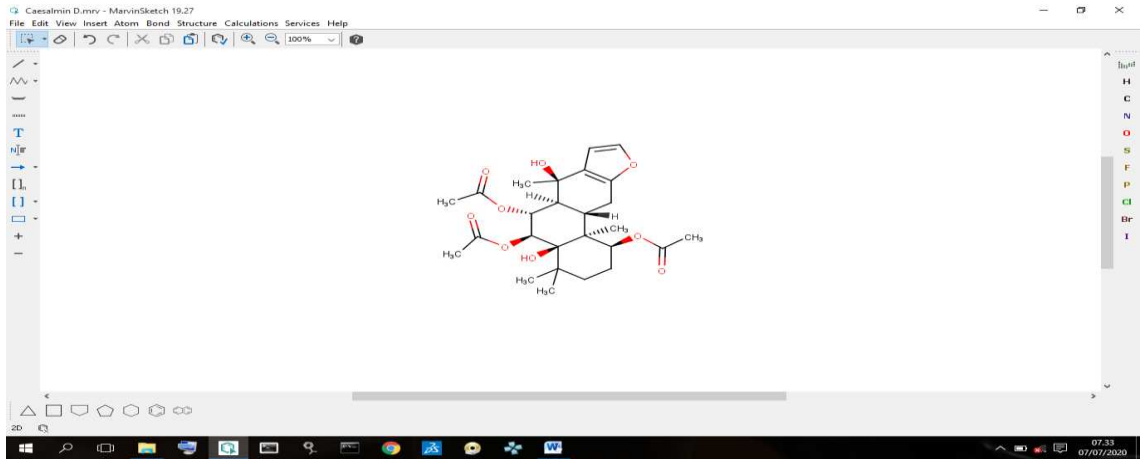
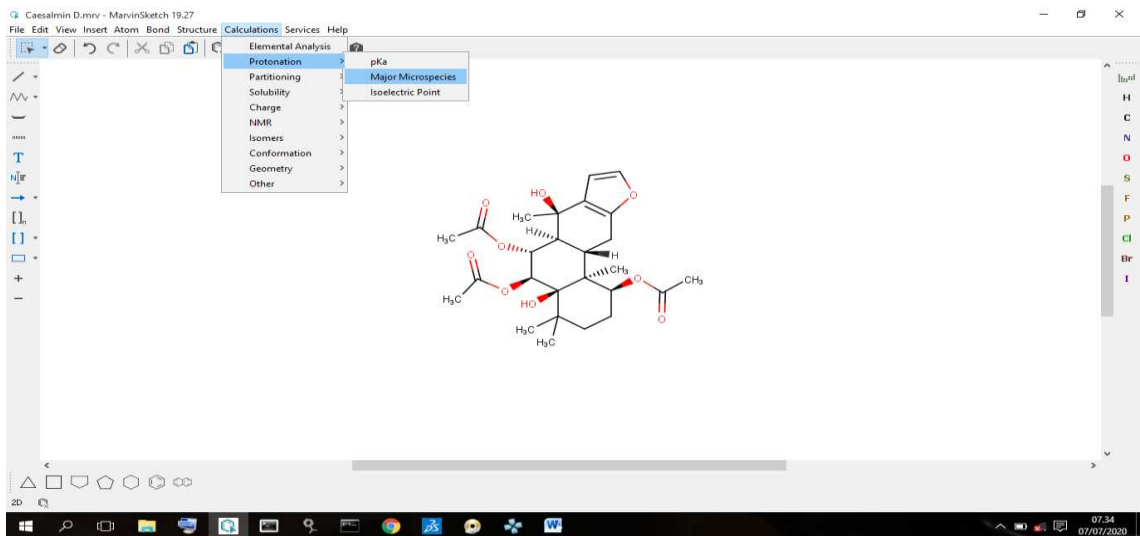


LAMPIRAN 1

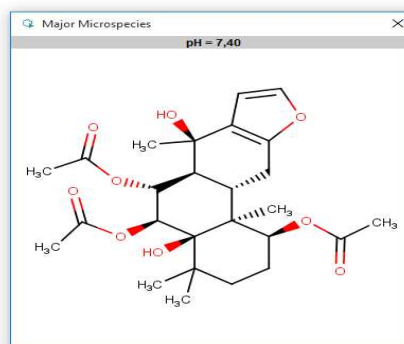
PREPARASI LIGAN



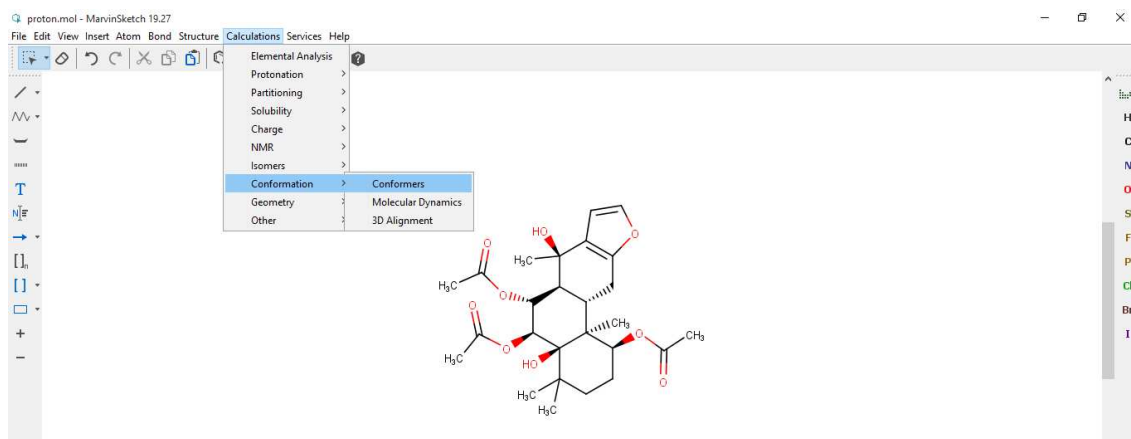
Pembuatan struktur ligan di MarvinSketch



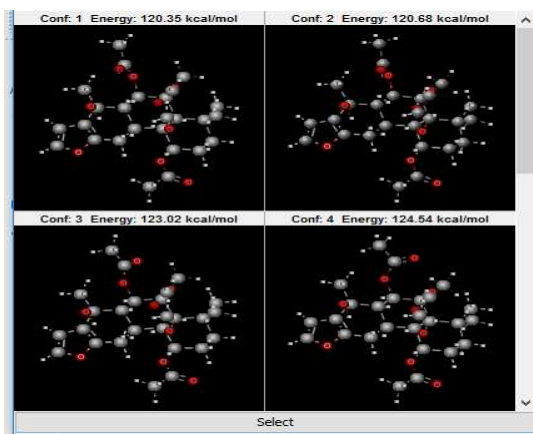
Ligan diprotonasi menggunakan software MarvinSketch 19.27



Ligan hasil protonasi



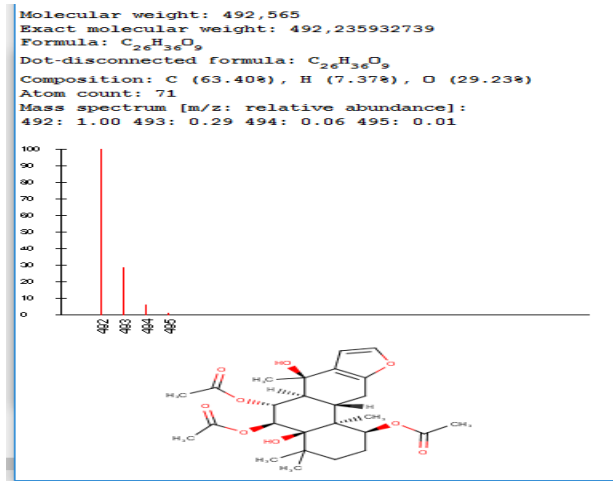
Ligan hasil protonasi dilakukan conformation



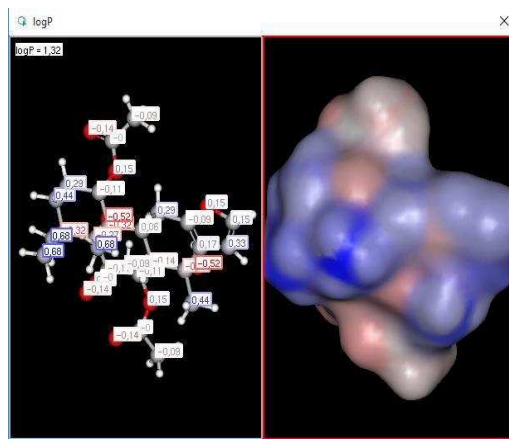
Ligan hasil konformasi

LAMPIRAN II

DRUG SCAN



Hasil berat molekul senyawa Favipiravir



Hasil logP senyawa Favipiravir

LAMPIRAN III

PREPARASI RESEPTOR

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Biological Assembly 1

1CET

CHLOROQUINE BINDS IN THE COFACTOR BINDING SITE OF PLASMODIUM FALCIPARUM LACTATE DEHYDROGENASE.

DOI: 10.2210/pdb1CET/pdb

Classification: OXIDOREDUCTASE
 Organism(s): Plasmodium falciparum
 Expression System: Escherichia coli
 Mutation(s): No

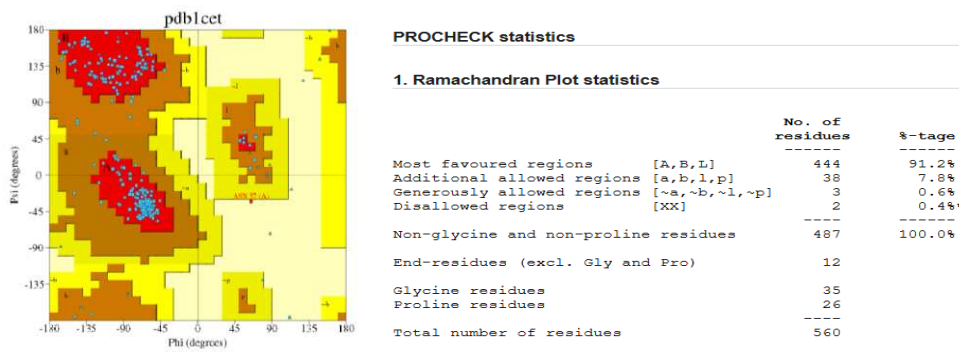
Deposited: 1999-03-10 Released: 1999-03-19
 Deposition Author(s): Read, J.A., Wilkinson, K.W., Tranter, R., Sessions, R.B., Brady, R.L.

Experimental Data Snapshot
 Method: X-RAY DIFFRACTION
 Resolution: 2.05 Å
 R-Value Free: 0.193
 R-Value Work: 0.154

wwPDB Validation
 Metric Percentile Ranks Value
 Clashscore 4
 Ramachandran outliers 0.3%
 Sidechain outliers 3.1%
 RSRZ outliers 2.3%

3D View: Structure | Electron Density | Ligand Interaction
 Global Symmetry: Dihedral - D2 (3D View)
 Global Stoichiometry: Homo 4-mer - A4

Pengunduhan reseptor 1CET melalui website <https://www.rcsb.org/>



Ramachandran Plot kode reseptor 1CET

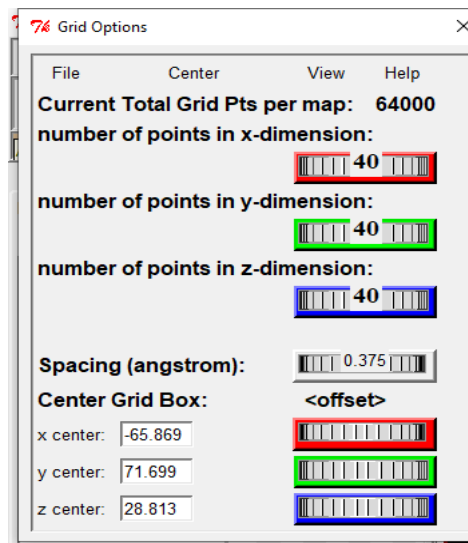
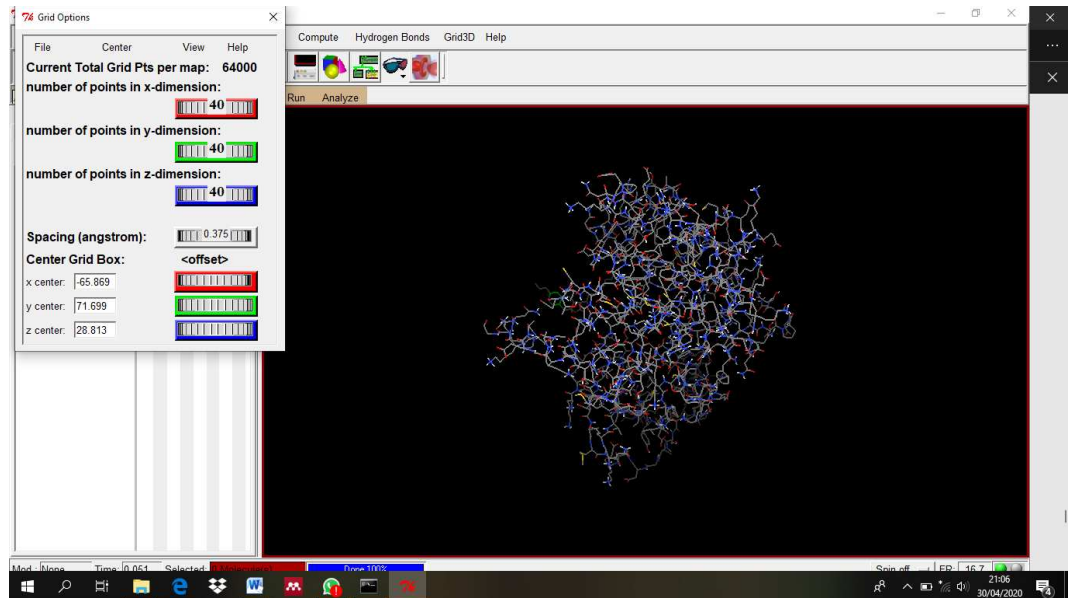
LAMPIRAN IV

VALIDASI DOCKING

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
6734						
6735						
6736						
6737						
6738						
6739	1	1	-7.25	0.00	2.46	RANKING
6740	1	2	-7.20	1.93	1.65	RANKING
6741	1	3	-7.13	1.52	1.80	RANKING
6742	1	4	-7.11	1.98	1.84	RANKING
6743	1	5	-7.08	1.03	2.11	RANKING
6744	1	6	-7.07	1.59	1.72	RANKING
6745	1	7	-7.07	1.37	1.87	RANKING
6746	1	8	-6.89	1.42	1.85	RANKING
6747	2	1	-7.04	0.00	2.88	RANKING
6748	3	1	-7.02	0.00	1.71	RANKING
6749	3	2	-7.01	1.49	1.26	RANKING
6750	3	3	-7.00	1.83	1.51	RANKING
6751	3	4	-6.89	1.51	1.47	RANKING
6752	3	5	-6.86	1.06	1.91	RANKING
6753	3	6	-6.86	1.47	1.68	RANKING
6754	3	7	-6.84	0.79	1.72	RANKING
6755	3	8	-6.69	1.11	1.90	RANKING
6756	3	9	-6.42	1.18	1.83	RANKING
6757	3	10	-6.35	1.16	1.69	RANKING
6758	4	1	-6.87	0.00	4.10	RANKING
6759	4	2	-5.87	1.20	3.59	RANKING
6760	5	1	-6.73	0.00	2.47	RANKING
6761	5	2	-6.56	0.98	2.48	RANKING
6762	5	3	-6.30	1.50	2.32	RANKING
6763	6	1	-6.38	0.00	3.34	RANKING
6764	6	2	-6.22	1.96	3.51	RANKING
6765	6	3	-5.87	1.70	3.79	RANKING
6766	7	1	-6.35	0.00	3.14	RANKING

Perolehan nilai binding affinity dan RMSD (Root Mean Square Deviation)

LAMPIRAN V
DOCKING LIGAN UJI DAN VISUALISASI



Pengaturan grid box untuk proses docking

```

Command Prompt
Microsoft Windows [Version 10.0.17763.1158]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Users\PC-HP>d:

D:\>cd monaspyridine B

D:\monaspyridine B>autogrid4.exe -p a.gpf -l a.dlg

autogrid4: Successful Completion.

D:\monaspyridine B>autodock4.exe -p a.dpf -l a.dlg

autodock4: Successful Completion on "LAPTOP-VN7274N8"

D:\monaspyridine B>

```

Proses docking senyawa Favipiravir melalui command prompt

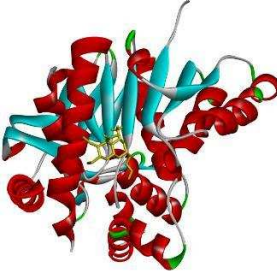
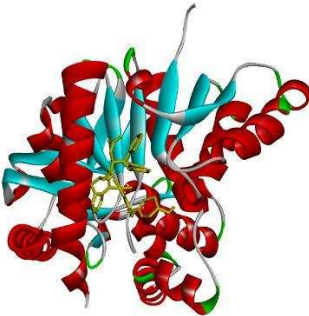
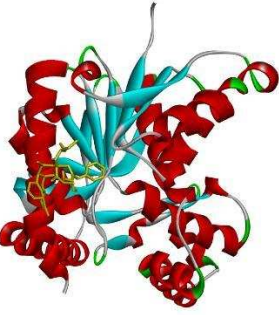
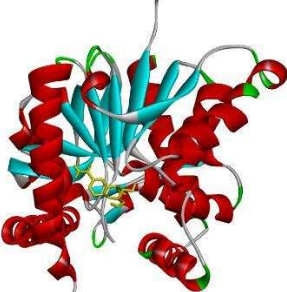
E:\senyawa\A.dlg - Notepad++

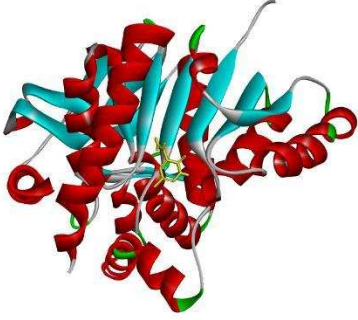
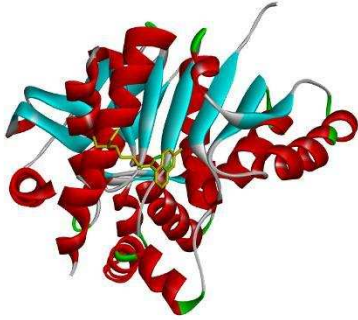
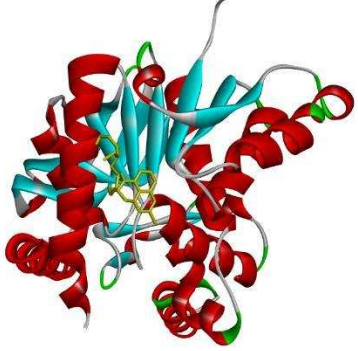
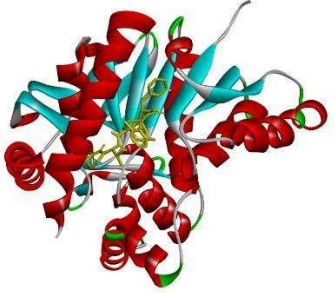
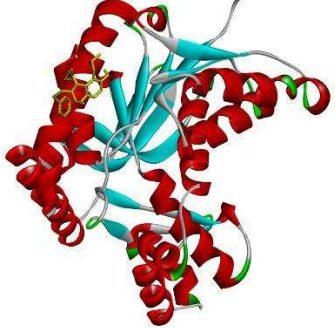
Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern	
7047							
7048							
7049							
7050							
7051							
7052							
7053							
7054	1	1	3	-9.71	0.00	33.21	RANKING
7055	1	2	24	-9.40	1.16	33.04	RANKING
7056	1	3	11	-7.88	1.93	31.83	RANKING
7057	1	4	9	-7.86	1.98	31.88	RANKING
7058	1	5	30	-7.79	1.90	31.88	RANKING
7059	1	6	16	-7.78	1.52	33.84	RANKING
7060	1	7	20	-7.32	1.74	32.37	RANKING
7061	2	1	26	-8.82	0.00	32.43	RANKING
7062	2	2	14	-8.73	1.06	32.54	RANKING
7063	2	3	15	-8.40	0.82	32.18	RANKING
7064	2	4	6	-8.36	0.81	32.81	RANKING
7065	2	5	29	-7.50	1.89	30.96	RANKING
7066	3	1	22	-8.65	0.00	32.36	RANKING
7067	3	2	13	-8.30	1.09	31.66	RANKING
7068	3	3	17	-8.18	0.68	31.98	RANKING
7069	3	4	21	-7.66	1.82	31.73	RANKING
7070	3	5	29	-7.65	1.68	31.84	RANKING
7071	3	6	7	-7.10	1.65	31.03	RANKING
7072	4	1	4	-7.22	0.00	32.03	RANKING
7073	4	2	10	-7.14	1.35	31.20	RANKING
7074	5	1	1	-7.11	0.00	29.61	RANKING
7075	5	2	8	-6.90	1.18	29.96	RANKING
7076	6	1	2	-6.90	0.00	30.02	RANKING
7077	6	2	28	-6.89	1.04	29.93	RANKING
7078	6	3	27	-6.08	1.93	29.92	RANKING
7079	6	4	18	-6.06	1.42	29.53	RANKING
7080	7	1	5	-6.45	0.00	29.32	RANKING
7081	8	1	19	-6.38	0.00	30.79	RANKING
7082	9	1	25	-5.97	0.00	29.94	RANKING
7083	10	1	12	-5.91	0.00	29.95	RANKING

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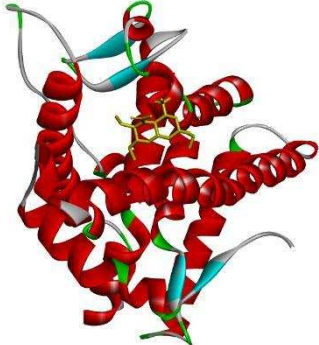
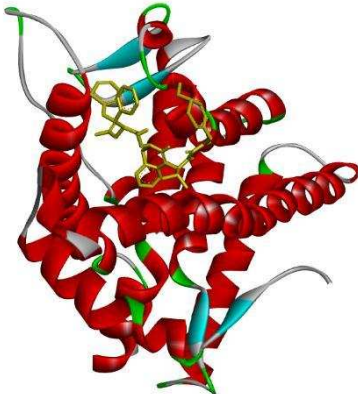
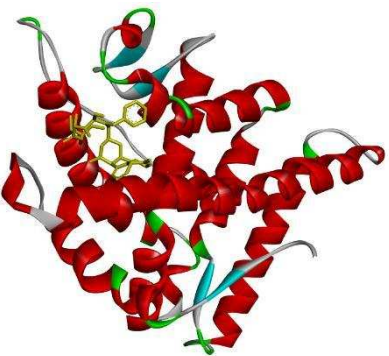
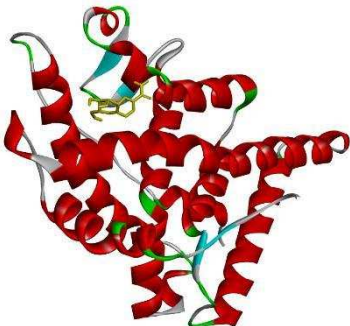
Perolehan nilai binding affinity hasil docking senyawa Favipiravir

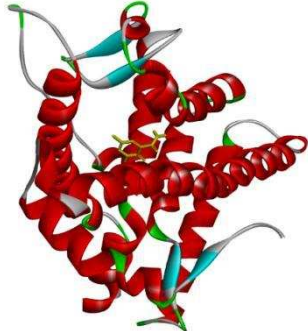
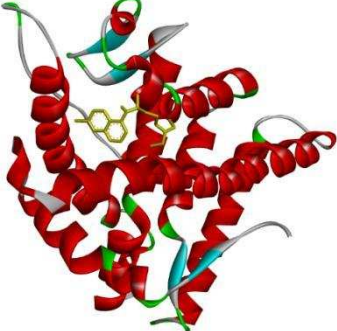
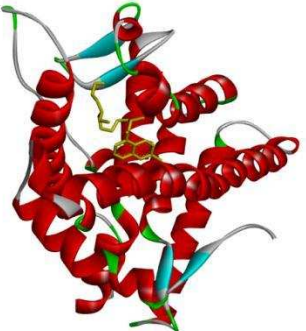
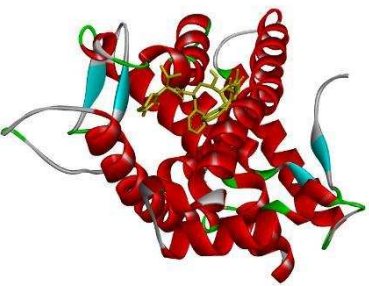
Tabel Hasil Visualisasi Kode Reseptor 1CET dengan Senyawa Uji
dalam Bentuk 3D

NO	NAMA SENYAWA	GAMBAR SENYAWA 3D
1	Oseltamivir	
2	Ritonavir	
3	Remdesivir	
4	Ribavirin	

5	Favipiravir	
6	Chloroquine	
7	Hydroxychloroquine	
8	Lopinavir	
9	Umifenovir hydrochloride	

Tabel Hasil Visualisasi Kode Reseptor 4UDC dengan Senyawa Uji
dalam Bentuk 3D

NO	NAMA SENYAWA	GAMBAR SENYAWA 3D
1	Oseltamivir	
2	Ritonavir	
3	Remdesivir	
4	Ribavirin	

5	Favipiravir	
6	Chloroquine	
7	Hydroxychloroquine	
8	Lopinavir	
9	Umifenovir hydrochloride	