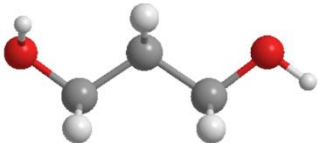
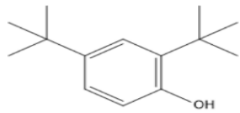
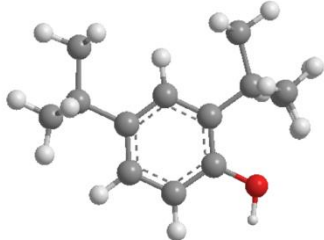
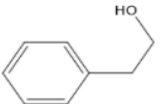
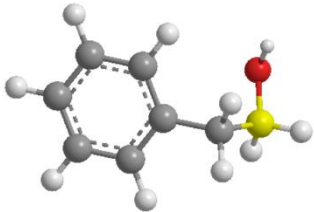
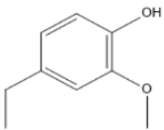
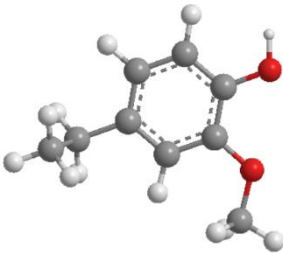
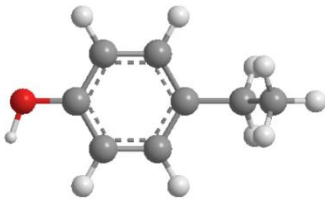
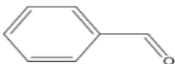
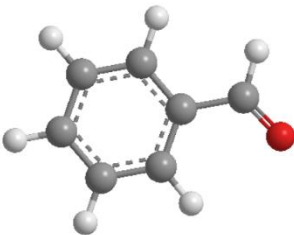
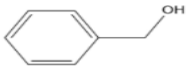
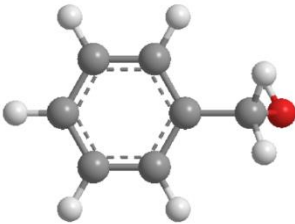
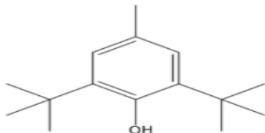
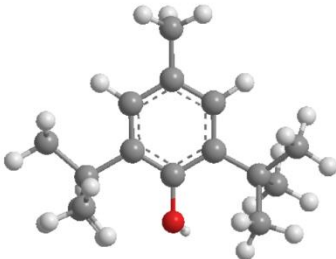
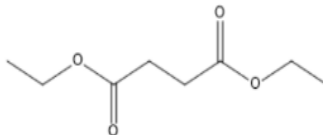
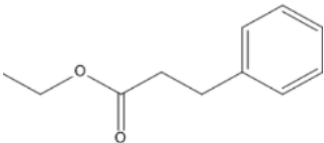
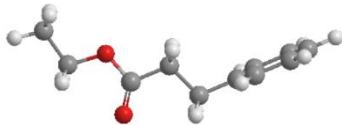
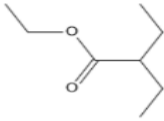
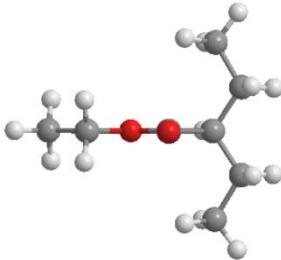
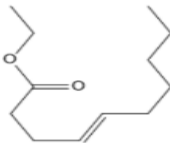
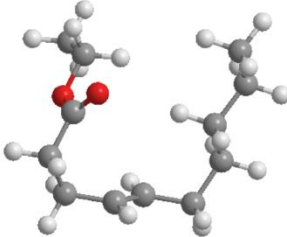
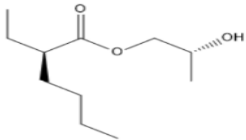
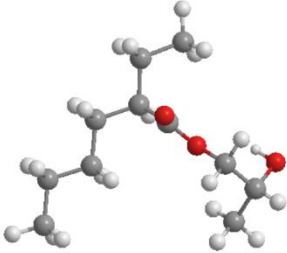


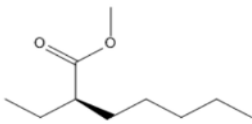
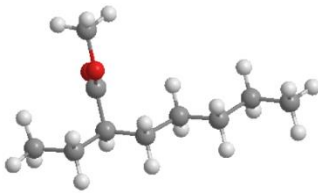
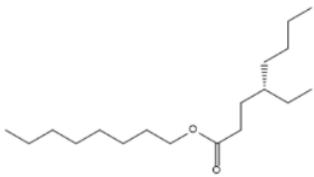
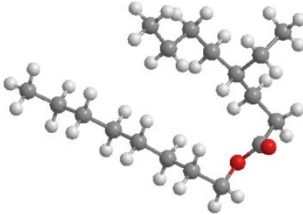
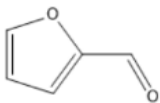
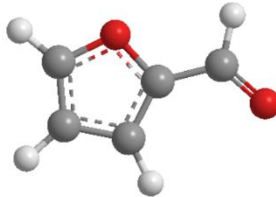
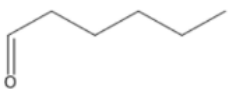
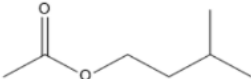
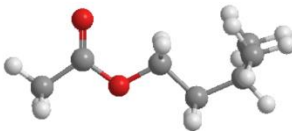
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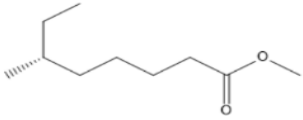
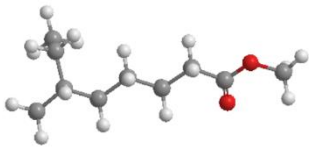
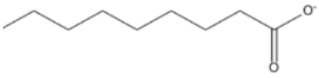
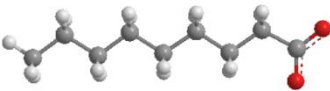
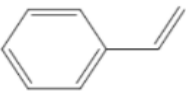
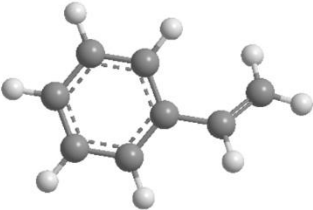
Lampiran 1. Daftar Senyawa Uji yang Digunakan Pada Penelitian

Kode Senyawa	Struktur 2D	Struktur 3D
S01		
1,3-Propanediol		
S02		
1-Octanol		
S03		
2,4-di-tert-butylphenol		
S04		
2-Phenylethanol		

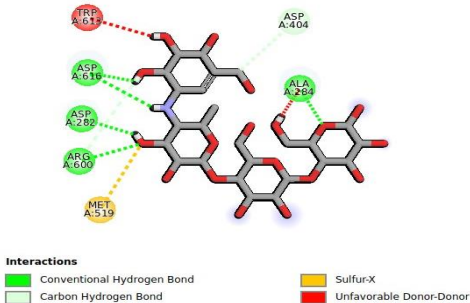
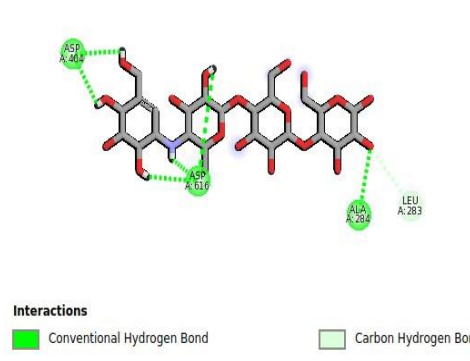
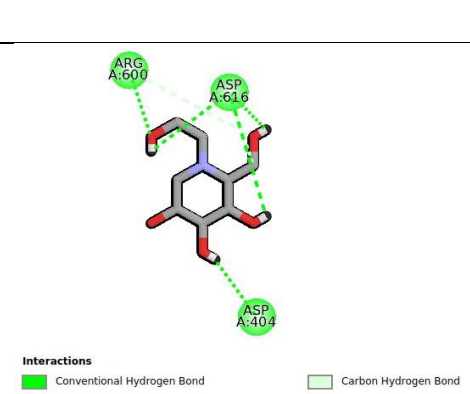
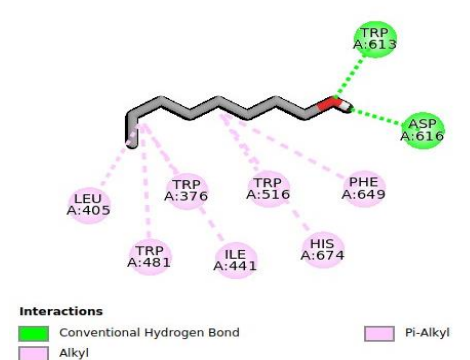
S05		
4-Ethylguaiacol		
S06		
4-Ethylphenol		
S07		
Benzaldehyde		
S08		
Benzyl alcohol		
S09		
ButylHydroxytoluene		

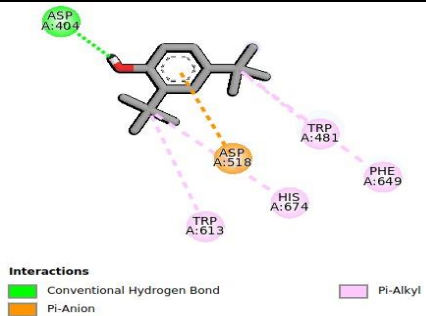
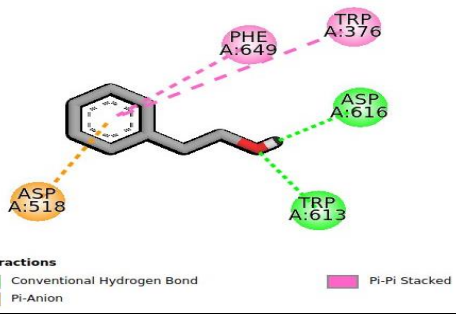
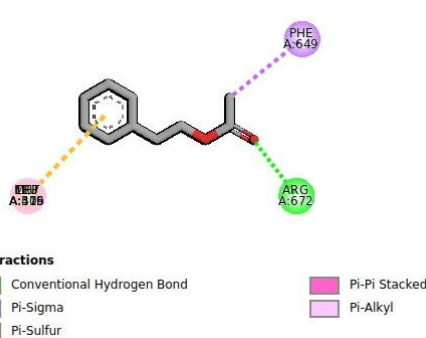
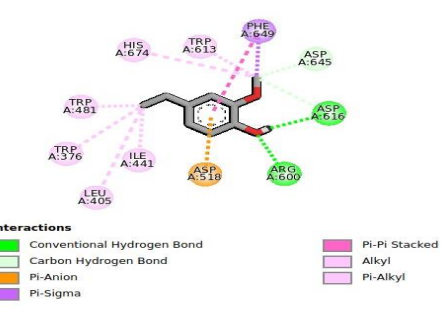
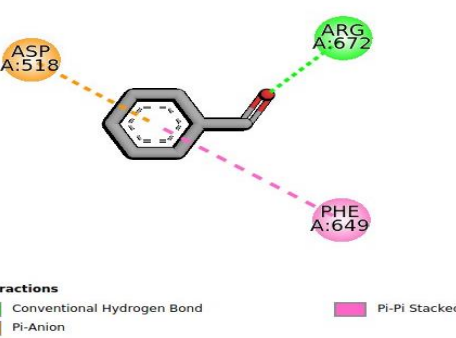
S10		
Diethyl Succinate		
S11		
Ethyl Benzenepropanoate		
S12		
Ethyl Butanoate		
S13		
Ethyl Decanoate		
S14		
Ethyl Hexanoate		

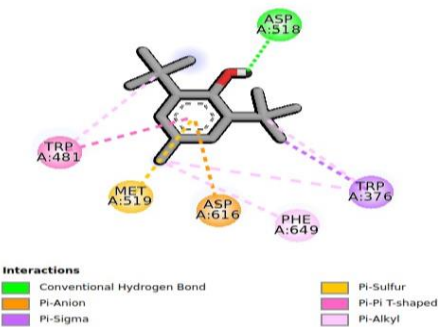
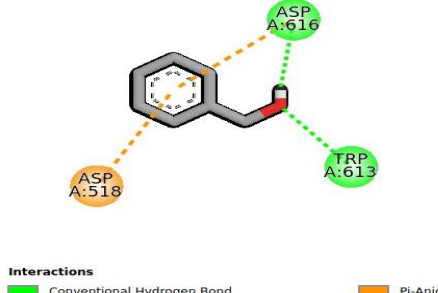
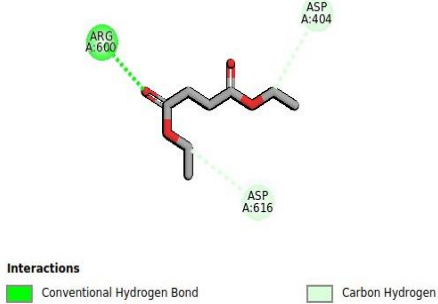
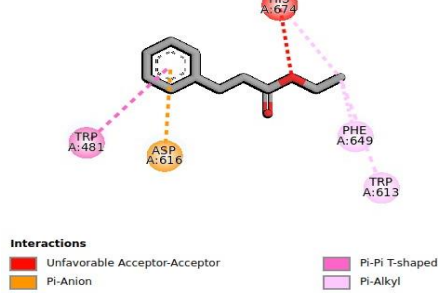
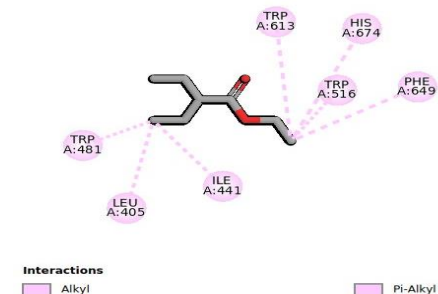
S15	 <chem>CCCCCOC(=O)CC</chem>	
Ethyl Heptanoate		
S16	 <chem>CCCCCOC(=O)CCCC</chem>	
Ethyl Octanoate		
S17	 <chem>O=Cc1ccoc1</chem>	
Furfural		
S18	 <chem>CCCCCC=O</chem>	
Hexanal		
S19	 <chem>CC(=O)OCC(C)CC</chem>	
Isoamyl Acetate		

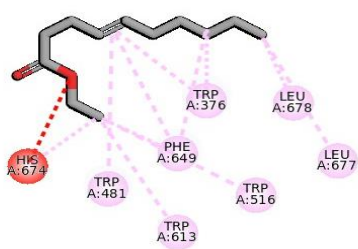
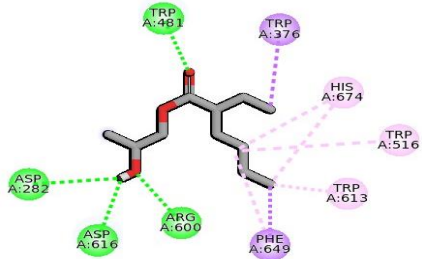
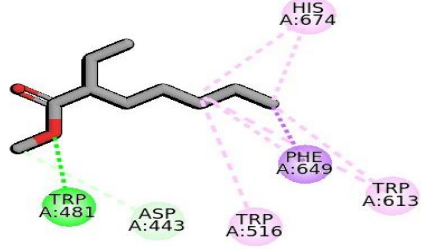
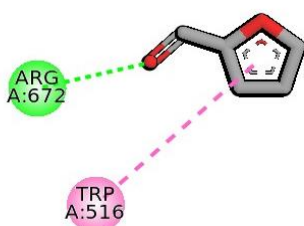
S20		
Methyl Octanoate		
S21		
Nonanoate		
S22		
Styrene		

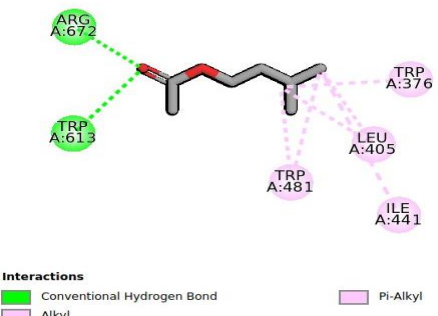
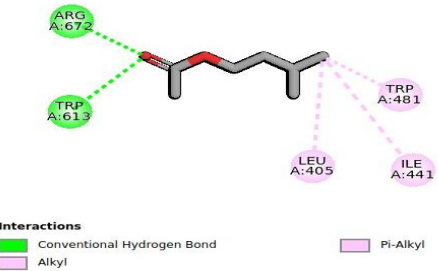
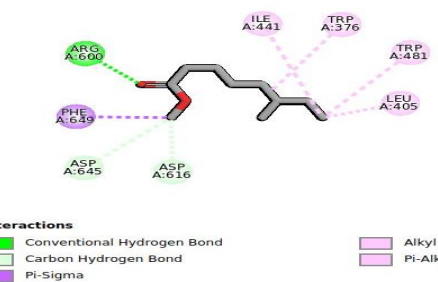
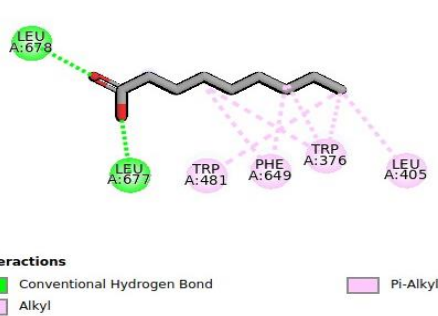
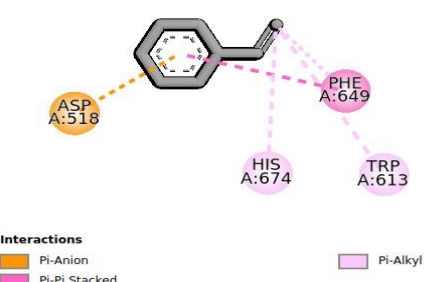
Lampiran 2. Visualisasi 2D dan 3D Interaksi Penambatan Molekul Ligan Uji

NL	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Sulfur-X - Unfavorable Donor-Donor	Hydrogen interaction = 4 ASP616,ASP282, ARG600,ALA284 Hidrofobik interaction =
ACR	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond	Hydrogen interaction = 3 ASP404,ASP616, ALA284 Hidrofobik interaction = 0
MGL	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond	Hydrogen interaction = 3 ASP616, ASP404, ALA284 Hidrofobik interaction = 0
S02	 Interactions - Conventional Hydrogen Bond - Alkyl - Pi-Alkyl	Hydrogen interaction = 2 TRP613, ASP616 Hidrofobik interaction =7 LEU405, TRP376, TRP516, PHE649, TRP481, ILE441, HIS674

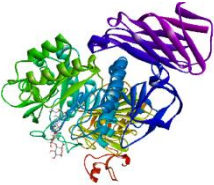
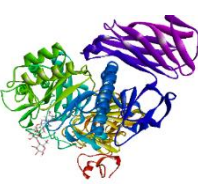
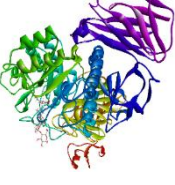
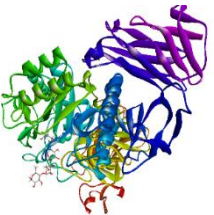
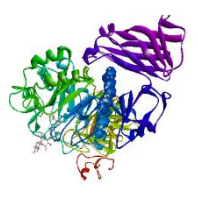
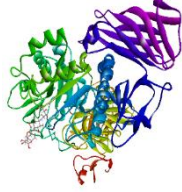
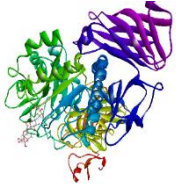
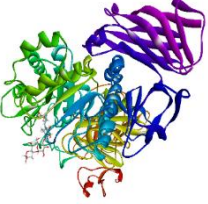
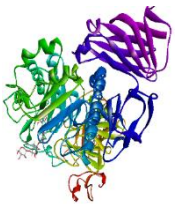
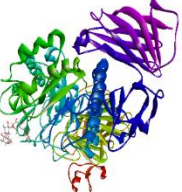
S03	 Interactions - Conventional Hydrogen Bond - Pi-Anion - Pi-Alkyl	Hydrogen interaction = 1 ASP404 Hidrofobik interaction = 4 TRP481, HIS674, PHE649, TRP613
S04	 Interactions - Conventional Hydrogen Bond - Pi-Anion - Pi-Pi Stacked	Hydrogen interaction = 2 ASP616, TRP613 Hidrofobik interaction = 2 PHE649, TRP376
S05	 Interactions - Conventional Hydrogen Bond - Pi-Sigma - Pi-Sulfur - Pi-Pi Stacked - Pi-Alkyl	Hydrogen interaction = 1 ARG672 Hidrofobik interaction = 2 PHE649, TRP376
S06	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Anion - Pi-Sigma - Pi-Pi Stacked - Alkyl - Pi-Alkyl	Hydrogen interaction = 2 ASP616, ARG600 Hidrofobik interaction = 7 PHE649, TRP613, TRP481, HIS674, TRP376, ILE441, LEU405
S07	 Interactions - Conventional Hydrogen Bond - Pi-Anion - Pi-Pi Stacked	Hydrogen interaction = 1 ARG672 Hidrofobik interaction = 1 PHE649

S08	 Interactions - Conventional Hydrogen Bond - Pi-Anion - Pi-Sulfur - Pi-Pi T-shaped - Pi-Alkyl	Hydrogen interaction = 2 ASP518 Hydrofobik interaction = 3 TRP481, TRP376, PHE649
S09	 Interactions - Conventional Hydrogen Bond - Pi-Anion	Hydrogen interaction = 2 ASP616, TRP613 Hydrofobik interaction = 0
S10	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond	Hydrogen interaction = 1 ARG600 Hydrofobik interaction = 0
S11	 Interactions - Unfavorable Acceptor-Acceptor - Pi-Anion - Pi-Pi T-shaped - Pi-Alkyl	Hydrogen interaction = 0 Hydrofobik interaction = 3 TRP481, PHE649, TRP613
S12	 Interactions - Alkyl - Pi-Alkyl	Hydrogen interaction = 0 Hydrofobik interaction = 7 TRP613, HIS674, TRP516, PHE649, TRP481, LEU405, ILE441

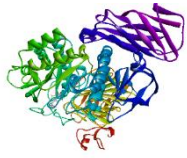
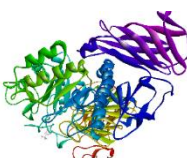
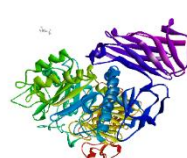
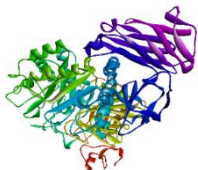
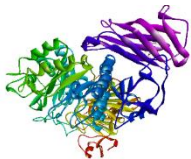
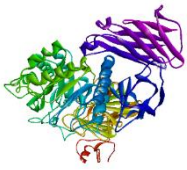
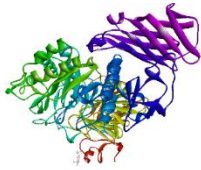
S13	 Interactions - Unfavorable Acceptor-Acceptor - Alkyl - Pi-Alkyl	Hydrogen interaction = 0 Hidrofobik interaction =7 TRP376, LEU678, LEU677, TRP516, PHE649, TRP481, TRP613
S14	 Interactions - Conventional Hydrogen Bond - Pi-Sigma - Pi-Alkyl	Hydrogen interaction = 4 TRP481, ASP282, ARG600, ASP616 Hidrofobik interaction =5 TRP376, HIS674, TRP516, TRP613, PHE649
S15	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Sigma - Pi-Alkyl	Hydrogen interaction =1 TRP481 Hidrofobik interaction =5 HIS674, PHE649, TRP613, TRP516, ASP443
S16	 Interactions - Conventional Hydrogen Bond - Pi-Pi T-shaped	Hydrogen interaction =1 ARG672 Hidrofobik interaction =1 TRP516

S18	 Interactions - Conventional Hydrogen Bond - Alkyl - Pi-Alkyl	Hydrogen interaction =2 ARG672, TRP613 Hidrofobik interaction =4 TRP376, LEU405, TRP481, ILE441
S19	 Interactions - Conventional Hydrogen Bond - Alkyl - Pi-Alkyl	Hydrogen interaction =2 ARG672, TRP613 Hidrofobik interaction =3 TRP481, LEU405, ILE441
S20	 Interactions - Conventional Hydrogen Bond - Carbon Hydrogen Bond - Pi-Sigma - Alkyl - Pi-Alkyl	Hydrogen interaction =1 ARG600 Hidrofobik interaction =5 ILE441, TRP376, TRP481, LEU405, PHE649
S21	 Interactions - Conventional Hydrogen Bond - Alkyl - Pi-Alkyl	Hydrogen interaction =2 LEU678, LEU677 Hidrofobik interaction =4 TRP481, PHE649, TRP376, LEU405
S22	 Interactions - Pi-Anion - Pi-Pi Stacked - Pi-Alkyl	Hydrogen interaction =0 Hidrofobik interaction =3 PHE649, HIS674, TRP613

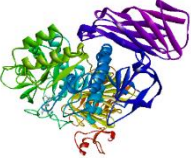
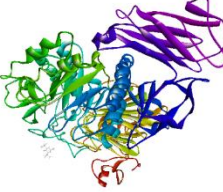
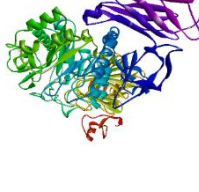
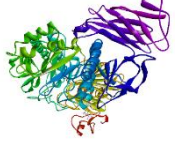
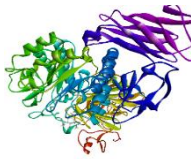
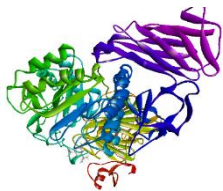
Lampiran 3. Analisis pergerakan ligan alami dan ligan uji per-ns

		
0 ns	10 ns	20 ns
		
30 ns	40 ns	50 ns
		
60 ns	70 ns	80 ns
		
90 ns	100 ns	

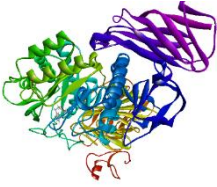
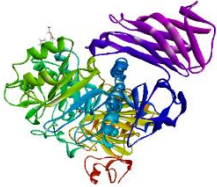
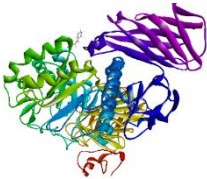
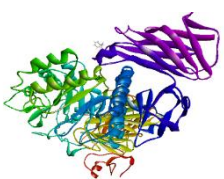
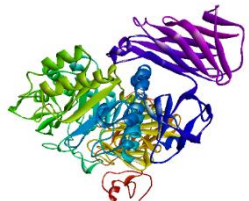
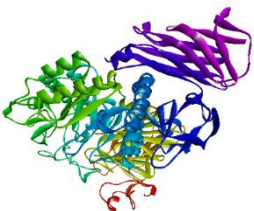
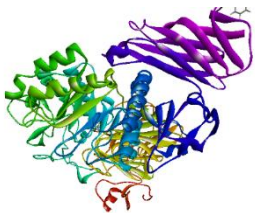
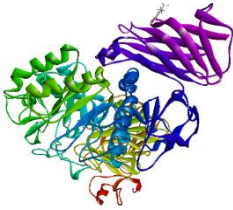
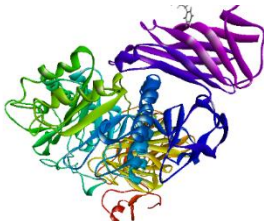
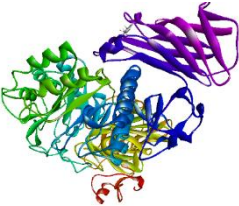
Lampiran 4. Analisis pergerakan ligan alami dan ligan uji S3 per-ns

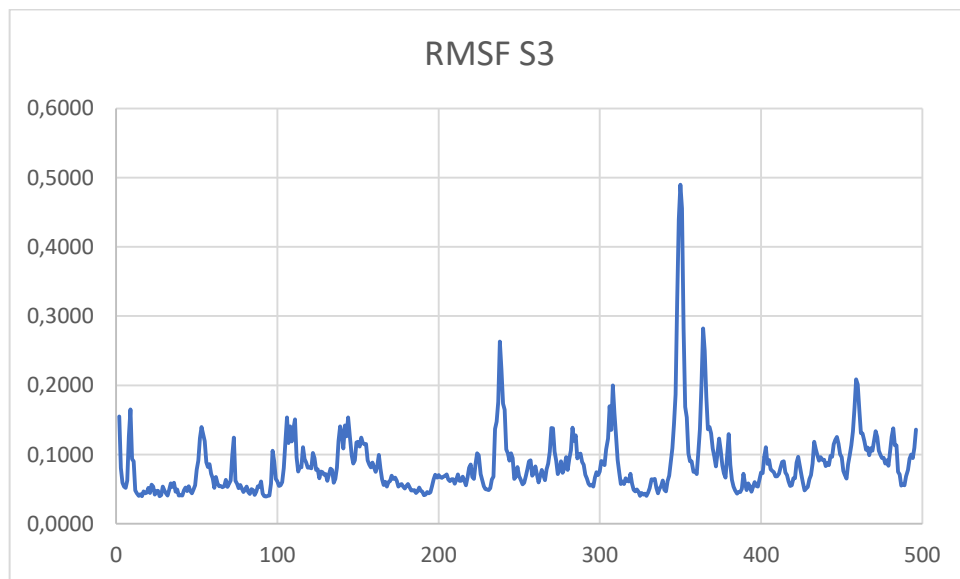
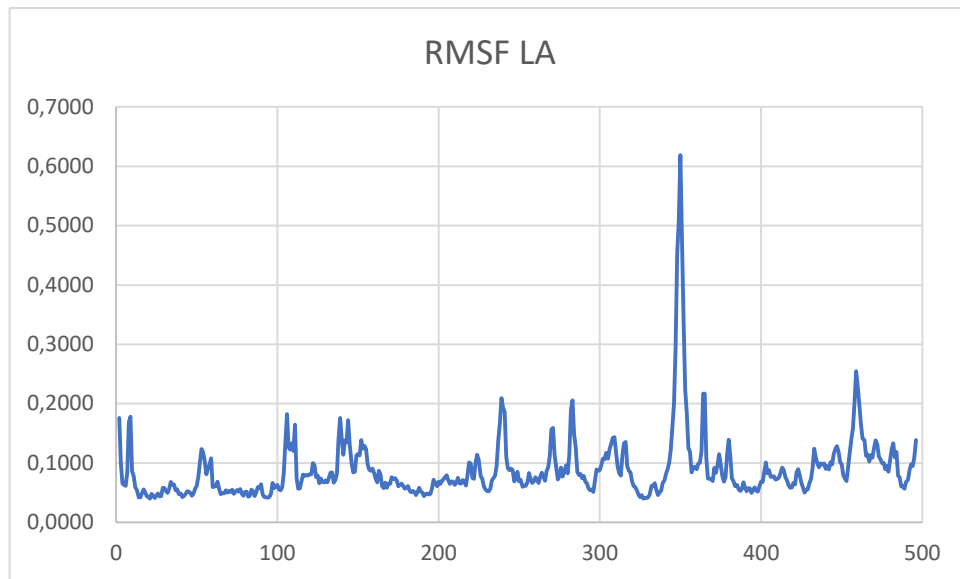
		
0 ns	10 ns	20 ns
		
30 ns	40 ns	50 ns
		
60 ns	70 ns	80 ns
		
90 ns	100 ns	

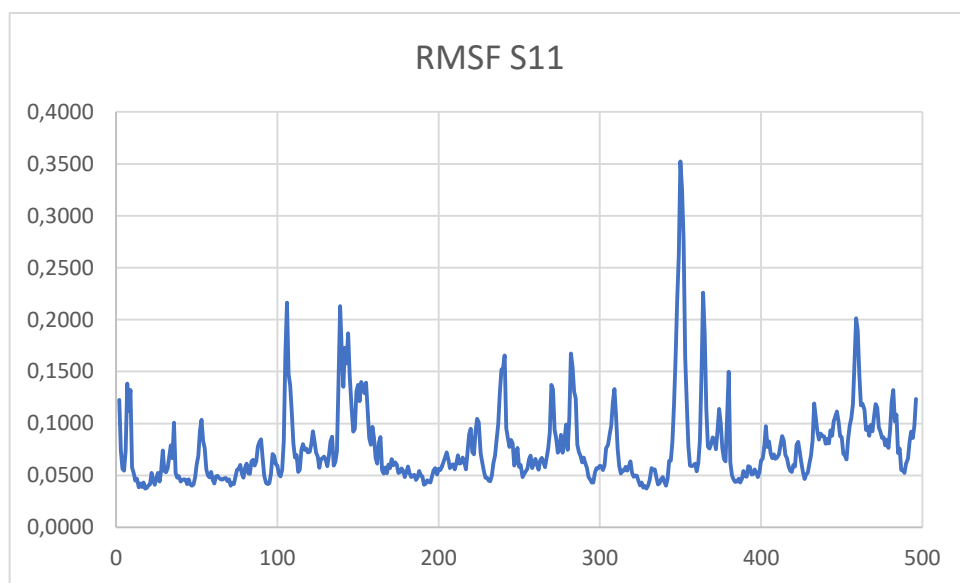
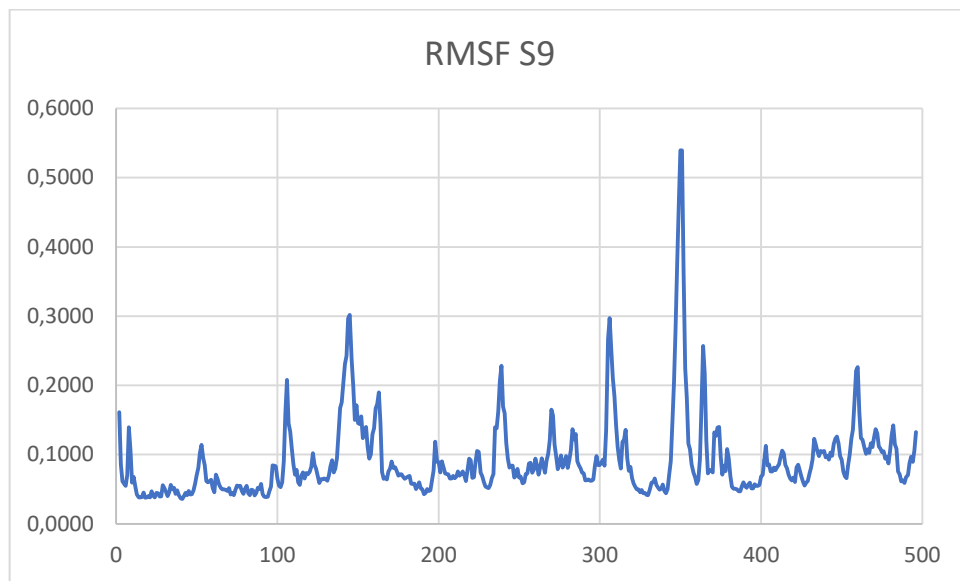
Lampiran 5. Analisis pergerakan ligan alami dan ligan uji S09 per-ns

		
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30 ns	40 ns	50 ns
		
60 ns	70 ns	80 ns
		
90 ns	100 ns	

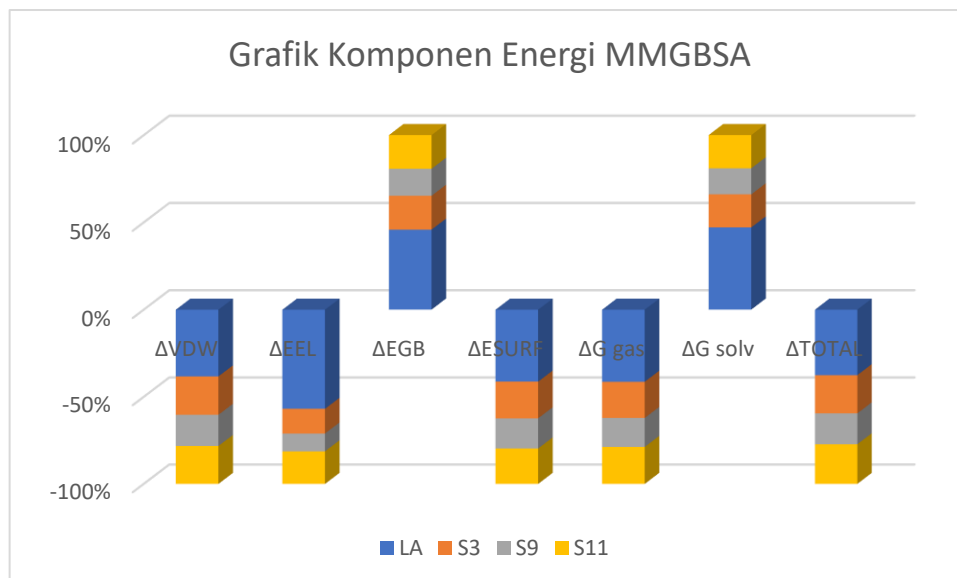
Lampiran 6. Analisis pergerakan ligan alami dan ligan uji S11 per-ns

		
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30 ns	40 ns	50 ns
		
60 ns	70 ns	80 ns
		
90 ns	100 ns	

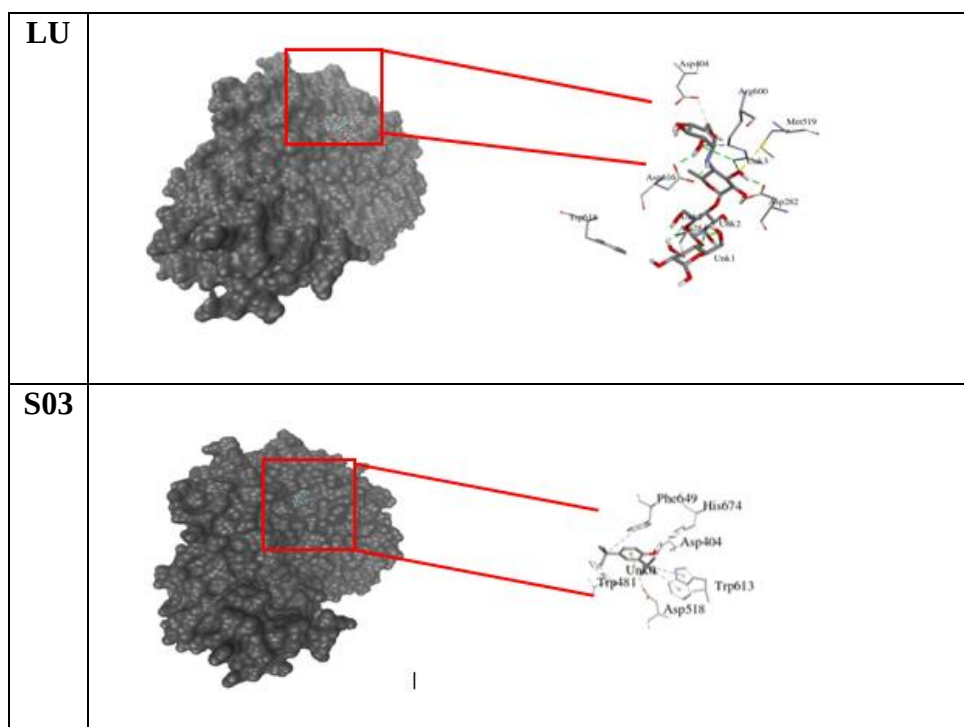
Lampiran 7. Fluktuasi Residu di Sekitar Atom

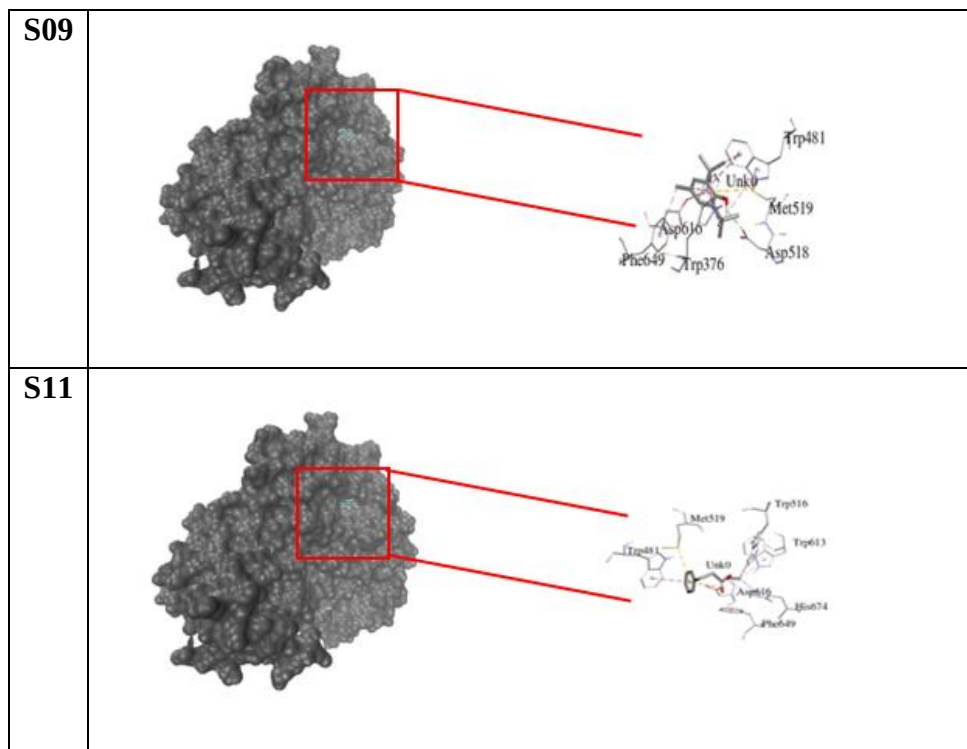


Lampiran 8. MMGBSA



Lampiran 9. Hasil Visualisasi VMD Docking Senyawa Uji





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Nama Mahasiswa	: Numalasari
NPM	: 201ff03083
Bidang Ilmu	: Analisis Farmasi dan Kimia Medisinal

No	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	22 / 02 / 2024	08.00	Lab Komputer lantai 1	Pelatihan docking	
2	25 / 03 / 2024	09.00	Lab Lantai 3	mencatat aturan kipinski senyawa	
3	26 / 03 / 2024	09.00	"	mengatur grid box	
4	27 / 03 / 2024	09.00	"	mengatur grid box	
5	22 / 04 / 2024	09.00	"	Validasi ulang menggunakan pc	
6	23 / 04 / 2024	09.00	"	optmali Senyawa uji	
7	25 / 04 / 2024	09.00	"	Docking Senyawa uji	
8	26 / 04 / 2024	09.00	"	Docking Senyawa uji	
9	08 / 05 / 2024	08.00	"	Tutorial MD	
10	13 / 05 / 2024	10.00	"	Pelatihan MD	
11	22 / 05 / 2024	09.00	"	Mengulang MD	
12	29 / 05 / 2024	09.00	"	Mengulang MD	
13	31 / 05 / 2024	09.00	"	Laporan Kemajuan 2	
14	25 / 06 / 2024	09.00	"	Presentasi	
15	09 / 07 / 2024	09.00	"	Laporan masalah MD	
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Nama Mahasiswa	: Numalasari
NPM	: 201ff03083
Bidang Ilmu	: Analisis Farmasi dan Kimia Medisinal

1	22 / 02 / 2024	00.00	Lab komputer Lantai 1	Pelatihan Docking	
2	25 / 03 / 2024	09.00	Lab Lantai 3	Mencatat aturan lipinski	Senyawa uji
3	26 / 03 / 2024	09.00	"	Mengatur grid box	
4	27 / 03 / 2024	09.00	"	mengatur ulang grid box	
5	22 / 04 / 2024	10.00	"	Validasi ulang menggunakan pc	
6	23 / 04 / 2024	09.00	"	Optimasi Senyawa uji	
7	25 / 04 / 2024	09.00	"	Docking senyawa uji	
8	29 / 04 / 2024	09.00	"	Visualisasi	
9	30 / 04 / 2024	12.00	"	Revisi laporan kemaguan 1	
10	01 / 05 / 2024	09.00	"	Pelatihan MD	
11	31 / 05 / 2024			Laporan kemaguan 2	
12	05 / 07 / 2024	09.00	"	Laporan mengenai MD	
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Domisili: Kab. Tangerang



Keahlian

- ◆ **Komunikasi**
- ◆ **Bahasa Inggris**
- ◆ **Orientasi Layanan**

Tentang Saya

Freshgraduate yang percaya diri, bersemangat, dan dapat bekerja dibawah tekanan dengan performa yang baik dan cepat.

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Pengalaman

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