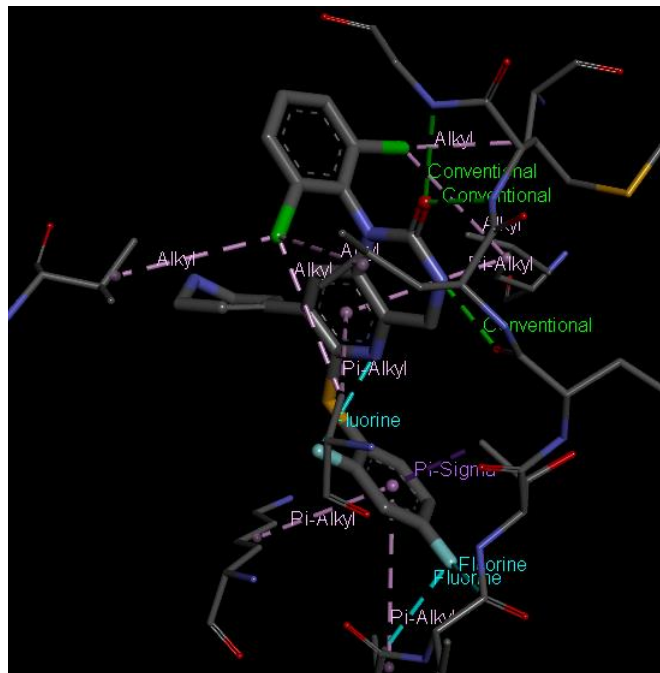
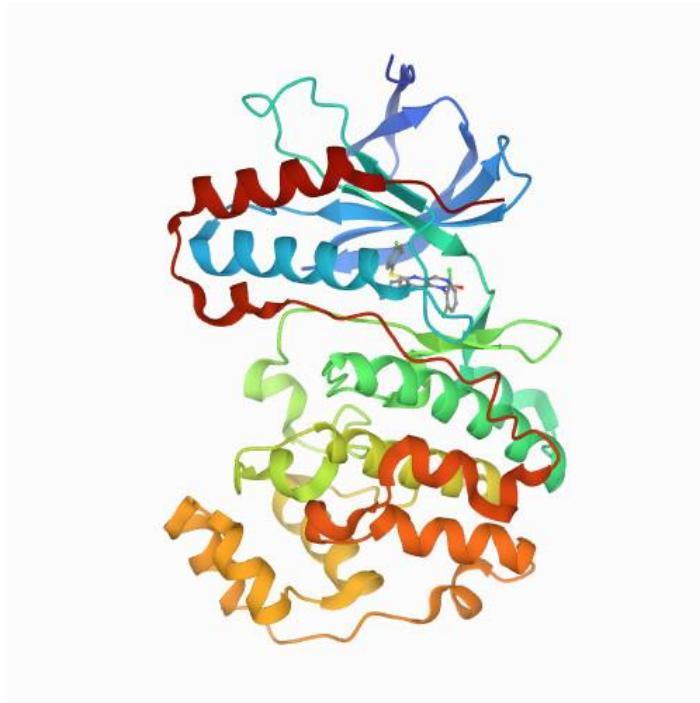
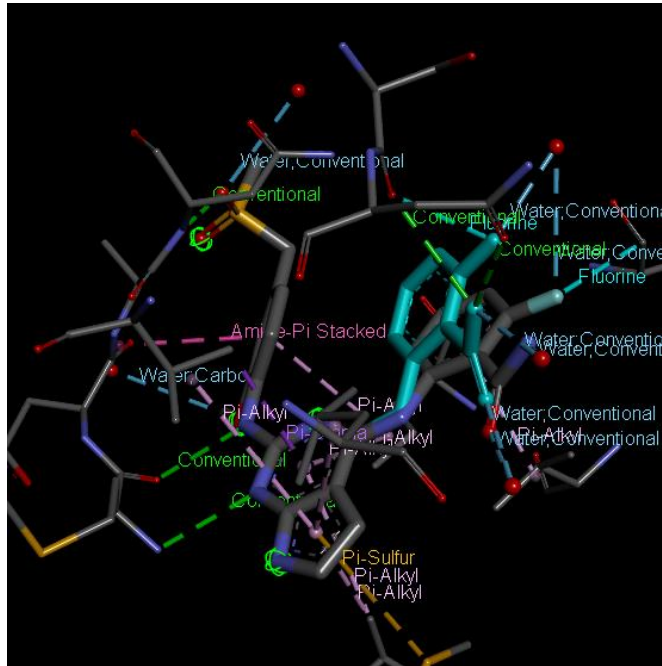
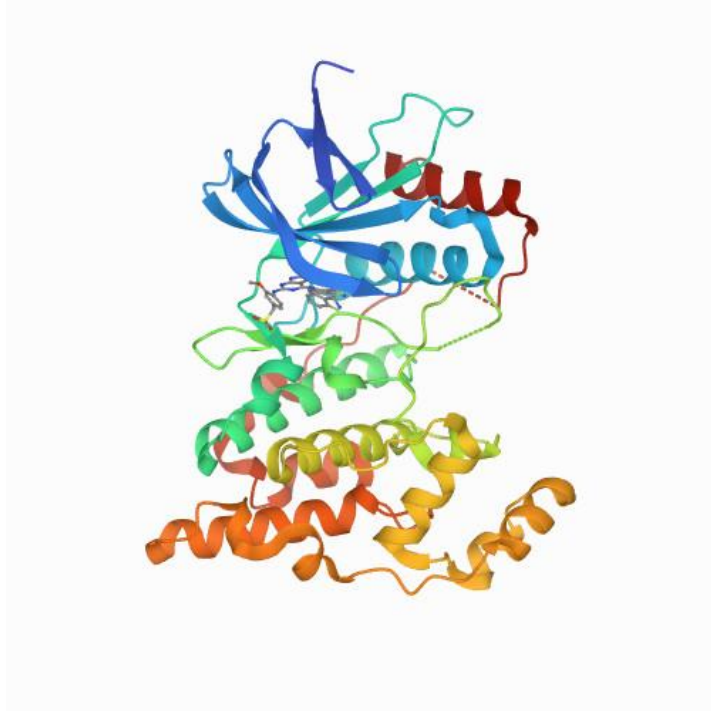
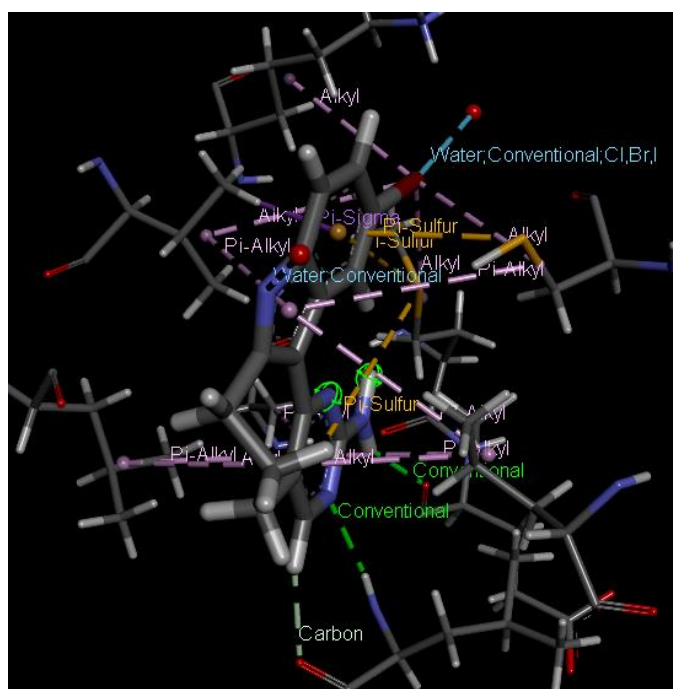
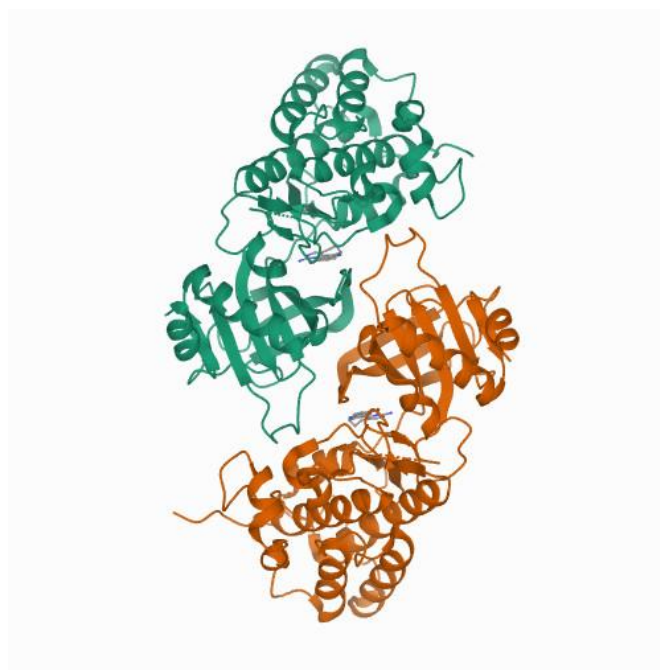


Lampiran 1. Struktur 3D makromolekul dan interaksi ligan asli

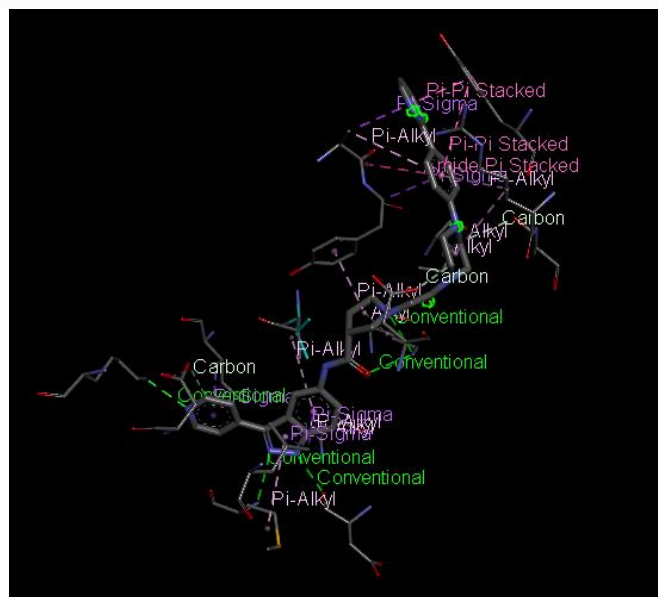
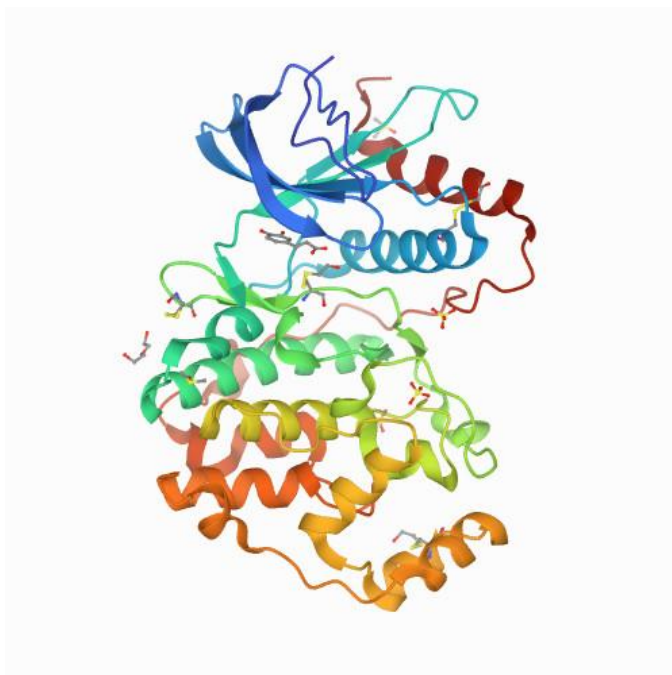
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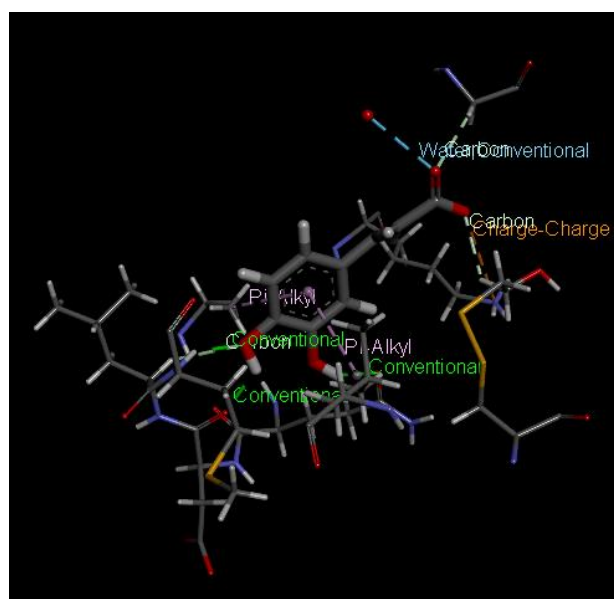
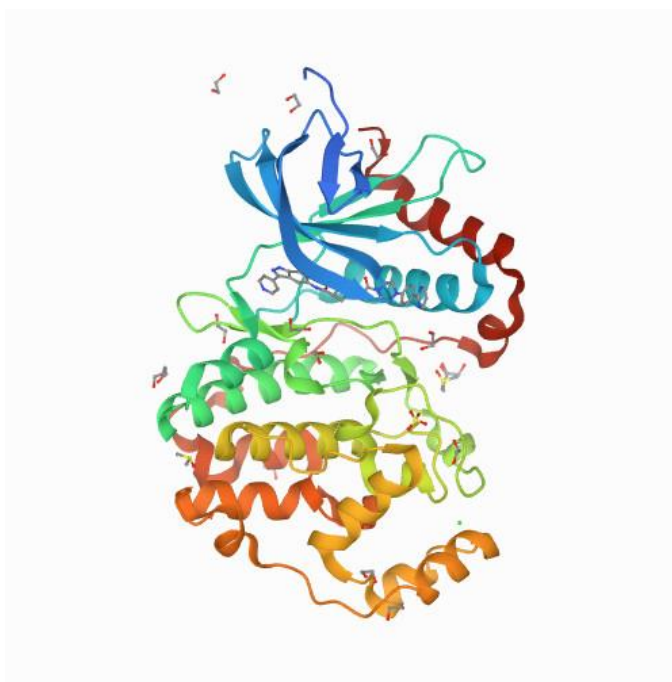
JNK1



Nf-Kb



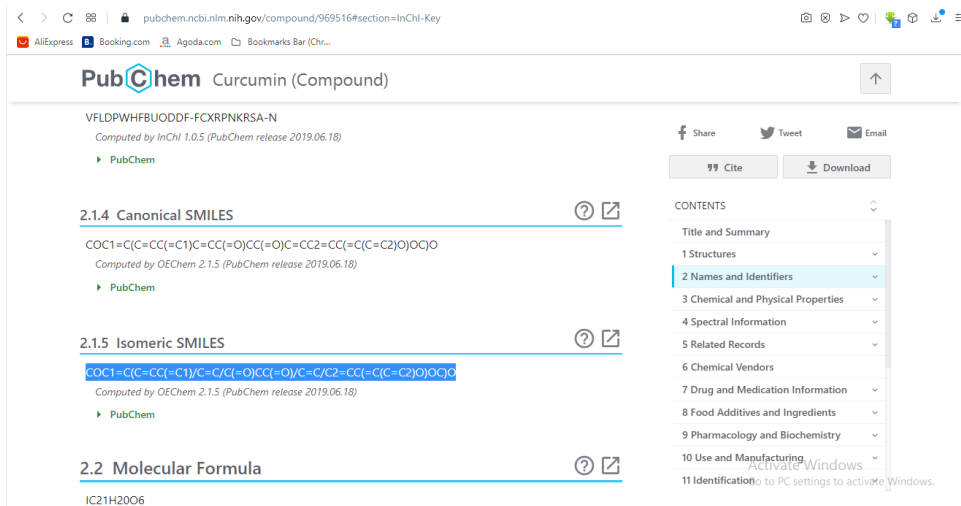
ERK2



ERK1

Lampiran 2. Prosedur Docking

1. Menggambar struktur ligan



pubchem.ncbi.nlm.nih.gov/compound/969516#section=InChI-Key

PubChem Curcumin (Compound)

VFLDPWHFBUODDF-FCXRPNKRSA-N
Computed by InChI 1.0.5 (PubChem release 2019.06.18)

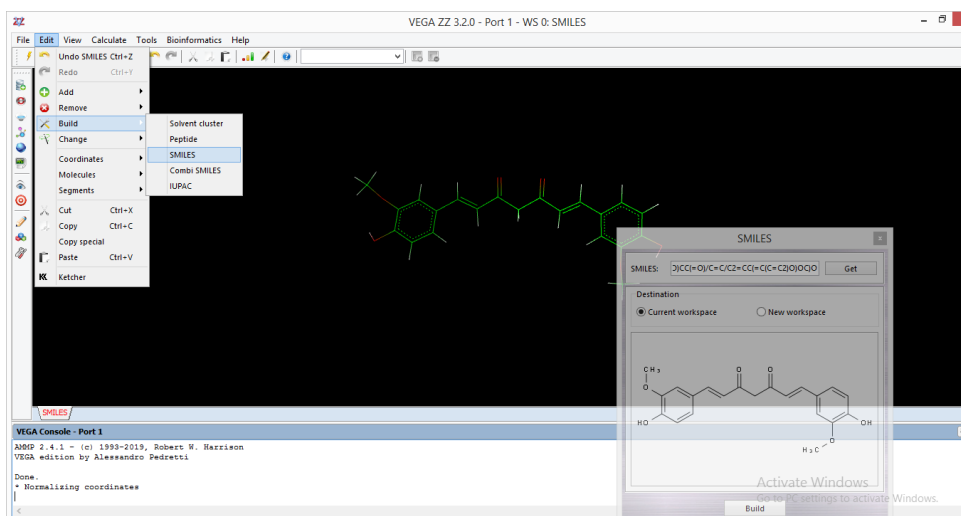
2.1.4 Canonical SMILES
COC1=C(C=CC(=C1)C=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC
Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

2.1.5 Isomeric SMILES
COC1=C(C=CC(=C1)/C=C/C(=O)CC(=O)/C=C/C2=CC(=C(C=C2)O)OC
Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

2.2 Molecular Formula
IC21H20O6

CONTENTS

- Title and Summary
- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Spectral Information
- 5 Related Records
- 6 Chemical Vendors
- 7 Drug and Medication Information
- 8 Food Additives and Ingredients
- 9 Pharmacology and Biochemistry
- 10 Use and Manufacturing
- 11 Identification



VEGA ZZ 3.2.0 - Port 1 - WS 0- SMILES

File Edit View Calculate Tools Bioinformatics Help

Undo SMILES Ctrl+Z
Redo Ctrl+Y
Add
Remove
Build
Change
Coordinates
Molecules
Segments
Cut Ctrl+X
Copy Ctrl+C
Copy special
Paste Ctrl+V
K Ketcher

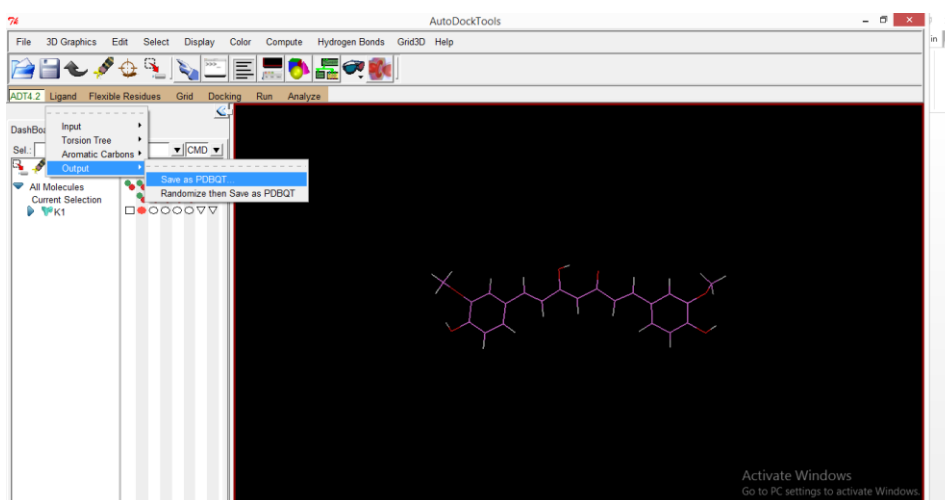
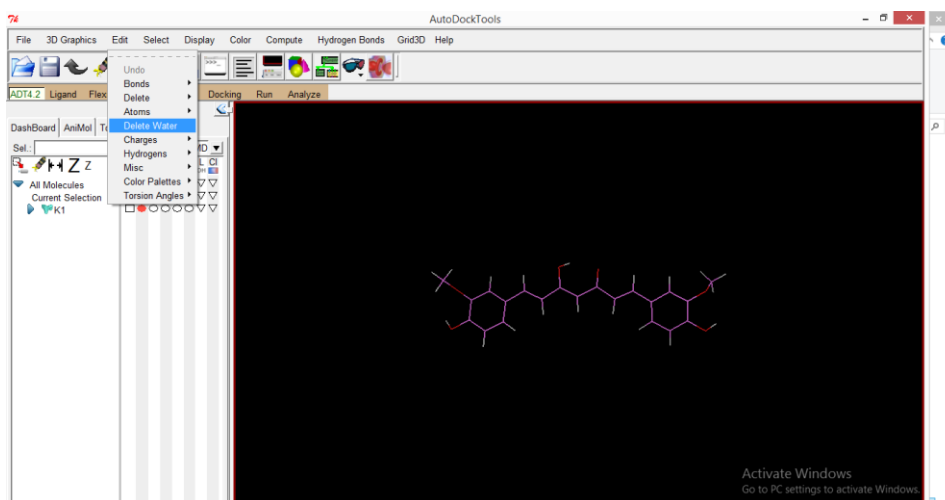
Solvent cluster
Peptide
SMILES
Combi SMILES
IUPAC

SMILES
SMILES: O=C1C=CC(=O)C=C(C=C1)OC Get
Destination
 Current workspace New workspace

VEGA Console - Port 1
A30IP 2.4.1 - (c) 1993-2019, Robert W. Harrison
VEGA edition by Alessandro Pedretti
Done
* Normalizing coordinates

Activate Windows
Go to PC settings to activate Windows.

2. Preparasi ligan uji



3. Mengetahui dan memisahkan ligan asli

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

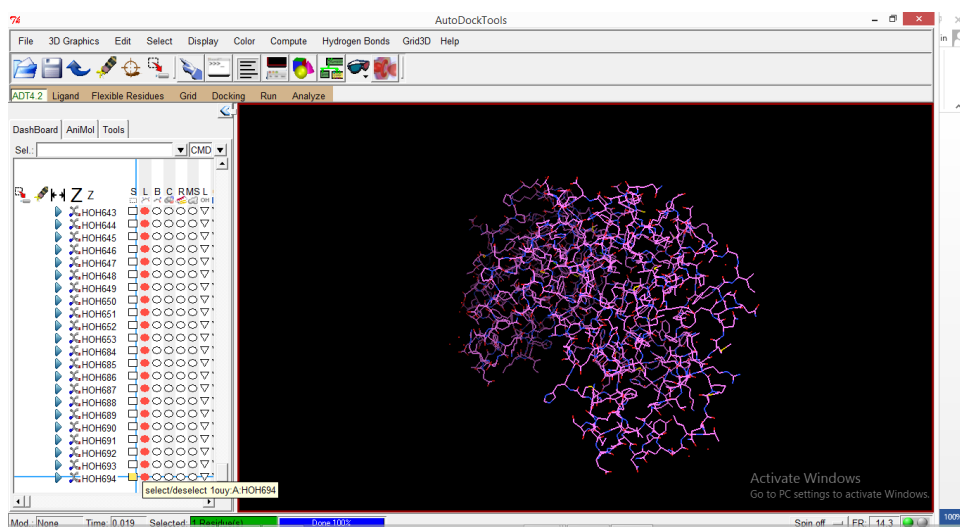
Reference Sequence 1OUY_1

PDB ENTITY SEQ 1OUY_1
UNPROT ALIGN Q16539
UNMODELED 1OUYA
ARTIFACT

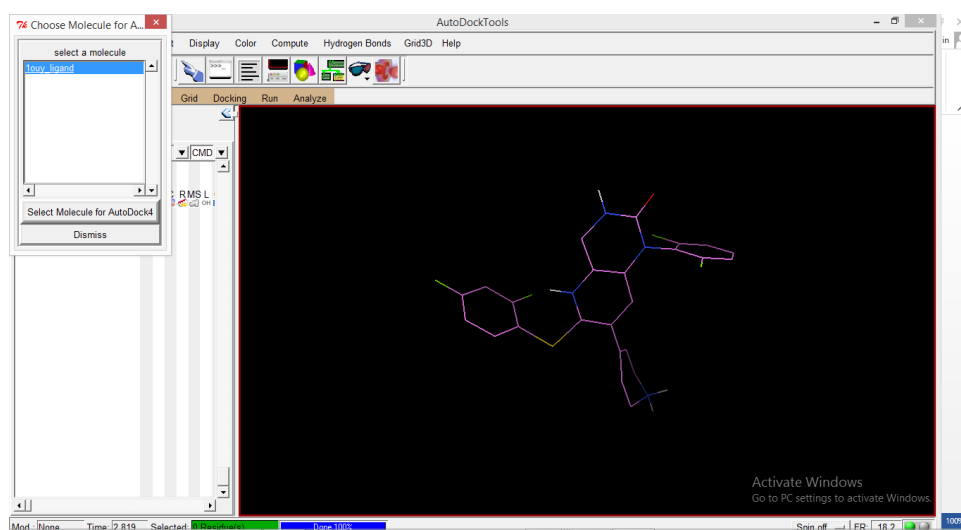
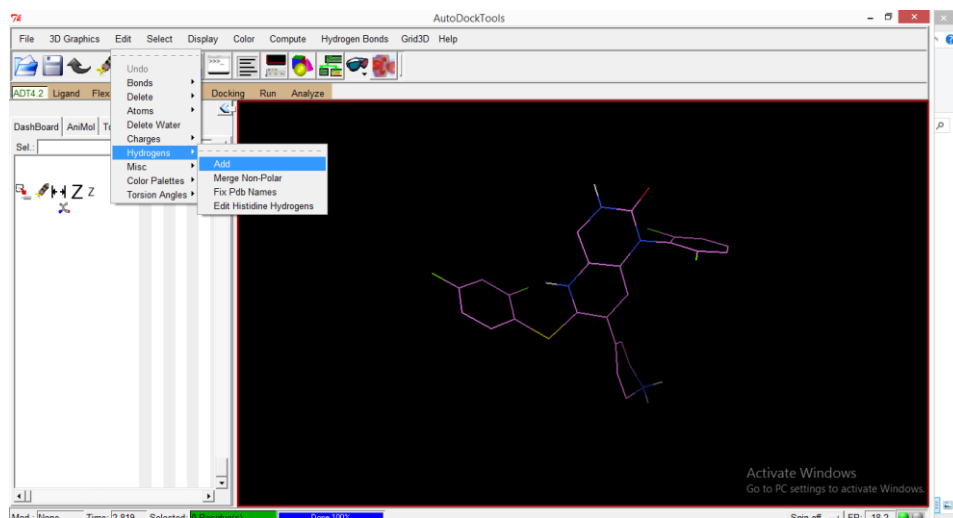
Small Molecules

Ligands 1 Unique

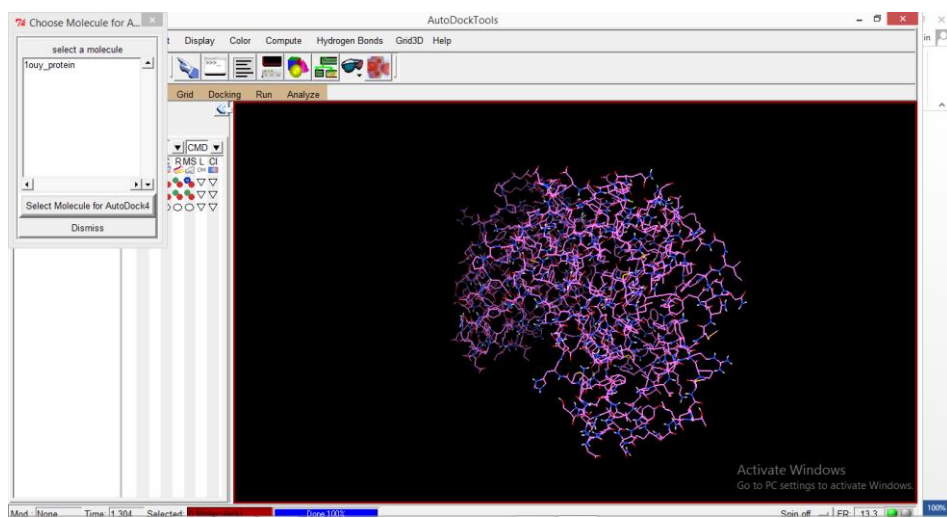
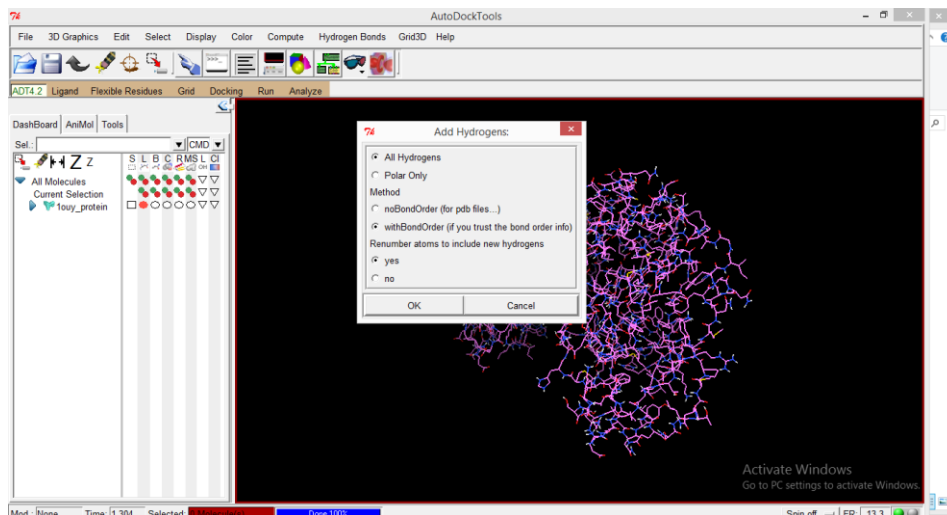
ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
094 Query on 094 Download CCD File	A	1-(2,6-DICHLOROPHENYL)-6-[[[2-(4-DIFLUOROPHENYL)SULFANYL]-7-(1,2,3,6-TETRAHYDRO-4-PYRIDINYL)-3,4-DIHYDROPYRIDO[3,2-D]PYRIMIDIN-2(1H)-ONE C ₂₄ H ₁₈ Cl ₂ F ₂ N ₄ O ₃ PZUXNWPJBLCKJB-UHFFFAOYSA-N		Ligand Interaction



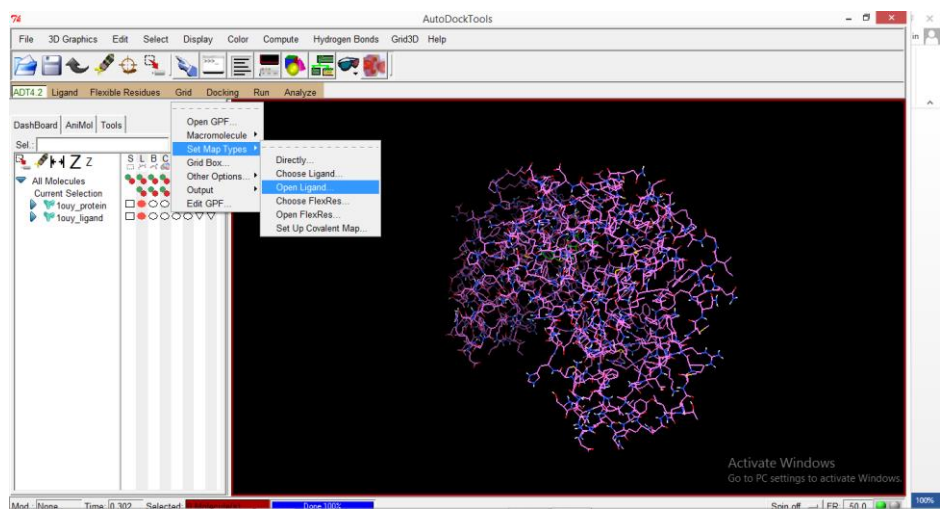
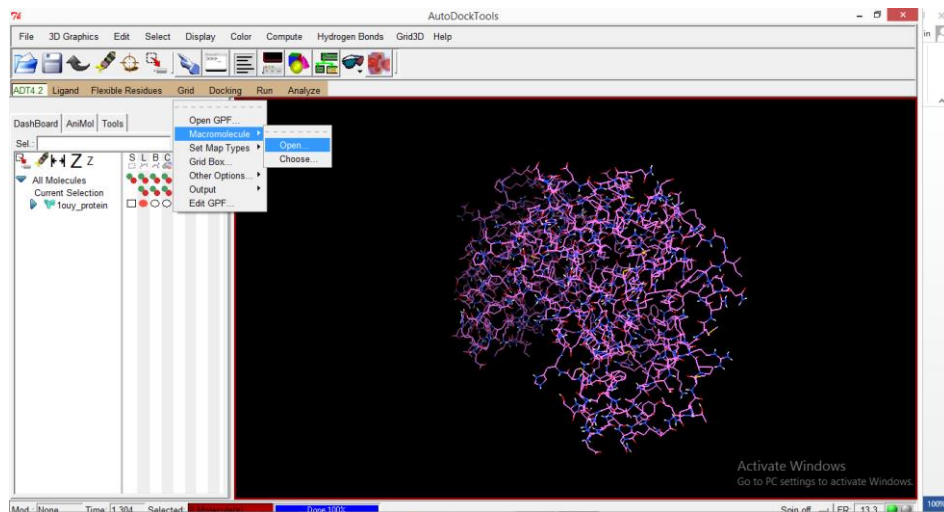
4. Preparasi ligan asli

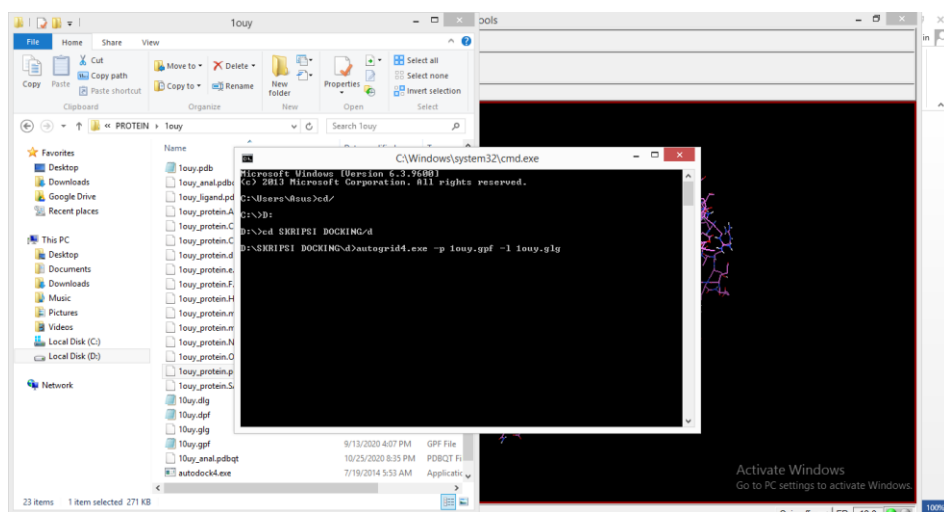
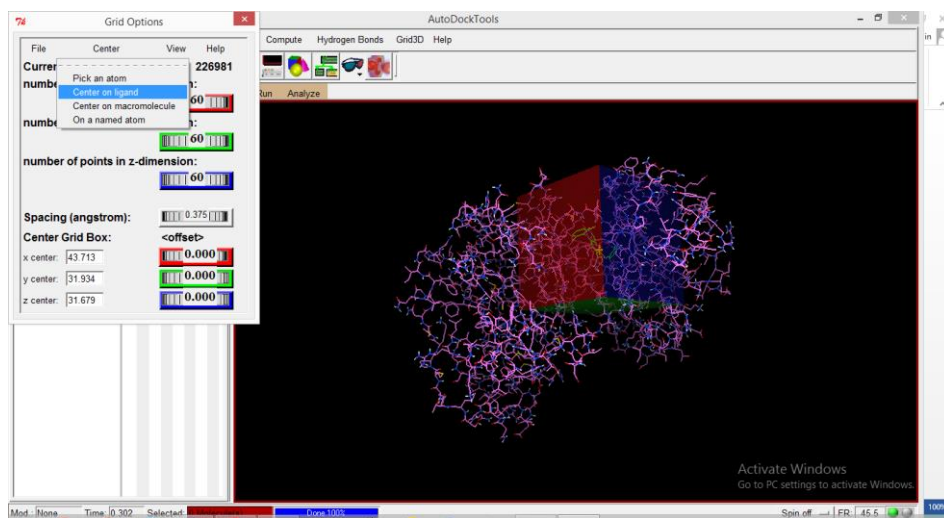


5. Preparasi protein

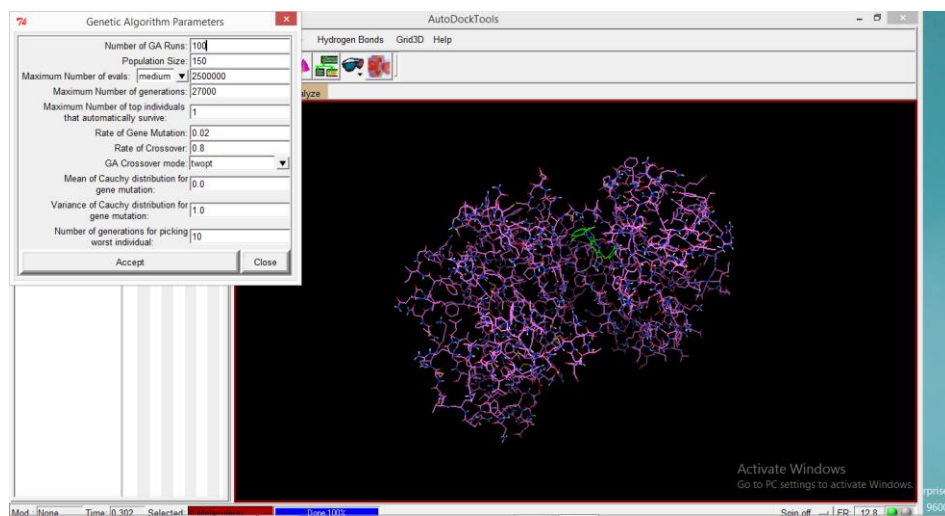
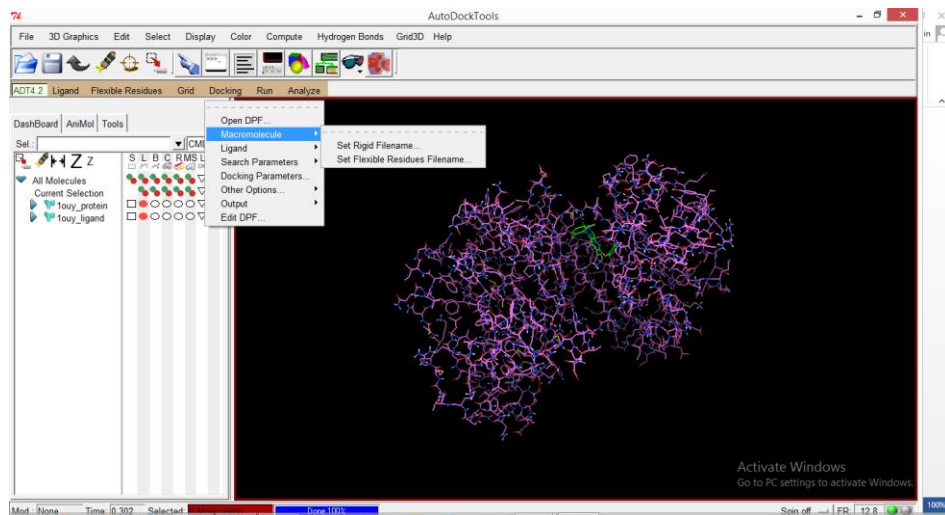


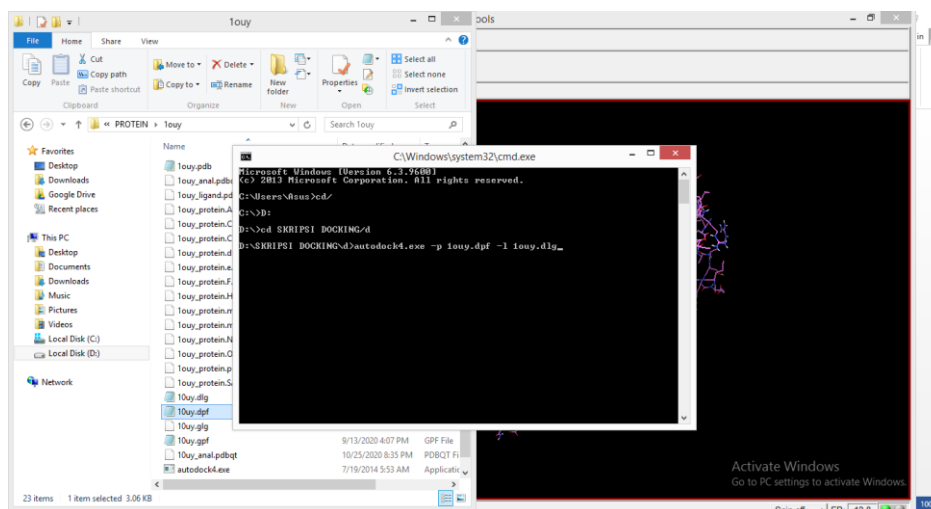
6. Preparasi gridbox



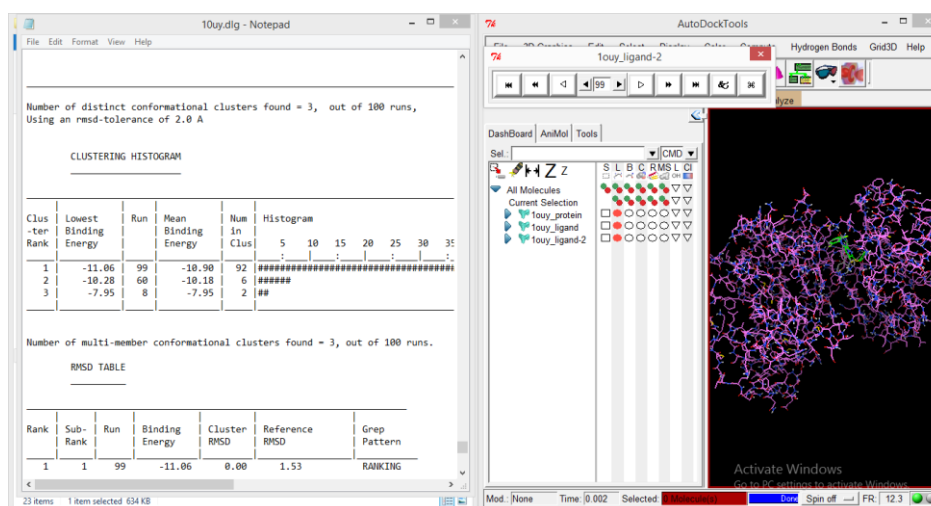


7. Validasi metode docking

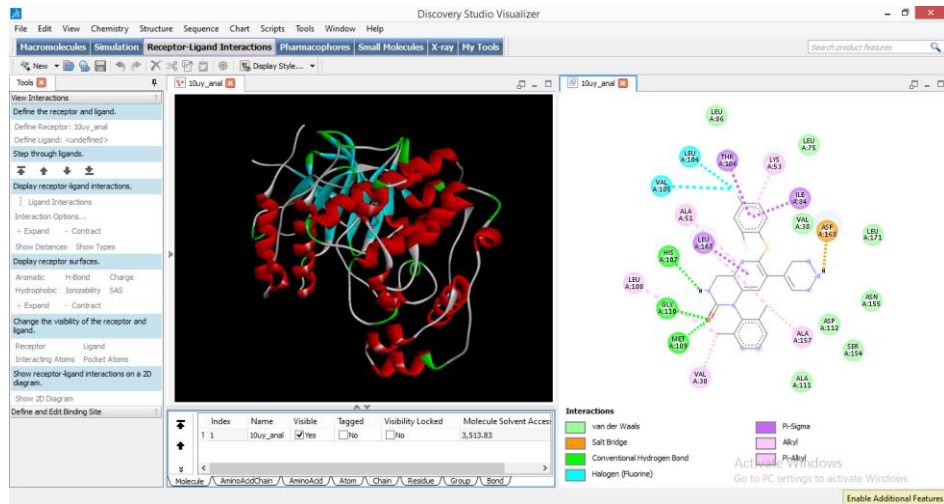




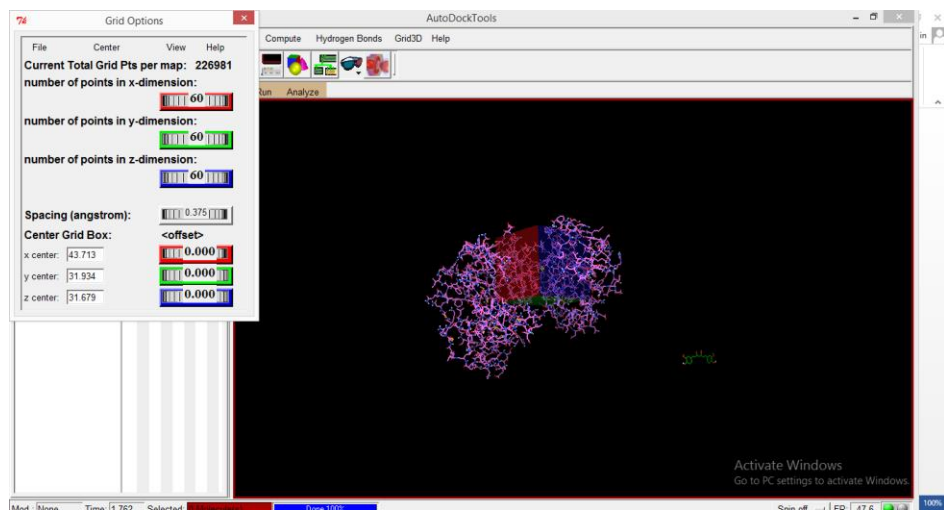
8. Pemilihan energi ikatan terbaik

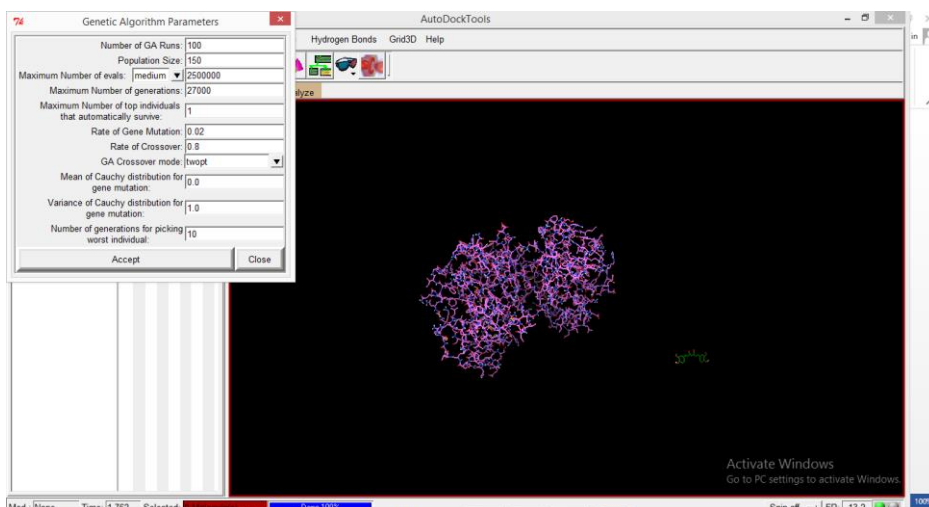


9. Visualisasi

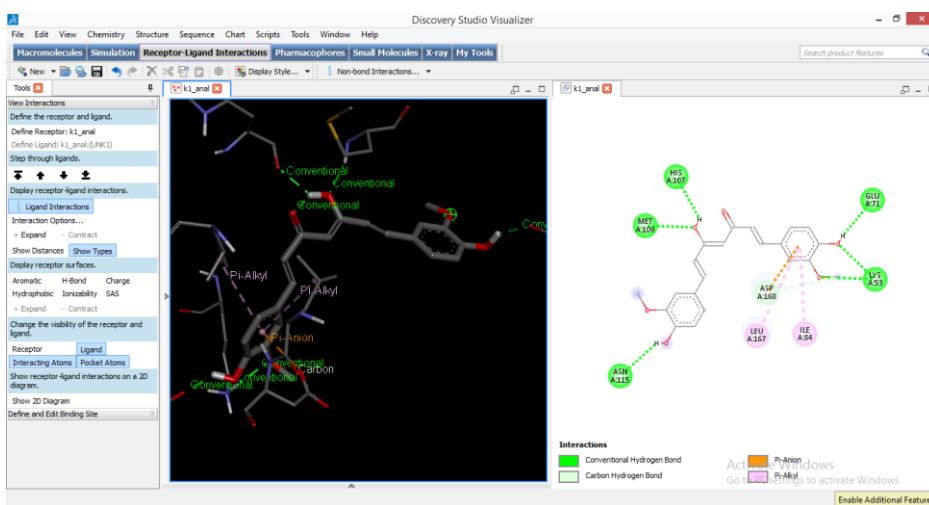
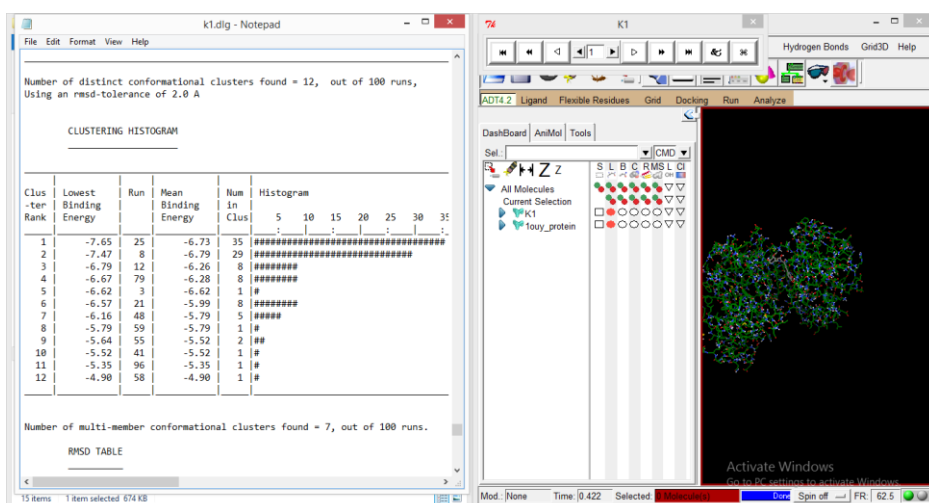


10. Docking dengan ligan uji





11. Visualisasi hasil docking



Lampiran 3. Hasil *docking*

Senyawa kunyit	Protein 1OUY				
	Rep1	Rep2	Rep3	Rata-rata	SD
Curcumin	-7.65	-7.79	-7.68	-7.71	0.073711
[1S-[1alpha,2beta,5beta(R*)]]-5-(1,5-Dimethyl-4-hexenyl)-2-methyl-3-cyclohexene-1,2-diol	-7.51	-7.61	-7.51	-7.54	0.057735
(+)-ar-Turmerone	-6.76	-6.85	-6.64	-6.75	0.105357
alpha-Turmerone	-6.89	-6.94	-6.81	-6.88	0.065574
Curlone	-7.28	-7.40	-7.27	-7.32	0.072342
Turmerone	-6.64	-6.62	-6.46	-6.57	0.098658
(+)-Curdione	-7.40	-7.40	-7.40	-7.40	1.09E-15
Dehydrocurdione	-7.23	-7.23	-7.23	-7.23	0
(E,E,E)-2-(4,8-Dimethyl-10-oxo-3,7-cyclodecadien-1-ylidene)-propanal	-7.35	-7.30	-7.36	-7.34	0.032146
Curcumenol	-7.14	-7.14	-7.14	-7.14	0
Procurcumadiol	-7.04	-7.05	-7.04	-7.04	0.005774
Zedoarondiol	-7.00	-7.01	-7.24	-7.08	0.135769
Procurcumenol	-7.63	-7.63	-7.63	-7.63	0
Bisacumol	-5.97	-5.87	-5.87	-5.90	0.057735
Curcumenone	-6.69	-6.69	-6.68	-6.69	0.005774
Isoprocurcumenol	-7.86	-7.86	-7.87	-7.86	0.005774
Turmeronol B	-6.60	-6.59	-6.60	-6.60	0.005774
bis-(4-hydroxycinnamoyl)methane	-7.10	-7.16	-7.23	-7.16	0.065064
Demethoxycurcumin	-7.28	-7.53	-7.39	-7.40	0.1253
Letestuienin A	-7.53	-7.50	-7.49	-7.51	0.020817
Letestuienin B	-7.55	-7.20	-7.55	-7.43	0.202073
Calebin A	-7.04	-7.32	-7.52	-7.29	0.241109
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	-6.02	-6.00	-6.02	-6.01	0.011547

Cetak tebal: hasil tiga terbaik

Senyawa kunyit	Protein 3ELJ				
	Rep1	Rep2	Rep3	Rata-rata	SD
Curcumin	-7.25	-7.37	-7.39	-7.34	0.075719
[1S-[1alpha,2beta,5beta(R*)]]-5-(1,5-Dimethyl-4-hexenyl)-2-methyl-3-cyclohexene-1,2-diol	-6.76	-6.74	-6.74	-6.75	0.011547
(+)-ar-Turmerone	-6.49	-6.49	-6.48	-6.49	0.005774
alpha-Turmerone	-6.86	-6.85	-6.84	-6.85	0.01
Curlone	-6.72	-6.81	-6.85	-6.79	0.066583
Turmerone	-6.38	-6.36	-6.37	-6.37	0.01
(+)-Curdione	-7.56	-7.56	-7.56	-7.56	0
Dehydrocurdione	-7.40	-7.40	-7.40	-7.40	1.09E-15
(E,E,E)-2-(4,8-Dimethyl-10-oxo-3,7-cyclodecadien-1-ylidene)-propanal	-6.99	-6.99	-6.99	-6.99	1.09E-15
Curcumenol	-6.82	-6.82	-6.82	-6.82	0
Procurcumadiol	-6.61	-6.61	-6.61	-6.61	0
Zedoarondiol	-7.47	-7.47	-7.47	-7.47	0
Procurcumenol	-7.19	-7.19	-7.19	-7.19	0
Bisacumol	-6.45	-6.44	-6.51	-6.47	0.037859
Curcumenone	-6.63	-6.63	-6.63	-6.63	0
Isoprocurcumenol	-7.15	-7.15	-7.15	-7.15	1.09E-15
Turmeronol B	-6.26	-6.26	-6.26	-6.26	1.09E-15
bis-(4-hydroxycinnamoyl)methane	-7.73	-7.89	-7.91	-7.84	0.098658
Demethoxycurcumin	-7.78	-7.78	-7.80	-7.79	0.011547
Letestuienin A	-7.90	-7.67	-7.80	-7.79	0.115326
Letestuienin B	-7.68	-7.54	-7.30	-7.51	0.19218
Calebin A	-7.72	-8.14	-8.06	-7.97	0.22301
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	-5.84			-5.84	

Cetak tebal: hasil tiga terbaik

Senyawa kunyit	Protein 3NPC				
	Rep1	Rep2	Rep3	Rata-rata	SD
Curcumin	-9.14	-9.12	-9.19	-9.15	0.036055513
[1S-[1alpha,2beta,5beta(R*)]]-5-(1,5-Dimethyl-4-hexenyl)-2-methyl-3-cyclohexene-1,2-diol	-7.65	-7.77	-7.72	-7.71	0.060277138
(+)-ar-Turmerone	-7.08	-7.09	-7.08	-7.08	0.005773503
alpha-Turmerone	-7.57	-7.57	-7.57	-7.57	0
Curlone	-7.50	-7.50	-7.50	-7.50	0
Turmerone	-6.96	-6.95	-6.94	-6.95	0.01
(+)-Curdione	-8.38	-8.38	-8.38	-8.38	0
Dehydrocurdione	-7.81	-7.81	-7.81	-7.81	0
(E,E,E)-2-(4,8-Dimethyl-10-oxo-3,7-cyclodecadien-1-ylidene)-propanal	-8.02	-8.02	-8.03	-8.02	0.005773503
Curcumenol	-7.20	-8.02	-8.02	-7.75	0.473427221
Procurcumadiol	-6.70	-6.70	-6.70	-6.70	0
Zedoarondiol	-7.35	-6.64	-7.34	-7.11	0.407062649
Procurcumenol	-7.14	-7.13	-7.14	-7.14	0.005773503
Bisacumol	-7.18	-7.18	-7.18	-7.18	0
Curcumenone	-7.64	-7.64	-7.63	-7.64	0.005773503
Isoprocurcumenol	-8.25	-8.25	-8.25	-8.25	0
Turmeronol B	-6.88	-6.88	-6.88	-6.88	0
bis-(4-hydroxycinnamoyl)methane	-8.70	-8.70	-8.70	-8.70	0
Demethoxycurcumin	-8.70	-8.64	-8.73	-8.69	0.045825757
Letestuanin A	-8.16	-8.63	-8.30	-8.36	0.241315837
Letestuanin B	-8.53	-8.50	-8.68	-8.57	0.096436508
Calebin A	-8.47	-8.44	-8.45	-8.45	0.015275252
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	-7.18	-7.18	-7.17	-7.18	0.005773503

Cetak tebal: hasil tiga terbaik

Senyawa kunyit	Protein 4IDT				
	Rep1	Rep2	Rep3	Rata-rata	SD
Curcumin	-8.13	-9.38	-9.16	-8.89	0.667308
[1S-[1alpha,2beta,5beta(R*)]]-5-(1,5-Dimethyl-4-hexenyl)-2-methyl-3-cyclohexene-1,2-diol	-6.78	-6.74	-6.78	-6.77	0.023094
(+)-ar-Turmerone	-6.92	-6.93	-6.38	-6.74	0.314696
alpha-Turmerone	-6.95	-7.12	-6.98	-7.02	0.090738
Curlone	-7.28	-7.36	-7.29	-7.31	0.043589
Turmerone	-6.21	-6.74	-6.78	-6.58	0.318172
(+)-Curdione	-7.64	-7.64	-7.64	-7.64	0
Dehydrocurdione	-6.98	-6.98	-6.98	-6.98	0
(E,E,E)-2-(4,8-Dimethyl-10-oxo-3,7-cyclodecadien-1-ylidene)-propanal	-7.43	-7.43	-7.43	-7.43	0
Curcumenol	-7.02	-7.02	-7.02	-7.02	0
Procurcumadiol	-7.00	-7.00	-7.00	-7.00	0
Zedoarondiol	-7.38	-7.38	-7.38	-7.38	0
Procurcumenol	-7.29	-7.29	-7.29	-7.29	0
Bisacumol	-6.48	-6.51	-6.52	-6.50	0.020817
Curcumenone	-6.86	-6.86	-6.85	-6.86	0.005774
Isoprocumumenol	-7.70	-7.70	-7.70	-7.70	0
Turmeronol B	-6.52	-6.51	-6.48	-6.50	0.020817
bis-(4-hydroxycinnamoyl)methane	-9.28	-9.29	-9.29	-9.29	0.005774
Demethoxycurcumin	-8.95	-9.00	-9.23	-9.06	0.149332
Letestuienin A	-7.47	-7.90	-8.26	-7.88	0.395517
Letestuienin B	-8.20	-7.72	-8.44	-8.12	0.366606
Calebin A	-7.53	-7.74	-7.46	-7.58	0.145717
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	-6.24	-6.24	-6.24	-6.24	1.09E-15

Cetak tebal: hasil tiga terbaik

Senyawa kunyit	Protein 4QTB				
	Rata-rata				SD
Curcumin	-8.81	-9.17	-9.01	-9.00	0.18037
[1S-[1alpha,2beta,5beta(R*)]]-5-(1,5-Dimethyl-4-hexenyl)-2-methyl-3-cyclohexene-1,2-diol	-7.52	-7.41	-7.22	-7.38	0.151767
(+)-ar-Turmerone	-7.34	-7.34	-7.33	-7.34	0.005774
alpha-Turmerone	-7.65	-7.67	-7.65	-7.66	0.011547
Curhone	-7.71	-7.72	-7.69	-7.71	0.015275
Turmerone	-7.22	-7.20	-7.23	-7.22	0.015275
(+)-Curdione	-8.10	-8.10	-8.11	-8.10	0.005774
Dehydrocurdione	-7.62	-7.62	-7.62	-7.62	0
(E,E,E)-2-(4,8-Dimethyl-10-oxo-3,7-cyclodecadien-1-ylidene)-propanal	-7.64	-7.64	-7.64	-7.64	0
Curcumenol	-7.21	-7.21	-7.21	-7.21	0
Procurcumadiol	-4.23			-4.23	
Zedoarondiol	-7.93	-7.93	-7.93	-7.93	0
Procurcumenol	-7.34	-7.34	-7.34	-7.34	0
Bisacumol	-7.23	-7.25	-7.24	-7.24	0.01
Curcumenone	-7.59	-7.62	-7.55	-7.59	0.035119
Isoprocurcumenol	-7.80	-7.80	-7.80	-7.80	0
Turmeronol B	-7.55	-7.57	-7.61	-7.58	0.030551
bis-(4-hydroxycinnamoyl)methane	-9.21	-9.23	-9.24	-9.23	0.015275
Demethoxycurcumin	-9.35	-9.28	-9.40	-9.34	0.060277
Letestuianin A	-9.16	-8.88	-9.04	-9.03	0.140475
Letestuianin B	-8.07	-8.95	-8.99	-8.67	0.52
Calebin A	-9.33	-9.11	-8.47	-8.97	0.446766
6-Methyl-7-(3-oxobutyl)-bicyclo[4.1.0]heptan-3-one	-6.54	-6.54	-6.54	-6.54	0

Cetak tebal: hasil tiga terbaik

Senyawa rosela	Protein IOUY				SD
	Rep1	Rep2	Rep3	Rata-rata	
Eugenol	-5.63			-5.63	
Myricetin	-6.89	-7.13	-7.20	-7.07	0.162583
Trigonelline	-3.9			-3.90	
3,4-Dihydroxybenzoic acid	-3.97			-3.97	
Cholesterol	-9.15	-9.20	-9.18	-9.18	0.025166
Ergosterol	-9.47	-9.52	-9.57	-9.52	0.05
Spinasterol	-9.94	-9.99	-9.88	-9.94	0.055076
Quercetin	-7.11	-7.17	-7.18	-7.15	0.037859
Gossypetin	-7.15	-7.17	-7.16	-7.16	0.01
Hibiscetin	-6.33	-6.69	-6.96	-6.66	0.31607
Hibiscetin 3-glucoside	-7.70	-7.64	-6.97	-7.44	0.405257
Delphinidin 3-sambubioside	-7.33	-6.30	-6.51	-6.71	0.544273
Citric acid	-3.26			-3.26	
D-(+)-Galactose	-4.56			-4.56	
alpha-Terpineol	-5.97			-5.97	
Daphniphylline	-9.21	-10.19	-9.28	-9.56	0.546717
Malic acid	-3.30			-3.30	

Cetak tebal: hasil tiga terbaik

Senyawa rosela	Protein 3ELJ				SD
	Rep1	Rep2	Rep3	Rata-rata	
Eugenol	-4.79			-4.79	
Myricetin	-6.97	-6.97	-6.96	-6.97	0.005774
Trigonelline	-4.29			-4.29	
3,4-Dihydroxybenzoic acid	-4.68			-4.68	
Cholesterol	-9.02	-8.95	-9.11	-9.03	0.080208
Ergosterol	-9.67	-9.66	-9.64	-9.66	0.015275
Spinasterol	-10.16	-10.18	-10.18	-10.17	0.011547
Quercetin	-6.91	-6.95	-6.92	-6.93	0.020817
Gossypetin	-6.57	-6.88	-6.89	-6.78	0.181934
Hibiscetin	-6.81	-6.77	-6.61	-6.73	0.10583
Hibiscetin 3-glucoside	-8.81	-8.69	-8.98	-8.83	0.145717
Delphinidin 3-sambubioside	-6.37	-7.19	-7.25	-6.94	0.491664
Citric acid	-2.78			-2.78	
D-(+)-Galactose	-2.28			-2.28	
alpha-Terpineol	-5.97			-5.97	
Daphniphylline	-5.86			-5.86	
Malic acid	-2.55			-2.55	

Cetak tebal: hasil tiga terbaik

Senyawa rosela	Protein 3NPC				
	Rep1	Rep2	Rep3	Rata-rata	SD
Eugenol	-5.72			-5.72	
Myricetin	-7.51	-7.51	-7.51	-7.51	1.08779E-15
Trigonelline	-5.4			-5.40	
3,4-Dihydroxybenzoic acid	-6.39	-6.37	-6.38	-6.38	0.01
Cholesterol	-11.23	-11.28	-11.26	-11.26	0.025166115
Ergosterol	-11.90	-11.87	-11.87	-11.88	0.017320508
Spinasterol	-11.97	-11.92	-11.93	-11.94	0.026457513
Quercetin	-7.58	-7.57	-7.53	-7.56	0.026457513
Gossypetin	-7.84	-7.77	-7.76	-7.79	0.043588989
Hibiscetin	-6.99	-7.00	-6.98	-6.99	0.01
Hibiscetin 3-glucoside	-6.24	-5.95	-6.16	-6.12	0.149777613
Delphinidin 3-sambubioside	-6.08	-5.92	-6.09	-6.03	0.09539392
Citric acid	-5.65			-5.65	
D-(+)-Galactose	-2.92			-2.92	
alpha-Terpineol	-6.64			-6.64	
Daphniphylline	-7.89	-7.37	-8.72	-7.99	0.680906259
Malic acid	-5.6			-5.60	

Cetak tebal: hasil tiga terbaik

Senyawa rosela	Protein 4IDT				SD
	Rep1	Rep2	Rep3	Rata-rata	
Eugenol	-4.79			-4.79	
Myricetin	-7.36	-7.37	-7.33	-7.35	0.020817
Trigonelline	-3.63			-3.63	
3,4-Dihydroxybenzoic acid	-3.97			-3.97	
Cholesterol	-10.02	-10.02	-10.03	-10.02	0.005774
Ergosterol	-10.62	-10.63	-10.63	-10.63	0.005774
Spinasterol	-9.72	-9.73	-9.70	-9.72	0.015275
Quercetin	-7.40	-7.58	-7.41	-7.46	0.10116
Gossypetin	-7.23	-7.22	-7.33	-7.26	0.060828
Hibiscetin	-7.38	-7.18	-7.19	-7.25	0.112694
Hibiscetin 3-glucoside	-7.67	-7.74	-7.74	-7.72	0.040415
Delphinidin 3-sambubioside	-7.58	-7.15	-6.95	-7.23	0.321921
Citric acid	-4.4			-4.40	
D-(+)-Galactose	-2.55			-2.55	
alpha-Terpineol	-5.67			-5.67	
Daphniphylline	-8.85	-8.86	-8.84	-8.85	0.01
Malic acid	-4.24			-4.24	

Cetak tebal: hasil tiga terbaik

Senyawa rosela	Protein 4QTB				SD
	Rep1	Rep2	Rep3	Rata-rata	
Eugenol	-5.28			-5.28	
Myricetin	-7.88	-7.90	-7.84	-7.87	0.030551
Trigonelline	-4.74			-4.74	
3,4-Dihydroxybenzoic acid	-5.34			-5.34	
Cholesterol	-11.16	-11.14	-11.15	-11.15	0.01
Ergosterol	-11.37	-11.37	-11.37	-11.37	0
Spinasterol	-11.20	-11.18	-11.20	-11.19	0.011547
Quercetin	-7.88	-7.92	-7.91	-7.90	0.020817
Gossypetin	-8.23	-8.24	-8.26	-8.24	0.015275
Hibiscetin	-7.87	-7.88	-7.88	-7.88	0.005774
Hibiscetin 3-glucoside	-9.37	-9.44	-9.48	-9.43	0.055678
Delphinidin 3-sambubioside	-8.61	-8.61	-8.6	-8.61	0.005774
Citric acid	-4.28			-4.28	
D-(+)-Galactose	-2.23			-2.23	
alpha-Terpineol	-5.86			-5.86	
Daphniphylline	-7.18	-7.17	-7.18	-7.18	0.005774
Malic acid	-4.29			-4.29	

Cetak tebal: hasil tiga terbaik