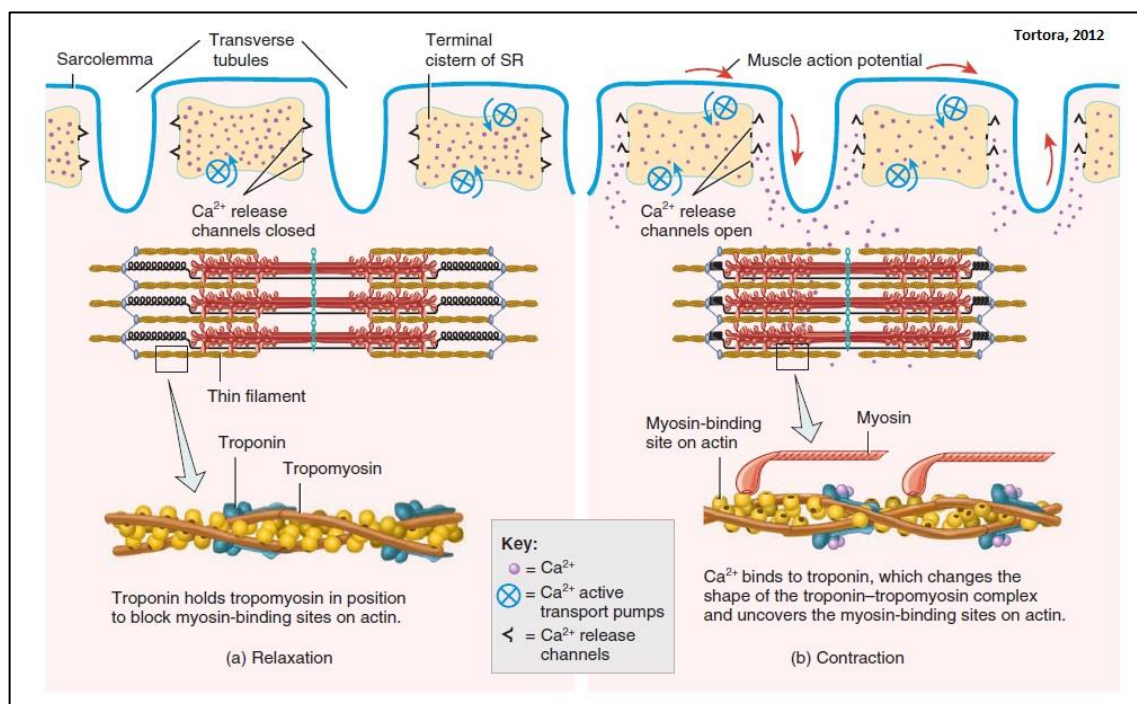
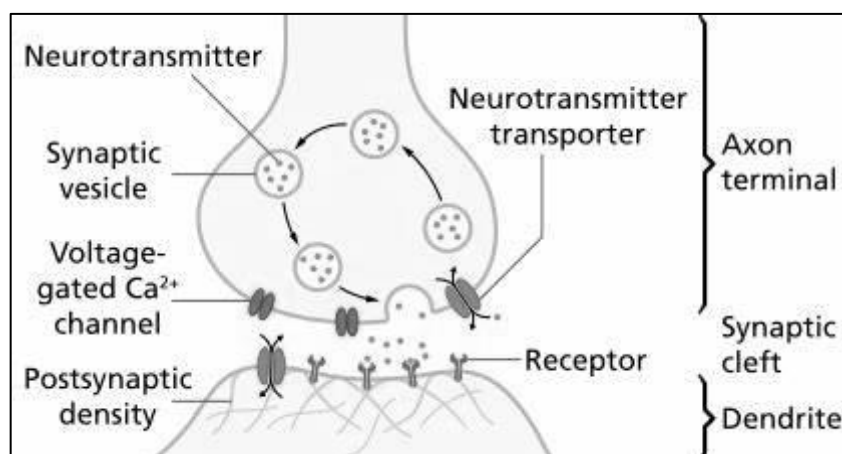


DAFTAR LAMPIRAN

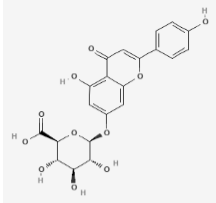
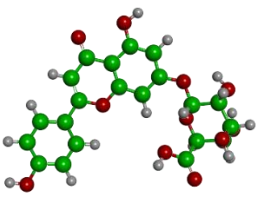
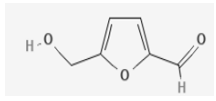
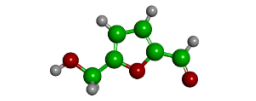


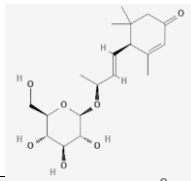
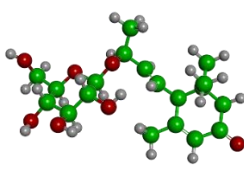
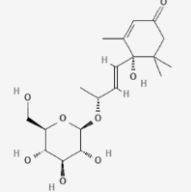
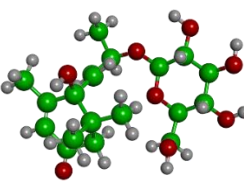
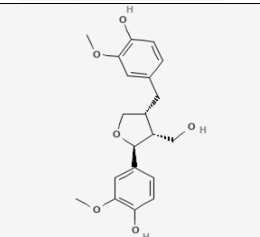
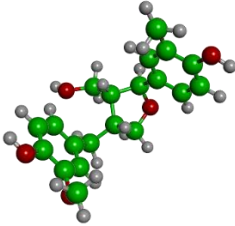
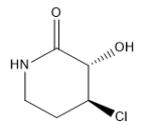
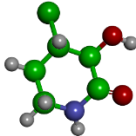
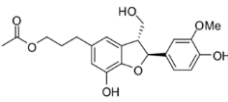
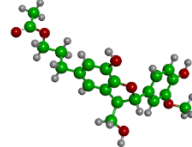
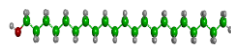
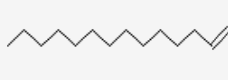
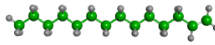
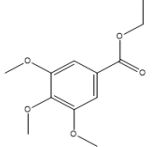
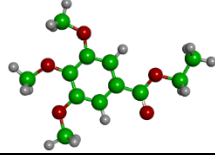
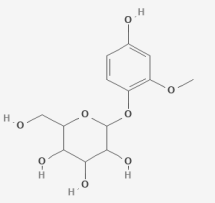
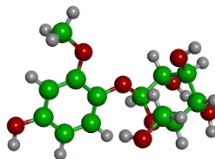
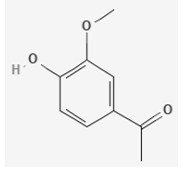
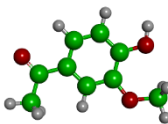
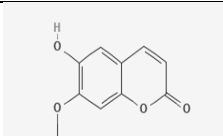
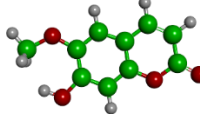
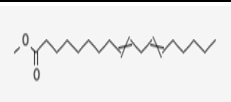
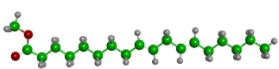
Gambar 0.1 Skema mekanisme kejang otot (tortora,2012)

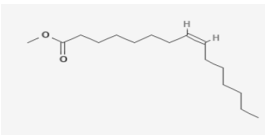
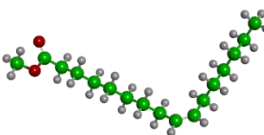
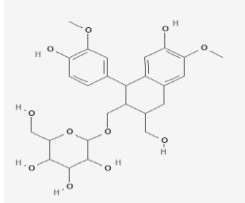
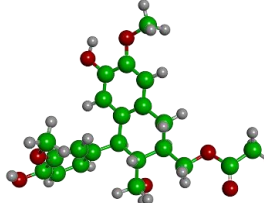
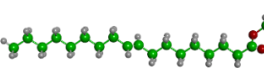
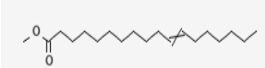
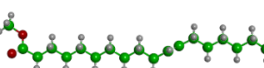
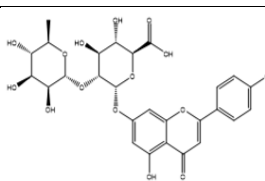
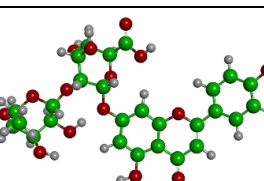
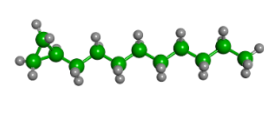
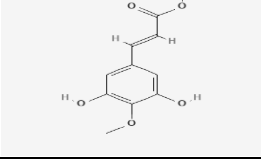
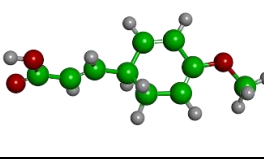
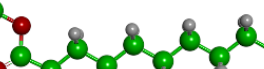
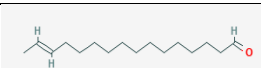
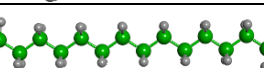
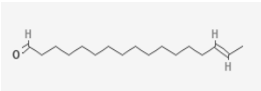
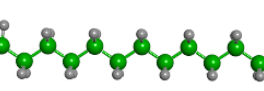
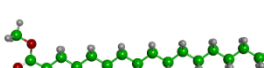
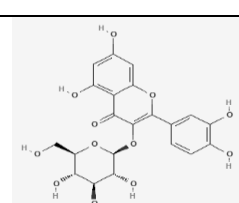
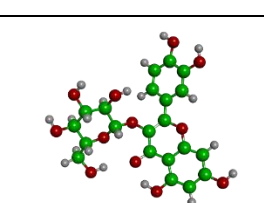
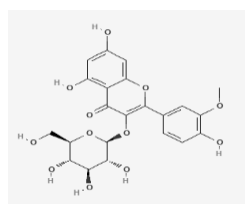
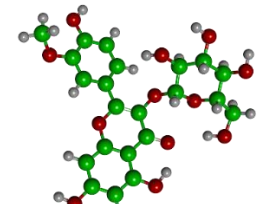


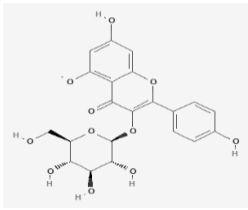
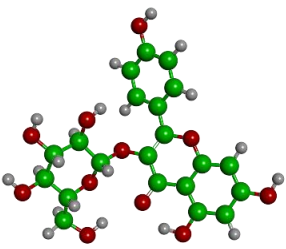
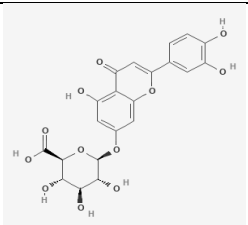
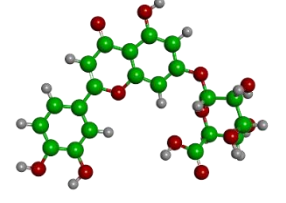
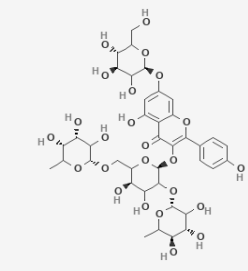
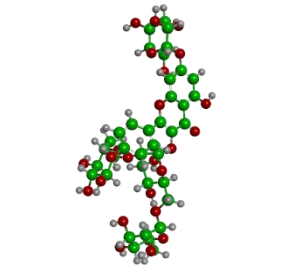
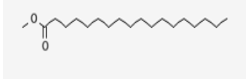
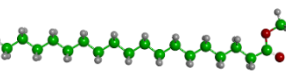
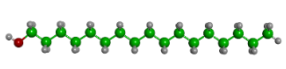
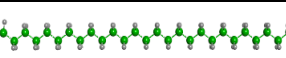
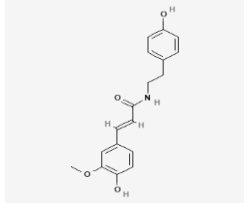
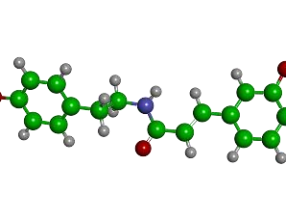
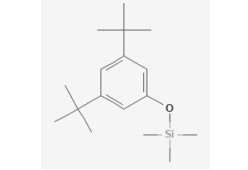
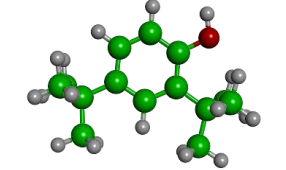
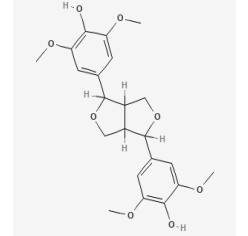
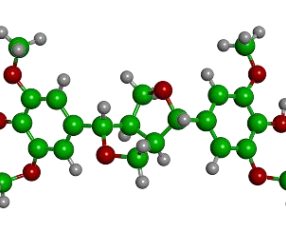
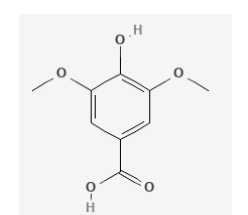
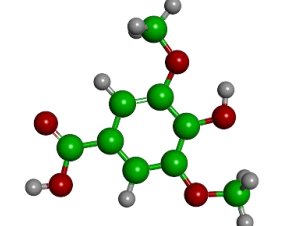
Gambar 0.2 Mekanisme penghantar Sinyal Neuron (tortora,2012)

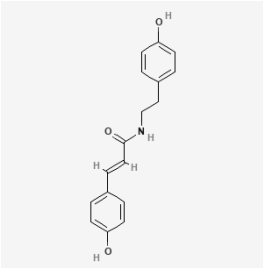
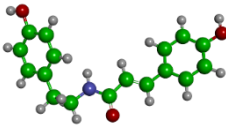
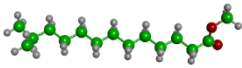
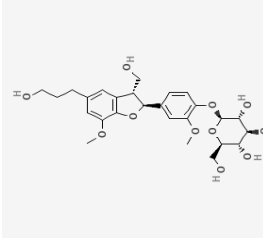
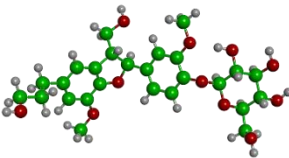
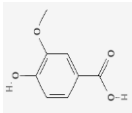
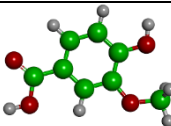
Lampiran 1 Struktur senyawa 2D dan 3D dari daun ginggiyang

NO	LIGAN UJI	SENYAWA		KELOMPOK	Referensi
		2D	3D		
1	Apigenin 7-O-glucuronide			Flavonol	(Md. Golam Mostofa, 2021)
2	5-hydroxymethylfurfural			Aldehid	(Md. Golam Mostofa, 2021)

3	(6S,9S)- Reseoside			sesquiterpenoid	(Md. Golam Mostofa, 2021)
4	(6S,9R)- roseoside			sesquiterpenoid	(Nay Lin Tun, 2019)
5	(+)- Lariciresinol			Lignan (fenolik)	(Nay Lin Tun, 2019)
6	(3S,4S)-4- chloro-3- hydroxy piperidin-2- one			Lactam	(Nay Lin Tun, 2019)
7	(7S,8R)-9'-O- acetylcedrusin			Neolignan (fenolik)	(Nay Lin Tun, 2019)
8	1- Heneicosanol			Alkohol rantai panjang	(Nay Lin Tun, 2019)
9	1-Tetradecene			alkena rantai panjang	(Nay Lin Tun, 2019)
10	3,4,5- trihydroxyben- zoic acid ethyl ester			Ester	(Nay Lin Tun, 2019)
11	4-hydroxy-2- methoxyphen- yl beta-D- glucopyranosi- de			glikosida (fenolik)	(Nay Lin Tun, 2019)
12	A- hydroxyaceto- vanillone			Fenolik	(Nay Lin Tun, 2019)
13	7-Hydroxy-6- methoxy-2H- chromen-2- one			Kumarin	(Nay Lin Tun, 2019)
14	9,12- Octadecadien- oic acid, methyl ester			Ester	(Md. Golam Mostofa, 2021)

15	9-Hexadecenoic acid, methyl ester, (Z)			Ester	(Nay Lin Tun, 2019)
16	9'-O-Acetylisolarici resinol			glikosida lignan (fenolik)	(Nay Lin Tun, 2019)
17	9-Octadecenoic acid methyl ester, (E)-			Ester	(Md. Golam Mostofa, 2021)
18	11-Octadecenoic acid, methyl ester			Ester	(Md. Golam Mostofa, 2021)
19	apigenin 7-O-(2-O-alpha-rhamnosyl) glucuronide			Flavonol	(NAHITM A GINTING, 2018)
20	Cyclopropane, nonyl-			Hidrokarbon siklik	(Md. Golam Mostofa, 2021)
21	dihydro-p-methoxy cinnamic acid			Fenolik	(Nay Lin Tun, 2019)
22	Dodecanoic acid, methyl ester			Ester	(Md. Golam Mostofa, 2021)
23	E-14-Hexadecenal			Aldehyd	(Nay Lin Tun, 2019)
24	E-15-Heptadecenal			Aldehyd	(Md. Golam Mostofa, 2021)
25	Hexadecanoic acid, methyl ester			Ester	(Md. Golam Mostofa, 2021)
26	Isoquercetin			Flavonol	(Md. Golam Mostofa, 2021)
27	Isorhamnetin-3-O-beta-D-Glucoside			Flavonol	(Md. Golam Mostofa, 2021)

28	Kaempferol 3-O-glucoside			Flavonol	(Md. Golam Mostofa, 2021)
29	Luteolin 7-O-glucuronide			Flavonol	(Md. Golam Mostofa, 2021)
30	Mauritianin 7-O-beta-D-glucopyranoside			antosianin	(Md. Golam Mostofa, 2021)
31	Methyl stearate			Ester	(Nay Lin Tun, 2019)
32	n-Heptadecanol-1			Fenolik	(Nay Lin Tun, 2019)
33	Nonacos-1-ene			Alkana	(Nay Lin Tun, 2019)
34	N-trans-feruloyltyramine			Alkaloid	(Md. Golam Mostofa, 2021)
35	Phenol, 2,4-bis(1,1-dimethylethyl)-			Fenolik	(Md. Golam Mostofa, 2021)
36	Syringaresinol			Lignan (fenolik)	(Md. Golam Mostofa, 2021)
37	syringic acid			asam fenolat	(Nay Lin Tun, 2019)

38	trans-n-p-coumaroyl tyramine			Alkaloid	(Nay Lin Tun, 2019)
39	Tridecanoic acid, 12-methyl-, methyl ester			Ester	(Md. Golam Mostofa, 2021)
40	Urolignoside			Lignan (fenolik)	(Nay Lin Tun, 2019)
41	vanillic acid			asam fenolat	(Nay Lin Tun, 2019)

Tabel 0.1 Hasil skrining data Lipinski rule of 5 daun ginggiyang

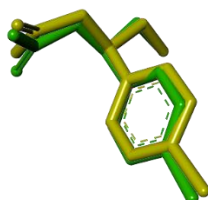
Kode Ligan	Lipinski Rule of Five				Kode Ligan	Lipinski Rule of Five			
	nilai CLogP	BM	donor Hidrogen	akseptor hidrogen		nilai CLogP	BM	donor Hidrogen	akseptor hidrogen
LG1	0.021	446.364	6	10	LG21	0.631	180.203	1	2
LG2	-0.122	126.111	1	3	LG22	4.964	214.349	0	1
LG3	0.085	370.442	4	7	LG23	5.724	238.415	0	1
LG4	-0.774	386.441	5	8	LG24	6.18	252.442	0	1
LG5	2.339	360.406	3	6	LG25	6.788	270.457	0	1
LG6	-1.149	149.574	2	2	LG26	-1.39	464.379	8	12
LG7	2.296	388.416	3	6	LG27	-1.127	478.406	7	12
LG8	8.761	312.582	1	1	LG28	-1.001	448.38	7	11
LG9	6.489	196.378	0	0	LG29	-0.368	462.363	7	11
LG10	1.813	240.255	0	4	LG30	-3.256	902.805	14	24
LG11	-0.711	302.279	5	8	LG31	7.7	298.511	0	1
LG12	1.064	166.176	1	3	LG32	6.937	256.474	1	1
LG13	1.309	192.17	1	3	LG33	13.329	406.783	0	0
LG14	6.231	294.479	0	1	LG34	2.624	313.353	3	4
LG15	6.074	268.441	0	1	LG35	5.227	206.329	1	1
LG16	2.46	402.443	3	6	LG36	1.68	418.442	2	8
LG17	6.986	296.495	0	1	LG37	1.096	198.174	2	4
LG18	6.986	296.495	0	1	LG38	2.751	283.327	3	3
LG19	-0.865	592.506	8	14	LG39	5.624	242.403	0	1
LG20	5.22	168.324	0	0	LG40	0.489	522.547	6	11
					LG41	1.355	168.148	2	3

Tabel 0.2 Hasil Optimasi geometri daun ginggiyang

Kode Ligan	Optimasi Geometri				Kode Ligan	Optimasi Geometri			
	Total Energi (a.u)	HOMO (a.u)	LUMO (a.u)	Gap Energi (a.u)		Total Energi (a.u)	HOMO (a.u)	LUMO (a.u)	Gap Energi (a.u)
LG1	-1638,00	-0,2226	-0,0624	0,160	LG21	-613,73	-0,20960	-0,05462	0,155
LG2	-457,73	-0,2455	-0,0678	0,178	LG22	-661,34	-0,26575	-0,00022	0,266
LG3	-1268,22	-0,23285	-0,05045	0,182	LG23	-702,81	-0,23383	-0,03668	0,197
LG4	-1343,40	-0,23173	-0,05215	0,180	LG24	-742,11	-0,23363	-0,03666	0,197
LG5	-1227,50	-0,20412	0,00087	0,205	LG25	-818,56	-0,26567	-0,00020	0,265
LG6	-860,62	-0,26629	-0,01815	0,248	LG26	-1714,39	-0,23062	-0,08822	0,142
LG7	-1340,83	-0,20502	-0,00282	0,202	LG27	-1753,67	-0,22994	-0,08736	0,143
LG8	-901,77	-0,26017	0,07083	0,331	LG28	-1639,19	-0,23235	-0,08787	0,144
LG9	-550,22	-0,24727	0,02114	0,268	LG29	-1713,18	-0,21497	-0,05733	0,158
LG10	-842,74	-0,20349	-0,03796	0,166	LG31	-897,16	-0,26565	-0,00019	0,265
LG11	-1107,59	-0,20273	-0,00051	0,202	LG32	-744,55	-0,26018	0,07082	0,331
LG12	-574,47	-0,21720	-0,05245	0,165	LG33	-1139,78	-0,24723	0,02116	0,268
LG13	-686,54	-0,22193	-0,07042	0,152	LG34	-1052,69	-0,21363	-0,05702	0,157
LG14	-894,69	-0,22276	-0,00054	0,222	LG35	-621,82	-0,21169	0,00501	0,217
LG15	-817,33	-0,23517	-0,00227	0,233	LG36	-1455,27	-0,20613	0,00509	0,211
LG16	-1380,15	-0,20039	-0,00125	0,199	LG37	-724,86	-0,21540	-0,04736	0,168
LG17	-895,94	-0,23545	-0,00203	0,233	LG38	-938,22	-0,21525	-0,05224	0,163
LG18	-895,94	-0,23486	-0,00199	0,233	LG39	-739,95	-0,26686	-0,00194	0,265
LG19	-2173,34	-0,22313	-0,06262	0,161	LG40	-1838,05	-0,20394	-0,00472	0,199
LG20	-471,60	-0,26961	0,08961	0,359	LG41	-610,37	-0,21870	-0,04816	0,171

Tabel 0.3 Parameter validasi penambatan molekul

Grid box			Grid spacing	Grid Center		
75	55	65	0,375 A	-21.333	17.880	-26.386
<i>Number of runs : 100</i>						
<i>Number of evals : medium</i>						
<i>Metode Algoritma : Lamarckian genetic algorithm</i>						



Hijau : ligan alami kristalografi sinar-x

Kuning : ligan alami Redocking

ΔG : -7,40 kcal/mol

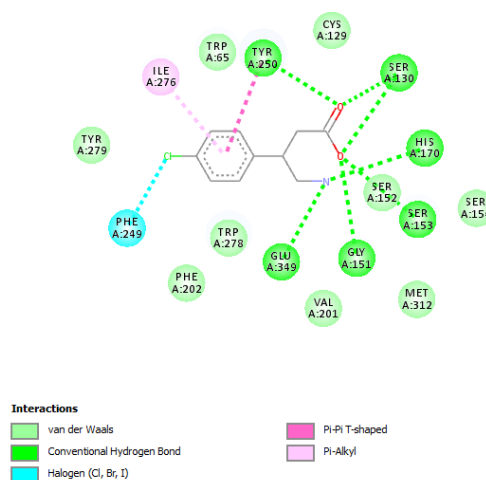
Ki : 3,77 μM

Run ke : 9

RMSD : 0.371

Gambar 0.3 Visualisasi tumpang tindih ligan alami hasil penmabatan ulang (kuning) dan kristalografi sinar-x (hijau)

Kompleks	Interaksi	Jarak Ikatan (A)	Residu Asam Amino
Kompleks : GABA (B) – 2C0 (baclofen)	Ikatan hidrogen		
	Tyr 250 – O	2,85	SER130, SER153, TYR250, GLY151, HIS170, GLU349, PHE249, TYR250, ILE276, TRP 278 dan TRP 65
	Ser 130 – O2	2,88 - 2,84	
	Ser 153 - O	3,34 - 2,97	
	His 170 – N	3,19	
	Gly 151 - N	3,04	
	Glu 349 - N	2,71	
ΔG (kcal/mol): -7,40 kcal/mol			
Ki (uM): 3,77 uM	Ikatan hidrofobik		
	Pi-akyl : Ile 276		
	Pi-pi T-shaped : Tyr 250		
	Halogen : Phe 249		
Interaksi van der waals:			
	Trp 278 dan Trp 65		



Gambar 0.4 Visualisasi Interaksi Reseptor GABA (B) - Ligan alami Baclofen (2C0)

Lampiran 2 Hasil simulasi penambatan ligan uji (e.bebas ikatan & konstanta inhibisi)

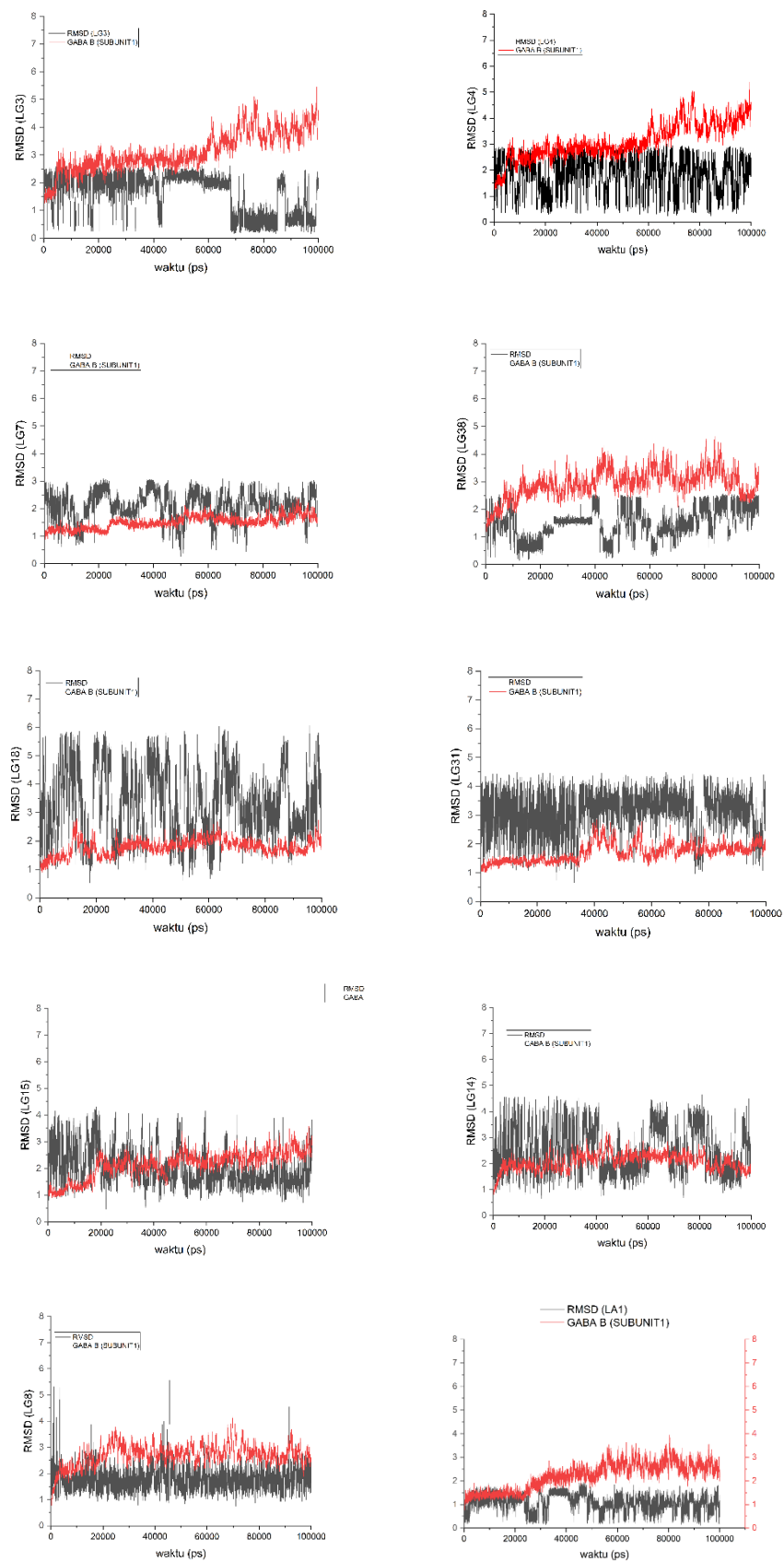
Kode ligan	Ligan Uji	Energi Bebas Ikatan (ΔG) kcal/mol	Konstanta Inhibisi (Ki) uM
2CO	BACLOFEN (LG ALAMI)	-7,40	3,77
LG4	(6S,9R)-roseoside	-9,46	0,11556
LG3	(6S,9S)-Reseoside	-8,70	0,4182
LG38	trans-n-p-coumaroyl tyramine	-8,43	0,66624
LG18	11-Octadecenoic acid, methyl ester	-8,41	0,68996
LG14	9,12-Octadecadienoic acid, methyl ester	-8,40	0,69675
LG8	1-Heneicosanol	-8,37	0,73057
LG15	9-Hexadecenoic acid, methyl ester, (Z)	-8,37	0,73675
LG31	Methyl stearate	-8,27	0,865
LG7	(7S,8R)-9'-O-acetylcedrusin	-8,23	0,93523
LG25	Hexadecanoic acid, methyl ester	-8,13	1,10
LG17	9-Octadecenoic acid methyl ester, (E)-	-8,12	1,11
LG34	N-trans-feruloyltyramine	-7,94	1,52
LG16	9'-O-Acetylisolariciresinol	-7,92	1,55
LG39	Tridecanoic acid, 12-methyl-, methyl ester	-7,86	1,73
LG24	E-15-Heptadecenal	-7,79	1,94
LG32	n-Heptadecanol-1	-7,74	2,13
LG40	Urolignoside	-7,57	2,81
LG23	E-14-Hexadecenal	-7,40	3,77
LG22	Dodecanoic acid, methyl ester	-7,20	5,28
LG35	Phenol, 2,4-bis(1,1- dimethylethyl)-	-7,15	5,73
LG21	dihydro-p-methoxy cinnamic acid	-6,78	10,75
LG19	apigenin 7-O-(2-O-a-rhamnosyl) glucuronide	-6,75	11,31
LG11	4-hydroxy-2-methoxyphenyl beta-D-glucopyranoside	-6,70	12,21
LG13	7-Hydroxy-6-methoxy-2H-chromen-2-one	-6,60	14,63
LG36	Syringaresinol	-6,54	15,99
LG9	1-Tetradecene	-6,50	17,06
LG10	3,4,5-trihydroxybenzoic acid ethyl ester	-6,49	17,39
LG5	(+)-Lariciresinol	-6,36	21,91
LG29	Luteolin 7-O-glucuronide	-6,25	26,3
LG28	Kaempferol 3-O-glucoside	-6,06	36,42
LG20	Cyclopropane, nonyl-	-5,91	46,3
LG12	A-hydroxyacetovanillone	-5,85	51,55
LG26	Isoquercetin	-5,82	54,52
LG41	vanillic acid	-5,74	61,81
LG1	Apigenin 7-O-glucuronide	-5,61	76,96
LG27	Isorhamnetin-3-O-beta-D-Glucoside	-5,31	128,09
LG37	syringic acid	-5,26	140,11
LG6	(3S,4S)-4-chloro-3-hydroxy piperidin-2-one	-5,13	172,55
LG2	5-hydroxymethylfurfural	-4,63	401,71
LG33	Nonacos-1-ene	-4,2	828,82

Lampiran 2 Hasil simulasi Penambatan ligan uji (Interaksi Ikatan Senyawa Uji)

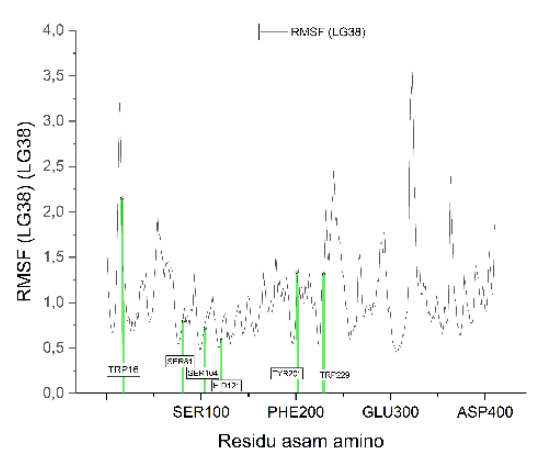
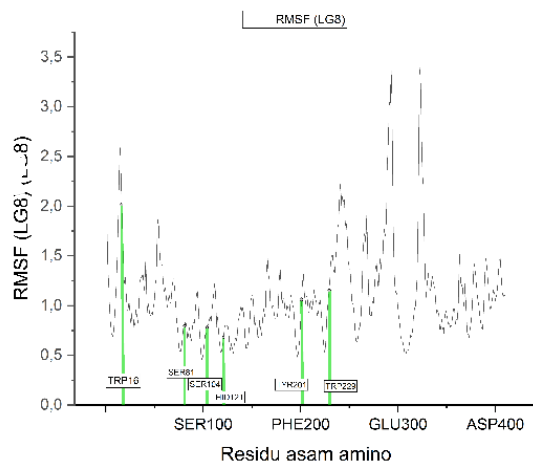
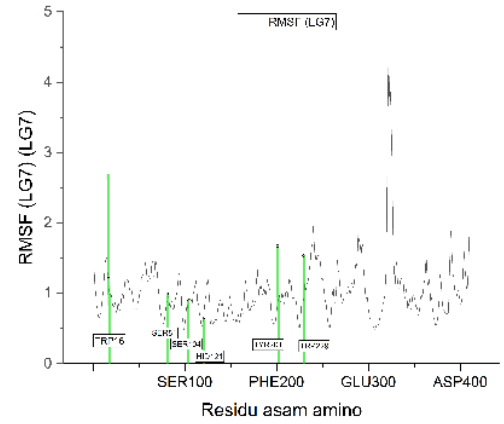
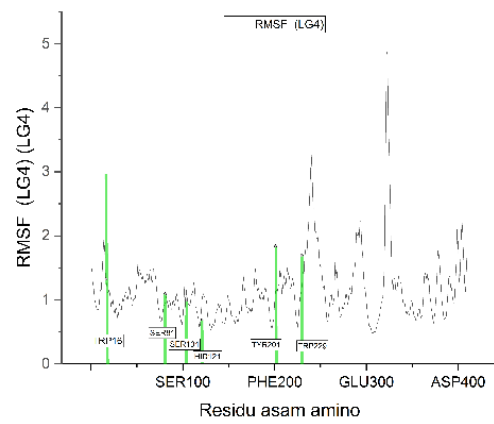
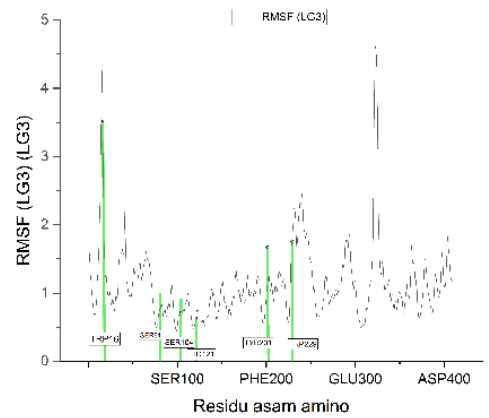
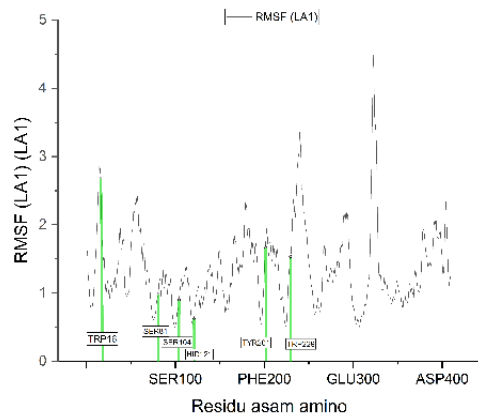
Kode ligan	Ligan Uji	Domain LB2		Domain LB1			
		TYR 250	TRP 278	SER 130	SER 153	TRP 65	HIS 170
LA1	BACLOFEN (LG ALAMI)	hydrogen bond	van der waals	hydrogen bond	hydrogen bond	van der waals	hydrogen bond
LG4	(6S,9R)-roseoside	×	hydrogen bond	hydrogen bond	van der waals	hydrogen bond	×
LG3	(6S,9S)-Reseoside	hydrogen bond	×	van der waals	hydrogen bond	×	van der waals
LG38	trans-n-p-coumaroyl tyramine	van der walls	van der walls	van der walls	×	×	van der walls
LG18	11-Octadecenoic acid, methyl ester	van der walls	×	hydrogen bond	hydrogen bond	×	van der walls
LG14	9,12-Octadecadienoic acid, methyl ester	van der walls	×	hydrogen bond	hydrogen bond	van der walls	×
LG8	1-Heneicosanol	hydrogen bond	van der waals	van der waals	van der waals	van der walls	van der waals
LG15	9-Hexadecenoic acid, methyl ester, (Z)	van der walls	×	hydrogen bond	hydrogen bond	×	van der walls
LG31	Methyl stearate	van der walls	van der walls	hydrogen bond	hydrogen bond	×	van der walls
LG7	(7S,8R)-9'-O-acetylcedrusin	hydrogen bond	×	van der waals	×	van der waals	van der waals
LG25	Hexadecanoic acid, methyl ester	van der walls	×	hydrogen bond	hydrogen bond	×	van der walls
LG17	9-Octadecenoic acid methyl ester, (E)-	hydrogen bond	×	hydrogen bond	hydrogen bond	×	van der walls
LG34	N-trans-feruloyltyramine	van der walls	van der walls	van der walls	×	×	van der walls
LG16	9'-O-Acetylisolariciresinol	×	×	hydrogen bond	hydrogen bond	×	van der walls
LG39	Tridecanoic acid, 12-methyl-, methyl ester	van der walls	van der walls	hydrogen bond	hydrogen bond	×	van der walls
LG24	E-15-Heptadecenal	hydrogen bond	×	hydrogen bond	van der walls	van der walls	van der walls
LG32	n-Heptadecanol-1	van der walls	van der walls	van der walls	van der walls	×	van der walls
LG40	Urolignoside	×	×	van der walls	×	×	×
LG23	E-14-Hexadecenal	van der walls	van der walls	van der walls	van der walls	van der walls	van der walls
LG22	Dodecanoic acid, methyl ester	van der walls	×	hydrogen bond	hydrogen bond	×	×
LG35	Phenol, 2,4-bis(1,1- dimethylethyl)-	×	×	van der walls	van der walls	×	×
LG21	dihydro-p-methoxy cinnamic acid	hydrogen bond	×	hydrogen bond	hydrogen bond	×	×
LG19	apigenin 7-O-(2-O-a-rhamnosyl) glucuronide	×	×	×	×	×	×
LG11	4-hydroxy-2-methoxyphenyl beta-D-glucopyranoside	hydrogen bond	×	hydrogen bond	hydrogen bond	×	×
LG13	7-Hydroxy-6-methoxy-2H-chromen-2-one	van der walls	van der walls	hydrogen bond	hydrogen bond	×	×
LG36	Syringaresinol	×	×	×	×	×	×
LG9	1-Tetradecene	van der waals	van der waals	van der waals	van der waals	×	van der waals
LG10	3,4,5-trihydroxybenzoic acid ethyl ester	van der waals	×	van der waals	hydrogen bond	×	van der waals
LG5	(+)-Lariciresinol	×	×	×	×	×	×
LG29	Luteolin 7-O-glucuronide	van der walls	×	×	×	×	×
LG28	Kaempferol 3-O-glucoside	×	×	×	×	×	×
LG20	Cyclopropane, nonyl-	van der walls	van der walls	van der walls	van der walls	×	van der walls

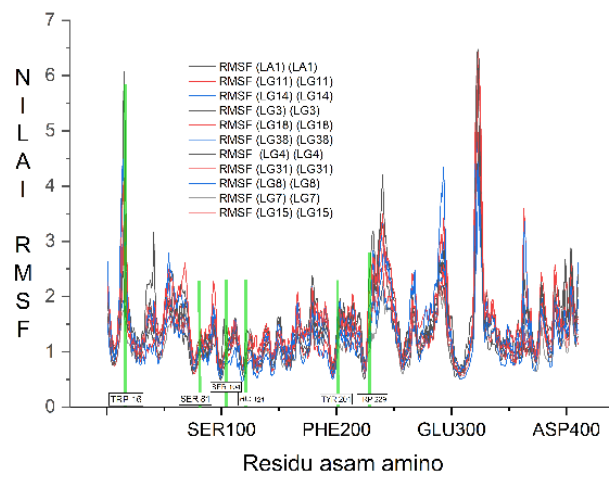
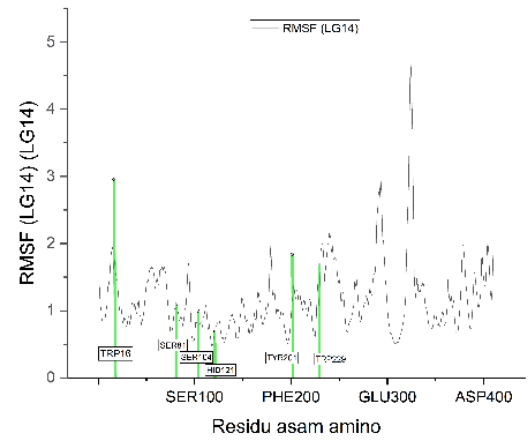
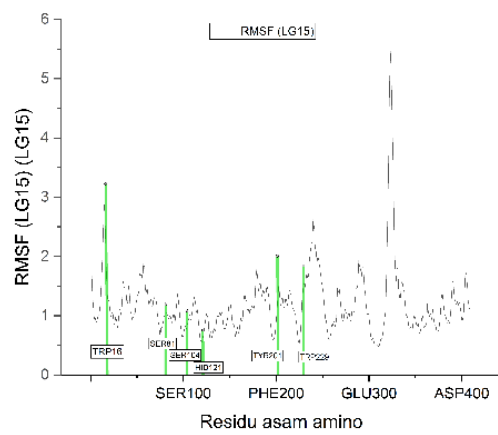
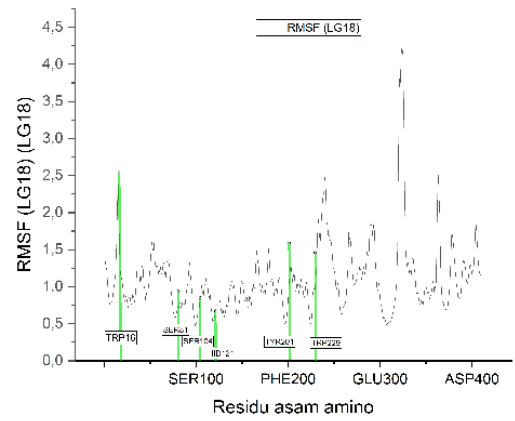
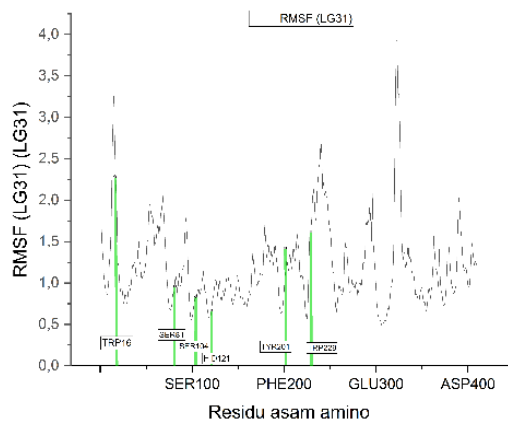
LG12	A-hydroxyacetovanillone	hydrogen bond	×	van der waals	×	×	van der waals
LG26	Isoquercetin	×	×	×	×	×	×
LG41	vanillic acid	hydrogen bond	×	×	van der walls	×	van der walls
LG1	Apigenin 7-O-glucuronide	×	×	×	×	×	×
LG27	Isorhamnetin-3-O-beta-D-Glucoside	×	×	×	×	×	×
LG37	syringic acid	hydrogen bond	van der walls	van der walls	×	van der walls	van der walls
LG6	(3S,4S)-4-chloro-3-hydroxy piperidin-2-one	hydrogen bond	×	hydrogen bond	hydrogen bond	van der waals	×
LG2	5-hydroxymethylfurfural	×	×	hydrogen bond	van der waals	×	×
LG33	Nonacos-1-ene	×	Van der walls	Van der walls	Van der walls	Van der walls	Van der walls

Lampiran 3 Grafik RMSD selama simulasi dinamika molekul



Lampiran 4 Grafik RMSF selama simulasi dinamika molekuler





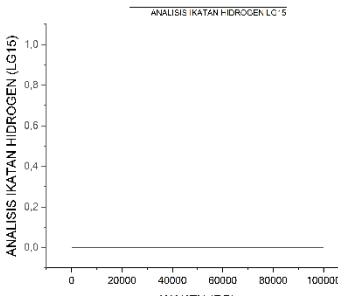
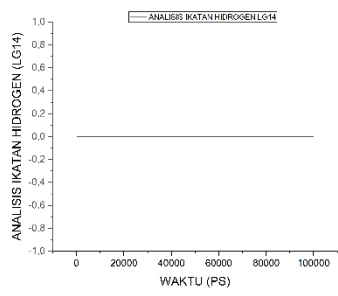
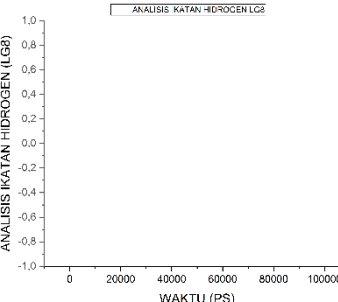
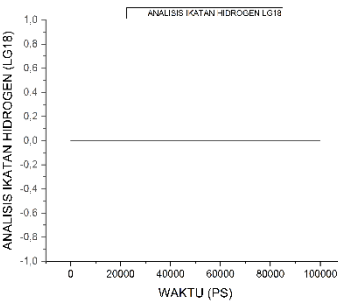
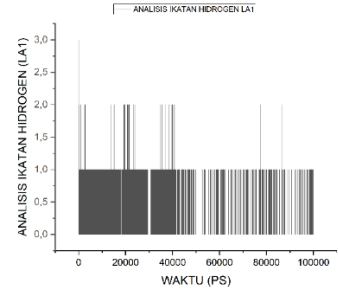
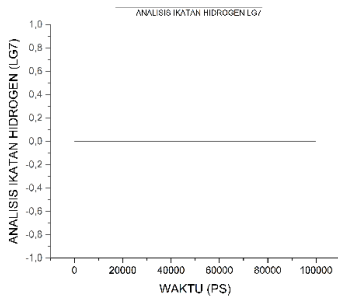
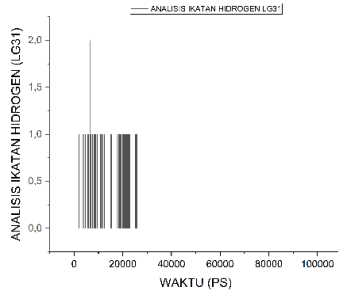
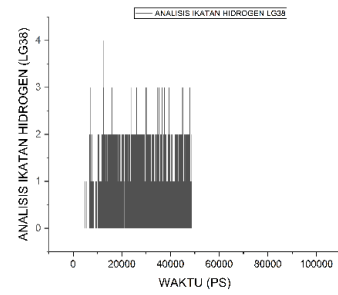
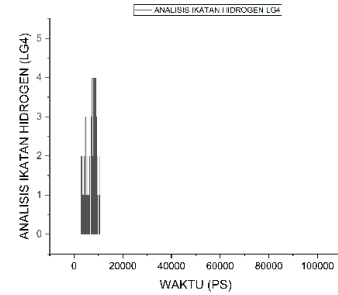
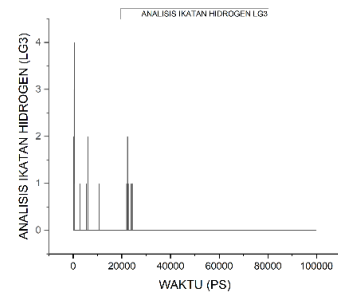
Lampiran 5 data occupancy ikatan hidrogen kompleks selama simulasi dinamika molekul

Kompleks ligan	Acceptor	Donor	Occupancy
(2CO) ALAMI	2C0_411@N	TYR_201@N	1,45
	2C0_411@O2	SER_104@N	1,24
	2C0_411@O1	SER_81@OG	1,01
	2C0_411@O1	SER_104@OG	0,94
	2C0_411@O2	SER_81@OG	0,59
	2C0_411@O2	SER_104@OG	0,39
	2C0_411@N	SER_81@OG	0,24
	2C0_411@O2	SER_81@N	0,21
	2C0_411@N	SER_104@OG	0,12
	2C0_411@O2	ALA_231@N	0,11
	2C0_411@O1	ALA_231@N	0,09
	2C0_411@O1	SER_82@N	0,08
	2C0_411@O1	SER_104@N	0,07
	2C0_411@O1	SER_81@N	0,07
	2C0_411@O1	THR_156@OG1	0,02
	2C0_411@O2	THR_156@OG1	0,01
	2C0_411@C	TYR_201@O	0,01
	2C0_411@O2	TRP_16@NE1	0,01
	2C0_411@O2	GLN_299@NE2	0,01
	2C0_411@N	TYR_201@OH	0,01
LG3	2C0_411@O1	TRP_16@NE1	0,01
	TRP_229@OE2	UNK_411@O8	0,15
	TRP_16@OE1	UNK_411@O9	0,12
	TRP_16@OE2	UNK_411@O8	0,11
	TRP_229@OE1	UNK_411@O8	0,08
	TRP_229@OE2	UNK_411@O9	0,07
	GLU_65@OE1	UNK_411@O9	0,06
	UNK_411@O7	LYS_53@NZ	0,05
	LYS_165@O	UNK_411@O9	0,05
	TRP_16@OE2	UNK_411@O9	0,04
	UNK_411@O26	TYR_62@OH	0,04
	UNK_411@O12	LYS_61@NZ	0,03
	TRP_16@OE1	UNK_411@O8	0,03
	GLU_65@OE1	UNK_411@O7	0,03
	ARG_1@O	UNK_411@O9	0,03
	ARG_324@O	UNK_411@O8	0,02
	UNK_411@O9	LYS_165@NZ	0,02
	UNK_411@O11	ALA_3@N	0,02
	UNK_411@O7	LYS_165@NZ	0,02
	UNK_411@O7	LYS_165@NZ	0,02
LG38	UNK_411@O7	LYS_165@NZ	0,02
	UNK_411@O9	LYS_53@NZ	0,02
	UNK_411@O26	HIE_49@N	0,02
	UNK_411@O9	LYS_53@NZ	0,01
	UNK_411@O11	LYS_61@NZ	0,01
	ASP_158@O	UNK_411@O27	0,03
	SER_366@O	UNK_411@O10	0,02
	THR_125@O	UNK_411@O27	0,02
	ASP_158@OD1	UNK_411@O9	0,02
	UNK_411@O9	ARG_163@NH1	0,01
	SER_389@O	UNK_411@O11	0,01
	SER_364@OG	UNK_411@O9	0,01
	UNK_411@O9	SER_389@OG	0,01
	UNK_411@O27	ASN_110@ND2	0,01
	GLN_112@OE1	UNK_411@O11	0,01
	SER_366@OG	UNK_411@O27	0,01
	UNK_411@O10	SER_364@OG	0,01
	UNK_411@O10	ASN_110@ND2	0,01
	UNK_411@O10	ARG_111@NH1	0,01
	UNK_411@O11	SER_389@OG	0,01
	UNK_411@O26	ASN_348@ND2	0,01
	UNK_411@O9	ARG_163@NH2	0,01
	UNK_411@O6	ARG_111@NH2	0,01
	UNK_411@O9	ARG_111@NH2	0,01
	UNK_411@O26	ALA_363@N	0,01
	GLN_112@OE1	UNK_411@O9	0,01
	UNK_411@O26	SER_109@OG	0,01
	UNK_411@O10	ALA_363@N	0,01
	UNK_411@O22	ARG_111@NH1	0,01
	UNK_411@O19	TYR_201@N	2,44
	UNK_411@O19	TRP_16@ND2	0,20
	UNK_411@O19	HID_121@NZ	0,06
	UNK_411@O19	LYS_317@NZ	0,05
	UNK_411@O20	ASN_274@ND2	0,04
	UNK_411@O19	LYS_317@NZ	0,03
	UNK_411@O19	ASN_274@ND2	0,03
	UNK_411@O20	GLU_353@N	0,03
	UNK_411@O19	ARG_36@NH1	0,03
	UNK_411@O19	ARG_36@NE	0,03
	UNK_411@O19	ILE_39@N	0,03
	UNK_411@O19	ASN_316@ND2	0,02
	UNK_411@O20	ASN_274@ND2	0,01
	UNK_411@O19	SER_351@OG	0,01
	UNK_411@O19	ARG_37@NH1	0,01
	UNK_411@O19	HIE_358@NE2	0,01
	UNK_411@O2	SER_104@NE2	18,87
	SER_81@OE1	UNK_411@O1	2,92
	UNK_411@O2	TYR_201@NE2	2,21
	UNK_411@O2	ARG_190@NH1	1,38
	GLN_191@OE1	UNK_411@N4	1,24

LG4	ARG_1@O	UNK_411@O7	0,01
	ARG_324@O	UNK_411@O11	0,01
	UNK_411@O8	LYS_165@NZ	0,01
	UNK_411@O11	LYS_165@NZ	0,01
	UNK_411@O9	LYS_165@NZ	0,01
	UNK_411@O8	LYS_289@NZ	0,01
	ARG_1@O	UNK_411@O11	0,01
	UNK_411@O7	LYS_61@NZ	0,01
	UNK_411@O8	LYS_165@NZ	0,01
	UNK_411@O12	GLN_58@NE2	0,01
	UNK_411@O7	GLN_58@NE2	0,01
	UNK_411@O12	LYS_53@NZ	0,01
	UNK_411@O26	SER_104@OG	0,85
	SER_104@OG	UNK_411@O11	0,78
	TYR_201@OD1	UNK_411@O11	0,63
	ASP_362@OD1	UNK_411@O11	0,47
	UNK_411@O27	ARG_163@NH2	0,36
	UNK_411@O9	SER_364@OG	0,32
	SER_389@OG	UNK_411@O9	0,31
	ASP_158@OD1	UNK_411@O10	0,29
	THR_390@OG1	UNK_411@O9	0,15
	UNK_411@O27	THR_125@OG1	0,15
	SER_109@OG	UNK_411@O10	0,14
	ASP_362@OD1	UNK_411@O9	0,11
	UNK_411@O26	ASN_110@ND2	0,09
	UNK_411@O27	ARG_163@NH1	0,07
	UNK_411@O26	GLN_112@N	0,07
	UNK_411@O22	ARG_111@NH2	0,06
	TRP_16@OE2	UNK_411@O27	0,06
	SER_109@OG	UNK_411@O11	0,05
	UNK_411@O10	ARG_111@NH2	0,05
	SER_109@OG	UNK_411@O9	0,05
	SER_109@OG	UNK_411@O22	0,04
	UNK_411@O26	ARG_111@N	0,04
	UNK_411@O27	SER_364@OG	0,04
	UNK_411@O11	SER_364@OG	0,03
	UNK_411@O10	ASN_110@ND2	0,03
	ASN_110@OD1	UNK_411@O10	0,03
	SER_366@O	UNK_411@O9	0,03

LG31	THR_172@O	UNK_411@O3	1,2
	UNK_411@O3	ARG_174@NH1	0,26
	UNK_411@O2	ASN_187@ND2	0,15
	UNK_411@O2	GLN_191@NE2	0,13
	GLU_170@OE1	UNK_411@O3	0,11
	ASP_192@OD2	UNK_411@O3	0,08
	UNK_411@O3	ARG_174@NE	0,06
	ARG_190@O	UNK_411@O1	0,06
	UNK_411@O2	ASN_187@ND2	0,05
	GLU_170@OE2	UNK_411@O3	0,05
	UNK_411@O3	SER_176@N	0,02
	ILE_171@O	UNK_411@O3	0,02
	UNK_411@O3	ARG_174@NH2	0,02
	ASN_187@OD1	UNK_411@O1	0,02
	ARG_190@O	UNK_411@O3	0,02
	UNK_411@O2	ARG_190@NH1	0,01
	UNK_411@O2	ARG_190@NH2	0,01
	GLU_161@OE2	UNK_411@O3	0,01
	UNK_411@O3	GLN_191@NE2	0,01
	GLN_191@NE2	UNK_411@N4	0,01
	UNK_411@O1	ARG_190@NE	0,01
	UNK_411@O3	ARG_174@N	0,01
	UNK_411@O17	ARG_92@NH1	0,01
	UNK_411@O17	ASN_335@ND2	0
	LG7		
	LG18		
	LG14		
	LG8		

Lampiran 6 grafik ikatan hidrogen kompleks selama simulasi dinamika molekul



Lampiran 7 Data hasil perhitungan MMGBSA

Kode ligan	ΔE_{vdw}	ΔE_{ele}	ΔG permukaan	ΔG pengikat
Ligan alami 2CO	-27,5267	-7,8815	-3,562	-17,3123
LG3	-18,0094	-3,965	-2,4544	-12,0731
LG4	-7,3652	-9,6286	-1,2345	-2,9015
LG7	-23,0532	-8,6168	-3,2366	-13,3278
LG8	-31,7986	-1,5147	-4,6086	-27,9437
LG14	-20,0255	-1,2247	-2,8607	-15,718
LG15	-21,5102	-2,6296	-3,0753	-16,5454
LG18	-22,9951	-2,1121	-3,2785	-17,3895
LG38	-18,4933	-9,562	-2,6431	-12,9181
LG31	-23,3005	-0,4927	-3,3886	-20,0819

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Lampiran 9 Kartu bimbingan



No. Dok.02.64.00/FRM-03/AKD-SPM



KARTU BIMBINGAN TUGAS AKHIR II

Pembimbing serta	: apt. Purwaniati, M.Si
Nama Mahasiswa	: Azriel nugraha
NPM	: 191ff03041
Bidang Ilmu	: S1 FARMASI (AFKM : KIMIA MEDISINAL)

N o	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	15/3/2023	11.30	Online (ZOOM)	Laporan mengenai reseptor target uji yg diganti	
2	14/4/2023	10.00	offline	presentasi kemajuan penelitian	
3	14/4/2023	10.00	offline	BIMBINGAN	
4	23/05/2023	08.00	Online (ZOOM)	laporan seminar kemajuan tugas 2 TA 2	
5	5/6/2023	08.00	Offline	BIMBINGAN TERKAIT PEMBAHASAN	
6	26/6/2023	12.00	ONLINE	Laporan terkait Validasi docking	
7	30/6/2023	10.00	ONLINE	laporan Revisi validasi docking	
8	6/7/2023	12.00	Offline	BIMBINGAN TERKAIT KEMAJUAN PENELITIAN	

Catatan : Kartu ini harus dibawa setiap kali melakukan bimbingan dan harus diisi oleh dosen pembimbing.



KARTU BIMBINGAN TUGAS AKHIR II

Pembimbing Utama	: Dr. apt. Fauzan Zein Muttaqin, M.Si
Nama Mahasiswa	: Azriel Nugraha
NPM	: 191ff03041
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[illegible]

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SMA : SMA 1 PURWAKARTA
S1 : UNIVERSITAS BHAKTI KENCANA
Pendidikan Sekarang : S1 Farmasi (Universitas Bhakti kencana)