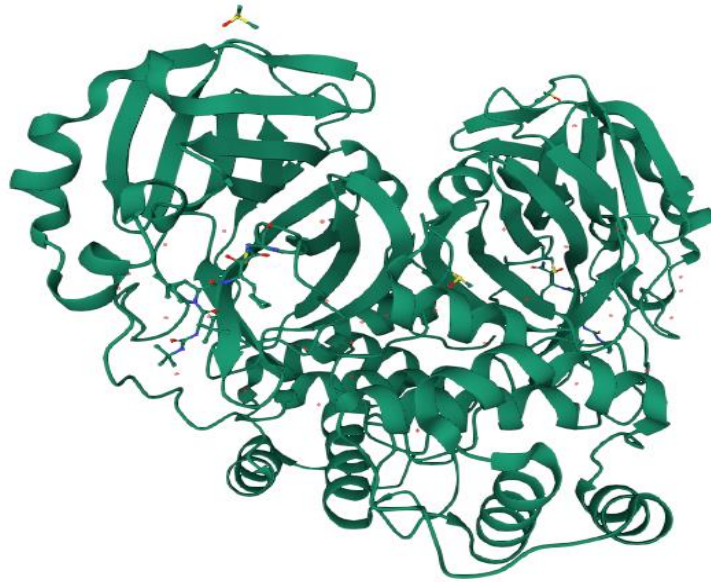


**LAMPIRAN I**  
**PREPARASI LIGAN DAN RESEPTOR**



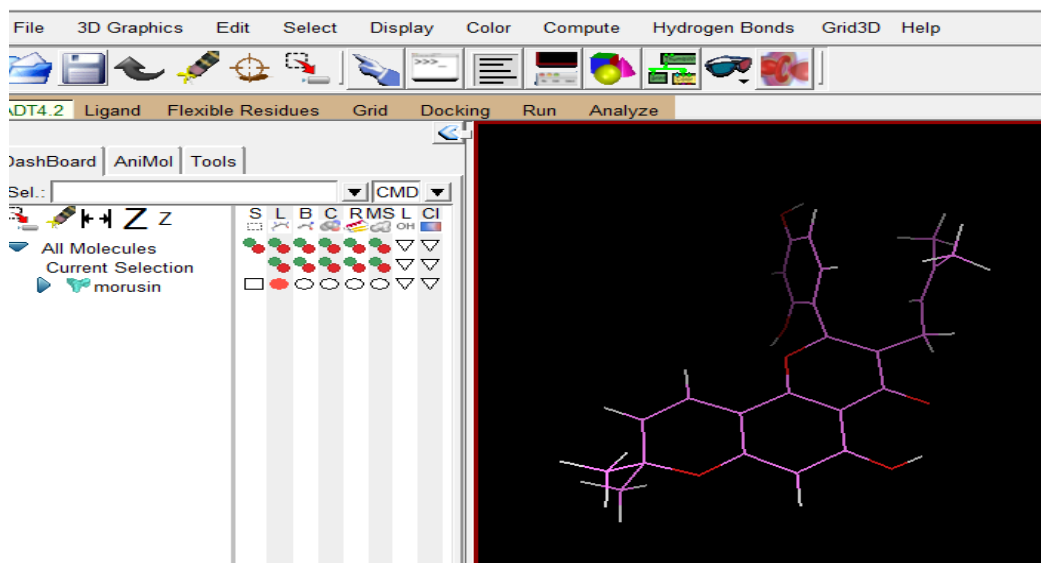
Reseptor 6ZRU dalam bentuk 3D



Reseptor 7CTT dalam bentuk 3D



Reseptor 6LZG dalam bentuk 3D



Preparasi ligan dan reseptor

## LAMPIRAN II

## VALIDASI METODE DOCKING

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	15	-14.36	0.00	1.76	RANKING
1	2	8	-14.19	0.65	1.65	RANKING
1	3	11	-14.14	0.44	1.62	RANKING
1	4	7	-13.30	1.62	1.47	RANKING
1	5	10	-10.47	1.97	2.20	RANKING
2	1	12	-12.49	0.00	2.80	RANKING
2	2	4	-11.47	1.59	2.92	RANKING
2	3	14	-11.23	1.65	2.46	RANKING
3	1	6	-11.18	0.00	2.45	RANKING
3	2	13	-9.88	2.00	2.84	RANKING

Nilai RMSD 6ZRU hasil docking menggunakan *Autodock*

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	8	-14.30	0.00	1.92	RANKING
1	2	3	-14.03	1.76	1.66	RANKING
1	3	13	-12.54	1.41	2.04	RANKING
2	1	10	-13.31	0.00	2.44	RANKING
2	2	4	-11.32	1.30	2.39	RANKING
3	1	2	-13.30	0.00	1.50	RANKING
3	2	7	-13.26	0.78	1.54	RANKING
4	1	14	-11.39	0.00	2.91	RANKING
5	1	11	-10.99	0.00	3.25	RANKING
5	2	15	-10.85	1.94	2.82	RANKING

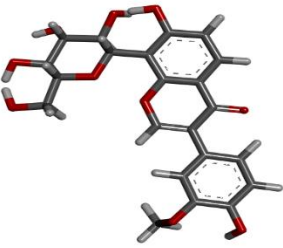
Nilai RMSD 7CTT hasil docking menggunakan *Autodock*

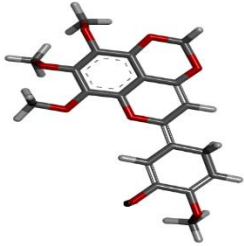
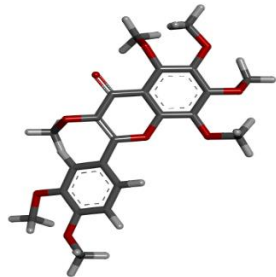
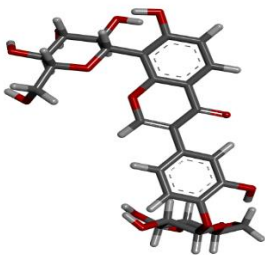
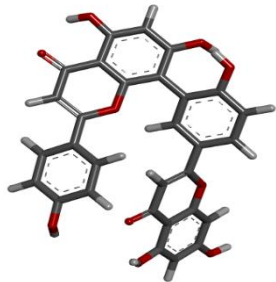
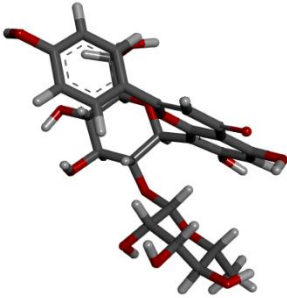
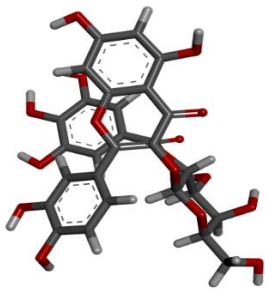
Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	4	-15.00	0.00	1.82	RANKING
1	2	12	-14.51	1.78	2.18	RANKING
1	3	5	-14.18	1.93	2.27	RANKING
1	4	13	-13.56	1.97	1.82	RANKING
2	1	10	-13.38	0.00	1.49	RANKING
3	1	9	-13.06	0.00	4.96	RANKING
3	2	11	-12.94	1.78	4.81	RANKING
3	3	3	-12.85	1.53	5.31	RANKING
3	4	1	-12.56	1.94	4.22	RANKING
3	5	7	-12.12	1.51	4.83	RANKING

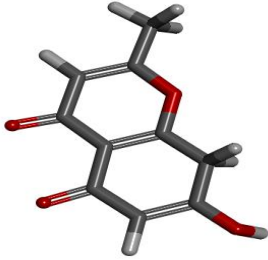
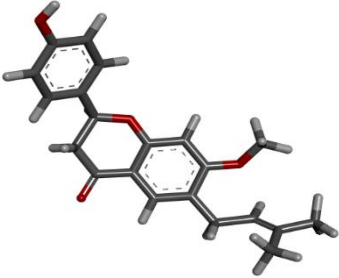
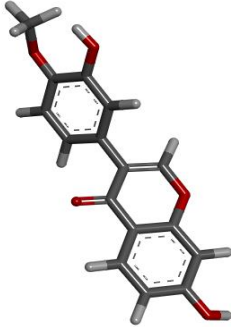
Nilai RMSD 6LZG hasil docking menggunakan *Autodock*

### LAMPIRAN III VIRTUAL SCREENING

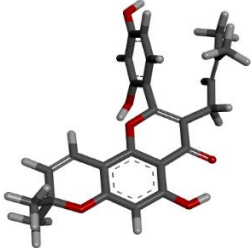
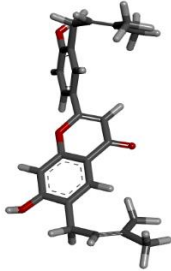
**Lampiran 3.1** Ligan terbaik hasil docking *Main Protease* (6ZRU)

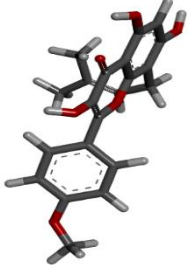
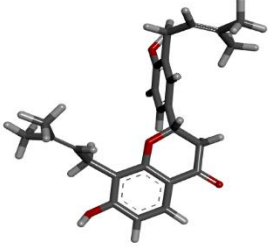
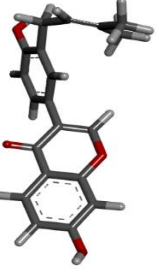
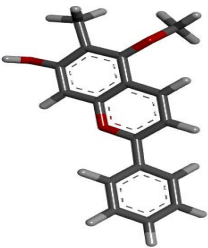
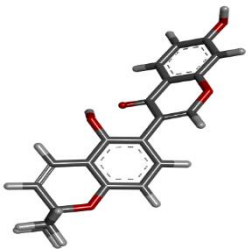
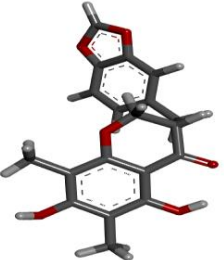
No	Nama Senyawa	Struktur Kimia
1.	3'_methoxypuearin	

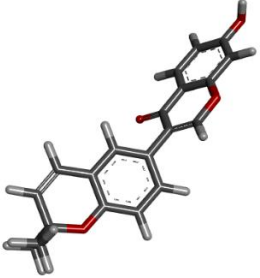
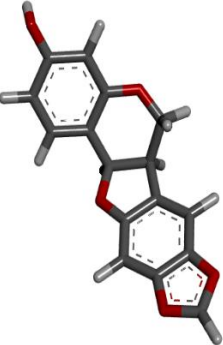
2.	3'- _hydroxy_5_6_7_8_4_pentamethoxyflavone	
3.	3_3_4_5_6_7_8_heptamethoxyflavone	
4.	3'_hydroxypuearin_glucoside	
5.	2_beta_2	
6.	2'_0_rhamnosylvitexin	
7.	2'_0_galloylhyperin_	

8.	Noreugenin	
9.	Bavachinin	
10.	Calycosin	


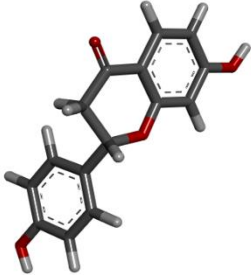
**Lampiran 1.2** Ligan terbaik hasil docking *RdRp* (7CTT)

No	Nama Senyawa	Gambar Ligan
1.	Morusin	
2.	Licoflavone B	

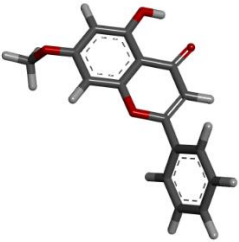
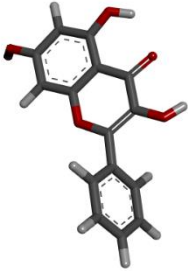
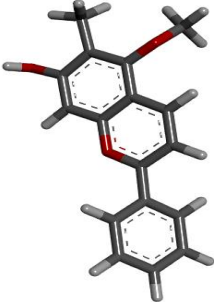
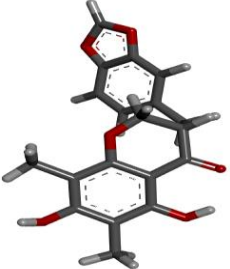
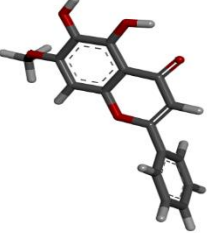
3.	Icaritin	
4.	Glabrol	
5.	Neobavaisoflavone	
6.	Dracorhodin percholate	
7.	Glabrone	
8.	Methylphlogonone_a	

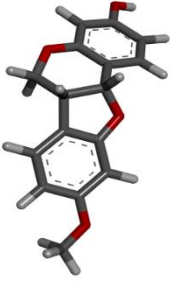
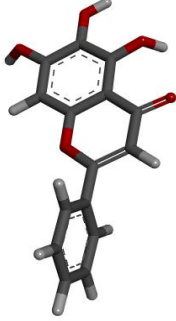
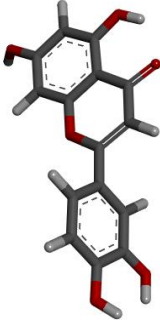
9.	Corvlin	
10.	Maackiain	

**Lampiran 1.3** Ligan terbaik hasil docking ACE2 (6LZG)

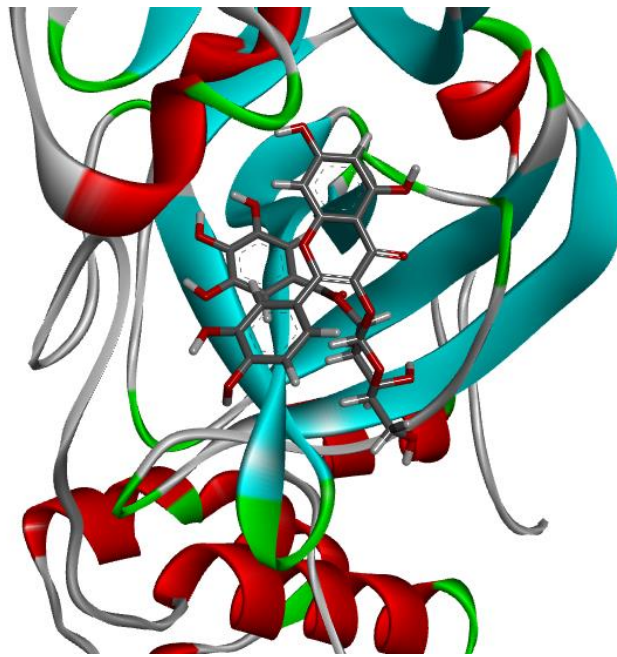
No	Senyawa	Gambar Ligan
1.	Noreugenin	
2.	Liquiritigenin	



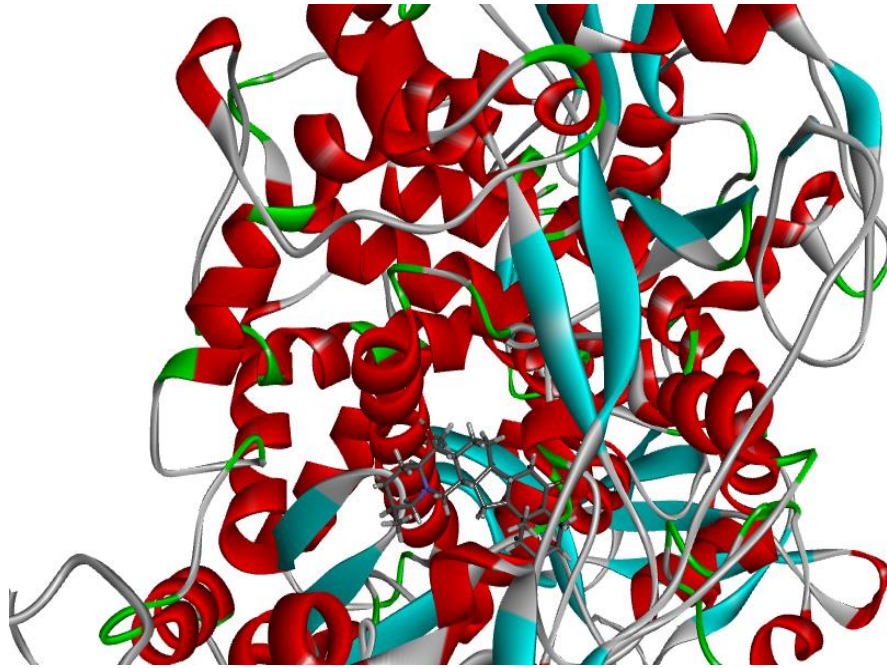
3.	Tectochrysin	
4.	Galangin	
5.	Diacorhodin_perchorate	
6.	Methylphiopogonone	
7.	Negletein	

8.	Medicarpin	 <p>A ball-and-stick model of Medicarpin, a flavanone. It features a central pyrone ring system with two phenyl rings attached at the 2 and 7 positions. The phenyl rings are substituted with hydroxyl groups at the 3 and 4 positions. The model uses grey for carbon, red for oxygen, and white for hydrogen atoms.</p>
9.	Baicalein	 <p>A ball-and-stick model of Baicalein, a flavone. It features a central pyrone ring system with two phenyl rings attached at the 2 and 7 positions. The phenyl rings are substituted with hydroxyl groups at the 3 and 4 positions. The model uses grey for carbon, red for oxygen, and white for hydrogen atoms.</p>
10.	Luteolin	 <p>A ball-and-stick model of Luteolin, a flavone. It features a central pyrone ring system with two phenyl rings attached at the 2 and 7 positions. The phenyl rings are substituted with hydroxyl groups at the 3 and 4 positions. The model uses grey for carbon, red for oxygen, and white for hydrogen atoms.</p>

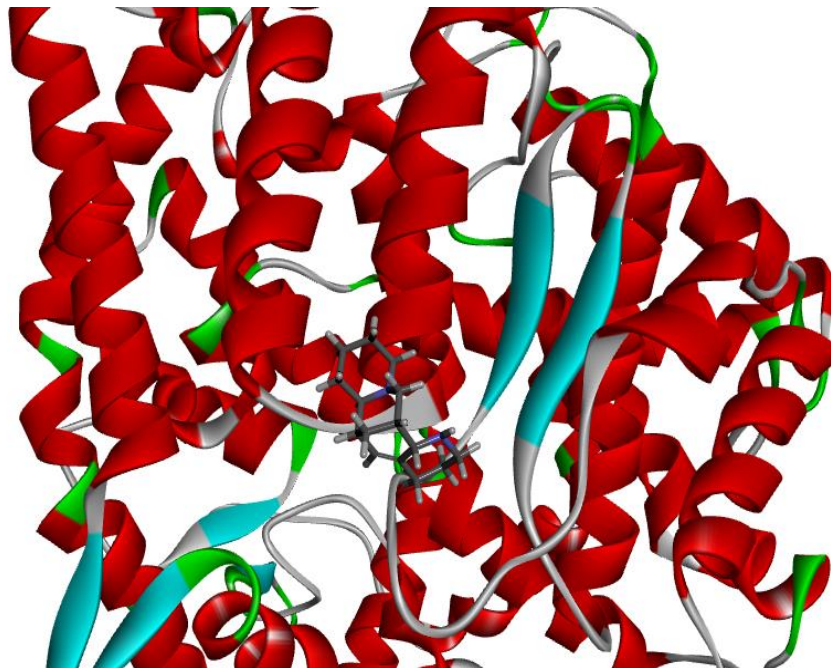
**LAMPIRAN IV**  
**VISUALISASI HASIL DOCKING**



Visualisasi 3D 6ZRU + 3'\_methoxypuearin

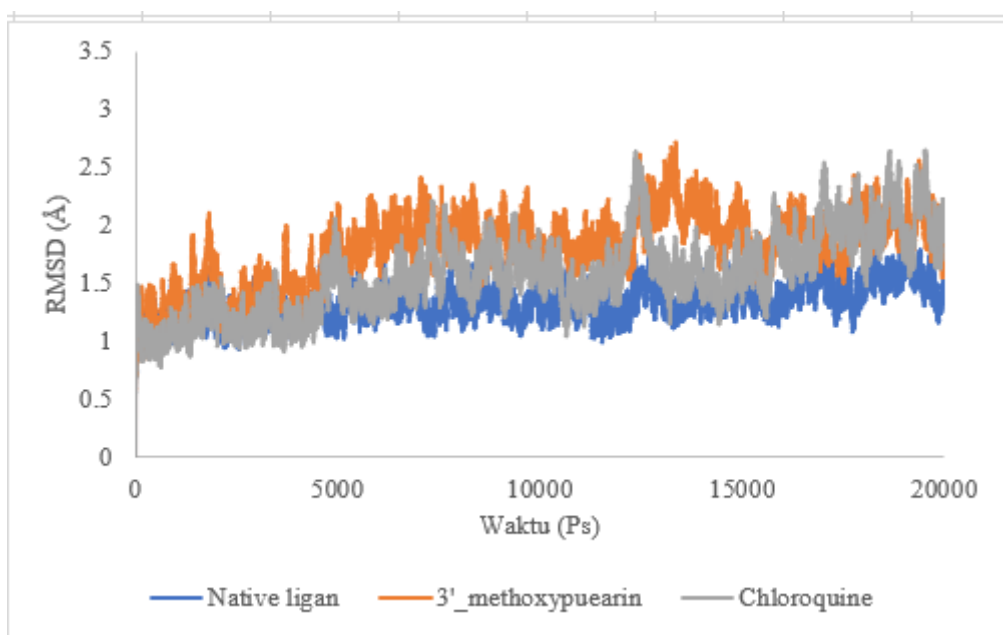


Visualisasi 3D 7CTT + morusin

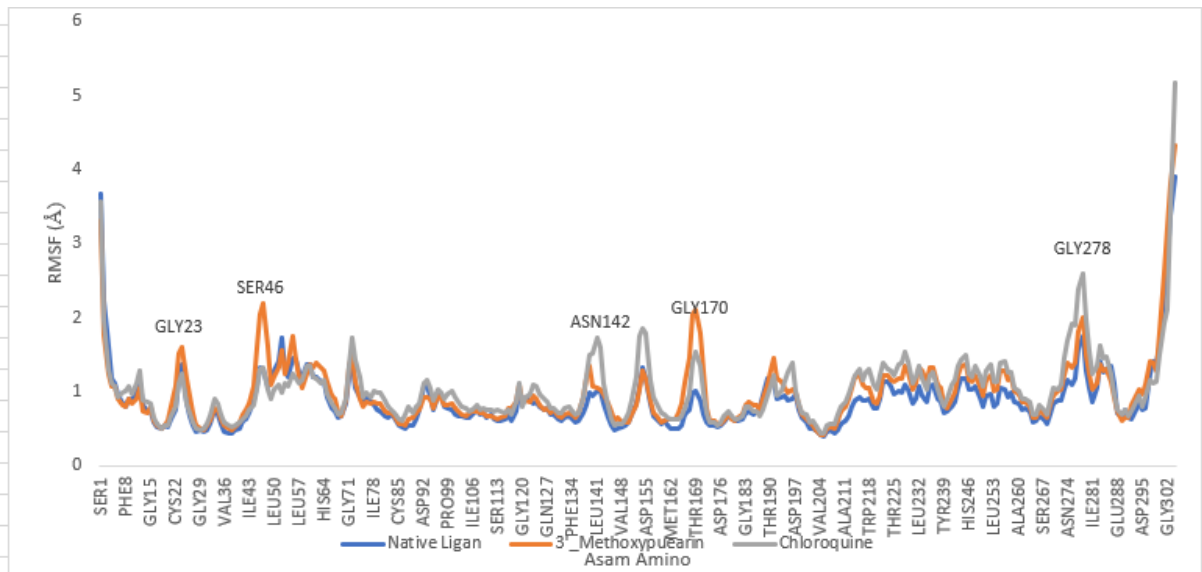


Visualisasi 3D 6LZG + noreugenin

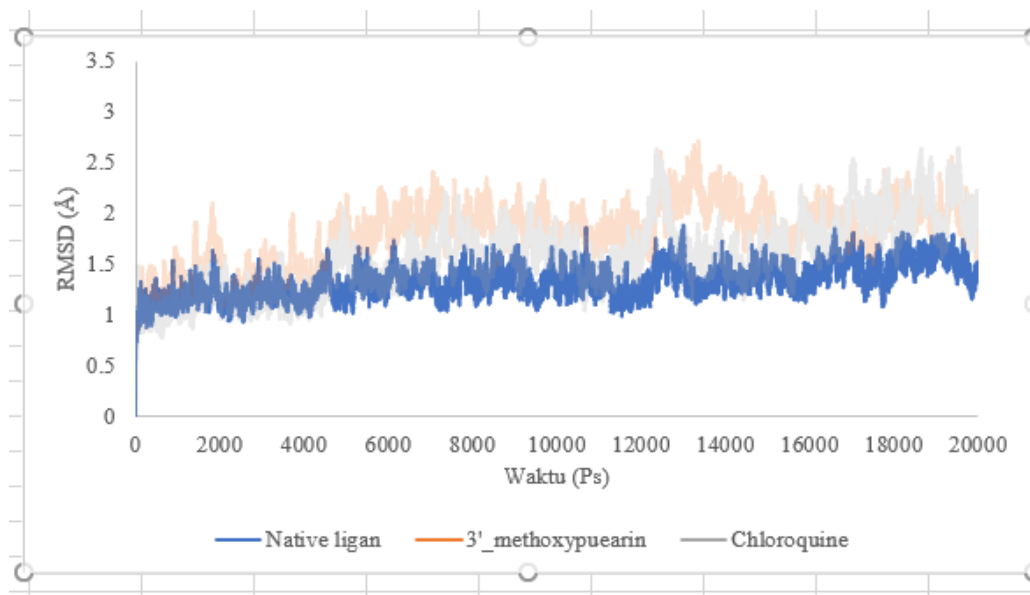
**LAMPIRAN V**  
**MOLECULAR DOCKING**



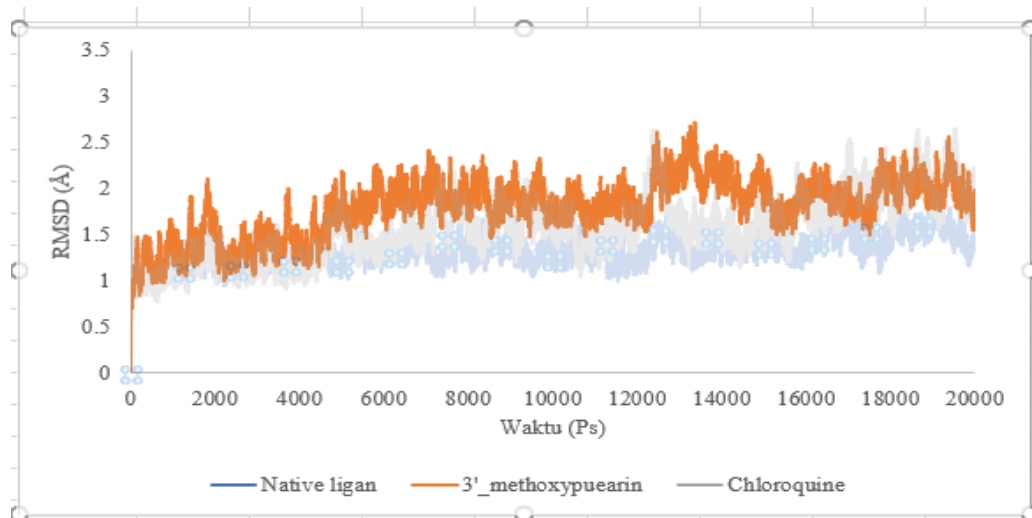
Grafik RMSD 6ZRU



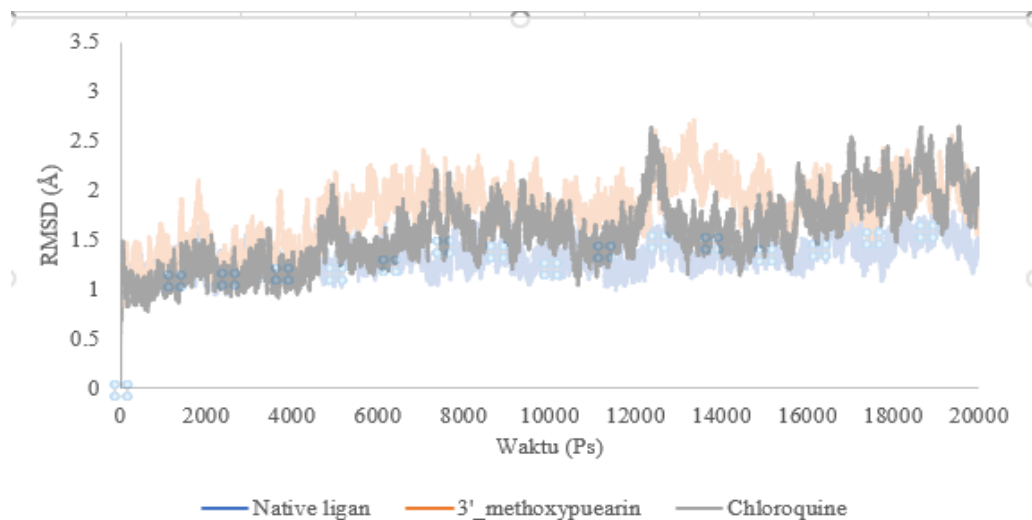
Grafik RMSF 6ZRU



Fluktuasi tinggi Native Ligand



Fluktuasi tertinggi 3'\_methoxypuearin



Fluktuasi tertinggi Chloroquine

1	Asam Amir	Native Lig
2	LEU205	0.3895
3	VAL204	0.4234
4	LEU208	0.4337

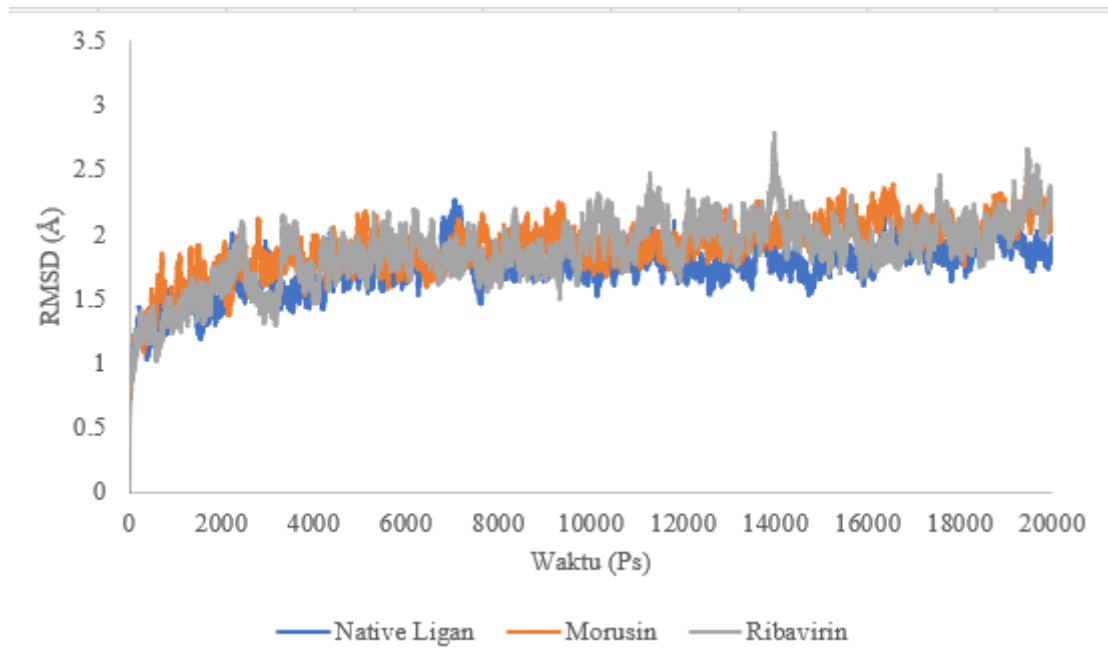
Fluktuasi terendah native ligand

1	Asam Amir	3'_Methoxypuear
2	LEU205	0.4151
3	VAL204	0.4262
4	CYS38	0.4783

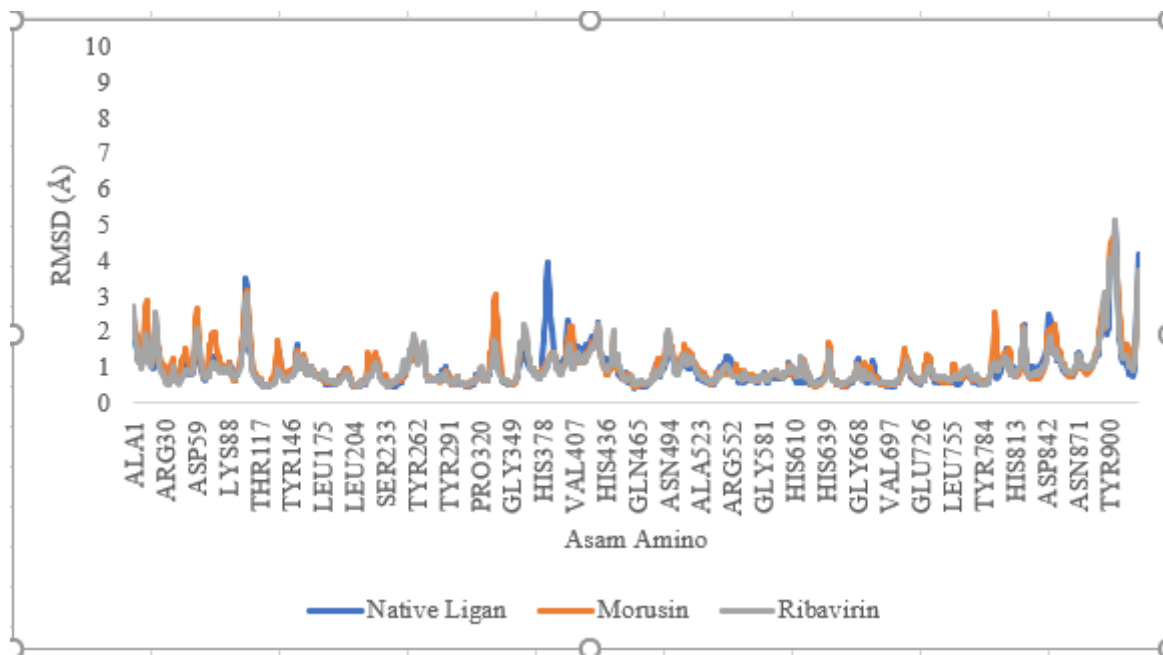
Fluktuasi terendah 3'\_methoxypuearin

1	Asam Amir	Chloroquin
2	LEU205	0.4339
3	VAL204	0.4415
4	GLY29	0.4802

Fluktuasi terendah Chloroquine

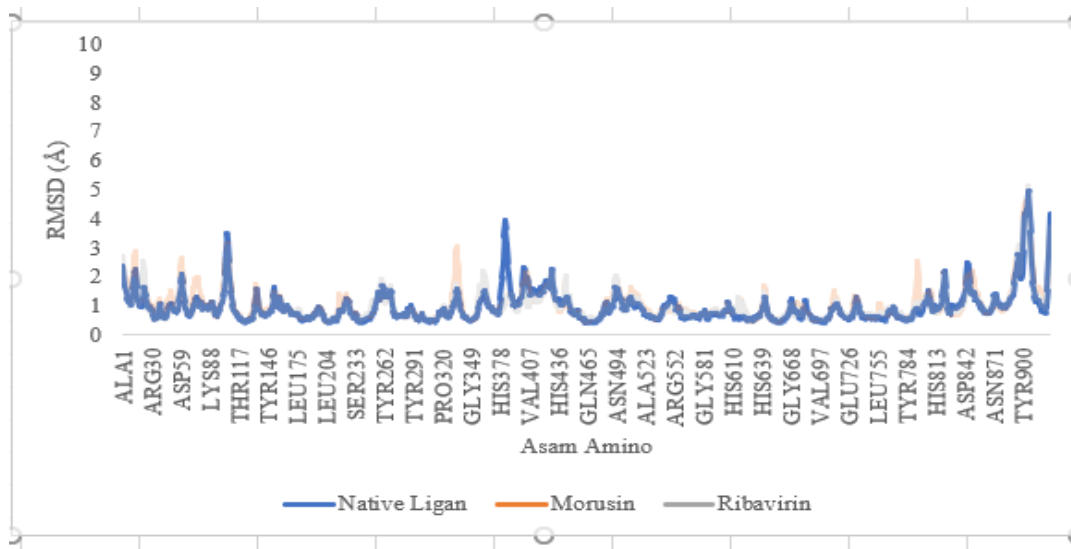


Grafik RMSD 7CTT

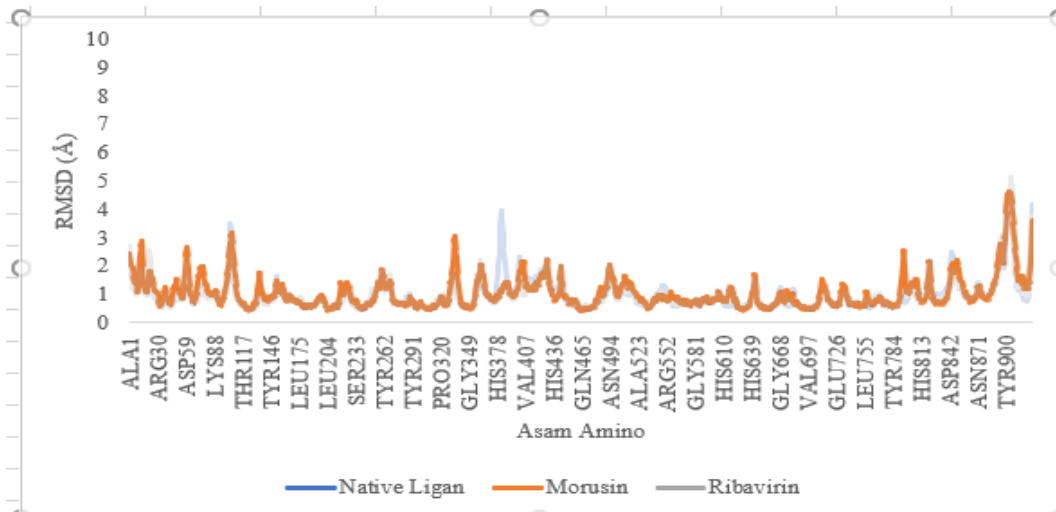


Grafik RMSF 7CTT

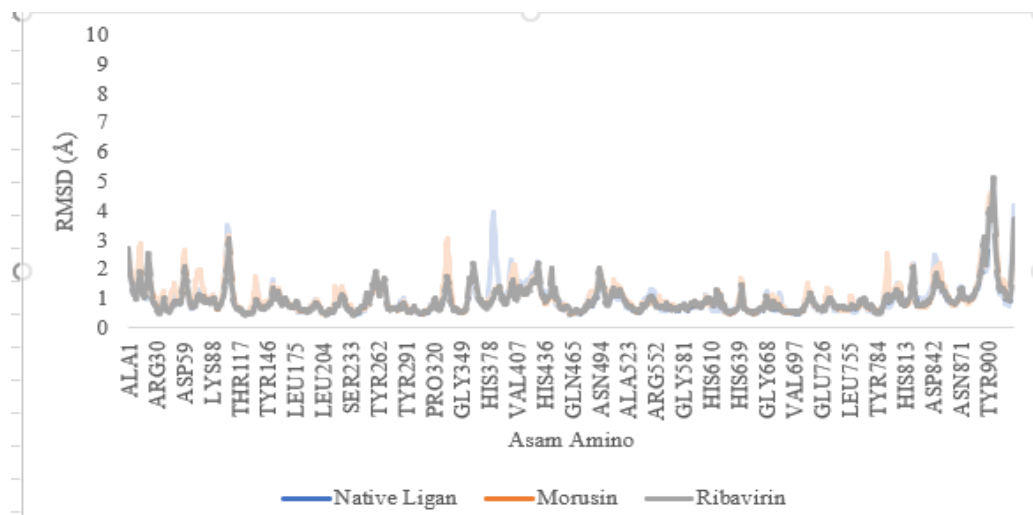




Fluktuasi tertinggi Native Ligand



Fluktuasi tertinggi Morusin



### Fluktuasi tertinggi Ribavirin

1	Asam Amir	Native Ligand
2	ASP462	0.4359
3	ALA122	0.4416
4	ASP205	0.4437

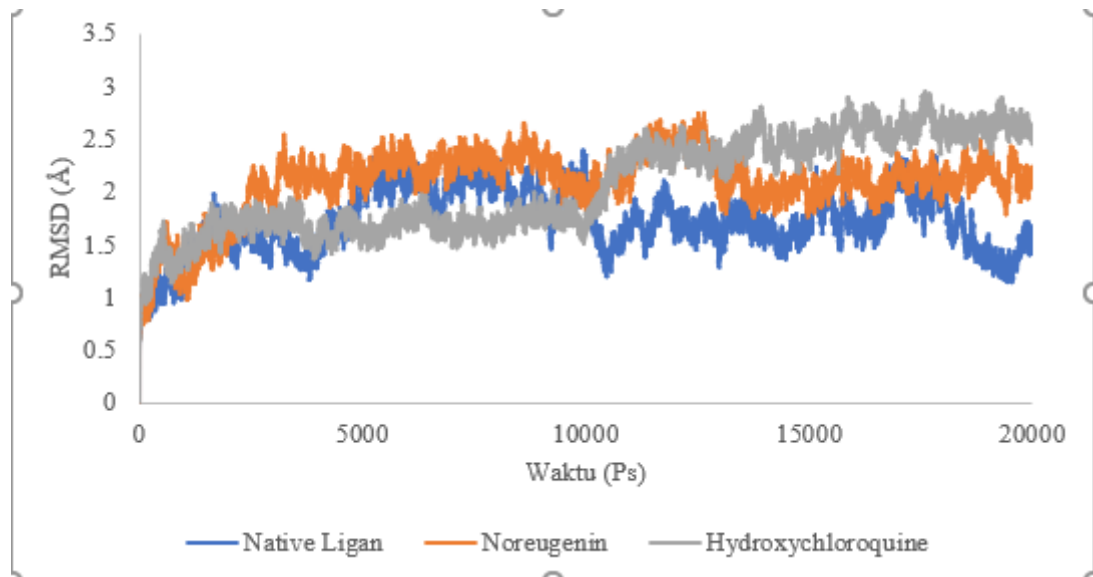
Fluktuasi terendah Native Ligand

1	Asam Amir	Morusin
2	ARG464	0.4636
3	ALA122	0.4674
4	LEU204	0.4721

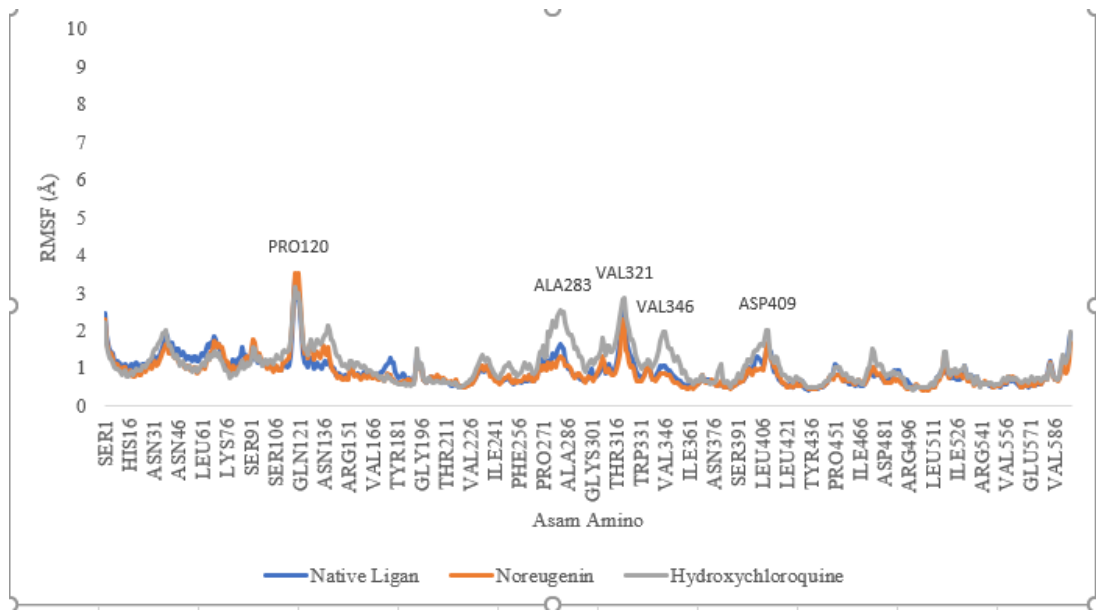
Fluktuasi terendah Morusin

1	Asam Amir	Ribavirin
2	ALA122	0.4554
3	TYR235	0.4597
4	MET121	0.4711

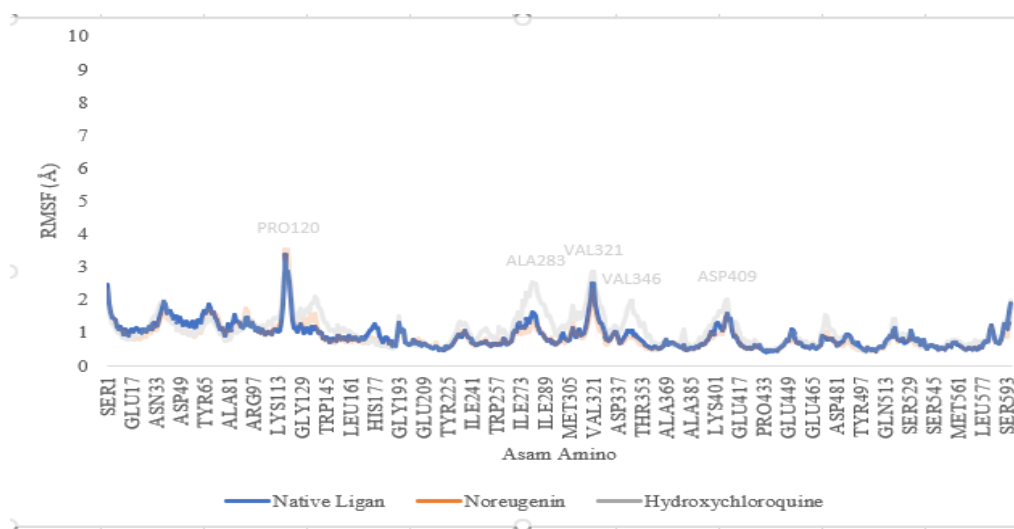
Fluktuasi terendah Ribavirin



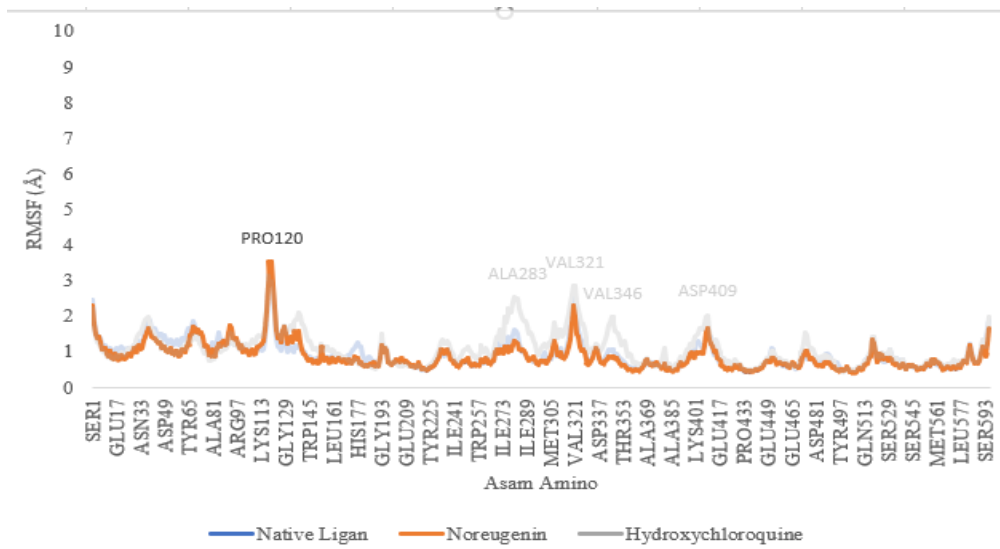
Grafik RMSD 6LZG



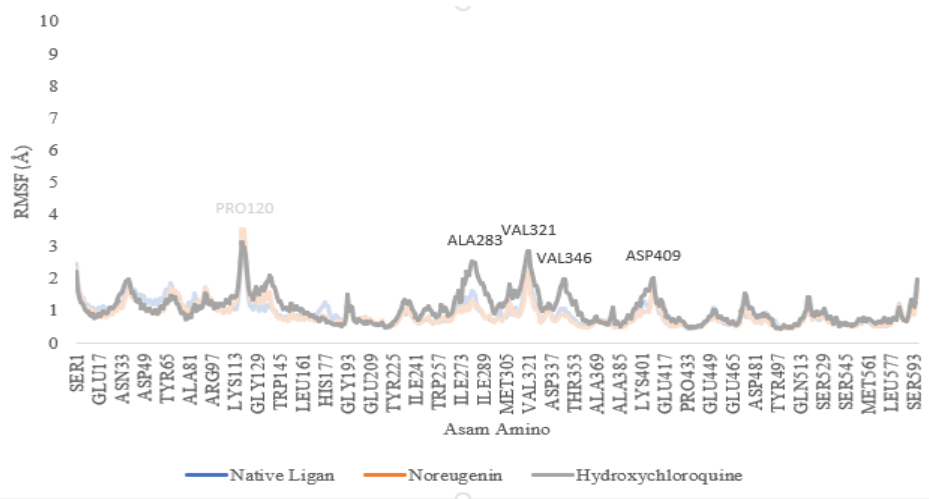
Grafik RMSF 6LZG



Fluktuasi tertinggi Native Ligand



Fluktuasi tertinggi Noreugenin



Fluktuasi tertinggi Hydroxychloroquine

	A	B
1	Asam Amir	Native Lig
2	PHE434	0.4287
3	PRO433	0.443
4	MET437	0.4463

Fluktuasi terendah Native Ligand

	A	B
1	Asam Amir	Noreugen
2	PHE507	0.4204
3	PHE505	0.4311
4	GLN504	0.4313

Fluktuasi terendah Noreugenin

	A	B
1	Asam Amir	Hydroxychloroquir
2	THR499	0.4275
3	TYR498	0.4585
4	ARG496	0.4786

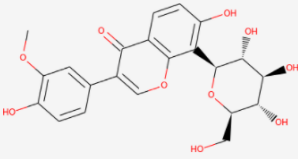
Fluktuasi terendah Hydroxychloroquine

## LAMPIRAN VI

### PREDIKSI PROFIL FARMAKOKINETIK DAN TOKSISITAS

pkCSM [Predict](#) [Theory](#) [Help](#) [Contact](#) [Acknowledgements](#) [Related Resources](#) [License](#)

**Molecule Depiction**



SMILES

**Molecule properties:**

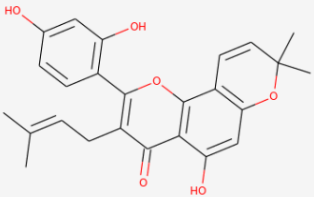
Descriptor	Value
Molecular Weight	446.408
LogP	0.3947
#Rotatable Bonds	4
#Acceptors	10
#Donors	6
Surface Area	180.678

Property	Model Name	Predicted Value	Unit
Absorption	Water solubility	-2.82	Numeric (log mol/L)
Absorption	Caco2 permeability	-0.803	Numeric (log Papp in 10 <sup>-6</sup> cm/s)
Absorption	Intestinal absorption (human)	39.533	Numeric (% Absorbed)
Absorption	Skin Permeability	-2.735	Numeric (log Kp)
Absorption	P-glycoprotein substrate	Yes	Categorical (Yes/No)
Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
Distribution	VDss (human)	0.033	Numeric (log L/kg)
Distribution	Fraction unbound (human)	0.132	Numeric (Fu)
Distribution	BBB permeability	-1.721	Numeric (log BB)
Distribution	CNS permeability	-4.119	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
Metabolism	CYP3A4 substrate	No	Categorical (Yes/No)
Metabolism	CYP1A2 inhibitor	No	Categorical (Yes/No)

Prediksi profil farmakokinetik dan toksisitas senyawa 3'-methoxypuearin menggunakan pkCSM

pkCSM [Predict](#) [Theory](#) [Help](#) [Contact](#) [Acknowledgements](#) [Related Resources](#) [License](#)

### Molecule Depiction



**SMILES**

#### Molecule properties:

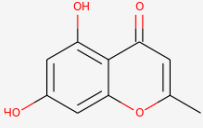
Descriptor	Value
Molecular Weight	420.461
LogP	5.2697
#Rotatable Bonds	3
#Acceptors	6
#Donors	3
Surface Area	178.897

Property	Model Name	Predicted Value	Unit
<b>Absorption</b>	Water solubility	-4.513	Numeric (log mol/L)
<b>Absorption</b>	Caco2 permeability	1.049	Numeric (log Papp in 10 <sup>-6</sup> cm/s)
<b>Absorption</b>	Intestinal absorption (human)	94.317	Numeric (% Absorbed)
<b>Absorption</b>	Skin Permeability	-2.737	Numeric (log Kp)
<b>Absorption</b>	P-glycoprotein substrate	Yes	Categorical (Yes/No)
<b>Absorption</b>	P-glycoprotein I inhibitor	Yes	Categorical (Yes/No)
<b>Absorption</b>	P-glycoprotein II inhibitor	Yes	Categorical (Yes/No)
<b>Distribution</b>	VDss (human)	-0.194	Numeric (log L/kg)
<b>Distribution</b>	Fraction unbound (human)	0.094	Numeric (Fu)
<b>Distribution</b>	BBB permeability	-1.045	Numeric (log BB)
<b>Distribution</b>	CNS permeability	-1.737	Numeric (log PS)
<b>Metabolism</b>	CYP2D6 substrate	No	Categorical (Yes/No)
<b>Metabolism</b>	CYP3A4 substrate	No	Categorical (Yes/No)
<b>Metabolism</b>	CYP1A2 inhibitor	Yes	Categorical (Yes/No)
<b>Metabolism</b>	CYP2C19 inhibitor	Yes	Categorical (Yes/No)

## Prediksi profil farmakokinetik dan toksisitas senyawa morusin menggunakan pkCSM

pkCSM [Predict](#) [Theory](#) [Help](#) [Contact](#) [Acknowledgements](#) [Related Resources](#) [License](#)

### Molecule Depiction



**SMILES**

#### Molecule properties:

Descriptor	Value
Molecular Weight	192.17
LogP	1.51262
#Rotatable Bonds	0
#Acceptors	4
#Donors	2
Surface Area	79.033

Property	Model Name	Predicted Value	Unit
<b>Absorption</b>	Water solubility	-2.282	Numeric (log mol/L)
<b>Absorption</b>	Caco2 permeability	1.364	Numeric (log Papp in 10 <sup>-6</sup> cm/s)
<b>Absorption</b>	Intestinal absorption (human)	93.09	Numeric (% Absorbed)
<b>Absorption</b>	Skin Permeability	-2.628	Numeric (log Kp)
<b>Absorption</b>	P-glycoprotein substrate	No	Categorical (Yes/No)
<b>Absorption</b>	P-glycoprotein I inhibitor	No	Categorical (Yes/No)
<b>Absorption</b>	P-glycoprotein II inhibitor	No	Categorical (Yes/No)
<b>Distribution</b>	VDss (human)	-0.048	Numeric (log L/kg)
<b>Distribution</b>	Fraction unbound (human)	0.343	Numeric (Fu)
<b>Distribution</b>	BBB permeability	-0.11	Numeric (log BB)
<b>Distribution</b>	CNS permeability	-2.907	Numeric (log PS)
<b>Metabolism</b>	CYP2D6 substrate	No	Categorical (Yes/No)
<b>Metabolism</b>	CYP3A4 substrate	No	Categorical (Yes/No)
<b>Metabolism</b>	CYP1A2 inhibitor	Yes	Categorical (Yes/No)

## Prediksi profil farmakokinetik dan toksisitas senyawa noreugenin menggunakan pkCSM

**Molecule properties:**

Descriptor	Value
Molecular Weight	446.408
LogP	0.3947
#Rotatable Bonds	4
#Acceptors	10
#Donors	6
Surface Area	180.678

*Lipinski's Rule of Five*  
senyawa 3'methoxypuearin

**Molecule properties:**

Descriptor	Value
Molecular Weight	420.461
LogP	5.2697
#Rotatable Bonds	3
#Acceptors	6
#Donors	3
Surface Area	178.897

*Lipinski's Rule of Five*  
senyawa morusin

**Molecule properties:**

Descriptor	Value
Molecular Weight	192.17
LogP	1.51262
#Rotatable Bonds	0
#Acceptors	4
#Donors	2
Surface Area	79.033

*Lipinski's Rule of Five*  
senyawa 3'methoxypuearin