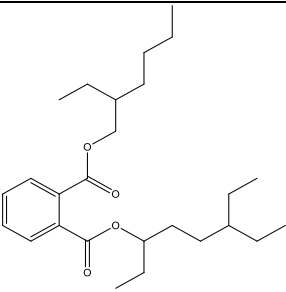
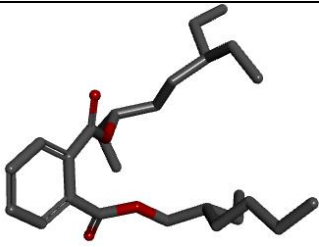
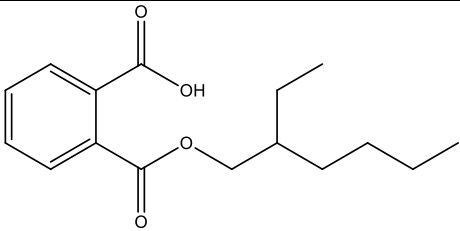
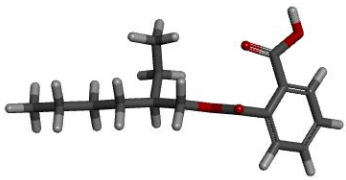
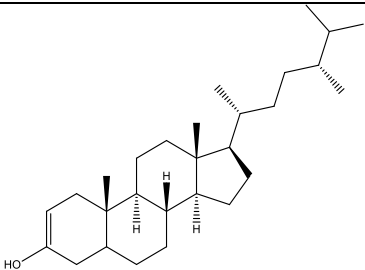
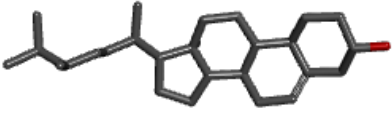
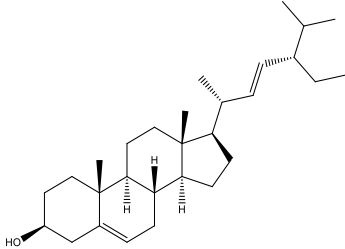
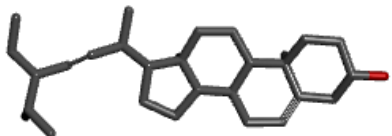


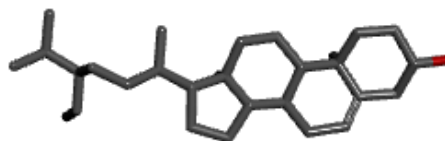
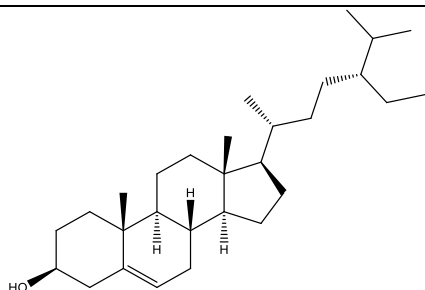
LAMPIRAN

Lampiran 1. Kandungan Senyawa dalam Kulit Buah Naga

Kode	2D	3D
Ligan		
1. PHT		
	<i>Phthalic acid, 6-ethyloct-3-yl 2-ethylhexyl ester</i>	
2. BEN		
	<i>1,2-Benzenedicarboxylic acid, mono (2-ethylhexyl) ester</i>	
3. CAM		
	<i>(3S,8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5,6-dimethylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol</i>	
4. STI		

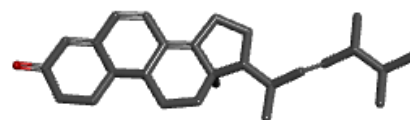
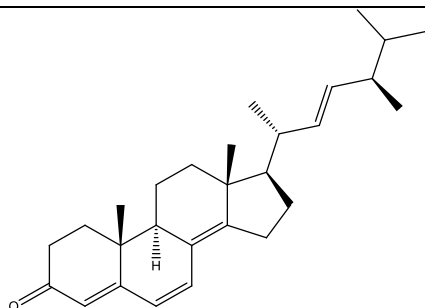
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(*E*,2*R*,5*S*)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-3-ol

5. BSI



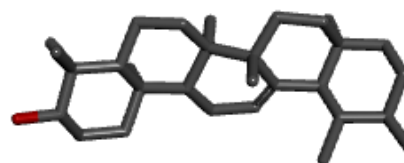
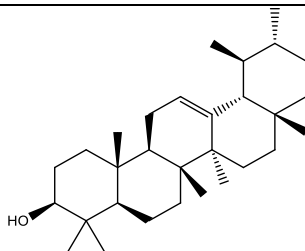
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(2*R*,5*R*)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-3-ol

8.ERG



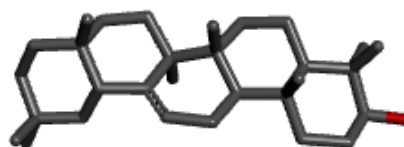
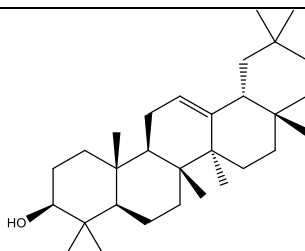
(9*R*,10*R*,13*R*,17*R*)-17-[(*E*,2*R*,5*R*)-5,6-dimethylhept-3-en-2-yl]-10,13-dimethyl-1,2,9,11,12,15,16,17-octahydrocyclopenta[*a*]phenanthren-3-one

9. AAM



(3*S*,4*aR*,6*aR*,6*bS*,8*aR*,11*R*,12*S*,12*aR*,14*aR*,14*bR*)-4,4,6*a*,6*b*,8*a*,11,12,14*b*-octamethyl-2,3,4*a*,5,6,7,8,9,10,11,12,12*a*,14,14*a*-tetradecahydro-1*H*-picen-3-ol

10. BAM



(3*S*,4*aR*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bR*)-4,4,6*a*,6*b*,8*a*,11,11,14*b*-octamethyl-1,2,3,4*a*,5,6,7,8,9,10,12,12*a*,14,14*a*-tetradecahydopicen-3-ol

Lampiran 2. Interaksi Hasil Penambatan Molekul dari Ligan Alami, Ligan Uji, dan Ligan Pembanding

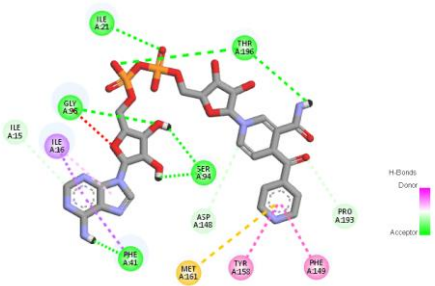
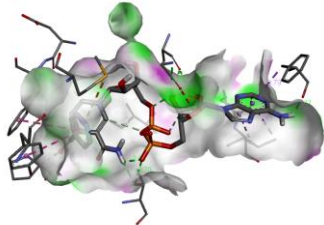
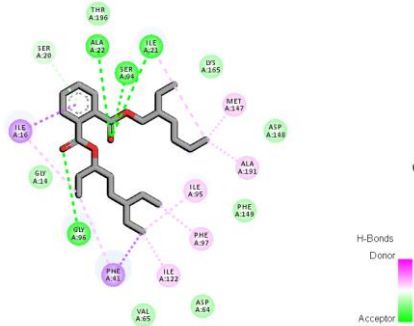
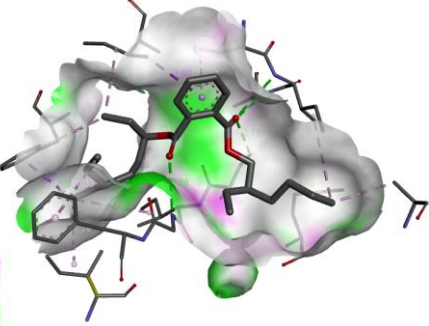
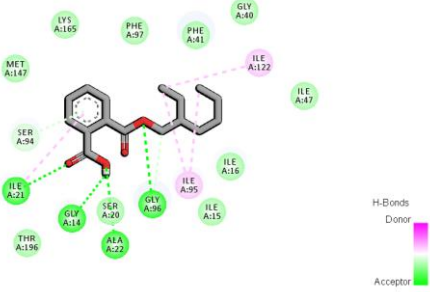
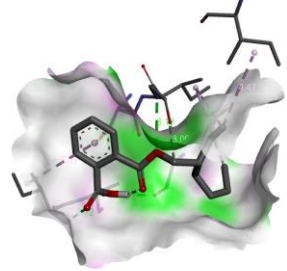
Kode Ligan	Interaksi	Jarak Ikatan (Å)	Residu Asam Amino
INH	Ikatan Hidrogen		
	ILE21:N	3,28207	ILE21, GLY96, THR196, THR196, PHE41, SER94, SER94, PRO193, ASP148, ILE15, ILE21, GLY96, THR196, THR196, PHE41, SER94, SER94, PRO193, ASP148, ILE15, ILE16, PHE4, MET161, PHE149, TYR158, ILE16.
	GLY96:N	3,38681	
	THR196:OG1	2,69850	
	THR196:OG1	2,07895	
	PHE41:O	1,76569	
	SER94:O	2,45510	
	SER94:O	2,57503	
	PRO193:CA	3,13003	
	ASP148:O	3,63397	
	ILE15:O	3,36226	
	ILE21:N	3,28207	
	GLY96:N	3,38681	
	THR196:OG1	2,69850	
	THR196:OG1	2,07895	
	PHE41:O	1,76569	
	SER94:O	2,45510	
	SER94:O	2,57503	
	PRO193:CA	3,13003	
	ASP148:O	3,63397	
	ILE15:O	3,36226	
	Ikatan Hidrofobik		
	π - <i>Sigma</i> : ILE16, PHE4		
	π - <i>Sulfur</i> : MET161		
	π - <i>T-shaped</i> : PHE149, TYR158		
	π - <i>Alkyl</i> : ILE16		
PHT	Ikatan Hidrogen		
	ILE21:N	3,32035	ILE21, ALA22, SER94, GLY96, SER20, ILE16, PHE41, PHE41, PHE97, ALA191, ILE95, ILE122, ILE16, ILE21, MET147, GLY14, THR196, LYS165, ASP148, PHE149, ASP64, VAL65
	ALA22:N	3,14143	
	SER94:OG	2,79297	
	GLY96:N	3,28103	
	SER20:OG	3,67687	

	Ikatan Hidrofobik <i>π-Sigma:</i> ILE16, PHE41 <i>π-Alkyl:</i> PHE41, PHE97 Alkyl: ALA191, ILE95, ILE122, ILE16, ILE21, MET147 Ikatan Van der Waals GLY14, THR196, LYS165, ASP148, PHE149, ASP64, VAL65.		
BEN	Ikatan Hidrogen ILE21:N ALA22:N GLY96:N GLY14:O GLY96:O SER94:OG Ikatan Hidrofobik <i>π-Alkyl:</i> ILE21 Alkyl: ILE95, ILE95, ILE122 Ikatan Van der Waals THR196, ILE15, ILE16, ILE47, GLY40, PHE41, PHE97, LYS165, MET147.	2,72229 3,14809 3,13160 1,93398 3,00385 3,38452	ILE21, ILE95, ILE95, ILE122, THR196, ILE15, ILE16, ILE47, GLY40, PHE41, PHE97, LYS165, MET147
CAM	Ikatan Hidrogen TYR158:OH Ikatan Hidrofobik <i>π-Alkyl:</i> PHE41 Alkyl: ILE21, ILE21, MET199, ILE21, ILE194, ILE21, ILE16, ILE95, ILE95, PHE41	2,25275	TYR158, PHE41, ILE21, ILE21, MET199, ILE21, ILE194, ILE21, ILE16, ILE95, ILE95, PHE41
STI	Ikatan Hidrogen TYR158:OH Ikatan Hidrofobik Alkyl: ILE21, ILE21, MET147, ILE21, MET199, ILE21, ILE194, ILE95, ILE16, ILE95, ILE122 Ikatan Van der Waals	2,10300	ILE21, ILE21, MET147, ILE21, MET199, ILE21, ILE194, ILE95, ILE16, ILE95, ILE122, SER20, PHE97, PHE41, ILE15, GLY14, GLY96, THR196, SER94, LYS165, PHE149, ALA191, GLY192, PRO193, LEU218, TYR158

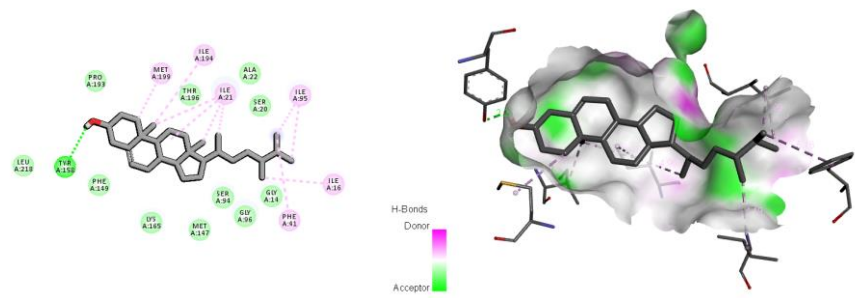
	SER20, PHE97, PHE41, ILE15, GLY14, GLY96, THR196, SER94, LYS165, PHE149, ALA191, GLY192, PRO193, LEU218		
BSI	Ikatan Hidrogen TYR158:OH Ikatan Hidrofobik <i>Alkyl:</i> ILE21, ILE21, MET199, ILE21, ILE194, ILE16, ILE95, PHE41. Ikatan Van der Waals THR196, SER20, GLY14, ILE15, GLY40, SER94, GLY96, MET147, LYS169, ALA191, PHE149, PRO193, GLY192, LEU218.	2,15792	TYR158, ILE21, ILE21, MET199, ILE21, ILE194, ILE16, ILE95, PHE41, THR196, SER20, GLY14, ILE15, GLY40, SER94, GLY96, MET147, LYS169, ALA191, PHE149, PRO193, GLY192, LEU218.
ERG	Ikatan Hidrogen VAL65:N Ikatan Hidrofobik <i>π-Alkyl:</i> PHE41 <i>Alkyl:</i> ILE95, ILE95, ILE122, ALA198, ILE16, LEU197, ILE16, LEU197. Ikatan Van der Waals ILE21, GLY96, PHE97, GLN66, ASP64, LEU63, GLY14, THR196, SER94, THR196, SER20, THR17, SER19.	2,77014	VAL65, PHE41, ILE95, ILE95, ILE122, ALA198, ILE16, LEU197, ILE16, LEU197, ILE21, GLY96, PHE97, GLN66, ASP64, LEU63, GLY14, THR196, SER94, THR196, SER20, THR17, SER19.
AAM	Ikatan Hidrogen MET98:O Ikatan Hidrofobik <i>π-Alkyl:</i> PHE149, PHE149, TYR158. <i>Alkyl:</i> MET103, MET161, ALA191, ALA191, ALA198, ALA198, ALA198, MET199, ILE202, MET161, PRO193, MET199, MET103, MET98, MET103, MET161, ILE21, ILE21, MET147, LYS165, LEU207, ILE194, PHE97, THR196, GLY192, ASP148.	2,19667	MET98, PHE149, PHE149, TYR158, MET103, MET161, ALA191, ALA191, ALA198, ALA198, ALA198, MET199, ILE202, MET161, PRO193, MET199, MET103, MET98, MET103, MET161, ILE21, ILE21, MET147, LYS165, LEU207, ILE194, PHE97, THR196, GLY192, ASP148.

	<i>Ikatan Van der Waals</i> LYS165, LEU207, ILE194, PHE97, THR196, GLY192, ASP148.		
BAM	<i>Ikatan Hidrogen</i> GLY192:O <i>Ikatan Hidrofobik</i> <i>Alkyl</i> : MET103, MET161, ALA191, ALA198, ALA198, ALA198, MET199, ILE21, ILE202, LEU207 <i>π-Alkyl</i> : PHE97, PHE149 <i>Ikatan Van der Waals</i> MET98, GLY96, TYR158, LYS165, PRO193, TRP230, THR196.	1,91242	GLY192, MET103, MET161, ALA191, ALA198, ALA198, ALA198, MET199, ILE21, ILE202, LEU207, PHE97, PHE149, MET98, GLY96, TYR158, LYS165, PRO193, TRP230, THR196.

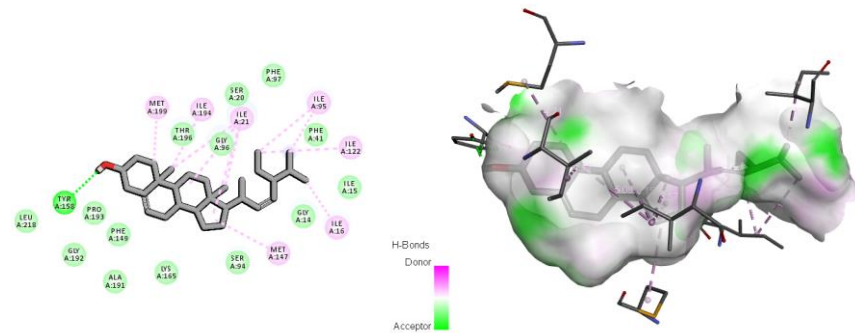
Lampiran 3. Visualisasi Interaksi Ligan dan Makromolekul

Kode	2D	3D
Ligan		
ISONIAZID		
PHT		
BEN		

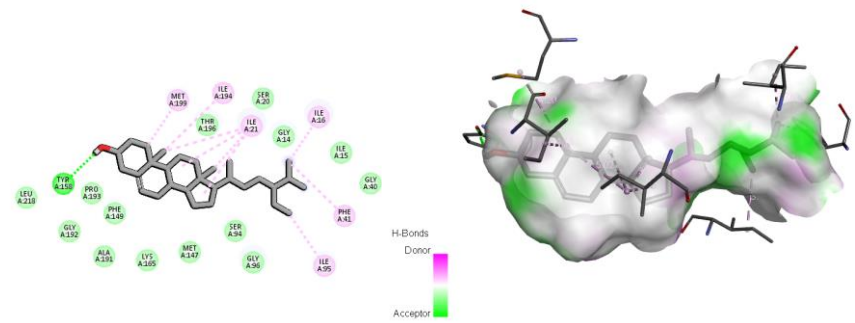
CAM



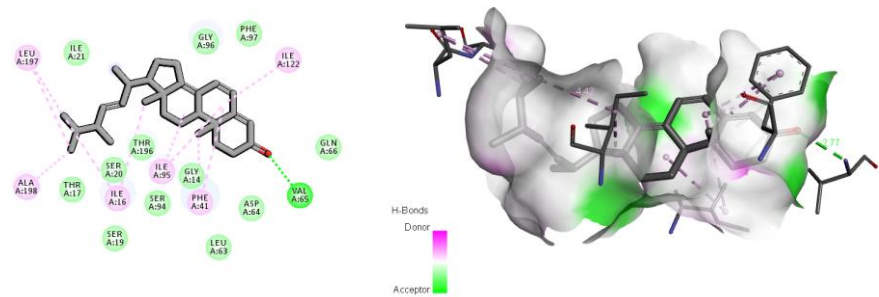
STI



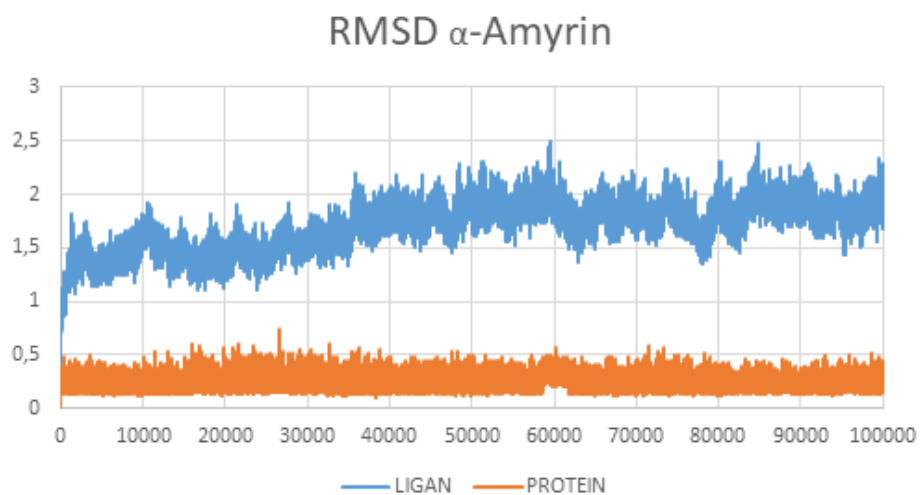
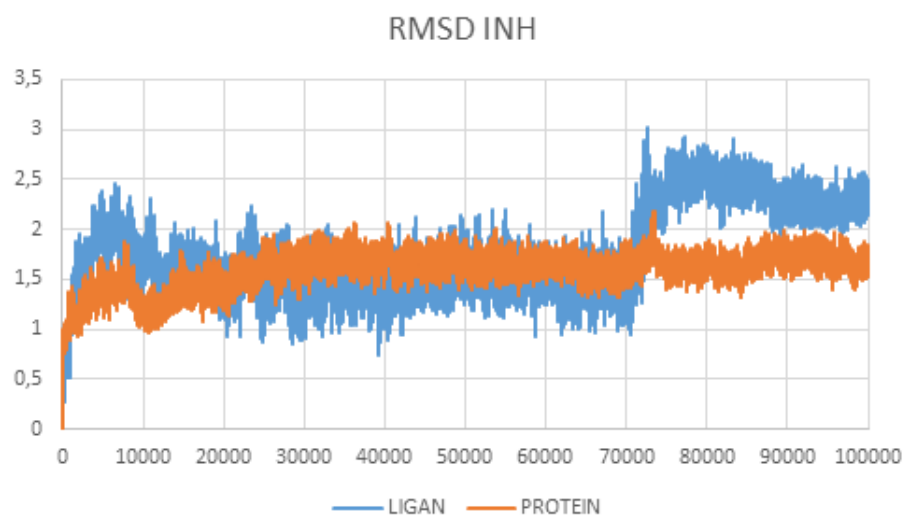
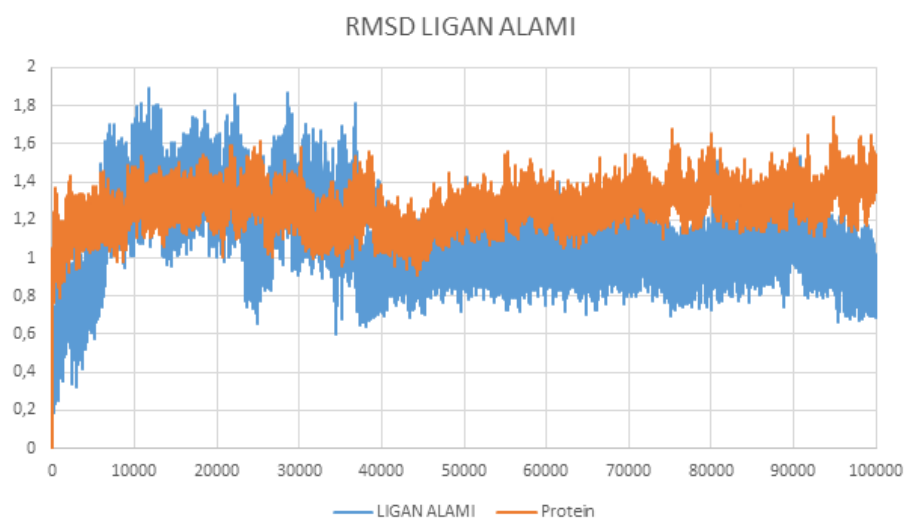
BSI

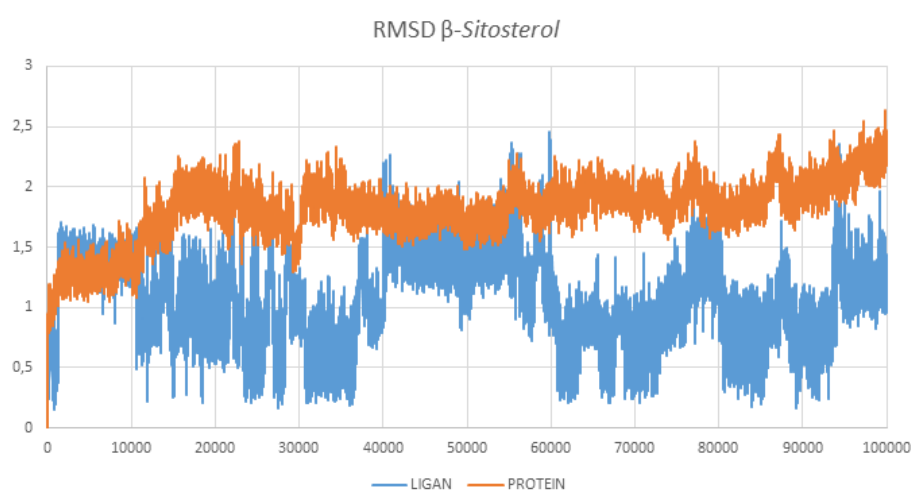
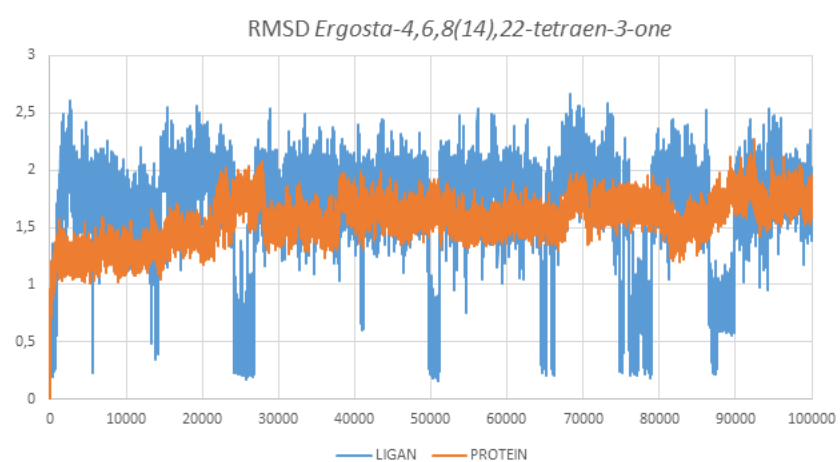


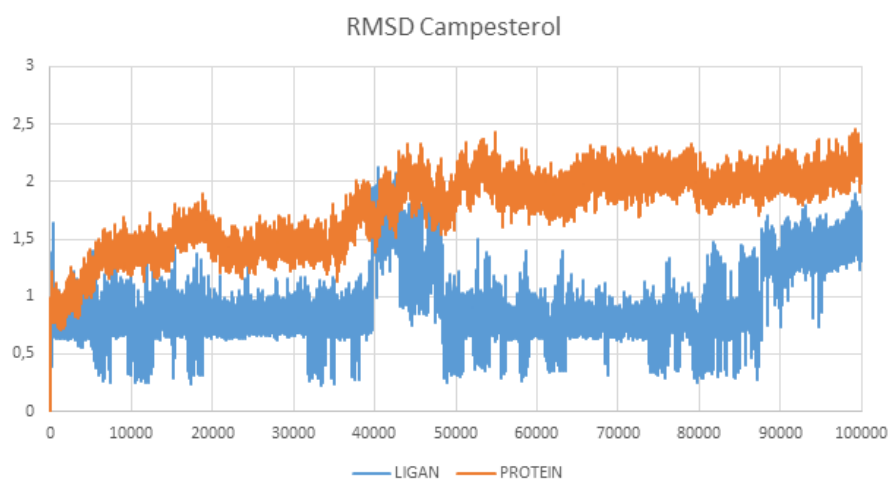
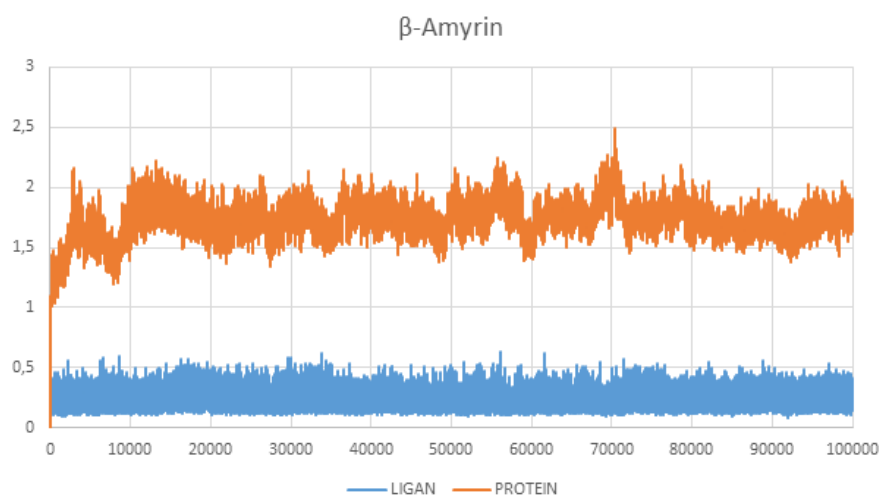
ERG



Lampiran 4. Grafik RMSD Hasil Simulasi Dinamika Molekul







Lampiran 5. Surat Pernyataan Bebas Plagiasi

SURAT PERNYATAAN

Yang bertanda tangan di bawah ini,

Nama : Sarah Stefanie Wijaya

N P M : 11181099

adalah mahasiswa Fakultas Farmasi, Universitas Bhakti Kencana, menyatakan dengan sesungguhnya bahwa Naskah Tugas Akhir/Skripsi yang saya tulis dengan judul:

**PENAMBATAN DAN SIMULASI DINAMIKA MOLEKUL SENYAWA
DARI KULIT BUAH NAGA (*Hylocereus polyrhizus*) TERHADAP NADH-
DEPENDENT ENOYL-ACP REDUCTASE (INHA) SEBAGAI
ANTITUBERKULOSIS**

adalah benar-benar merupakan hasil karya saya sendiri. Apabila di kemudian hari diketahui bahwa isi Naskah Skripsi ini merupakan hasil plagiasi, maka saya bersedia menerima sanksi berupa pembatalan kelulusan dan atau pencabutan gelar yang saya peroleh.

Demikian surat pernyataan ini saya buat untuk dapat dipergunakan sebagaimana mestinya.

Bandung, 31 Juli 2022

Yang membuat pernyataan,



(Sarah Stefanie Wijaya)

NPM. 11181099

Lampiran 6. Surat Persetujuan untuk Dipublikasikan di Media Online

SURAT PERNYATAAN

Yang bertanda tangan di bawah ini,

Nama : Sarah Stefanie Wijaya

N P M : 11181099

Menyatakan bahwa demi kepentingan perkembangan ilmu pengetahuan, saya menyetujui abstrak Skripsi yang saya tulis dengan judul:

**PENAMBATAN DAN SIMULASI DINAMIKA MOLEKUL SENYAWA
DARI KULIT BUAH NAGA (*Hylocereus polyrhizus*) TERHADAP NADH-
DEPENDENT ENOYL-ACP REDUCTASE (INHA) SEBAGAI
ANTITUBERKULOSIS**

Untuk dipublikasikan atau ditampilkan di internet atau media lain yaitu Digital Library Perpustakaan Universitas Bhakti Kencana untuk kepentingan akademik, sebatas sesuai dengan Undang-Undang Hak Cipta.

Demikian surat pernyataan ini saya buat untuk dapat dipergunakan sebagaimana mestinya.

Bandung, 31 Juli 2022

Yang membuat pernyataan,



(Sarah Stefanie Wijaya)

NPM. 11181099