



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

SKRIPSI

**Untuk Memenuhi Persyaratan Dalam Rangka
Menyelesaikan Program Studi Sarjana Farmasi**

Oleh

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UNIVERSITAS BORNEO LESTARI
BANJARBARU**

MEI 2024

PERNYATAAN

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Banjarbaru, 23 April 2024



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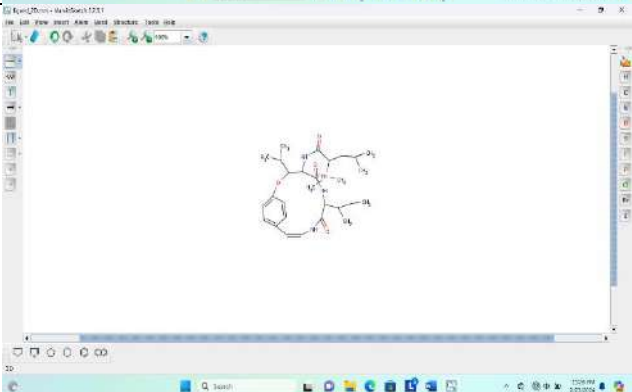
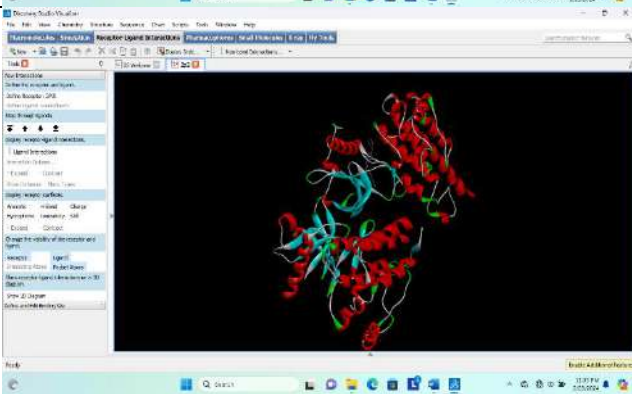
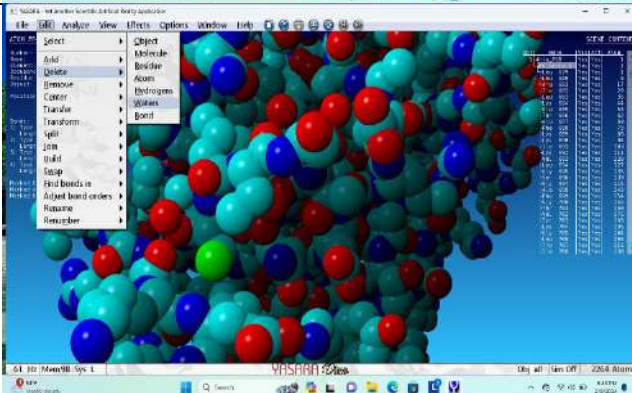
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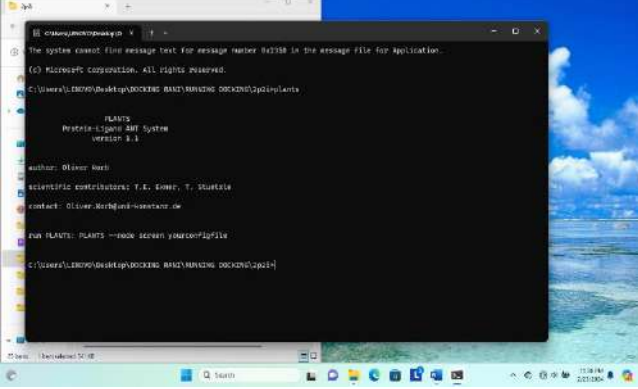
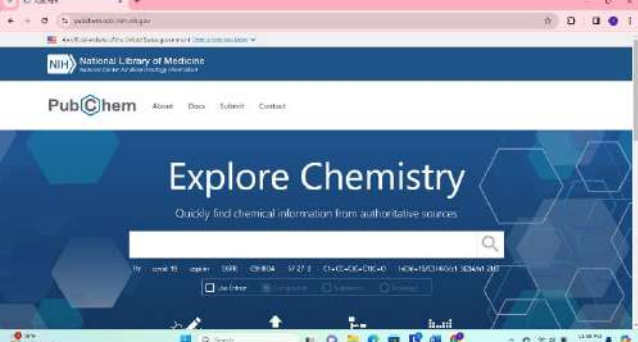
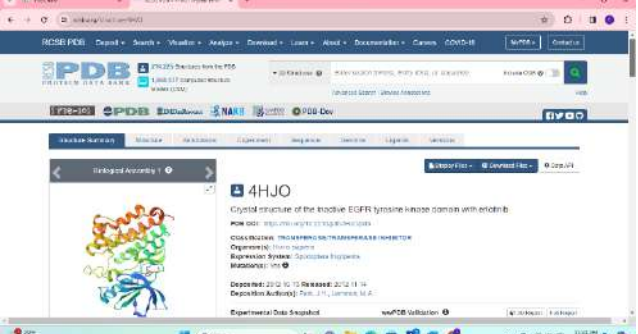

DAFTAR SINGKATAN

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


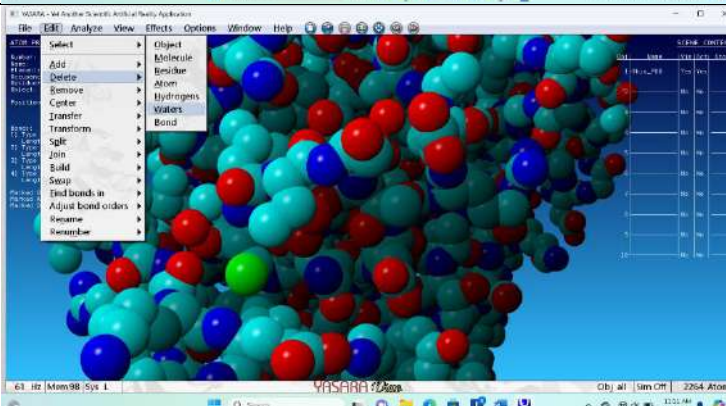
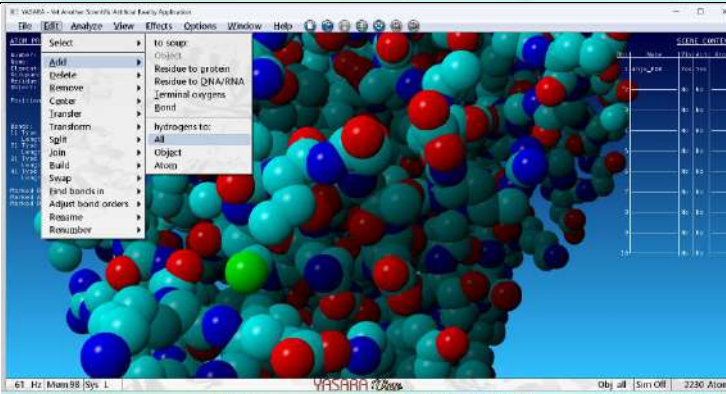
LAMPIRAN

Lampiran 1. Aplikasi dan Web Penunjang yang Digunakan

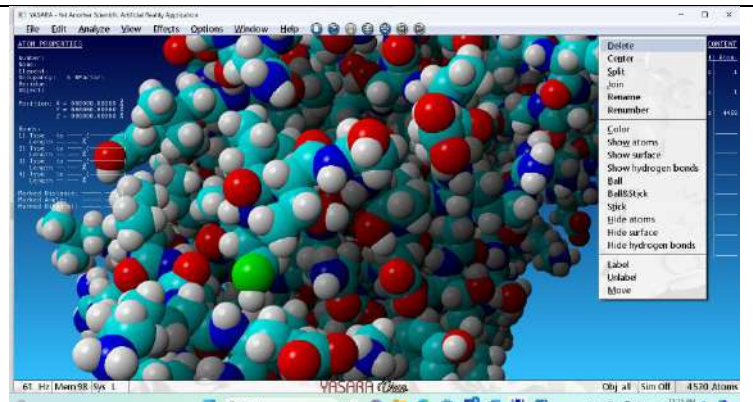
Icon Aplikasi		
Dalam Aplikasi	Marvin Sketch	
	Discovery Studio	
	Yasara	

	<p><i>PLANTS</i></p>	
<p>Web Penunjang</p>	<p>Pubchem</p>	
	<p>PDB</p>	
	<p><i>Uji Lipinski</i></p>	

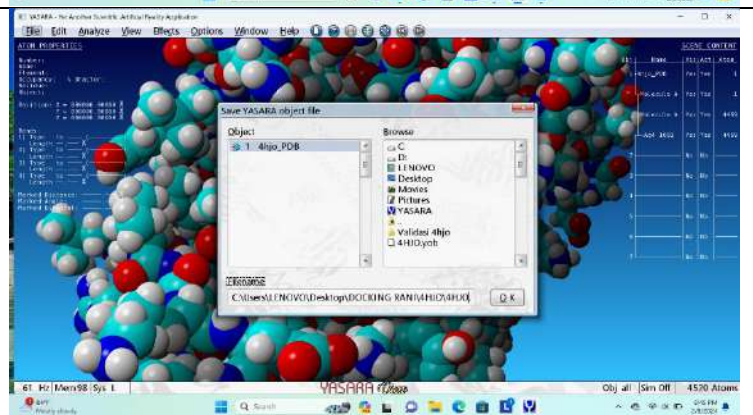
Lampiran 2. Tahapan Preparasi Protein dan *Native Ligand*

Load File Protein	
Penghapusan Air	
Penambahan Hidrogen	

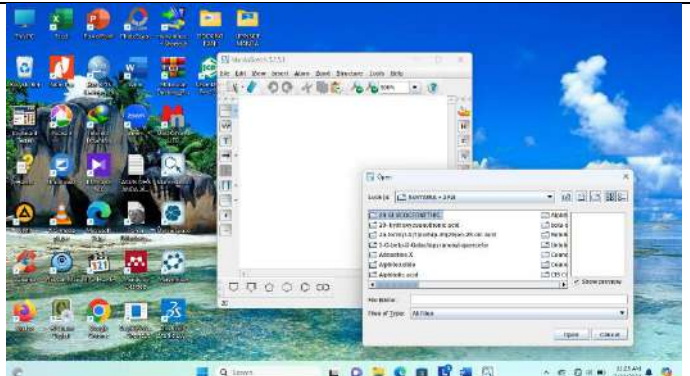
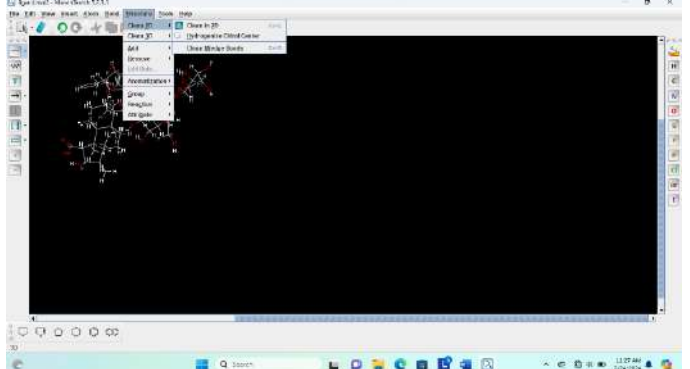
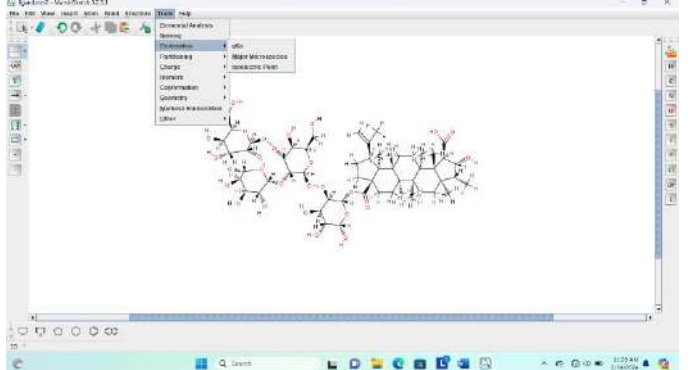
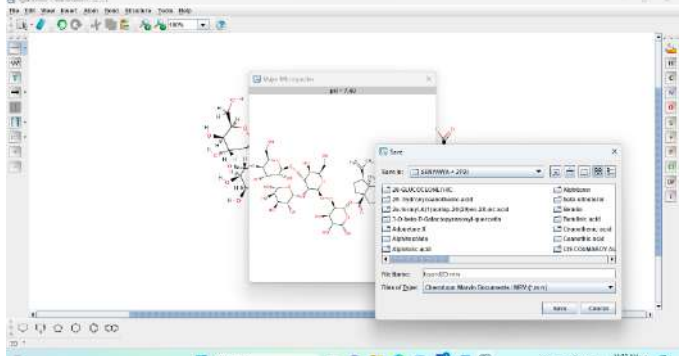
Penghapusan Rantai yang tidak digunakan (Preparasi Protein); Penghapusan protein (sisakan *native ligand*)

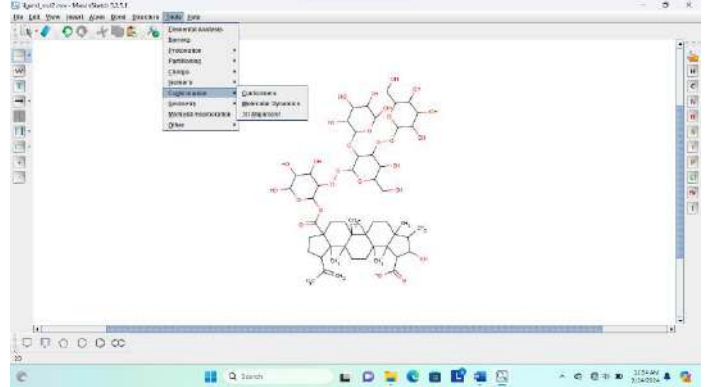
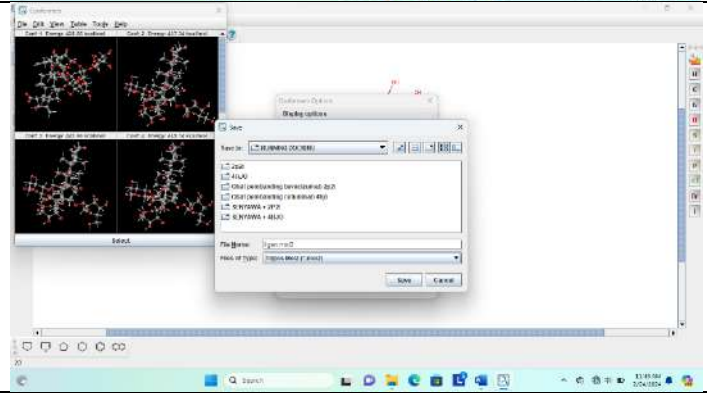


Penyimpanan Hasil Preparasi

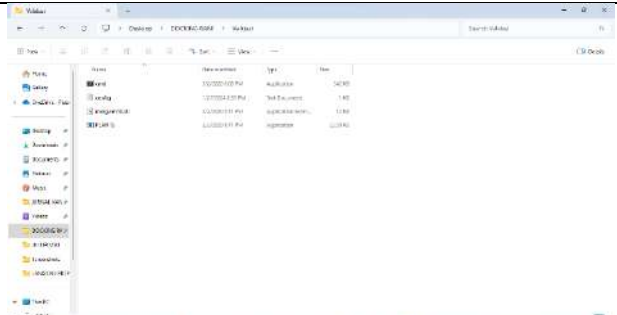
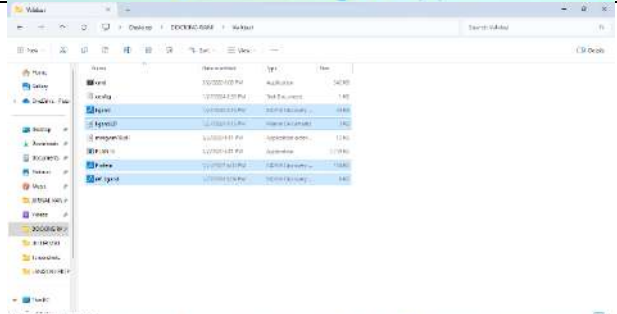
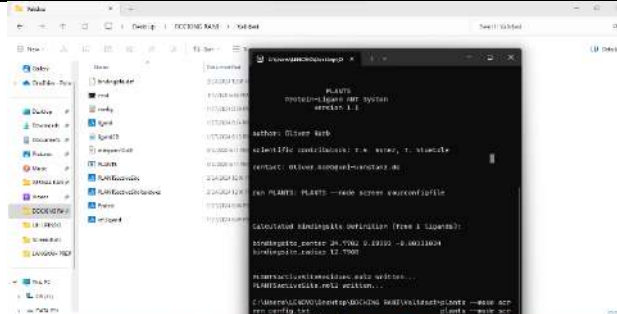
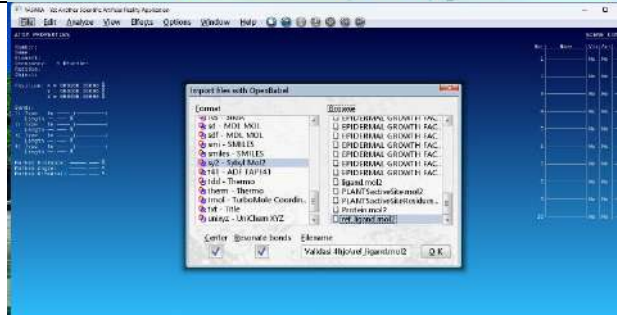


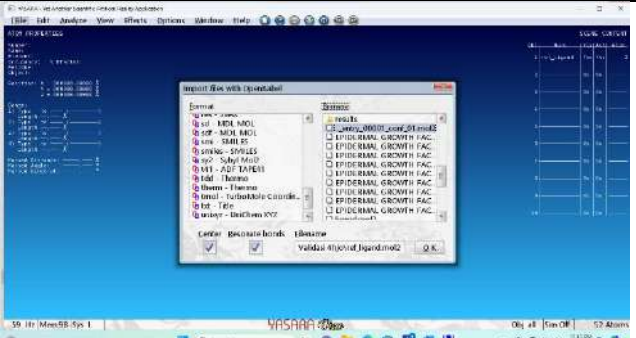
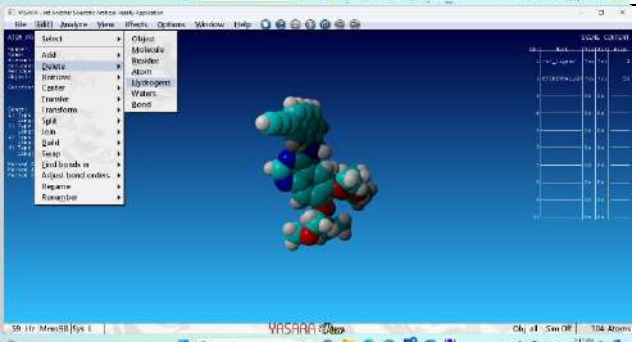
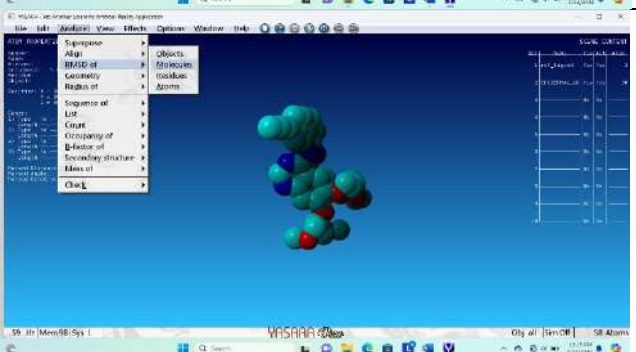
Lampiran 3. Tahapan Preparasi Ligand Senyawa Pembanding dan Senyawa Uji

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

<p>Pembuatan Konformasi</p>	 <p>The screenshot shows the Avogadro software interface. A large ball-and-stick model of a complex organic molecule is displayed in the center. The 'Conformation' menu is open, showing options like 'Randomize', 'Minimize Strain', and 'Relaxation'. The molecule consists of several fused and linked rings, including what appears to be a sugar-like structure.</p>
<p>Penyimpanan Hasil Konformasi dengan nama ligan.mol2</p>	 <p>The screenshot shows the Avogadro software interface with a 'Save' dialog box open. The dialog box has 'File name' set to 'ligan.mol2' and 'File type' set to 'Mol2 (*.mol2)'. There are 'Save' and 'Cancel' buttons at the bottom of the dialog. In the background, a window titled 'Conformation' is visible, showing a 3D view of the molecule.</p>

Lampiran 4. Tahapan Validasi Protein dan Penetapan RMSD

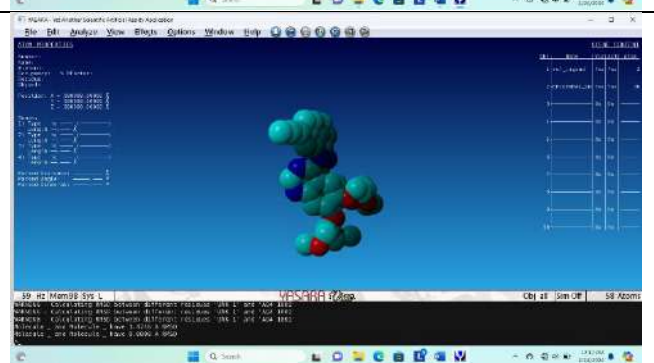
Validasi Protein	Siapkan Folder Untuk Validasi Protein dengan PLANTS	
	Masukkan ke Folder File Protein dan <i>Ligand Native</i> yang sudah dipreparasi	
	Docking Senyawa <i>Native Ligand</i> dengan PLANTS	
Penetapan RMSD	Load File <i>ref_ligand.mol2</i>	

	<p>Load <i>ligand native</i> hasil docking</p>	
	<p>Hapus Hydrogen</p>	
	<p>Klik analys kemudian RMSD of molecules</p>	

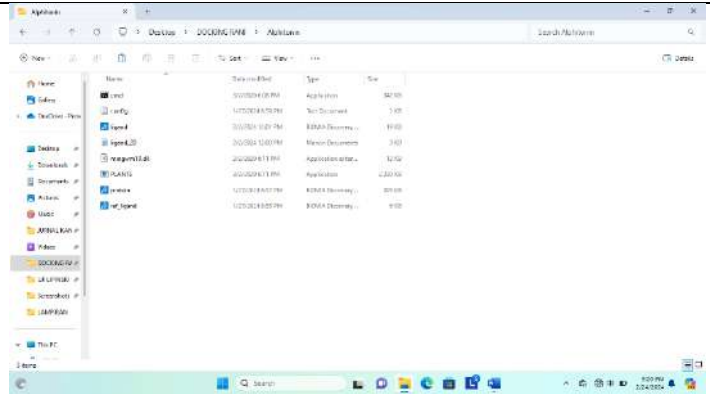
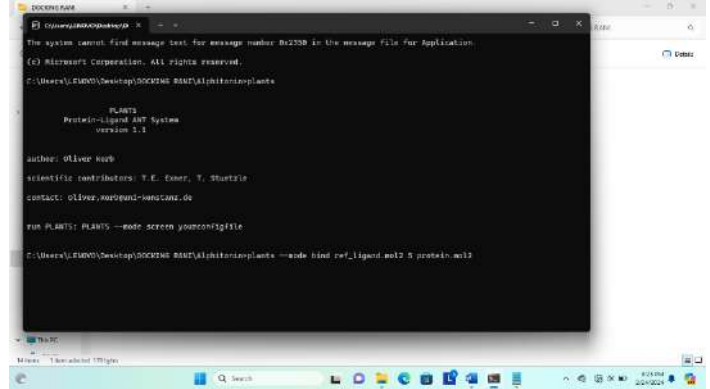
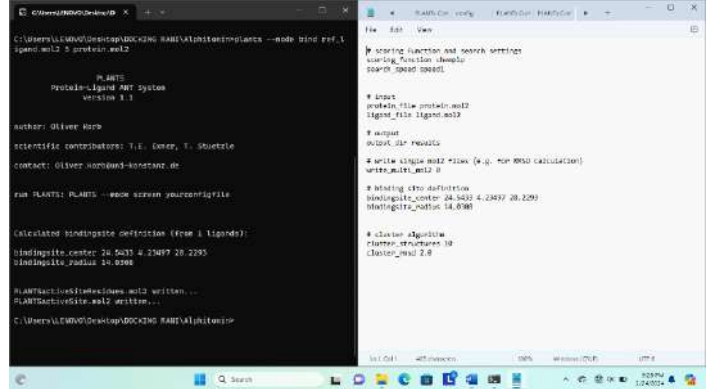
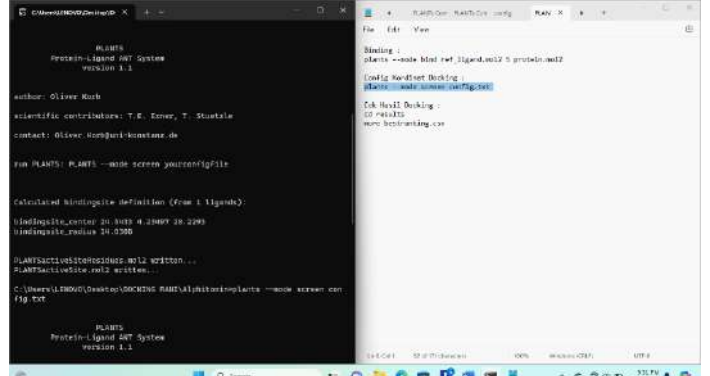
Sesuaikan Parameter

The image displays three sequential screenshots of the VASARA software interface. Each screenshot shows a dialog box for selecting molecules based on RMSD. The first dialog, titled 'Select molecules in best RMSD range', has a 'Sequnce' column with values 1 and 2, and a 'Name' column with values 1 and 2. The second dialog, also titled 'Select molecules in best RMSD range', shows a 'References to select' list with options: All, AminoAcid, Protein, Nucleotide, Polysaccharide, Water, City 1, and City 2. The third dialog, titled 'Set parameters', has two checked options: 'Match atoms, consider only those present in both selected' and 'Use chemically equivalent groups to minimize RMSD'. Below these options are radio buttons for 'Use an RMSD per: Object', 'Molecule', 'Residue', and 'Atom', with 'Molecule' selected. The background of all screenshots shows the VASARA software interface with various panels and a taskbar.

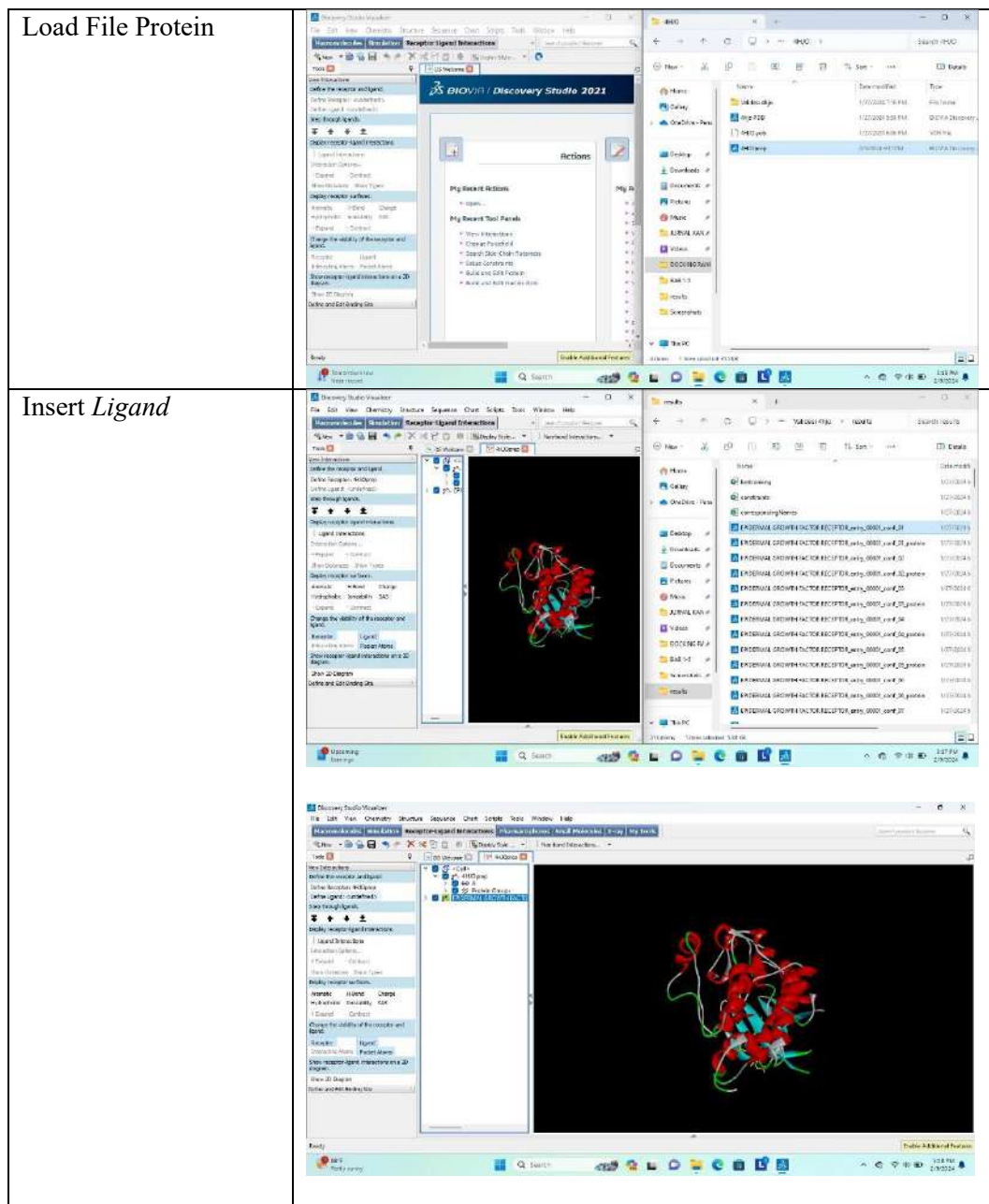
Lihat Hasil



Lampiran 5. Tahapan Docking Senyawa

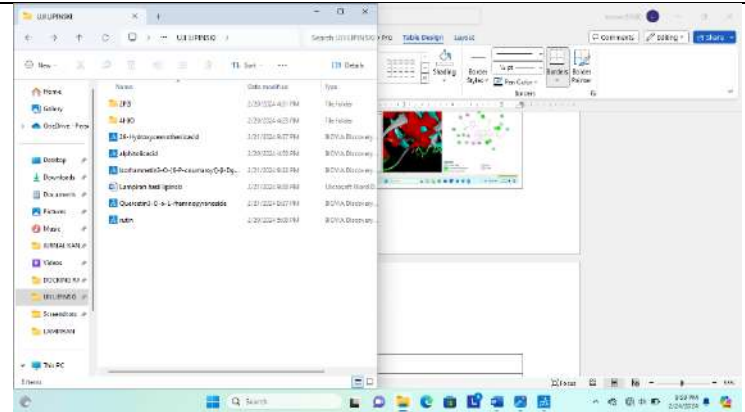

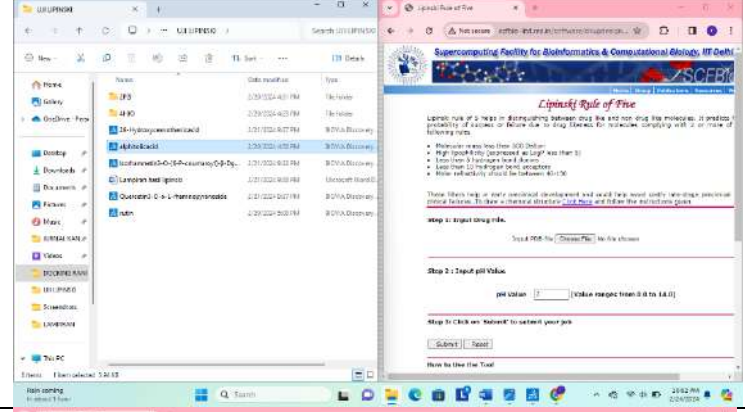
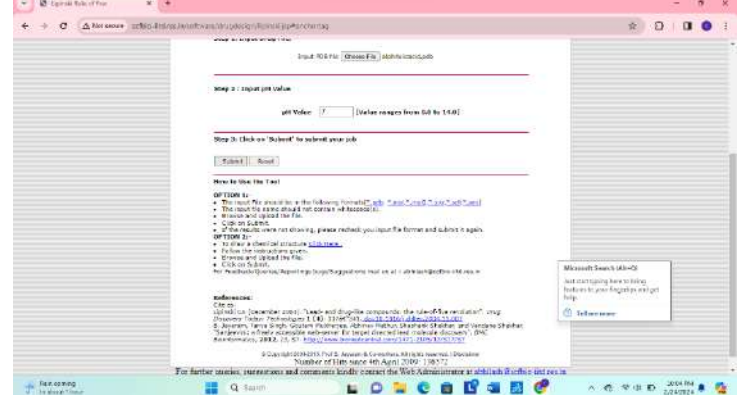
<p>Siapkan Folder dan File</p>	
<p>Masukkan perintah “plants—mode bind ref_ligand.mol2 5 protein.mol2”</p>	
<p>Ubah Kordinat protein di File Config dengan di layer plants</p>	
<p>Masukkan perintah “plants==mode screen config.txt”</p>	

Lampiran 6. Tahapan Visualisasi Ikatan Senyawa dan Protein

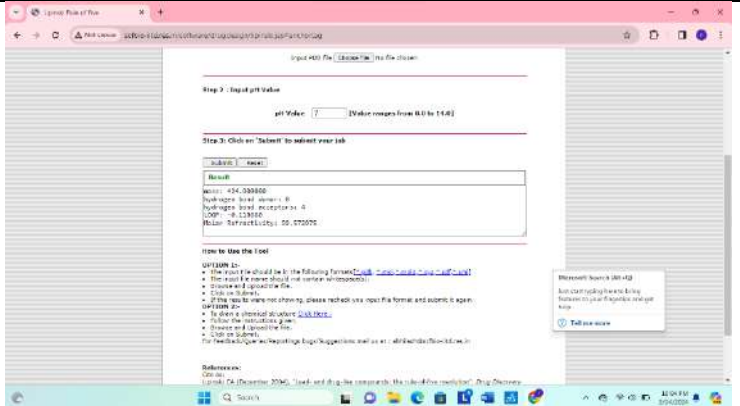


<p>Atur Parameter</p>	
<p>Show 2D</p>	

Lampiran 7. Tahapan Uji Lipinski

<p>Siapkan Ligand Dalam Bentuk .pdb</p>	
<p>Buka Website Uji Lipinski</p>	
<p>Pilih File Ligand</p>	
<p>Submit</p>	

Cek Result



The screenshot shows a web browser window with a URL starting with 'https://www.ijournal.uin-suka.ac.id'. The main content area is titled 'Input File' and contains a form for 'Step 3: Input pH Value'. The pH value is set to 7. Below the form, there is a 'Result' section with the following data:

- Acid: 434.000000
- Buffering: 0
- pH: 7.000000
- pKa: 11.130000
- Molar: 0.000000

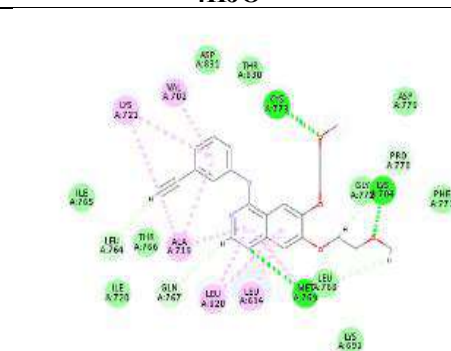
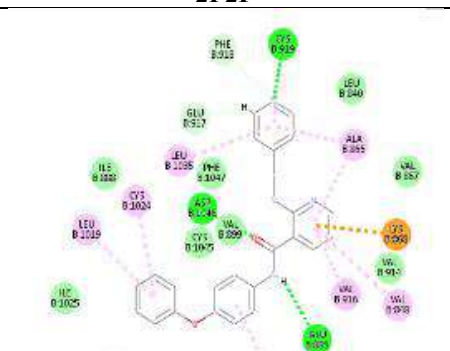
Below the results, there is a 'References' section with a list of links and a 'Tell me more' button on the right.

Lampiran 8. Hasil RMSD Protein Kanker Kolorektal

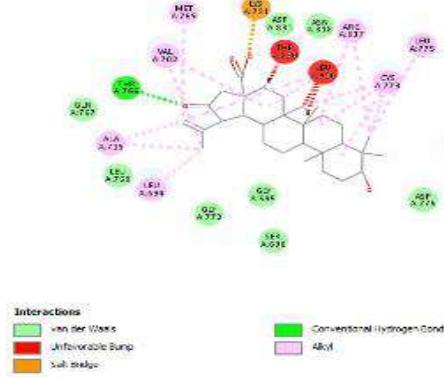
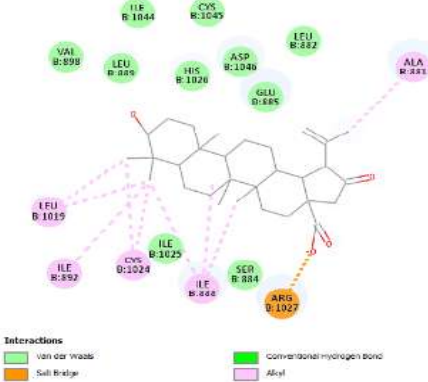
Protein (Reseptor)	Konformasi	Skor Docking	RMSD
4HJO	1	-103.046	1.4746
<i>(Epidermal Growth Factor Reseptor)</i>	2	-103.022	1.4720
	3	-102.489	1.5304
	4	-102.611	1.4335
	5	-102.363	1.4688
	6	-102.969	1.4942
	7	-102.671	1.4658
	8	-100.297	1.9648
	9	-101.972	1.4679
	10	-102.529	1.5809
	2P2I	1	-113.492
<i>(Vascular Endothelial Growth Factor Receptor)</i>	2	-111.546	0.8169
	3	-115.511	1.5294
	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

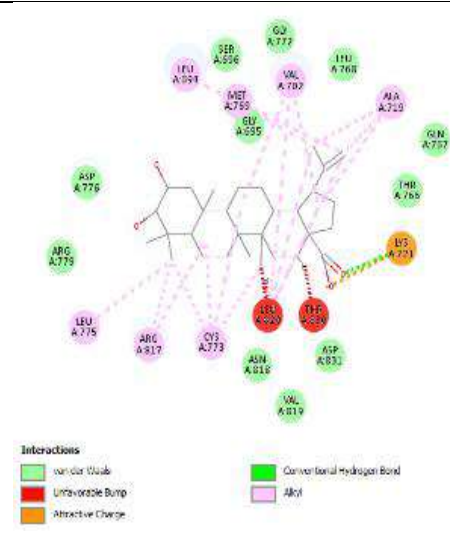
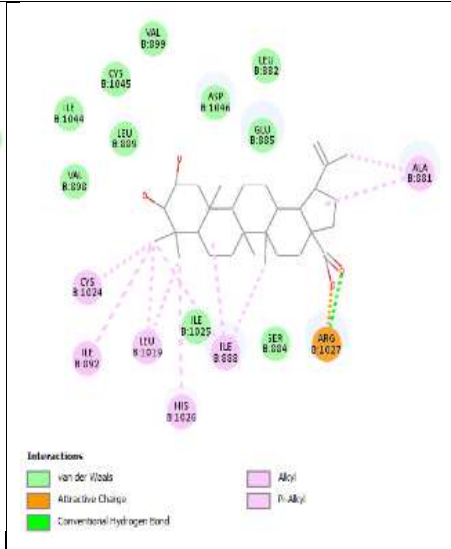
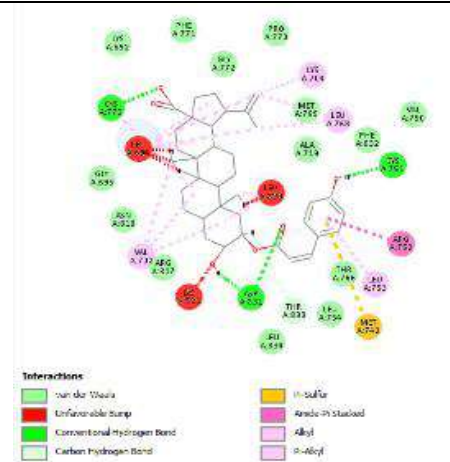
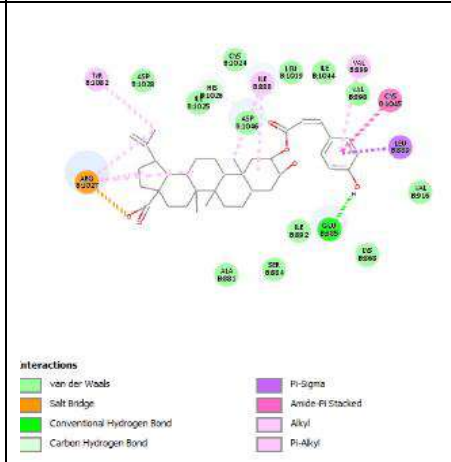
Keterangan : Nilai yang terpilih dan memenuhi parameter RMSD <2

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

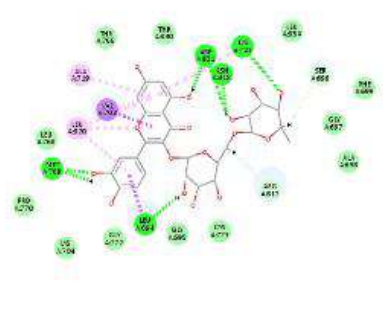
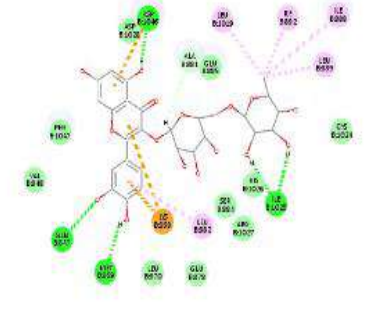
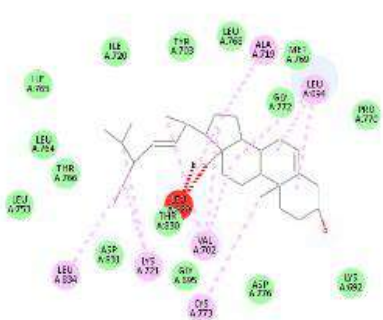
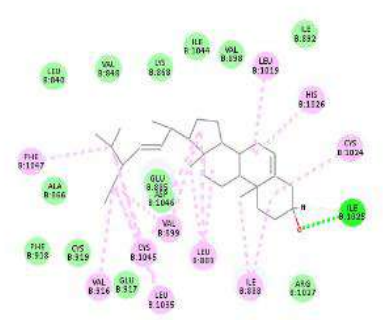
No	Senyawa/ Ligand	Conformer	Protein		Visualisasi		Residu Asam Amino	
			4HJO	2P2I	4HJO	2P2I	4HJO	2P2I
1	Native	1	-103.046	-113.492			LYS A:721 VAL A:702 ALA A:719 LEU A:820 LEU A:694	CYS B:1024 LEU B:1019 LEU B:1035 ALA B:866 VAL B:916 VAL B:848 LEU B:889
		2	-103.022	-111.546			LEU A: 764 GLN A: 767	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	-

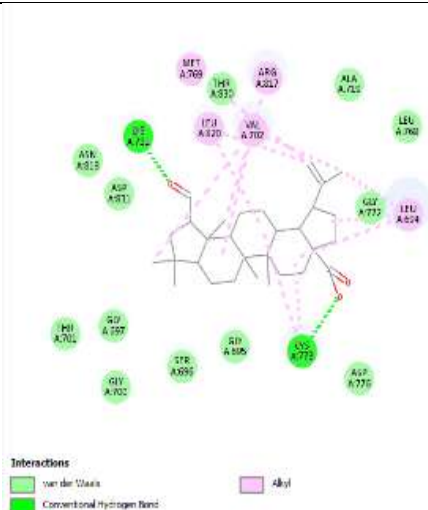
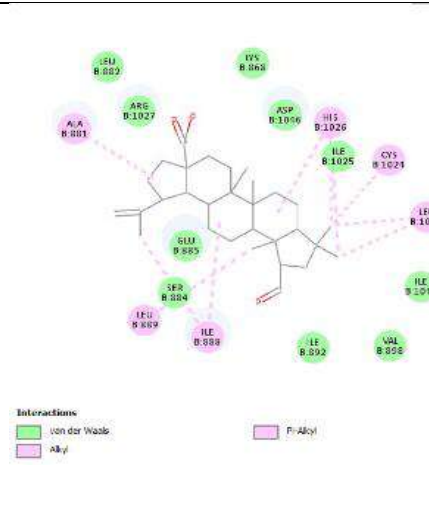
					<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon-Hydrogen Bond Unfavorable Acceptor-Acceptor Pi-Action Alkyl Pi-Alkyl 	MET A:742 LEU A: 753 LEU A:764 LEU A:834 LYS A:721 VAL A:702 LEU A: 694	
		2	-102.208	-		ASP A:831	-
		3	-96.5392	-		PHE A:832	-
		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			

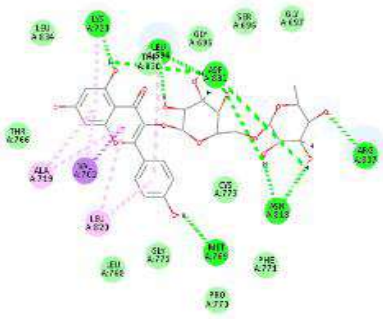
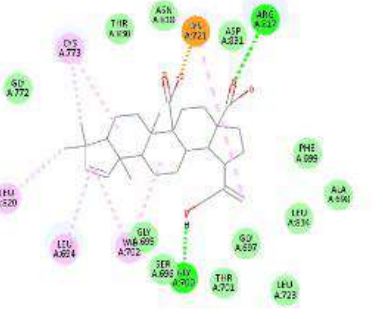
		6	-86.0733	-82.0079				
		7	-86.0323	-81.6469				
		8	-85.8145	-81.4153				
		9	-85.9173	-82.4718				
		10	-85.9905	-82.6294				
5	<i>2-Ketobetulinic acid</i>	1	-67.634	-73.7887			THR A: 766	ARG B: 1027
		2		-72.2763			ALA A:719 ARG A: 817 CYS A: 773 LEU A: 775 LEU A:694 ME T A: 769 VAL A: 702	ALA B: 881 CYS B: 1024 ILE B: 888 ILE B: 892 LEU B: 1019
		3	-65.3384	-73.8581				
		4	-67.1968	-73.1844				
		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	<i>Alphitollic acid</i>	1	-66.9985	-74.2965			LYS A: 721	ARG B: 1027
		2					THR A: 830 LEU A: 820	ALA A: 881 CYS B: 1024 ILE B: 892 ILE
			-66.9249	-74.1826				

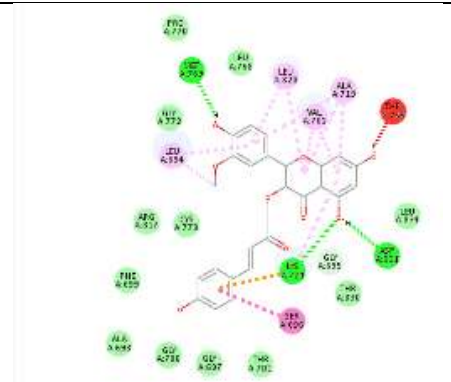
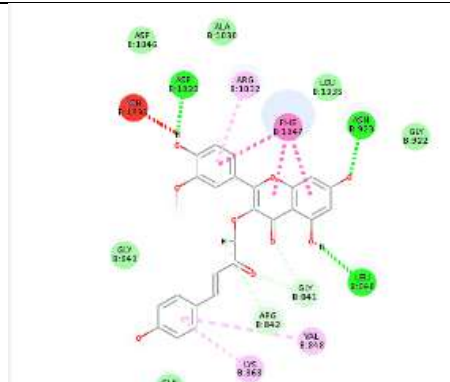
					 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Unfavorable Bump Attractive Charge Conventional Hydrogen Bond Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Alkyl Pi-Alkyl 		<p>B: 888 LEU B: 1019 HIS B: 1026</p>
		3	-68.411	-73.4419				
		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				
7	<i>3-O-Cis-p-Coumaroyl aphitolic acid</i>	1	-87.6377	-85.0584	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Unfavorable Bump Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sulfur Amide-Pi Stacked Alkyl Pi-Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Salt Bridge Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sigma Amide-Pi Stacked Alkyl Pi-Alkyl 		<p>ALA A:719 AR G A: 817 CYS A: 773 LEU A: 775 LEU A: 694 MET A: 769 VAL A: 702</p>
		2	-86.79	-88.3605				
		3	-88.2855	-85.9986				
		4	-86.0648	-88.7478				
		5	-93.266	-87.2428				
		6	-84.8468	-88.4604				
		7	-84.7635	-88.6802				
		8	-90.8286	-88.5672				
		9	-82.7416	-83.6603				
		10	-82.8859	-82.4549				
								<p>LYS A: 721</p>
								<p>CYS A: 751 CYS A:773 ASP A: 831</p>
								<p>LEU A: 820 LEU A: 694 LYS A:721</p>
								<p>GLU B:885 ARG B:1027 HIS B:1026 CYS B:1045</p>
								<p>VAL B:899 TYR B:1082 ILE B:888 LEU B:889</p>
								<p>ARG A: 752 THR A: 830</p>
								<p>LEU A: 753 LEU</p>

							A:768 LYS A:704 VAL A: 702	
8	<i>3-O-p-Trans-7-Coumaroyl aphitolic acid</i>	1	-84.1539	-82.4614	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Carbon Hydrogen Bond Unfavorable Negative-Negative Pi-Alkyl 			
		2	-84.3599	-82.9554				
		3	-88.6126	-79.2032				
		4	-88.5996	-78.309				
		5	-88.7004	-78.5425				
		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	<i>Rutin</i>	1	-104.489	-78.788	<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Alkyl 	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		

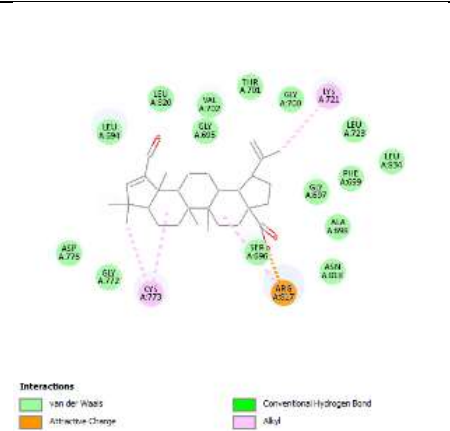
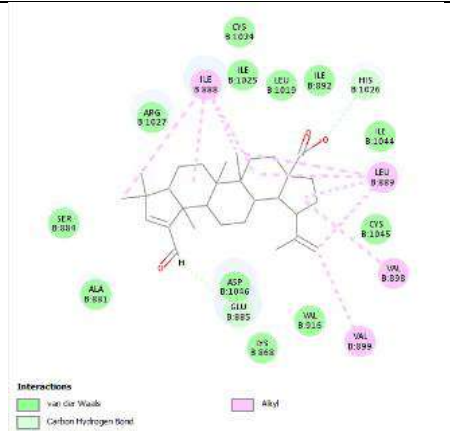
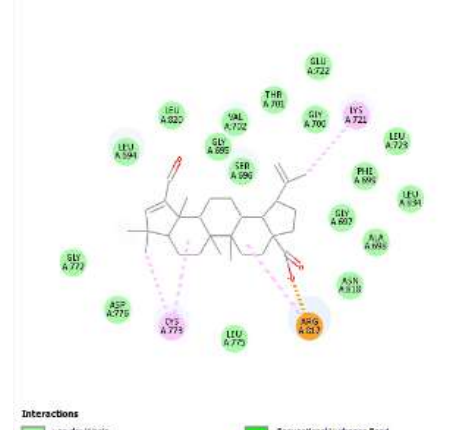
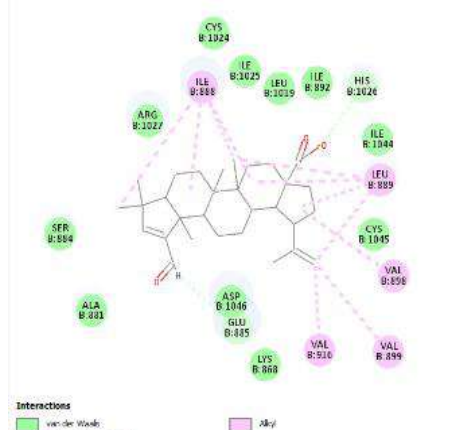
					 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventioneel Hydrogen Bond Carbon Hydrogen Bond Pi-Sigma Pi-Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventioneel Hydrogen Bond Carbon Hydrogen Bond Pi-Alkyl Pi-Alone Pi-Sigma Alkyl Pi-Alkyl Pi-Cation 	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	<i>Stigmasterol</i>	1	-95.7533	-83.6522			ALA A:719 CYS	ILE B:1025
		2	-94.6749	-79.6349			A: 773 LEU	ILE B: 1025
		3	-96.0936	-83.5991	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Unfavorable Bump Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventioneel Hydrogen Bond Carbon Hydrogen Bond Alkyl Pi-Alkyl 	A: 773 LEU A: 694 LEU A: 834 LYS A: 721 VAL A: 702	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	<i>2α-Formyl-A(1)norlup-20(29)-en-28- oic acid</i>	1	-63.8425	-65.297	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Pi-Allyl 				
		2	-64.8717	-65.1465					
		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	<i>Kaempferol-3-rutinoside</i>	1	-96.6792	-81.0359	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Pi-Allyl 				
		2	-92.0206	-81.2006					
		3	-98.3471	-81.5223					
		4	-101.451	-81.1558					
		5	-90.0179	-81.6199					
								CYS A: 773 LYS A: 721 ARG A: 817 LEU A: 694 LEU A: 820 MET A: 769 VAL A: 702	ALA B: 881 CYS B:1024 HI S B: 1026 LEU B: 889 LEU B:1019 ILE B:888
								ALA A: 719 LEU A:820 ASN A: 818 ARG A: 817 ASP A: 831 LEU A: 694 LYS A: 721 MET A: 769 VAL A: 702	ILE B: 888 LEU B: 889 LYS B: 868 VAL B: 916 VAL B: 914 ASP B: 1046 CYS B: 1045 ILE B: 1044

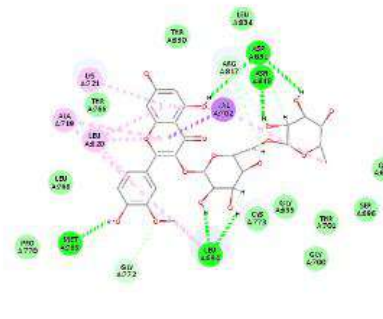
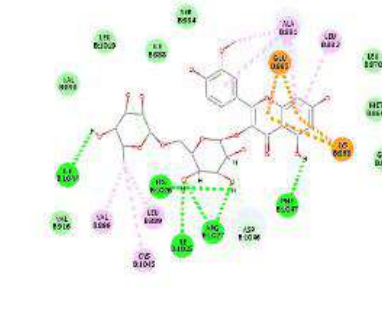
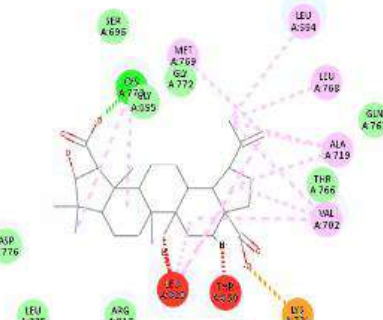
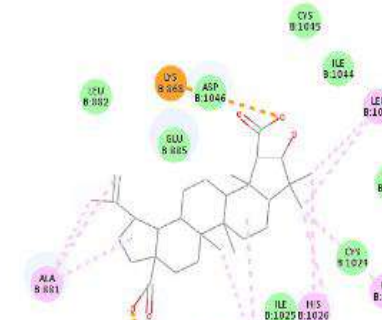
		6	-98.9981	-81.9695	 <p>Interactions:</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Carbon-Hydrogen Bond PI-Sigma PI-Alkyl 		ALA B: 881 SER B: 884	
		7	-94.6642	-81.9707			HIS B: 1026 GLU B: 885	
		8	-96.2757	-82.0085				
		9	-95.9779	-78.5779				
		10	-99.4359	-71.3232				
13	29-Hydroxyceanothe nic acid	1	-62.2838	-70.191	 <p>Interactions:</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Salt Bridge Alkyl Carbon-Hydrogen Bond 		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				GLY A: 700 ARG A: 817
		3	-65.7841	-70.518				ASP B: 1024
		4	-65.6273	-71.0135				ASP B: 1024
		5	-65.4392	-70.795				ARG B: 1027 LYS B: 8

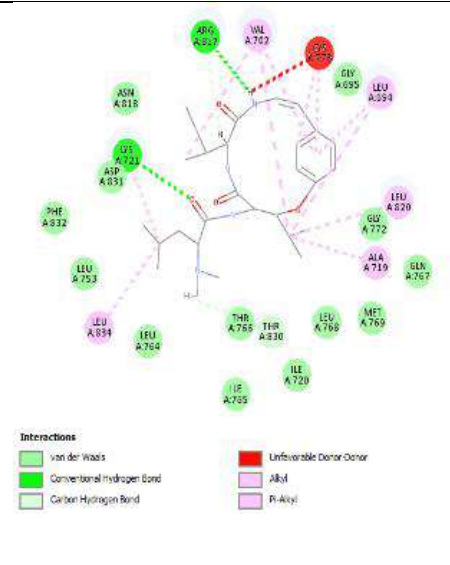
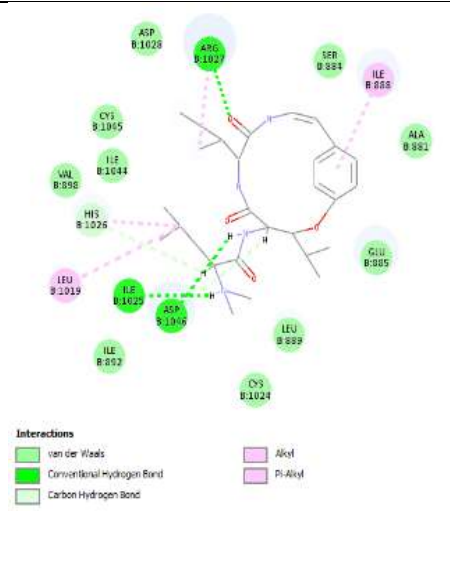
		6	-61.8453	-70.5191			LYS A: 721	SER B: 884	
		7	-64.5875	-71.2725					
		8	-65.6295	-71.8428					
		9	-65.0515	-70.0557					
		10	-70.9519	-71.8839					
14	<i>Isorhamnetin 3-O-[6-P-coumaroyl]-β-D-glucopyranoside</i>	1	-94.1843	-67.86				SER A: 696	GLY B: 841 ARG B: 842
		2	-89.3218	-76.6866					
		3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

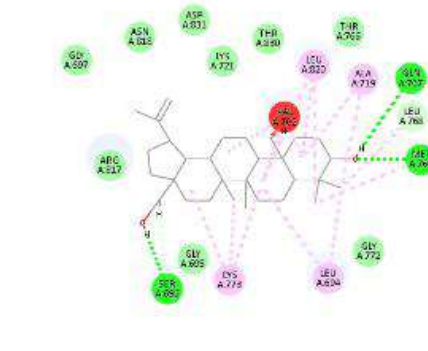
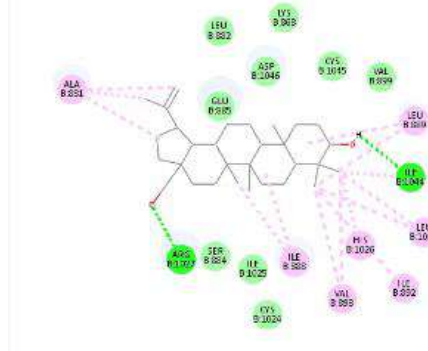
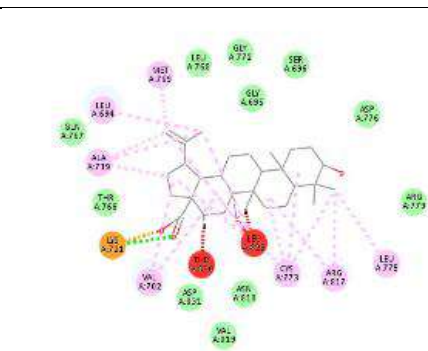
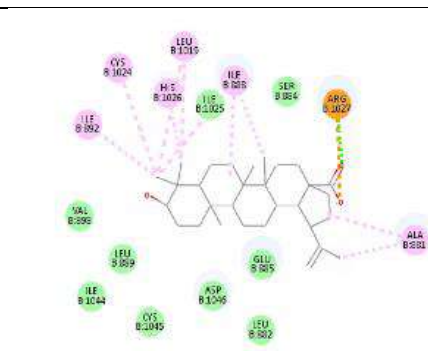
		2	-94.495	-88.3768	<p>Interactions</p> <ul style="list-style-type: none"> von der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sigma Pi-Alkyl 	<p>Interactions</p> <ul style="list-style-type: none"> von der Waals Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Carbon Alkyl Pi-Alkyl 	721 GLY A: 700 MET A: 769 THR A: 766	LYS B:868 PHE B:918
		3	-97.6928	-82.8513			LEU A: 694	VAL B:916 VAL B:848 ALA B:866 LEU B:1035 CYS B:1045 PHE B:1047
		4	-97.2976	-82.1932			ALA A: 719 VAL A: 702	
		5	-96.1914	-87.2556				
		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	<i>Quercetin 3-O-α-L-rhamnopyranoside</i>	1			-62.5748	-73.267
2	-62.0981			-71.974	ARG A: 817	HIS B: 1026 GLU B: 885		
3	-62.9055			-73.3643				
4	-62.0243			-72.7641				
5	-62.8054			-73.4887				
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	<i>Zizyberenic acid</i>	1	-61.8626	-72.4532			ARG A: 817	LEU B:
		2	-61.9684	-73.1799			LYS A:	889 ILE B:
		3	-62.9595	-73.4741			A: 773	888 VAL B:
		4	-61.841	-72.3894				916 VAL B:
		5	-62.2234	-72.8737				899 VAL B:
		6	-62.3306	-72.626				
		7	-63.9997	-72.222				
		8	-64.2479	-72.4952				HIS B:
		9	-62.6185	-72.4685				1026, GLU B:
		10	-62.4948	-72.1486				885
18	<i>Ceanothenic acid</i>	1	-62.7768	-70.099			CYS A:	ARG B:
							773 LEU A:	1027 LYS B:
							820 LEU A:	868

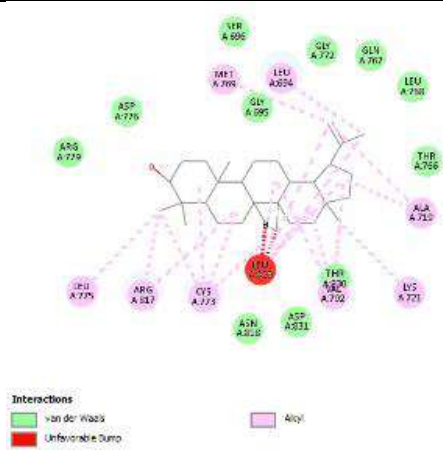
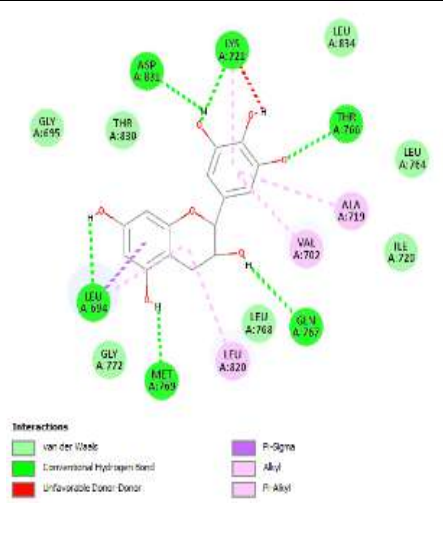
		2	-61.5657	-69.9324			A:694 VAL A: 702	
		3	-64.6444	-70.0756			LYS A: 721	HIS B: 1026 VAL B: 898 VAL B: 899 LEU B: 889
		4	-65.5028	-69.921			LYS A: 721	ARG B: 1027
		5	-62.1194	-70.1319				
		6	-63.1049	-70.1574				
		7	-65.342	-70.1583				
		8	-63.9933	-70.0934				
		9	-60.6763	-69.5346				
		10	-65.7592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

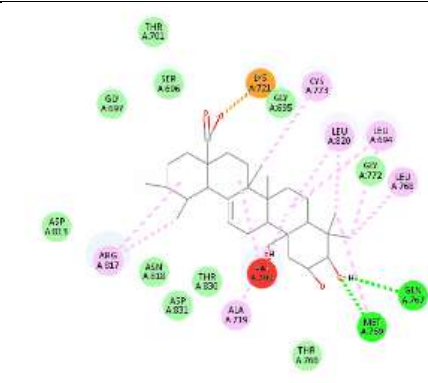
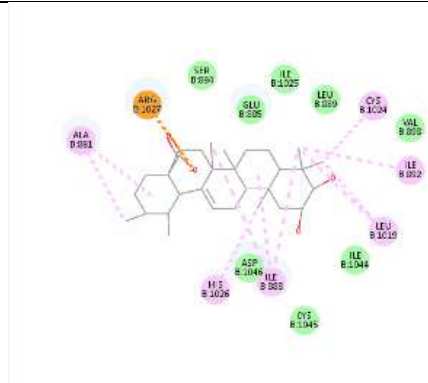
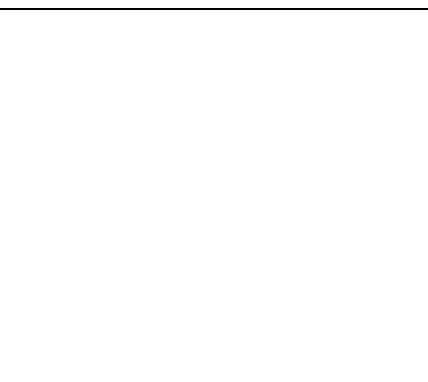
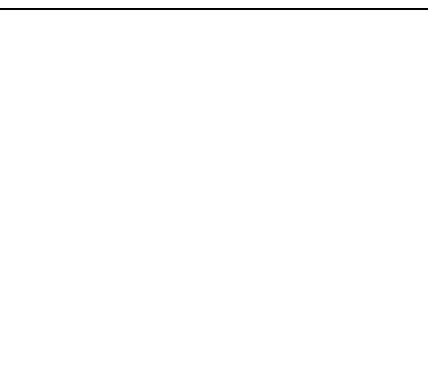
		7		-75.7752				ARG B:1027 HIS B:1026 ILE B:1025 PH E B:1047 ILE B:1044
		8	-103.472	-80.2518				
		9	-95.4106	-75.3317				
		10	-90.2581	-77.3643				
			-95.3586					
20	<i>Ceanothic acid</i>	1	-64.2546	-67.9354			LEU A: 820 THR A: 830	ARG B: 1027 LYS B: 868
		2	-64.548	-67.7097			CYS A: 773	HIS B: 1026 ILE B: 888 LEU B: 889 ILE B: 892 LEU B: 1019 ALA B: 892
		3	-62.2885	-69.1971			MET A: 769 LEU A: 694 LEU A: 768 ALA A: 719 VAL A: 702	LEU B: 1019 VAL B: 898 CYS B: 1021 ILE B: 1020 HIS B: 892 LEU B: 889
		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				

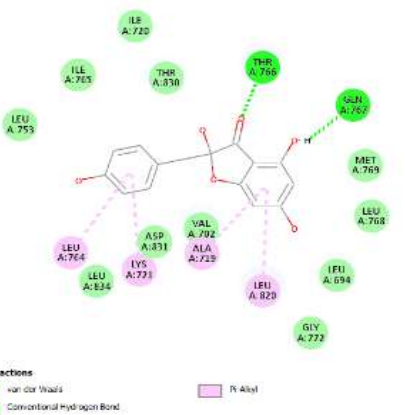
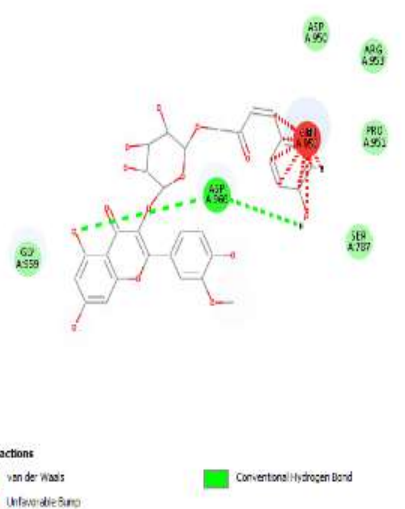
		9	-63.2424	-68.0841				
		10	-63.7382	-67.6861				
21	<i>Adouetine X</i>	1	-75.7101	-89.4698			ARG A: 817 LYS A: 721	ARG B:1027 ILE B: 1025 ASP B:1046
		2	-80.8638	-77.0234			THR A: 830	LEU B:1019 ILE B:888
		3	-70.04	-88.275			ARG A:817	HIS B:1026
		4	-71.0035	-85.7145			ALA A: 719 LEU A: 820 LEU A: 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	<i>Betulin</i>	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			

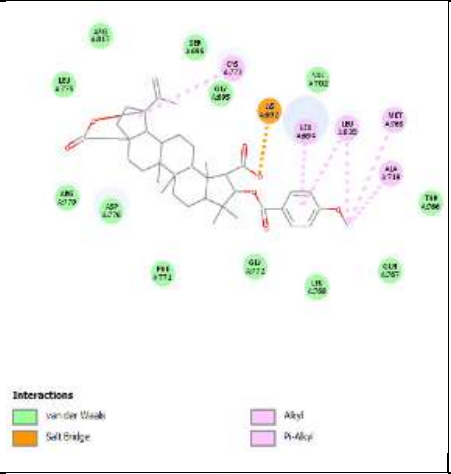
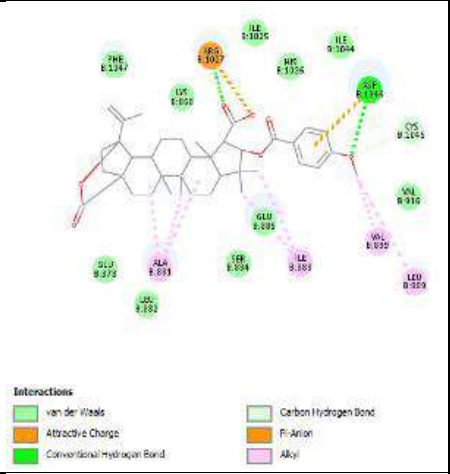
		3	-73.2387	-67.2655	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Unfavorable Bump Conventional Hydrogen Bond Carbon Hydrogen Bond Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Conventional Hydrogen Bond Alkyl Pi-Alkyl 	LEU A: 768	ALA B:				
		4	-71.5011	-68.2996			MET A: 769 GLN A: 767 SER A: 696	881 LEU B: 889 LEU B: 1019 HIS B: 1026 ILE B: 892 VAL B: 898 ILE B: 888				
		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	<i>Betulinic acid</i>	1			-67.6676	-71.1653	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Unfavorable Bump Attractive Charge Conventional Hydrogen Bond Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Alkyl Pi-Alkyl 	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	<i>Platanic acid</i>	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	<i>Lupeol</i>	1	-68.3782	-70.4803			LEU A: 820	ILE B: 888 VAL A: 899 LEU B: 889	
		2	-69.9271	-70.2604					
		3	-69.359	-71.1807					
		4	-70.5221	-69.2313				ALA A: 719 LEU A: 694	VAL A:

						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		ALAA: 719 VAL A: 702 LEU A: 820	LEU B:840 ASN B:923 CYS B:919 GLU B:917	
		2	-84.1628	-86.27				
		3	-83.5686	-86.3297				
		4	-83.0882	-86.2466				
		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				

27	<i>Corosolic acid</i>	10	-83.3826	-85.6531			VAL A: 702	ARG B: 1027
		1	-67.9092	-66.6492			GLN A: 767 MET A: 769	ALA B: 881 HIS B: 1026 ILE B: 888
		2	-67.8021	-66.5047			ARG A: 817 ALA A: 719	LEU B: 1019 LEU B: 892
		3	-67.8114	-63.1136			A: 694 LEU A: 820 CYS A: 773	CYS B: 1024
		4	-64.282	-69.0099			LYS A: 721	
		5	-65.5333	-60.4023				
		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	<i>Maesopsin</i>	1	-85.4452	-78.5049			LEU A: 820 ALA A: 719	PHE B: 1047
		2	-85.2406	-80.5067			LYS A: 721 LEU 764 764	GLU B: 917 ASP B: 1046 LYS B:
		3	-85.2331	-80.8398			THR A: 766 GLN A: 767	868 ALA B: 866
		4	-85.4479	-77.6907				LEU B: 1035 CYS B: 919
		5	-85.3693	-80.5155				CYS B: 1045 VAL

					 <p>Interactions ■ van der Waals ■ Conventional Hydrogen Bond ■ Pi-Alkyl</p>			
		6	-85.4493	-80.6725				B: 916 VAL B: 848
		7	-85.4199	-78.8763				
		8	-85.2116	-79.6688				
		9	-85.3704	-78.1647				
		10	-85.2596	-77.2723				
29	<i>Isorhamn etin3-O- (6''-O-(Z)-p-coumaroy l)-β-D-glucopyranoside</i>	1	-87.8293	-89.148	 <p>Interactions ■ van der Waals ■ Conventional Hydrogen Bond ■ Carbon Hydrogen Bond ■ Pi-Cation ■ Unfavorable Bump</p>		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	<i>Alphitoxolide</i>	1	-65.6741	-74.7165			LYS A: 692	ARG B: 1027

		2	-62.7882	-73.8794	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Alkyl Pi-Alkyl 	 <p>Interactions</p> <ul style="list-style-type: none"> van der Waals Attractive Charge Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Alkyl 	ALA A: 719 MET A: 769 LEU A: 820 LEU A: 694 CYS A: 773	ASP B: 1046 CYS B: 1045 ALA B: 881 ILE B: 888 VAL B: 899 LEU B: 889
		3	-65.8147	-74.2504				
		4	-64.9095	-74.4416				
		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				
2	-80.2845			-69.849				
3	-81.2921			-69.8069				
4	-80.8568			-69.6303				
5	-81.44			-70.0478				
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	<i>3-O-beta-D-Galactopyranosyl-quercetin</i>	1	-94.0572	-80.9045				
		2	-93.2175	-80.2223				
		3	-94.3898	-80.5791			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 AS P B: 1046
		4	-94.1567	-80.0277			ALA A: 719 LEU A: 820 VAL A: 702	ILE B: 888 CYS B: 1024
		5	-94.0227	-79.423			LYS A: 721	GLU B: 885
		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	<i>β-Sitosterol</i>	1	-93.6912	-84.8849				
		2	-91.7533	-81.5029		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	
		3	-91.8599	-81.338				

					<p>Interactions</p> <ul style="list-style-type: none"> van der Waals Alkyl 																															
					<p>Interactions</p> <ul style="list-style-type: none"> Van der Waals Unfavorable Bump Conventional Hydrogen Bond Carbon Hydrogen Bond Alkyl Pi-Alkyl 	<table border="1"> <tr> <td>VAL A: 702</td> <td>CYS B:1045</td> </tr> <tr> <td></td> <td>ILE B:888</td> </tr> <tr> <td></td> <td>CYS B:1024</td> </tr> <tr> <td></td> <td>LEU B:1019</td> </tr> <tr> <td></td> <td>LEU B:889</td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> <tr> <td></td> <td></td> </tr> </table>	VAL A: 702	CYS B:1045		ILE B:888		CYS B:1024		LEU B:1019		LEU B:889																				
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																																