STUDI *IN SILICO* AKTIVITAS SENYAWA DARI GENUS *ALPHITONIA* SEBAGAI ANTI-KANKER KOLOREKTAL MENGGUNAKAN *PLANTS*®

SKRIPSI

Untuk Memenuhi Persyaratan Dalam Rangka
Menyelesaikan Program Studi Sarjana Farmasi

Oleh

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PROGRAM STUDI SARJANA FARMASI
UNIVERSITAS BORNEO LESTARI
BANJARBARU

MEI 2024

PERNYATAAN

Dengan ini saya menyatakan bahwa dalam skripsi ini tidak terdapat karya yang pernah diajukan untuk memperoleh gelar kesarjanaan di suatu Perguruan Tinggi, dan sepanjang pengetahuan saya juga tidak terdapat karya atau pendapat yang pernah ditulis atau diterbitkan oleh orang lain, kecuali yang secara tertulis diacu dalam naskah ini dan disebutkan dalam Daftar Pustaka.

Banjarbaru, 23 April 2024

Rani Fatika Sari
NIM. SF20084

DAFTAR ISI

DAFTAR TABEL

Tabel Halaman

DAFTAR GAMBAR

Gambar Halaman

DAFTAR LAMPIRAN

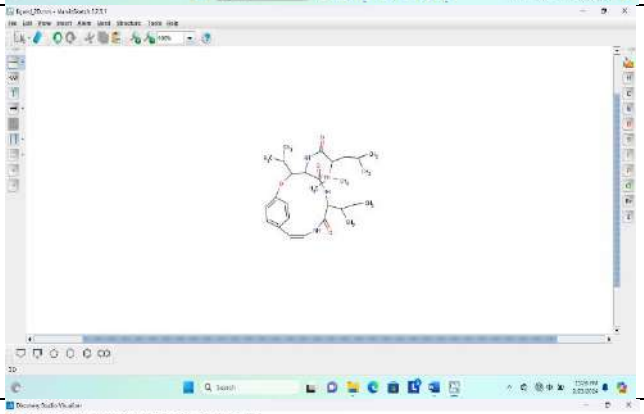
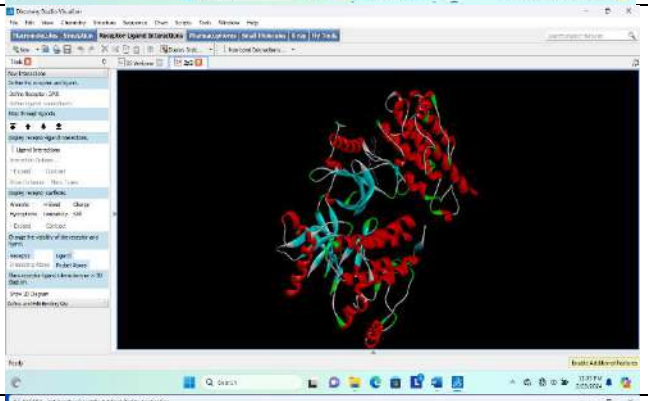
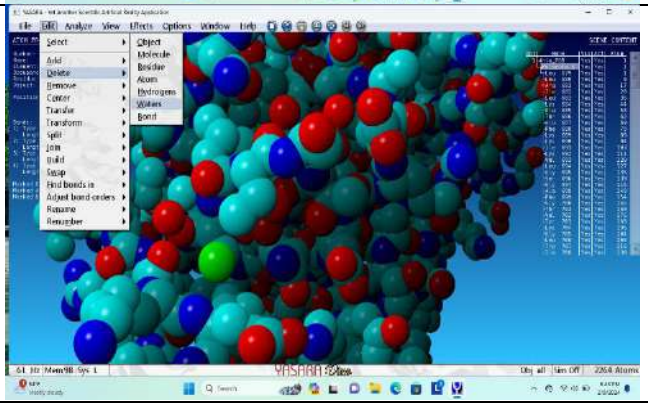
Lampiran Halaman

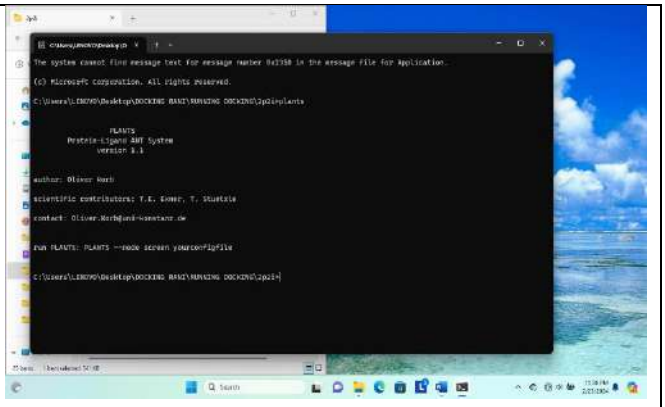
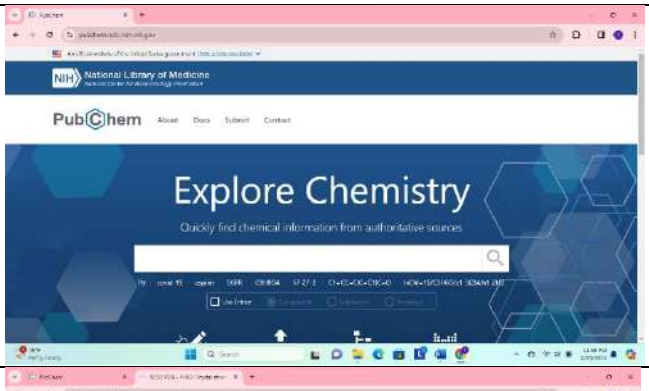
DAFTAR SINGKATAN

Singkatan	Kepanjangan
APR	: *Abdomino Perianal Resection*
CPT	: *carriage paid to*
DNA	: *Deoxyribo Nucleic Acid*
EGFR	: *Epidermal Growth Factor Receptor*
FAP	: *Familial Adenomatous Polyposis*
FDA	: *Food and Drug Administration*
FOLFIRI	: 5-fluorouracil, Leucovorin dan Irinotecan
GIST	: *Gastro Intestinal Stromal Tumor*
Gy	: Gray
HNPCC	: *Hereditary Nonpolyposis Colorectal Cancer*
KKR	: Kanker Kolorektal
KRAS	: *Kirsten Rat Sarcoma*
LAR	: *Low Anterior Resection*
MAPK	: *mitogen activated protein kinase*
PDB	: Protein Data Bank
PI3K	: *phosphoinositide 3-kinase inhibitors*
PLANTS	: *Protein-Ligan ANT System*
PTEN/AKT	: *phospatase and tensin homolog/threonin kinase*
RAF	: *rapidly accelerated fibrosarcoma*
RMSD	: *Root Mean Square Deviation*
SRC	: *Steroid Receptor Coactivator*
TGFα	: *Transforming Growth Factor α*
TKR	: *Tirosin Kinase Receptor*
TP	: Timidin Fosforilase
VEGFR	: *Vascular Endothelial Growth Factor Receptor*

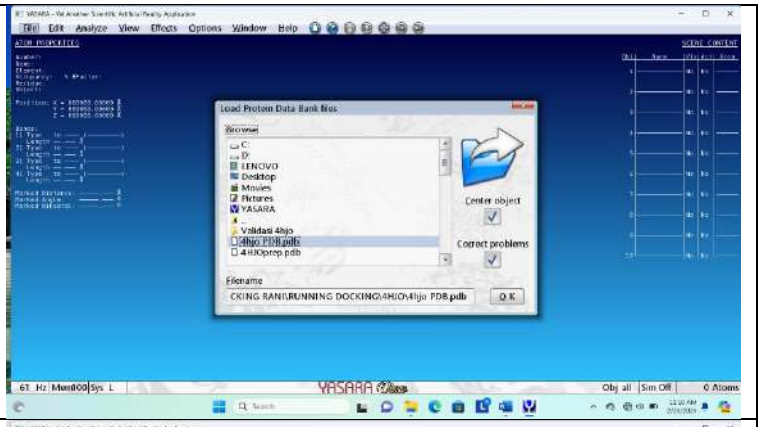
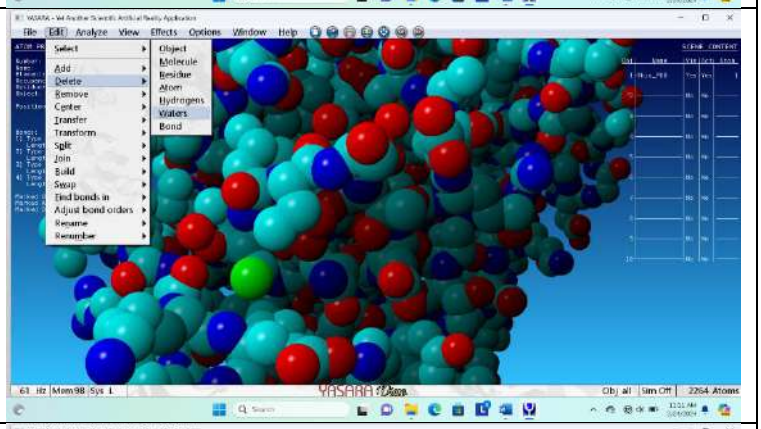
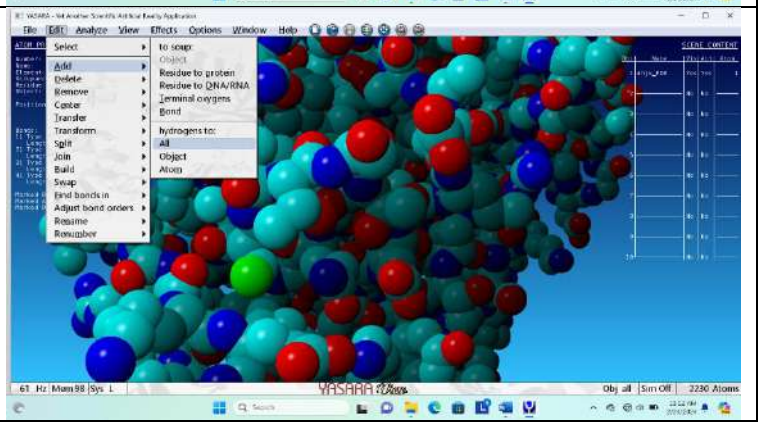
LAMPIRAN

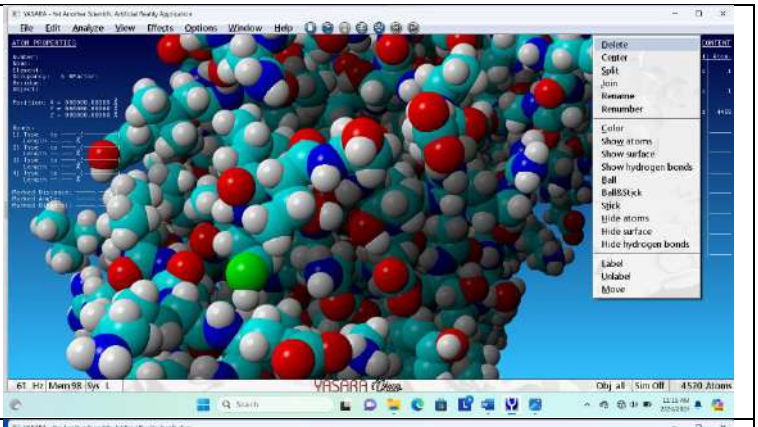
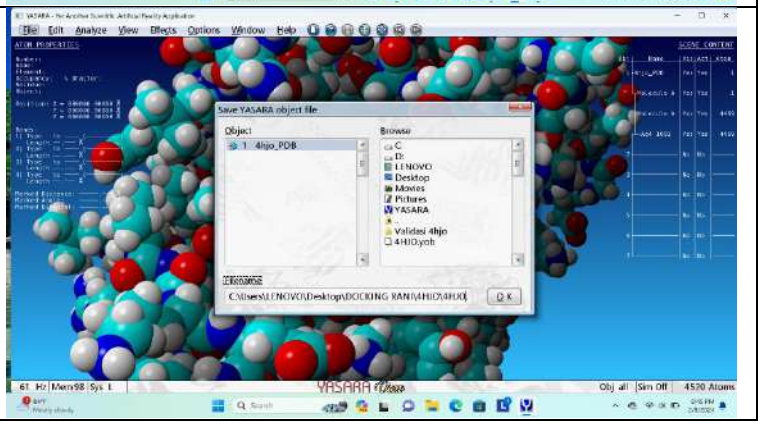
Lampiran 1. Aplikasi dan Web Penunjang yang Digunakan

Icon Aplikasi		
Dalam Aplikasi	*Marvin Sketch*	
	Discovery Studio	
	Yasara	

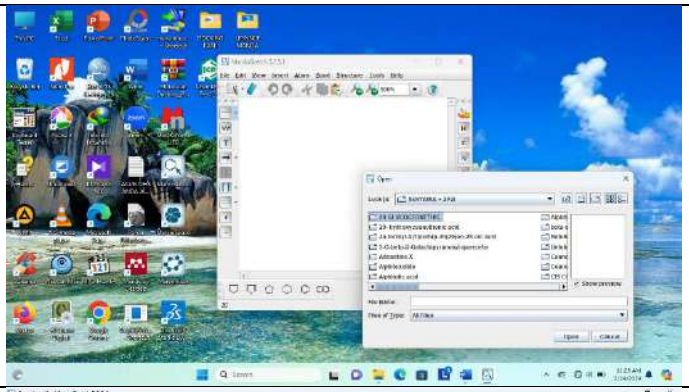
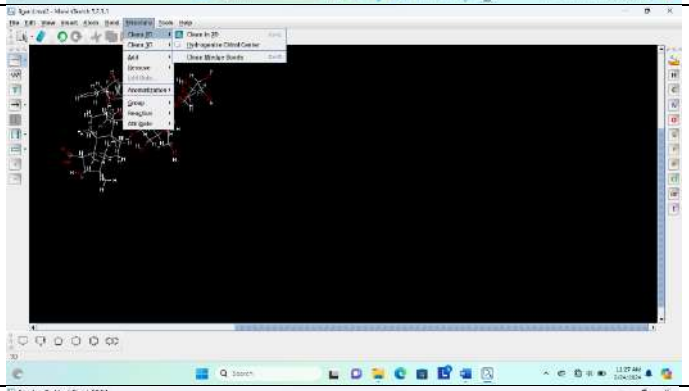
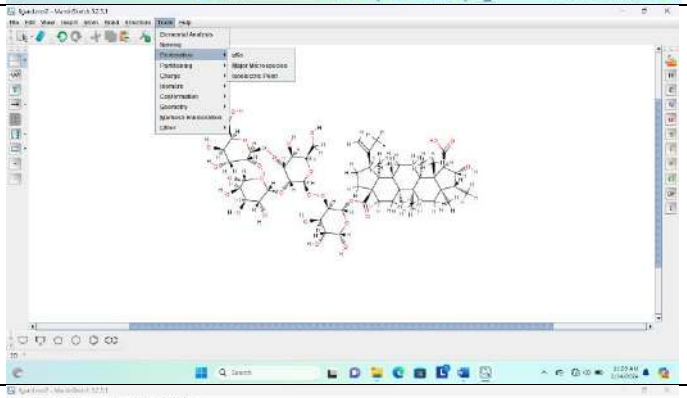
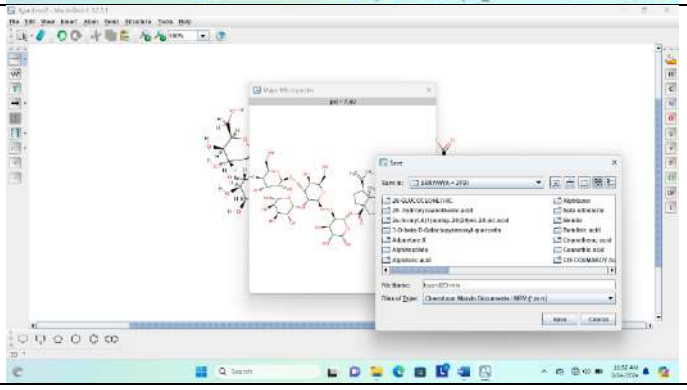
	PLANTS	
Web Penunjang	Pubchem	
	PDB	
	Uji *Lipinski*	

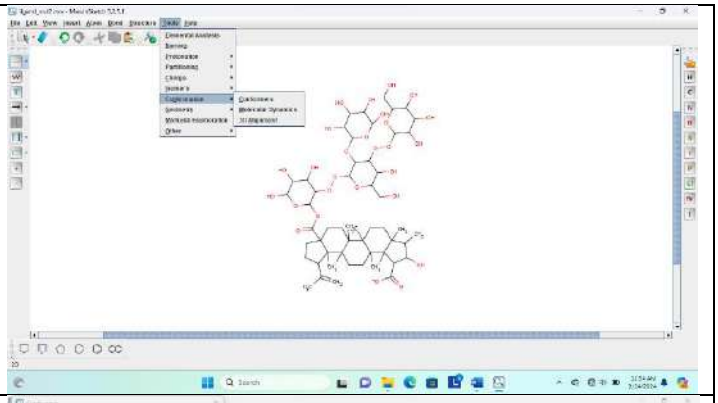
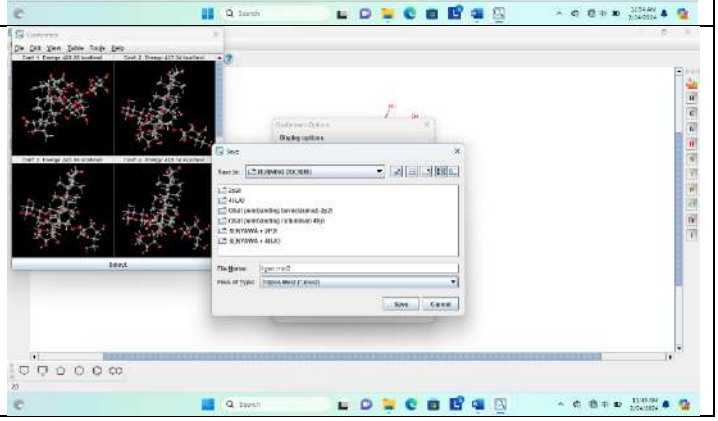
Lampiran 2. Tahapan Preparasi Protein dan *Native Ligand*

Load File Protein	
Penghapusan Air	
Penambahan Hidrogen	

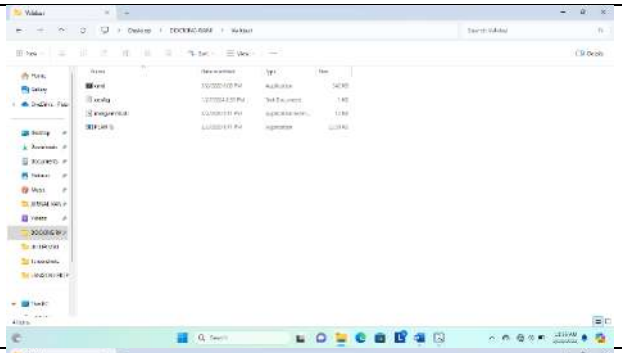
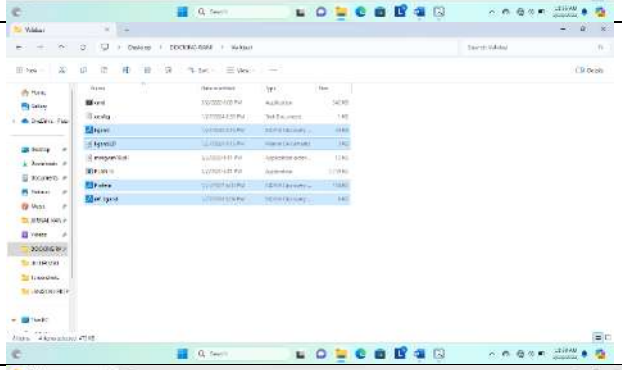
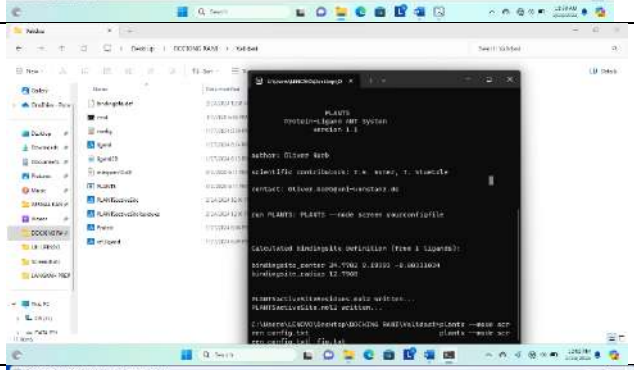
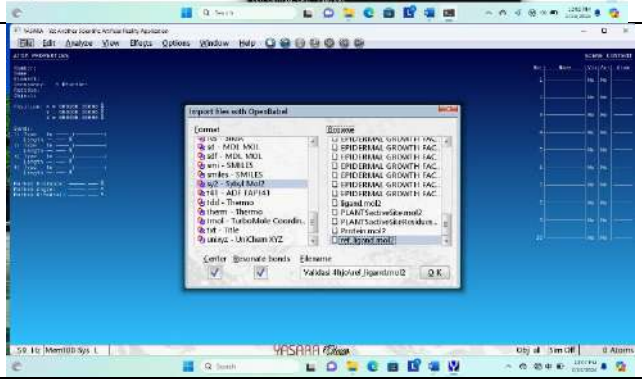
Penghapusan Rantai yang tidak digunakan (Preparasi Protein); Penghapusan protein (sisakan *native ligand*)	
Penyimpanan Hasil Preparasi	

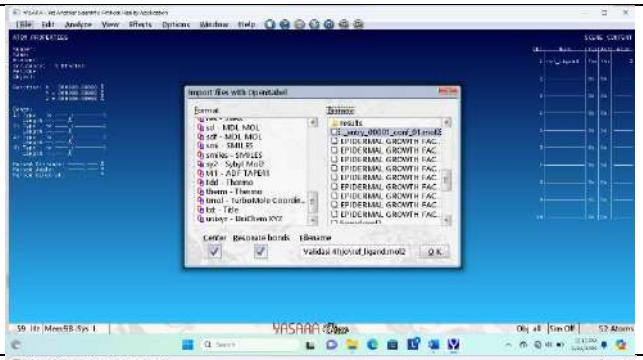
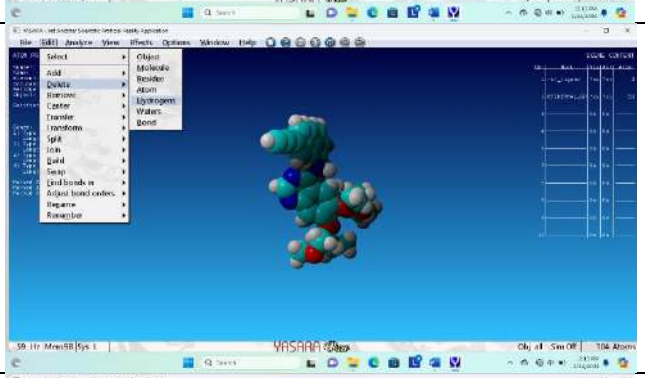
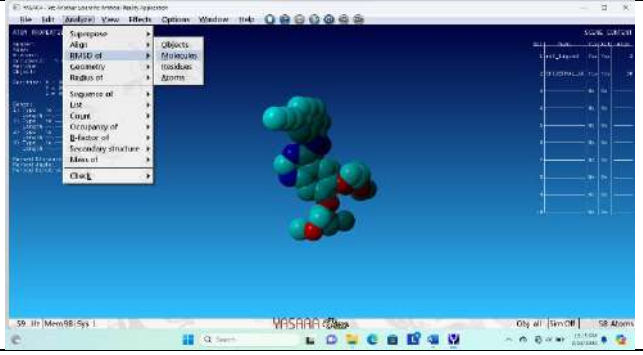
Lampiran 3. Tahapan Preparasi Ligand Senyawa Pembanding dan Senyawa Uji

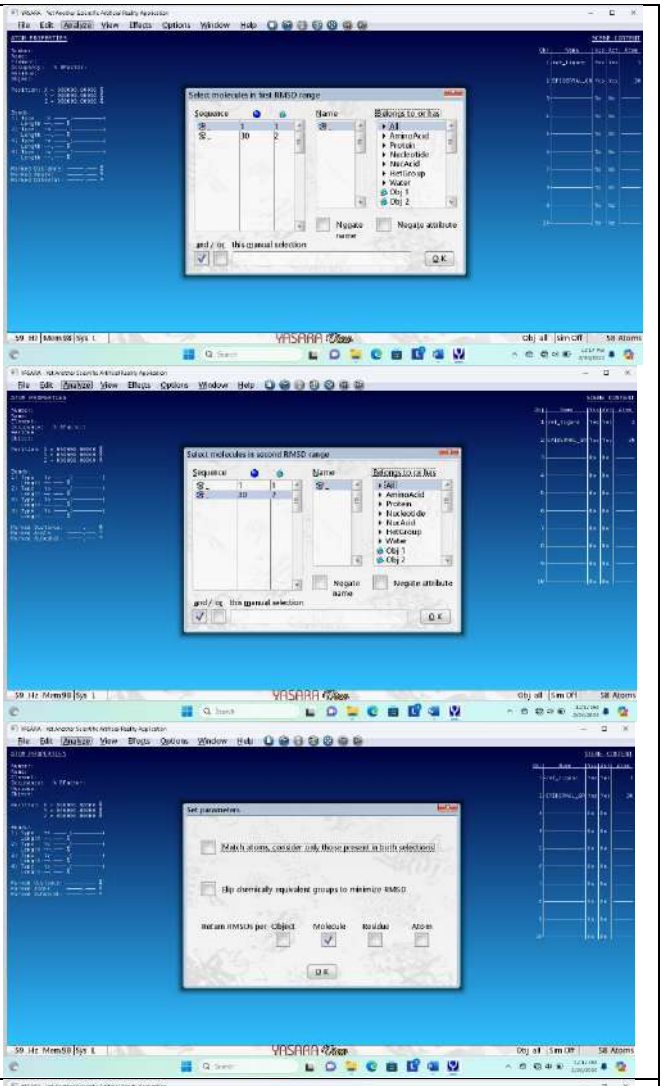
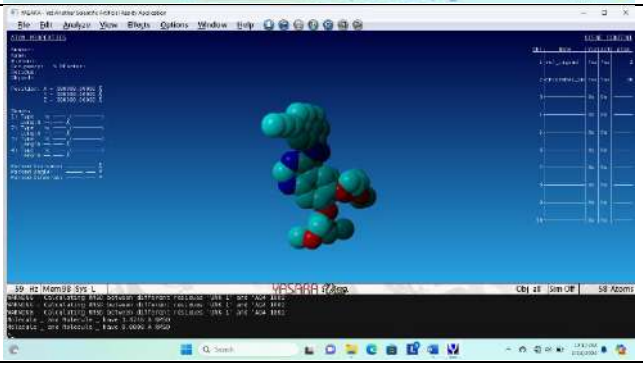
Buka *Marvin Sketch*, Load File Protein/Gambar Struktur Ligan	
Clean 2D ligand	
Protonasi di PH 7,4	
Simpan Hasil Preparasi dengan Nama ligand2D.mrv	

Pembuatan Konformasi	
Penyimpanan Hasil Konformasi dengan nama ligan.mol2	

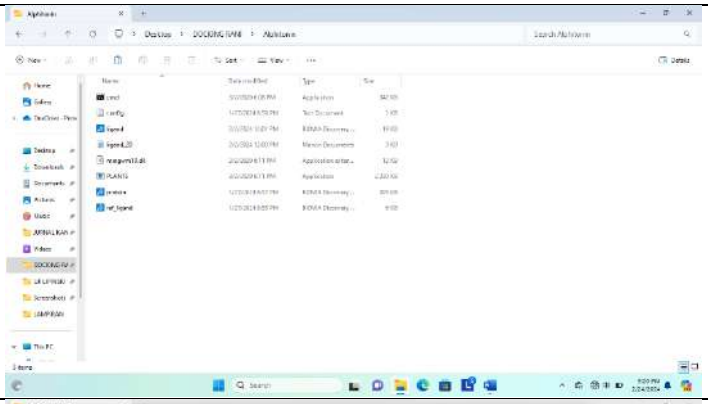
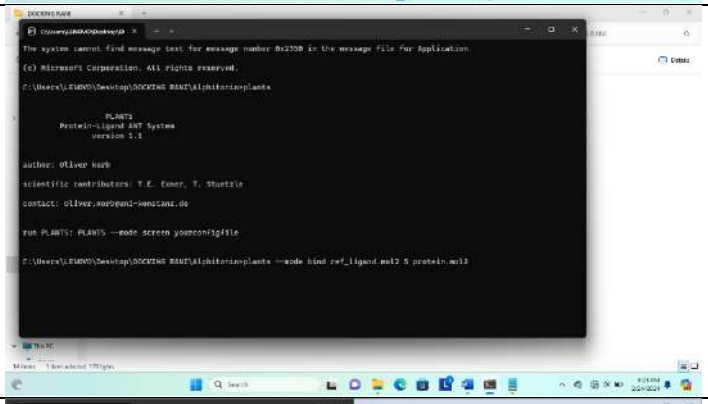
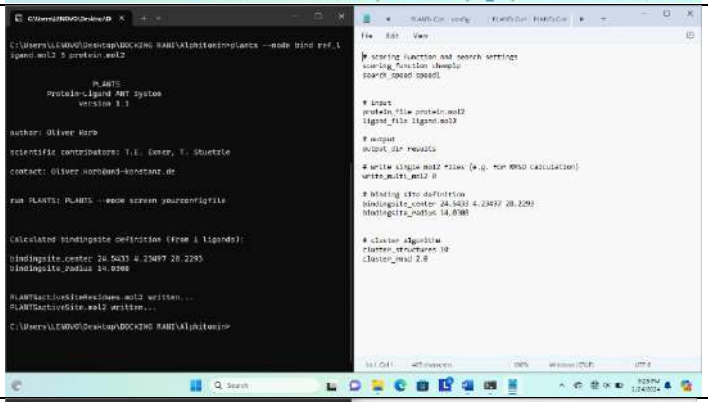
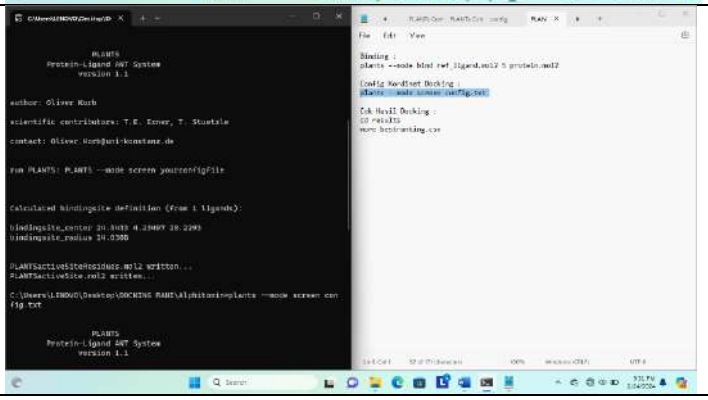
Lampiran 4. Tahapan Validasi Protein dan Penetapan RMSD

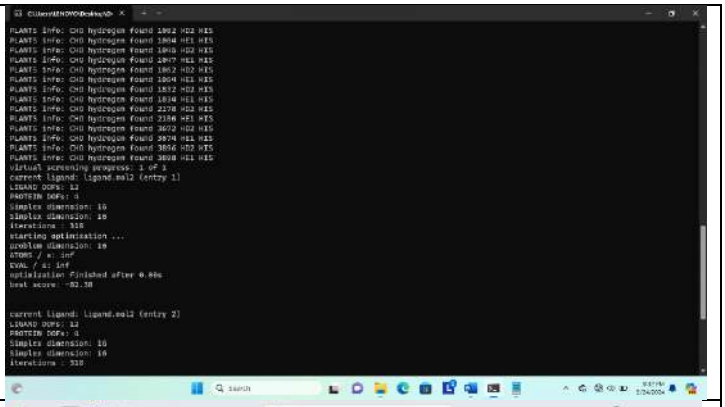
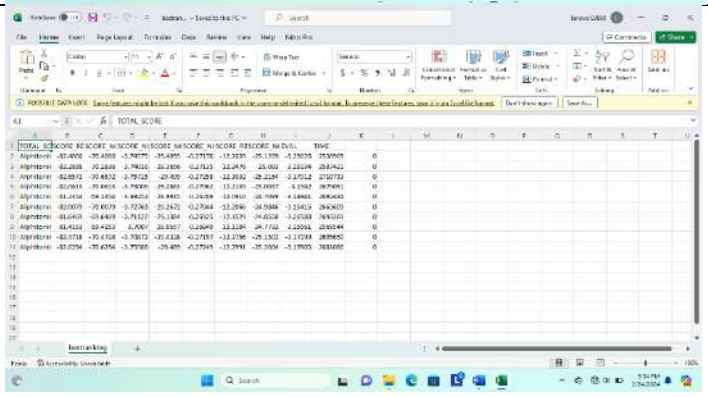
Validasi Protein	Siapkan Folder Untuk Validasi Protein dengan PLANTS	
	Masukkan ke Folder File Protein dan *Ligand Native* yang sudah dipreparasi	
	Docking Senyawa *Native Ligand* dengan PLANTS	
Penetapan RMSD	Load File ref_ligand.mol2	

	Load *ligand native* hasil docking	
	Hapus Hydrogen	
	Klik analys kemudian RMSD of molecules	

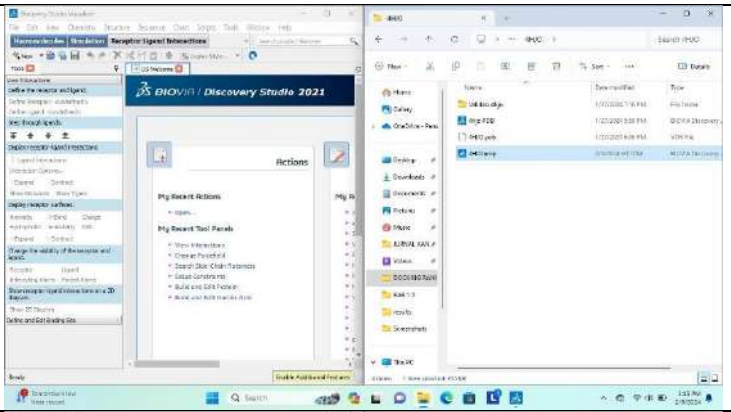
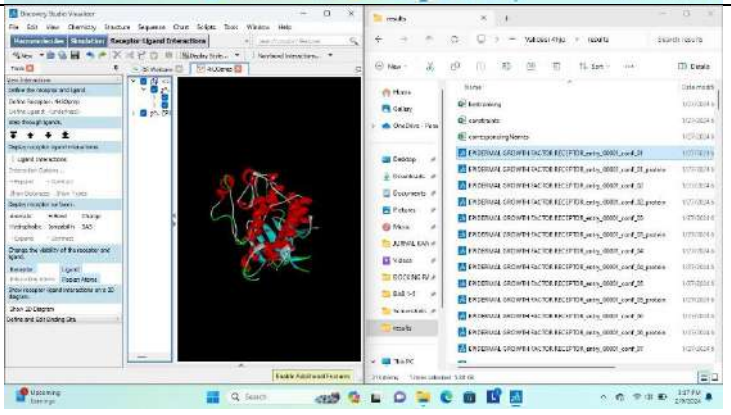
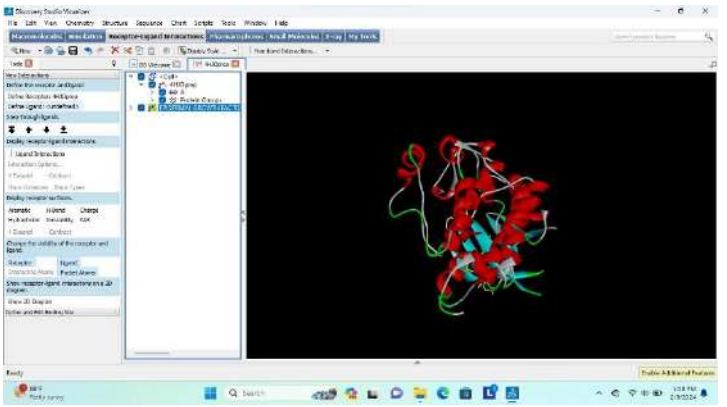
	Sesuaikan Parameter	
	Lihat Hasil	

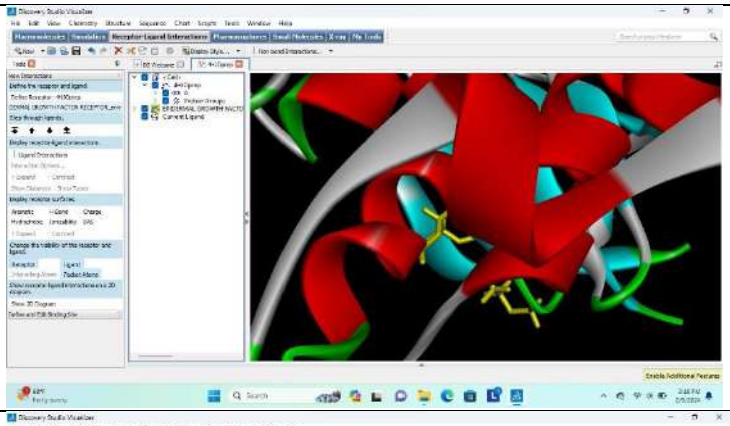
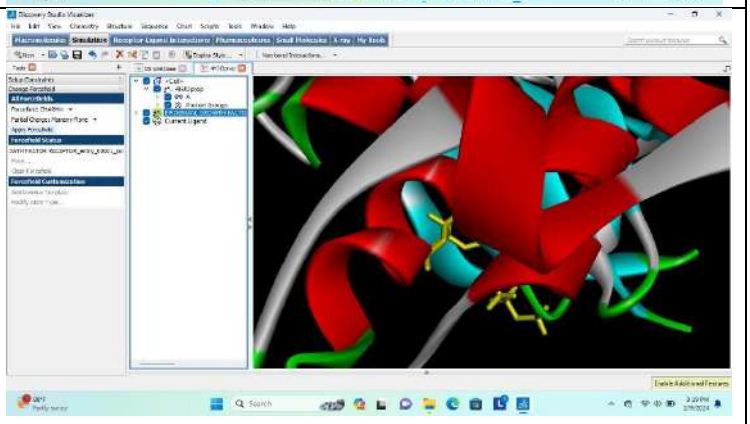
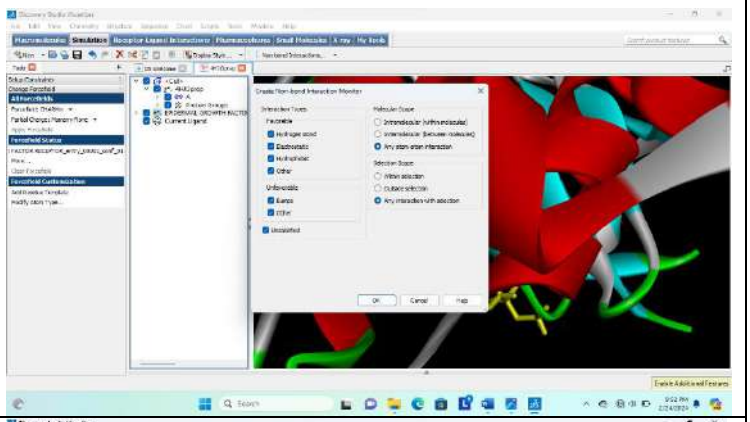
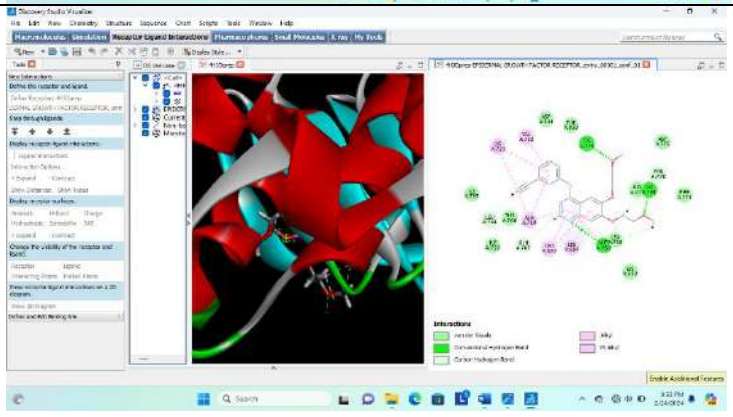
Lampiran 5. Tahapan Docking Senyawa

Siapkan Folder dan File	
Masukkan perintah “plants—mode bind ref_ligand.mol2 5 protein.mol2”	
Ubah Kordinat protein di File Config dengan di layer plants	
Masukkan perintah “plants==mode screen config.txt”	

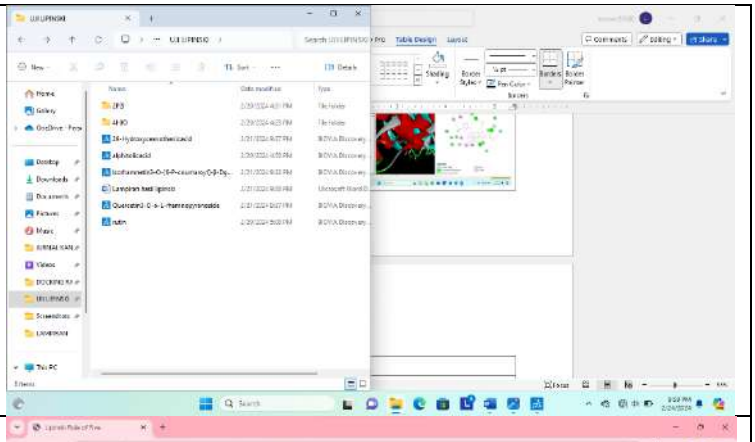
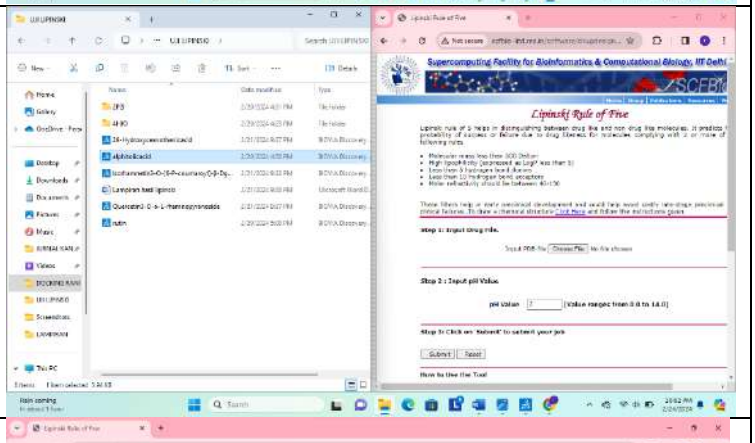
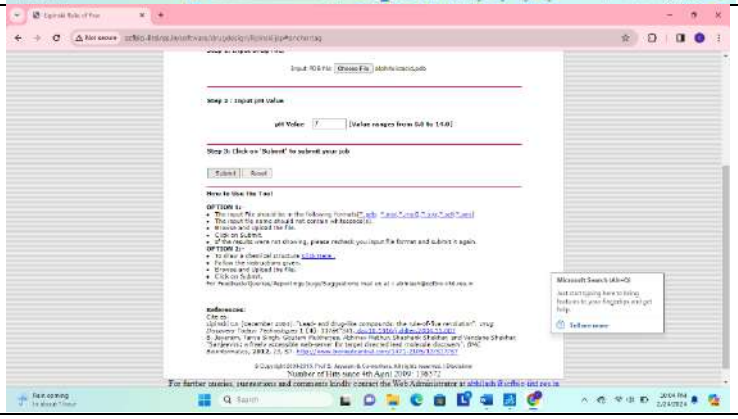
Tunggu Proses *Docking*	
Lihat Hasil di Folder “result/best ranking”	

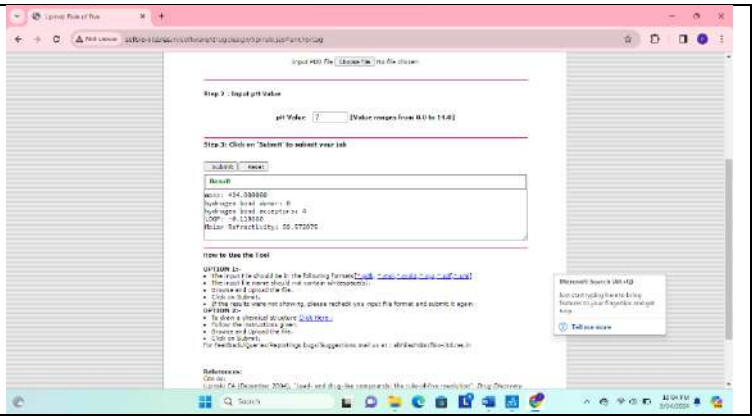
Lampiran 6. Tahapan Visualisasi Ikatan Senyawa dan Protein

Load File Protein	
Insert *Ligand*	 

	
Atur Parameter	 
Show 2D	

Lampiran 7. Tahapan Uji Lipinski

Siapkan Ligand Dalam Bentuk .pdb	
Buka Website Uji *Lipinski*	
Pilih File *Ligand*	
Submit	

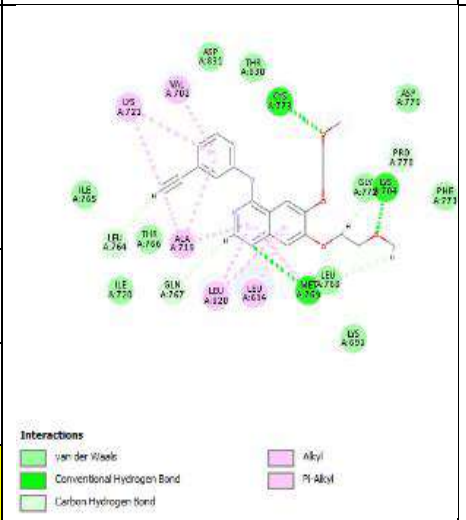
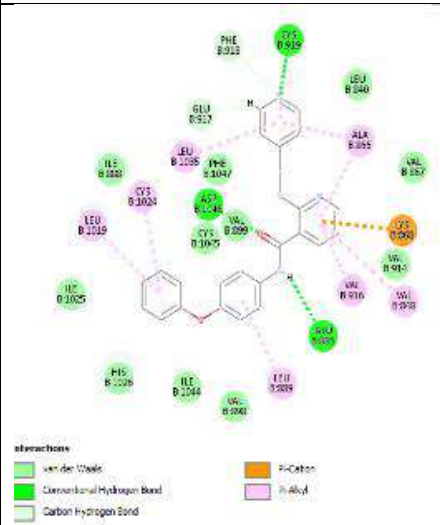
Cek Result	

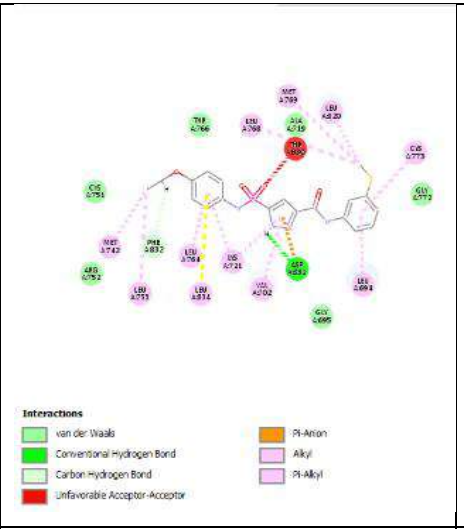
Lampiran 8. Hasil RMSD Protein Kanker Kolorektal

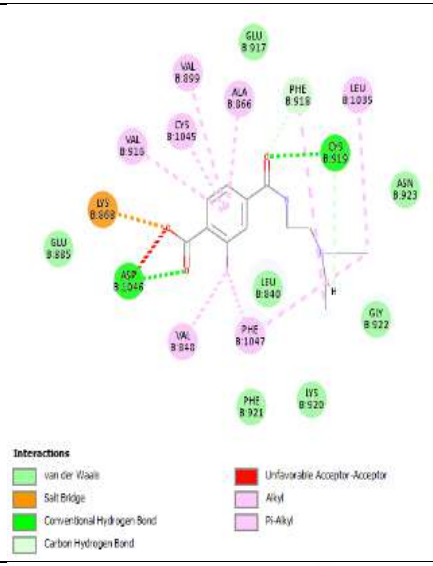
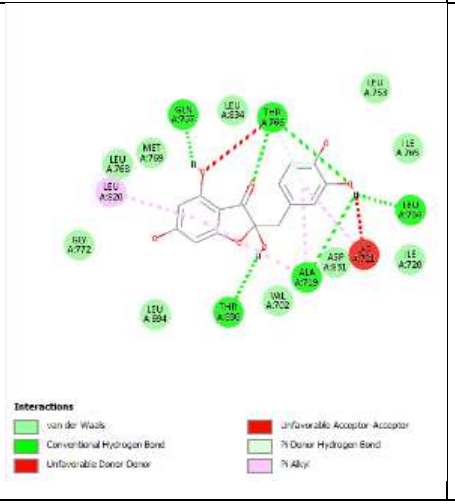
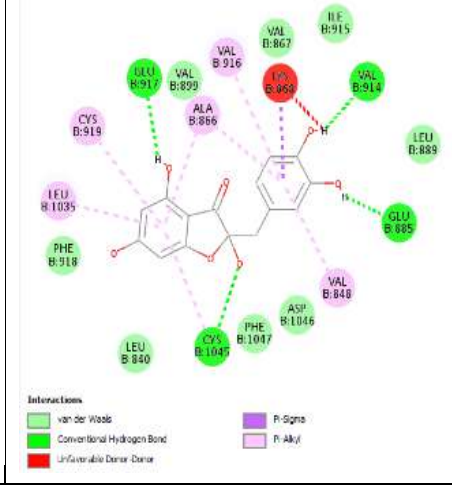
Protein (Reseptor)	Konformasi	Skor Docking	RMSD
4HJO	1	-103.046	1.4746
(Epidermal Growth	2	-103.022	1.4720
Factor Reseptor)	3	-102.489	1.5304
	4	-102.611	1.4335
	5	-102.363	1.4688
	6	-102.969	1.4942
	7	-102.671	1.4658
	8	-100.297	1.9648
	9	-101.972	1.4679
	10	-102.529	1.5809
2P2I	1	-113.492	1.0514
(Vascular Endothelial	2	-111.546	0.8169
Growth Factor	3	-115.511	1.5294
Receptor)	4	-119.197	1.4272
	5	-116.343	1.0921
	6	-115.201	1.0961
	7	-117.339	1.1748
	8	-112.438	1.3510
	9	-118.818	1.0809
	10	-117.435	1.2152

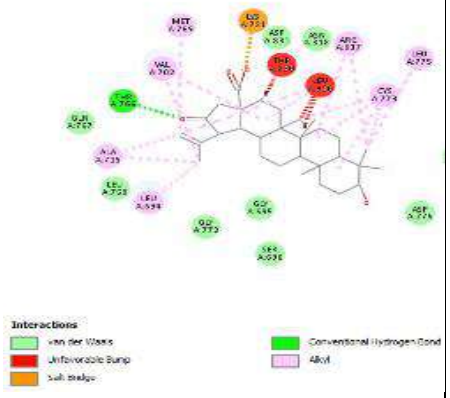
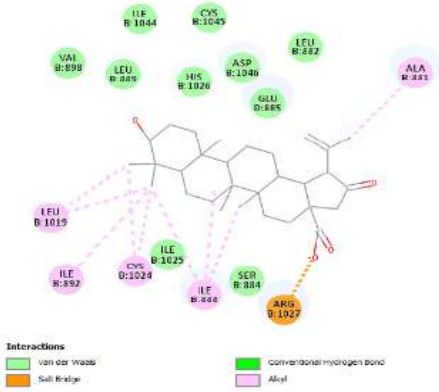
Keterangan : Nilai yang terpilih dan memenuhi parameter RMSD <2

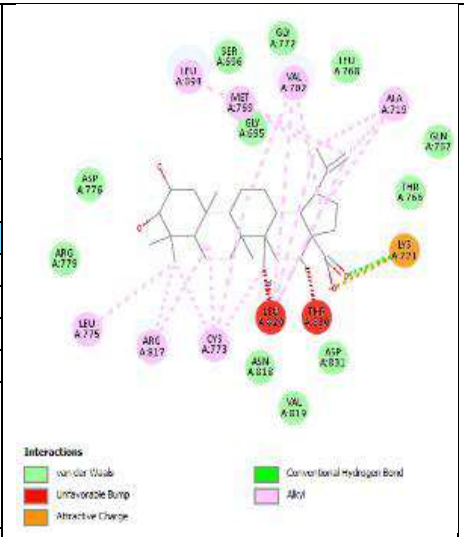
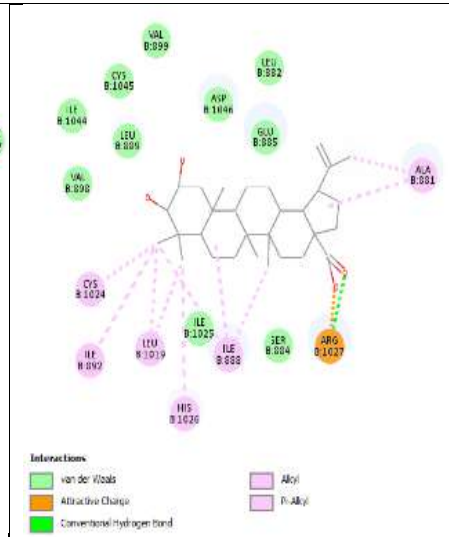
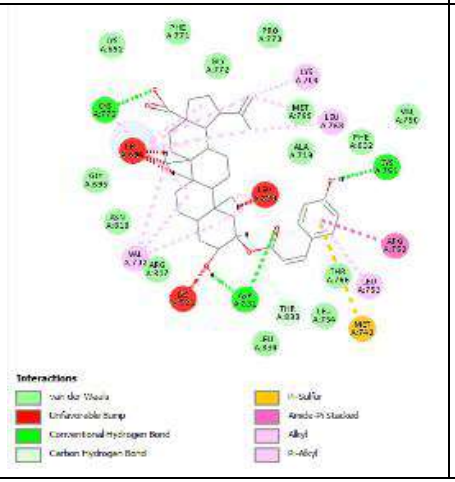
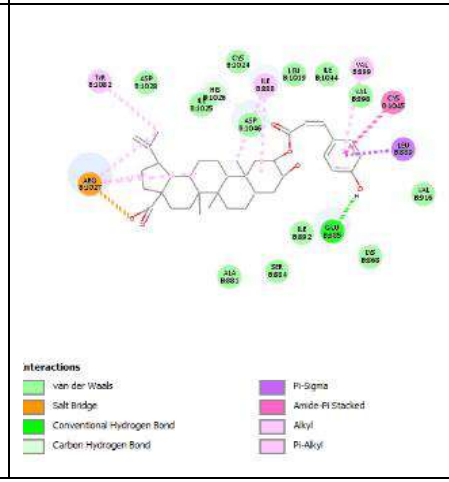
Lampiran 9. Hasil Docking, Visualisasi, dan Residu Asam Amino Senyawa Genus *Alphitonia*

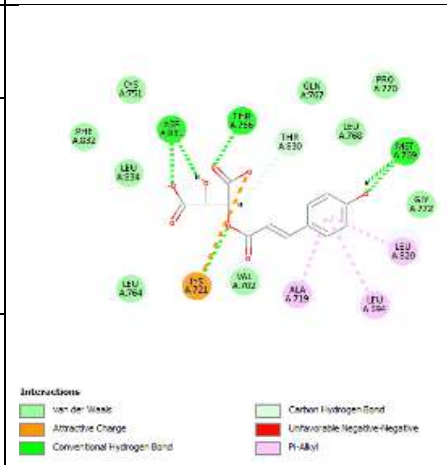
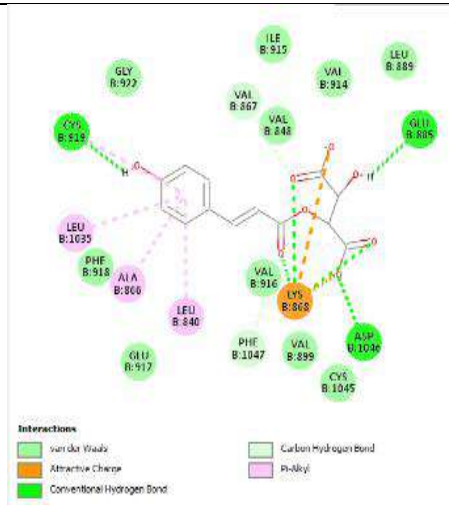
No	Senyawa/ Ligand	Conformer	Protein		Visualisasi		Residu Asam Amino	
			4HJO	2P2I	4HJO	2P2I	4HJO	2P2I
1	*Native*	1	-103.046	-113.492			LYS A:721 | VAL A:702 | ALA A:719 | LEU A:820 | LEU A:694	CYS B:1024 | LEU B:1019 | LEU B:1035 | ALA B:866 | VAL B:916 | VAL B:848 | LEU B:889
		2	-103.022	-111.546			LEU A: 764 | GLN A: 767	PHE B:918 | GLU B:917
		3	-102.489	-115.511			CYS A:773 | MET A:769 | LYS A:704	CYS B: 919 | GLU B: 885
		4	-102.611	-119.197			LEU A: 768 | GLY A: 772	VAL B: 899
		5	-102.363	-116.343				
		6	-102.969	-115.201				
		7	-102.671	-117.339				
		8	-100.297	-112.438				
		9	-101.972	-118.818				
		10	-102.529	-117.435				
2	Cetuximab	1	-100.435	-		-	LEU A:768 | MET A:769 | LEU A:820 | CYS A:773 | LEU A:694 |	-

							MET A:742 | LEU A: 753 | LEU A:764 | LEU A:834 | LYS A:721 | VAL A:702 LEU A: 694	
		2	-102.208	-			ASP A:831	-
		3	-96.5392	-			PHE A:832	-
		4	-96.5	-			THP A:830	-
		5	-101.637	-				-
		6	-99.8231	-				-
		7	-102.28	-				-
		8	-103.618	-				-
		9	-100.211	-				-
		10	-98.2228	-				-
3	Bevacizumab	1	-	-82.5468	-		-	ALA B:866 | CYS B:1045 | VAL B:916 | VAL B:899 | LEU B:1035 | PHE B:1047 | VAL B:848
		2	-	-82.8146			-	CYS B: 919 | ASP B:1046
		3	-	-83.0241			-	LYS B:868
		4	-	-83.0043			-	PHE B:918
		5	-	-82.7775			-	
		6	-	-83.0624			-	

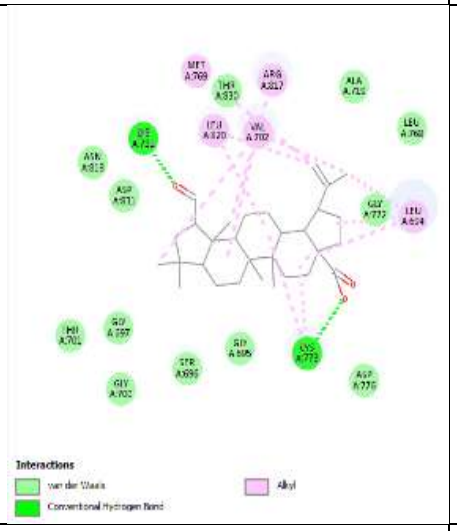
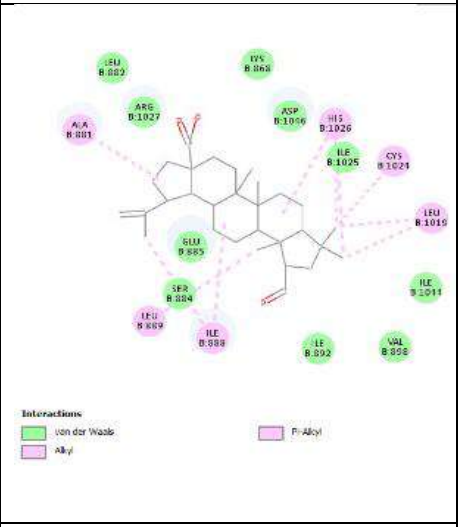
		7	-	-82.4448			-	
		8	-	-81.5948			-	
		9	-	-83.1842			-	
		10	-	-82.2371			-	
4	*Alphitonin*	1	-86.0803	-82.4066			THR A:766	GLU B: 917 | VAL B: 914 | GLU B: 885 | CYS B: 1045
		2	-86.202	-82.2836			THR A: 830 | GLN A: 767 | THR A: 766 | LEU A: 764 | ALA A: 719	ALA B: 866 | CYS B:919 | LEU B: 1035 | VAL B: 848 | VAL B: 916
		3	-86.0102	-82.6572			LEU A:820	LYS B: 868
		4	-85.8695	-82.0613			LYS A:721	LYS B: 868
		5	-85.659	-81.2354				

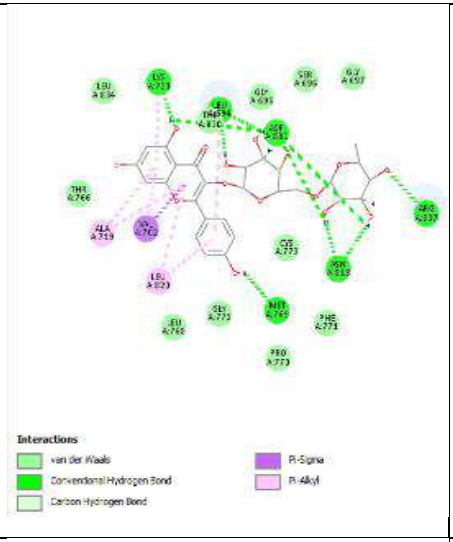
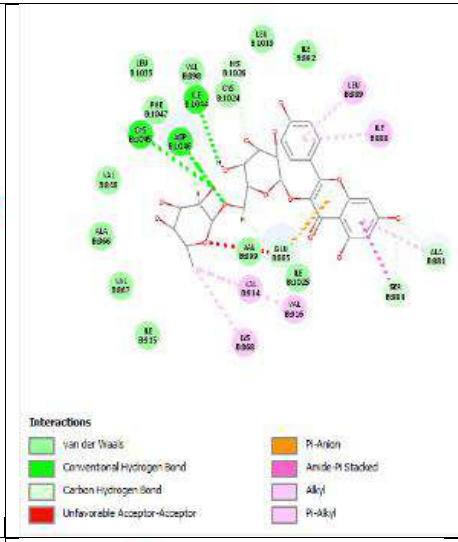
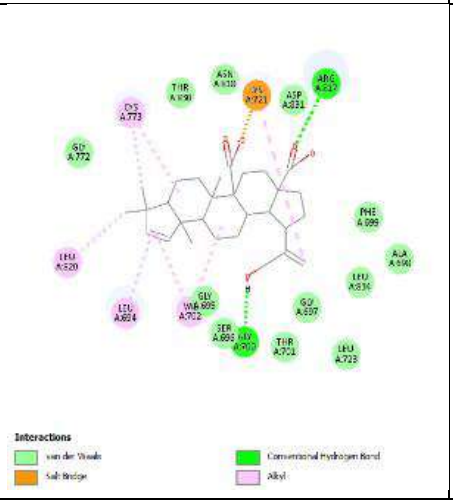
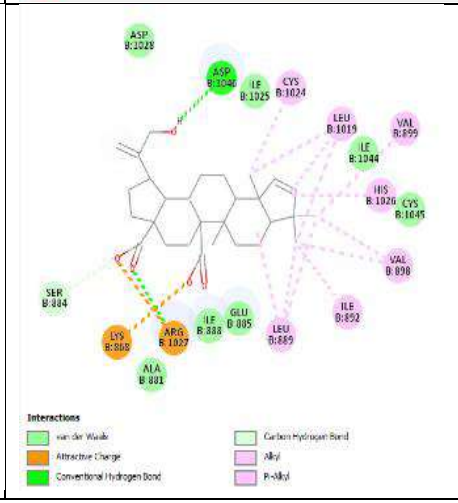
		6	-86.0733	-82.0079				
		7	-86.0323	-81.6469				
		8	-85.8145	-81.4153				
		9	-85.9173	-82.4718				
		10	-85.9905	-82.6294				
5	*2-Ketobetulinic acid*	1	-67.634	-73.7887			THR A: 766	ARG B: 1027
		2	-68.9177	-72.2763			ALA A:719 | ARG A: 817 | CYS A: 773 | LEU A: 775 | LEU A:694 | MET A: 769 | VAL A: 702	ALA B: 881 | CYS B: 1024 | ILE B: 888 | ILE B: 892 | LEU B: 1019
		3	-65.3384	-73.8581			LYS A: 721	
		4	-67.1968	-73.1844			THR A: 830 | LEU A:820	
		5	-65.6779	-74.0362				
		6	-64.237	-72.3278				
		7	-63.6233	-72.1531				
		8	-64.5664	-71.5721				
		9	-65.6164	-73.0385				
		10	-64.1166	-71.6005				
6	*Alphitolic acid*	1	-66.9985	-74.2965			LYS A: 721	ARG B: 1027
		2	-66.9249	-74.1826			THR A: 830 | LEU A: 820	ALA A: 881 | CYS B: 1024 | ILE B: 892 | ILE

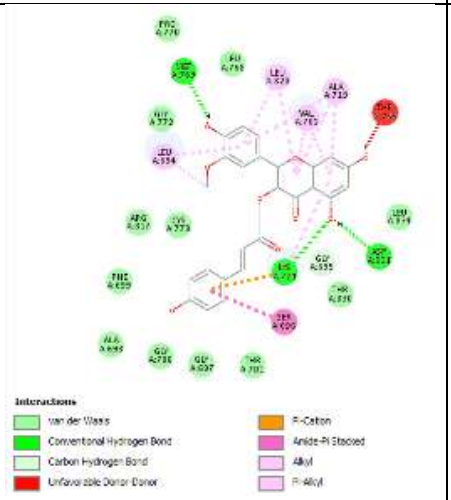
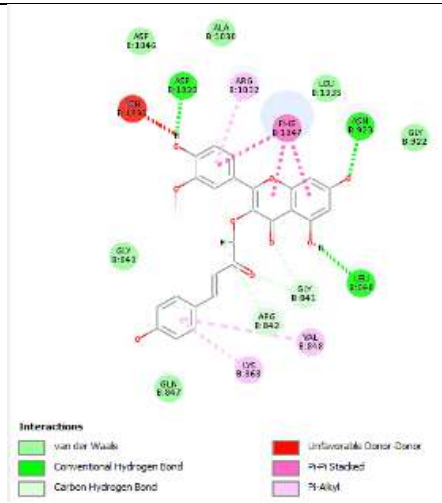
								B: 888 | LEU B: 1019 | HIS B: 1026
		3	-68.411	-73.4419			ALA A:719 | ARG A: 817 | CYS A: 773 | LEU A: 775 | LEU A: 694 | MET A: 769 | VAL A: 702	ARG B: 1027
		4	-67.3483	-74.4963				
		5	-66.9935	-74.0681				
		6	-67.8034	-74.384				
		7	-67.9811	-72.7907				
		8	-67.0314	-74.1228				
		9	-68.7571	-71.7842				
		10	-67.5214	-74.2374			LYS A: 721	
7	*3-O-Cis-p-Coumaroyl aphitolic acid*	1	-87.6377	-85.0584			CYS A: 751 | CYS A:773 | ASP A: 831	GLU B:885
		2	-86.79	-88.3605				ARG B:1027
		3	-88.2855	-85.9986				HIS B:1026
		4	-86.0648	-88.7478				CYS B:1045
		5	-93.266	-87.2428			LEU A: 820 | LEU A: 694 | LYS A:721	VAL B:899 | TYR B:1082 | ILE B:888
		6	-84.8468	-88.4604				LEU B:889
		7	-84.7635	-88.6802				
		8	-90.8286	-88.5672			ARG A: 752	
		9	-82.7416	-83.6603			THR A: 830	
		10	-82.8859	-82.4549			LEU A: 753 | LEU	

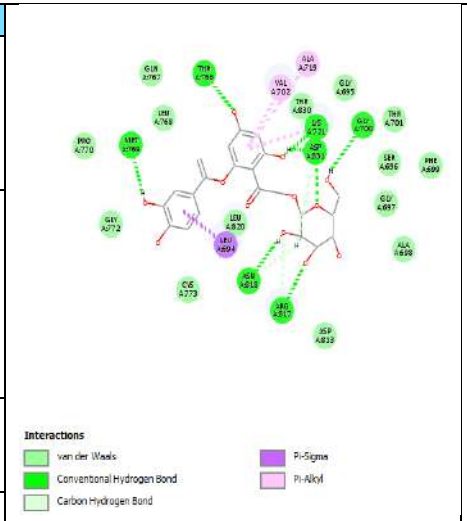
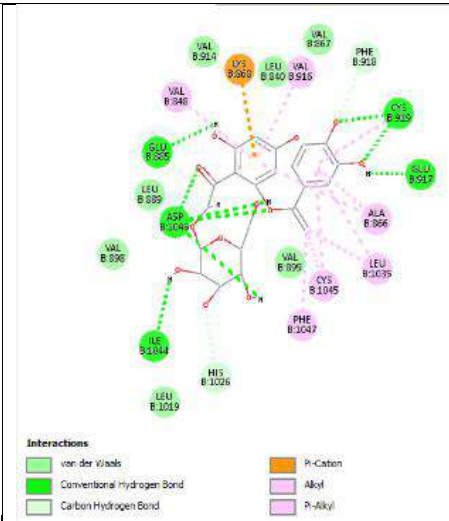
							A:768 | LYS A:704 | VAL A: 702	
8	*3-O-p-Trans-7-Coumaroyl aphitolic acid*	1	-84.1539	-82.4614			THR A: 830	CYS B:919 GLU B:885 ASP B:1046
		2	-84.3599	-82.9554			ASP A: 831 | MET A: 769 | THR A: 766 | LYS A: 721	LYS B:868
		3	-88.6126	-79.2032			ALA A: 719 | LEU A: 694 | LEU A: 820	LEU B:1035 ALA B:866 LEU B:840
		4	-88.5996	-78.309			LYS A: 721	PHE B:1047 VAL B:867
		5	-88.7004	-78.5425				VAL B:848 VAL B:916
		6	-88.401	-75.172				
		7	-84.2853	-84.0819				
		8	-83.5137	-84.3679				
		9	-88.4057	-77.5611				
		10	-84.2864	-80.0858				
9	*Rutin*	1	-104.489	-78.788			ALA A:719 | LEU A:820	LYS B: 868
		2	-99.421	-76.6357			VAL A:702	ILE B: 1019 | ILE B: 892 | ILE
		3	-97.9603	-75.1807			MET A:769 LEU A:694	

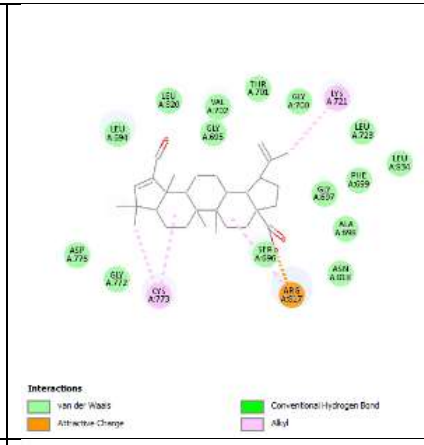
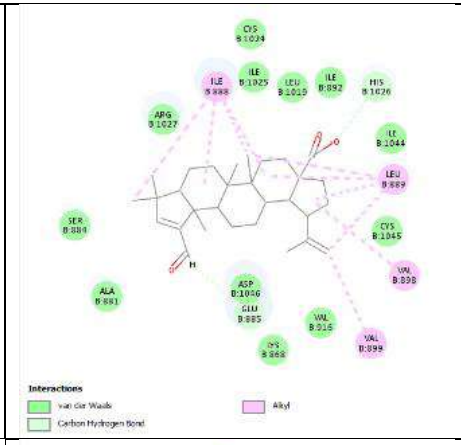
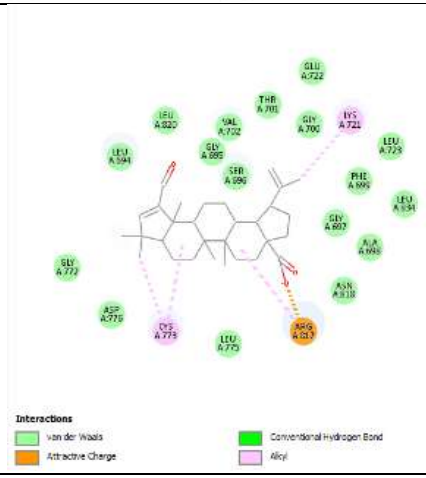
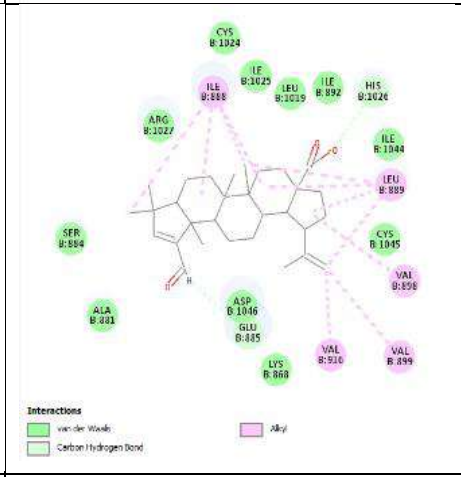
							ASP A:831 ASN A:818 LYS A:721	B: 888 | LEU B: 889 | LEU B:882
		4	-98.8269	-73.4409			ARG A:817 SER A:696	ILE B: 1025 | ASP B: 1046 | GLN B:847 | ME T B: 869
		5	-97.6836	-73.3849				ALA B: 881
		6	-100.31	-76.7891				
		7	-104.646	-81.0856				
		8	-98.8224	-76.4757				
		9	-99.7808	-75.1797				
		10	-98.5519	-80.8015				
10	*Stigmasterol*	1	-95.7533	-83.6522			ALA A:719 | CYS A: 773 | LEU A: 694 | LEU A: 834 | LYS A: 721 | VAL A: 702	ILE B:1025
		2	-94.6749	-79.6349				ILE B: 1025
		3	-96.0936	-83.5991				VAL B:899 VAL B:916 ILE B:888 LEU B:889 CYS B:1045 PHE B:1047 LEU B:1035 CYS B:1024 HIS B: 1026 | LEU B:1019
		4	-96.0782	-83.6963			LEU A: 820	
		5	-95.5731	-85.3837				
		6	-95.7595	-82.4836				

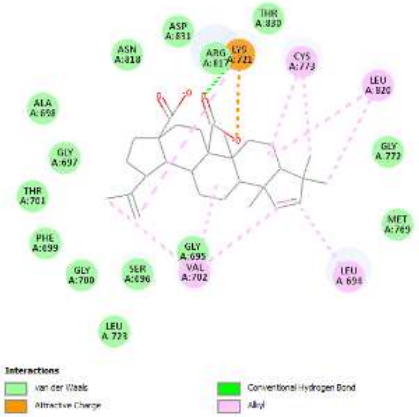
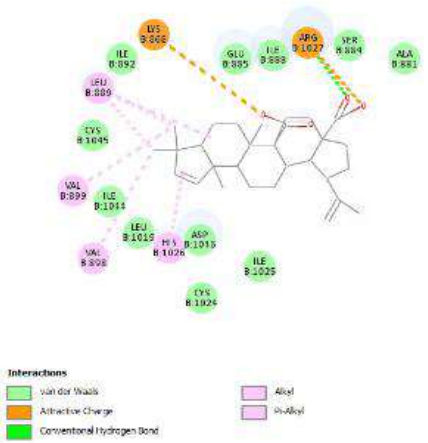
		7	-95.5554	-82.6402				
		8	-94.9074	-83.8036				
		9	-94.6798	-84.7883				
		10	-94.97	-80.9184				
11	*2α-Formyl-A(1)norlup-20 (29)-en-28- oic acid*	1	-63.8425	-65.297			CYS A: 773 | LYS A: 721	ALA B: 881 | CYS B:1024 | HIS B: 1026 | LEU B: 889 | LEU B:1019 | ILE B:888
		2	-64.8717	-65.1465			ARG A: 817 | LEU A: 694 | LEU A: 820 | MET A: 769 | VAL A: 702	
		3	-64.0649	-65.2696				
		4	-64.0966	-65.7025				
		5	-65.5495	-65.3963				
		6	-64.6864	-66.0064				
		7	-64.4113	-66.3795				
		8	-67.5873	-65.3946				
		9	-66.574	-65.1002				
		10	-64.7808	-63.0723				
12	*Kaempferol-3-rutinoside*	1	-96.6792	-81.0359			ALA A: 719 | LEU A:820	ILE B: 888 | LEU B: 889 | LYS B: 868 | VAL B: 916 | VAL B: 914
		2	-92.0206	-81.2006			ASN A: 818 | ARG A: 817 | ASP A: 831 | LEU A: 694 | LYS A: 721 | MET A: 769	ASP B: 1046 | CYS B: 1045 | ILE B: 1044
		3	-98.3471	-81.5223				
		4	-101.451	-81.1558				
		5	-90.0179	-81.6199			VAL A: 702	

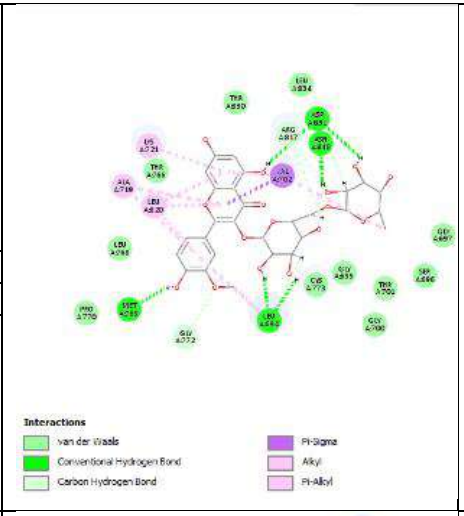
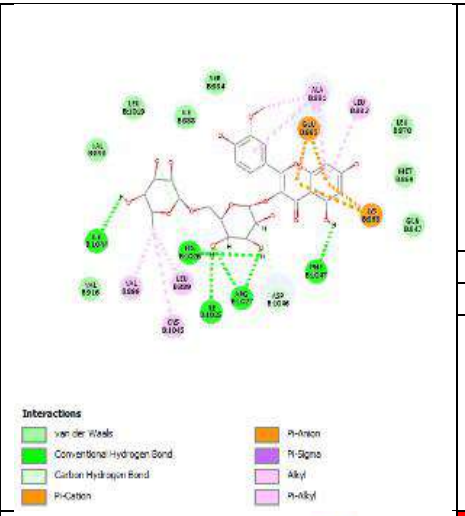
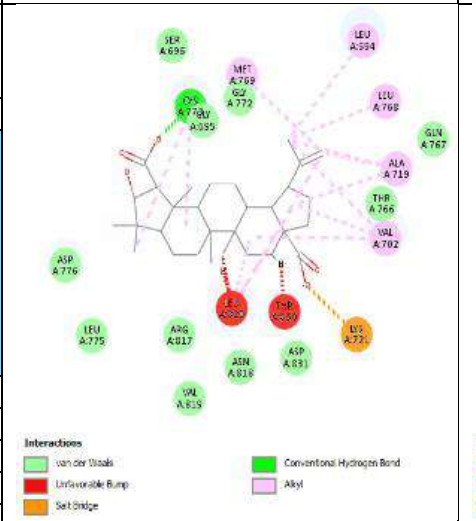
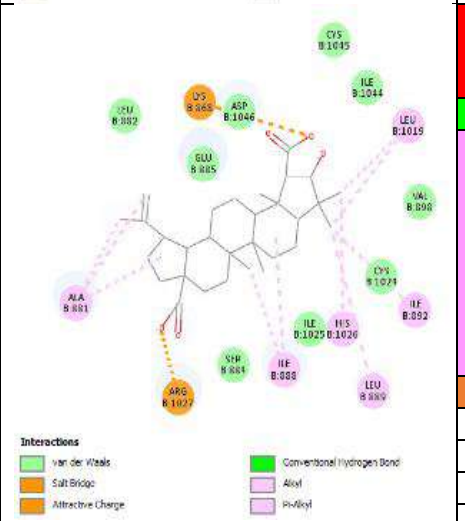
		6	-98.9981	-81.9695				ALA B: 881 | SER B: 884
		7	-94.6642	-81.9707				HIS B: 1026 | GLU B:885
		8	-96.2757	-82.0085				
		9	-95.9779	-78.5779				
		10	-99.4359	-71.3232				
13	*29-Hydroxyceanothenic acid*	1	-62.2838	-70.191			CYS A: 773 | LEU A: 820 | LEU A: 694 | VAL A: 702	CYS B: 1024 | LEU B: 1019 | VAL B: 899 | HIS B: 1026 | VAL B: 898 | ILE B: 892 | LEU B: 889
		2	-65.1637	-70.9446				
		3	-65.7841	-70.518				
		4	-65.6273	-71.0135			GLY A: 700 | ARG A: 817	ASP B: 1024
		5	-65.4392	-70.795				ARG B: 1027 | LYS B: 8

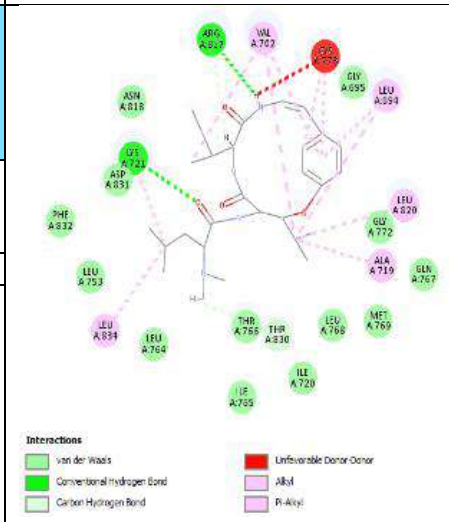
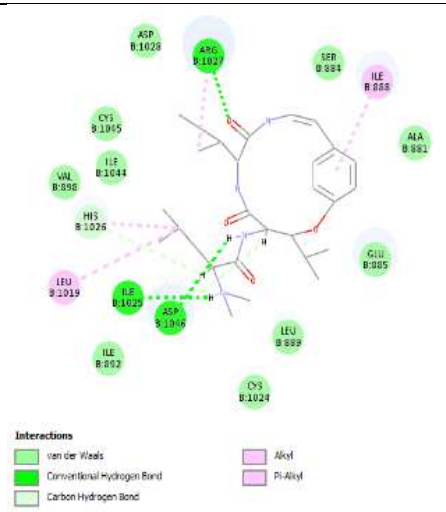
		6	-61.8453	-70.5191			LYS A: 721	SER B: 884
		7	-64.5875	-71.2725				
		8	-65.6295	-71.8428				
		9	-65.0515	-70.0557				
		10	-70.9519	-71.8839				
14	*Isorhamnetin3-O-[6-P-coumaroyl]- β –Dglucopyranoside*	1	-94.1843	-67.86			SER A: 696	GLY B: 841 | ARG B: 842
		2	-89.3218	-76.6866			ALA A: 719 | LEU A; 820 | LEU A: 694 | VAL A: 702	LEU B: 840 | ASN B: 923 | ASP B:1028
		3	-89.7033	-67.6864				
		4	-92.6322	-71.202				
		5	-92.2492	-71.7929			ASP A: 831 | LYS A: 721 | MET A: 769	PHE B: 1047
		6	-94.169	-77.4794			THR A: 766	ARG B: 1032 | LYS B: 868 | VAL B: 848
		7	-99.4354	-78.4724				
		8	-98.8743	-76.6659				
		9	-95.063	-77.3537				ASN B: 1033
		10	-97.1218	-76.7542				
15	*Quercetin 3-O-β-D-glucopyranoside*	1	-90.6375	-82.1864			ASN A: 818 | ARG A: 817 | ASP A: 831 | LYS A:	ASP B:1046 GLU B:885 CYS B:919 GLU B:917 ILE B:1044

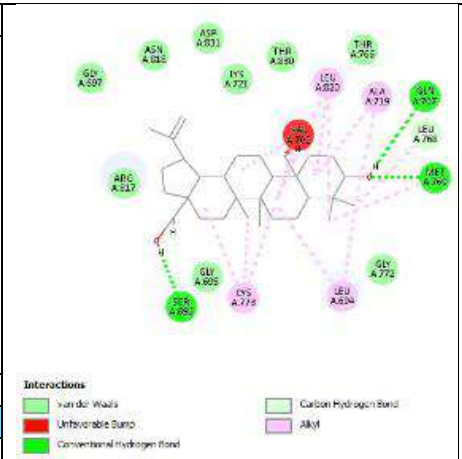
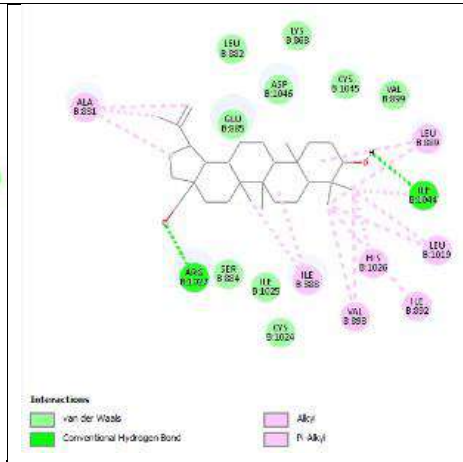
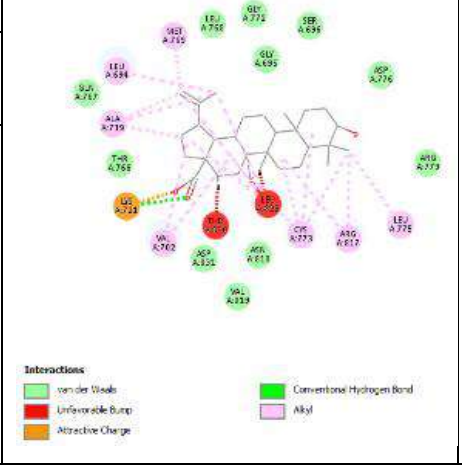
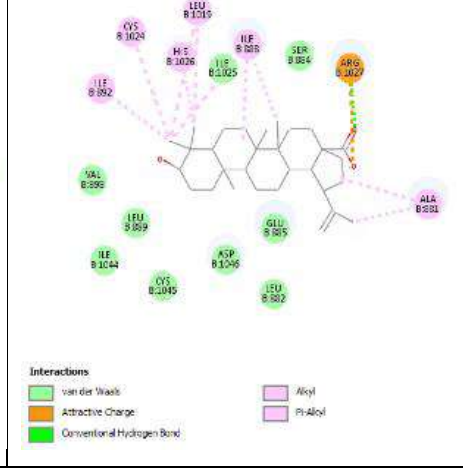
		2	-94.495	-88.3768			721 | GLY A: 700 | MET A: 769 | THR A: 766	LYS B:868 PHE B:918
		3	-97.6928	-82.8513				
		4	-97.2976	-82.1932			LEU A: 694	VAL B:916 VAL B:848 ALA B:866 LEU B:1035 CYS B:1045 PHE B:1047
		5	-96.1914	-87.2556			ALA A: 719 | VAL A: 702	
		6	-91.5309	-82.5479				
		7	-94.5005	-84.7332				
		8	-93.7521	-83.5942				
		9	-98.8391	-82.1786				
		10	-99.3072	-81.383				
16	*Quercetin 3-O-α-L-rhamnopyranoside*	1	-62.5748	-73.267			CYS A: 773 | LYS A: 721	VAL B: 898 | VAL B:899 | LEU B:889 | ILE B:888
		2	-62.0981	-71.974			ARG A: 817	
		3	-62.9055	-73.3643				
		4	-62.0243	-72.7641				
		5	-62.8054	-73.4887				HIS B: 1026 | GLU B: 885
		6	-63.8583	-72.2509				
		7	-62.3402	-72.4392				
		8	-62.4401	-72.2213				
		9	-63.7464	-71.9854				

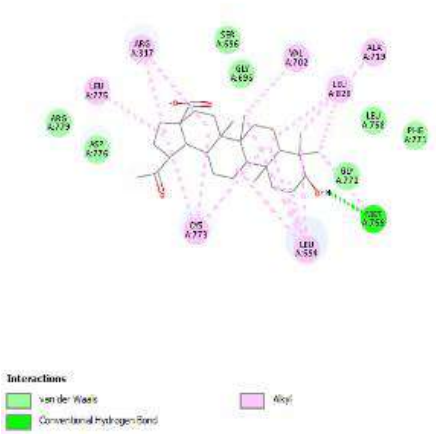
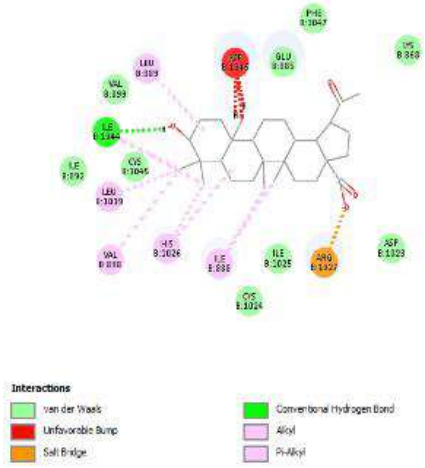
		10	-62.4672	-71.8779				
17	*Zizyberenalic acid*	1	-61.8626	-72.4532			ARG A: 817	LEU B: 889 | ILE B: 888 | VAL B: 916 | VAL B: 899 | VAL B: 898
		2	-61.9684	-73.1799			LYS A: 721 | CYS A: 773	
		3	-62.9595	-73.4741				
		4	-61.841	-72.3894				HIS B: 1026, GLU B: 885
		5	-62.2234	-72.8737				
		6	-62.3306	-72.626				
		7	-63.9997	-72.222				
		8	-64.2479	-72.4952				
		9	-62.6185	-72.4685				
		10	-62.4948	-72.1486				
18	*Ceanothenic acid*	1	-62.7768	-70.099			CYS A: 773 | LEU A: 820 | LEU	ARG B: 1027 | LYS B: 868

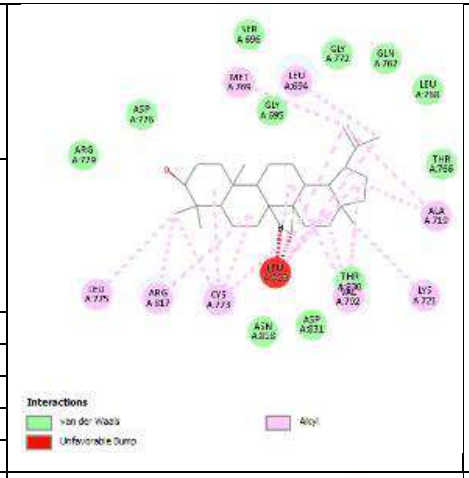
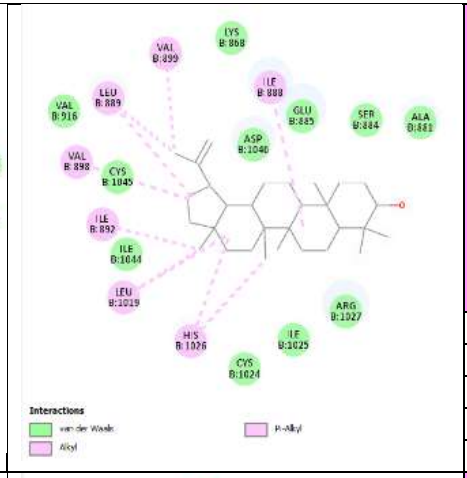
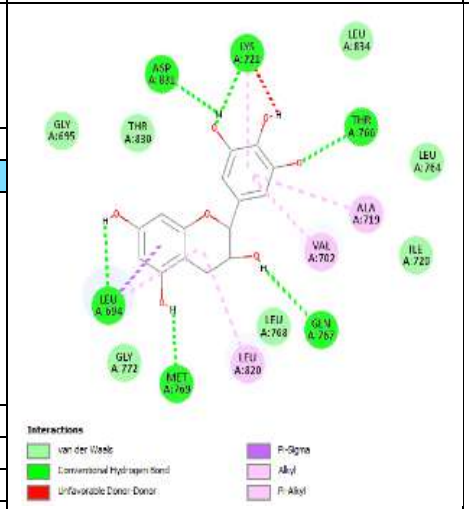
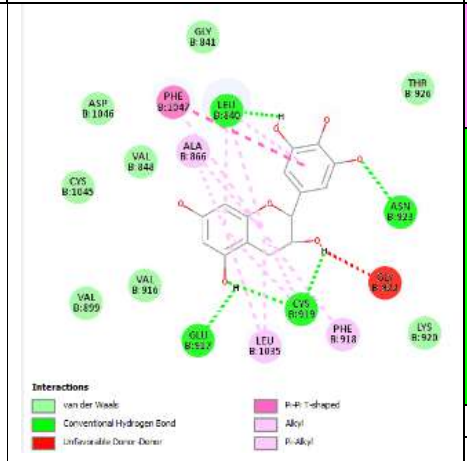
							A:694 | VAL A: 702	
		2	-61.5657	-69.9324			LYS A: 721	HIS B: 1026 | VAL B: 898 | VAL B: 899 | LEU B: 889
		3	-64.6444	-70.0756			LYS A: 721	ARG B: 1027
		4	-65.5028	-69.921				
		5	-62.1194	-70.1319				
		6	-63.1049	-70.1574				
		7	-65.342	-70.1583				
		8	-63.9933	-70.0934				
		9	-60.6763	-69.5346				
		10	-65.7592	-69.375				
19	*Isorhamnetin 3-O-rutinoside*	1	-103.678	-76.2502			LEU A:820 ALA A:719 LYS A:721 VAL A:702	LYS B: 868 | GLU B: 885
		2	-104.705	-80.6413				
		3	-106.34	-77.9292			MET A:769 LEU A:694 ASN A:818 ASP A:831	LEU B: 882 | ALA B: 881 | LEU B: 889 | CYS B: 1045 | VAL B: 899
		4	-103.509	-76.227			ARG A:817	
		5	-103.268	-73.5739				
		6	-101.867	-81.2263				ASP B: 1046

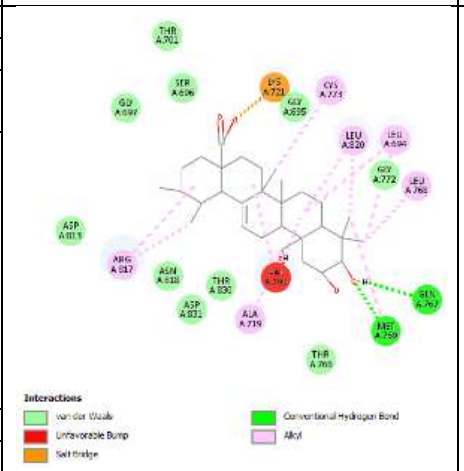
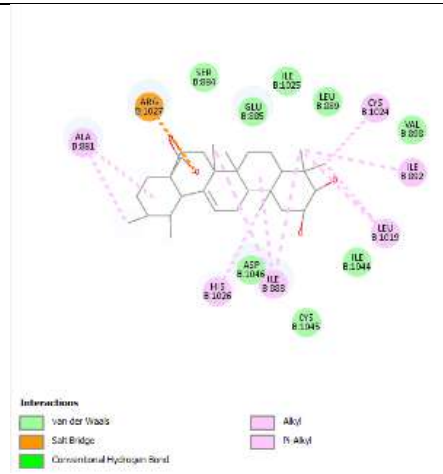
		7	-103.472	-75.7752				ARG B:1027 | HIS B: 1026 | ILE B:1025 | PHE B: 1047 | ILE B:1044
		8	-95.4106	-80.2518				
		9	-90.2581	-75.3317				
		10	-95.3586	-77.3643				
20	*Ceanothic acid*	1	-64.2546	-67.9354			LEU A: 820 | THR A: 830	ARG B: 1027 | LYS B: 868
		2	-64.548	-67.7097			CYS A: 773	HIS B: 1026 | ILE B: 888 | LEU B: 889 | ILE B:892 | LEU B: 1019 | ALA B: 881
		3	-62.2885	-69.1971			MET A: 769 | LEU A: 694 | LEU A: 768 | ALA A: 719 | VAL A: 702	
		4	-63.3863	-68.2668			LYS A: 721	
		5	-62.2229	-68.2457				
		6	-64.6381	-67.8106				
		7	-64.072	-68.0767				
		8	-62.5907	-68.2239				

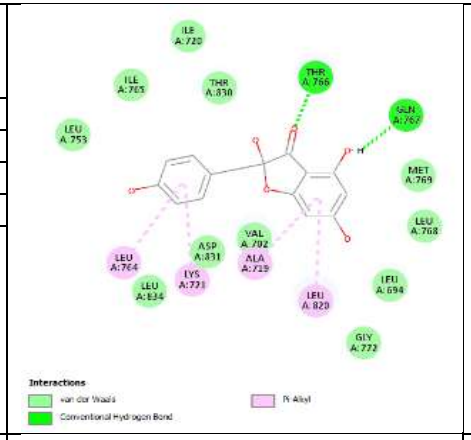
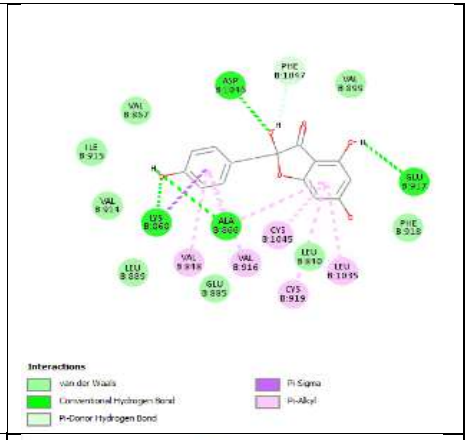
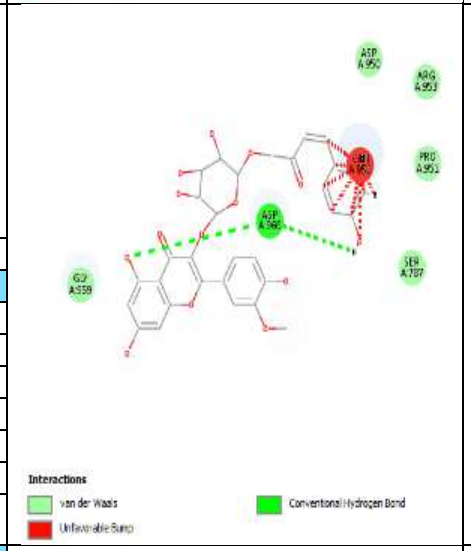
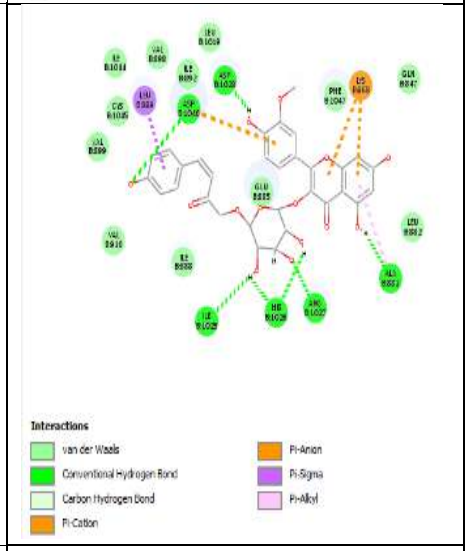
		9	-63.2424	-68.0841				
		10	-63.7382	-67.6861				
21	*Adouetine X*	1	-75.7101	-89.4698			ARG A: 817 | LYS A: 721	ARG B:1027 | ILE B: 1025 | ASP B:1046
		2	-80.8638	-77.0234			THR A: 830	LEU B:1019 | ILE B:888
		3	-70.04	-88.275			ARG A:817	HIS B:1026
		4	-71.0035	-85.7145			ALA A: 719 | LEU A: 820 | LEU A: 694 | LEU A: 834 | VAL A: 702	
		5	-69.5667	-85.1106				
		6	-68.6836	-82.4631				
		7	-75.0857	-84.3491				
		8	-71.5003	-84.9554				
		9	-71.1606	-81.4203				
		10	-71.0804	-83.0354				
22	*Betulin*	1	-71.5164	-67.5525			ALA A:719 | LEU A: 820 | LEU A:694 | CYS A: 773	ARG B: 1027 | ILE B:1044
		2	-71.7878	-67.8553			VAL A: 702	

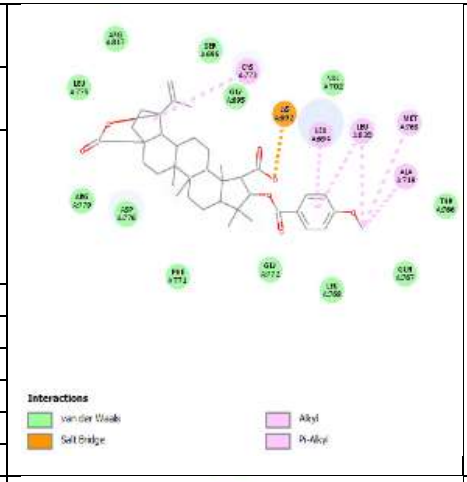
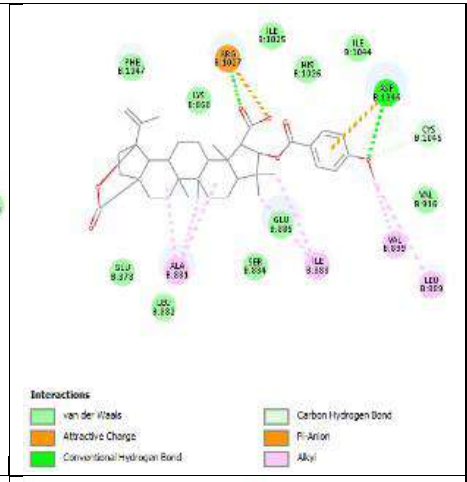
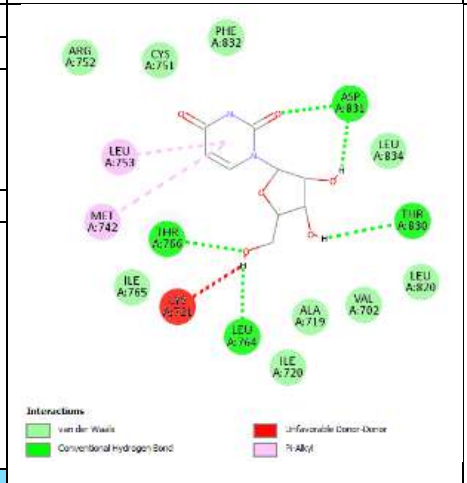
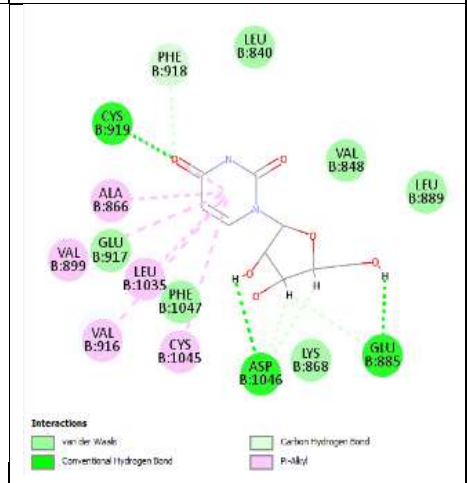
		3	-73.2387	-67.2655			LEU A: 768 MET A: 769 | GLN A: 767 | SER A: 696	ALA B: 881 | LEU B: 889 | LEU B: 1019 | HIS B: 1026 | ILE B: 892 | VAL B: 898 | ILE B: 888
		4	-71.5011	-68.2996				
		5	-73.1186	-67.2935				
		6	-70.7842	-68.9487				
		7	-72.2218	-67.5662				
		8	-72.2062	-67.7237				
		9	-70.8184	-68.7823				
		10	-72.0121	-67.531				
23	*Betulinic acid*	1	-67.6676	-71.1653			LYS A: 721	ARG B: 1027
		2	-68.4486	-72.5581			LEU A: 820 | THR A: 830	ILE B: 888 | LEU B: 1019 | HIS B: 1026 | CYS B: 1024 | ILE B: 892 | ALA B: 881
		3	-66.8775	-72.9659			LEU A: 775 | ARG A: 817 | CYS A:773 | VAL A:702 | ALA A: 719 | LEU A: 694 | MET A: 769	

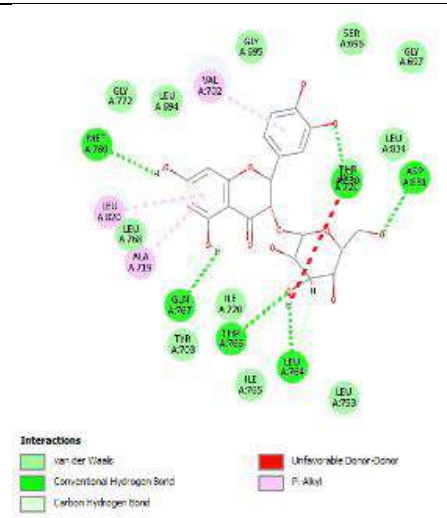
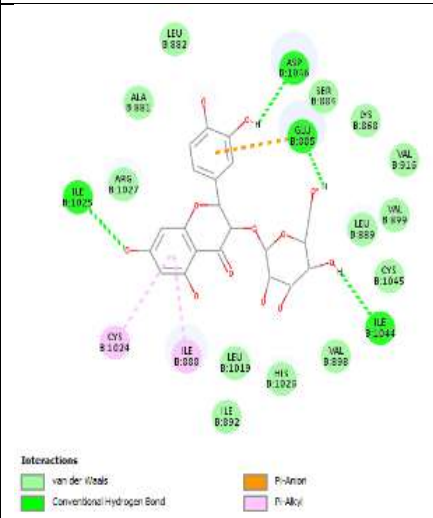
		4	-66.0482	-71.3324			LYS A:721	
		5	-65.4721	-73.8353				
		6	-68.6616	-71.1752				
		7	-68.9017	-71.8649				
		8	-66.2626	-72.7139				
		9	-64.8378	-73.2217				
		10	-64.0679	-73.2851				
24	*Platanic acid*	1	-55.7656	-62.7682			MET A: 769	ARG B: 1027
		2	-55.9121	-60.9436				ILE B: 1044
		3	-55.9728	-61.3251			CYS A: 773 | LEU A:694 | LEU A: 775 | ARG A:817 | VAL A: 702 | LEU A: 820 | ALA A: 719	ILE B: 888 | HIS B: 1026 | VAL B: 898 | LEU B: 1019 | LEU B:889
		4	-56.8945	-59.8211				
		5	-56.2509	-62.8389				
		6	-56.6517	-63.3495				
		7	-57.628	-62.2835				
		8	-58.8327	-63.9969				
		9	-58.4874	-63.1373				
		10	-58.181	-64.7459				
25	*Lupeol*	1	-68.3782	-70.4803			LEU A: 820	ILE B: 888 | VAL A: 899 | LEU B: 889 VAL A:
		2	-69.9271	-70.2604			ALA A: 719 | LEU A: 694	
		3	-69.359	-71.1807				
		4	-70.5221	-69.2313				

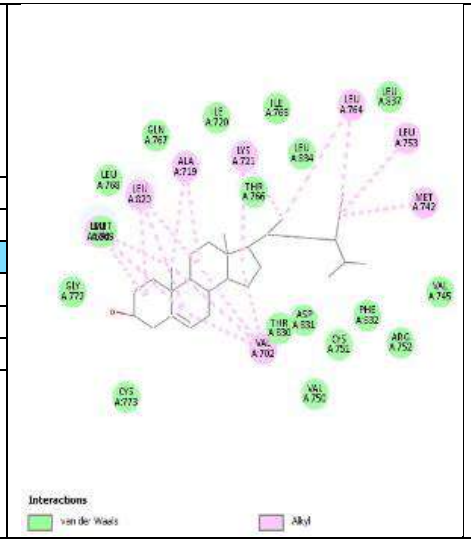
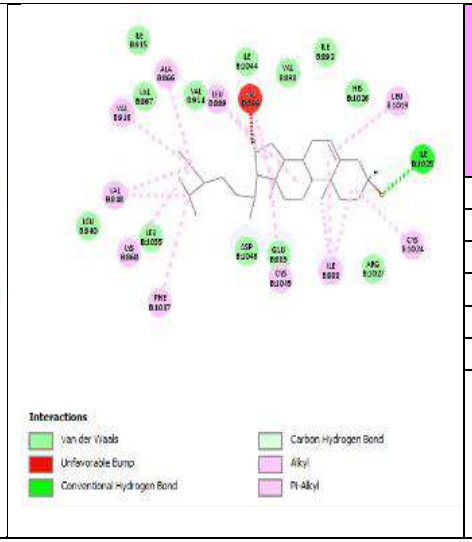
							|MET A:769| LYS A: 721|VAL A: 702|CYS A: 773 |ARG A: 817 |LEU A: 775	898|ILE B: 892|LEU B: 1019 |HIS B: 1026
		5	-68.2541	-70.1003				
		6	-68.7616	-70.4307				
		7	-68.4646	-69.1893				
		8	-68.6821	-69.0015				
		9	-68.7187	-70.7679				
		10	-69.6924	-69.5555				
26	*(+)-Gallocatechin*	1	-84.0953	-86.2747			ALA A: 719| VAL A: 702| LEU A: 820	LEU B:840 ASN B:923 CYS B:919 GLU B:917
		2	-84.1628	-86.27			GLN A: 767|MET A: 769 |LEU A:694|THR A: 766 |LYS A: 721|ASP A: 831	PHE B:1047
		3	-83.5686	-86.3297				GLY B:922
		4	-83.0882	-86.2466				PHE B:1047 LEU B:1035 ALA B:866
		5	-83.7997	-86.2316				
		6	-84.4365	-86.3052				
		7	-83.2543	-85.9805				
		8	-84.2259	-86.2099				
		9	-83.4358	-85.9173				

		10	-83.3826	-85.6531				
27	*Corosolic acid*	1	-67.9092	-66.6492			VAL A: 702	ARG B: 1027
		2	-67.8021	-66.5047			GLN A: 767 | MET A: 769	ALA B: 881 | HIS B: 1026 | ILE B: 888 | LEU B: 1019 | LEU B: 892 | CYS B: 1024
		3	-67.8114	-63.1136			ARG A: 817 | ALA A: 719 | LEU A: 768 | LEU A: 694 | LEU A: 820 | CYS A: 773	
		4	-64.282	-69.0099				
		5	-65.5333	-60.4023			LYS A: 721	
		6	-66.555	-64.5637				
		7	-60.8429	-67.4118				
		8	-62.6081	-68.4156				
		9	-63.6732	-70.4398				
		10	-63.977	-73.7348				
28	*Maesopsin*	1	-85.4452	-78.5049			LEU A: 820 | ALA A: 719 | LYS A: 721 | LEU 764 | 764	PHE B: 1047
		2	-85.2406	-80.5067				GLU B: 917 | ASP B: 1046 | LYS B: 868 | ALA B: 866
		3	-85.2331	-80.8398				
		4	-85.4479	-77.6907			THR A: 766 | GLN A: 767	
		5	-85.3693	-80.5155				LEU B: 1035 | CYS B:919 | CYS B: 1045 | VAL

								B: 916 | VAL B: 848
		6	-85.4493	-80.6725				
		7	-85.4199	-78.8763				
		8	-85.2116	-79.6688				
		9	-85.3704	-78.1647				
		10	-85.2596	-77.2723				
29	*Isorhamn etin3-O- (6''-O-(Z)-p-coumaroy l)-β-D-glucopyranoside*	1	-87.8293	-89.148			GLN A: 952	ASP B:1046 ASP B:1028 ILE B:1025 HIS B:1026 | ARG B: 1027 ALA B:881
		2	-82.94	-78.808			ASP A: 960	LYS B:868
		3	-90.2937	-89.6252				LEU B:889
		4	-79.6792	-88.2339				ALA B:881
		5	-89.4271	-89.4431				
		6	-91.0269	-89.3831				
		7	-78.7192	-81.3176				
		8	-77.7314	-85.5314				
		9	-76.8687	-83.7469				
		10	-77.6259	-82.8692				
30	*Alphitexolide*	1	-65.6741	-74.7165			LYS A: 692	ARG B: 1027

		2	-62.7882	-73.8794			ALA A: 719 | MET A: 769 | LEU A: 820 | LEU A: 694 | CYS A: 773	ASP B: 1046
		3	-65.8147	-74.2504				CYS B: 1045
		4	-64.9095	-74.4416				ALA B: 881 | ILE B: 888 | VAL B: 899 | LEU B: 889
		5	-62.5045	-73.6452				
		6	-62.8695	-73.7185				
		7	-64.9855	-73.8383				
		8	-65.3226	-73.7268				
		9	-59.9774	-72.3338				
		10	-60.1943	-72.3205				
31	*Uridine*	1	-80.713	-69.8187			THR A: 830 | LEU A: 764 | THR A: 766 | ASP A: 831	GLU B: 885 | ASP B: 1046 | CYS B:919
		2	-80.2845	-69.849				
		3	-81.2921	-69.8069				
		4	-80.8568	-69.6303			LYS A:721	PHE B: 918
		5	-81.44	-70.0478			LEU A: 753 | MET A: 742	CYS B: 1045 | LEU B: 1035 | VAL 916 | VAL B: 899 | ALA B: 866
		6	-79.8883	-70.0753				
		7	-76.4837	-69.627				
		8	-76.8318	-69.8913				

		9	-76.7153	-69.8692				
		10	-76.2269	-69.5925				
32	*3-O-beta-D-Galactopyranosyl-quercetin*	1	-94.0572	-80.9045			MET A: 769 | THR A: 721 | ASP A: 831 | GLN A: 767 | THR A: 766 | LEU A: 764	GLU B: 885 | ILE B: 1044 | ILE B:1025 | ASP B: 1046
		2	-93.2175	-80.2223			ALA A: 719 | LEU A: 820 | VAL A: 702	ILE B: 888 | CYS B: 1024
		3	-94.3898	-80.5791			LYS A: 721	GLU B: 885
		4	-94.1567	-80.0277				
		5	-94.0227	-79.423				
		6	-93.9333	-79.019				
		7	-94.2703	-80.7465				
		8	-94.9645	-79.6008				
		9	-93.633	-79.2735				
		10	-92.826	-79.1919				
33	*β- Sitosterol*	1	-93.6912	-84.8849			ALA A: 719 | LYS A: 721 | LEU A:764 | LEU A: 753 | MET A: 742 | LEU A: 820	ILE B:1025 VAL B:899 ALA B:866 VAL B: 916 VAL B:848 LYS B:868 PHE B:1047 |
		2	-91.7533	-81.5029				
		3	-91.8599	-81.338				

							VAL A: 702	CYS B:1045 ILE B:888 CYS B:1024 LEU B:1019 LEU B:889
		4	-89.7542	-83.0922				
		5	-93.2728	-85.1163				
		6	-93.3453	-86.2919				
		7	-93.401	-82.3892				
		8	-92.4317	-81.1126				
		9	-93.2833	-84.869				
		10	-95.6451	-83.1141				