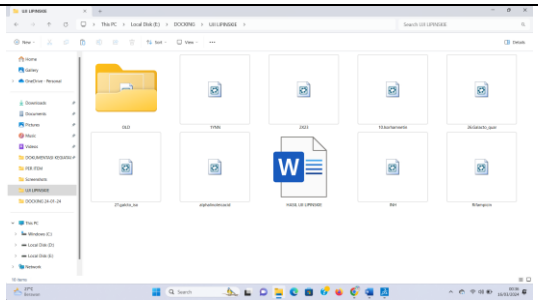
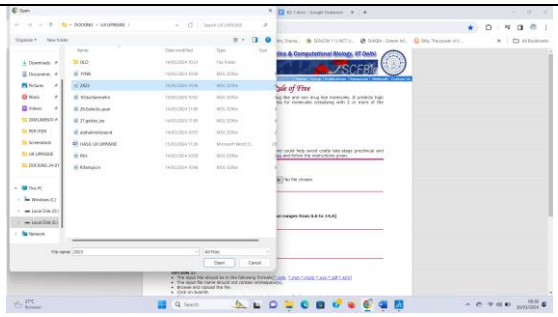
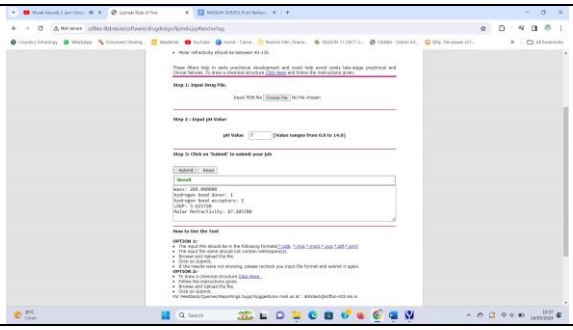
3.	Ubah koordinat protein di file config sesuai dengan layar PLANTs	
4.	Masukkan kode **“plants --mode screen config.txt”**	
5.	Tunggu proses docking	
6.	Lihat hasil melalui file excel otomatis “bestrangking”	

Lampiran 5. Tahapan Visualisasi Ikatan Protein dengan Senyawa Uji

No	Tahapan	Dokumentasi
1.	Visualisasi dilakukan di aplikasi Discovery Studio. Input file protein yang sudah dipreparasi dengan cara : File → Open → file protein	
2.	Input *native ligand*/obat pembanding/senyawa uji. Dengan cara : Pindahkan file langsung ke layar discovery (insert *ligand)*	
3.	Atur parameter dengan cara - *Receptor-Ligand Interaction* → Klik define ligand - *Simulation* → Klik Apply Forcefield - *Non bond Interaction* → ceklis seperti di gambar - *Receptor-Ligand Interaction* → klik show 2D	 

Lampiran 6. Tahapan Pengujian *Rules Of Five Lipinskie*

No	Tahapan	Dokumentasi
1.	Siapkan ligand dalam bentuk sdf	
2.	Buka website lipinskie melalui : http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp	
3.	Input file dengan cara : Choose file → pilih file	
4.	Submit → lihat hasil	

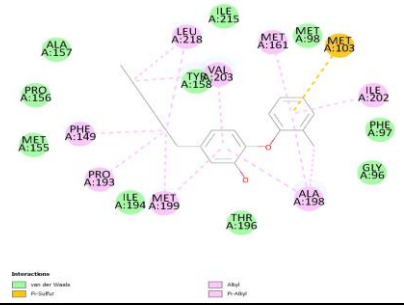
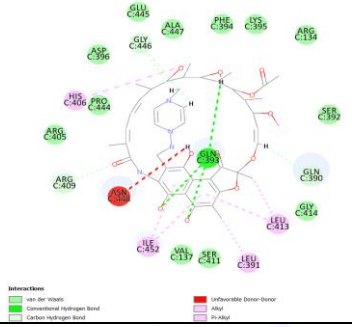
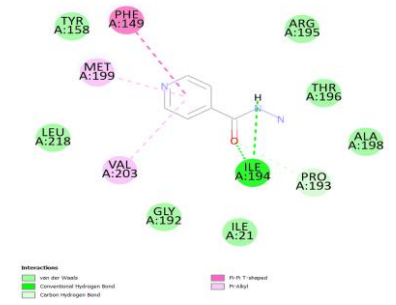
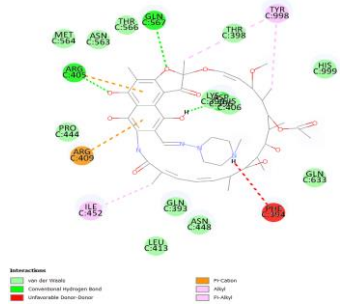
Lampiran 7. Hasil RMSD Protein *Enoyl-Acyl Carrier Protein Reductase* / InhA

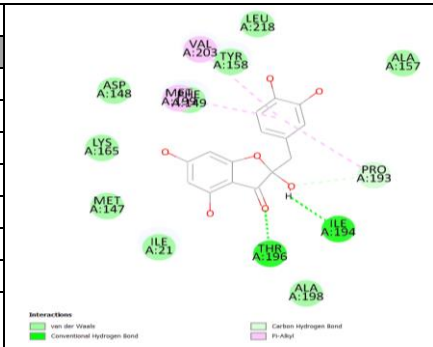
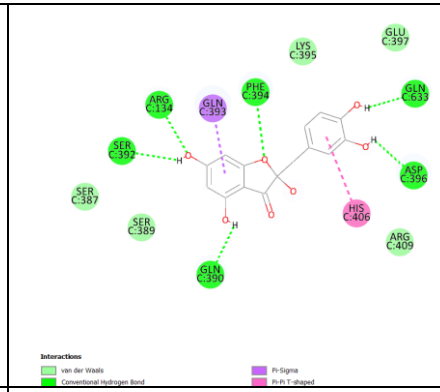
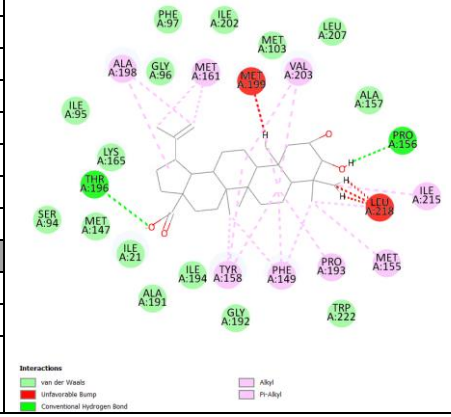
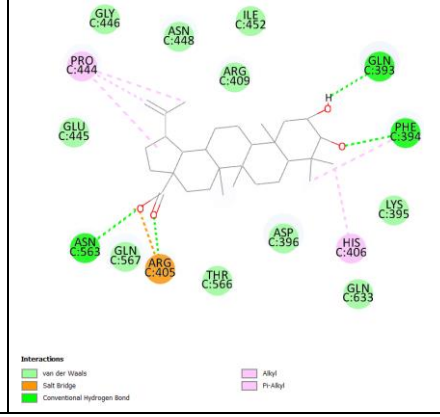
Conformer	**Protein**			**RMSD**		
	1ENY	**2NV6**	**2X23**	**1ENY**	**2NV6**	**2X23**
1	-130.635	-110.184	-98.812	9.339	15.446	1.640
2	-128.094	-111.048	-98.513	9.856	5.716	1.645
3	-130.916	-106.142	-95.322	11.674	12.612	1.830
4	-131.304	-105.281	-95.095	11.170	14.197	3.271
5	-123.486	-97.539	-93.995	6.861	5.208	1.238
6	-129.290	-109.244	-94.704	11.977	16.085	1.175
7	-124.159	-110.503	-94.012	4.897	16.079	1.162
8	-128.769	-99.631	-92.974	3.045	13.009	3.252
9	-132.402	-109.775	-94.870	11.715	15.795	1.251
10	-130.752	-96.291	-93.709	9.545	14.592	2.938

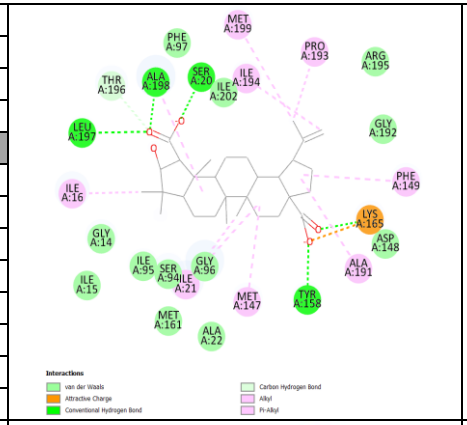
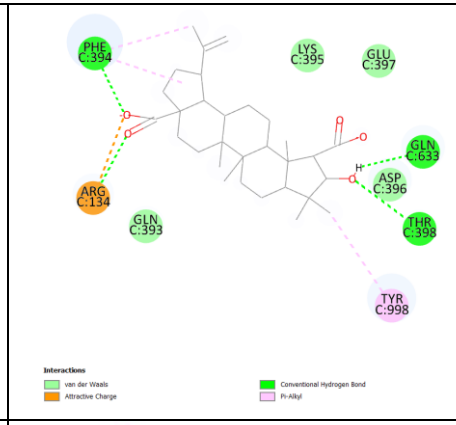
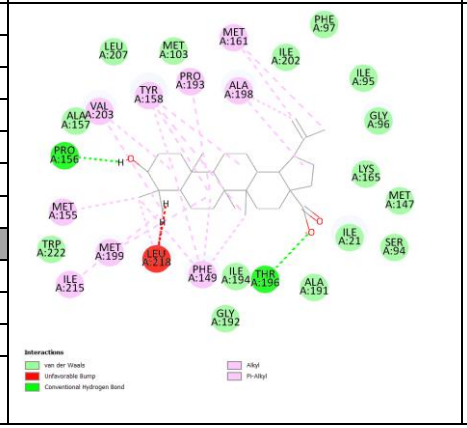
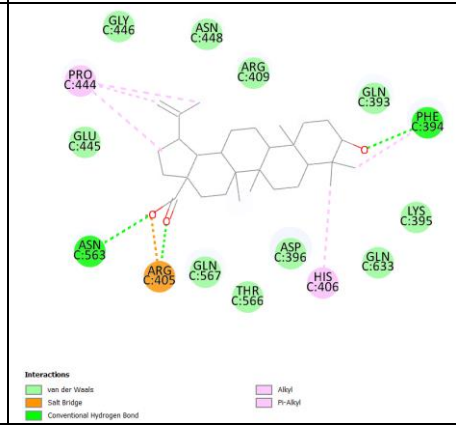
Lampiran 8. Hasil RMSD Protein *RNA Polymerase* (RNAP)

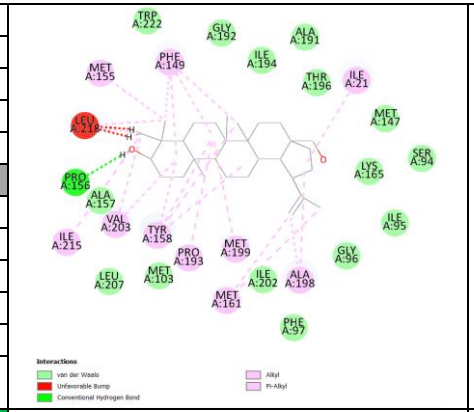
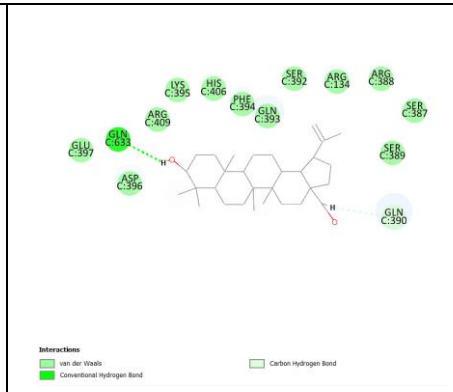
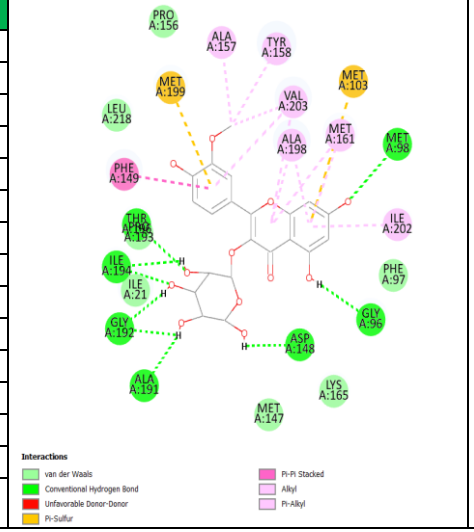
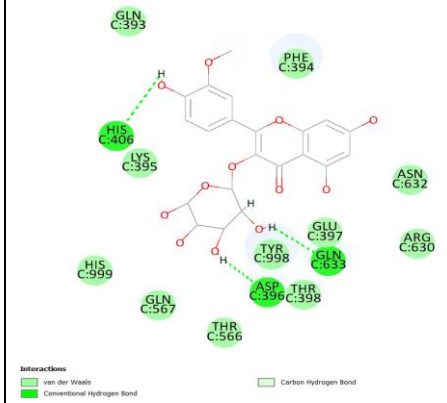
Conformer	Protein			RMSD		
	3H87	**1I6V**	**1YNN**	**3H87**	**1I6V**	**1YNN**
1	-32.86	-74.936	-86.298	0.308	8.242	2.240
2		-71.996	-86.277		8.461	2.249
3		-76.718	-79.412		8.310	1.971
4		-72.945	-79.267		7.228	1.988
5		-78.618	-80.367		8.631	2.085
6		-73.006	-79.598		8.533	2.059
7		-77.114	-81.480		7.316	4.452
8		-77.839	-79.697		8.379	1.928
9		-72.715	-79.536		6.388	1.894
10		-72.386	-79.580		8.529	1.949

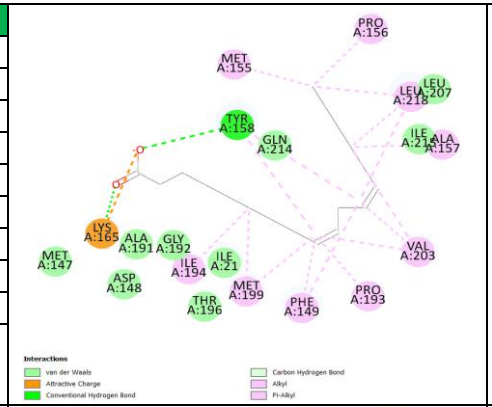
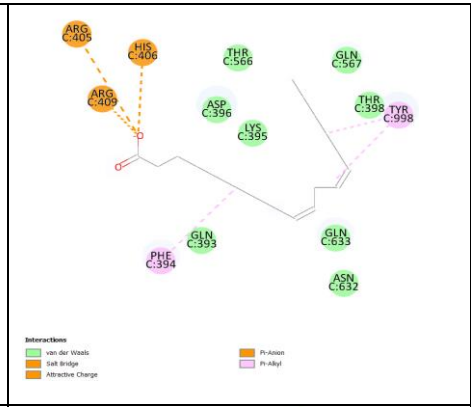
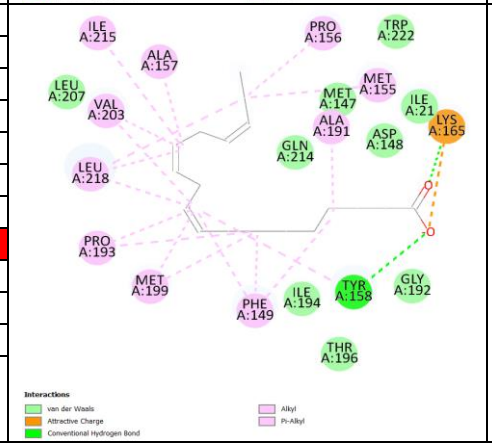
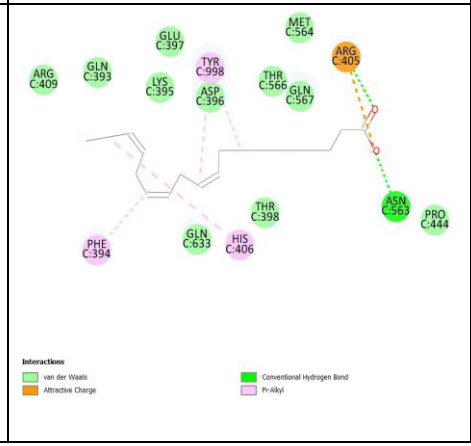
Lampiran 9. Hasil *Docking*, Visualisasi dan Residu Asam Amino Senyawa Genus Alphitonia

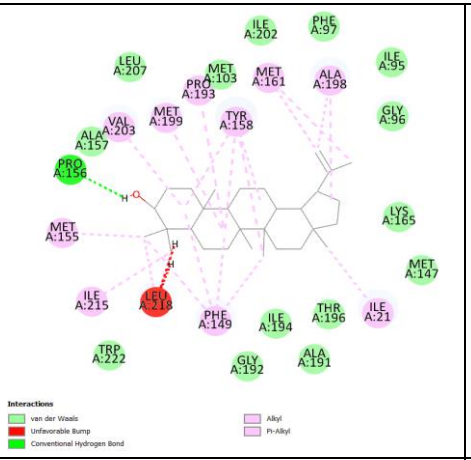
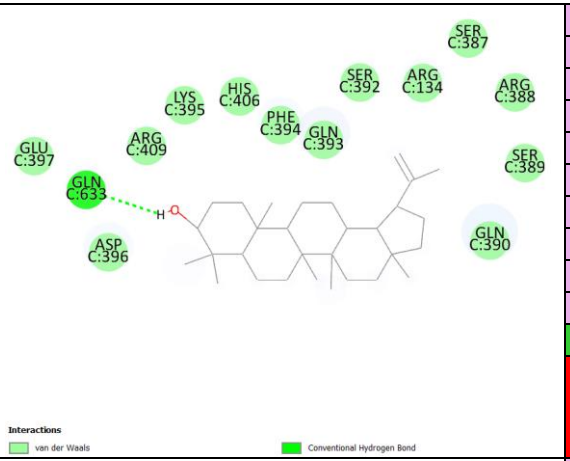
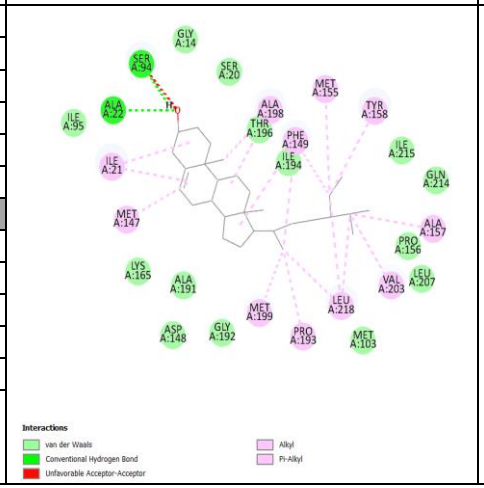
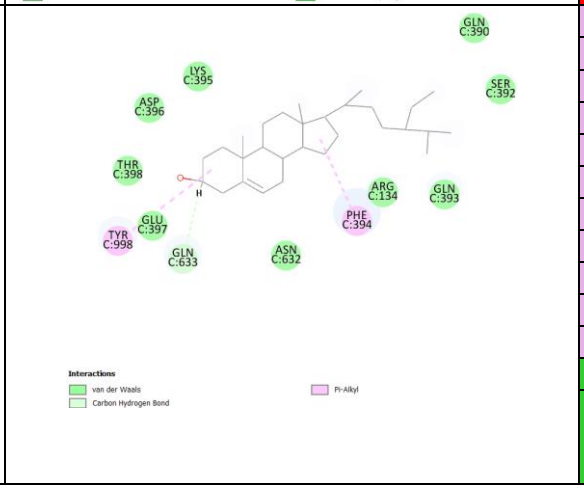
No	Senyawa/*Ligand*	*Conformer*	Protein		Visualisasi		Residu Asam Amino	
			2X23	1YNN	2X23	1YNN	2X23	1YNN
1.	Native	1	-98.812	-86.298			PHE A:149	LEU C:413
		2	-98.513	-86.277			PRO A:193	LEU C:391
		3	-95.322	-79.412			MET A:199	ILE C:452
		4	-95.095	-79.267			LEU A:218	HIS C:406
		5	-93.995	-80.367			VAL A:203	ASN C:448
		6	-94.704	-79.598			ALA A:198	GLN C:393
		7	-94.012	-81.480			MET A:161	GLY C:446
		8	-92.974	-79.697			ILE A:202	ARG C:409
		9	-94.870	-79.536			MET A:103	GLN C:390
		10	-93.709	-79.580				
2.	Obat Pembanding	1	-65.484	-79.449			PHE A:149	TYR C:998
		2	-65.448	-79.705			MET A:199	ILE C:452
		3	-65.504	-79.560			VAL A:203	PHE C:394
		4	-65.269	-79.922			ILE A:194	ARG C:409
		5	-65.375	-77.678				GLN C:567
		6	-65.412	-78.361				ARG C:405
		7	-65.442	-78.109				ASP :396
		8	-65.373	-78.937				
		9	-65.406	-79.622				
		10	-65.378	-79.825				

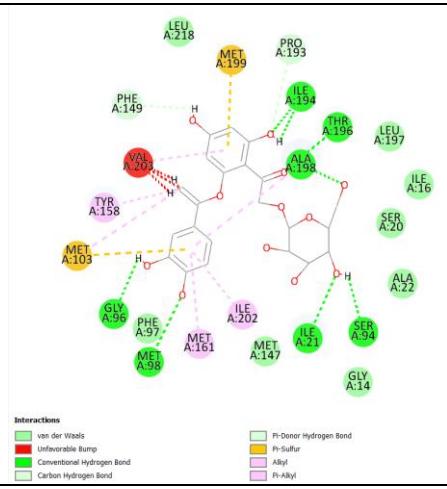
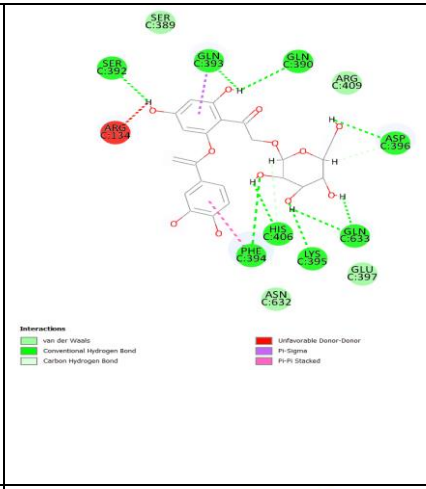
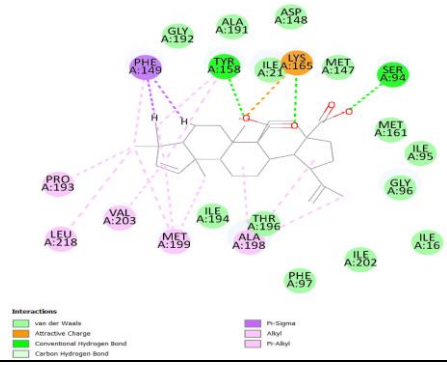
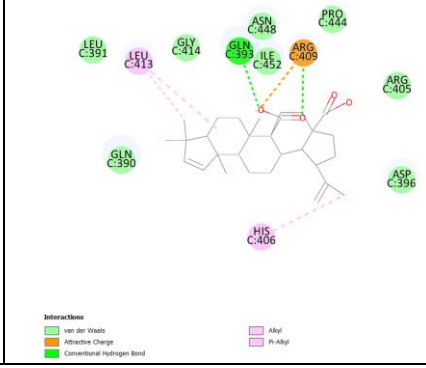
3.	*Alphitonin*	1	-84.351	-78.666			VAL A:203	GLN C:393
		2	-84.678	-78.693			MET A:199	HIS C:406
		3	-85.364	-77.802			ILE A:194	GLN C:633
		4	-85.359	-76.493			THR A:196	ASP C:396
		5	-84.621	-78.007			PRO A:193	PHE C:394
		6	-85.395	-77.993				ARG C:134
		7	-85.263	-78.363				SER C:392
		8	-85.189	-78.316				GLN C:390
		9	-85.244	-78.661				
		10	-85.590	-78.627				
4.	*Alphitolic acid*	1	-64.892	-65.195			ALA A:198	PRO C:444
		2	-65.423	-63.643			MET A:161	HIS C:406
		3	-66.796	-68.509			VAL A:203	GLN C:393
		4	-66.125	-66.657			ILE A:215	PHE C:394
		5	-65.234	-64.960			MET A:155	ASN C:563
		6	-67.085	-66.653			PRO A:193	ARG C:405
		7	-67.979	-69.374			PHE A:149	
		8	-66.195	-66.738			TYR A:158	
		9	-68.422	-70.275			PRO A:156	
		10	-66.420	-66.636			THR A:196	
							MET A:199	
							LEU A:218	

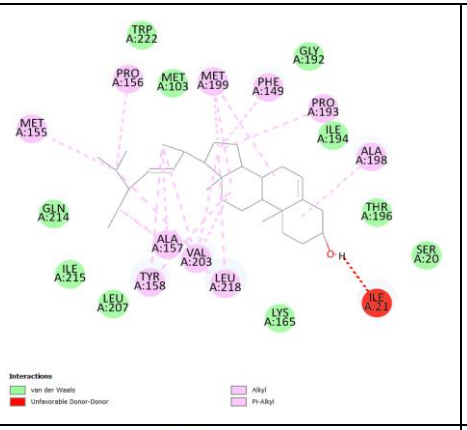
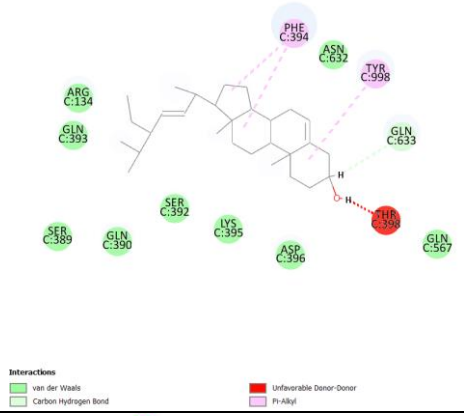
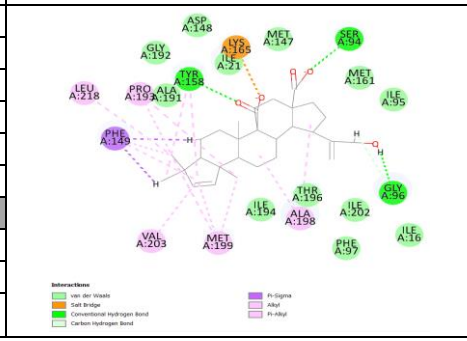
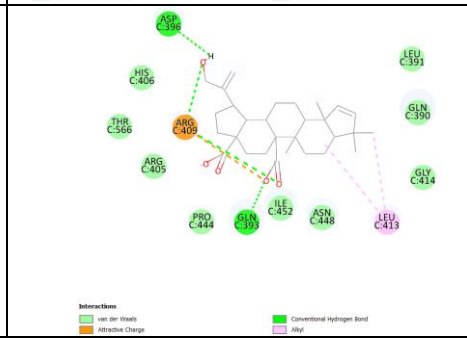
5.	*Ceanothic acid*	1	-67.922	-60.297			ILE A:16	TYR C:998
		2	-68.663	-62.754			ILE A:21	ARG C:134
		3	-69.857	-63.662			MET A:147	PHE C:394
		4	-67.741	-63.719			ALA A:191	GLN C:633
		5	-68.144	-64.025			PHE A:149	THR C:398
		6	-68.457	-62.924			PRO A:193	
		7	-68.531	-63.210			ILE A:194	
		8	-67.589	-63.792			MET A:199	
		9	-68.753	-63.193			TYR A:158	
		10	-67.907	-63.375			SER A:20	
							ALA A:198	
							LEU A:197	
							LYS A:165	
6.	*Betulinic acid*	1	-73.932	-64.809			MET A:161	PRO C:444
		2	-74.109	-66.684			ALA A:198	HIS C:406
		3	-74.341	-65.176			PRO A:193	ARG C:405
		4	-73.613	-60.567			TYR A:158	ASN C:563
		5	-75.066	-66.126			VAL A:203	PHE C:394
		6	-74.520	-66.873			MET A:155	
		7	-74.201	-65.594			MET A:199	
		8	-74.907	-66.953			ILE A:215	
		9	-75.316	-66.150			PHE A:149	
		10	-75.534	-65.929			PRO A:156	
							THR A:196	
							LEU A:218	

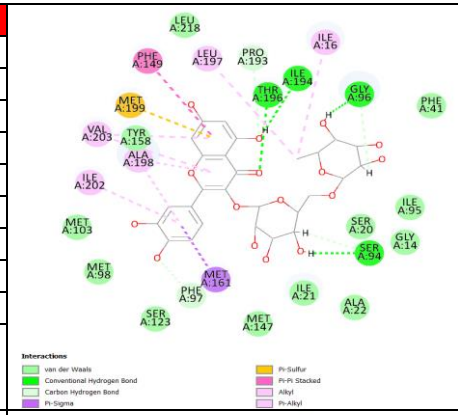
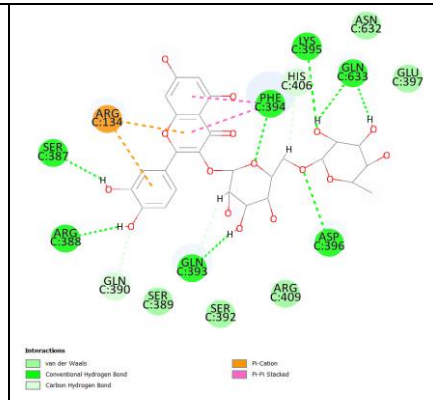
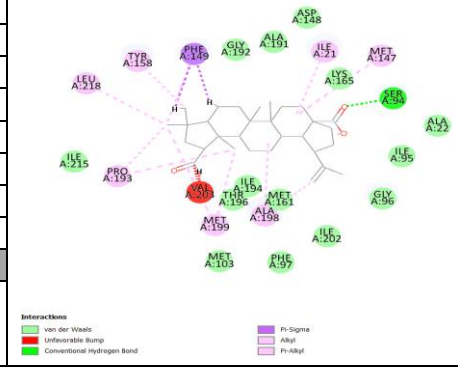
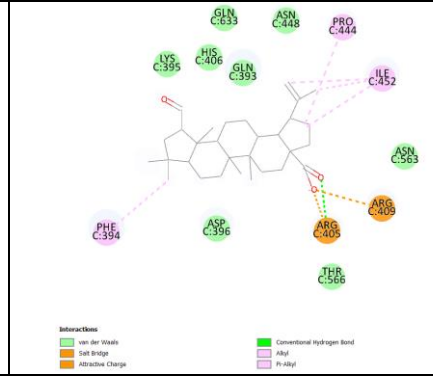
7.	*Betulin*	1	-72.429	-64.160			ILE A:21	GLN C:633
		2	-72.604	-64.613			PHE A:149	GLN C:390
		3	-73.217	-63.401			MET A:155	
		4	-72.219	-62.921			ILE A:215	
		5	-73.376	-63.244			VAL A:203	
		6	-73.019	-65.103			TYR A:158	
		7	-73.667	-63.829			PRO A:193	
		8	-74.455	-63.443			MET A:199	
		9	-74.822	-63.812			MET A:161	
		10	-74.461	-64.512			ALA A:198	
							PRO A:156	
							LEU A:218	
8.	*Isorhamnetin 3-O-β-D-glucopyranoside*	1	-87.231	-80.203			ILE A:202	HIS C:406
		2	-94.349	-69.052			MET A:161	ASP C:396
		3	-88.700	-79.208			ALA A:198	GLN C:633
		4	-88.527	-75.910			VAL A:203	
		5	-94.094	-72.387			TYR A:158	
		6	-93.407	-72.771			ALA A:157	
		7	-90.645	-74.820			PHE A:149	
		8	-86.646	-79.632			MET A:98	
		9	-86.583	-79.782			THR A:196	
		10	-87.719	-77.757			ILE A:194	
							GLY A:192	
							ALA A:191	
							ASP A:148	
							MET A:98	
							MET A:103	
							MET A:199	

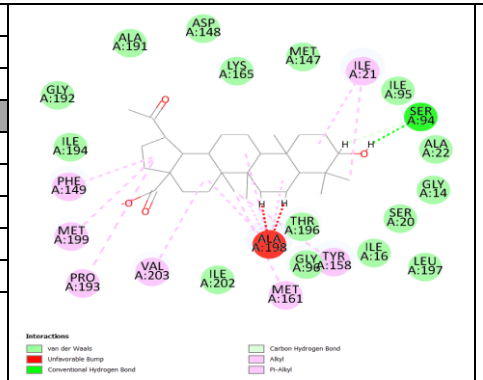
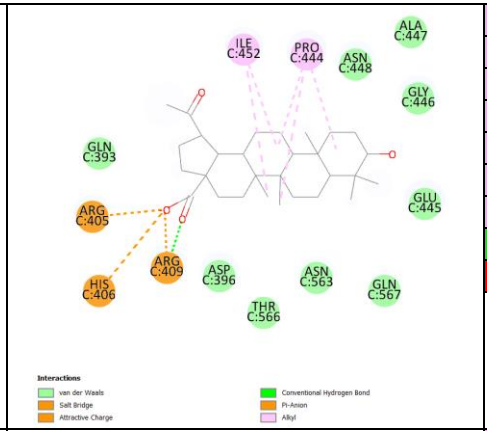
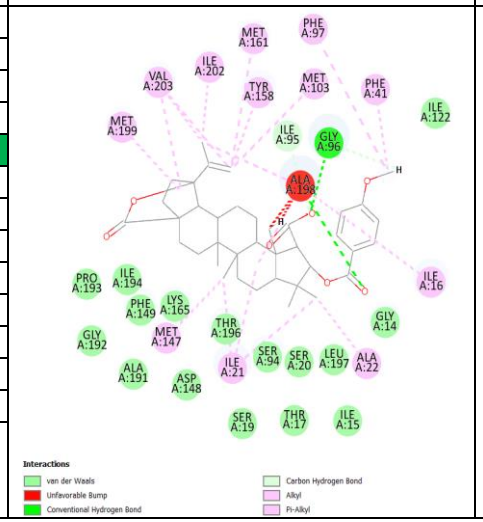
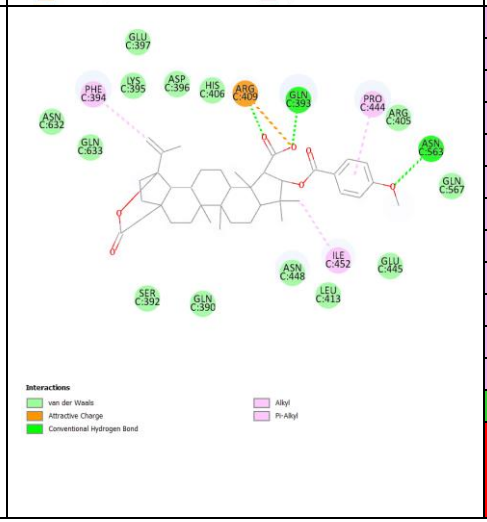
9.	*Linoleic acid*	1	-107.022	-83.562			MET A:155	TYR C:998
		2	-104.893	-76.696			PRO A:156	PHE C:394
		3	-104.682	-79.790			LEU A:218	HIS C:406
		4	-104.902	-79.583			ALA A:157	ARG C:409
		5	-104.920	-77.618			VAL A:203	ARG C:405
		6	-104.278	-77.582			PRO A:193	
		7	-104.991	-81.072			PHE A:149	
		8	-104.766	-78.327			MET A:199	
		9	-105.490	-76.541			ILE A:194	
		10	-104.386	-80.300			TYR A:158	
							LYS A:165	
10.	*α- Linoleic acid*	1	-105.898	-83.950			ALA A:191	TYR C:998
		2	-105.023	-80.682			MET A:155	PHE C:394
		3	-105.031	-79.095			PRO A:156	HIS C:406
		4	-103.600	-85.018			ALA A:157	ARG C:405
		5	-104.764	-76.149			ILE A:215	ASN C:563
		6	-104.965	-83.371			VAL A:203	
		7	-105.398	-79.433			LEU A:218	
		8	-103.729	-86.792			PRO A:193	
		9	-103.352	-85.875			MET A:199	
		10	-103.295	-78.480			PHE A:149	
							TYR A:158	
							LYS A:165	

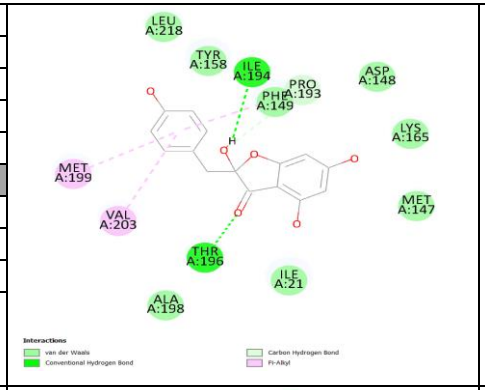
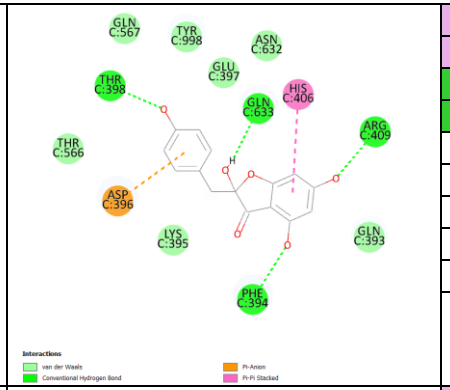
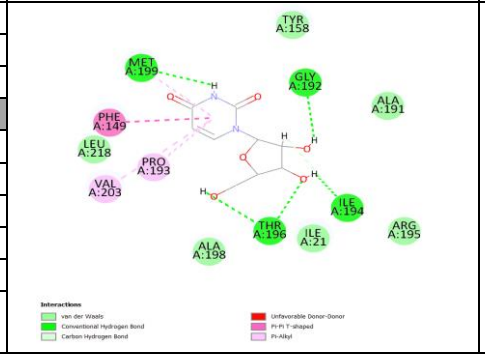
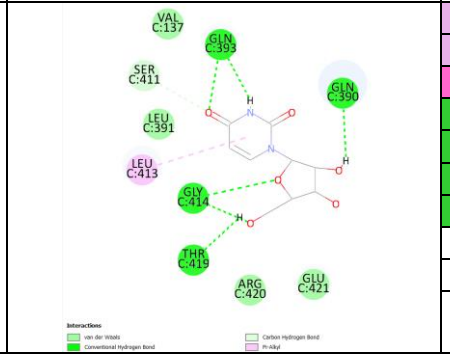
11.	*Lupeol*	1	-75.465	-61.917			ALA A:198	GLN C:633
		2	-74.687	-64.936			MET A:161	
		3	-74.218	-62.767			TYR A:158	
		4	-75.592	-64.080			PRO A:193	
		5	-75.745	-63.727			MET A: 199	
		6	-74.969	-64.422			VAL A:203	
		7	-74.713	-63.712			MET A:155	
		8	-75.353	-64.000			ILE A:215	
		9	-75.571	-63.568			PHE A:149	
		10	-75.046	-64.667			ILE A:21	
							PRO A:156	
							LEU A:218	
12.	*β -Sitosterol*	1	-99.416	-71.395			TYR A:158	TYR C:998
		2	-100.171	-77.976			MET A:155	PHE C:394
		3	-100.918	-78.980			PHE A:149	GLN C:633
		4	-100.635	-77.097			ALA A:198	
		5	-100.425	-73.013			ILE A:21	
		6	-102.141	-77.161			MET A:147	
		7	-100.703	-79.484			MET A:199	
		8	-100.738	-79.205			PRO A:193	
		9	-100.129	-78.366			LEU A:218	
		10	-99.355	-79.434			VAL A:203	
							ALA A:157	
							SER A:94	
							ALA A:22	

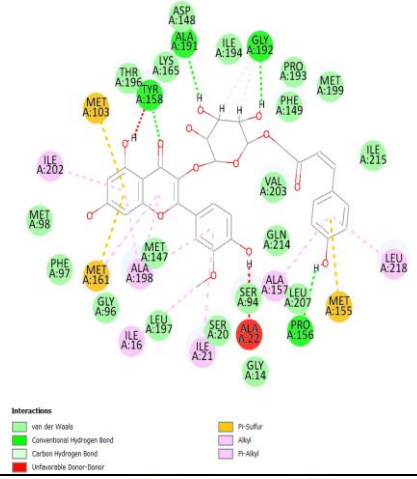
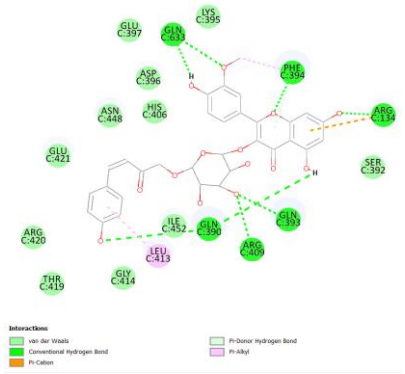
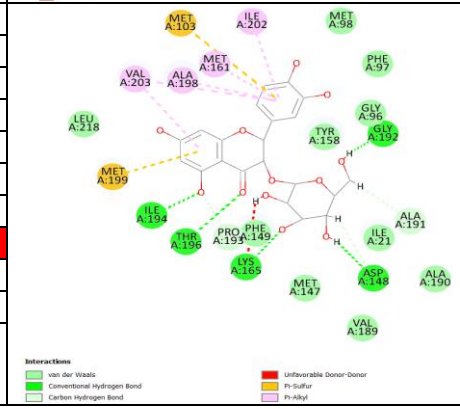
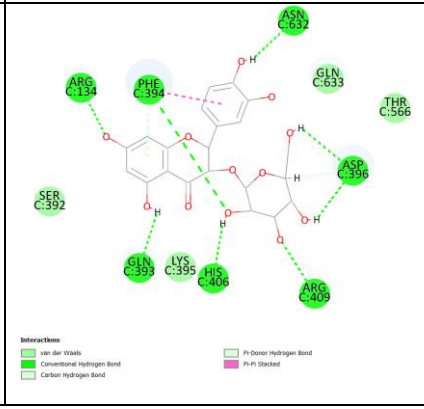
13.	*Quarcetin 3-O-β-D-glucopyranoside*	1	-89.934	-75.970			ILE A:202	ARG C:134
		2	-96.088	-77.818			MET A:161	SER C:392
		3	-99.774	-77.732			TYR A:158	GLN C:393
		4	-98.601	-83.317			GLY A:96	GLN C:390
		5	-94.736	-77.763			MET A:98	ASP C:396
		6	-94.390	-74.661			ILE A:21	GLN C:633
		7	-93.892	-80.110			SER A:94	LYS C:395
		8	-92.082	-73.709			ALA A:198	HIS C:406
		9	-100.388	-84.593			THR A:196	PHE C:394
		10	-100.641	-86.920			ILE A:194	
							MET A:199	
							MET A:103	
							VAL A:203	
14.	*Ceanothenic acid*	1	-81.812	-59.803			PRO A:193	LEU C:413
		2	-81.079	-60.158			LEU A:218	HIS C:406
		3	-81.207	-60.018			VAL A:203	ARG C:409
		4	-81.627	-59.172			MET A:199	GLN C:393
		5	-81.065	-60.138			ALA A:198	
		6	-82.027	-58.831			PHE A:149	
		7	-81.408	-59.410			TYR A:158	
		8	-81.178	-59.146			SER A:94	
		9	-81.693	-60.193			LYS A:165	
		10	-80.883	-59.446				

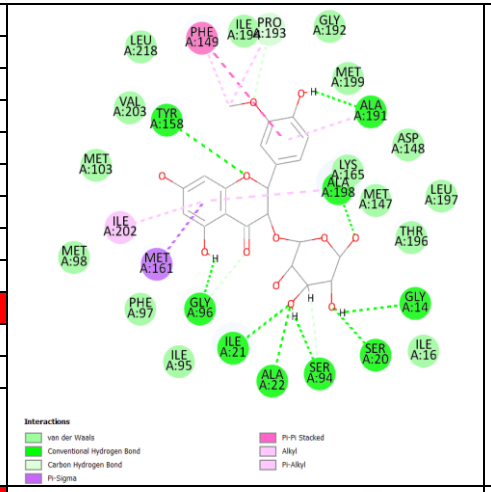
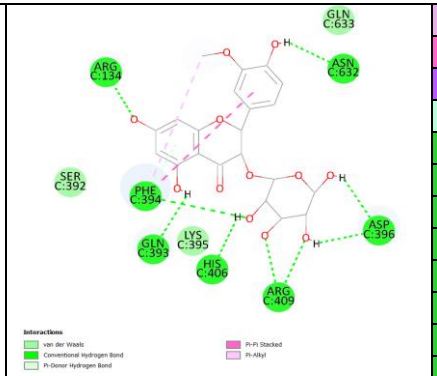
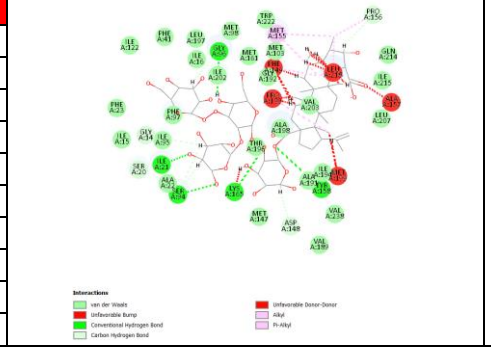
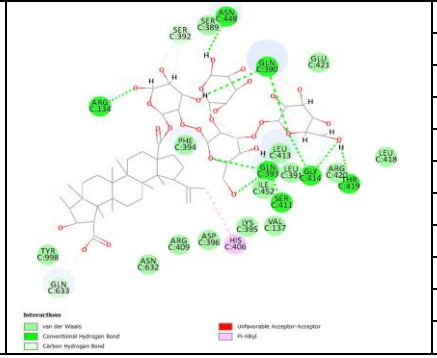
15.	*Stigmasterol*	1	-98.374	-77.339			ALA A:198	GLN C:633
		2	-97.744	-78.732			PRO A:193	PHE C:394
		3	-97.249	-77.711			PHE A:149	TYR C:998
		4	-99.192	-77.343			MET A:199	THR C:398
		5	-99.486	-77.034			PRO A:156	
		6	-98.684	-77.145			MET A:155	
		7	-98.861	-77.038			TYR A:158	
		8	-99.928	-77.902			ALA A:157	
		9	-98.356	-76.400			VAL A:203	
		10	-98.056	-78.048			LEU A:218	
							ILE A:21	
16.	*29-Hydroxyceanothenic acid*	1	-86.596	-65.821			PRO A:193	ARG C:409
		2	-86.329	-61.168			LEU A:218	ASP C:396
		3	-87.359	-64.599			VAL A:203	GLN C:393
		4	-86.460	-60.359			MET A:199	LEU C:413
		5	-85.707	-65.106			ALA A:198	
		6	-85.483	-64.691			PHE A:149	
		7	-85.446	-65.911			TYR A:158	
		8	-85.744	-65.422			GLY A:96	
		9	-84.369	-62.814			SER A:94	
		10	-82.651	-63.293			LYS A:165	

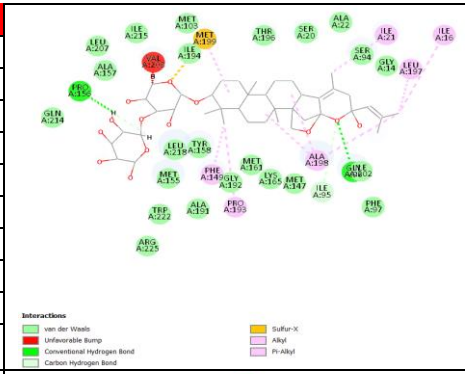
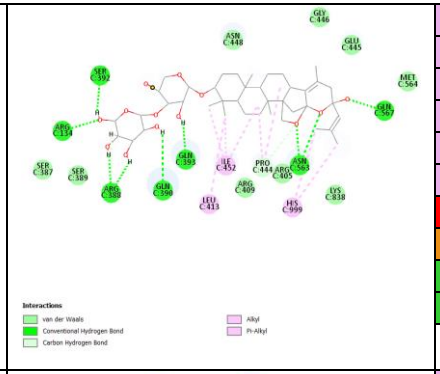
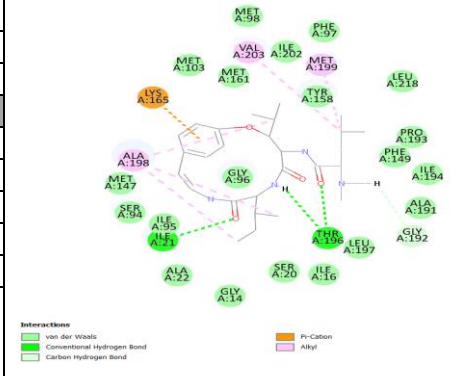
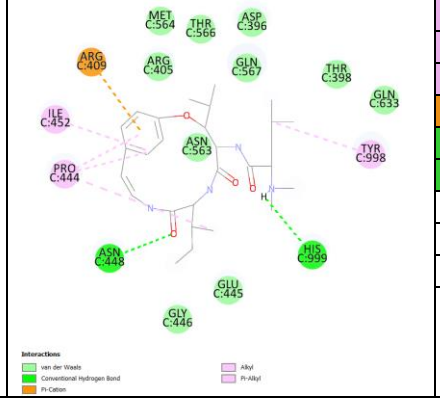
17.	*Rutin*	1	-111.556	-94.255			ILE A:16	ARG C:134
		2	-102.391	-90.324			LEU A:197	SER C:387
		3	-99.679	-89.760			VAL A:203	ARG C:388
		4	-100.090	-89.866			ALA A:198	GLN C:393
		5	-100.564	-91.600			ILE A:202	ASP C:396
		6	-101.613	-90.867			PHE A:149	GLN C:633
		7	-107.594	-93.317			MET A:161	LYS C:395
		8	-101.803	-91.731			SER A:94	PHE C:394
		9	-101.803	-93.946			GLY A:96	GLN C:390
		10	-106.836	-90.880			ILE A:194	HIS C:406
							THR A:196	
18.	*2α-formyl-A(1)norlup-20(29)en-28-oic acid.*	1	-71.694	-61.278			MET A:147	ARG C:409
		2	-72.601	-61.049			ILE A:21	ARG C:405
		3	-72.551	-60.950			TYR A:158	PHE C:394
		4	-73.443	-60.924			LEU A:218	PRO C:444
		5	-72.275	-61.466			PRO A:193	ILE C:452
		6	-73.351	-60.862			MET A:199	
		7	-68.717	-65.186			ALA A:198	
		8	-69.500	-65.236			PHE A:149	
		9	-70.219	-66.108			SER A:94	
		10	-72.868	-62.267			VAL A:203	

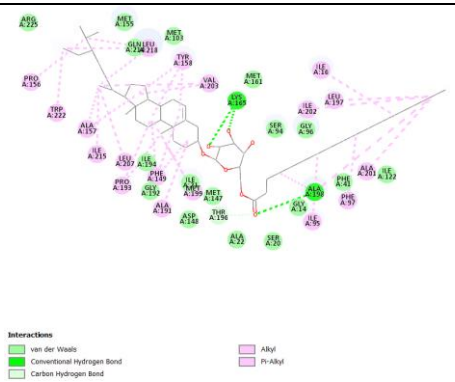
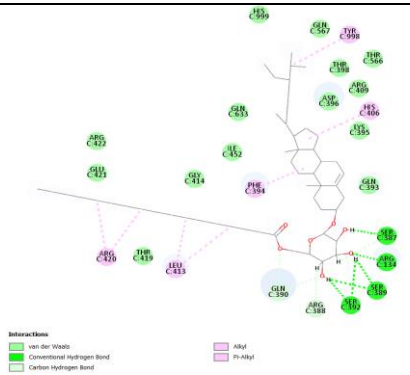
19.	*Platanic acid*	1	-76.064	-63.288			ILE A:21	ARG C:405
		2	-79.939	-64.535			PHE A:149	ARG C:409
		3	-80.542	-64.377			MET A:199	HIS C:406
		4	-71.480	-65.732			PRO A:193	ILE C:452
		5	-77.919	-64.230			VAL A:203	PRO C:444
		6	-75.074	-64.748			MET A:161	
		7	-78.352	-64.468			TYR A:158	
		8	-73.506	-64.805			SER A:94	
		9	-75.605	-65.065			ALA A:198	
		10	-72.266	-65.290				
20.	*Alphitexolide*	1	-72.057	-78.043			PHE A:41	PRO C:444
		2	-68.300	-71.055			PHE A:97	ILE C:452
		3	-68.310	-76.949			MET A:103	PHE C:394
		4	-70.357	-77.546			TYR A:158	ARG C:409
		5	-69.248	-81.065			MET A:161	GLN C:393
		6	-67.237	-80.695			ILE A:202	ASN C:563
		7	-66.564	-75.470			VAL A:203	
		8	-67.302	-77.127			MET A:199	
		9	-63.599	-79.017			MET A:147	
		10	-64.069	-80.159			ILE A:21	
							ALA A:22	
							ILE A:16	
							GLY A:96	
							ALA A:198	

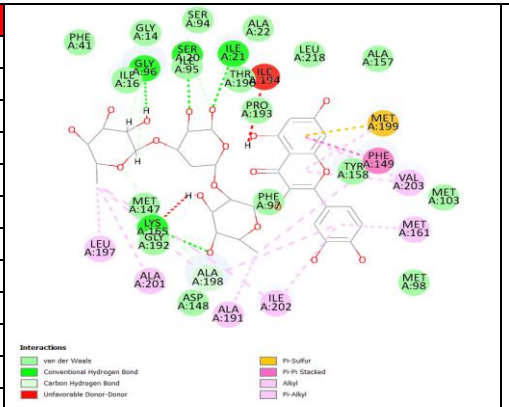
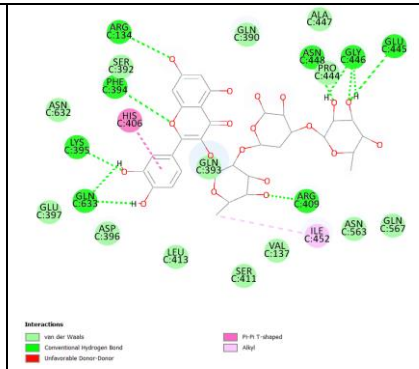
21.	*Maesopsin*	1	-84.787	-75.506			MET A:199	HIS C:406
		2	-85.389	-75.176			VAL A:203	THR C:398
		3	-85.726	-72.463			THR A:196	GLN C:633
		4	-85.561	-75.574			ILE A:194	ARG C:409
		5	-85.851	-70.950				PHE C:394
		6	-85.680	-75.815				ASP C:396
		7	-84.890	-74.511				
		8	-84.622	-74.070				
		9	-84.832	-75.591				
		10	-85.256	-75.460				
22.	*Uridin*	1	-75.048	-65.430			PRO A:193	LEU C:413
		2	-75.124	-65.373			VAL A:203	GLN C:393
		3	-75.305	-62.513			PHE A:149	GLN C:390
		4	-76.567	-66.121			MET A:199	GLY C:414
		5	-75.216	-62.636			GLY A:192	THR C:419
		6	-75.115	-63.642			ILE A:194	SER C:411
		7	-73.803	-60.230			THR A:196	
		8	-73.953	-60.412				
		9	-73.772	-60.475				
		10	-74.783	-60.072				

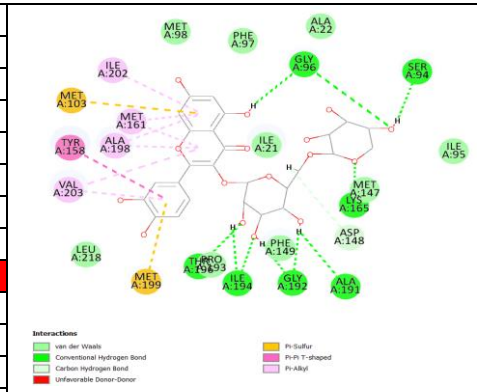
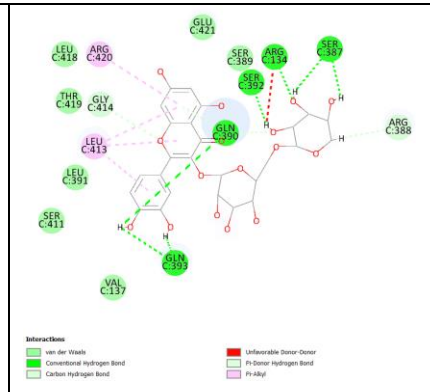
23.	*Isorhamnetin 3-O-(6''-O-(Z)-p-coumaroyl)-β-D-glucopyranoside*	1	-107.785	-95.570			LEU A:218	LEU C:413
		2	-107.315	-90.031			ALA A:157	GLN C:390
		3	-108.232	-85.155			ILE A:21	ARG C:409
		4	-99.024	-89.933			ILE A:16	GLN C:393
		5	-104.296	-92.734			ALA A:198	ARG C:134
		6	-111.918	-91.952			ILE A:202	PHE C:394
		7	-109.692	-85.765			TYR A:158	GLN C:633
		8	-104.966	-77.488			ALA A:191	
		9	-106.425	-88.718			GLY A:192	
		10	-106.984	-82.155			PRO A:156	
							MET A:103	
							MET A:161	
							MET A:155	
							ALA A:22	
24.	*3-O-β-D-Galactopyranosyl-quercetin*	1	-106.195	-79.408			ILE A:202	ASN C:632
		2	-106.052	-79.379			MET A:161	ASP C:396
		3	-105.585	-80.657			ALA A:198	ARG C:409
		4	-105.931	-79.704			VAL A:203	HIS C:406
		5	-105.116	-79.195			GLY A:192	GLN C:393
		6	-104.835	-78.787			ASP A:148	ARG C:134
		7	-105.753	-79.476			LYS A:165	PHE C:394
		8	-105.816	-89.045			THR A:196	
		9	-104.029	-81.248			ILE A:194	
		10	-103.895	-87.615			MET A:199	
							MET A:103	

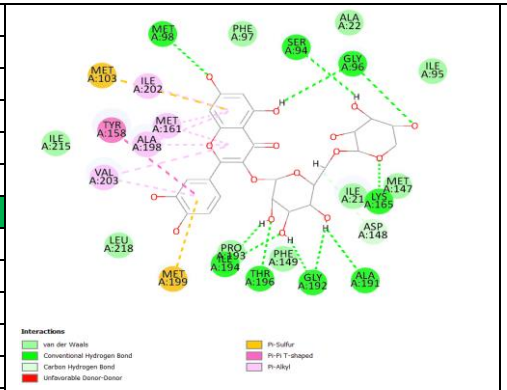
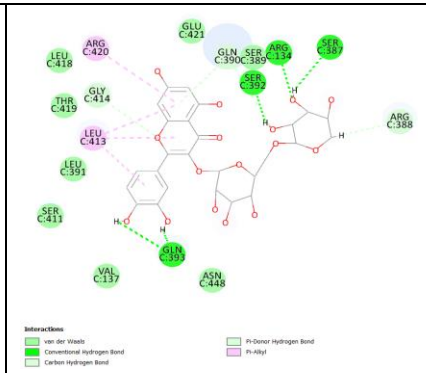
25.	*3-O-β-D-Galactopyranosyl-isorhamnetin*	1	-100.378	-88.404			ILE A:202	ASN C:632
		2	-100.803	-81.917			PHE A:149	ASP C:396
		3	-100.031	-81.515			MET A:161	ARG C:409
		4	-99.813	-81.726			PRO A:193	HIS C:406
		5	-100.257	-82.014			ALA A:191	GLN C:393
		6	-100.972	-83.885			ALA A:198	ARG C:134
		7	-99.509	-81.909			GLY A:14	PHE C:394
		8	-100.586	-81.623			SER A:20	
		9	-97.960	-81.714			SER A:94	
		10	-100.020	-89.052			ALA A:22	
							ILE A:21	
							GLY A:96	
							TYR A:158	
26.	*28-O-β-D-Glucopyranosyl-(1→3)-[β-Dglucopyranosyl-(1→2)]-β-D-lucopyranosyl-(1→2)-β-D-glucopyranosylceanothic acid*	1	153.399	-113.046				HIS C:406
		2	80.704	-111.461				ARG C:134
		3	133.154	-104.334				ASN C:448
		4	137.016	-102.792				GLN C:390
		5	140.122	-102.179				THR C:419
		6	146.056	-111.044				GLY C:414
		7	163.690	-102.287				GLN C:393
		8	93.983	-102.551				SER C:411
		9	135.539	-96.168				ARG C:420
		10	152.377	-106.870				SER C:392
								GLN C:633

27.	*3-O-β-D-Glucopyranosyl-(1→3)-α-arabinopyranosyl-17,20-didehydro-20-deoxyjujubogenin*	1	-68.835	-87.615			ILE A:21	LEU C:413
		2	-69.895	-84.572			ILE A:16	ILE C:452
		3	-70.299	-81.982			LEU A:197	HIS C:999
		4	-70.499	-85.010			ALA A:198	GLN C:567
		5	-70.684	-82.836			PRO A:193	ASN C:563
		6	-70.325	-81.152			PHE A:149	GLN C:393
		7	-70.738	-84.607			VAL A:203	GLN C:390
		8	-71.665	-85.716			MET A:199	ARG C:388
		9	-70.360	-85.723			GLY A:96	ARG C:134
		10	-58.980	-82.968			PRO A:156	SER C:392
								PRO C:444
28.	*Adouetine X*	1	-100.250	-73.872			VAL A:203	
		2	-101.353	-75.543			MET A:199	
		3	-103.081	-73.521			ALA A:198	
		4	-105.980	-76.235			LYS A:165	
		5	-99.334	-69.630			THR A:196	
		6	-96.481	-67.001			ILE A:21	
		7	-101.414	-71.424				
		8	-94.565	-74.344				
		9	-102.146	-72.682				
		10	-98.457	-72.376				

29.	*6'-Heptadecanoyl-3-O-β-Dglucopyranosylsitosterol*	1	-125.413	-125.417			ILE A:16	TYR C:998
		2	-129.815	-118.308			LEU A:197	HIS C:406
		3	-106.737	-111.446			ILE A:202	PHE C:394
		4	-114.487	-108.322			ALA A:201	LEU C:413
		5	6.665	-116.472			PHE A:97	ARG C:420
		6	-130.934	-119.773			ILE A:95	SER C:387
		7	-98.845	-112.524			MET A:199	ARG C:134
		8	-94.323	-109.465			ALA A:191	SER C:389
		9	-87.549	-108.570			PHE A:149	SER C:392
		10	-108.587	-112.235			PRO A:193	ARG C:388
							LEU A:207	GLN C:490
							ILE A:215	
							ALA A:157	
							TRP A:222	
							PRO A:156	
							LEU A:218	
							TYR A:158	
							VAL A:203	
							ALA A:198	
							LYS A:165	

30.	*Quercetin 3-O-α-L-rhamnopyranosyl (1→2)-α-L arabinopyranosyl (1→2)-α-L-rhamnopyranoside*	1	-102.704	-96.245			LEU A:197	ILE C:452
		2	-80.489	-86.476			ALA A:201	HIS C:406
		3	-75.318	-84.044			ALA A:191	GLU C:445
		4	-98.533	-94.939			ILE A:202	GLY C:446
		5	-79.304	-77.702			MET A:161	ASN C:448
		6	-80.976	-87.449			VAL A:203	ARG C:134
		7	-80.083	-96.038			PHE A:149	PHE C:394
		8	-79.880	-90.194			ILE A:194	LYS C:395
		9	-78.755	-82.634			MET A:199	GLN C:633
		10	-74.835	-81.487			LYS A:165	ARG C:409
							GLY A:96	
							SER A:20	
							ILE A:21	
							ILE A:16	
							ILE A:95	
							MET A:147	

31.	*3-O-α-L-Arabinopyranosyl-(1→2)-α-Lrhamnopyranosylkaempferol*	1	-101.732	-80.507			ILE A:202	ARG C:420
		2	-101.446	-79.795			MET A:161	LEU C:413
		3	-99.909	-74.484			ALA A:198	SER C:387
		4	-100.221	-73.552			VAL A:203	ARG C:134
		5	-101.761	-74.994			TYR A:158	SER C:392
		6	-101.413	-82.208			MET A:103	GLN C:390
		7	-97.687	-74.401			MET A:199	GLN C:393
		8	-97.431	-76.223			GLY A:96	GLY C:414
		9	-99.845	-86.996			SER A:94	ARG C:388
		10	-98.593	-77.071			LYS A:165	
							ALA A:191	
							GLY A:192	
							ILE A:194	
							THR A:196	
							ASP A:148	

32.	*3-O-β-D-Xylopyranosyl-(1→2)-α-Lrhamnopyranosylkaempferol*	1	-98.492	-73.165			ILE A:202	ARG C:420
		2	-101.486	-80.189			MET A:161	LEU C:413
		3	-99.854	-78.511			ALA A:198	SER C:387
		4	-101.435	-72.174			VAL A:203	ARG C:134
		5	-101.329	-82.182			TYR A:158	SER C:392
		6	-99.993	-76.621			MET A:103	GLN C:393
		7	-97.814	-83.367			MET A:199	GLN C:390
		8	-97.724	-78.863			MET A:98	ARG C:388
		9	-100.292	-77.116			SER A:94	GLY C:414
		10	-98.460	-77.690			GLY A:96	
							LYS A:165	
							ALA A:191	
							GLY A:192	
							THR A:196	
							ILE A:194	
							ASP A:148	