

LAMPIRAN 1

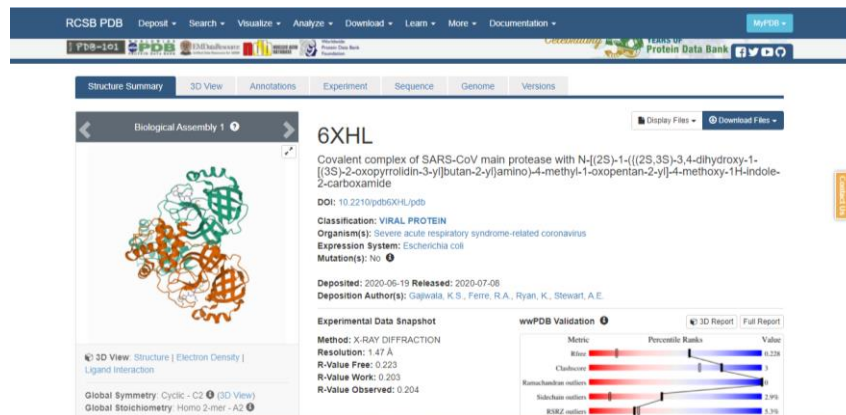
Analisis Reseptor Main Protease



Lamp 1.1 Reseptor 6XHM



Lamp 1.2 Reseptor 6XHN



Lamp 1.3 Reseptor 6XHL

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100 YEARS OF Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

Biological Assembly 1

6MOK

The crystal structure of COVID-19 main protease in complex with an inhibitor 11b

DOI: 10.2210/pdb6MOK/pdb

Classification: VIRAL PROTEIN
 Organism(s): Severe acute respiratory syndrome coronavirus 2
 Expression System: Escherichia coli BL21(DE3)
 Mutation(s): No

Deposited: 2020-02-22 Released: 2020-04-29
 Deposition Author(s): Zhang, B., Zhao, Y., Ji, Z., Liu, X., Yang, H., Liu, H., Rao, Z., Jiang, H.
 Funding Organization(s): Chinese Academy of Sciences, National Natural Science Foundation of China (NSFC)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
 Resolution: 1.50 Å
 R-Value Free: 0.193
 R-Value Work: 0.179
 R-Value Observed: 0.180

wwPDB Validation

Metric	Percentile Rank	Value
R-factors	100	0.197
Clashscore	100	0
Ramachandran outliers	100	0
Sidechain outliers	100	1.5%
RSRZ outliers	100	9.2%

3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View)

Lamp 1.4 Receptor 6MOK

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation MyPDB

100 YEARS OF Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

Biological Assembly 1

6LZE

The crystal structure of COVID-19 main protease in complex with an inhibitor 11a

DOI: 10.2210/pdb6LZE/pdb

Classification: VIRAL PROTEIN
 Organism(s): Severe acute respiratory syndrome coronavirus 2
 Expression System: Escherichia coli BL21(DE3)
 Mutation(s): No

Deposited: 2020-02-19 Released: 2020-04-29
 Deposition Author(s): Zhang, B., Zhang, Y., Jing, Z., Liu, X., Yang, H., Liu, H., Rao, Z., Jiang, H.
 Funding Organization(s): National Natural Science Foundation of China (NSFC), Chinese Academy of Sciences

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
 Resolution: 1.50 Å
 R-Value Free: 0.199
 R-Value Work: 0.176
 R-Value Observed: 0.177

wwPDB Validation

Metric	Percentile Rank	Value
R-factors	100	0.203
Clashscore	100	0
Ramachandran outliers	100	0.8%
Sidechain outliers	100	7.6%
RSRZ outliers	100	7.6%

3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Cyclic - C2 (3D View)

Lamp1.4 Receptor 6LZE

LAMPIRAN II

Validasi Metode *Docking*

D:\pejuang 5\ldocking\validasi reseptor\6XHM\prot.dlg - Notepad++

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
6743						
6744						
6745						
6746						
6747						
6748						
6749						
6750						
6751						
6752	1	1	94	-3.70	0.00	6.73
6753	1	2	55	-3.37	1.09	6.24
6754	1	3	90	-3.37	1.08	6.24
6755	1	4	98	-3.37	1.08	6.38
6756	1	5	7	-3.37	1.09	6.25
6757	1	6	53	-3.36	1.07	6.28
6758	1	7	43	-3.36	1.10	6.43
6759	1	8	36	-3.36	1.10	6.40
6760	1	9	67	-3.35	1.10	6.22
6761	1	10	85	-3.35	1.08	6.25
6762	1	11	45	-3.34	1.06	6.35
6763	1	12	15	-3.33	1.07	6.31
6764	1	13	96	-3.32	1.14	6.36
6765	1	14	35	-3.32	1.11	6.29
6766	1	15	72	-3.32	1.12	6.42
6767	1	16	61	-3.32	1.07	6.30
6768	1	17	9	-3.31	1.13	6.22
6769	1	18	99	-3.31	1.14	6.25
6770	1	19	44	-3.31	1.15	6.41
6771	1	20	3	-3.31	1.16	6.37
6772	1	21	63	-3.30	1.16	6.35
6773	1	22	75	-3.30	1.08	6.39
6774	1	23	5	-3.29	1.17	6.42
6775	1	24	89	-3.29	1.17	6.37
6776	1	25	4	-3.29	1.10	6.23
6777	1	26	30	-3.29	1.19	6.41
6778	1	27	65	-3.29	1.15	6.23
6779	1	28	17	-3.28	1.13	6.28
6780	1	29	42	-3.28	1.10	6.27

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Lamp 2.1 Hasil Redocking Reseptor 6XHM

D:\pejuang 5\ldocking\validasi reseptor\6XHM\prot.dlg - Notepad++

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
6744						
6745						
6746						
6747						
6748						
6749						
6750						
6751						
6752	1	1	22	-3.33	0.00	6.54
6753	1	2	81	-3.31	0.09	6.52
6754	1	3	19	-3.30	0.16	6.49
6755	1	4	10	-3.29	0.17	6.47
6756	1	5	57	-3.27	0.32	6.44
6757	1	6	53	-3.26	0.34	6.43
6758	1	7	74	-3.25	0.94	6.62
6759	1	8	6	-3.24	0.40	6.62
6760	1	9	89	-3.24	0.25	6.62
6761	1	10	43	-3.23	0.40	6.61
6762	1	11	4	-3.21	0.40	6.64
6763	1	12	26	-3.18	0.44	6.43
6764	1	13	9	-3.18	0.30	6.54
6765	1	14	94	-3.17	0.29	6.70
6766	1	15	62	-3.16	0.53	6.39
6767	1	16	98	-3.16	0.58	6.76
6768	1	17	50	-3.14	0.63	6.78
6769	1	18	21	-3.13	0.49	6.43
6770	1	19	33	-3.12	0.62	6.43
6771	1	20	79	-3.10	0.75	6.77
6772	1	21	1	-3.09	0.84	6.84
6773	1	22	11	-3.08	0.72	6.67
6774	1	23	2	-3.08	0.85	6.85
6775	1	24	73	-3.07	1.07	6.92
6776	1	25	45	-3.07	0.85	6.78
6777	1	26	40	-3.06	1.07	6.92
6778	1	27	71	-3.06	1.23	7.09
6779	1	28	95	-3.05	1.01	6.97
6780	1	29	13	-3.05	1.28	6.97

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Lamp 2.2 Hasil Redocking Reseptor 6XHN

D:\pejuang 5\ldocking\6XHL docking\6XHL\prot.dlg - Notepad++

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
13449						
13450						
13451						
13452						
13453						
13454						
13455						
13456						
13457	1	1	49	-14.43	0.00	1.44
13458	1	2	30	-14.42	0.71	1.51
13459	1	3	36	-13.52	1.63	1.81
13460	1	4	67	-13.33	0.82	1.66
13461	1	5	91	-13.30	1.77	1.98
13462	1	6	4	-13.27	1.87	2.06
13463	1	7	86	-13.27	1.49	1.69
13464	1	8	61	-13.24	1.74	1.69
13465	1	9	9	-13.17	1.65	1.44
13466	1	10	42	-13.13	1.99	2.07
13467	1	11	45	-13.10	1.60	1.97
13468	1	12	82	-12.99	1.49	1.64
13469	1	13	6	-12.87	1.75	1.54
13470	1	14	21	-12.86	1.99	2.10
13471	1	15	52	-12.85	1.96	1.72
13472	1	16	58	-12.72	1.63	1.96
13473	1	17	35	-12.41	0.96	1.59
13474	1	18	8	-12.43	1.98	2.08
13475	1	19	43	-12.31	1.45	1.58
13476	1	20	16	-12.20	1.44	1.66
13477	1	21	59	-12.16	1.80	1.81
13478	1	22	79	-11.97	1.78	1.77
13479	1	23	33	-11.96	1.80	1.80
13480	1	24	24	-11.80	1.96	1.68
13481	1	25	74	-11.73	1.99	1.72
13482	1	26	75	-11.66	1.98	1.75
13483	1	27	89	-11.61	1.73	1.62
13484	1	28	48	-11.60	1.73	1.74
13485	1	29	50	-11.54	1.88	1.73

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Lamp 2.3 Hasil Redocking Kode Reseptor 6XHL

D:\pejuang S1\docking\6MOK docking\6MOK\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg

12034
12035
12036
12037
12038
12039

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern	
12042	1	1	14	-14.06	0.00	1.22	RANKING
12044	1	2	2	-14.04	0.39	1.10	RANKING
12045	1	3	40	-13.61	1.20	1.84	RANKING
12046	1	4	57	-13.41	1.16	1.59	RANKING
12047	1	5	38	-13.33	1.65	2.00	RANKING
12048	1	6	94	-13.30	1.52	1.52	RANKING
12049	1	7	13	-13.07	1.61	1.99	RANKING
12050	1	8	20	-12.67	1.97	2.30	RANKING
12051	1	9	99	-12.19	1.63	1.62	RANKING
12052	1	10	96	-11.82	1.95	1.94	RANKING
12053	1	11	17	-11.59	1.82	2.17	RANKING
12054	2	1	41	-13.97	0.00	4.25	RANKING
12055	2	2	50	-13.94	0.49	4.27	RANKING
12056	2	3	60	-13.93	0.89	4.14	RANKING
12057	2	4	43	-13.73	0.28	4.21	RANKING
12058	2	5	58	-13.70	0.46	4.33	RANKING
12059	2	6	36	-13.69	0.71	4.24	RANKING
12060	2	7	69	-13.68	0.34	4.15	RANKING
12061	2	8	37	-13.54	0.73	4.18	RANKING
12062	2	9	23	-13.42	1.37	4.33	RANKING
12063	2	10	18	-13.04	0.85	4.18	RANKING
12064	2	11	70	-12.99	0.76	4.18	RANKING
12065	2	12	78	-12.98	1.86	4.13	RANKING
12066	2	13	91	-12.90	1.60	4.32	RANKING
12067	2	14	28	-12.77	1.39	4.13	RANKING
12068	2	15	19	-12.56	1.90	4.11	RANKING
12069	2	16	95	-12.28	1.50	4.33	RANKING
12070	2	17	67	-12.23	1.45	4.24	RANKING
12071	2	18	72	-12.21	1.56	4.28	RANKING

Normal text file length: 853.632 lines: 14.181 Ln: 12.034 Col: 1 Pos: 709.973 Windows (CR LF) UTF-8 INS

Lamp 2.4 Hasil Redocking kode reseptor 6MOK

D:\pejuang S1\docking\validasi reseptor\6LZE\protein.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg

11913
11914
11915
11916
11917
11918
11919
11920
11921

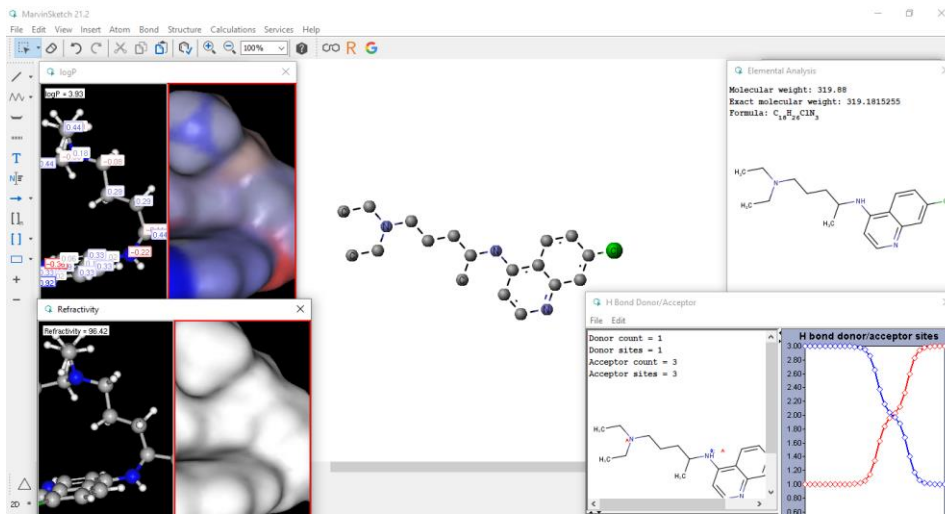
RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern	
11922	1	1	69	-15.64	0.00	3.99	RANKING
11923	1	2	88	-15.53	1.51	4.43	RANKING
11924	1	3	46	-15.12	1.69	4.23	RANKING
11925	1	4	13	-15.06	1.63	3.91	RANKING
11926	1	5	60	-15.04	1.47	3.95	RANKING
11927	1	6	72	-14.93	1.72	3.92	RANKING
11928	1	7	15	-14.92	1.72	4.15	RANKING
11929	1	8	76	-14.89	1.75	4.17	RANKING
11930	1	9	48	-14.85	1.57	3.96	RANKING
11931	1	10	36	-14.82	1.34	4.19	RANKING
11932	1	11	6	-14.73	1.76	3.92	RANKING
11933	1	12	85	-14.66	1.55	4.28	RANKING
11934	1	13	32	-14.62	1.59	4.45	RANKING
11935	1	14	19	-14.58	1.85	4.16	RANKING
11936	1	15	99	-14.51	1.72	3.97	RANKING
11937	1	16	37	-14.43	1.62	3.98	RANKING
11938	1	17	79	-14.36	1.58	4.02	RANKING
11939	1	18	67	-14.27	1.92	4.20	RANKING
11940	1	19	90	-14.25	1.65	3.76	RANKING
11941	1	20	40	-14.24	1.80	4.14	RANKING
11942	1	21	66	-14.22	1.42	4.19	RANKING
11943	1	22	73	-14.21	1.76	3.92	RANKING
11944	1	23	70	-14.20	1.59	3.77	RANKING
11945	1	24	50	-14.09	1.73	3.90	RANKING
11946	1	25	52	-14.00	1.45	3.82	RANKING
11947	1	26	14	-13.84	1.99	4.08	RANKING
11948	1	27	12	-13.82	1.47	3.86	RANKING
11949	1	28	27	-13.74	1.78	3.93	RANKING
11950	1	29	29	-13.72	1.75	4.24	RANKING

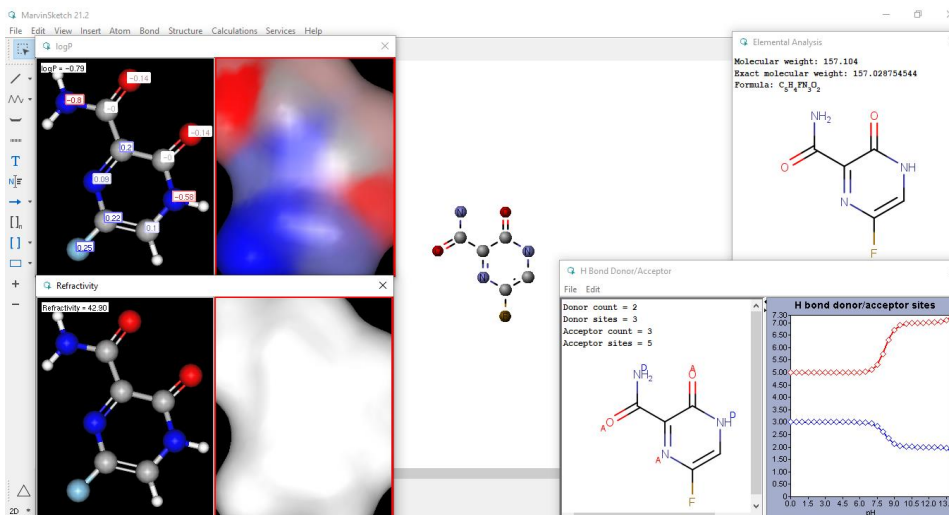
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Lamp 2.5 Hasil redocking Reseptor 6LZE

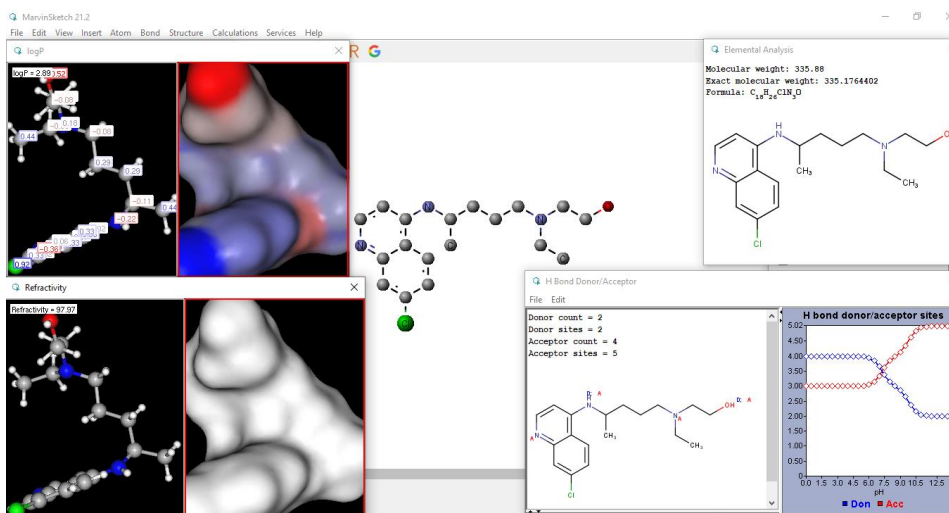
Lampiran III PENGAMATAN OBAT (*DRUG SCAN*)



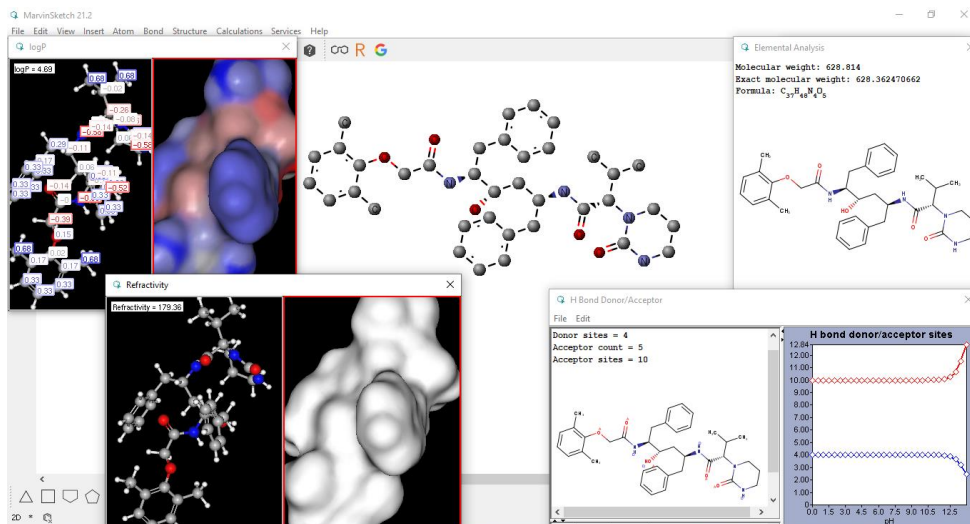
Lamp 3.1 Drug Scan Klorokuin



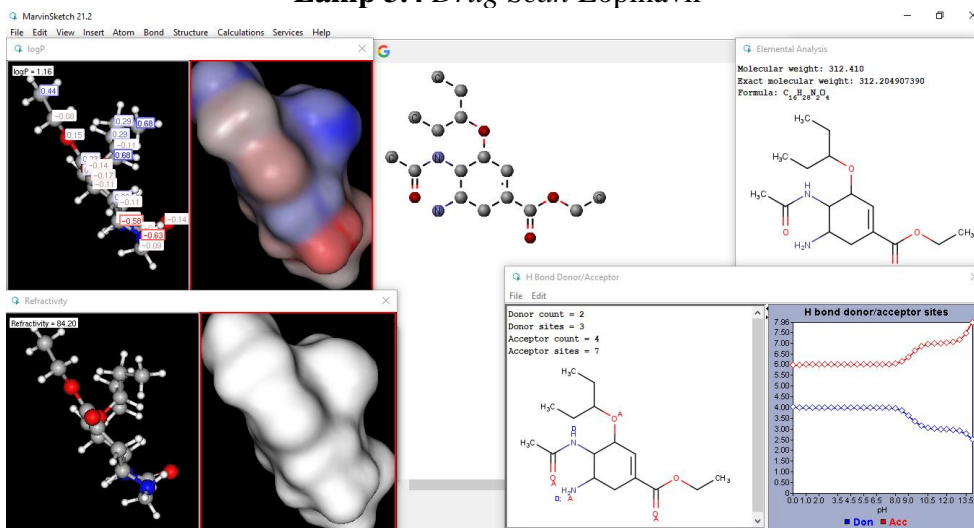
Lamp 3.2 Drug Scan Favipiravir



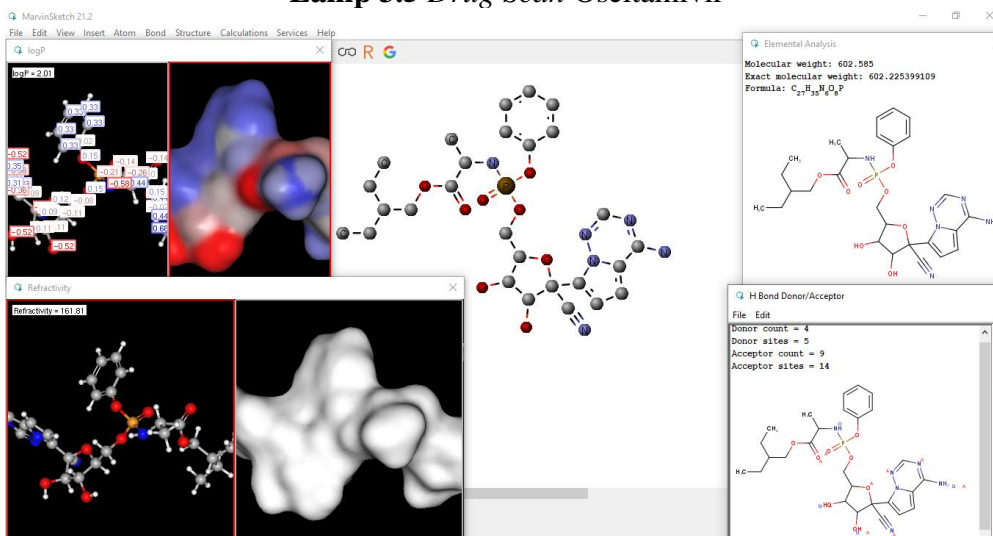
Lamp 3.3 Drug Scan Hidroksiklorokuin



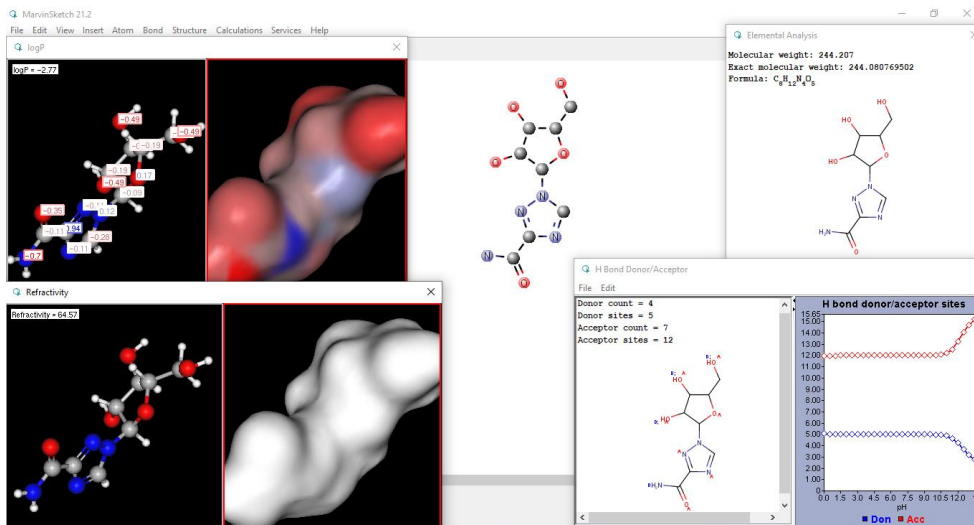
Lamp 3.4 Drug Scan Lopinavir



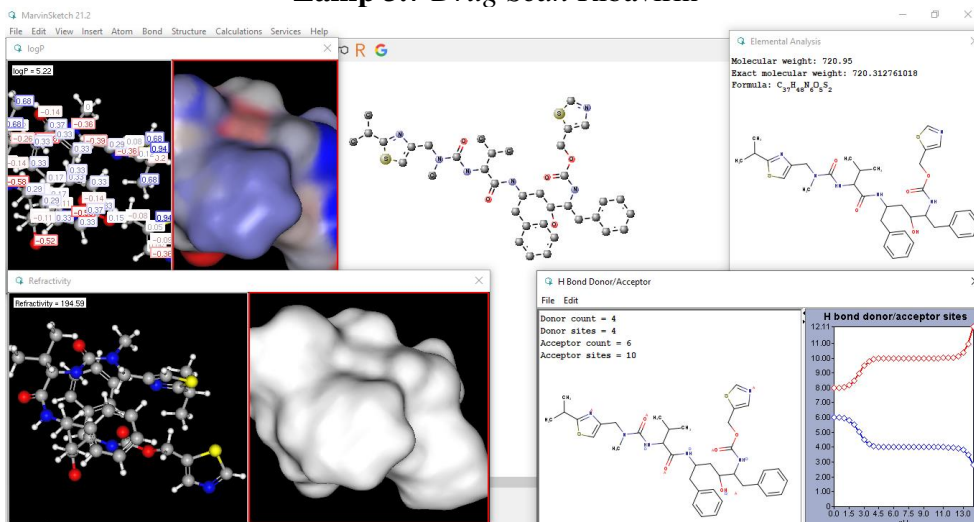
Lamp 3.5 Drug Scan Oseltamivir



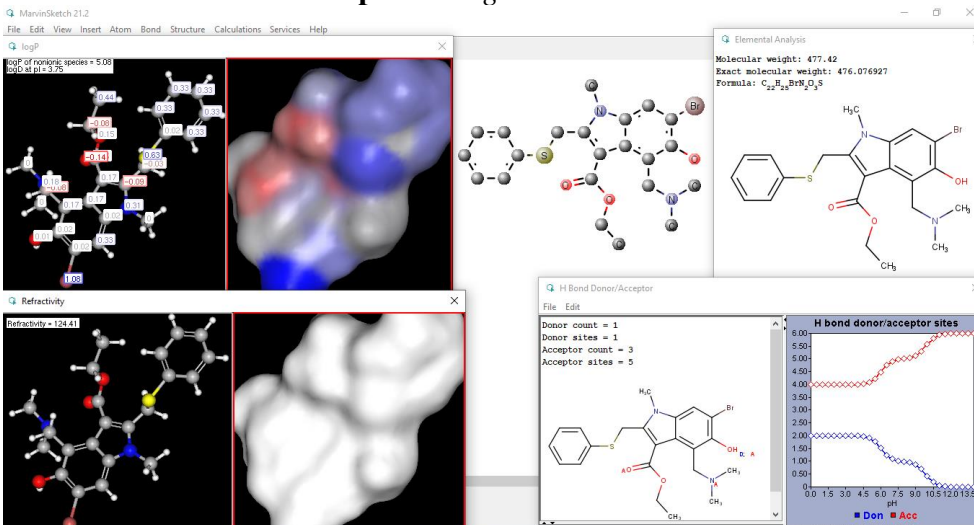
Lamp 3.6 Drug Scan Remdesivir



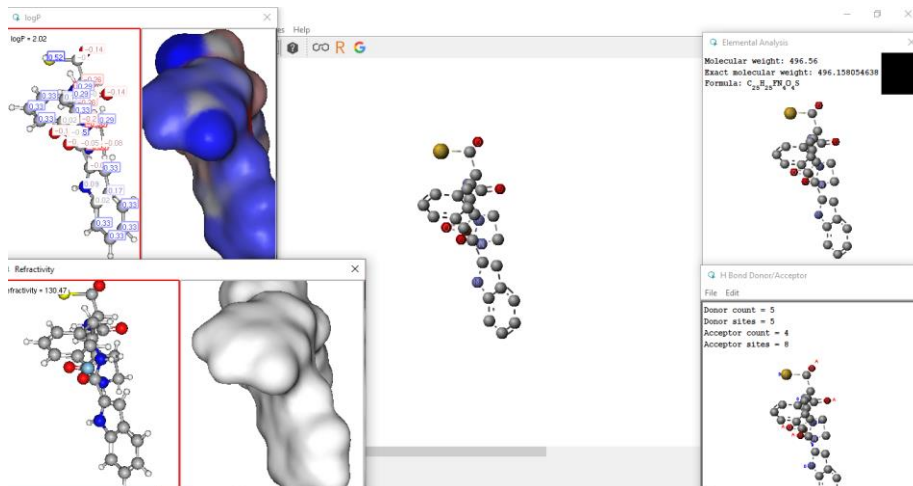
Lamp 3.7 Drug Scan Ribavirin



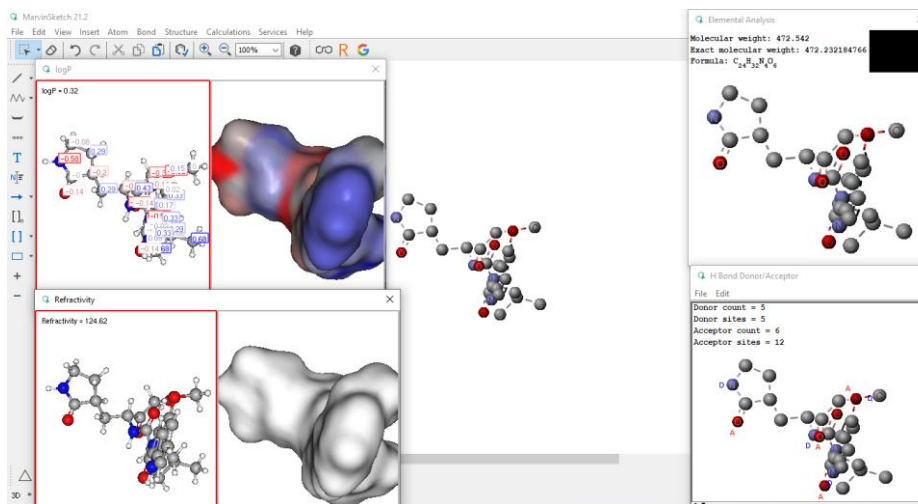
Lamp 3.8 Drug Scan Ritonavir



Lamp 3.9 Drug Scan Umifenovir



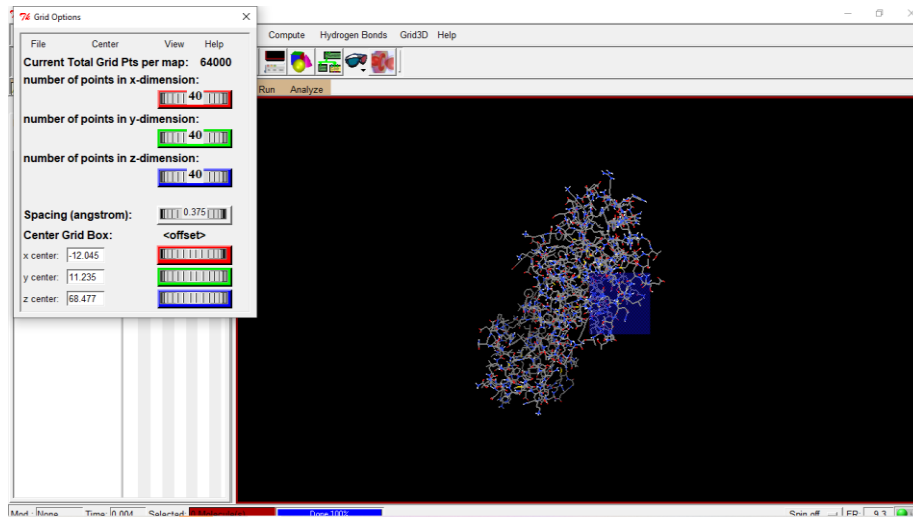
Lamp 3.10 *Drug Scan* Nativ Ligan FJC dari kode 6M0K



Lamp 3.11 *Drug Scan* Nativ Ligan V2M dari kode 6XH

LAMPIRAN IV

Molecular Docking



Lamp 4.1 Pengaturan Gridbox Reseptor 6M0K

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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern
10200						
10201						
10202						
10203						
10204						
10205						
10206						
10207	1	49	-9.40	0.00	69.35	RANKING
10208	1	2	-9.25	0.73	69.42	RANKING
10209	1	3	-9.16	0.96	69.43	RANKING
10210	1	4	-9.11	1.39	69.53	RANKING
10211	1	5	-9.10	1.78	69.06	RANKING
10212	1	6	-9.09	0.63	69.49	RANKING
10213	1	7	-9.05	0.85	69.39	RANKING
10214	1	8	-9.04	0.89	69.40	RANKING
10215	1	9	-9.04	0.82	69.34	RANKING
10216	1	10	-9.01	0.88	69.46	RANKING
10217	1	11	-8.99	1.00	69.60	RANKING
10218	1	12	-8.90	0.93	69.60	RANKING
10219	1	13	-8.75	1.72	69.55	RANKING
10220	1	14	-8.74	0.90	69.54	RANKING
10221	1	15	-8.74	1.37	69.74	RANKING
10222	1	16	-8.73	1.40	69.62	RANKING
10223	1	17	-8.69	1.16	69.29	RANKING
10224	1	18	-8.64	1.46	69.50	RANKING
10225	1	19	-8.64	1.21	69.73	RANKING
10226	1	20	-8.63	1.29	69.48	RANKING
10227	1	21	-8.58	1.02	69.48	RANKING
10228	1	22	-8.54	1.06	69.74	RANKING
10229	1	23	-8.54	1.56	69.73	RANKING
10230	1	24	-8.53	1.25	69.82	RANKING
10231	1	25	-8.49	1.54	69.70	RANKING
10232	1	26	-8.42	1.75	69.44	RANKING
10233	1	27	-8.41	1.47	69.62	RANKING
10234	1	28	-8.39	1.43	69.68	RANKING
10235	1	29	-8.36	1.83	69.32	RANKING
10236	1	30	-8.34	1.70	69.59	RANKING
10237						

Lamp 4.2 Hasil Docking senyawa klorokuin dengan kode 6M0K

D:\pejuang ST\docking\6M0K docking\favipiravir\prot.dlg - Notepad++

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern
7053						
7054						
7055						
7056						
7057						
7058						
7059						
7060						
7061	1	99	-7.75	0.00	74.65	RANKING
7062	1	2	-7.75	0.05	74.67	RANKING
7063	1	3	-7.75	0.05	74.67	RANKING
7064	1	4	-7.75	0.04	74.66	RANKING
7065	1	5	-7.75	0.03	74.66	RANKING
7066	1	6	-7.75	0.03	74.66	RANKING
7067	1	7	-7.75	0.03	74.66	RANKING
7068	1	8	-7.75	0.06	74.67	RANKING
7069	1	9	-7.75	0.06	74.66	RANKING
7070	1	10	-7.75	0.04	74.67	RANKING
7071	1	11	-7.75	0.02	74.65	RANKING
7072	1	12	-7.75	0.08	74.66	RANKING
7073	1	13	-7.75	0.03	74.66	RANKING
7074	1	14	-7.75	0.06	74.66	RANKING
7075	1	15	-7.75	0.03	74.64	RANKING
7076	1	16	-7.74	0.04	74.66	RANKING
7077	1	17	-7.74	0.13	74.65	RANKING
7078	1	18	-7.74	0.04	74.66	RANKING
7079	1	19	-7.74	0.12	74.67	RANKING
7080	1	20	-7.74	0.06	74.67	RANKING
7081	1	21	-7.74	0.09	74.66	RANKING
7082	1	22	-7.74	0.03	74.66	RANKING
7083	1	23	-7.74	0.13	74.67	RANKING
7084	1	24	-7.74	0.12	74.67	RANKING
7085	1	25	-7.74	0.11	74.67	RANKING
7086	1	26	-7.74	0.06	74.66	RANKING
7087	1	27	-7.74	0.06	74.63	RANKING
7088	1	28	-7.74	0.12	74.66	RANKING
7089	1	29	-7.74	0.03	74.66	RANKING

Lamp 4.3 Hasil Docking senyawa Favipiravir dengan kode 6M0K

D:\pejuang ST\docking\6MOK docking\hydroxychloroquine\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg x1 prot.dlg x2 prot.dlg x3 prot.dlg x4 prot.dlg x5 prot.dlg x6 prot.dlg x7 prot.dlg x8 prot.dlg x9

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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	50	-14.97	0.00	69.85	RANKING
1	2	82	-14.46	1.91	69.53	RANKING
1	3	61	-14.45	1.90	69.47	RANKING
1	4	31	-13.00	1.94	69.23	RANKING
1	5	95	-13.74	1.62	69.67	RANKING
1	6	41	-13.28	1.46	70.17	RANKING
1	7	37	-12.83	1.41	69.91	RANKING
1	8	36	-12.69	2.00	69.11	RANKING
1	9	59	-12.65	1.59	69.66	RANKING
1	10	68	-12.65	1.85	69.50	RANKING
1	11	24	-11.52	1.92	70.18	RANKING
2	1	89	-14.65	0.00	69.70	RANKING
3	1	60	-14.56	0.00	69.93	RANKING
3	2	76	-12.60	1.99	69.68	RANKING
3	3	16	-12.59	1.81	69.75	RANKING
4	1	57	-14.56	0.00	69.93	RANKING
5	1	49	-14.48	0.00	68.43	RANKING
5	2	91	-13.52	1.47	68.16	RANKING
6	1	40	-14.39	0.00	69.05	RANKING
6	2	84	-12.80	1.72	69.19	RANKING
6	3	23	-12.68	1.99	69.27	RANKING
6	4	47	-11.91	1.64	68.69	RANKING
6	5	53	-11.28	1.92	68.99	RANKING
7	1	28	-14.26	0.00	70.14	RANKING
8	1	56	-14.12	0.00	69.52	RANKING
9	1	20	-14.01	0.00	69.76	RANKING
10	1	10	-13.98	0.00	69.76	RANKING
10	2	97	-13.15	1.91	69.55	RANKING
11	1	68	-13.69	0.00	69.53	RANKING

Normal text file length: 1.335.605 lines: 21.269 Ln: 15.450 Col: 89 Pos: 921.046 Windows (CR LF) UTF-8 INS

Lamp 4.4 Hasil Docking senyawa Hidroksiklorokuin dengan kode 6MOK

D:\pejuang ST\docking\6MOK docking\lopinavir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg x1 prot.dlg x2 prot.dlg x3 prot.dlg x4 prot.dlg x5 prot.dlg x6 prot.dlg x7 prot.dlg x8 prot.dlg x9

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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	6	-16.36	0.00	70.45	RANKING
1	2	83	-12.17	1.61	69.97	RANKING
2	1	25	-15.24	0.00	69.85	RANKING
2	2	65	-13.64	1.86	69.90	RANKING
2	3	71	-12.46	1.92	69.57	RANKING
3	1	86	-14.56	0.00	69.43	RANKING
3	2	63	-14.17	1.62	69.52	RANKING
3	3	50	-13.53	1.65	69.53	RANKING
4	1	56	-14.47	0.00	69.04	RANKING
4	2	46	-13.79	1.89	69.51	RANKING
5	1	30	-14.45	0.00	68.45	RANKING
6	1	93	-14.45	0.00	69.99	RANKING
6	2	85	-14.33	1.92	69.76	RANKING
6	3	79	-14.12	1.71	69.38	RANKING
6	4	99	-12.99	1.67	69.79	RANKING
7	1	41	-14.39	0.00	69.24	RANKING
8	1	59	-14.31	0.00	70.52	RANKING
9	1	53	-14.27	0.00	69.70	RANKING
9	2	68	-14.14	1.91	70.37	RANKING
10	1	49	-14.20	0.00	70.88	RANKING
10	2	16	-12.67	1.76	69.81	RANKING
10	3	59	-11.81	1.98	69.69	RANKING
11	1	54	-14.19	0.00	69.47	RANKING
11	2	69	-11.42	1.95	68.47	RANKING
11	3	29	-11.25	1.89	67.92	RANKING
12	1	88	-14.13	0.00	69.24	RANKING
13	1	48	-14.08	0.00	71.72	RANKING
13	2	82	-12.20	2.00	70.46	RANKING
13	3	87	-10.96	1.95	70.96	RANKING

Normal text file length: 1.333.845 lines: 21.269 Ln: 15.450 Col: 21 Pos: 919.923 Windows (CR LF) UTF-8 INS

Lamp 4.5 Hasil Docking senyawa Lopinavir dengan kode 6MOK

D:\pejuang ST\docking\6MOK docking\oseltamvir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg x1 prot.dlg x2 prot.dlg x3 prot.dlg x4 prot.dlg x5 prot.dlg x6 prot.dlg x7 prot.dlg x8 prot.dlg x9

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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	71	-10.53	0.00	74.56	RANKING
1	2	17	-10.06	0.97	74.33	RANKING
1	3	67	-9.72	1.27	74.46	RANKING
1	4	99	-9.49	1.01	74.29	RANKING
1	5	40	-9.43	1.14	74.51	RANKING
1	6	2	-9.30	0.86	74.50	RANKING
1	7	74	-9.21	0.87	74.35	RANKING
1	8	14	-9.20	1.52	74.85	RANKING
1	9	4	-9.10	1.25	74.38	RANKING
1	10	75	-9.09	0.86	74.53	RANKING
1	11	22	-9.98	1.24	74.35	RANKING
1	12	91	-9.98	1.93	73.16	RANKING
1	13	81	-9.95	1.78	73.76	RANKING
1	14	26	-9.76	1.98	73.13	RANKING
1	15	82	-9.74	1.57	74.33	RANKING
1	16	76	-9.61	1.64	74.62	RANKING
1	17	96	-9.54	1.80	73.46	RANKING
1	18	90	-9.54	1.82	73.64	RANKING
1	19	70	-9.46	1.57	73.94	RANKING
1	20	20	-9.42	1.92	73.07	RANKING
1	21	36	-9.39	1.82	73.47	RANKING
1	22	59	-9.30	1.80	73.57	RANKING
1	23	93	-9.09	1.97	72.77	RANKING
2	1	2	-9.99	0.89	74.70	RANKING
2	1	95	-9.42	0.00	74.92	RANKING
2	2	42	-9.37	0.56	75.06	RANKING
2	3	33	-9.27	0.45	74.58	RANKING
2	4	85	-9.04	0.86	75.24	RANKING
2	5	45	-9.00	0.84	74.98	RANKING
2	6	32	-8.97	0.91	75.03	RANKING

Normal text file length: 635.767 lines: 11.375 Ln: 10.733 Col: 21 Pos: 596.200 Windows (CR LF) UTF-8 INS

Lamp 4.6 Hasil Docking senyawa Oseltamvir dengan kode 6MOK

D:\pejuang 51\docking\6MOK docking\remdesivir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

Normal text file length: 1.287.622 lines: 20.857 Ln: 15.250 Col: 21 Pos: 891.844 Windows (CR LF) UTF-8

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
15215						
15216						
15217						
15218						
15219						
15220						
15221						
15222						
15223						
15224	1	1	86	-13.65	0.00	66.84
15225	1	2	71	-11.59	1.62	66.10
15226	2	1	66	-12.90	0.00	67.83
15227	2	2	47	-11.19	1.61	68.60
15228	2	3	59	-11.04	1.80	69.78
15229	3	1	89	-12.86	0.00	67.45
15230	4	1	50	-12.50	0.00	67.69
15231	5	1	31	-12.48	0.00	67.41
15232	5	2	16	-9.73	1.89	66.86
15233	6	1	45	-12.16	0.00	67.74
15234	7	1	87	-12.13	0.00	68.07
15235	8	1	39	-12.02	0.00	68.42
15236	8	2	13	-10.24	0.85	68.77
15237	9	1	10	-11.91	0.00	67.19
15238	9	2	32	-11.12	1.58	67.67
15239	10	1	36	-11.90	0.00	68.50
15240	11	1	63	-11.77	0.00	67.48
15241	11	2	23	-10.60	1.43	68.06
15242	11	3	72	-9.16	1.75	67.14
15243	12	1	2	-11.75	0.00	65.84
15244	13	1	73	-11.71	0.00	68.52
15245	13	2	71	-11.41	1.94	67.96
15246	13	3	94	-11.05	1.68	67.77
15247	14	1	19	-11.58	0.00	67.69
15248	15	1	95	-11.51	0.00	65.91
15249	16	1	19	-11.38	0.00	68.08
15250	16	2	6	-9.63	1.79	68.12
15251	16	3	90	-9.20	1.81	68.61

Lamp 4.7 Hasil Docking senyawa Remdesivir dengan kode 6MOK

D:\pejuang 51\docking\6MOK docking\ribavirin\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

Normal text file length: 550.988 lines: 9.974 Ln: 9.419 Col: 1 Pos: 517.920 Windows (CR LF) UTF-8

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
9383						
9384						
9385						
9386						
9387						
9388						
9389						
9390						
9391						
9392	1	1	37	-9.33	0.00	72.91
9393	1	2	32	-9.32	0.20	72.83
9394	1	3	7	-9.29	0.33	72.76
9395	1	4	49	-9.27	0.25	72.82
9396	1	5	62	-9.16	1.69	72.30
9397	1	6	41	-9.15	1.65	72.36
9398	1	7	21	-9.14	1.63	72.38
9399	1	8	68	-9.13	0.59	72.83
9400	1	9	35	-9.13	1.55	72.42
9401	1	10	83	-9.12	0.63	72.83
9402	1	11	94	-9.11	1.67	72.36
9403	1	12	93	-9.11	1.58	72.38
9404	1	13	50	-9.11	1.71	72.30
9405	1	14	76	-9.11	0.28	72.82
9406	1	15	52	-9.11	0.50	72.88
9407	1	16	15	-9.10	1.42	72.50
9408	1	17	52	-9.10	1.72	72.32
9409	1	18	13	-9.10	1.72	72.33
9410	1	19	44	-9.10	0.45	72.59
9411	1	20	54	-9.10	0.66	72.74
9412	1	21	91	-9.09	1.72	72.33
9413	1	22	36	-9.08	1.70	72.34
9414	1	23	31	-9.08	1.62	72.37
9415	1	24	28	-9.08	1.32	72.56
9416	1	25	30	-9.07	1.72	72.37
9417	1	26	71	-9.06	1.72	72.38
9418	1	27	51	-9.06	1.70	72.35
9419	1	28	56	-9.06	1.69	72.31
9420	1	29	47	-9.06	1.69	72.37

Gambar 4.8 Hasil Docking senyawa Ribavirin dengan kode 6MOK

D:\pejuang 51\docking\6MOK docking\ritonavir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

Normal text file length: 1.609.728 lines: 25.287 Ln: 17.000 Col: 21 Pos: 1.010.928 Windows (CR LF) UTF-8

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
16964						
16965						
16966						
16967						
16968						
16969						
16970						
16971						
16972						
16973	1	1	12	-14.94	0.00	64.83
16974	2	1	55	-14.25	0.00	65.48
16975	3	1	83	-14.24	0.00	65.49
16976	4	1	4	-14.00	0.00	64.42
16977	5	1	2	-13.97	0.00	66.01
16978	6	1	65	-13.94	0.00	66.54
16979	7	1	94	-13.94	0.00	64.94
16980	8	1	89	-13.79	0.00	63.85
16981	9	1	64	-13.68	0.00	64.06
16982	10	1	94	-13.68	0.00	64.40
16983	11	1	77	-13.60	0.00	65.47
16984	12	1	99	-13.53	0.00	65.88
16985	13	1	50	-13.50	0.00	65.42
16986	14	1	96	-13.35	0.00	64.69
16987	15	1	10	-13.31	0.00	66.65
16988	15	2	87	-11.12	1.99	65.88
16989	16	1	43	-13.24	0.00	64.20
16990	16	2	40	-9.26	1.85	64.25
16991	17	1	90	-13.19	0.00	65.89
16992	18	1	6	-13.09	0.00	64.79
16993	19	1	39	-13.01	0.00	66.65
16994	20	1	93	-12.90	0.00	65.31
16995	21	1	5	-12.89	0.00	65.07
16996	22	1	8	-12.81	0.00	65.79
16997	23	1	58	-12.71	0.00	65.94
16998	24	1	100	-12.64	0.00	66.13
16999	25	1	45	-12.62	0.00	64.38
17000	26	1	28	-12.53	0.00	66.75
17001	27	1	84	-12.52	0.00	65.27

Lamp 4.9 Hasil Docking senyawa Ritonavir dengan kode 6MOK

D:\docking\6XHL docking\chloroquine\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

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RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern
10211	1	30	-10.14	0.00	62.05	RANKING
10212	1	47	-9.73	1.16	62.32	RANKING
10213	1	66	-9.64	0.65	62.39	RANKING
10214	1	23	-9.54	1.27	62.70	RANKING
10215	1	28	-9.48	1.37	62.89	RANKING
10216	1	15	-9.46	1.00	62.02	RANKING
10217	1	71	-9.40	1.51	62.49	RANKING
10218	1	52	-9.38	1.01	62.41	RANKING
10219	1	20	-9.33	1.00	62.47	RANKING
10220	1	81	-9.33	1.98	61.05	RANKING
10221	1	12	-9.26	1.92	62.96	RANKING
10222	1	45	-9.26	1.66	62.56	RANKING
10223	1	58	-9.15	1.49	63.21	RANKING
10224	1	91	-9.08	0.97	62.41	RANKING
10225	1	10	-8.98	1.57	63.32	RANKING
10226	1	56	-8.98	1.57	62.37	RANKING
10227	1	89	-8.93	1.89	63.44	RANKING
10228	1	93	-8.84	1.55	62.99	RANKING
10229	1	24	-8.78	1.77	63.50	RANKING
10230	1	4	-8.78	1.23	61.90	RANKING
10231	1	32	-8.75	1.67	61.00	RANKING
10232	1	73	-8.67	1.29	62.50	RANKING
10233	1	48	-8.61	1.56	61.69	RANKING
10234	1	9	-8.57	1.55	63.43	RANKING
10235	1	72	-8.53	1.41	61.94	RANKING
10236	1	74	-8.52	1.69	63.18	RANKING
10237	1	57	-8.47	1.57	63.10	RANKING
10238	1	25	-8.44	1.86	63.08	RANKING
10239	1	82	-8.40	1.76	62.46	RANKING

Normal text file length: 643.247 lines: 11.477 Ln: 10.169 Col: 21 Sel: 5 | 1 Windows (CR LF) UTF-8 INS

Lamp 4.13 Hasil Docking Favipiravir dengan kode reseptor 6XHL

D:\docking\6XHL docking\hydroxychloroquine\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

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RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern
15426	1	99	-16.46	0.00	61.85	RANKING
15427	1	73	-16.00	1.97	61.15	RANKING
15428	1	80	-15.24	1.90	61.84	RANKING
15429	1	63	-14.62	1.95	61.69	RANKING
15430	1	47	-14.10	1.80	62.18	RANKING
15431	2	75	-14.05	0.00	61.39	RANKING
15432	2	71	-14.93	1.57	61.77	RANKING
15433	2	55	-13.74	1.61	61.58	RANKING
15434	3	45	-15.88	0.00	62.82	RANKING
15435	3	37	-15.74	1.90	63.88	RANKING
15436	3	18	-13.12	1.86	63.12	RANKING
15437	4	27	-15.84	0.00	61.52	RANKING
15438	4	52	-14.45	1.99	61.57	RANKING
15439	5	40	-15.76	0.00	61.99	RANKING
15440	5	43	-14.42	1.62	61.81	RANKING
15441	6	89	-15.40	0.00	63.46	RANKING
15442	7	34	-15.39	0.00	61.95	RANKING
15443	8	11	-15.23	0.00	61.67	RANKING
15444	8	2	-15.26	1.85	61.14	RANKING
15445	8	21	-13.31	1.87	62.42	RANKING
15446	8	69	-13.04	1.81	62.32	RANKING
15447	9	92	-14.53	0.00	62.42	RANKING
15448	9	2	-13.36	1.95	62.55	RANKING
15449	10	1	-14.52	0.00	61.97	RANKING
15450	10	70	-12.19	1.93	62.08	RANKING
15451	11	1	-14.32	0.00	62.21	RANKING
15452	12	1	-14.29	0.00	63.37	RANKING
15453	12	42	-15.02	1.92	62.78	RANKING
15454	13	1	-14.29	0.00	63.12	RANKING

Normal text file length: 1.352.901 lines: 21.512 Ln: 15.453 Col: 1 Sel: 0 | 0 Windows (CR LF) UTF-8 INS

Lamp 4.14 Hasil Docking Hidroksiklorokuin dengan kode reseptor 6XHL

D:\docking\6XHL docking\lopinavir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

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RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Group Pattern
15423	1	9	-17.96	0.00	62.95	RANKING
15424	1	50	-13.88	1.98	63.48	RANKING
15425	1	87	-13.21	1.98	63.19	RANKING
15426	2	82	-16.15	0.00	60.73	RANKING
15427	2	90	-15.00	1.71	61.57	RANKING
15428	2	33	-14.48	1.60	61.77	RANKING
15429	3	16	-16.10	0.00	61.42	RANKING
15430	4	34	-15.95	0.00	61.57	RANKING
15431	4	87	-14.34	1.86	62.15	RANKING
15432	5	10	-15.71	0.00	61.31	RANKING
15433	5	39	-15.23	1.81	61.88	RANKING
15434	5	70	-15.09	1.68	61.72	RANKING
15435	5	73	-13.64	1.84	61.88	RANKING
15436	5	60	-11.79	2.00	61.86	RANKING
15437	6	22	-15.41	0.00	61.87	RANKING
15438	6	77	-14.97	1.87	62.20	RANKING
15439	7	72	-15.38	0.00	61.32	RANKING
15440	7	69	-14.02	1.91	60.43	RANKING
15441	8	71	-15.35	0.00	60.84	RANKING
15442	9	91	-15.19	0.00	62.25	RANKING
15443	9	58	-14.13	1.81	61.40	RANKING
15444	10	1	-14.87	0.00	62.13	RANKING
15445	10	2	-13.85	1.33	62.88	RANKING
15446	11	20	-14.94	0.00	62.37	RANKING
15447	12	1	-14.61	0.00	62.05	RANKING
15448	13	1	-14.46	0.00	60.24	RANKING
15449	13	2	-12.97	1.78	60.95	RANKING
15450	13	3	-12.97	1.78	60.58	RANKING
15451	13	4	-11.97	1.92	60.05	RANKING

Normal text file length: 1.333.943 lines: 21.269 Ln: 15.450 Col: 44 Sel: 0 | 0 Windows (CR LF) UTF-8 INS

Lamp 4.15 Hasil Docking Lopinavir dengan kode reseptor 6XHL

D:\docking\6XHL_docking\ritonavir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg x1 prot.dlg x2 prot.dlg x3 prot.dlg x4 prot.dlg x5 prot.dlg x6 prot.dlg x7 prot.dlg x8 prot.dlg x9

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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	83	-14.76	0.00	61.62	RANKING
2	1	111	-15.30	0.00	61.44	RANKING
3	1	36	-14.27	0.00	60.80	RANKING
4	1	96	-14.08	0.00	60.37	RANKING
5	1	94	-13.79	0.00	60.59	RANKING
5	2	99	-12.99	1.71	60.68	RANKING
5	3	95	-11.86	1.99	60.61	RANKING
6	1	59	-13.71	0.00	60.26	RANKING
7	1	37	-13.49	0.00	61.54	RANKING
8	1	62	-13.47	0.00	63.03	RANKING
9	1	77	-13.41	0.00	62.57	RANKING
10	1	22	-13.25	0.00	62.06	RANKING
11	1	35	-13.20	0.00	62.47	RANKING
12	1	67	-13.18	0.00	60.91	RANKING
13	1	85	-13.12	0.00	62.06	RANKING
14	1	91	-12.92	0.00	62.02	RANKING
15	1	25	-12.86	0.00	62.86	RANKING
16	1	57	-12.80	0.00	62.19	RANKING
17	1	84	-12.74	0.00	61.77	RANKING
18	1	49	-12.59	0.00	60.83	RANKING
19	1	30	-12.46	0.00	62.07	RANKING
20	1	45	-12.41	0.00	61.16	RANKING
20	2	16	-12.17	1.69	61.33	RANKING
21	1	28	-12.35	0.00	61.82	RANKING
22	1	89	-12.22	0.00	61.77	RANKING
23	1	55	-12.20	0.00	62.48	RANKING
24	1	29	-12.19	0.00	61.46	RANKING
25	1	6	-12.01	0.00	61.61	RANKING
26	1	79	-12.00	0.00	64.51	RANKING

Normal text file length: 1.603.694 lines: 25.202 Ln: 16.963 Col: 1 Set: 0|0 Windows (CR LF) UTF-8 INS

Lamp 4.19 Hasil Docking Ritonavir dengan kode reseptor 6XHL

D:\docking\6XHL_docking\umifenovir\prot.dlg - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

prot.dlg x1 prot.dlg x2 prot.dlg x3 prot.dlg x4 prot.dlg x5 prot.dlg x6 prot.dlg x7 prot.dlg x8 prot.dlg x9

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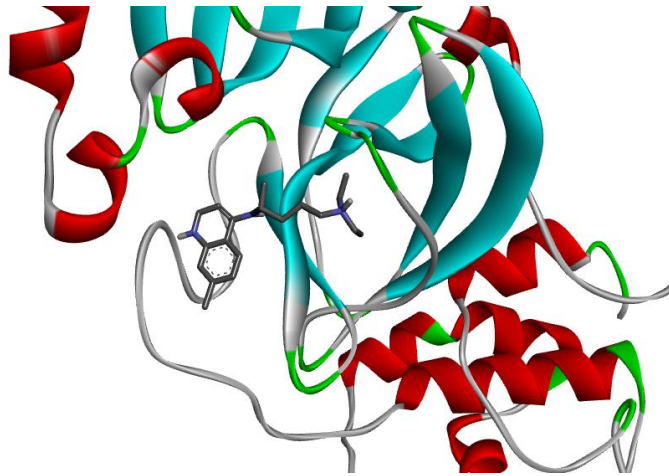
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Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	33	-12.86	0.00	62.47	RANKING
1	2	78	-12.54	1.46	62.11	RANKING
1	3	81	-12.46	1.54	62.36	RANKING
2	1	44	-12.69	0.00	63.40	RANKING
2	2	10	-12.50	0.58	63.37	RANKING
2	3	22	-12.39	0.79	63.20	RANKING
2	4	77	-12.20	0.64	63.52	RANKING
2	5	89	-12.12	0.92	63.72	RANKING
2	6	93	-10.96	1.07	63.21	RANKING
2	7	46	-9.67	1.89	63.21	RANKING
2	8	31	-9.65	1.75	63.34	RANKING
2	9	91	-9.63	1.73	63.12	RANKING
2	10	17	-9.63	1.92	63.24	RANKING
2	11	40	-9.51	1.88	63.18	RANKING
2	12	30	-9.38	1.82	63.61	RANKING
2	13	61	-9.36	1.99	62.69	RANKING
3	1	12	-12.59	0.00	64.25	RANKING
3	2	8	-12.04	1.96	65.54	RANKING
3	3	70	-11.85	1.63	65.44	RANKING
3	4	7	-11.77	1.24	64.59	RANKING
3	5	34	-11.76	1.26	64.88	RANKING
3	6	37	-11.45	1.30	64.84	RANKING
4	1	41	-12.25	0.00	63.86	RANKING
4	2	38	-11.86	0.58	64.03	RANKING
4	3	43	-11.71	0.83	63.93	RANKING
4	4	25	-11.62	1.19	64.60	RANKING
4	5	2	-11.61	1.13	64.36	RANKING
4	6	60	-11.17	1.10	63.94	RANKING
4	7	28	-10.86	1.64	64.58	RANKING

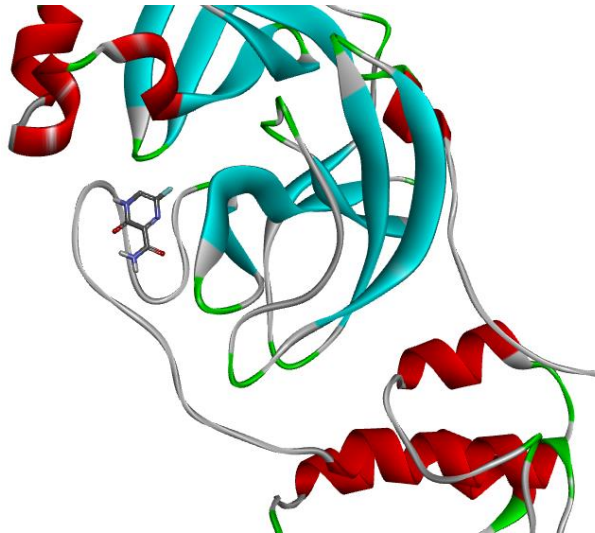
Normal text file length: 717.947 lines: 12.391 Ln: 10.752 Col: 1 Set: 0|0 Windows (CR LF) UTF-8 INS

Lamp 4.20 Hasil Docking Umifenovir dengan kode reseptor 6XHL

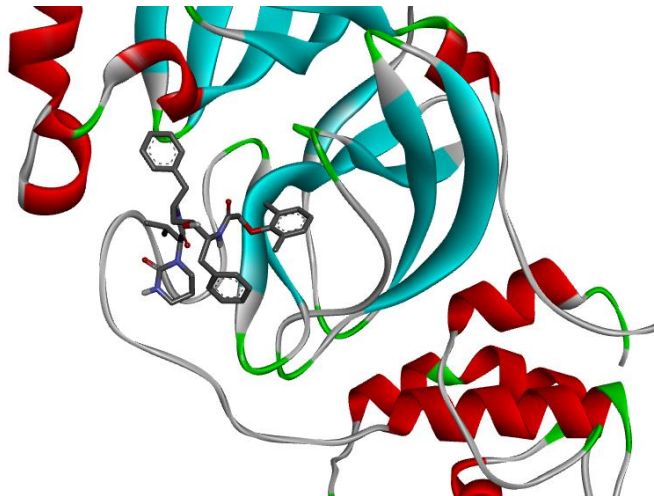
LAMPIRAN V
VISUALISASI DOCKING



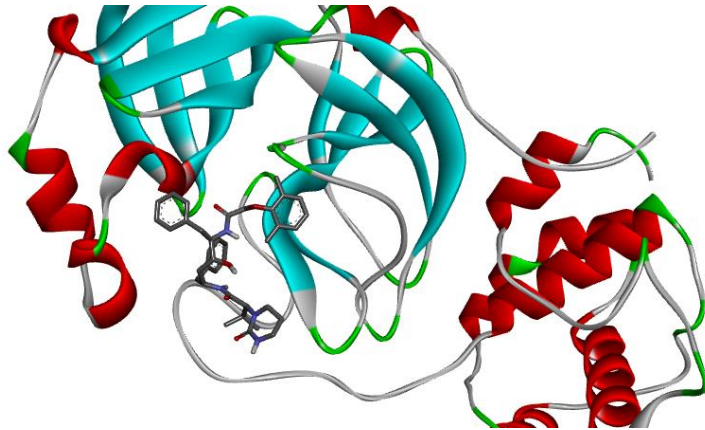
Lamp 5.1 Visualisasi Interaksi 3D Klorokuin 6M0K



Lamp 5.2 Visualisasi Interaksi 3D Favipiravir 6M0K



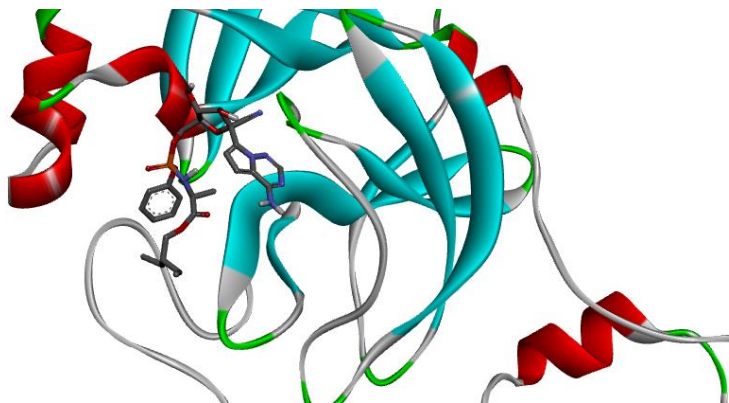
Lamp 5.3 Visualisasi Interaksi 3D Hidroksiklorokuin 6M0K



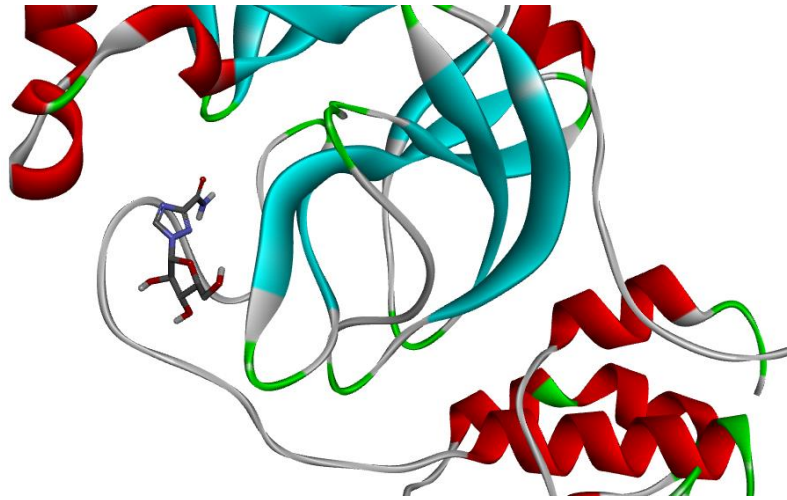
Lamp 5.4 Visualisasi Interaksi 3D Lopinavir 6M0K



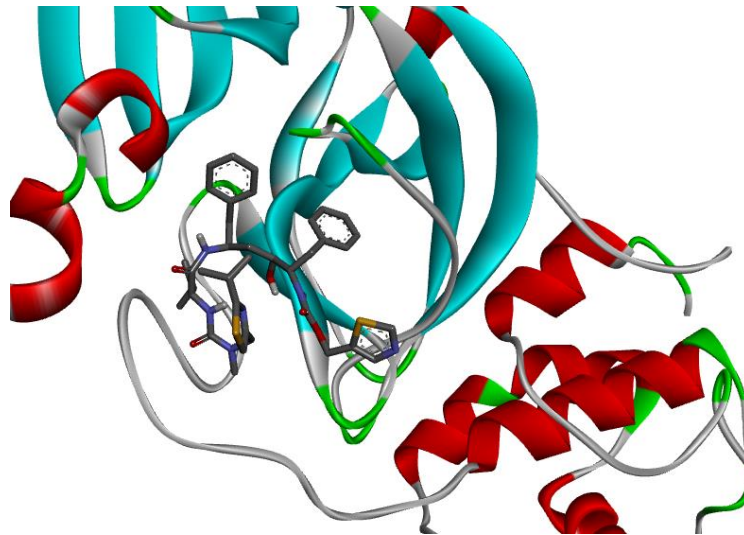
Lamp 5.5 Visualisasi Interaksi 3D Oseltamivir 6M0K



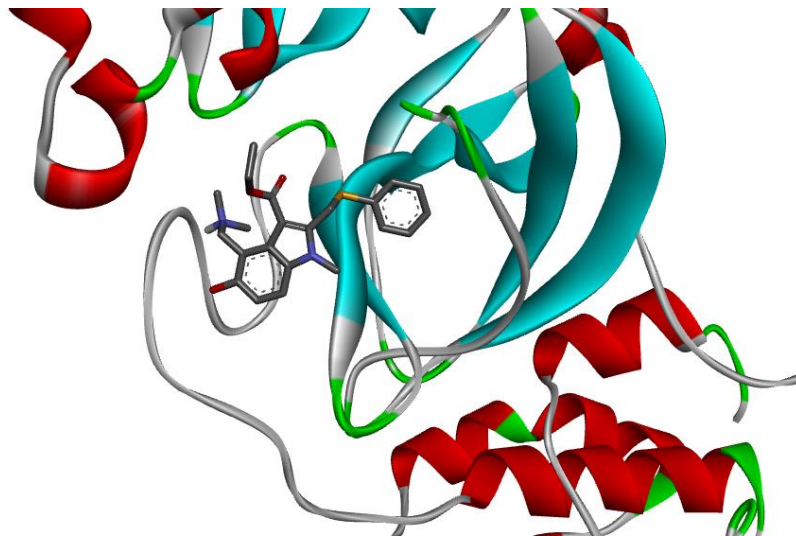
Lamp 5.6 Visualisasi Interaksi 3D Remdesivir 6M0K



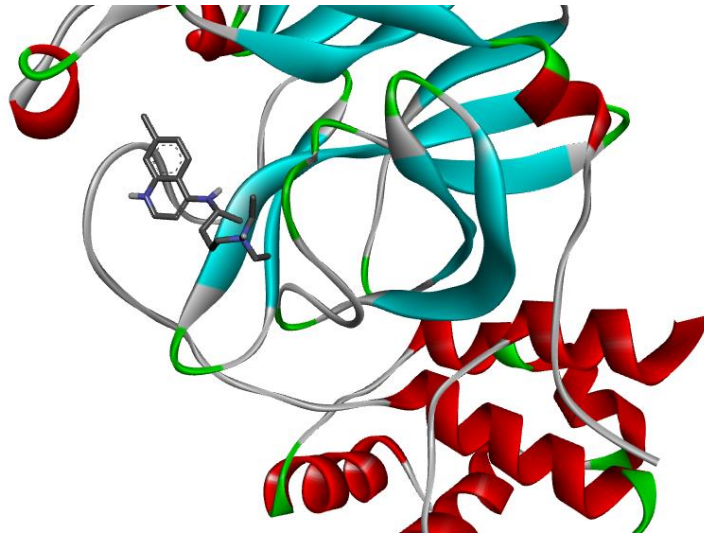
Lamp 5.7 Visualisasi Interaksi 3D Ribavirin 6M0K



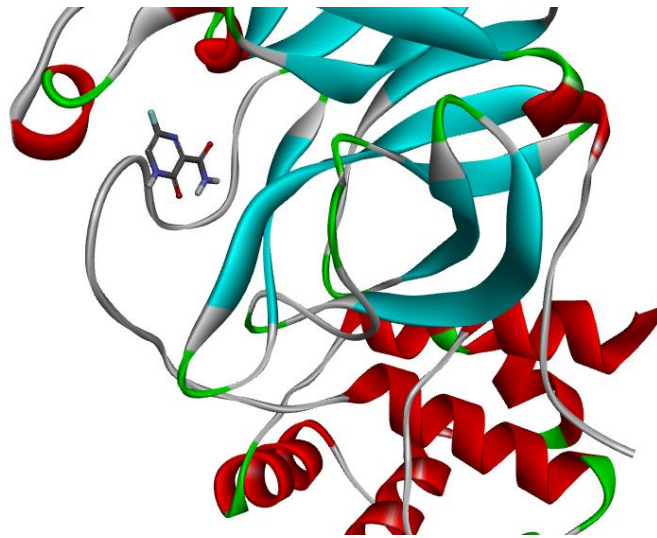
Lamp 5.8 Visualisasi Interaksi 3D Ritonavir 6M0K



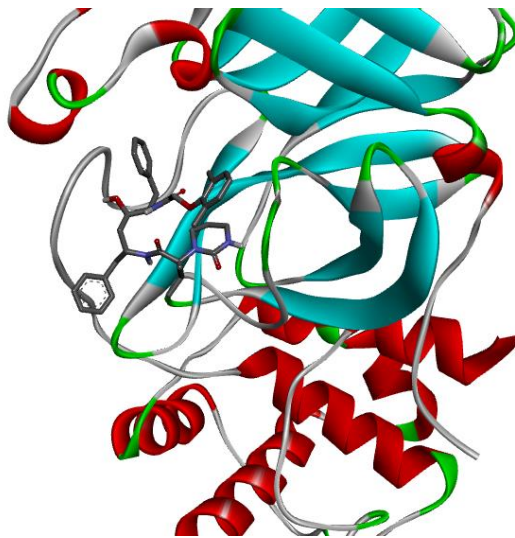
Lamp 5.9 Visualisasi Interaksi 3D Umifenovir 6M0K



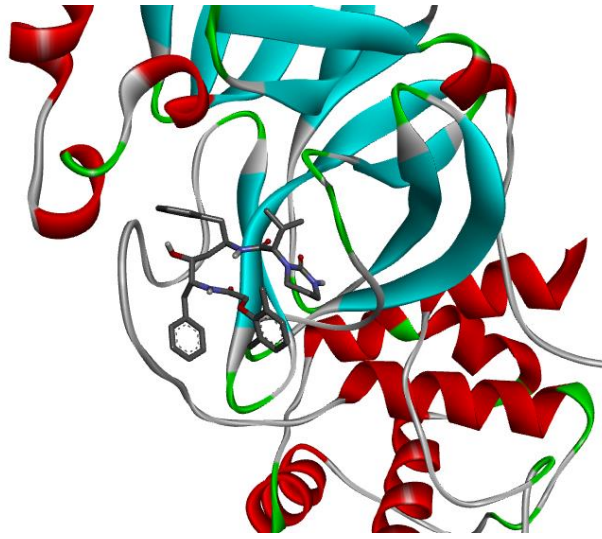
Lamp 5.10 Visualisasi Interaksi 3D Klorokuin 6XHL



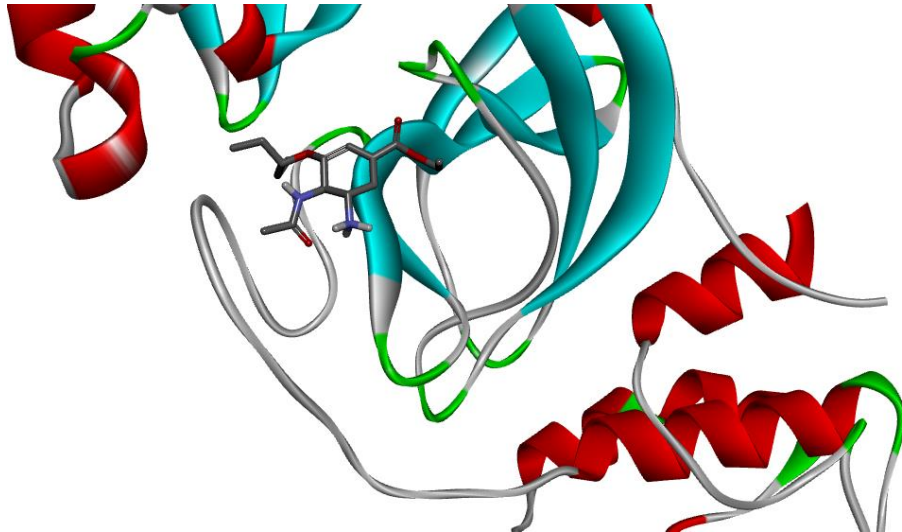
Lamp 5.11 Visualisasi Interaksi 3D favipiravir 6XHL



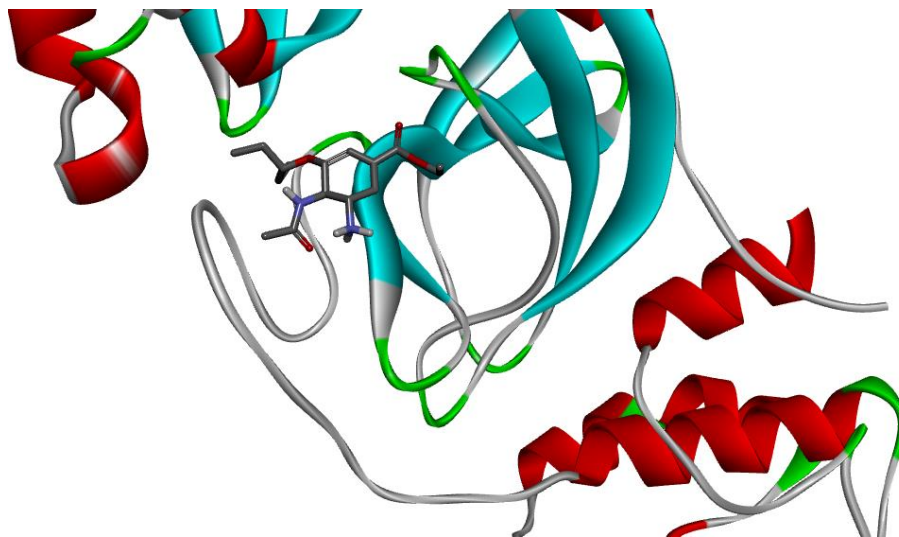
Lamp 5.12 Visualisasi Interaksi 3D Hidroksiklorokuin 6XHL



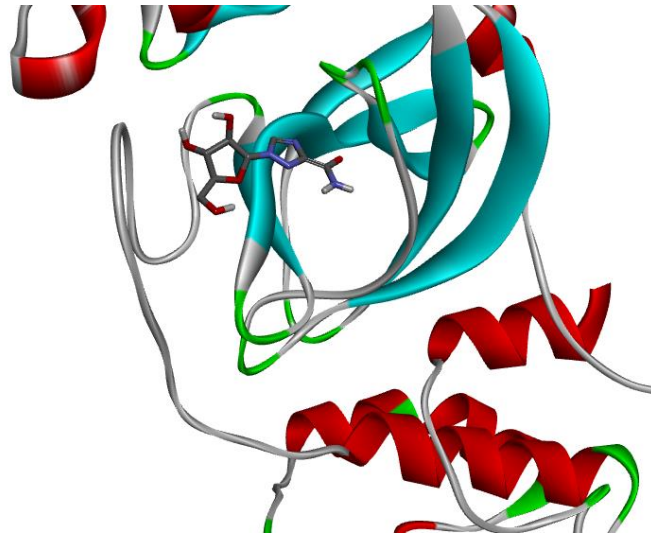
Lamp 5.13 Visualisasi Interaksi 3D Lopinavir 6XHL



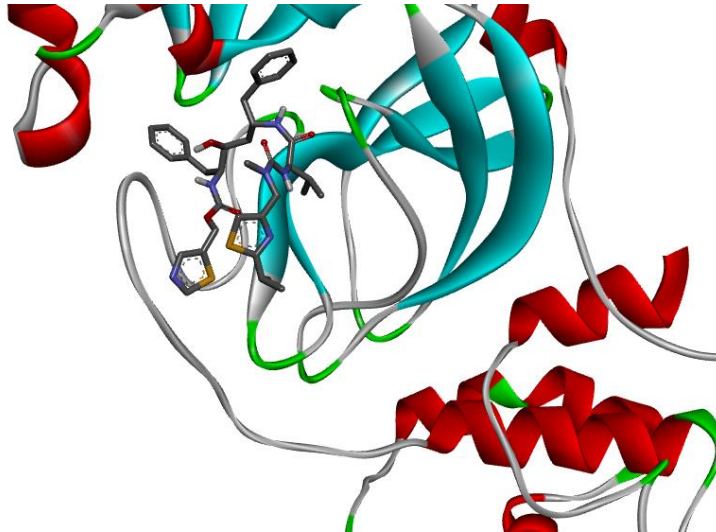
Lamp 5.14 Visualisasi Interaksi 3D Oseltamivir 6XHL



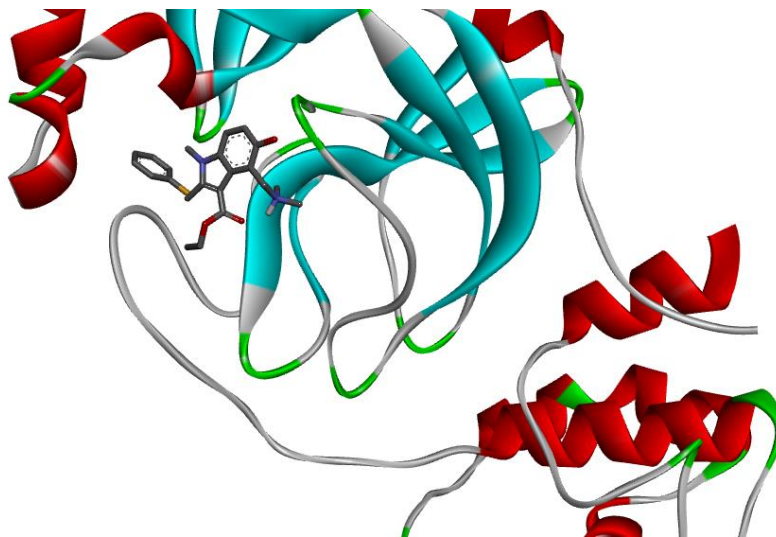
Lamp 5.15 Visualisasi Interaksi 3D Remdesivir 6XHL



Lamp 5.16 Visualisasi Interaksi 3D Ribavirin 6XHL

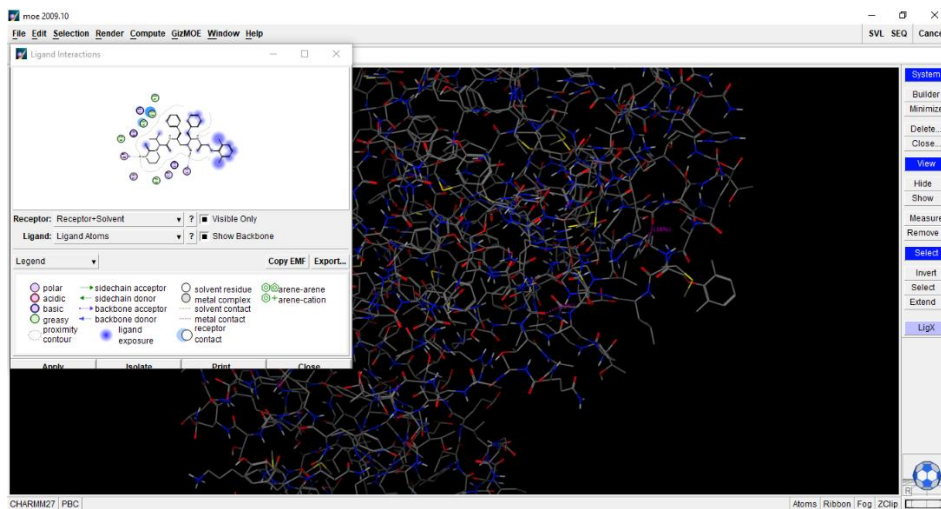


Lamp 5.17 Visualisasi Interaksi 3D Ritonavir 6XHL

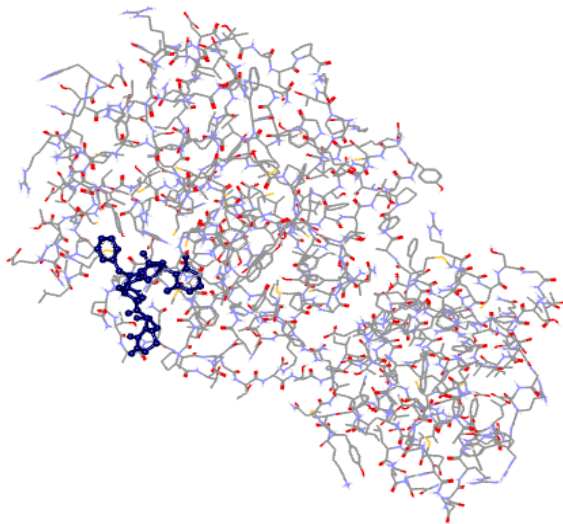


Lamp 5.18 Visualisasi Interaksi 3D Umifenovir 6XHL

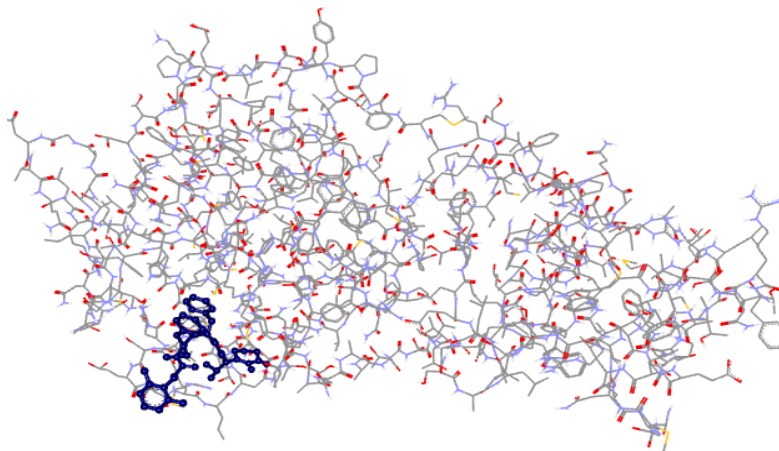
LAMPIRAN VI MOLECULAR DYNAMIC



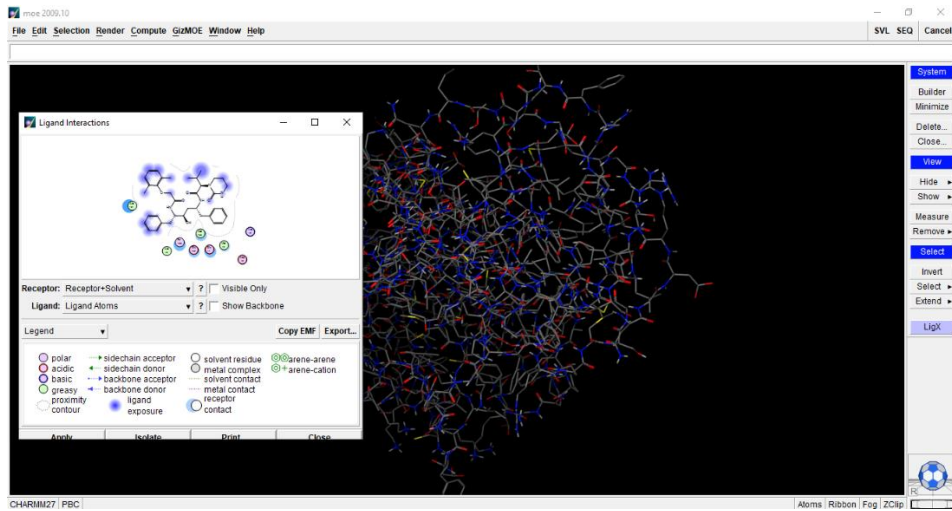
Lamp 6.1 Hasil Simulasi MD Lopinavir dengan kode reseptor 6M0K



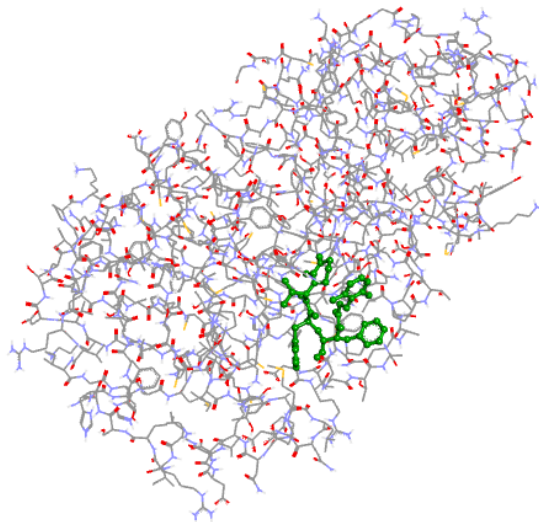
Lamp 6.2 Gambar Sebelum simulasi MD pada kompleks lopinavir



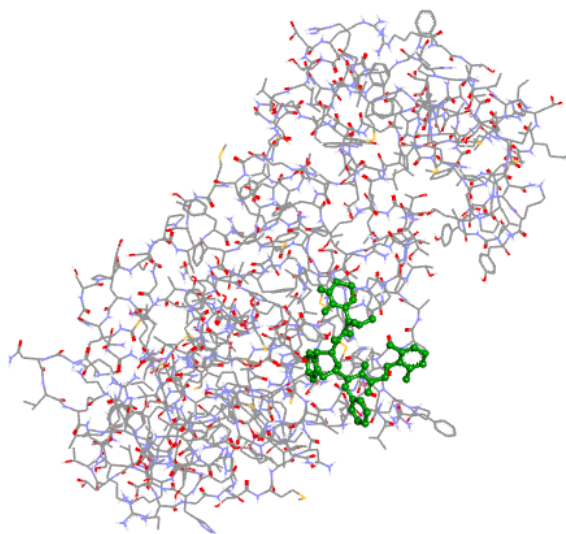
Lamp 6.3 Gambar Sebelum simulasi MD pada kompleks lopinavir



Lamp 6.4 Hasil Simulasi MD Lopinavir dengan kode reseptor 6XHL



Lamp 6.5 Sebelum Simulasi MD Lopinavir dengan kode reseptor 6XHL



Lamp 6.6 Setelah Simulasi MD Lopinavir dengan kode reseptor 6XHL