LAMPIRAN

Lampiran 1 Daftar Senyawa Uji yang Digunakan Pada Penelitian

Pubchem CID	Nama Senyawa	Nama Senyawa (IUPAC Name)	Rumus Kimia
5493444	Aliskiren	(2S,4S,5S,7S)-5-amino-N-(3-amino-2,2-dimethyl-3-oxopropyl)-4-hydroxy-7-[[4-methoxy-3-(3-methoxypropoxy)phenyl]methyl]-8-methyl-2-propan-2-ylnonanamide	$C_{30}H_{53}N_3O_6$
10277042	3-Epimasclinic Acid	(4aS,6aS,6bR,12aR)-10,11-dihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_4$
5280443	Apigenin	5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	$C_{15}H_{10}O_5$
73641	Arjunolic acid	(4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_5$
119034	Asiatic acid	(1S,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	$C_{30}H_{48}O_5$
16212811	Asiaticoside	[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6R)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl] (1S,2R,4aS,6aR,6aS,6bR,9R,10R,11R,12aR)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	$C_{48}H_{78}O_{19}$
5282102	Astragalin	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	$C_{21}H_{20}O_{11}$
12305221	Bayogenin	(4aS,6aR,6aS,6bR,8aR,9R,10R,11S,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_5$
5281515	Beta caryophyllene	(1R,4E,9S)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene	$C_{15}H_{24}$

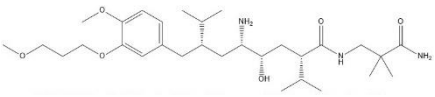
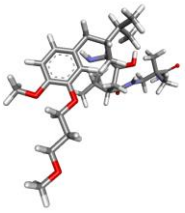
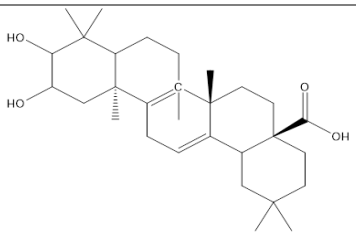
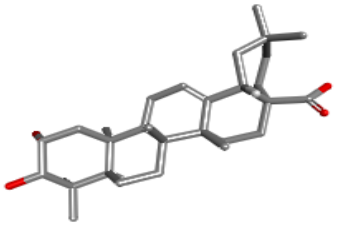
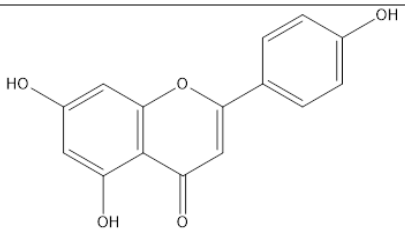
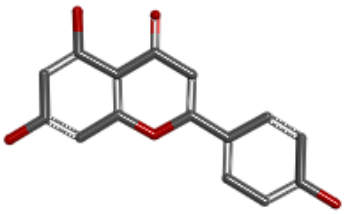
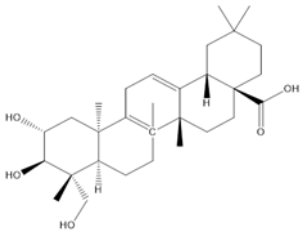
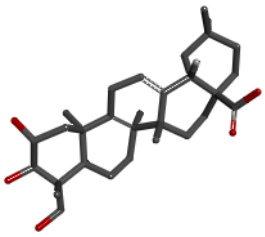
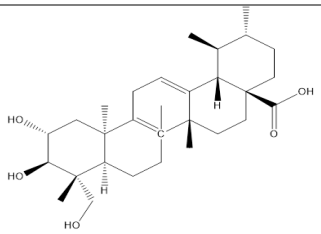
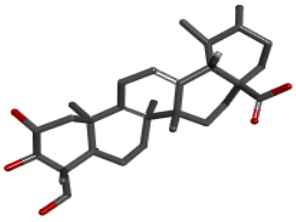
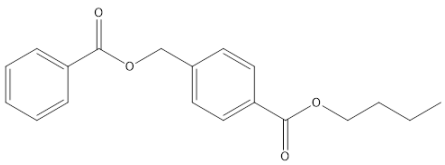
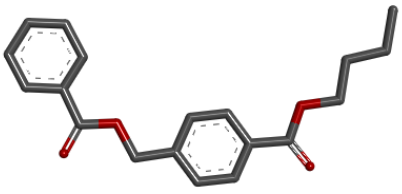
6918391	Beta elemene	(1S,2S,4R)-1-ethenyl-1-methyl-2,4-bis(prop-1-en-2-yl)cyclohexane	$C_{15}H_{24}$
64971	Betulinic acid	(1R,3aS,5aR,5bR,7aR,9S,11aR,11bR,13aR,13bR)-9-hydroxy-5a,5b,8,8,11a-pentamethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid	$C_{30}H_{48}O_3$
56842786	Bicycloelemene	(1R,2R,3S,6R)-3-ethenyl-3,7,7-trimethyl-2-prop-1-en-2-ylbicyclo[4.1.0]heptane	$C_{15}H_{24}$
64685	Borneol	1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	$C_{10}H_{18}O$
17757599	Cadiyenol	methyl 5-[(9E)-6,15-dihydroxy-8-methoxyheptadeca-9,16-dien-11,13-diyn-7-yl]oxypentanoate	$C_{24}H_{36}O_6$
173183	Campesterol	(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	$C_{28}H_{48}O$
6616	Camphene	2,2-dimethyl-3-methylidenebicyclo[2.2.1]heptane	$C_{10}H_{16}$
7438	Carveol	2-methyl-5-prop-1-en-2-ylcyclohex-2-en-1-ol	$C_{10}H_{16}O$
14350	Caryophyllene Epoxide	4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.04,6]dodecane	$C_{15}H_{24}O$
102394640	Castillicetin	[2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxochromen-3-yl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	$C_{24}H_{16}O_{10}$
10526707	Castilliferol	[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxochromen-3-yl] (E)-3-(4-hydroxyphenyl)prop-2-enoate	$C_{24}H_{16}O_8$
9064	Catechin	(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol	$C_{15}H_{14}O_6$
73196815	Centellasapogenol A	10,11-dihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_5$
21633803	Centellasaponin A	[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl] (4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR)-10,11-dihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14-tetradecahydropicene-4a-carboxylate	$C_{48}H_{78}O_{19}$
85411973	Centellasaponin B	[3,4,5-trihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl] 8,10,11-	$C_{42}H_{68}O_{16}$

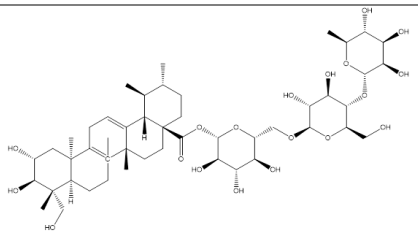
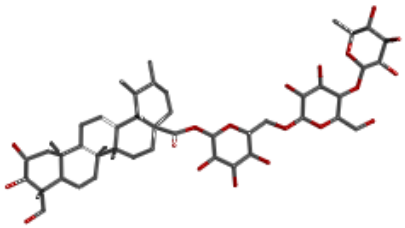
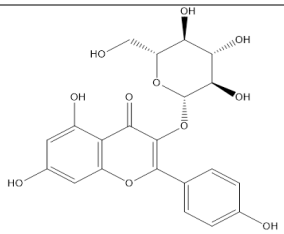
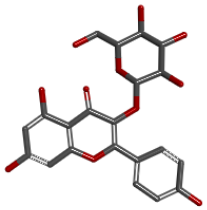
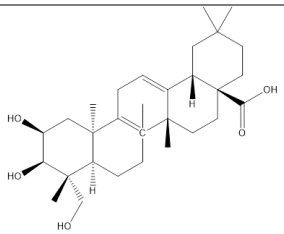
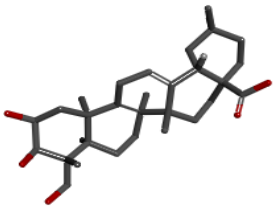
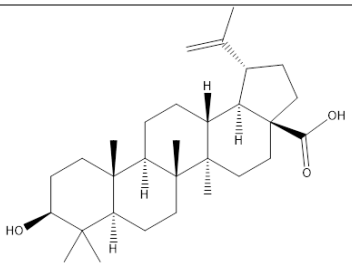
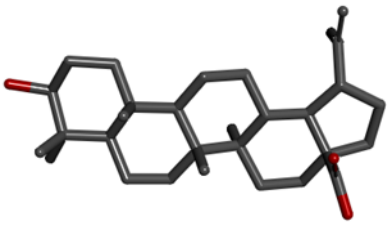
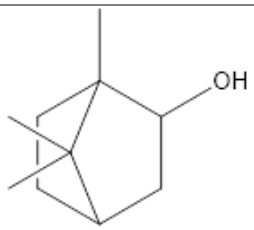
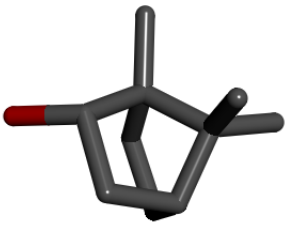
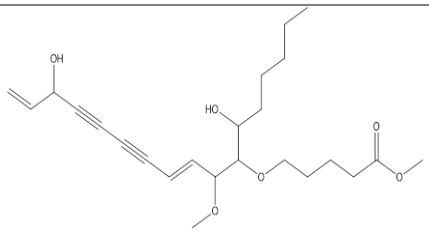
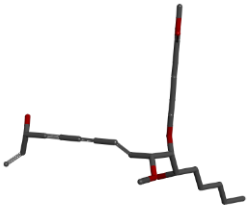
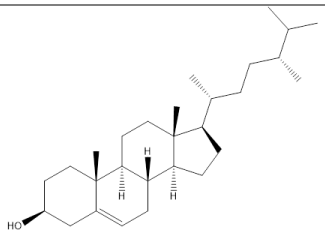
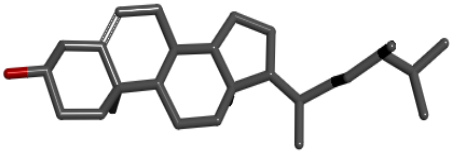
		trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	
163184102	Centellin	[(7E)-3-hydroxytrideca-1,7-dien-4-yn-6-yl] acetate	$C_{15}H_{22}O_3$
101568838	Centelloside E	[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl] (1S,2R,4aS,6aR,6aR,6bR,8aR,9R,10R,11R,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,8a,10,11,12,13,14b-dodecahydro-1H-picene-4a-carboxylate	$C_{48}H_{76}O_{19}$
1794427	Chlorogenic acid	(1S,3R,4R,5R)-3-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-1,4,5-trihydroxycyclohexane-1-carboxylic acid	$C_{16}H_{18}O_9$
6918774	Corosolic Acid	(1S,2R,4aS,6aR,6aS,6bR,8aR,10R,11R,12aR,14bS)-10,11-dihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	$C_{30}H_{48}O_4$
11141699	Galanolactone	(3E)-3-[2-[(1R,2S,4aS,8aS)-5,5,8a-trimethylspiro[3,4,4a,6,7,8-hexahydro-1H-naphthalene-2,2'-oxirane]-1-yl]ethylidene]oxolan-2-one	$C_{20}H_{30}O_3$
1549026	Geranyl Acetate	[(2E)-3,7-dimethylocta-2,6-dienyl] acetate	$C_{12}H_{20}O_2$
9548706	Germacrene A	(1*E*,5*E*,8*S*)-1,5-dimethyl-8-prop-1-en-2-ylcyclodeca-1,5-diene	$C_{15}H_{24}$
9896928	Ginsenoside MC	(2R,3S,4S,5R,6S)-2-[[(2R,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-6-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-en-2-yl]oxyoxane-3,4,5-triol	$C_{41}H_{70}O_{12}$
5280804	Isoquercitrin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	$C_{21}H_{20}O_{12}$
12302703	Isothankunic Acid	8,8a,10-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-	$C_{30}H_{48}O_6$

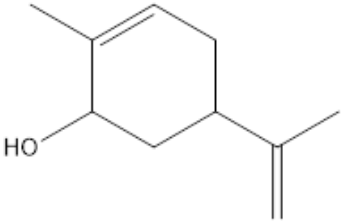
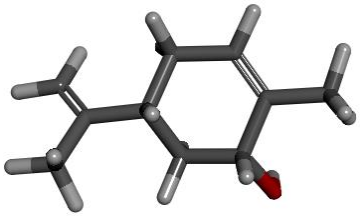
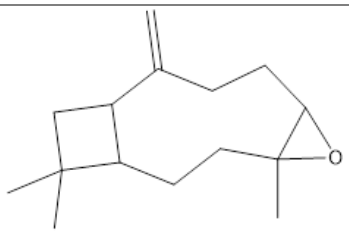
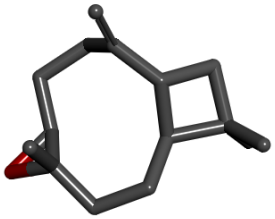
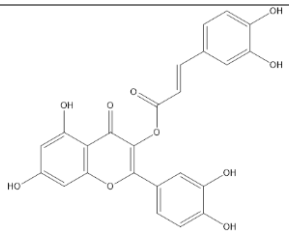
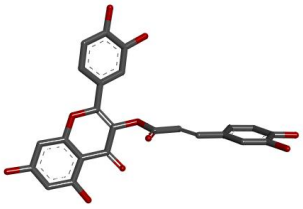
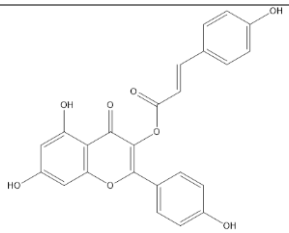
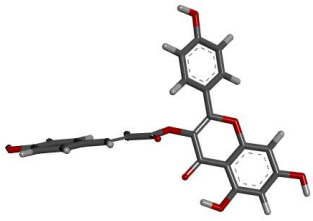
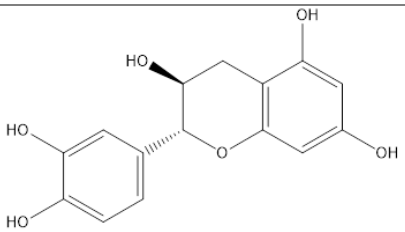
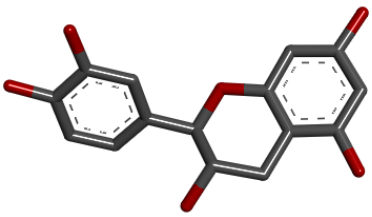
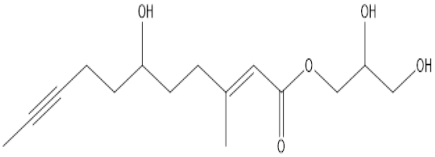
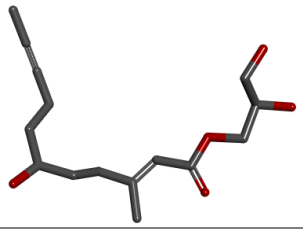
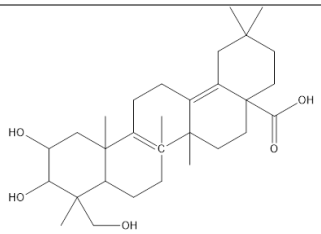
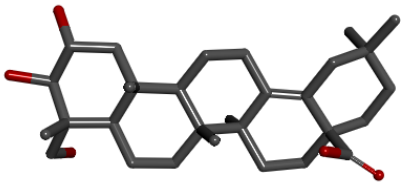
		1,2,3,4,5,6,6a,7,8,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	
5280863	Kaempferol	3,5,7-trihydroxy-2-(4-hydroxyphenyl)chromen-4-one	$C_{15}H_{10}O_6$
25079965	Kaempferol-7-rhamnoside	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one	$C_{21}H_{20}O_{10}$
6549	Linalool	3,7-dimethylocta-1,6-dien-3-ol	$C_{10}H_{18}O$
5280445	Luteolin	-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one	$C_{15}H_{10}O_6$
23132225	Madasiatic Acid	8,10,11-trihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	$C_{30}H_{48}O_5$
73412	Madecassic Acid	(1S,2R,4aS,6aR,6aS,6bR,8R,8aR,9R,10R,11R,12aR,14bS)-8,10,11-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	$C_{30}H_{48}O_6$
45356919	Madecassoside	[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl] (1S,2R,4aS,6aR,6aR,6bR,8R,8aR,9R,10R,11R,12aR,14bS)-8,10,11-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	$C_{48}H_{78}O_{20}$
21672634	Methyl Asiatate	methyl (1S,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	$C_{31}H_{50}O_5$
5281672	Myricetin	3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)chromen-4-one	$C_{15}H_{10}O_8$
442428	Naringin	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	$C_{27}H_{32}O_{14}$
7463	P-cymene	1-methyl-4-propan-2-ylbenzene	$C_{10}H_{14}$ atau $CH_3C_6H_4CH(CH_3)_2$
5281678	Patuletin	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-6-methoxychromen-4-one	$C_{16}H_{12}O_8$

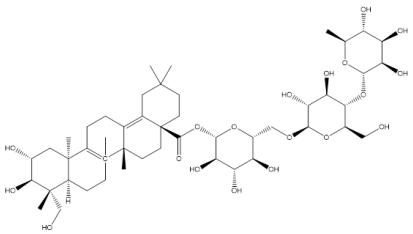
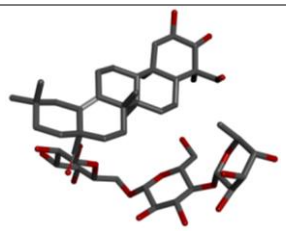
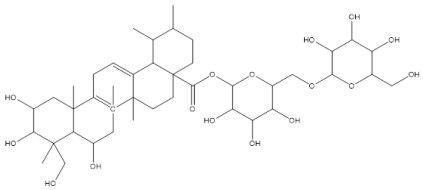
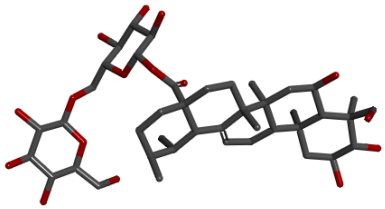
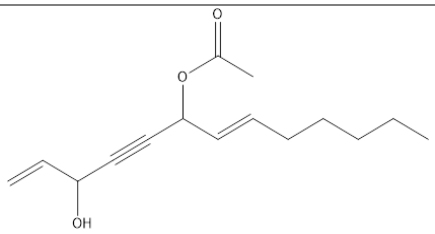
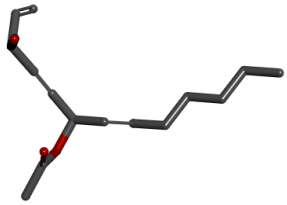
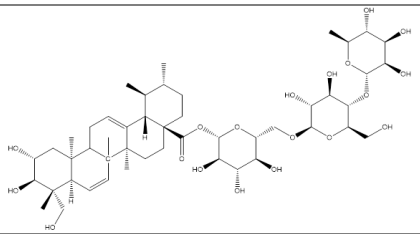
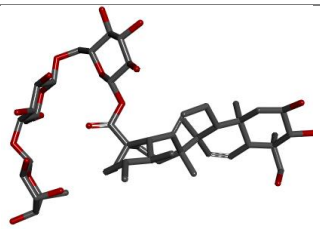
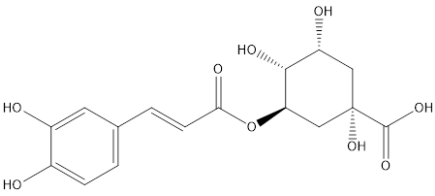
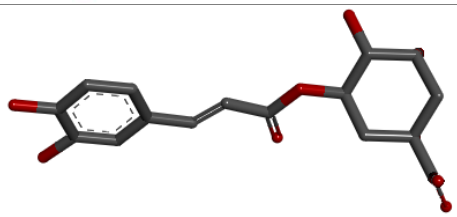
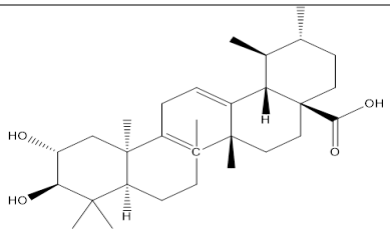
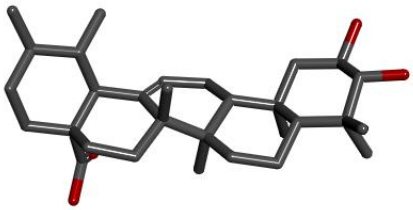
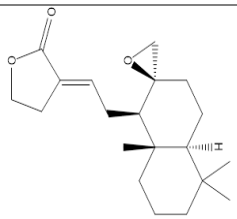
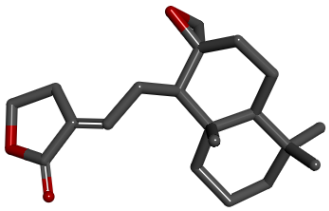
15837102	Pinene	2,6,6-trimethylbicyclo[3.1.1]hept-1-ene	$C_{10}H_{16}$
382831	Pomolic Acid	(1R,2R,4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-1,10-dihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_4$
5280343	Quercetin	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one	$C_{15}H_{10}O_7$
5280805	Rutin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxychromen-4-one	$C_{27}H_{30}O_{16}$
5280794	Stigmasterol	(3S,8S,9S,10R,13R,14S,17R)-17-[(E,2R,5S)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	$C_{29}H_{48}O$
12314613	Terminolic Acid	(4aS,6aR,6aS,6bR,8R,8aR,9R,10R,11R,12aR,14bS)-8,10,11-trihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	$C_{30}H_{48}O_6$
64945	Ursolic Acid	(1S,2R,4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-10-hydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	$C_{30}H_{48}O_3$
12303902	α_copaene	(1R,2S,6S,7S,8S)-1,3-dimethyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene	$C_{15}H_{24}$

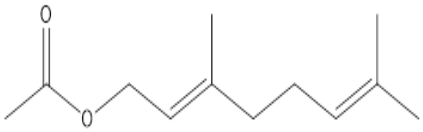
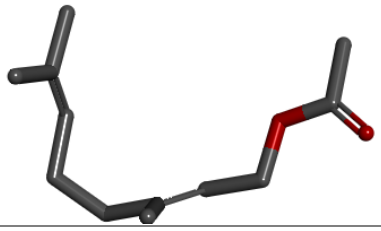
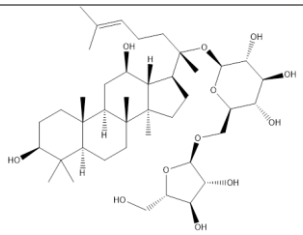
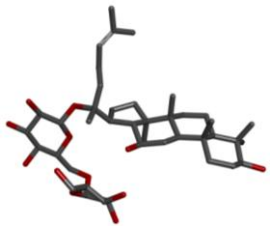
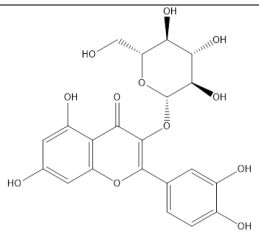
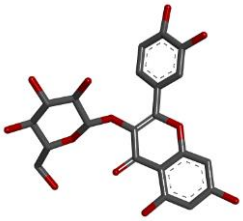
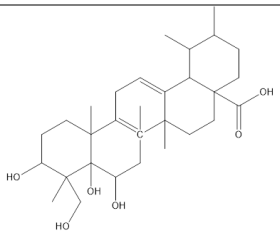
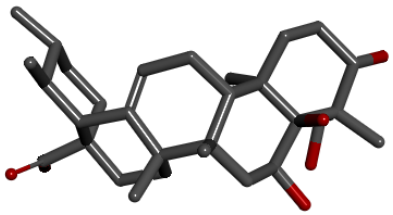
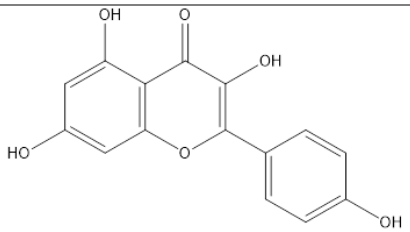
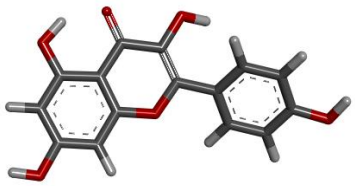
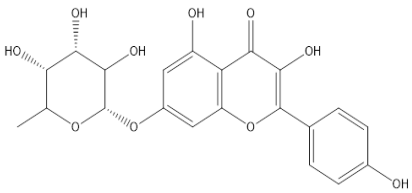
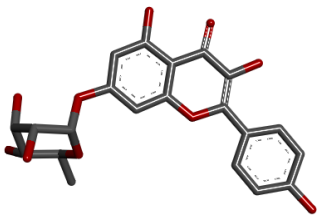
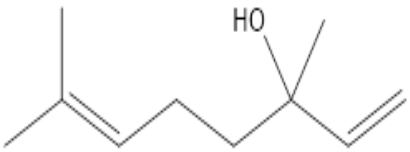
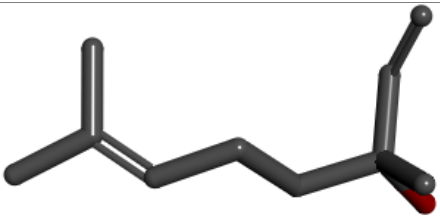
Lampiran 2 Struktur Dua Dimensi (2D) dan 3 Dimensi (3D) Senyawa Uji

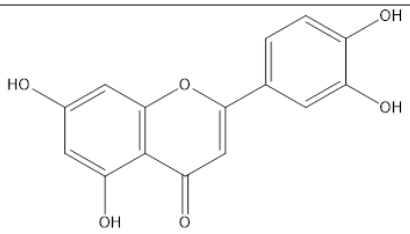
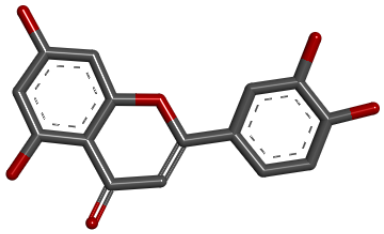
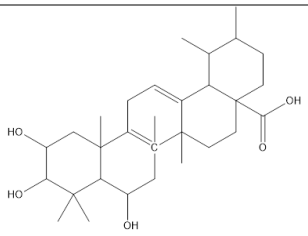
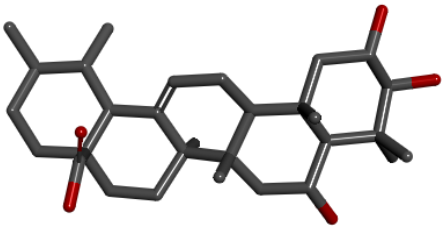
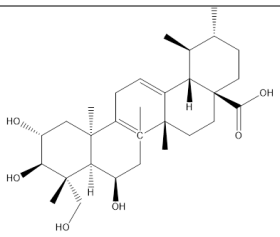
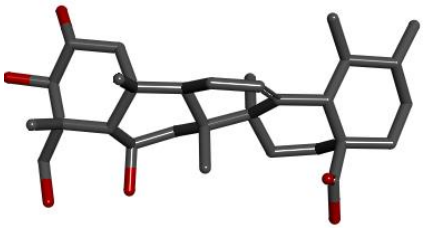
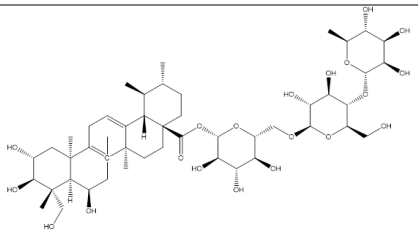
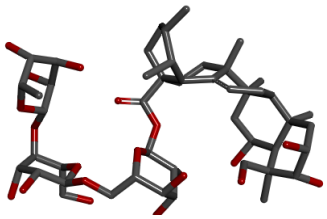
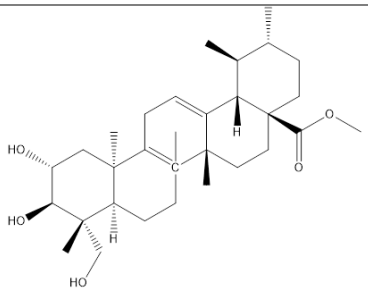
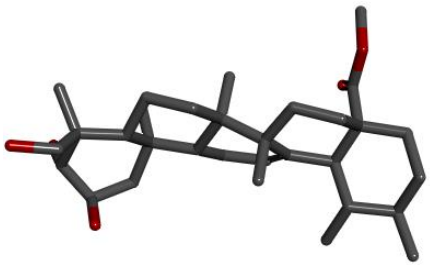
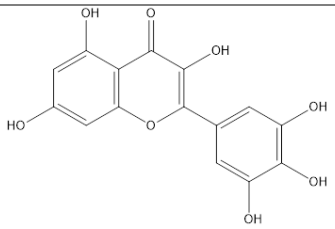
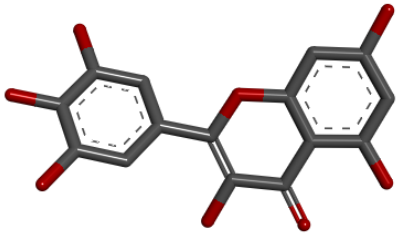
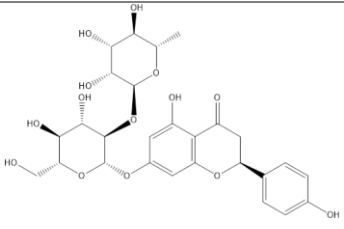
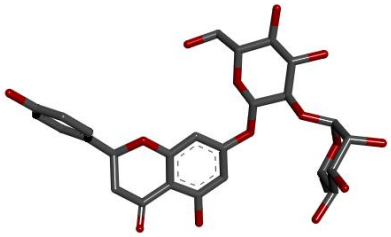
Nama Senyawa	Struktur 2D	Struktur 3D
Aliskiren (LA)		
3-Epimasclinic Acid (SU1)		
Apigenin (SU2)		
Arjunolic acid (SU3)		
Asiatic acid (SU4)		
Asiaticin (SU5)		

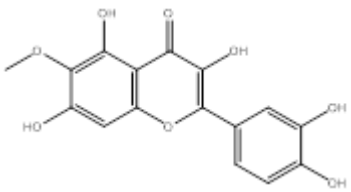
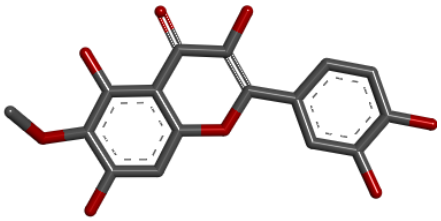
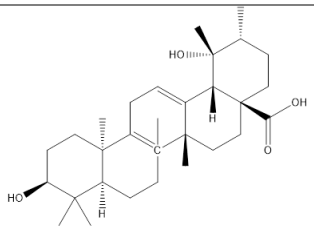
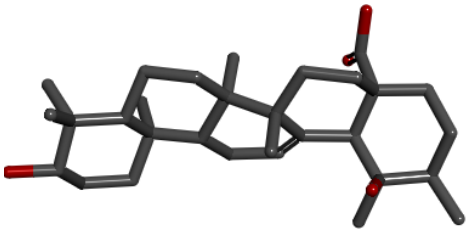
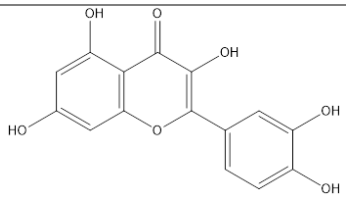
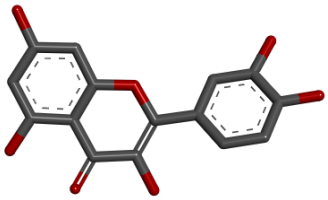
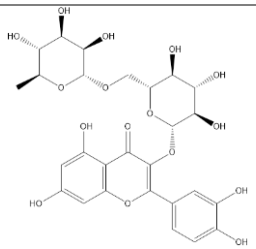
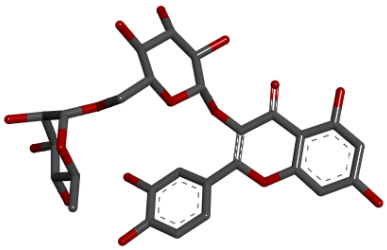
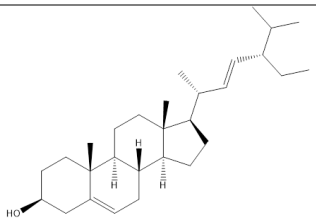
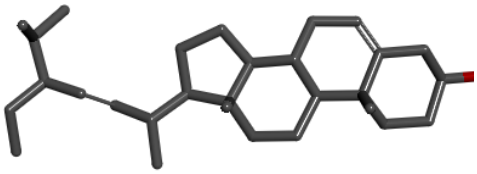
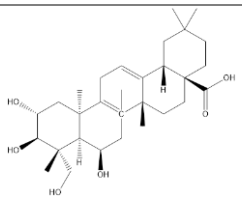
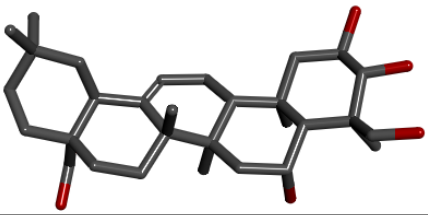
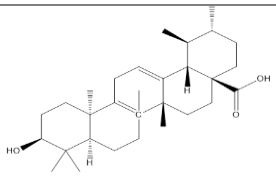
Asiaticoside (SU6)		
Astragalin (SU7)		
Bayogenin (SU8)		
Betulinic acid (SU9)		
Borneol (SU10)		
Cadiyenol (SU11)		
Campesterol (SU12)		

Carveol (SU13)		
Caryophyllene Epoxide (SU14)		
Castillicetin (SU15)		
Castilliferol (SU16)		
Catechin (SU17)		
Cenetellicin (SU18)		
Centellasapogenol A (SU19)		

Centellasaponin A (SU20)		
Centellasaponin B (SU21)		
Centellin (SU22)		
Centelloside E (SU23)		
Chlorogenic acid (SU24)		
Corosolic Acid (SU25)		
Galanolactone (SU26)		

Geranyl Acetate (SU27)		
Ginsenoside MC (SU28)		
Isoquercitrin (SU29)		
Isothankunic Acid (SU30)		
Kaempferol (SU31)		
Kaempferol-7-rhamnoside (SU32)		
Linalool (SU33)		

Luteolin (SU34)		
Madasiatic Acid (SU35)		
Madecassic Acid (SU36)		
Madecassoside (SU37)		
Methyl Asiatate (SU38)		
Myricetin (SU39)		
Naringin (SU40)		

Patuletin (SU41)		
Pomolic Acid (SU42)		
Quercetin (SU43)		
Rutin (SU44)		
Stigmasterol (SU45)		
Terminolic Acid (SU46)		
Ursolic Acid (SU47)		

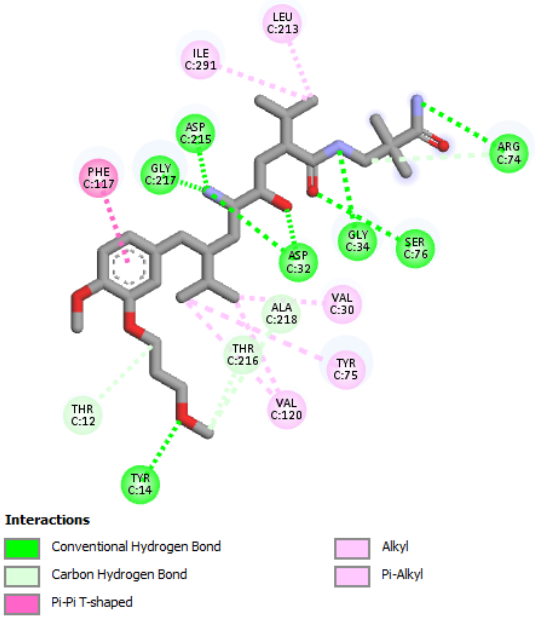
Lampiran 3 Tabel RMSD Penambatan Ulang Ligan Alami

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	35	-11.37	0.00	1.30	RANKING
1	2	64	-10.27	1.46	1.93	RANKING
1	3	33	-7.82	1.68	1.85	RANKING
2	1	6	-9.81	0.00	5.04	RANKING
3	1	25	-9.69	0.00	3.94	RANKING
3	2	41	-8.91	1.82	3.30	RANKING
4	1	50	-9.32	0.00	2.12	RANKING
4	2	75	-7.62	1.99	2.65	RANKING
4	3	13	-7.62	1.59	2.22	RANKING
4	4	40	-6.75	1.99	2.46	RANKING
5	1	43	-9.16	0.00	2.15	RANKING
5	2	68	-8.33	1.86	1.65	RANKING
5	3	4	-6.62	1.88	2.29	RANKING
6	1	49	-8.89	0.00	4.46	RANKING
7	1	100	-8.80	0.00	4.62	RANKING
8	1	77	-8.68	0.00	1.68	RANKING
8	2	44	-6.04	1.94	1.81	RANKING
9	1	48	-8.58	0.00	5.42	RANKING
10	1	37	-8.57	0.00	2.54	RANKING
10	2	5	-7.98	1.92	2.32	RANKING
11	1	55	-8.50	0.00	2.41	RANKING
12	1	45	-8.45	0.00	4.85	RANKING
12	2	60	-7.08	1.49	4.64	RANKING
12	3	21	-6.82	1.45	4.65	RANKING
13	1	38	-8.40	0.00	5.09	RANKING
13	2	58	-6.93	1.65	4.52	RANKING
13	3	27	-6.84	1.86	5.43	RANKING
13	4	10	-6.52	1.90	4.58	RANKING
14	1	71	-8.25	0.00	2.93	RANKING
14	2	53	-7.50	1.90	2.58	RANKING
15	1	70	-8.17	0.00	5.02	RANKING
15	2	12	-7.74	1.92	5.16	RANKING
15	3	7	-7.09	1.47	4.79	RANKING
15	4	63	-7.00	1.96	4.77	RANKING
16	1	47	-8.05	0.00	2.05	RANKING
17	1	95	-7.89	0.00	4.87	RANKING
17	2	65	-6.95	1.89	4.99	RANKING
17	3	29	-6.37	1.79	4.95	RANKING
18	1	92	-7.88	0.00	2.91	RANKING
18	2	59	-7.86	1.95	2.61	RANKING
19	1	34	-7.80	0.00	3.71	RANKING

19	2	51	-7.53	1.82	3.49	RANKING
20	1	39	-7.71	0.00	3.24	RANKING
21	1	62	-7.63	0.00	4.79	RANKING
21	2	79	-6.94	1.82	4.45	RANKING
21	3	9	-6.26	1.82	4.50	RANKING
22	1	85	-7.57	0.00	3.97	RANKING
22	2	57	-6.44	1.93	4.17	RANKING
22	3	15	-5.57	1.74	4.21	RANKING
23	1	84	-7.43	0.00	2.36	RANKING
24	1	97	-7.41	0.00	4.16	RANKING
25	1	78	-7.37	0.00	5.18	RANKING
25	2	91	-7.31	1.66	5.35	RANKING
26	1	69	-7.25	0.00	2.38	RANKING
26	2	86	-6.58	1.54	2.32	RANKING
26	3	3	-6.05	1.90	2.88	RANKING
26	4	61	-5.53	1.94	2.76	RANKING
27	1	26	-7.06	0.00	2.40	RANKING
28	1	31	-6.95	0.00	4.42	RANKING
28	2	42	-6.84	1.83	4.30	RANKING
29	1	24	-6.93	0.00	3.51	RANKING
30	1	93	-6.82	0.00	4.85	RANKING
31	1	76	-6.67	0.00	2.53	RANKING
32	1	66	-6.65	0.00	4.76	RANKING
32	2	98	-6.53	1.88	4.70	RANKING
32	3	11	-5.57	1.77	5.56	RANKING
32	4	20	-5.22	1.71	4.66	RANKING
33	1	96	-6.59	0.00	5.73	RANKING
34	1	16	-6.57	0.00	3.85	RANKING
34	2	67	-6.22	1.94	3.10	RANKING
35	1	72	-6.56	0.00	3.07	RANKING
36	1	99	-6.47	0.00	2.43	RANKING
37	1	36	-6.41	0.00	3.90	RANKING
38	1	73	-6.38	0.00	2.61	RANKING
39	1	83	-6.38	0.00	4.29	RANKING
40	1	54	-6.28	0.00	4.97	RANKING
41	1	82	-6.26	0.00	2.83	RANKING
42	1	32	-6.02	0.00	3.89	RANKING
42	2	14	-5.83	1.99	3.56	RANKING
43	1	74	-5.99	0.00	4.51	RANKING
44	1	30	-5.99	0.00	5.83	RANKING
45	1	46	-5.90	0.00	4.94	RANKING
46	1	18	-5.88	0.00	4.77	RANKING
47	1	23	-5.88	0.00	3.90	RANKING
48	1	88	-5.84	0.00	4.60	RANKING
49	1	56	-5.67	0.00	5.35	RANKING
50	1	28	-5.60	0.00	3.50	RANKING

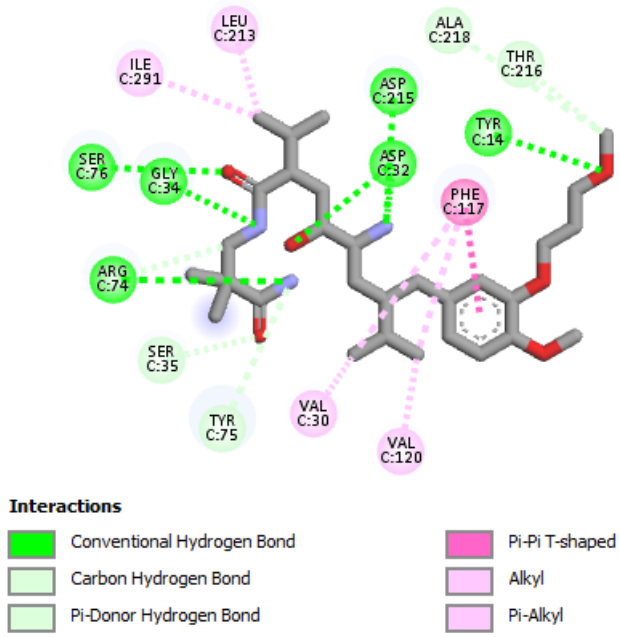
51	1	94	-5.53	0.00	3.80	RANKING
51	2	1	-5.44	1.99	4.25	RANKING
52	1	90	-5.52	0.00	3.17	RANKING
53	1	81	-5.51	0.00	3.13	RANKING
54	1	8	-5.44	0.00	4.60	RANKING
54	2	80	-4.36	1.97	4.24	RANKING
55	1	89	-5.42	0.00	4.79	RANKING
56	1	19	-5.30	0.00	3.46	RANKING
57	1	2	-5.26	0.00	3.61	RANKING
58	1	87	-5.25	0.00	3.89	RANKING
59	1	22	-4.51	0.00	4.30	RANKING
60	1	17	-4.48	0.00	2.74	RANKING
61	1	52	-2.46	0.00	4.53	RANKING

Lampiran 4 Interaksi Ligan Alami Hasil Kristalografi Sinar-X dengan Target Kerja



Kode Ligan	Interaksi	Jarak ikatan	Residu Asam Amino
Ligan Alami	**Ikatan Hidrogen** • **Conventional H-Bond** C:TYR14:N - C:C411328:O2 C:SER76:N - C:C411328:O31 C:C411328:N22 - C:ASP32:OD1 C:C411328:N22 - C:ASP215:OD1 C:C411328:N22 - C:GLY217:O C:C411328:O24 - C:ASP32:OD2 C:C411328:N32 - C:GLY34:O C:C411328:N39 - C:ARG74:O • **Carbon H-Bond** C:C411328:C1 - C:THR216:O C:C411328:C1 - C:ALA218:O C:C411328:C5 - C:THR12:O C:C411328:C33 - C:ARG74:O **Ikatan Hidrofobik** • **π-π T-shaped** C:PHE117 - C:C411328 • **Alkyl** C:C411328:C18 - C:VAL30 C:C411328:C18 - C:VAL120 C:C411328:C19 - C:VAL120 C:C411328:C29 - C:LEU213 C:C411328:C29 - C:ILE291 • **π-Alkyl** C:TYR75 - C:C411328:C19	 3,0 2,9 3,0 2,8 3,0 2,7 3,0 3,0 3,2 3,4 3,3 3,8 5,1 3,9 3,8 4,5 4,5 4,5 4,1	**Tyr14, Arg74, Gly 34, Ser76, Asp215, Asp32**, Gly 217, Thr216, Al218, Thr12, Phe117, Val30, Val120, Leu213, Ile291, Tyr75,

Lampiran 5 Interaksi Ligan Alami Pose Terbaik dengan Target Kerja



Kode Ligan	Interaksi	Jarak ikatan	Residu Asam Amino
Ligan Alami	**Ikatan Hidrogen** • **Conventional H-Bond** C:C411328:N39 – C:Arg74:O C:C411328:N32 – C:Gly34:O C:Ser76:N – C:C411328:O31 C:C411328:N22 – C:Asp215:Od1 C:C411328:N22 – C:Asp32:Od1 C:Tyr14:N – C:C411328:O2 • **Carbon H-Bond** C:Ser35:Cb – C:C411328:O38 C:C411328:C1 – C:Thr216:O C:C411328:C1 – C:Ala218:O C:C411328:C33 – C:Arg74:O • **π-Donor H-Bond** C:C411328:N39 – C:Tyr75 **Ikatan Hidrofobik** • **π-π T-shaped** C:Phe117 – C:C411328 • **Alkyl** C:C411328:C18 – C:Val120 C:C411328:C19 – C:Val30 C:C411328:C28 – C:Leu213 C:C411328:C28 – C:Ile291 • **II-Alkyl** C:Phe117 – C:C411328:C18 C:Phe117 – C:C411328:C19	 3,2 3,3 2,8 2,7 2,7 2,9 3,1 3,2 3,6 3,3 3,6 5,2 3,7 3,3 4,4 4,1 5,2 4,7	**Arg74, Gly 34, Ser76, Asp215, Asp32, Tyr14,** Ser35, Thr216, Ala218, Tyr75, Phe117, Val120, Val30, Leu213, Ile291

Lampiran 6 Interaksi Senyawa Uji dengan Target Kerja

Nama Senyawa	Interaksi	Jarak ikatan	Residu Asam Amino
3-Epimasclinic Acid (SU1)	**Ikatan Hidrogen** • **Conventional H-Bond** C:SER219:OG - :UNK0:O :UNK0:H - C:TYR220:OH :UNK0:H - C:TYR220:OH • **Carbon H-Bond** C:THR12:CB - :UNK0:O • **π-Donor H-Bond** :UNK0:H - C:TYR75 **Ikatan Hidrofobik** • **Alkyl** C:VAL30 - :UNK0 :UNK0:C - C:PRO111 :UNK0:C - C:PRO111 :UNK0:C - C:LEU114 • **π-Alkyl** C:TYR75 - :UNK0 C:TYR75 - :UNK0:C C:PHE117 - :UNK0 C:PHE117 - :UNK0:C	 3,1 2,0 2,0 3,4 3,0 5,0 4,5 4,7 4,4 4,8 5,0 5,1 5,	 Tyr220, Ser219, Thr12, **Tyr75, Phe117,** Pro111, Val30, Leu114
Apigenin (SU2)	**Ikatan Hidrogen** • **Conventional H-Bond** d:RES1:H30 - C:TYR155:OH d:RES1:H30 - C:THR216:O d:RES1:H28 - C:THR77:OG1 d:RES1:H29 - C:PRO111:O • **π-Donor H-Bond** C:TYR14:N - d:RES1 **Ikatan Hidrofobik** • **π-Sigma** C:GLN13:CA - d:RES1 • **Amide π- Stacked** C:GLY217:C,O;ALA218:N - d:RES1 • **π-Alkyl** d:RES1 - C:PRO111 d:RES1 - C:ALA115 d:RES1 - C:VAL30	 2,6 2,0 3,0 2,0 4,0 4,0 3,7 5,1 5,3 4,6	 Tyr155, **Thr216**, Pro111, Thr77, **Tyr14, Ala218**, Ala115, Gln13, Gly217, **Val30**
Arjunolic acid (SU3)	**Ikatan Hidrogen** • **Conventional H-Bond** d:RES1:H82 - C:GLN13:OE1 d:RES1:H74 - C:THR12:OG1 d:RES1:H75 - C:TYR220:OH d:RES1:H83 - C:THR77:OG1	 1,8 2,9 2,1 1,7	 Tyr220, Thr77, Thr12, Gln13, Leu114, **Phe117**, Pro111, Phe112,

	Ikatan Hidrofobik		Val120, **Val30**, **Tyr75**
	• **Alkyl**		
	C:PRO111 - d:RES1	5,2	
	C:PRO111 - d:RES1	4,9	
	C:VAL120 - d:RES1	5,2	
	d:RES1:C20 - C:PRO111	3,6	
	d:RES1:C31 - C:LEU114	4,7	
	d:RES1:C35 - C:VAL30	4,3	
	d:RES1:C35 - C:VAL120	4,3	
	• **π-Alkyl**		
	C:TYR75 - d:RES1	4,2	
	C:TYR75 - d:RES1:C34	4,5	
	C:PHE112 - d:RES1	5,0	
	C:PHE117 - d:RES1:C26	4,0	
Asiatic acid (SU4)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:OG - :UNK0:O	2,8	
	:UNK0:H - C:TYR220:OH	2,1	
	:UNK0:H - C:TYR220:OH	2,2	
	Ikatan Hidrofobik		Tyr220, ser219, leu114, pro111, ala115, phe117, val30, tyr75
	• **Alkyl**		
	C:VAL30 - :UNK0	5,1	
	C:PRO111 - :UNK0	5,2	
	C:ALA115 - :UNK0:C	4,5	
	:UNK0:C - C:PRO111	4,7	
	:UNK0:C - C:LEU114	4,8	
	:UNK0:C - C:LEU114	4,7	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	5,0	
	C:PHE117 - :UNK0	5,0	
	C:PHE117 - :UNK0:C	4,4	
Asiaticin (SU5)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:TYR220:N - :UNK0:O	2,8	
	Ikatan Hidrofobik		Tyr220, Ser219, Leu114, Pro111, Ala115, **Phe117, Val30, Tyr75**
	• **π-Sigma**		
	C:ALA218:CB - :UNK0	3,1	
	C:MET289:CE - :UNK0	3,4	
	• **π-Alkyl**		
	:UNK0 - C:ALA300	4,4	
	Ikatan Lain		
	• **π-Sulfur**		
	C:MET289:SD - :UNK0	3,4	
Asiaticoside (SU6)	**Ikatan Hidrogen**		ala300, arg74, asp290, gln128,
	• **Conventional H-Bond**		
	C:SER76:N - :UNK0:O	3,4	

	C:SER219:N - :UNK0:O	3,2	gly217, ile291,
	:UNK0:H - C:GLY217:O	2,0	leu213,
	:UNK0:H - C:TYR75:O	2,0	met289,
	:UNK0:H - C:ARG74:O	2,5	phe117,
	:UNK0:H - C:GLN128:OE1	2,2	pro292, ser76,
	• **Carbon H-Bond**		Ser219, tyr75
	C:TYR75:CA - :UNK0:O	3,6	
	C:PRO292:CD - :UNK0:O	3,2	
	C:PRO292:CD - :UNK0:O	2,7	
	:UNK0:C - C:TYR75:O	3,7	
	:UNK0:C - C:ASP290:O	3,3	
	:UNK0:C - C:SER76:O	3,6	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:LEU213 - :UNK0	4,3	
	C:ILE291 - :UNK0	4,6	
	C:ALA300 - :UNK0	5,0	
	C:ALA300 - :UNK0:C	3,4	
	:UNK0:C - C:MET289	4,4	
	:UNK0:C - C:ILE291	3,7	
	:UNK0:C - C:LEU213	3,2	
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	4,6	
	C:PHE117 - :UNK0:C	4,2	
Astragalin (SU7)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:THR77:OG1 - :UNK0:O	2,4	
	C:SER219:OG - :UNK0:O	3,0	
	:UNK0:H - C:PRO111:O	2,0	
	:UNK0:H - C:GLN13:OE1	2,1	
	:UNK0:H - C:SER219:OG	2,0	
	:UNK0:H - C:THR12:O	2,1	
	:UNK0:H - C:THR77:OG1	2,4	gln13, **phe117,** pro111, ser219, thr77, Thr12, **tyr75, val30**
	Ikatan Hidrofobik		
	• **π-π Stacked**		
	C:PHE117 - :UNK0	5,2	
	C:PHE117 - :UNK0	5,5	
	• **π-π T-Shaped**	4,7	
	C:TYR75 - :UNK		
	• **π-Alkyl**		
	:UNK0 - C:VAL30	4,5	
Bayogenin (SU8)	**Ikatan Hidrogen**		gln13, leu114,
	• **Conventional H-Bond**		**phe117**,
	:UNK0:H - C:GLN13:OE1	1,9	phe112,
	:UNK0:H - C:TYR220:OH	1,9	pro111, thr77,

	:UNK0:H - C:TYR220:OH	1,7	**tyr75,** Tyr220,
	:UNK0:H - C:THR77:OG1	1,7	**val30, val120**
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:PRO111 - :UNK0	5,2	
	C:PRO111 - :UNK0	5,9	
	C:VAL120 - :UNK0	5,1	
	:UNK0:C - C:PRO111	3,5	
	:UNK0:C - C:LEU114	5,3	
	:UNK0:C - C:VAL30	4,3	
	:UNK0:C - C:VAL120	3,9	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,2	
	C:PHE112 - :UNK0	4,9	
	C:PHE117 - :UNK0:C	4,2	
Betulinic acid (SU9)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:OG - :UNK0:O	2,6	
	:UNK0:H - C:TYR220:OH	2,0	
	• **Carbon H-Bond**		
	C:THR12:CB - :UNK0:O	3,2	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:VAL30 - :UNK0	5,4	Ala115,
	C:PRO111 - :UNK0	5,0	leu114,
	C:ALA115 - :UNK0:C	4,4	phe112,
	:UNK0 - C:LEU114	5,1	**phe117,**
	:UNK0:C - C:VAL30	3,3	pro111, ser219,
	:UNK0:C - C:VAL120	3,6	thr12, tyr220,
	:UNK0:C - C:PRO111	5,1	**val30, val120**
	:UNK0:C - C:LEU114	4,8	
	:UNK0:C - C:PRO111	4,1	
	:UNK0:C - C:LEU114	3,6	
	• **π-Alkyl**		
	C:PHE112 - :UNK0:C	4,9	
	C:PHE117 - :UNK0	4,7	
	C:PHE117 - :UNK0:C	4,4	
	C:PHE117 - :UNK0:C	4,3	
Borneol (SU10)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:ARG74:N - :UNK0:O	2,9	
	:UNK0:H - C:ARG74:O	1,9	**Arg74,** ile130, **tyr75**
	Ikatan Hidrofobik		
	• **Alkyl**		
	:UNK0:C - C:ILE130	4,7	

	:UNK0:C - C:ILE130	4,3	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,7	
Cadiyenol (SU11)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:TYR14:N - :UNK0:O	2,8	
	C:TYR14:N - :UNK0:O	2,8	
	C:THR77:OG1 - :UNK0:O	3,2	
	:UNK0:H - C:ASP215:OD1	2,1	Ala115, **ala218, asp215,** leu114, pro111, thr77, **thr216, tyr14**
	• **Carbon H-Bond**		
	:UNK0:C - C:THR216:O	3,1	
	:UNK0:C - C:ALA218:O	3,3	
	:UNK0:C - C:THR77:OG1	3,3	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:ALA115 - :UNK0:C	4,5	
	:UNK0:C - C:PRO111	5,4	
	:UNK0:C - C:LEU114	4,8	
Campesterol (SU12)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:THR295:OG1	1,8	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	:UNK0:C - C:TYR75	3,6	**Ala218, ile291,** phe112, **phe117,** pro111, thr295, **tyr75, val120**
	• **Alkyl**		
	C:ALA218 - :UNK0	4,3	
	C:ILE291 - :UNK0	4,7	
	:UNK0:C - C:PRO111	4,7	
	:UNK0:C - C:VAL120	4,2	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	5,4	
	C:TYR75 - :UNK0:C	4,5	
	C:PHE112 - :UNK0:C	4,7	
	C:PHE112 - :UNK0:C	4,5	
	C:PHE117 - :UNK0:C	4,7	
Carveol (SU13)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER36:N - :UNK0:O	2,9	
	:UNK0:H - C:ASN37:OD1	1,8	
	Ikatan Hidrofobik		Asn37, **arg74,** ile130, leu73, **tyr75,** ser36
	• **Alkyl**		
	:UNK0 - C:LEU73	3,9	
	:UNK0 - C:ILE130	4,6	
	:UNK0:C - C:LEU73	4,1	
	:UNK0:C - C:ARG74	4,5	
	:UNK0:C - C:ILE130	4,7	

	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,1	
	C:TYR75 - :UNK0:C	4,5	
Caryophyllene Epoxide (SU14)	**Ikatan Hidrofobik**		
	• **π-Sigma**		
	:UNK0:C - C:TYR75	3,8	
	:UNK0:C - C:TYR75	3,4	
	• **Alkyl**		
	C:ALA218 - :UNK0:C	4,3	
	:UNK0:C - C:VAL120	4,1	**Ala218,** phe112, pro111, trp39, **tyr75, val120**
	:UNK0:C - C:PRO111	4,9	
	• **π-Alkyl**		
	C:TRP39 - :UNK0:C	5,3	
	C:TRP39 - :UNK0:C	5,5	
	C:TYR75 - :UNK0	4,8	
	C:TYR75 - :UNK0:C	4,9	
	C:TYR75 - :UNK0:C	4,6	
	C:PHE112 - :UNK0:C	5,3	
	C:PHE112 - :UNK0:C	5,0	
Castillicetin (SU15)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,0	
	:UNK0:H - C:ASP32:OD2	1,8	
	:UNK0:H - C:GLY34:O	2,7	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - C:TYR155:OH	2,9	
	:UNK0:H - C:THR216:O	2,3	
	:UNK0:H - :UNK0:O	1,7	
	:UNK0:H - C:GLN13:OE1	2,5	**Asp32, asp215,** gln13, **gly34,** leu114, **thr216, tyr14, tyr75,** tyr155, ser219, **val30**
	:UNK0:H - C:LEU114:O	2,2	
	Electrostatic		
	• **π-Anion**		
	C:ASP215:OD1 - :UNK0	4,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	3,9	
	• **π-π T-shaped**		
	C:TYR75 - :UNK0	3,3	
	• **π-Alkyl**		
	:UNK0 - C:VAL30	4,5	
Castilliferol (SU16)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		**Ala218, asp215,** gln13, **gly217,** leu114, **phe117, thr216, tyr14, tyr75,** tyr155, **val30**
	:UNK0:H - C:TYR155:OH	2,2	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - :UNK0:O	1,7	
	:UNK0:H - C:GLN13:OE1	2,5	
	:UNK0:H - C:LEU114:O	2,8	
	• **Carbon H-Bond**		

	C:TYR14:N - :UNK0	3,8	
	Electrostatic		
	• **π-Anion**		
	C:ASP215:OD1 - :UNK0	4,3	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	4,0	
	C:TYR75:CB - :UNK0	3,8	
	• **π-π T-shaped**		
	C:PHE117 - :UNK0	4,4	
	• **Amide-π Stacked**		
	C:GLY217:C,O;ALA218:N - :UNK0	3,7	
	• **π-Alkyl**		
	:UNK0 - C:VAL30	4,6	
Catechin (SU17)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	2,9	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - C:TYR155:OH	2,4	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - C:GLY217:O	1,8	
	:UNK0:H - C:PRO111:O	2,0	
	• **Carbon H-Bond**		Ala115, **ala218,** gln13, **gly217,** pro111, ser219, **thr216, tyr14,** tyr155, **val30**
	:UNK0:C - C:SER219:OG	3,0	
	• **π-Donor H-Bond**		
	C:TYR14:N - :UNK0	3,8	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	3,8	
	• **Amide-π Stacked**		
	C:GLY217:C,O;ALA218:N - :UNK0	3,8	
	• **π-Alkyl**		
	:UNK0 - C:PRO111	5,2	
	:UNK0 - C:ALA115	5,2	
	:UNK0 - C:VAL30	4,5	
Cenetellicin (SU18)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER36:N - :UNK0:O	3,0	Asn37, gln128, ser36, **ser76**
	:UNK0:H - C:ASN37:OD1	2,1	
	:UNK0:H - C:GLN128:O	1,8	
	:UNK0:H - C:SER76:OG	2,1	
Centellasapogenol A (SU19)	**Ikatan Hidrogen**		Gln13, Leu114, **phe117,** pro111, thr77, **tyr75,** tyr220
	• **Conventional H-Bond**		
	:UNK0:H - C:LEU114:O	2,1	
	:UNK0:H - C:TYR220:OH	2,2	
	:UNK0:H - C:THR77:OG1	1,7	
	• **Carbon H-Bond**		

	:UNK0:C - C:GLN13:OE1	2,7	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:PRO111 - :UNK0	5,4	
	C:PRO111 - :UNK0	5,2	
	:UNK0:C - C:PRO111	3,7	
	:UNK0:C - C:LEU114	4,2	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,7	
	C:PHE117 - :UNK0:C	4,4	
Centellasaponin A (SU20)	**Ikatan Hidrogen**		**Arg74. Asp215, gly217, ile291,** leu114, **phe117,** pro111, pro292, **ser76, tyr75**
	• **Conventional H-Bond**		
	:UNK0:H - C:GLY217:O	2,1	
	:UNK0:H - :UNK0:O	1,6	
	:UNK0:H - :UNK0:O	1,8	
	:UNK0:H - C:ARG74:O	1,8	
	:UNK0:H - :UNK0:O	2,1	
	• **Carbon H-Bond**		
	:UNK0:C - C:SER76:OG	3,2	
	:UNK0:C - C:ASP215:OD1	2,8	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	:UNK0:C - C:TYR75	3,6	
	• **Alkyl**		
	C:PRO111 - :UNK0	5,3	
	C:PRO111 - :UNK0	4,5	
	C:LEU114 - :UNK0	5,5	
	:UNK0:C - C:PRO111	4,7	
	:UNK0:C - C:LEU114	3,4	
	:UNK0:C - C:PRO111	5,0	
	:UNK0:C - C:LEU114	4,7	
	:UNK0:C - C:ILE291	4,3	
	:UNK0:C - C:PRO292	5,0	
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	4,5	
	C:PHE117 - :UNK0:C	4,5	
Centellasaponin B (SU21)	**Ikatan Hidrogen**		**Arg74, asp32, asp215, gly34,** leu114, phe112, **phe117,** pro111, **ser76, ser35,** thr77, **tyr75,** tyr220, **val30, val120**
	• **Conventional H-Bond**		
	C:SER76:N - :UNK0:O	2,8	
	C:SER76:OG - :UNK0:O	2.6	
	C:THR77:OG1 - :UNK0:O	3,0	
	:UNK0:H - C:GLY34:O	2,8	
	:UNK0:H - :UNK0:O	1,7	
	:UNK0:H - C:ARG74:O	1,9	
	:UNK0:H - C:ARG74:O	2,2	
	:UNK0:H - C:ASP215:OD1	1,8	
	:UNK0:H - C:THR77:OG1	2,2	
	:UNK0:H - C:TYR220:OH	1,9	

	• **Carbon H-Bond**		
	C:GLY34:CA - :UNK0:O	3,7	
	C:SER35:CB - :UNK0:O	3,2	
	:UNK0:C - C:ASP32:OD2	3,1	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:PRO111 - :UNK0	5,2	
	C:VAL120 - :UNK0	4,7	
	:UNK0:C - C:PRO111	4,4	
	:UNK0:C - C:PRO111	4,5	
	:UNK0:C - C:LEU114	4,8	
	:UNK0:C - C:VAL30	3,1	
	:UNK0:C - C:VAL120	3,8	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,8	
	C:PHE112 - :UNK0:C	4,2	
	C:PHE117 - :UNK0	5,2	
	C:PHE117 - :UNK0:C	5,1	
	C:PHE117 - :UNK0:C	4,5	
Centellin (SU22)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	2,9	
	:UNK0:H - C:TYR14:O	2,2	**Ala218,** phe112, ser219, **tyr14, tyr 75**
	• **Carbon H-Bond**		
	C:ALA218:CA - :UNK0:O	3,1	
	Ikatan Hidrofobik		
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	4,4	
	C:PHE112 - :UNK0:C	4,9	
Centelloside E (SU23)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:ARG74:N - :UNK0:O	3,1	
	C:SER76:OG - :UNK0:O	3,3	
	C:THR77:N - :UNK0:O	3,0	
	C:THR77:OG1 - :UNK0:O	2,5	
	C:SER219:OG - :UNK0:O	3,4	**Arg74, asp215,** gln13, **gly34,** ile130, leu114, met289, **phe117,** pro111, **ser76,** ser219, thr77, **tyr75,** tyr220, **val30, val120**
	C:TYR220:OH - :UNK0:O	3,0	
	:UNK0:H - C:GLN13:OE1	2,6	
	:UNK0:H - C:LEU114:O	2,2	
	:UNK0:H - :UNK0:O	1,8	
	:UNK0:H - C:ARG74:O	2,2	
	:UNK0:H - C:ARG74:O	2,2	
	:UNK0:H - C:ASP215:OD1	2,1	
	• **Carbon H-Bond**		
	:UNK0:C - C:SER76:OG	3,3	
	:UNK0:C - C:GLY34:O	3,3	
	:UNK0:C - C:ARG74:O	2,6	

	Ikatan Lain		
	• **Sulfur-x**		
	C:MET289:SD - :UNK0:O	3,2	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:PRO111 - :UNK0	4,5	
	C:PRO111 - :UNK0	5,0	
	C:VAL120 - :UNK0	5,5	
	:UNK0:C - C:PRO111	4,1	
	:UNK0:C - C:LEU114	4,0	
	:UNK0:C - C:VAL30	4,1	
	:UNK0:C - C:VAL30	3,8	
	:UNK0:C - C:VAL120	3,7	
	:UNK0:C - C:ILE130	4,7	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,8	
	C:PHE117 - :UNK0:C	4,1	
	C:PHE117 - :UNK0:C	4,9	
Chlorogenic acid (SU24)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:THR77:OG1 - :UNK0:O	3,0	
	C:THR77:OG1 - :UNK0:O	3,2	
	:UNK0:H - C:SER76:OG	1,9	
	:UNK0:H - C:SER76:OG	1,9	
	:UNK0:H - C:GLY217:O	2,1	**Asp215,**
	:UNK0:H - C:SER219:OG	2,2	**gly217, ser76,**
	• **Carbon H-Bond**		ser219, thr77
	:UNK0:C - C:GLY217:O	2,9	
	Electrostatic		
	• **π-Anion**		
	C:ASP215:OD1 - :UNK0	4,6	
Corosolic Acid (SU25)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:OG - :UNK0:O	2,8	
	:UNK0:H - C:TYR220:OH	2,3	
	:UNK0:H - C:ASP32:OD2	2,0	
	:UNK0:H - C:ASP32:OD2	2,7	**Asp32,** his287,
	• **Carbon H-Bond**		met289,
	C:THR12:CB - :UNK0:O	3,3	phe112,
	Ikatan Lain		**phe117,**
	• **π-Lone Pair**		ser219, thr12,
	:UNK0:O - C:TYR75	2,9	**tyr75,** tyr220,
	Ikatan Hidrofobik		**val30, val120**
	• **π-Sigma**		
	:UNK0:C - C:TYR75	4,0	

	• **Alkyl**		
	:UNK0:C - C:VAL30	4,1	
	:UNK0:C - C:VAL120	3,9	
	:UNK0:C - C:MET289	5,2	
	• **π-Alkyl**		
	C:PHE112 - :UNK0:C	4,3	
	C:PHE117 - :UNK0	5,1	
	C:PHE117 - :UNK0:C	5,0	
	C:PHE117 - :UNK0:C	4,4	
	C:PHE117 - :UNK0:C	4,4	
	C:TYR220 - :UNK0	4,6	
	C:TYR220 - :UNK0:C	5,2	
	C:TYR220 - :UNK0:C	5,0	
	C:HIS287 - :UNK0	5,0	
	C:HIS287 - :UNK0:C	3,6	
Galanolactone (SU26)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,0	
	C:SER219:OG - :UNK0:O	3,3	
	Ikatan Hidrofobik		Ala303,
	• **Alkyl**		Phe112,
	C:ALA303 - :UNK0	4,4	**Phe117,**
	:UNK0:C - C:PRO111	4,0	Pro111,
	:UNK0:C - C:PRO111	5,0	Ser219, ,
	• **π-Alkyl**		**Tyr75, Tyr14**
	C:TYR75 - :UNK0:C	5,2	
	C:PHE112 - :UNK0:C	4,1	
	C:PHE117 - :UNK0	4,9	
	C:PHE117 - :UNK0:C	4,4	
	C:PHE117 - :UNK0:C	5,3	
Geranyl Acetate (SU27)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:TYR220:N - :UNK0:O	3,1	
	Ikatan Hidrofobik		Ala303,
	• **Alkyl**		**Tyr14,**
	C:ALA303 - :UNK0:C	3,6	Tyr155,
	:UNK0:C - C:VAL30	4,2	Tyr220, **Val30**
	• **π-Alkyl**		
	C:TYR14 - :UNK0:C	4,7	
	C:TYR155 - :UNK0:C	4,9	
	C:TYR155 - :UNK0:C	5,1	
Ginsenoside MC (SU28)	**Ikatan Hidrogen**		**Ala218,**
	• **Conventional H-Bond**		**Asp32,** gln13,
	C:SER76:OG - :UNK0:O	2,7	gln128,
	C:THR77:OG1 - :UNK0:O	3,3	**leu213,**
	C:SER219:N - :UNK0:O	3,0	met289,
	C:SER219:OG - :UNK0:O	2,9	phe112,
	C:TYR220:N - :UNK0:O	3,2	pro111**, ser76,**

	:UNK0:H - :UNK0:O	1,7	ser219, thr12, thr77, tyr75, tyr220
	:UNK0:H - C:TYR220:OH	2,1	
	:UNK0:H - C:SER219:OG	2,2	
	:UNK0:H - :UNK0:O	2,2	
	:UNK0:H - C:GLN128:O	2,0	
	:UNK0:H - C:ASP32:OD2	1,7	
	• **Carbon H-Bond**		
	C:THR12:CB - :UNK0:O	3,1	
	:UNK0:C - C:GLN13:OE1	3,0	
	Ikatan Lain		
	• **Sulfur-x**		
	C:MET289:SD - :UNK0:O	2,7	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:ALA218 - :UNK0:C	3,6	
	:UNK0:C - C:LEU213	4,6	
	:UNK0:C - C:PRO111	4,8	
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	5,1	
	C:TYR75 - :UNK0:C	4,3	
	C:PHE112 - :UNK0:C	5,3	
Isoquerc7trin (SU29)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:THR77:OG1 - :UNK0:O	3,0	Gln13, leu114, **phe117,** pro111, thr77, **tyr14, tyr75, val30**
	:UNK0:H - C:GLN13:OE1	2,5	
	:UNK0:H - C:LEU114:O	2,2	
	:UNK0:H - C:GLN13:OE1	2,3	
	:UNK0:H - C:TYR14:O	2,1	
	:UNK0:H - C:THR77:OG1	2,4	
	:UNK0:H - :UNK0:O	2,1	
	• **Carbon H-Bond**		
	:UNK0:C - C:PRO111:O	3,0	
	Ikatan Hidrofobik		
	• **π-π Stacked**		
	C:PHE117 - :UNK0	5,8	
	• **π-π T-shaped**		
	C:TYR75 - :UNK0	4,9	
	• **π-Alkyl**		
	:UNK0 - C:VAL30	4,6	
Isothankunic Acid (SU30)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		Leu114, **phe117**, pro111, ser219, **tyr75, val30**
	C:SER219:OG - :UNK0:O	3,2	
	:UNK0:H - C:PRO111:O	2,1	
	:UNK0:H - :UNK0:O	1,8	

	Ikatan Hidrofobik		
	• **Alkyl**		
	:UNK0:C - C:VAL30	3,9	
	:UNK0:C - C:PRO111	4,8	
	:UNK0:C - C:LEU114	4,5	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,9	
	C:TYR75 - :UNK0:C	5,2	
	C:PHE117 - :UNK0	5,1	
	C:PHE117 - :UNK0:C	4,1	
Kaempferol (SU31)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,0	
	:UNK0:H - C:TYR155:OH	2,5	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - C:GLY217:O	2,0	
	:UNK0:H - :UNK0:O	1,7	
	:UNK0:H - C:PRO111:O	2,0	Ala115, **ala218,** gln13, **gly217,** pro111, ser219, **thr216, tyr14,** tyr155, **val30**
	• **π-Donor H-Bond**		
	C:TYR14:N - :UNK0	4,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	4,0	
	• **Amide-π Stacked**		
	C:GLY217:C,O;ALA218:N - :UNK0	5,1	
	• **π-Alkyl**		
	:UNK0 - C:PRO111	5,1	
	:UNK0 - C:ALA115	5,4	
	:UNK0 - C:VAL30	4,6	
Kaempferol-7-rhamnoside (SU32)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER76:N - :UNK0:O	3,0	
	C:SER76:OG - :UNK0:O	2,7	
	C:SER219:N - :UNK0:O	2,9	
	:UNK0:H - C:GLY34:O	2,0	
	:UNK0:H - C:ASP215:OD1	2,2	
	:UNK0:H - :UNK0:O	2,2	Ala115, **Ala218, asp32, asp215, gly34,** met289, **phe117,** pro111, **ser76,** ser219,
	:UNK0:H - C:ASP32:OD2	1,9	
	:UNK0:H - :UNK0:O	1,8	
	:UNK0:H - C:PRO111:O	2,1	
	:UNK0:H - C:SER219:OG	1,9	
	Ikatan Hidrofobik		
	• **π-π T-shaped**		
	C:PHE117 - :UNK0	5,4	
	• **π-Alkyl**		
	:UNK0 - C:ALA218	5,2	
	:UNK0 - C:ALA218	4,4	
	:UNK0 - C:MET289	5,4	

	:UNK0 - C:PRO111	4,6	
	:UNK0 - C:ALA115	5,3	
Linalool (SU33)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:THR12:O	2,1	
	:UNK0:H - C:SER219:OG	2,1	
	Ikatan Hidrofobik		Ala303, ser219, thr12, **tyr14,** tyr155, **val30**
	• **Alkyl**		
	C:ALA303 - :UNK0:C	3,7	
	:UNK0:C - C:VAL30	4,0	
	• **π-Alkyl**		
	C:TYR14 - :UNK0:C	4,9	
	C:TYR155 - :UNK0:C	4,8	
	C:TYR155 - :UNK0:C	5,1	
Luteolin (SU34)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:TYR155:OH	2,3	
	:UNK0:H - C:THR216:O	2,3	
	:UNK0:H - C:THR216:O	2,2	
	:UNK0:H - :UNK0:O	1,9	
	:UNK0:H - C:GLN13:OE1	2,4	
	:UNK0:H - C:LEU114:O	2,2	Ala115, **ala218,** gln13, **gly217,** leu114 **phe117, thr216, tyr14,** tyr155, **val30**
	• **Carbon H-Bond**		
	C:TYR14:N - :UNK0	4,0	
	Ikatan Hidrofobik		
	• **π-π T-shaped**		
	C:PHE117 - :UNK0	4,5	
	C:PHE117 - :UNK0	4,7	
	• **Amide-π Stacked**		
	C:GLY217:C,O;ALA218:N - :UNK0	3,6	
	• **π-Alkyl**		
	:UNK0 - C:ALA115	4,7	
	:UNK0 - C:VAL30	4,8	
Madasiatic Acid (SU35)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:THR77:OG1	2,0	
	:UNK0:H - C:TYR220:OH	2,7	
	:UNK0:H - C:GLN13:OE1	2,0	
	:UNK0:H - C:LEU114:O	2,8	
	:UNK0:H - C:GLN13:OE1	2,1	**Ala218,** gln13, leu114, pro111, thr77, **tyr 75,** tyr 220
	:UNK0:H - C:LEU114:O	1,9	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:ALA218 - :UNK0	3,9	
	C:ALA218 - :UNK0:C	4,2	
	C:ALA218 - :UNK0	5,2	
	:UNK0:C - C:PRO111	4,4	

	:UNK0:C - C:LEU114	5,0	
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	3,9	
Madecassic Acid (SU36)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:THR12:OG1 - :UNK0:O	3,0	
	:UNK0:H - C:GLN13:OE1	2,1	
	:UNK0:H - C:TYR220:OH	2,2	
	:UNK0:H - C:GLN13:OE1	1,7	
	:UNK0:H - C:TYR220:OH	2,0	
	Ikatan Hidrofobik		gln13, leu114, **phe117,**
	• **Alkyl**		pro111, thr12, **tyr75,** tyr220, **val30**
	C:VAL30 - :UNK0	5,2	
	C:PRO111 - :UNK0	5,0	
	:UNK0:C - C:PRO111	5,0	
	:UNK0:C - C:PRO111		
	:UNK0:C - C:LEU114	4,4	
	• **π-Alkyl**	4,1	
	C:TYR75 - :UNK0		
	C:TYR75 - :UNK0:C	4,0	
	C:PHE117 - :UNK0	4,5	
	C:PHE117 - :UNK0:C	5,0	
		4,6	
Madecassoside (SU37)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER76:N - :UNK0:O	2,8	
	C:SER76:OG - :UNK0:O	3,3	
	C:THR77:N - :UNK0:O	2,8	
	C:THR77:OG1 - :UNK0:O	2,3	
	:UNK0:H - C:PRO111:O	2,1	
	:UNK0:H - C:ASP215:OD1	2,1	
	:UNK0:H - C:THR295:OG1	2,2	**Arg74, asp215,**
	:UNK0:H - C:GLN128:O	2,1	gln128, **gly34,**
	:UNK0:H - C:ASP215:OD1	1,7	ile130, phe112, **phe117,**
	• **Carbon H-Bond**		pro111, **ser76,**
	C:GLY34:CA - :UNK0:O	3,4	ser219, thr77, thr29, trp39,
	:UNK0:C - C:SER219:OG	3,8	**tyr75, val30, val120**
	:UNK0:C - C:THR295:OG1	3,0	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:VAL120 - :UNK0	5,2	
	:UNK0:C - C:VAL30	4,3	
	:UNK0:C - C:VAL120	4,1	
	:UNK0:C - C:ILE130	5,3	
	• **π-Alkyl**		
	C:TRP39 - :UNK0:C	5,3	
	C:TRP39 - :UNK0:C	5,0	
	C:TYR75 - :UNK0	3,8	

	C:TYR75 - :UNK0:C	4,1	
	C:PHE112 - :UNK0:C	4,1	
	C:PHE112 - :UNK0:C	4,7	
	C:PHE117 - :UNK0	5,0	
	C:PHE117 - :UNK0:C	3,9	
	C:PHE117 - :UNK0:C	4,6	
Methyl Asiatate (SU38)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:OG - :UNK0:O	2,8	
	:UNK0:H - C:TYR220:OH	2,1	
	:UNK0:H - C:TYR220:OH	2,2	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	:UNK0:C - C:TYR75	4,0	Ala115, leu114, **phe117,** pro111, ser219, **tyr75,** tyr220, **val30**
	• **Alkyl**		
	C:VAL30 - :UNK0	5,2	
	C:PRO111 - :UNK0	5,2	
	C:ALA115 - :UNK0:C	4,5	
	:UNK0:C - C:PRO111	4,8	
	:UNK0:C - C:LEU114	4,7	
	:UNK0:C - C:LEU114	4,7	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	5,1	
	C:PHE117 - :UNK0	5,0	
	C:PHE117 - :UNK0:C	4,5	
Myricetin (SU39)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,0	
	:UNK0:H - C:THR216:O	2,0	
	:UNK0:H - C:TYR14:O	1,8	
	:UNK0:H - C:TYR14:O	1,8	
	:UNK0:H - C:GLY217:O	2,1	Gln13, **gly217,** pro111, ser219, **thr216, tyr14, val30**
	:UNK0:H - :UNK0:O	1,7	
	:UNK0:H - C:PRO111:O	2,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	3,9	
	• **π-Alkyl**		
	:UNK0 - C:PRO111	5,1	
	:UNK0 - C:VAL30	4,5	
Naringin (SU40)	**Ikatan Hidrogen**		**Ala218,** ala300, **asp215,** gln13, **ile291,** leu114, Met289, **phe117,** pro111, **ser76,**
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,3	
	C:TYR220:N - :UNK0:O	3,0	
	:UNK0:H - :UNK0:O	1,9	
	:UNK0:H - C:THR77:OG1	1,8	
	:UNK0:H - C:GLN13:OE1	1,8	

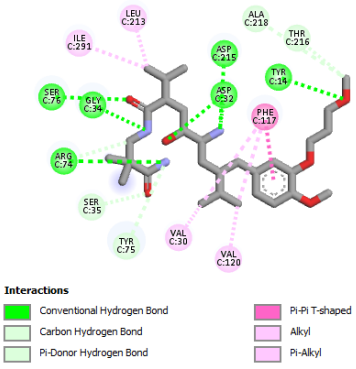
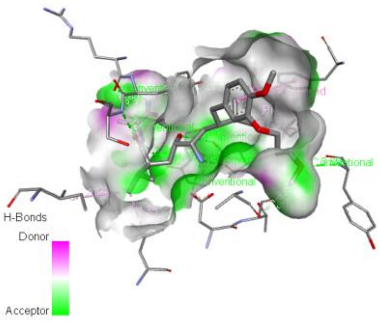
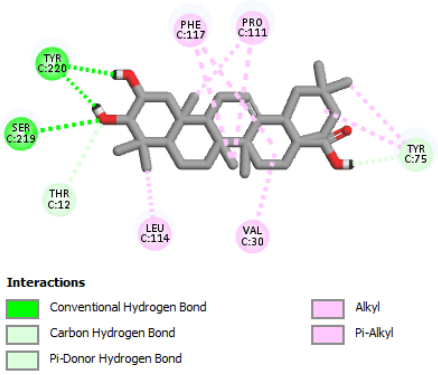
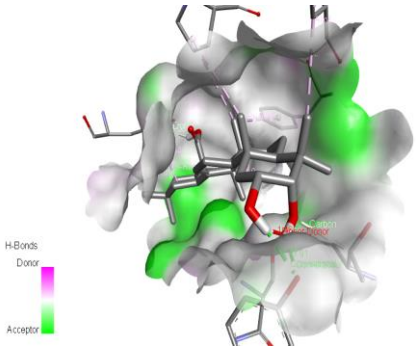
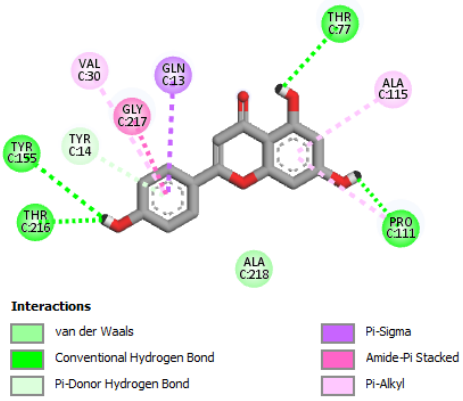
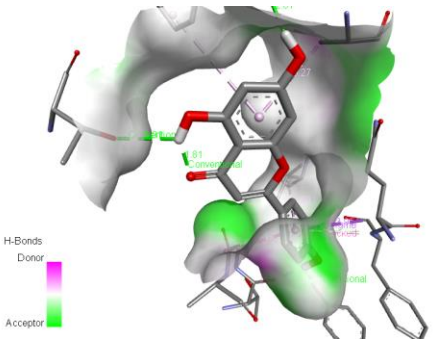
	:UNK0:H - C:PRO111:O	2,3	ser219, thr77, tyr220, **val120**
	:UNK0:H - C:GLN13:OE1	2,2	
	:UNK0:H - C:LEU114:O	2,4	
	• **Carbon H-Bond**		
	C:SER76:OG - :UNK0	3,6	
	Elektrostatik		
	• **π-Anion**		
	C:ASP215:OD1 - :UNK0	3,3	
	Ikatan Hidrofobik		
	• **Alkyl**		
	:UNK0:C - C:VAL120	4,1	
	• **π-Alkyl**		
	C:PHE117 - :UNK0:C	4,7	
	:UNK0 - C:ALA218	4,9	
	:UNK0 - C:ALA218		
	:UNK0 - C:MET289	5,3	
	:UNK0 - C:ILE291	5,0	
	:UNK0 - C:ALA300	5,0	
		4,4	
Patuletin (SU41)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:THR216:O	2,1	Ala115, gln13, pro111, ser219, **thr216, tyr14,** tyr115, **val30**
	:UNK0:H - C:TYR155:OH	2,7	
	:UNK0:H - C:THR216:O	2,1	
	:UNK0:H - C:SER219:OG	2,4	
	:UNK0:H - C:PRO111:O	2,1	
	• **π-Donor H-Bond**		
	C:TYR14:N - :UNK0	4,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	3,9	
	• **π-Alkyl**		
	:UNK0 - C:PRO111	5,3	
	:UNK0 - C:ALA115	5,5	
	:UNK0 - C:VAL30	4,4	
Pomolic Acid (SU42)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:OG - :UNK0:O	2,5	Gln13, leu114, phe112, **phe117,** pro111, ser219, **tyr75,** tyr220, **val30, val120**
	:UNK0:H - C:TYR220:OH	2,0	
	:UNK0:H - C:GLN13:OE1	2,2	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:PRO111 - :UNK0	5,0	
	:UNK0:C - C:PRO111	4,6	
	:UNK0:C - C:VAL30	3,8	
	:UNK0:C - C:VAL120	3,6	

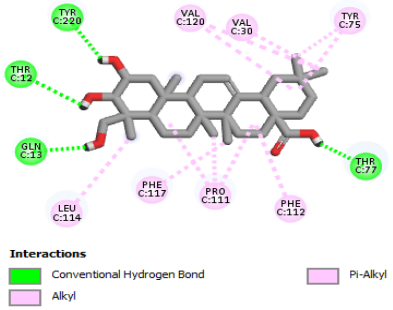
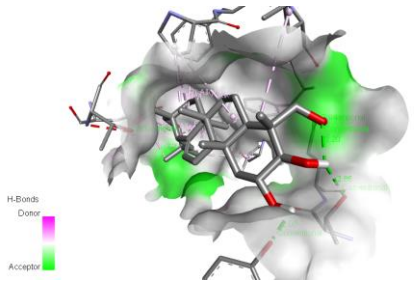
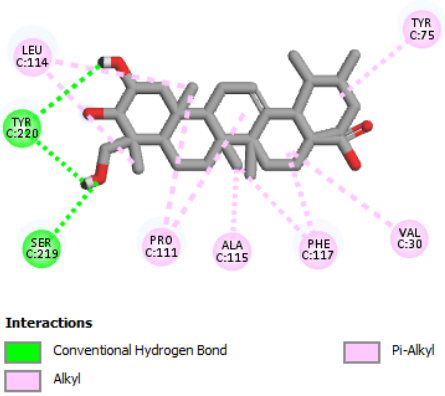
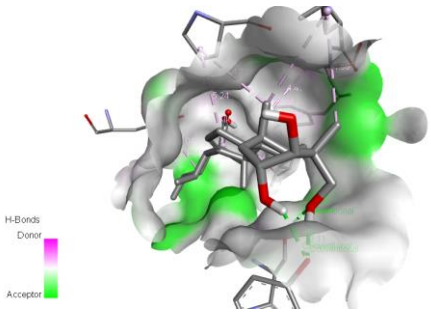
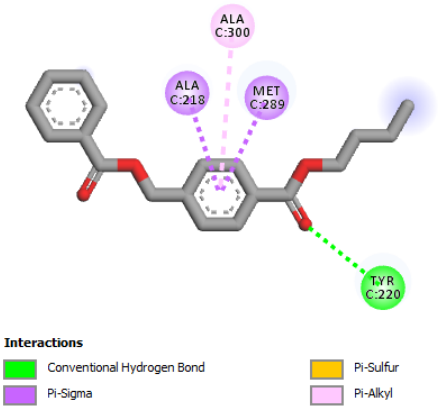
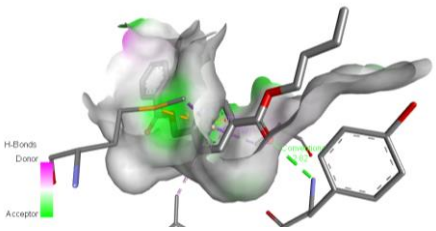
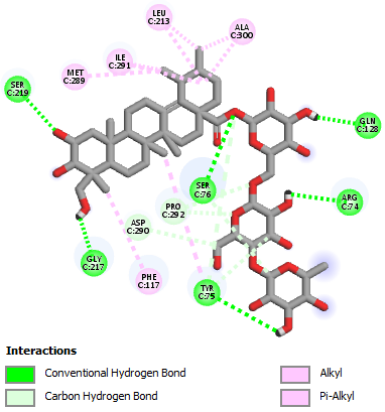
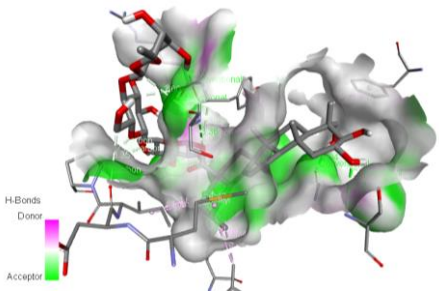
	:UNK0:C - C:LEU114	3,2	
	• **π-Alkyl**		
	C:TYR75 - :UNK0:C	4,3	
	C:PHE112 - :UNK0:C	4,4	
	C:PHE117 - :UNK0	5,0	
	C:PHE117 - :UNK0:C	4,4	
	C:PHE117 - :UNK0:C	4,5	
Quercetin (SU43)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER219:N - :UNK0:O	3,0	
	:UNK0:H - C:THR216:O	2,1	
	:UNK0:H - C:TYR155:OH	2,5	
	:UNK0:H - C:THR216:O	2,1	
	:UNK0:H - C:GLY217:O	1,9	
	:UNK0:H - :UNK0:O	1,7	**Gly217,** gln13,
	:UNK0:H - C:PRO111:O	2,0	pro111, ser219,
	• **π-Donor H-Bond**		**thr216, tyr14,**
	C:TYR14:N - :UNK0	4,0	tyr155, **val30**
	Ikatan Hidrofobik		
	• **π-Sigma**		
	C:GLN13:CA - :UNK0	4,0	
	• **π-Alkyl**		
	:UNK0 – C:PRO111	5,3	
	:UNK0 – C:VAL30	4,3	
Rutin (SU44)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	C:SER76:N - :UNK0:O	3,1	
	:UNK0:H - C:TYR220:O	2,7	
	:UNK0:H - C:SER219:OG	2,1	
	:UNK0:H - :UNK0:O	2,0	
	:UNK0:H - C:ASP32:OD2	2,2	
	:UNK0:H - C:SER219:OG	1,8	
	:UNK0:H - C:SER219:OG	2,0	
	:UNK0:H - C:ASP32:OD2	1,8	**ala218,** ala300,
	:UNK0:H - C:SER35:OG	3,0	**asp32, asp215,**
	• **Carbon H-Bond**		**gly217, ile291,**
	:UNK0:C - C:GLY217:O	3,8	**leu213,**
	• **π-Donor H-Bond**		met289,
	C:SER76:OG - :UNK0	2,9	**phe117, ser35,**
	C:SER76:OG - :UNK0	3,8	**ser76,** ser219,
			tyr220, **val30**
	Electrostatic		
	• **π-Anion**		
	C:ASP215:OD1 - :UNK0		
	C:ASP215:OD1 - :UNK0	3,3	
		4,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		

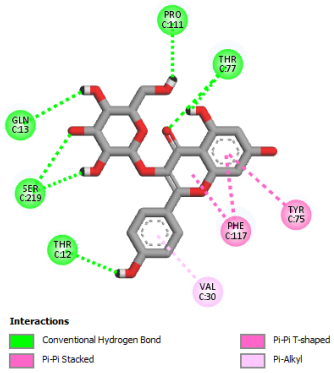
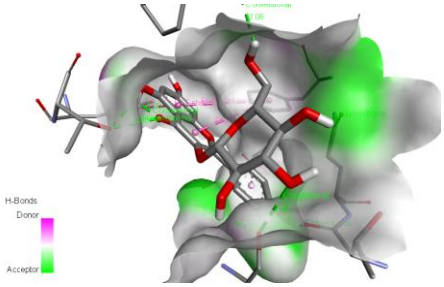
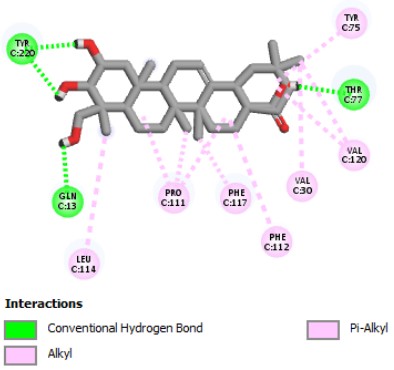
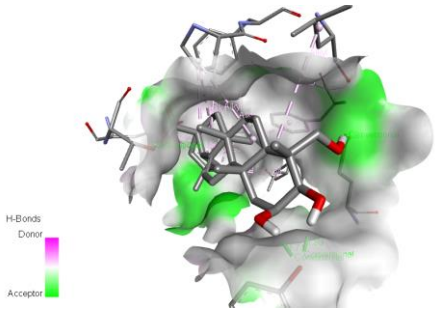
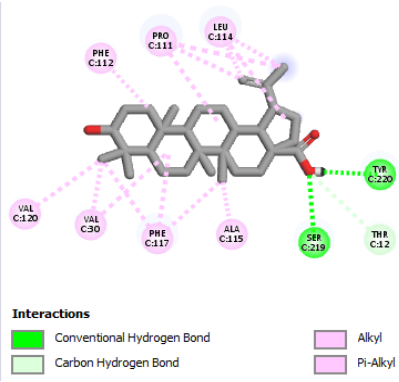
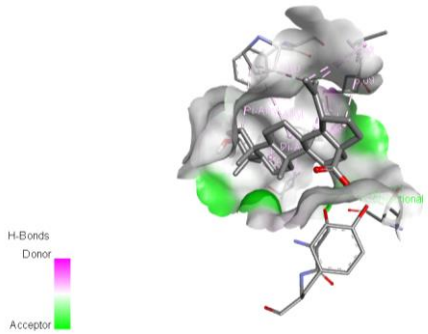
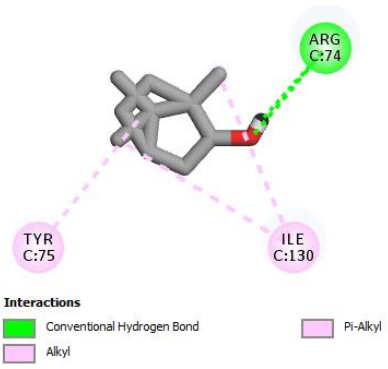
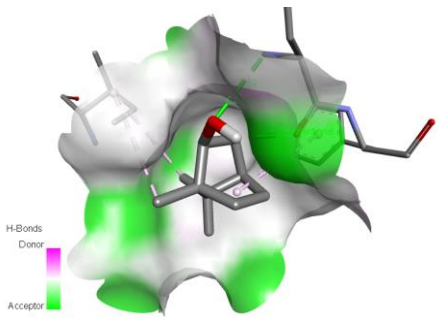
	C:ALA218:CB - :UNK0		
	C:MET289:CE - :UNK0	3,6	
	• **Alkyl**	3,7	
	:UNK0:C - C:VAL30		
	• **π-Alkyl**	4,0	
	C:PHE117 - :UNK0:C		
	:UNK0 - C:ALA218	4,9	
	:UNK0 - C:MET289	5,2	
	:UNK0 - C:LEU213	5,3	
	:UNK0 - C:ILE291	5,4	
	:UNK0 - C:ALA300	4,4	
		5,1	
Stigmasterol (SU45)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:GLN128:OE1	2,8	
	:UNK0:H - C:THR295:OG1	2,0	
	Ikatan Hidrofobik		
	• **π-Sigma**		
	:UNK0:C - C:TYR75	3,7	
	• **Alkyl**		**Ala218,**
	C:ALA218 - :UNK0	4,4	gln128, **ile291,**
	C:ILE291 - :UNK0	4,5	phe112,
	:UNK0:C - C:VAL120	4,2	**phe117,**
	:UNK0:C - C:VAL120	3,8	pro111, thr295,
	:UNK0:C - C:PRO111	4,6	trp29, **tyr75,**
	• **π-Alkyl**		**val120**
	C:TRP39 - :UNK0:C	5,2	
	C:TRP39 - :UNK0:C	5,1	
	C:TYR75 - :UNK0	5,5	
	C:TYR75 - :UNK0:C	4,3	
	C:TYR75 - :UNK0:C	4,8	
	C:PHE112 - :UNK0:C	4,7	
	C:PHE112 - :UNK0:C	5,0	
	C:PHE117 - :UNK0:C	5,4	
Terminolic Acid (SU46)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:GLN13:OE1	1,8	
	:UNK0:H - C:LEU114:O	2,9	
	:UNK0:H - C:THR12:OG1	2,7	Gln13, leu114,
	:UNK0:H - :UNK0:O	2,2	phe112,
	:UNK0:H - C:TYR220:OH	2,1	**phe117,**
	:UNK0:H - C:THR77:OG1	1,7	pro111, thr12,
			thr12, **tyr75,**
	Ikatan Hidrofobik		tyr220, **val30,**
	• **Alkyl**		**val120**
	C:PRO111 - :UNK0	4,8	
	:UNK0:C - C:PRO111	3,6	
	:UNK0:C - C:LEU114	4,7	
	:UNK0:C - C:VAL30	4,6	

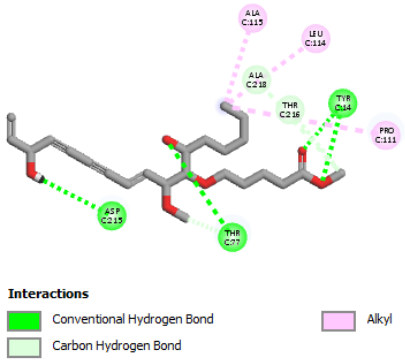
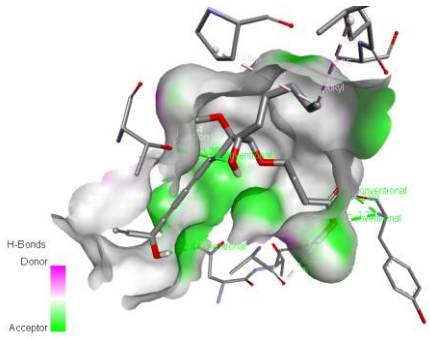
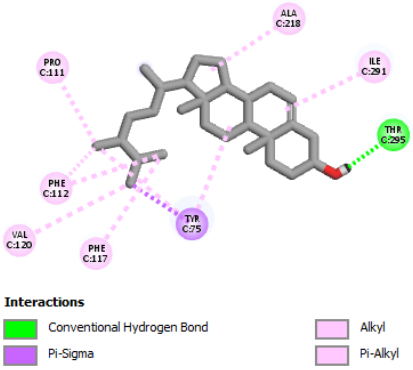
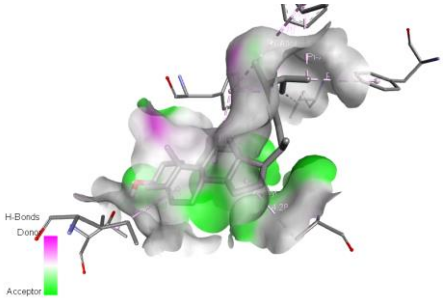
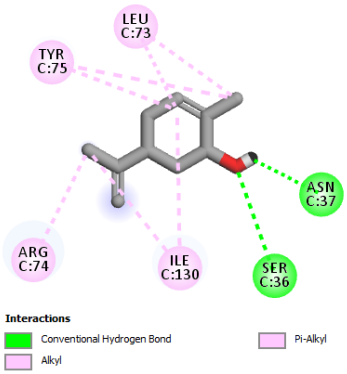
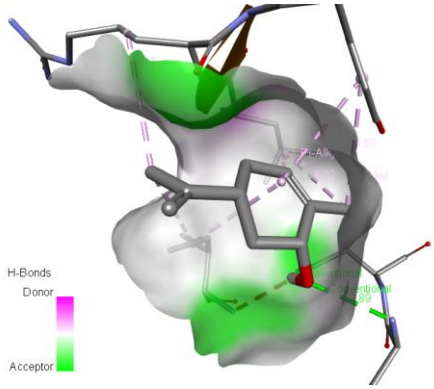
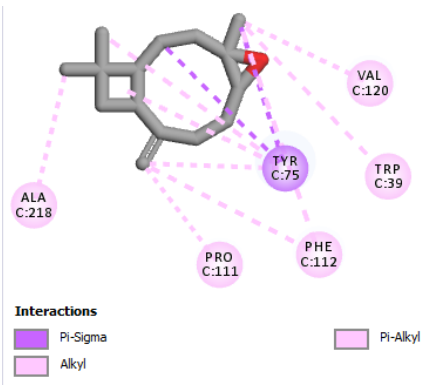
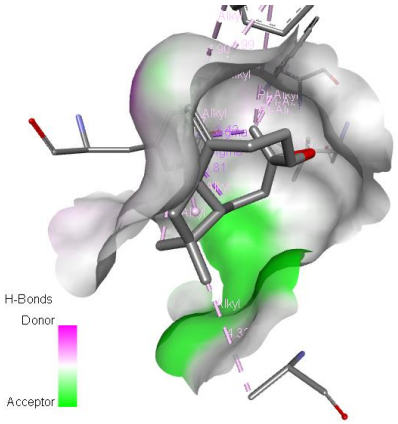
	:UNK0:C - C:VAL120	4,2	
	• **π-Alkyl**		
	C:TYR75 - :UNK0	4,3	
	C:PHE112 - :UNK0	5,0	
	C:PHE117 - :UNK0:C	4,2	
Ursolic Acid (SU47)	**Ikatan Hidrogen**		
	• **Conventional H-Bond**		
	:UNK0:H - C:TYR220:OH	1,9	
	Ikatan Hidrofobik		
	• **Alkyl**		
	C:VAL30 - :UNK0	5,2	
	C:PRO111 - :UNK0	5,3	
	C:LEU114 - :UNK0	4,8	Leu114,
	:UNK0:C - C:PRO111	4,6	phe112,
	:UNK0:C - C:VAL120	4,9	**phe117,**
	:UNK0:C - C:VAL30	3,7	pro111, tyr220,
	:UNK0:C - C:VAL120	3,8	**val30, val120**
	:UNK0:C - C:PRO111	5,0	
	:UNK0:C - C:LEU114	3,7	
	:UNK0:C - C:LEU114	3,1	
	• **π-Alkyl**		
	C:PHE112 - :UNK0:C	4,7	
	C:PHE117 - :UNK0	4,6	
	C:PHE117 - :UNK0:C	4,5	
	C:PHE117 - :UNK0:C	4,1	

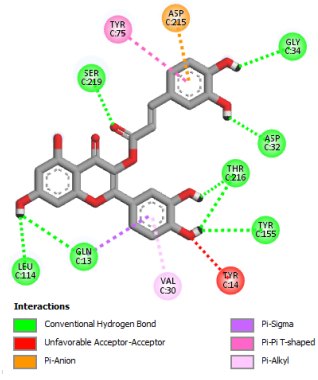
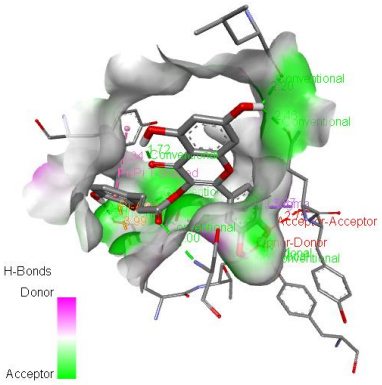
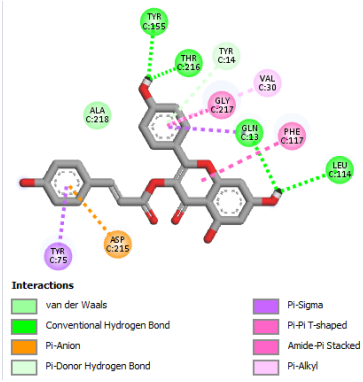
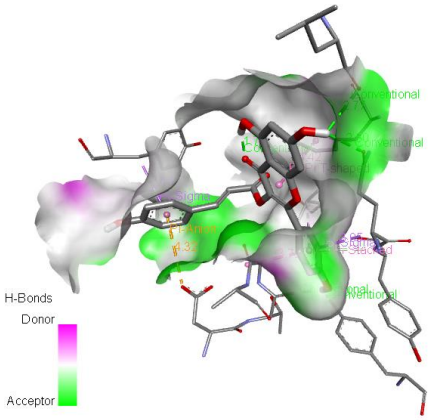
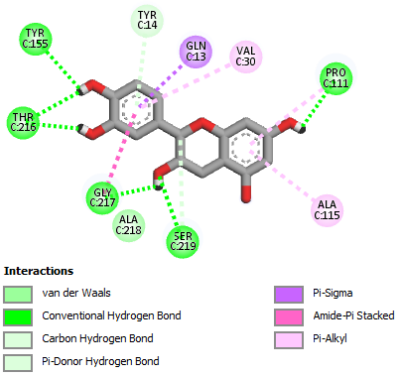
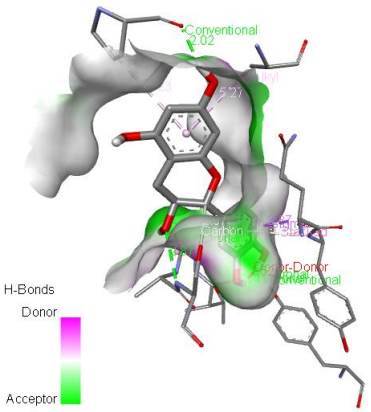
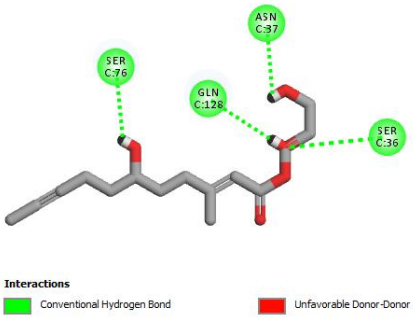
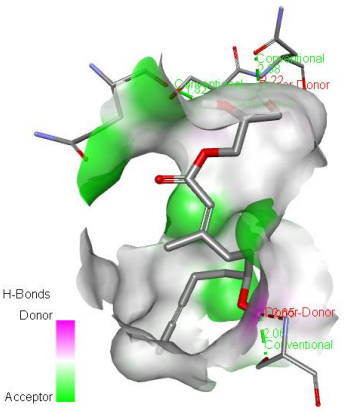
Lampiran 7 Visualisasi 2D dan 3D Interaksi Senyawa Uji Pose Terbaik dengan Protein Target Hasil Penambatan Molekul

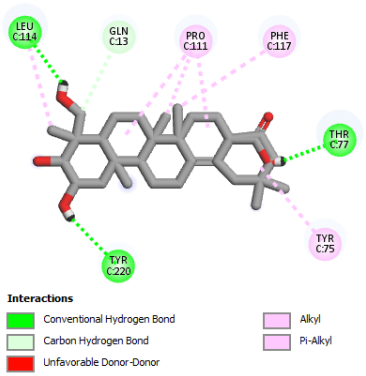
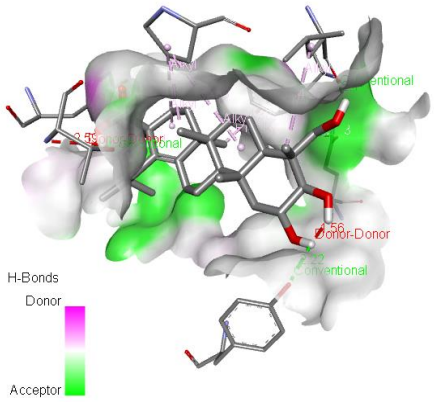
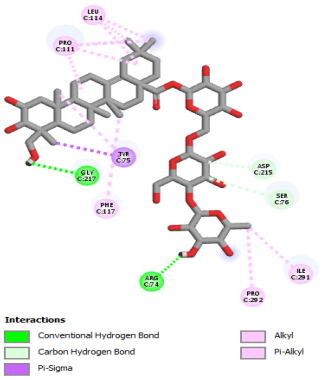
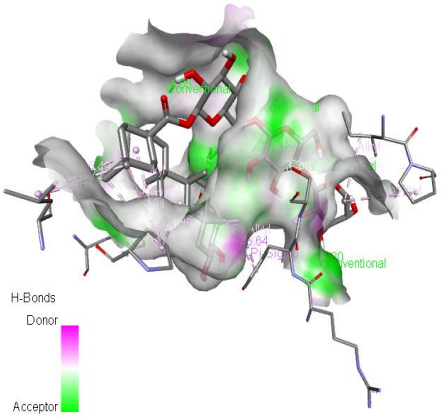
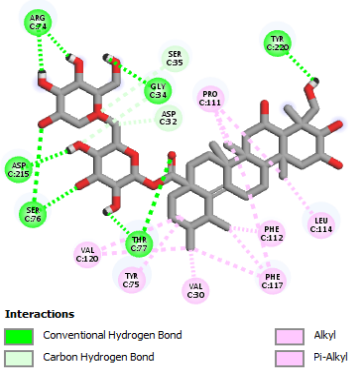
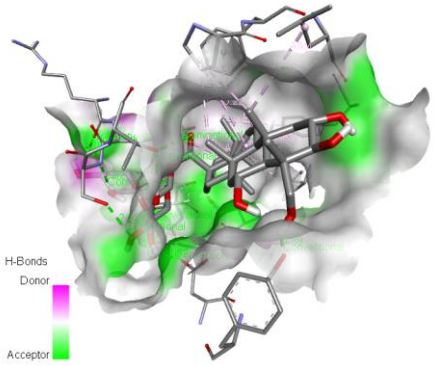
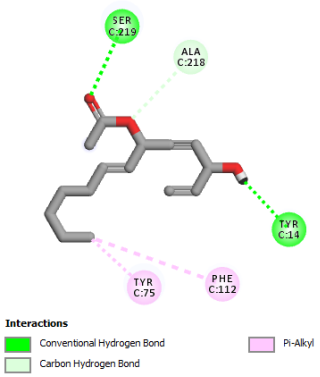
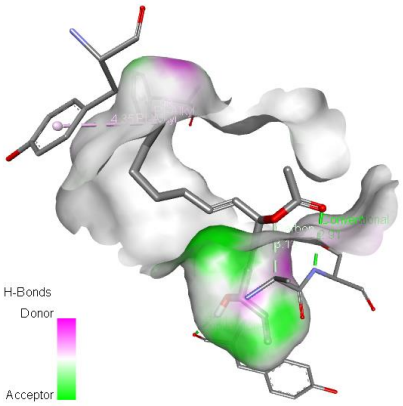
Nama Senyawa	Visualisasi	
	2D	3D
Aliskiren (Ligan Alami)		
3-Epimasclinic Acid (SU1)		
Apigenin (SU2)		

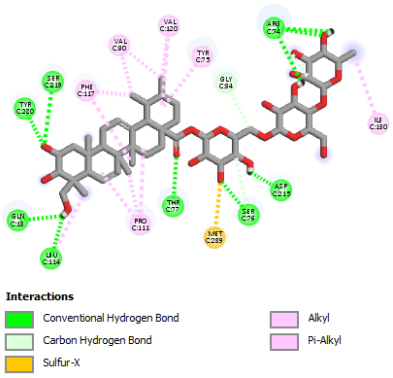
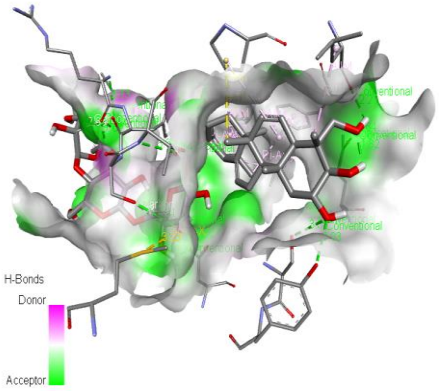
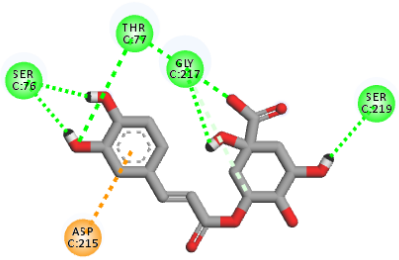
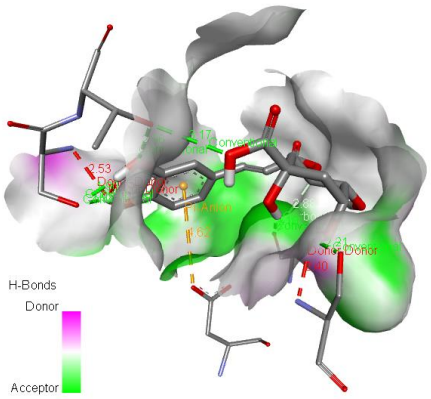
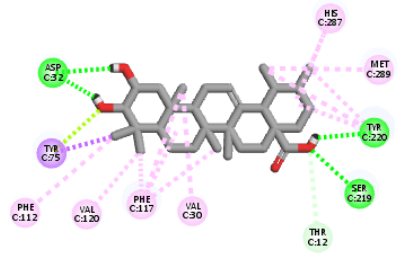
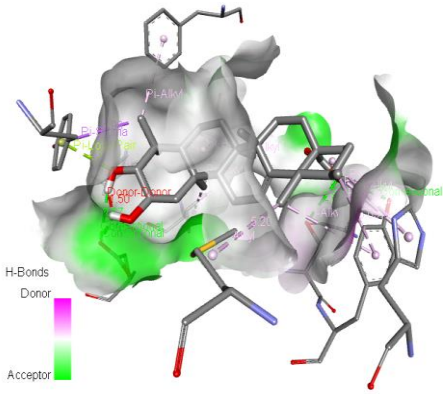
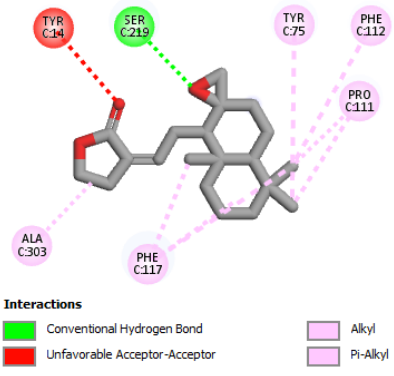
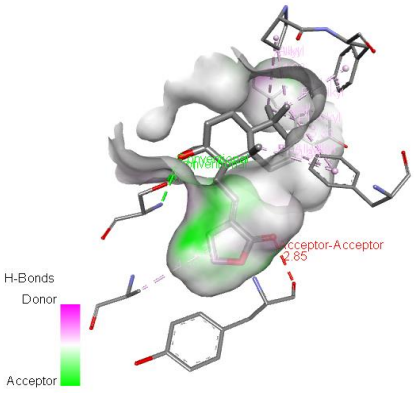
Arjunolic acid (SU3)		
Asiatic acid (SU4)		
Asiaticin (SU5)		
Asiaticoside (SU6)		

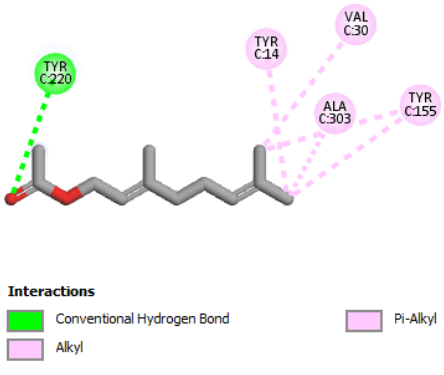
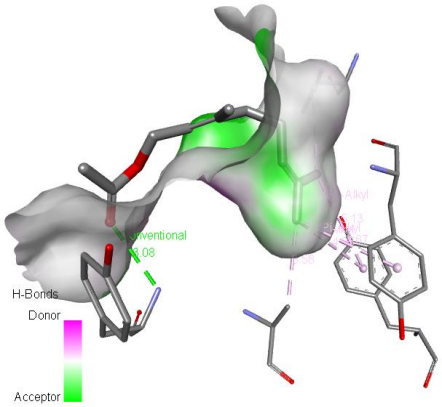
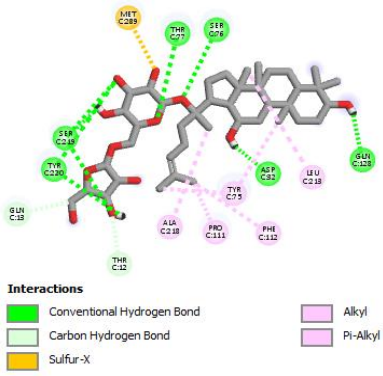
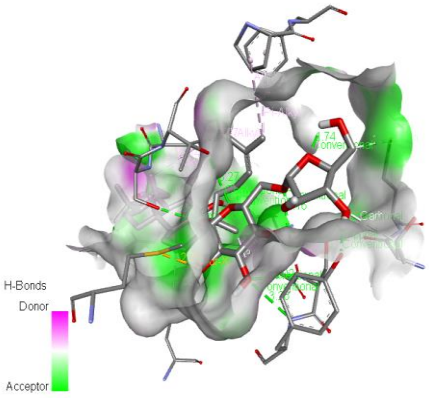
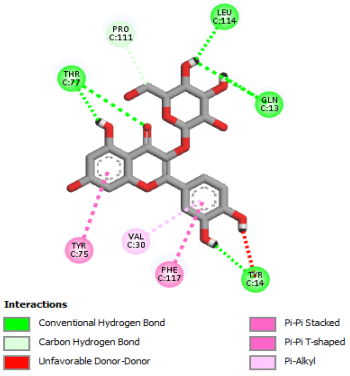
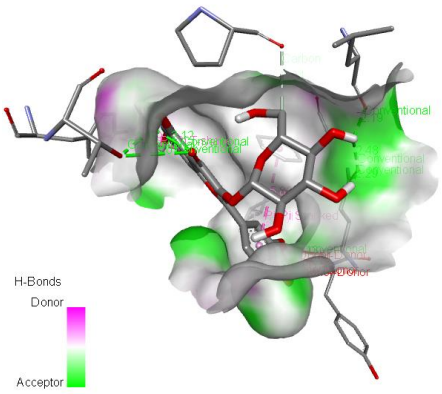
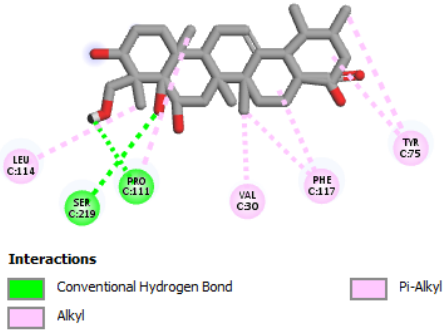
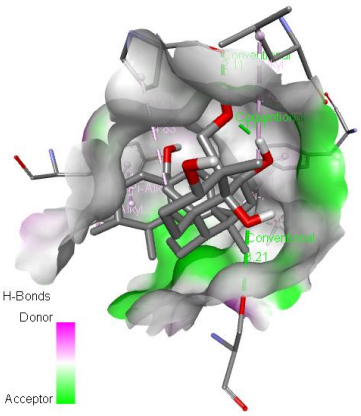
Astragalin (SU7)		
Bayogenin (SU8)		
Betulinic acid (SU9)		
Borneol (SU10)		

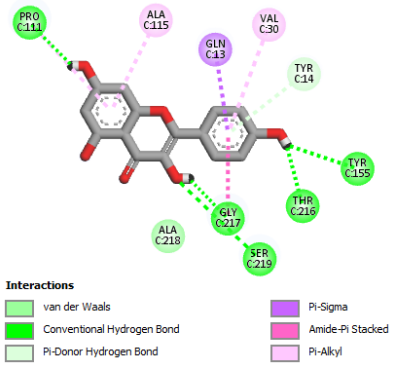
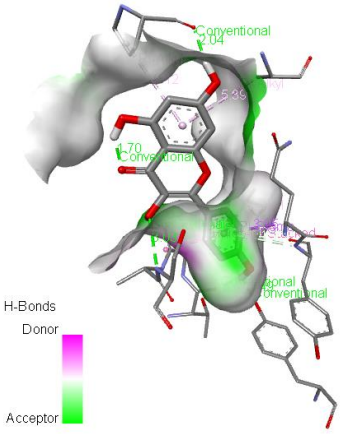
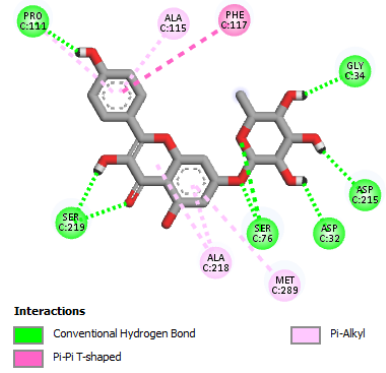
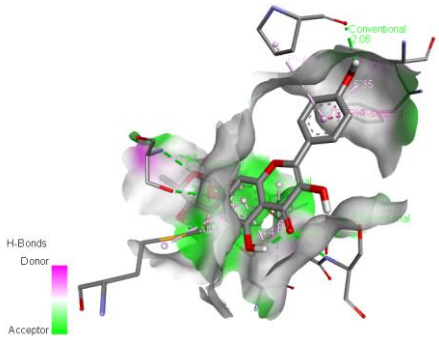
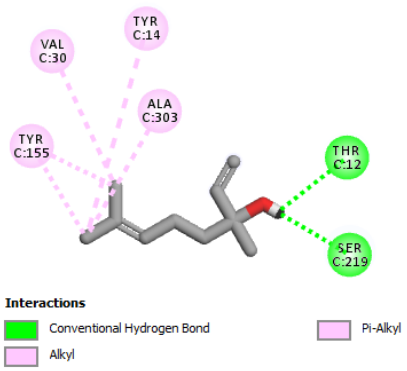
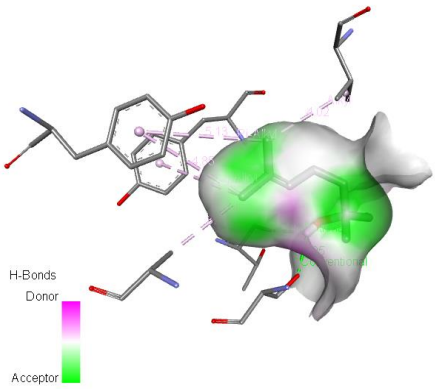
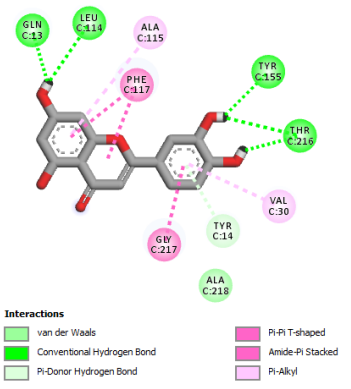
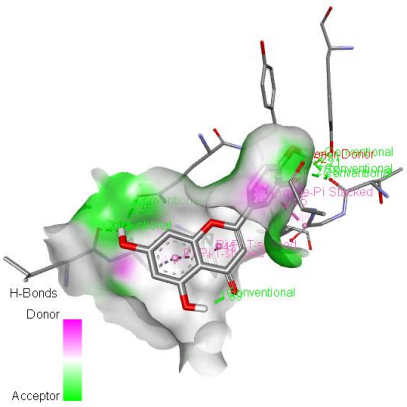
Cadiyenol (SU11)		
Campesterol (SU12)		
Carveol (SU13)		
Caryophyllene Epoxide (SU14)		

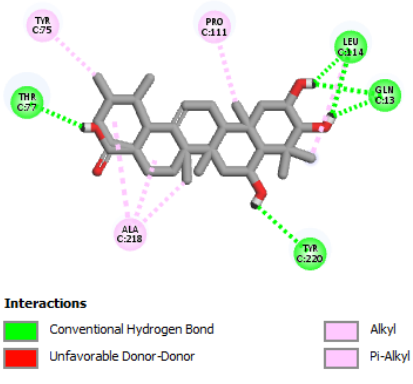
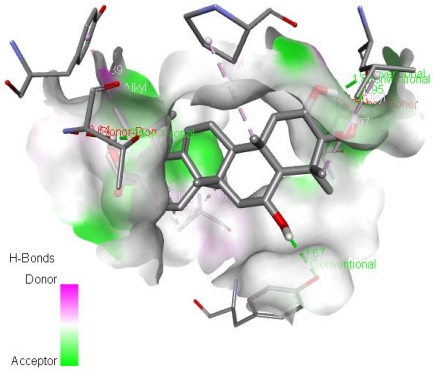
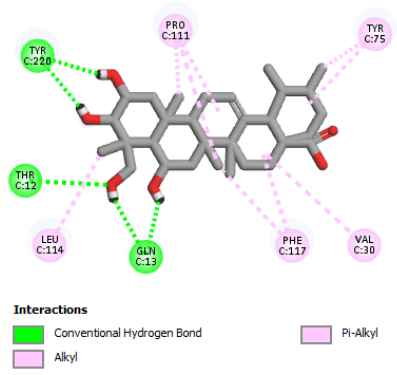
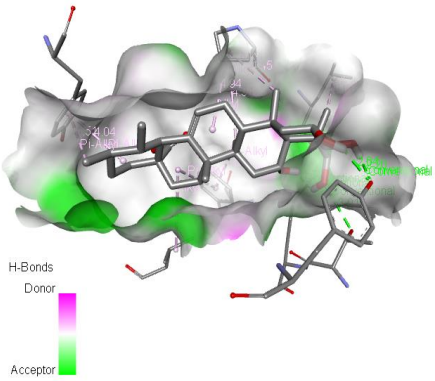
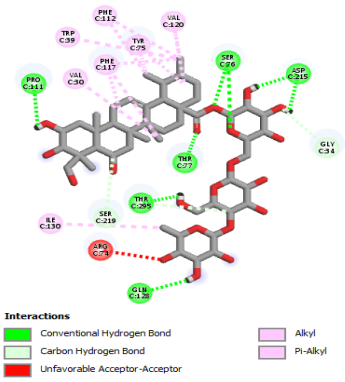
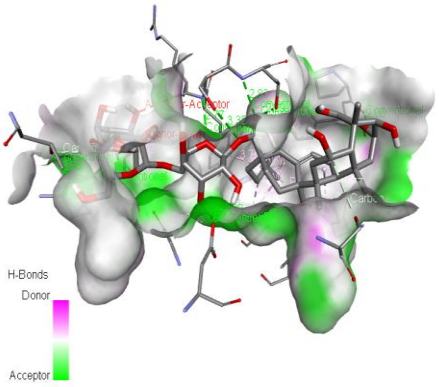
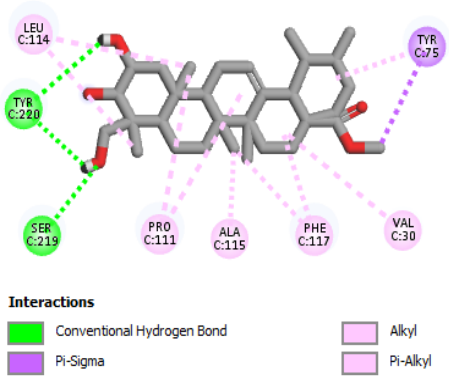
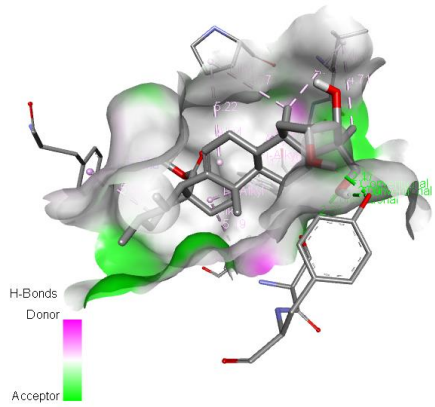
Castillicetin (SU15)		
Castilliferol (SU16)		
Catechin (SU17)		
Cenetellicin (SU18)		

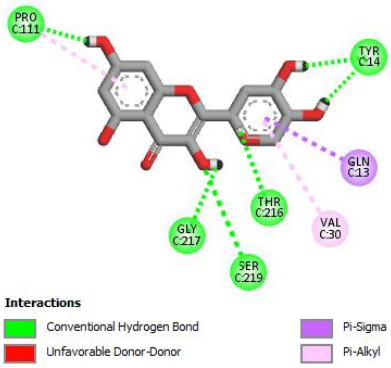
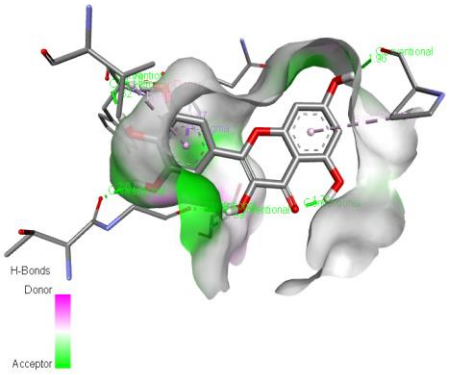
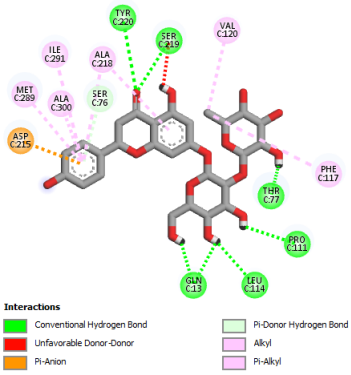
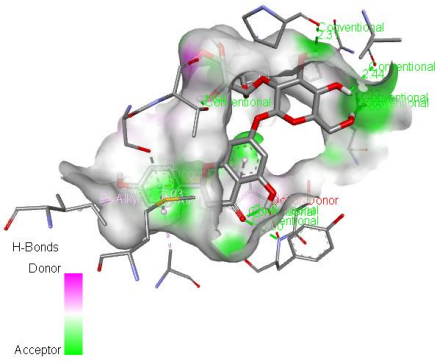
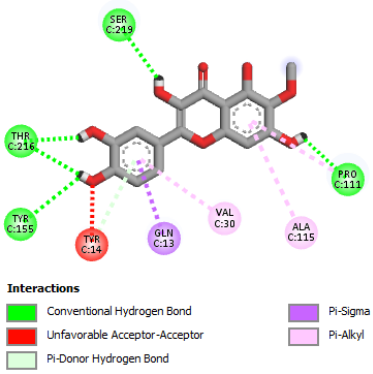
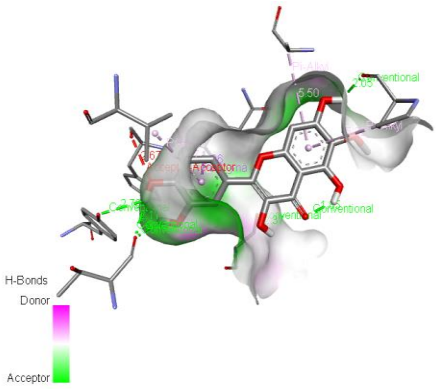
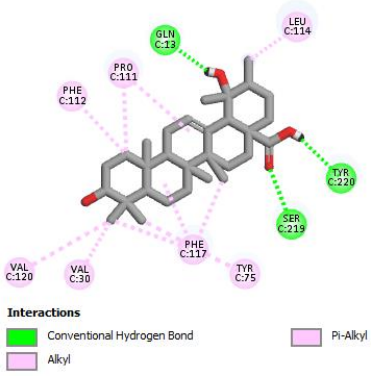
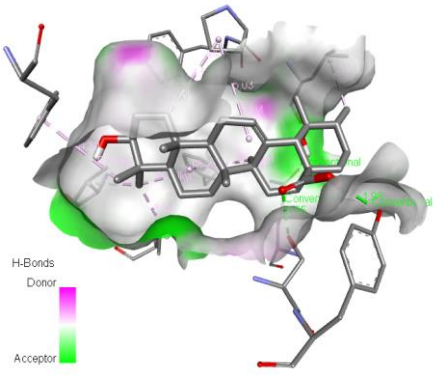
Centellasapogenol A (SU19)		
Centellasaponin A (SU20)		
Centellasaponin B (SU21)		
Centellin (SU22)		

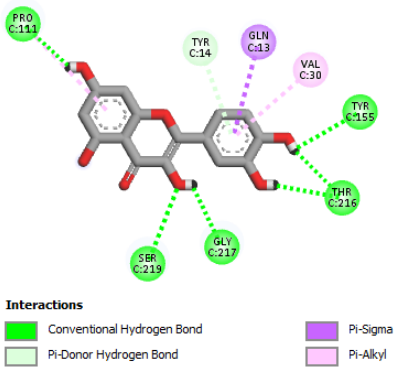
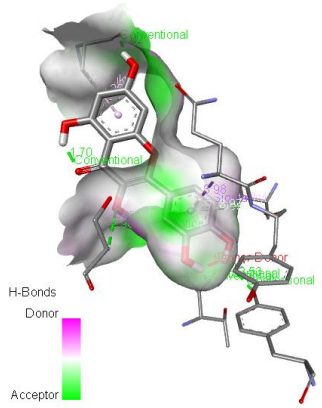
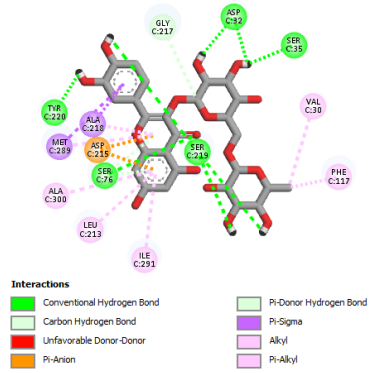
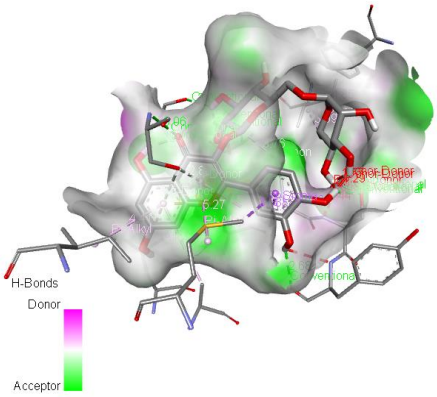
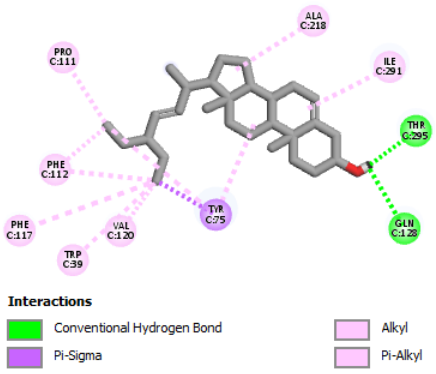
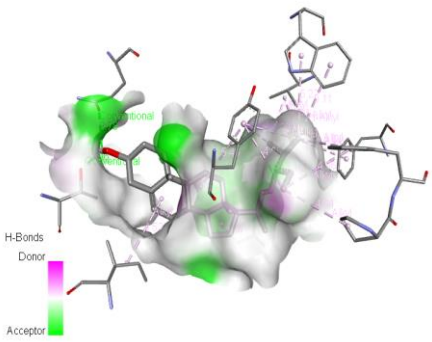
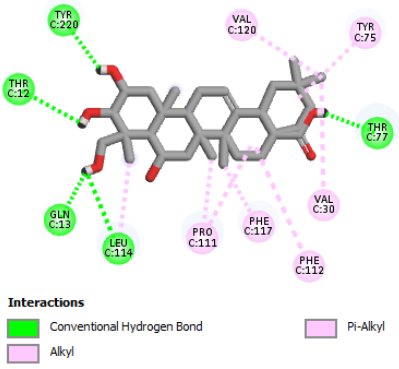
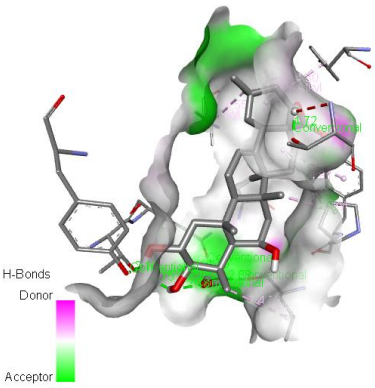
Centelloside E (SU23)		
Chlorogenic acid (SU24)		
Corosolic Acid (SU25)		
Galanolactone (SU26)		

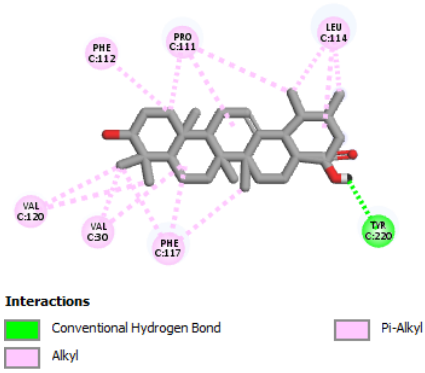
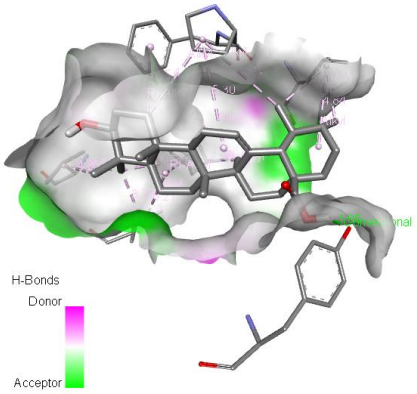
Geranyl Acetate (SU27)		
Ginsenoside MC (SU28)		
Isoquercitrin (SU29)		
Isothankunic Acid (SU30)		

Kaempferol (SU31)		
Kaempferol-7-rhamnoside (SU32)		
Linalool (SU33)		
Luteolin (SU34)		

Madasiatic Acid (SU35)		
Madecassic Acid (SU36)		
Madecassoside (SU37)		
Methyl Asiatate (SU38)		

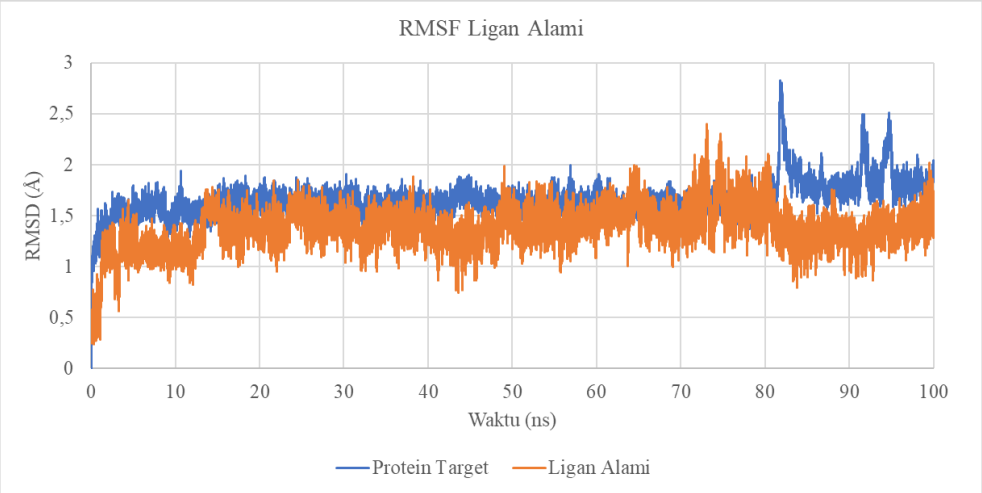
Myricetin (SU39)		
Naringin (SU40)		
Patuletin (SU41)		
Pomolic Acid (SU42)		

Quercetin (SU43)		
Rutin (SU44)		
Stigmasterol (SU45)		
Terminolic Acid (SU46)		

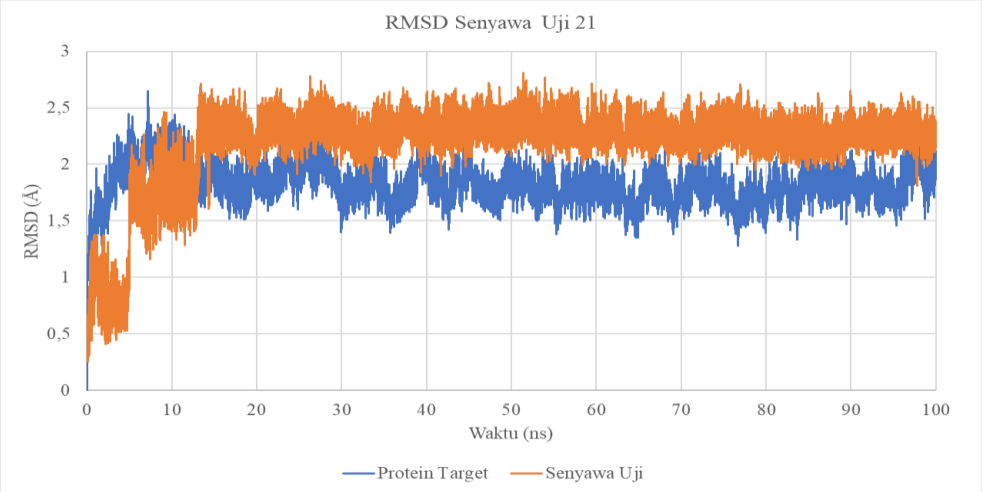
Ursolic Acid (SU47)		

Lampiran 8 Grafik RMSD Hasil Simulasi Dinamika Molekul

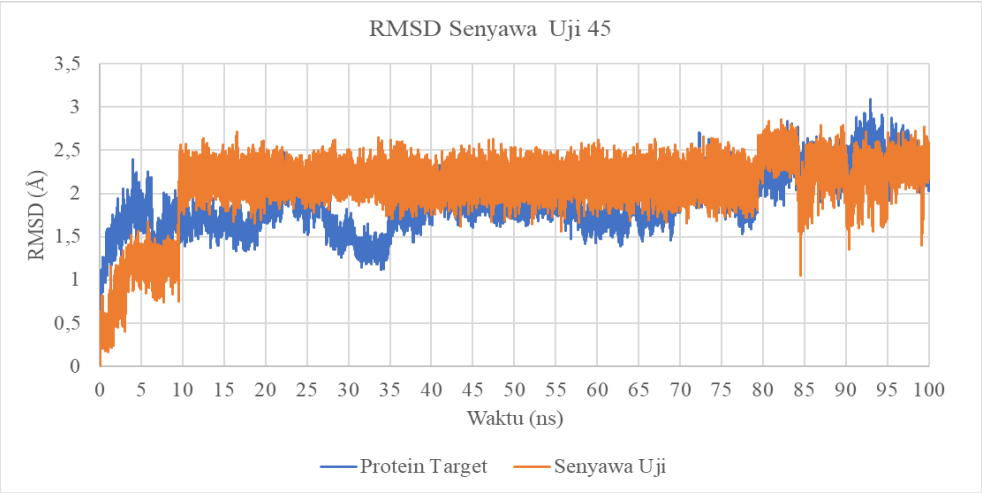
Ligan Alami



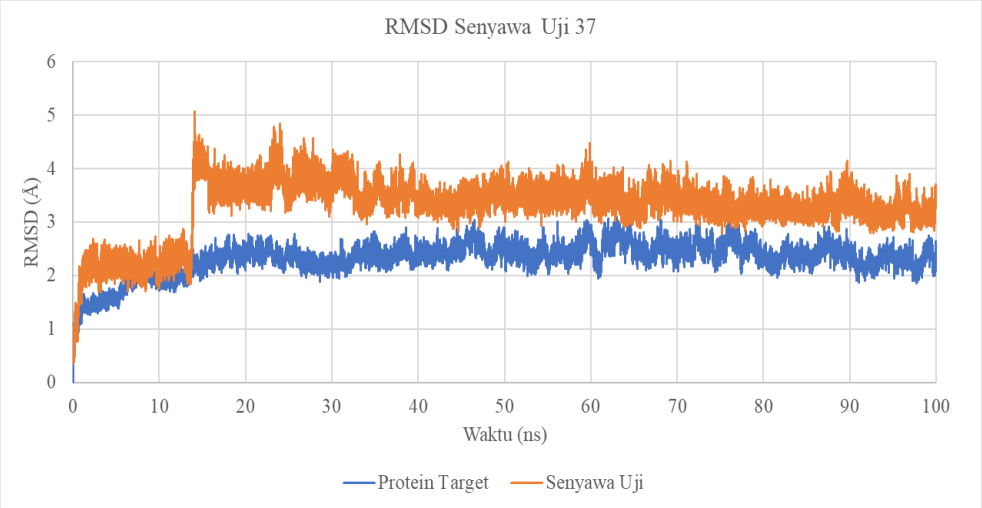
RMSD Senyawa Uji 21



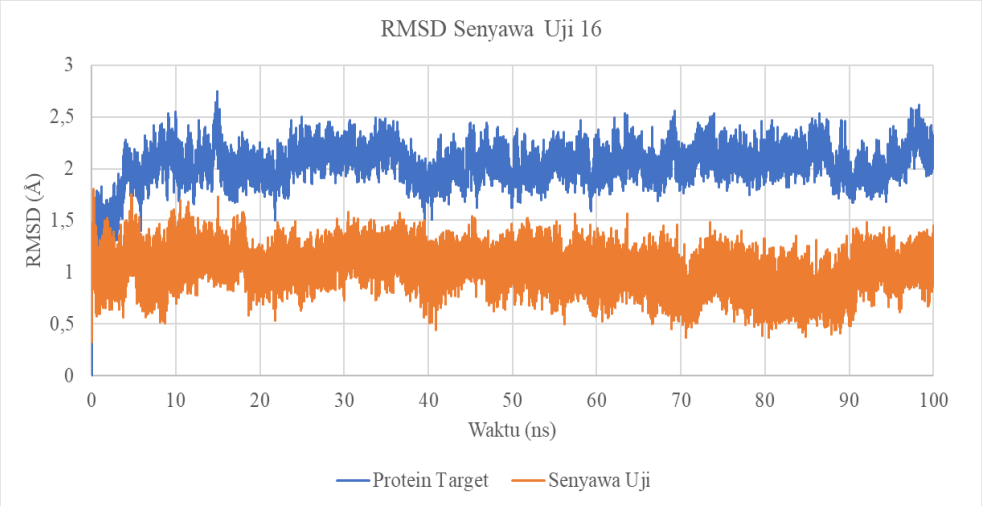
RMSD Senyawa 45



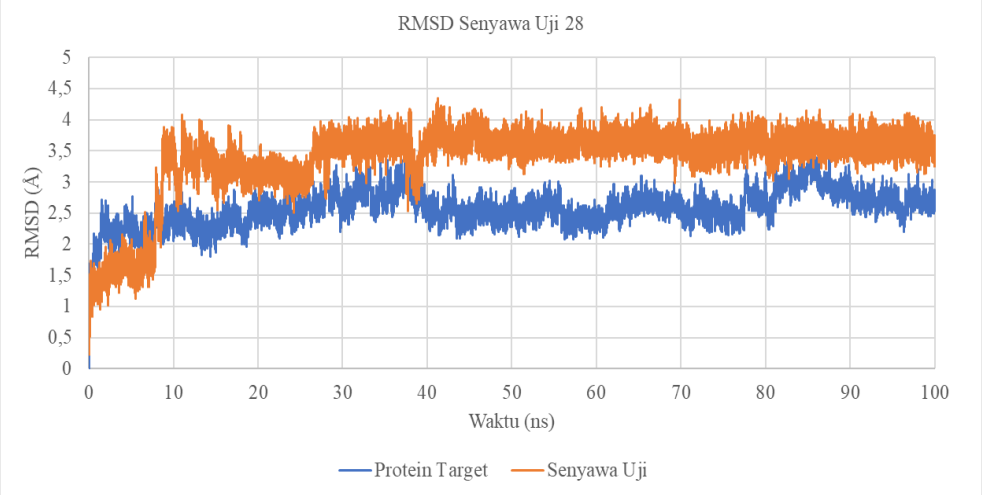
RMSD Senyawa 37



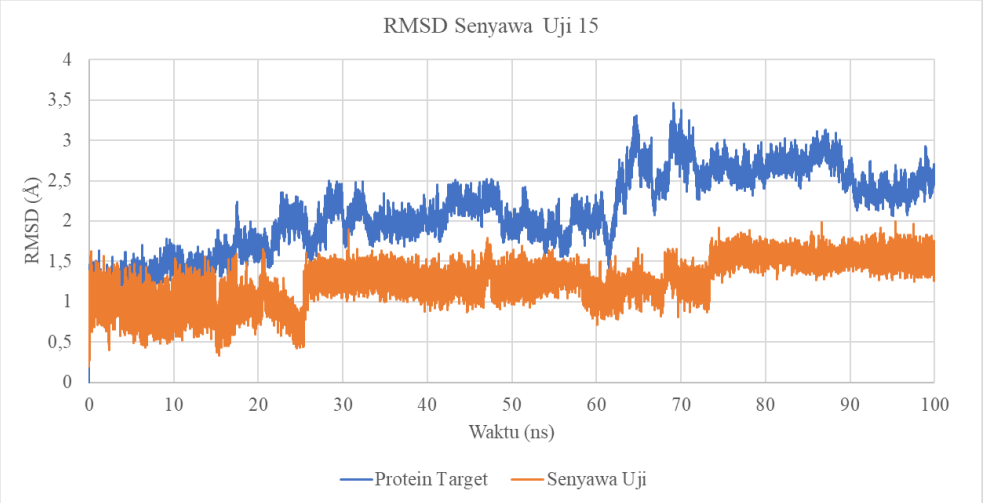
RMSD Senyawa 16



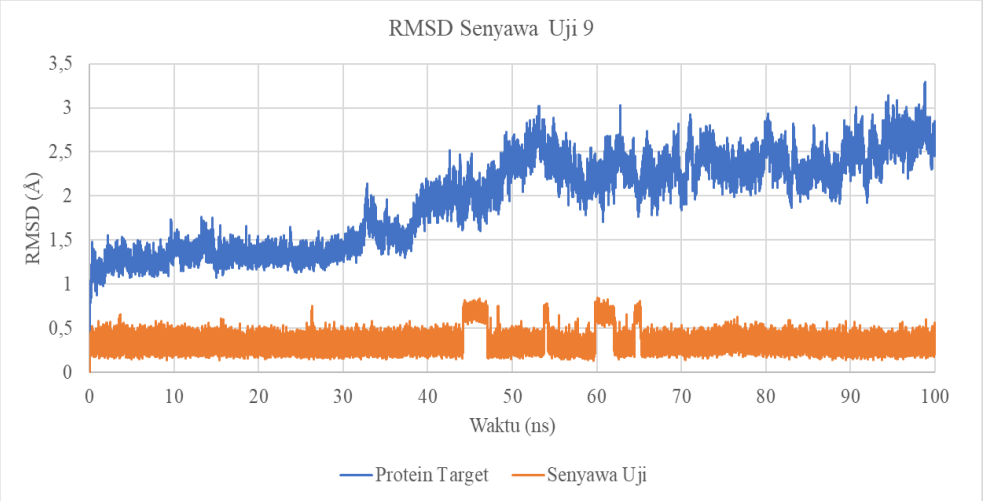
RMSD Senyawa 28



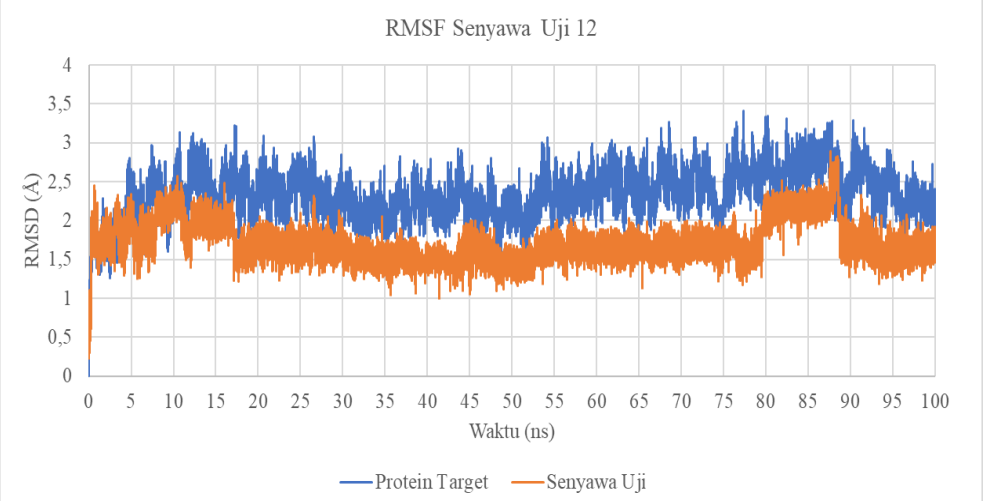
RMSD Senyawa 15



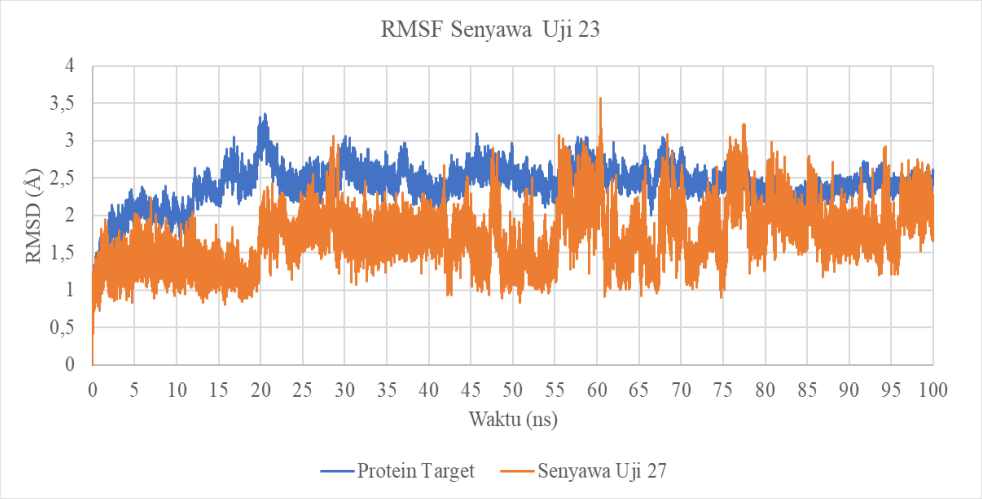
RMSD Senyawa 9



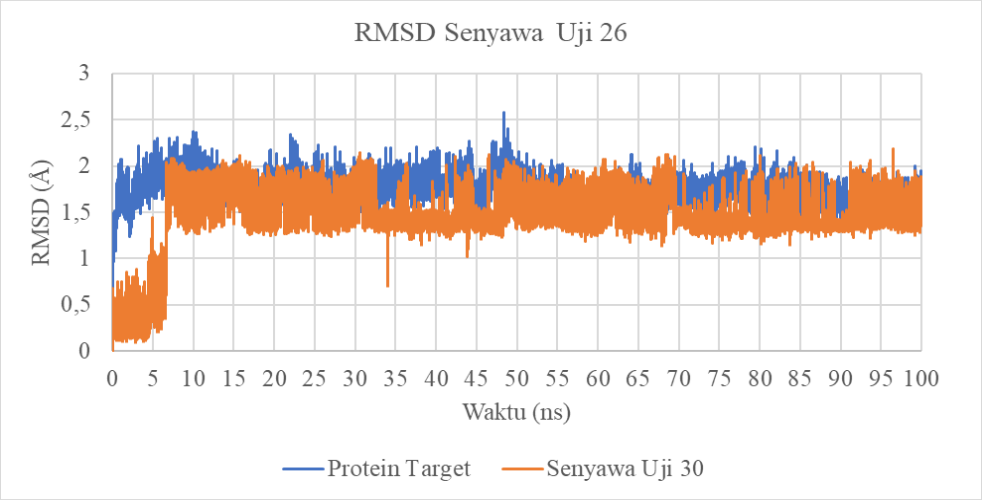
RMSD Senyawa 12



RMSD Senyawa 23

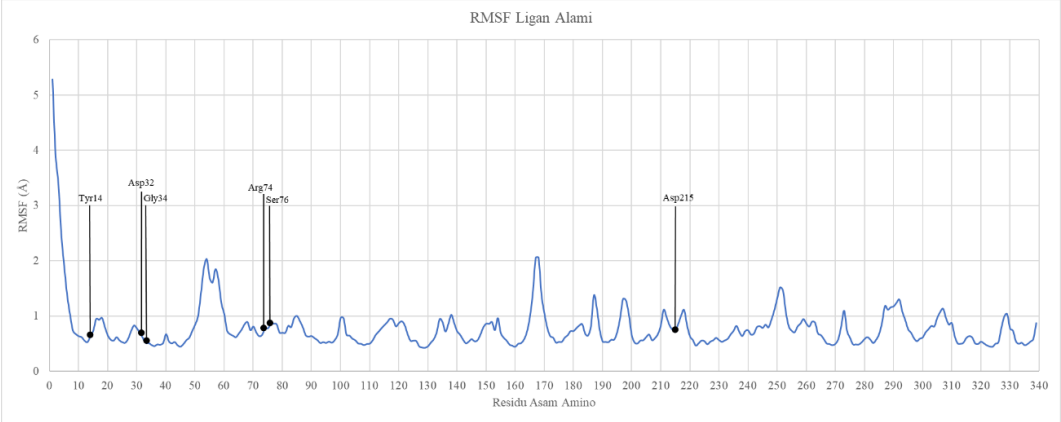


RMSD Senyawa 26

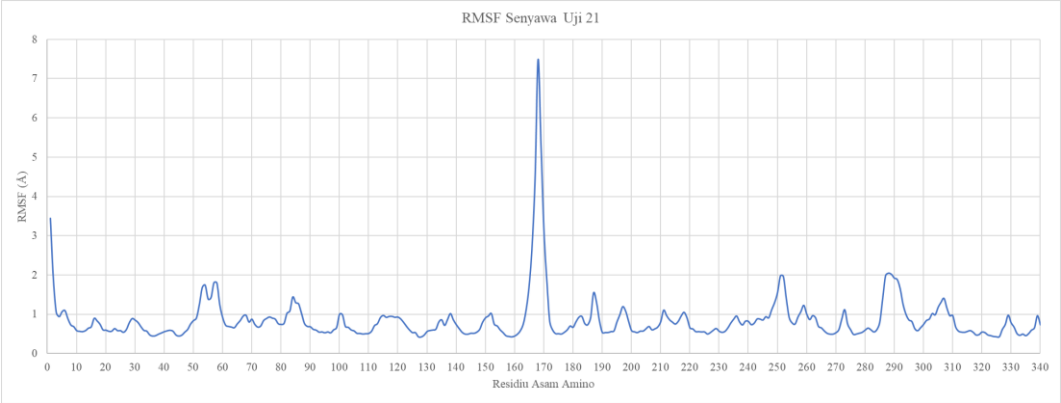


Lampiran 9 Grafik RMSD Hasil Simulasi Dinamika Molekul

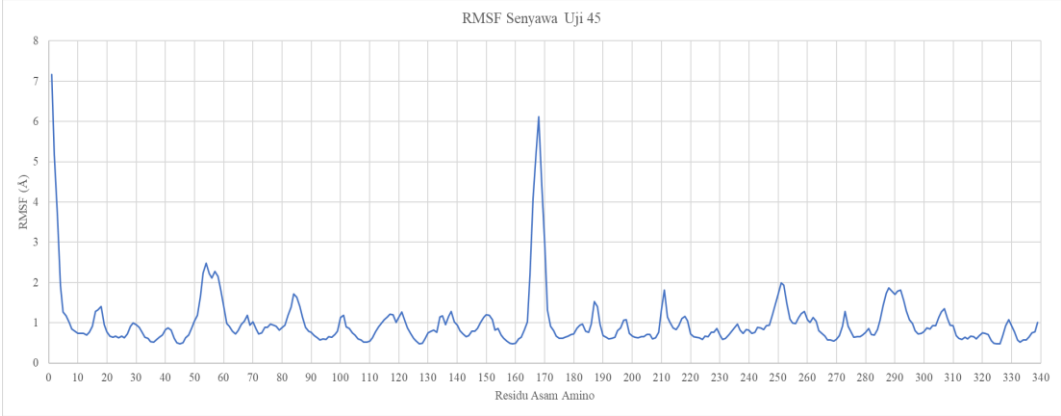
RMSF Ligan Alami



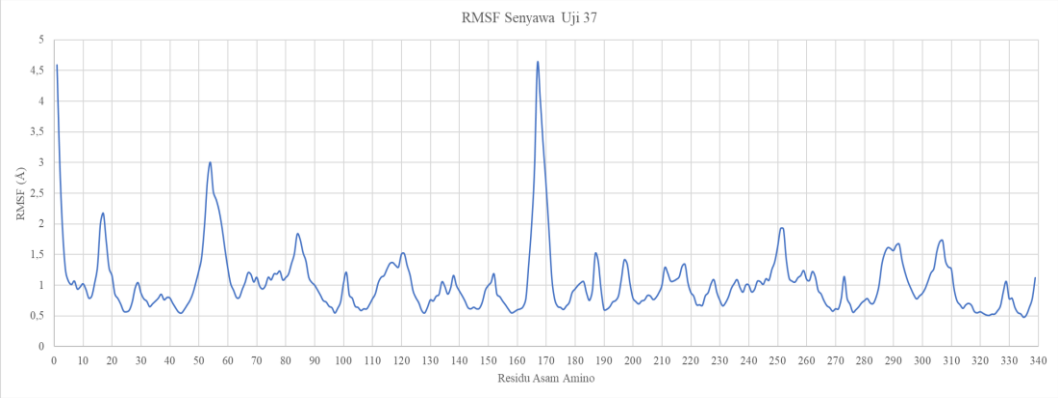
RMSF Senyawa Uji 21



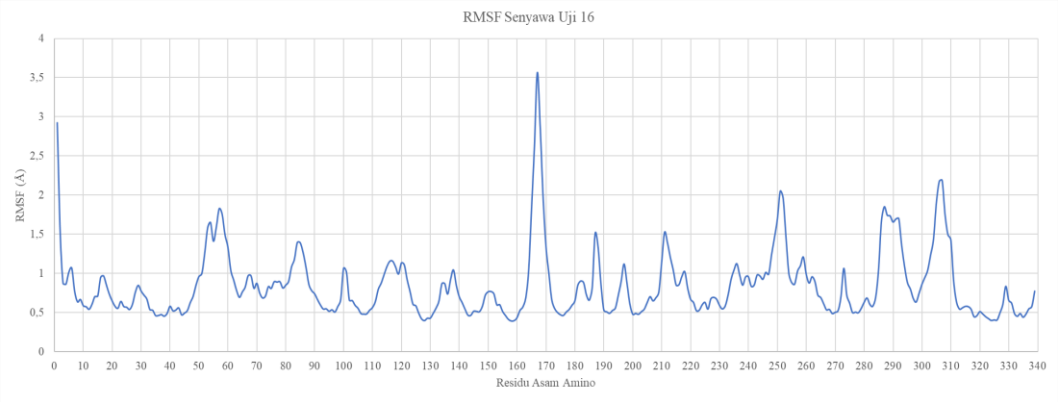
RMSF Senyawa 45



RMSF Senyawa 37



RMSF Senyawa 16



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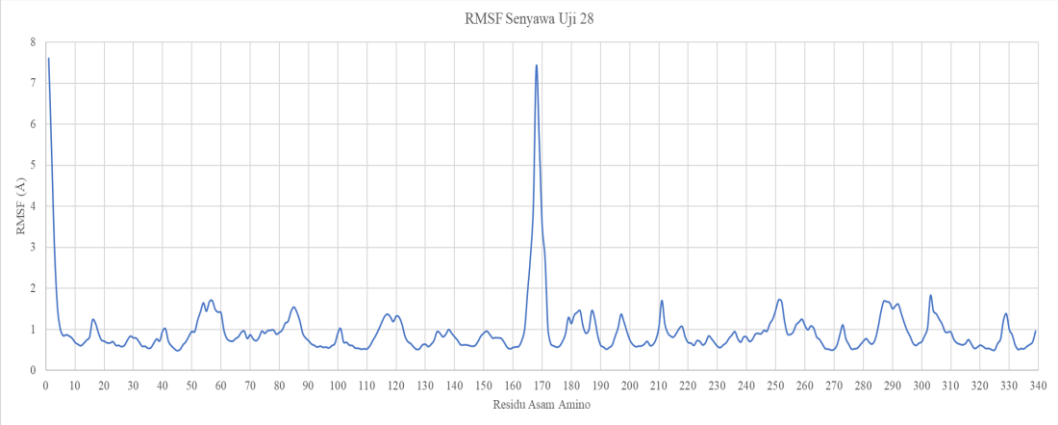

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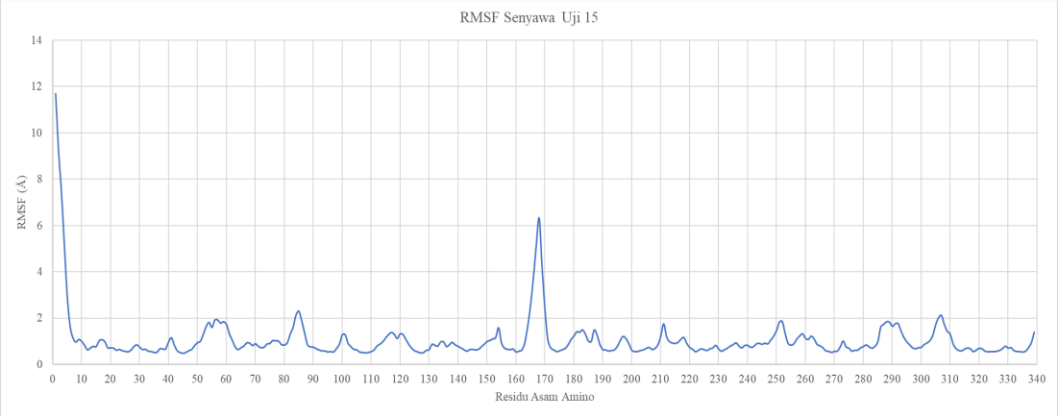
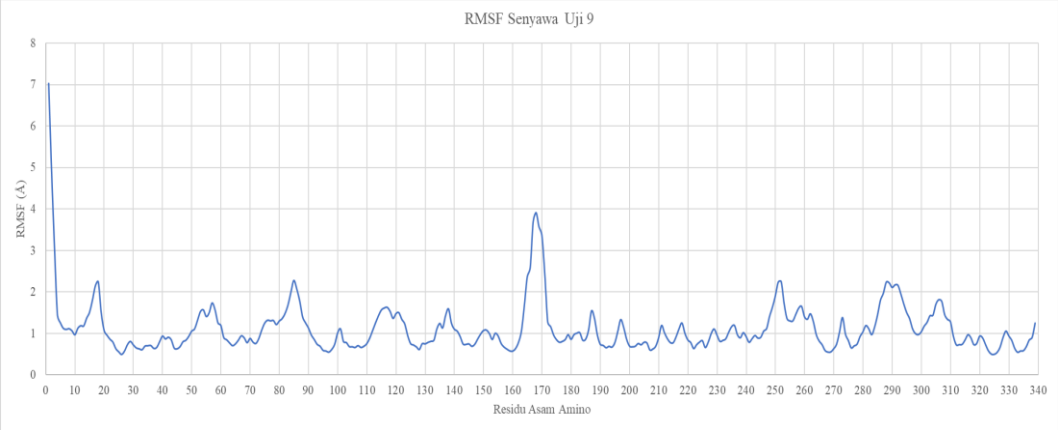
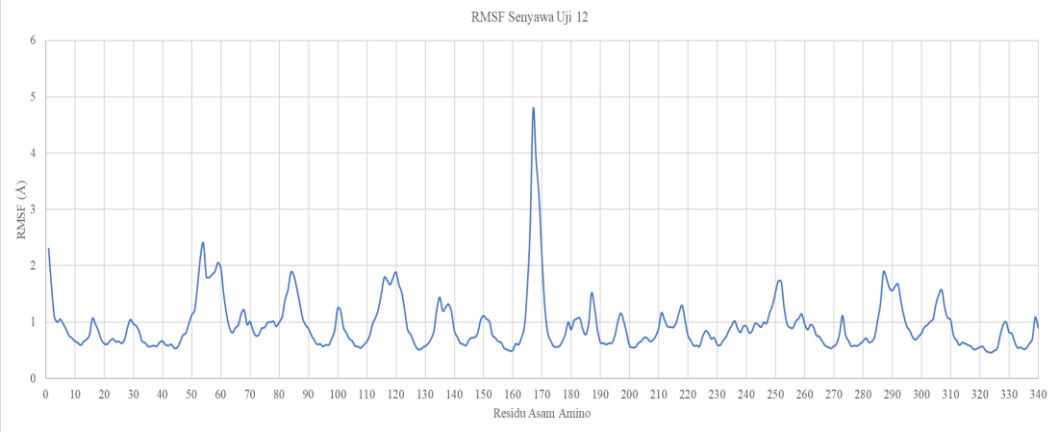


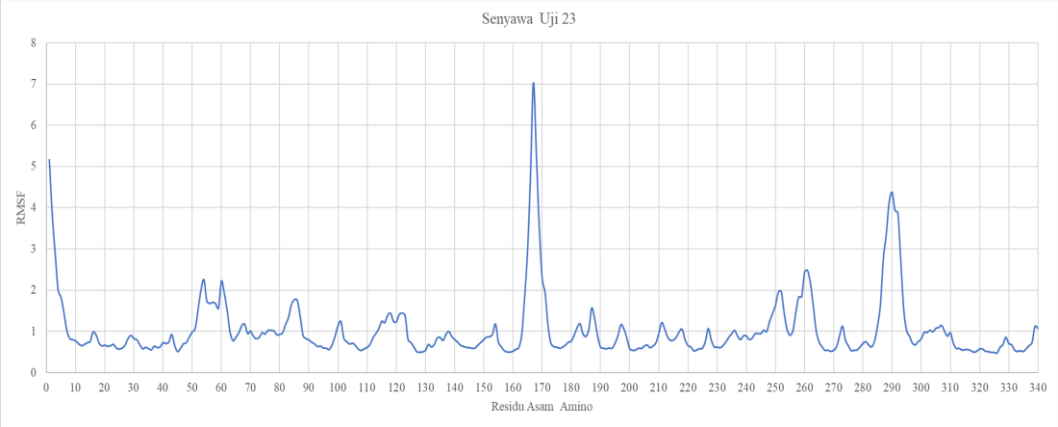
RMSF Senyawa 9



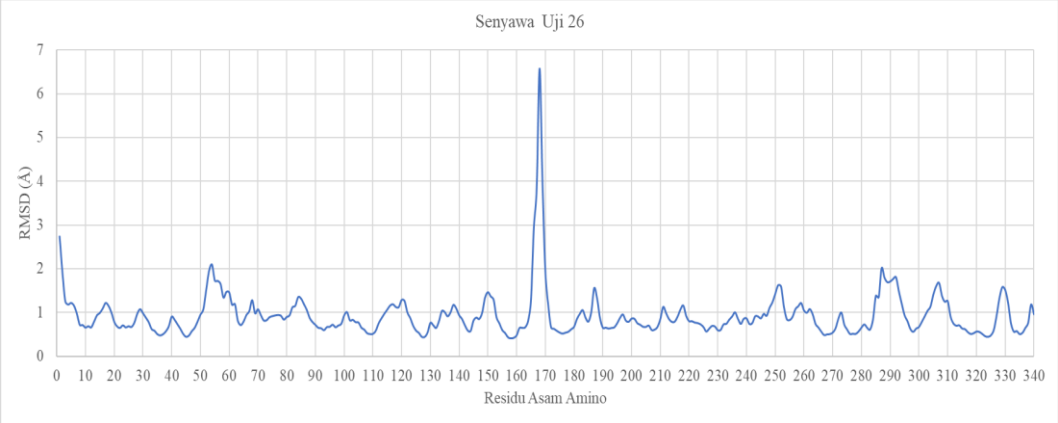
RMSF Senyawa 12



RMSF Senyawa 23



RMSF Senyawa 26



Lampiran 10 Data Analisis Ikatan Hidrogen

Kompleks	Akseptpr	Donor	Waktu (ns)	Jarak (Å)	Sudut Ikatan
2V0Z-LA	ALA228 N	LA H29	0,004	2,9407	139,8228
	ALA228 N	LA H30	0,018	2,9346	143,4299
	ARG82 N	LA H53	0,001	2,9026	136,1678
	ARG82 NH1	LA H53	0,011	2,909	153,9496
	ARG82 NH2	LA H53	0,016	2,9463	150,0659
	ARG82 O	LA H52	11,884	2,8404	153,5773
	ARG82 O	LA H53	0,604	2,8722	160,5666
	ASP225 OD1	LA H29	0,102	2,9105	151,8358
	ASP225 OD1	LA H30	0,314	2,9063	154,1484
	ASP225 OD1	LA H32	0,015	2,8164	166,7049
	ASP225 OD2	LA H29	9,098	2,8778	152,4484
	ASP225 OD2	LA H30	18,458	2,8753	153,2379
	ASP225 OD2	LA H32	12,704	2,7335	160,2351
	ASP38 OD1	LA H29	14,462	2,8575	157,681
	ASP38 OD1	LA H30	12,198	2,8492	159,0018
	ASP38 OD1	LA H32	22,516	2,7773	152,5618
	ASP38 OD2	LA H29	0,451	2,9057	156,3972
	ASP38 OD2	LA H30	0,137	2,9119	157,2678
	ASP38 OD2	LA H32	15,856	2,7835	149,7692
	GLN135 NE2	LA H52	0,001	2,9032	140,8072
	GLN135 NE2	LA H53	0,001	2,8827	142,6005
	GLN135 OE1	LA H52	0,492	2,8584	150,0955
	GLN135 OE1	LA H53	0,071	2,8679	153,4517
	GLY227 O	LA H29	0,445	2,9141	153,6378
	GLY227 O	LA H30	0,205	2,9179	155,9821
	GLY40 O	LA H43	2,121	2,8955	162,8741
	GLY40 O	LA H52	0,432	2,8558	154,4966
	GLY40 O	LA H53	0,262	2,8646	156,0311
	LA N22	ALA228 H	0,002	2,9489	144,6563
	LA N39	ARG82 HE	0,002	2,9257	150,2197
	LA N39	THR308 HG1	0,001	2,7493	169,4193
	LA O13	GLN19 HE22	1,152	2,8948	149,2196
	LA O2	TYR20 H	3,177	2,9165	156,1686
	LA O2	SER229 HG	0,187	2,8248	153,7448
	LA O31	SER84 H	57,148	2,8625	161,1199
	LA O31	SER84 HG	29,495	2,7569	161,5905
	LA O38	ARG82 H	3,029	2,8637	150,1806
	LA O38	ARG82 HH11	1,865	2,8217	157,1282
	LA O38	THR308 HG1	1,082	2,7439	157,9323
	LA O38	GLN135 HE22	1,000	2,8552	159,1284
	LA O38	ARG82 HH21	0,740	2,8312	151,7005
	LA O38	ARG82 HE	0,714	2,8616	151,9954
	LA O38	GLN135 HE21	0,142	2,8499	158,8475
	LA O38	SER84 HG	0,034	2,7732	158,26
	LA O38	ARG82 HH12	0,010	2,885	148,3688
	LA O38	ARG82 HH22	0,003	2,8423	152,9507
	LA O6	GLN19 HE22	0,291	2,9125	153,5988

	LA O6	GLN19 HE21	0,001	2,8621	138,341
	SER84 N	LA H52	0,001	2,9891	143,015
	SER84 OG	LA H52	1,174	2,8906	156,7812
	SER84 OG	LA H53	0,015	2,8604	149,2443
	THR308 OG1	LA H52	0,013	2,9228	146,0615
	THR308 OG1	LA H53	0,038	2,8935	154,0041
	TYR83 O	LA H52	0,001	2,9147	159,5346
	TYR83 O	LA H53	0,001	2,9457	137,6104
2V0Z-SU11	ASP38 OD1	SU11 H49	0,549	2,7981	152,6205
	ASP38 OD2	SU11 H49	0,005	2,7387	157,9344
	PHE252 O	SU11 H	0,005	2,8847	139,1524
	SER229 OG	SU11 H	0,002	2,753	155,6724
	SU11 O	TYR230 HH	0,001	2,7528	162,0115
	SU11 O1	HIE300 HE2	0,001	2,9131	152,1725
	SU11 O1	GLN19 HE21	0,098	2,9229	142,1127
	SU11 O1	THR18 HG1	0,088	2,8993	163,1104
	SU11 O1	SER229 HG	32,414	2,9326	141,1899
	SU11 O2	TYR83 HH	4,456	2,8484	158,3164
	SU11 O2	SER41 HG	0,012	2,9028	143,4147
	TYR83 OH	SU11 H49	0,007	2,8799	144,616
2V0Z-SU15	ALA136 O	SU15 H	19,140	2,8267	163,6384
	GLN135 OE1	SU15 H	0,093	2,8327	156,0356
	GLN201 OE1	SU15 H	0,006	2,7832	161,2148
	GLY198 O	SU15 H	0,039	2,7722	157,3219
	SU15 O	TRP200 H	0,040	2,9107	157,9339
	SU15 O	GLN135 HE22	0,064	2,9215	155,3381
	SU15 O	THR308 HG1	0,057	2,8735	166,4396
	THR308 OG1	SU15 H	0,013	2,8169	163,8703
	TRP200 O	SU15 H	0,018	2,8816	143,8481
2V0Z-SU19	ALA301 O	SU19 H2	0,006	2,7874	147,5941
	ASP225 OD1	SU19 H2	0,005	2,653	165,4395
	ASP225 OD1	SU19 H	0,388	2,6854	161,5486
	ASP225 OD2	SU19 H2	0,099	2,6228	166,2134
	ASP225 OD2	SU19 H	0,004	2,6465	165,932
	ASP38 OD1	SU19 H2	0,245	2,7066	160,0618
	ASP38 OD1	SU19 H	0,128	2,7274	151,5433
	ASP38 OD2	SU19 H2	0,079	2,6733	158,7465
	ASP38 OD2	SU19 H	0,039	2,7905	149,7927
	GLN19 NE2	SU19 H6	0,016	2,8844	157,2115
	GLN19 OE1	SU19 H3	0,811	2,7268	163,1518
	GLY227 O	SU19 H4	0,171	2,7452	148,7103
	GLY227 O	SU19 H3	7,589	2,7685	150,8239
	GLY227 O	SU19 H	0,092	2,7767	158,1692
	HIE300 ND1	SU19 H2	0,001	2,82	161,4415
	HIE300 ND1	SU19 H	0,554	2,7421	163,7421
	LEU121 O	SU19 H6	0,311	2,7501	156,8777
	MET302 O	SU19 H2	0,065	2,5949	140,3498

	PRO118 O	SU19 H6	0,022	2,9221	150,5967
	SER229 OG	SU19 H3	0,003	2,7087	141,6037
	SER232 OG	SU19 H2	1,682	2,8068	161,6195
	SER232 OG	SU19 H	0,856	2,8551	149,4514
	SER84 OG	SU19 H	0,073	2,8461	160,3248
	SU19 O	GLN19 HE21	0,015	2,9189	150,4354
	SU19 O	GLN19 HE22	0,007	2,9353	144,5048
	SU19 O	THR18 HG1	0,086	2,9418	161,9657
	SU19 O1	TYR230 HH	0,034	2,7913	159,0384
	SU19 O1	THR85 HG1	0,001	2,7999	161,9945
	SU19 O1	SER84 HG	0,003	2,7709	162,2133
	SU19 O1	HIE300 HE2	2,729	2,8648	161,044
	SU19 O1	THR18 HG1	0,004	2,7506	153,8228
	SU19 O2	THR85 HG1	0,063	2,8956	148,3655
	SU19 O3	THR18 HG1	0,001	2,7785	160,2726
	SU19 O3	THR85 HG1	0,008	2,8034	159,2849
	SU19 O3	TYR230 HH	3,399	2,8357	158,3099
	SU19 O3	HIE300 HE2	35,559	2,8643	147,7843
	SU19 O4	SER84 HG	0,004	2,8229	159,4778
	SU19 O4	SER232 HG	0,064	2,8954	156,5272
	SU19 O4	SER84 H	43,863	2,972	142,7257
	SU19 O5	SER232 HG	0,001	2,8483	155,8559
	SU19 O5	SER84 HG	19,225	2,9004	161,5843
	SU19 O6	SER229 H	1,279	2,9095	152,8771
	SU19 O6	SER229 HG	0,024	2,8341	154,6579
	SU19 O6	THR18 HG1	0,586	2,8465	156,6378
	SU19 O6	TYR20 H	0,001	2,9296	157,5398
	SU19 O6	GLN19 HE21	0,780	2,9498	160,7912
	SU19 O7	TYR20 H	0,477	2,9245	158,0419
	SU19 O7	SER229 H	0,382	2,9262	148,9629
	SU19 O7	THR18 HG1	78,324	2,801	159,9299
	SU19 O9	GLN19 HE22	13,842	2,9488	153,0016
	SU19 O9	GLN19 HE21	0,271	2,9453	144,1858
	THR18 O	SU19 H4	0,009	2,7411	152,3985
	THR18 O	SU19 H3	0,021	2,7277	162,5537
	THR18 OG1	SU19 H4	0,001	2,8506	143,6526
	THR18 OG1	SU19 H3	0,091	2,8361	154,5562
	TYR162 OH	SU19 H4	6,054	2,9992	135,7571
	TYR20 O	SU19 H4	2,666	2,7349	151,85
	TYR230 O	SU19 H2	66,845	2,832	163,2255
	TYR230 OH	SU19 H3	7,412	2,8409	155,6006
2V0Z-SU20	ASP253 OD1	SU20 H4	2,683	2,6657	164,4843
	ASP253 OD2	SU20 H4	0,555	2,662	164,7862
	ASP38 OD1	SU20 H	0,02	2,7157	160,6308
	ASP38 OD2	SU20 H	0,306	2,6824	164,413
	GLN19 O	SU20 H2	0,02	2,7772	158,7832
	GLY227 O	SU20 H2	0,005	2,7576	165,3242

	HIE300 ND1	SU20 H3	45,614	2,8472	151,245
	SU20 O	SER229 HG	0,001	2,9067	142,396
	SU20 O	GLN19 HE21	0,043	2,8357	152,7308
	SU20 O	GLN19 HE22	0,025	2,9296	149,3834
	SU20 O1	THR85 HG1	0,008	2,7997	158,4997
	SU20 O1	SER229 H	0,002	2,9177	154,0094
	SU20 O1	HIE300 HE2	0,063	2,8605	147,4265
	SU20 O1	TYR230 H	0,001	2,9917	171,9591
	SU20 O3	GLN19 HE22	0,001	2,838	141,7001
	SU20 O4	TYR83 HH	1,965	2,8447	161,4065
	SU20 O5	TYR20 H	8,746	2,9326	154,204
	SU20 O5	GLU123 H	26,709	2,9304	152,8796
	SU20 O5	PHE124 H	6,827	2,9216	150,055
	SU20 O6	HIE300 HE2	0,081	2,8963	146,6895
	SU20 O7	TYR230 HH	91,667	2,8694	151,8896
	SU20 O7	THR18 HG1	0,327	2,8527	157,8404
	THR18 OG1	SU20 H4	0,004	2,8036	164,3001
	TYR20 O	SU20 H2	97,149	2,6875	158,5185
	TYR230 OH	SU20 H4	0,009	2,8419	156,0251
2V0Z-SU25	ARG82 NH2	SU25 H7	1,385	2,9687	137,6192
	ARG82 O	SU25 H9	0,176	2,7812	155,1515
	ARG82 O	SU25 H8	0,005	2,7351	160,8924
	ARG82 O	SU25 H7	0,003	2,7897	156,4434
	ARG82 O	SU25 H	0,128	2,7602	155,0254
	ASP225 OD1	SU25 H69	0,043	2,7115	159,6957
	ASP225 OD1	SU25 H11	1,469	2,6603	162,2838
	ASP225 OD1	SU25 H10	0,091	2,7206	162,4931
	ASP225 OD2	SU25 H69	0,383	2,7515	157,7713
	ASP225 OD2	SU25 H11	0,128	2,6473	164,9276
	ASP225 OD2	SU25 H10	0,008	2,7631	156,8662
	ASP253 OD1	SU25 H73	0,185	2,7724	151,9881
	ASP253 OD1	SU25 H71	0,078	2,7115	153,1622
	ASP253 OD2	SU25 H73	0,064	2,7866	151,4818
	ASP253 OD2	SU25 H71	0,004	2,7594	145,4984
	ASP303 O	SU25 H	0,616	2,8228	151,9014
	ASP38 OD1	SU25 H10	0,052	2,8566	158,4732
	ASP38 OD2	SU25 H10	0,007	2,9684	151,2364
	GLN135 NE2	SU25 H8	0,002	2,905	149,949
	GLN135 NE2	SU25 H7	0,078	2,9575	157,5536
	GLN135 O	SU25 H7	0,067	2,7819	154,2867
	GLN135 O	SU25 H	0,853	2,7693	159,4174
	GLN135 OE1	SU25 H9	0,572	2,7855	154,7385
	GLN135 OE1	SU25 H8	0,571	2,7638	159,0478
	GLN135 OE1	SU25 H7	0,258	2,7611	153,9572
	GLN19 NE2	SU25 H72	0,115	2,881	155,5846
	GLY40 O	SU25 H9	0,018	2,7082	155,7946
	GLY40 O	SU25 H8	0,010	2,8077	155,9961
	GLY40 O	SU25 H7	0,005	2,8403	156,2646

GLY40 O	SU25 H10	0,004	2,9549	169,0993
GLY40 O	SU25 H	0,003	2,7837	156,8124
HIE300 ND1	SU25 H70	0,003	2,8816	161,5316
HIE300 NE2	SU25 H70	0,001	2,9349	154,2429
LEU121 O	SU25 H72	0,001	2,788	159,5464
MET302 O	SU25 H10	0,355	2,783	154,7981
PHE252 O	SU25 H73	0,325	2,8284	150,4429
PHE252 O	SU25 H71	0,158	2,8339	151,304
PRO305 O	SU25 H	0,101	2,8145	159,34
SER229 OG	SU25 H71	0,093	2,8639	138,665
SER229 OG	SU25 H70	0,026	2,8441	158,2939
SER232 OG	SU25 H69	0,021	2,9506	166,2273
SER232 OG	SU25 H11	0,013	2,8262	154,3556
SER41 OG	SU25 H9	0,709	2,7985	153,9899
SER41 OG	SU25 H	0,185	2,8094	152,3944
SER84 N	SU25 H	0,032	2,9572	153,7347
SER84 OG	SU25 H10	0,014	2,8169	157,5653
SER84 OG	SU25 H	0,001	2,8337	151,8125
SU25 O	THR85 HG1	0,027	2,8159	159,5614
SU25 O	SER84 HG	0,002	2,7351	162,5671
SU25 O	THR85 H	0,002	2,9454	157,4277
SU25 O1	SER84 H	0,002	2,9379	149,7726
SU25 O10	SER232 HG	0,136	2,8215	160,7783
SU25 O10	HIE300 HE2	0,525	2,934	148,6834
SU25 O11	ALA228 H	0,003	2,8905	145,2149
SU25 O11	HIE300 HE2	0,317	2,9213	152,6105
SU25 O12	SER229 H	0,003	2,9178	157,6499
SU25 O12	HIE300 HE2	0,008	2,8963	148,9375
SU25 O12	TYR230 H	12,122	2,939	162,7643
SU25 O13	SER229 HG	0,099	2,8523	151,7216
SU25 O13	TYR230 HH	0,160	2,8448	153,4962
SU25 O13	GLN19 HE21	0,637	2,92	160,3628
SU25 O13	THR18 HG1	0,063	2,8605	138,2249
SU25 O14	GLN19 HE21	0,327	2,8843	151,7588
SU25 O14	GLN19 HE22	0,392	2,9014	148,328
SU25 O3	SER84 H	0,298	2,9363	160,3724
SU25 O3	SER84 HG	0,054	2,8607	171,3151
SU25 O4	SER84 H	0,534	2,9017	141,9451
SU25 O4	SER84 HG	0,405	2,8627	148,998
SU25 O5	SER84 HG	0,013	2,835	160,7878
SU25 O5	THR308 HG1	0,016	2,8124	160,344
SU25 O5	TYR83 HH	0,002	2,7963	157,6734
SU25 O5	ARG82 HH11	2,154	2,8715	154,0532
SU25 O5	SER84 H	0,012	2,905	149,7812
SU25 O5	ARG82 H	0,576	2,9257	147,0843
SU25 O5	ARG82 HH12	13,101	2,9048	150,8892

	SU25 O5	ARG82 HH22	0,488	2,8333	154,1259
	SU25 O5	ARG82 HH21	0,026	2,9072	153,3026
	SU25 O5	ARG82 HE	0,083	2,9305	158,2578
	SU25 O5	SER42 H	0,001	2,9657	158,3443
	SU25 O5	GLN135 HE22	2,225	2,88	144,3042
	SU25 O5	THR308 H	0,005	2,8876	148,8251
	SU25 O6	GLN135 HE22	0,003	2,8875	156,1393
	SU25 O6	ARG82 H	1,630	2,911	149,957
	SU25 O6	THR308 HG1	0,012	2,842	160,0049
	SU25 O6	GLN135 HE21	0,332	2,8882	159,0087
	SU25 O6	ARG82 HE	70,491	2,8976	157,539
	SU25 O6	ARG82 HH21	29,988	2,9028	148,8575
	SU25 O6	ARG82 HH12	0,002	2,8609	148,3977
	SU25 O6	ARG82 HH11	3,416	2,9032	153,2333
	SU25 O7	GLN135 HE22	82,801	2,8915	151,6796
	SU25 O7	ARG82 H	0,221	2,9165	151,7938
	SU25 O7	THR308 HG1	3,011	2,8212	162,9344
	SU25 O7	GLN135 HE21	0,658	2,9125	150,8222
	SU25 O7	ARG82 HH22	0,011	2,9365	137,3746
	SU25 O8	GLN135 HE21	0,001	2,8847	157,9853
	SU25 O8	THR308 HG1	0,001	2,8318	149,1442
	SU25 O8	SER84 H	0,013	2,8708	144,6842
	SU25 O8	GLN135 HE22	0,015	2,944	140,9467
	SU25 O9	SER84 HG	9,502	2,8307	157,6612
	THR18 O	SU25 H71	0,012	2,7333	151,3575
	THR18 O	SU25 H70	0,061	2,8783	149,0276
	THR18 OG1	SU25 H71	1,305	2,8135	155,7879
	THR308 OG1	SU25 H9	0,054	2,8643	160,6216
	THR308 OG1	SU25 H8	1,699	2,8209	161,5796
	THR308 OG1	SU25 H7	0,005	2,7984	162,0504
	THR308 OG1	SU25 H	5,352	2,7863	162,2746
	TYR230 OH	SU25 H71	0,342	2,8821	158,331
	TYR83 O	SU25 H	0,150	2,811	155,8008
	TYR83 OH	SU25 H	0,006	2,8368	145,1599
2V0Z-SU27	ARG82 O	SU27 H80	1,992	2,9146	176,2674
	ARG82 O	SU27 H79	1,895	2,7549	146,1476
	ARG82 O	SU27 H78	0,293	2,7584	157,9323
	ARG82 O	SU27 H77	0,011	2,7787	150,2223
	ARG82 O	SU27 H12	0,008	2,7941	151,9177
	ARG82 O	SU27 H11	1,714	2,7332	155,4718
	ASP225 OD1	SU27 H82	0,015	2,6839	166,0775
	ASP225 OD1	SU27 H81	2,660	2,7068	159,0426
	ASP225 OD1	SU27 H10	0,439	2,7028	163,5853
	ASP225 OD2	SU27 H82	0,125	2,7262	165,2642
	ASP225 OD2	SU27 H81	0,026	2,7119	157,7495
	ASP225 OD2	SU27 H10	0,005	2,714	163,6865
	ASP303 O	SU27 H80	0,001	2,9984	145,7759
	GLN135 NE2	SU27 H78	0,002	2,9091	145,3761

GLN135 NE2	SU27 H77	5,675	2,8907	149,5055
GLN135 NE2	SU27 H11	0,062	2,9054	157,8138
GLN135 O	SU27 H77	0,006	2,7557	155,6392
GLN135 OE1	SU27 H78	0,481	2,7876	154,6126
GLN135 OE1	SU27 H77	0,418	2,7714	154,8972
GLN135 OE1	SU27 H11	0,289	2,772	158,0135
GLN19 OE1	SU27 H9	0,735	2,8305	160,3156
GLY227 O	SU27 H10	0,535	2,7479	160,4781
GLY40 O	SU27 H11	0,006	2,7723	156,8844
LEU121 O	SU27 H9	0,204	2,8643	155,8449
LEU121 O	SU27 H8	0,091	2,8552	150,5754
LEU121 O	SU27 H	0,016	2,7494	160,4942
PHE252 O	SU27 H9	0,009	2,8259	159,323
PHE252 O	SU27 H8	0,004	2,8274	149,1796
PRO118 O	SU27 H	0,003	2,7012	168,5408
PRO305 O	SU27 H80	6,663	2,8669	160,6369
PRO305 O	SU27 H78	2,157	2,7584	160,0354
PRO305 O	SU27 H12	0,108	2,7559	158,0558
PRO306 O	SU27 H78	0,056	2,7855	159,4906
PRO306 O	SU27 H77	0,003	2,7342	169,099
PRO306 O	SU27 H12	0,002	2,7897	153,4033
SER232 OG	SU27 H82	0,001	2,8627	152,0551
SER232 OG	SU27 H81	0,001	2,8365	155,9252
SER84 OG	SU27 H80	0,642	2,798	158,1049
SER84 OG	SU27 H79	0,104	2,8509	149,8058
SU27 O10	THR308 HG1	0,075	2,8418	151,6736
SU27 O11	THR308 HG1	0,064	2,7819	155,9445
SU27 O12	ARG82 H	0,025	2,8903	157,5737
SU27 O12	THR308 H	0,011	2,9252	149,259
SU27 O12	THR308 HG1	0,009	2,8024	156,7392
SU27 O12	ARG82 HH21	6,412	2,8627	167,796
SU27 O12	ARG82 HE	0,133	2,8685	146,1424
SU27 O12	ARG82 HH22	0,097	2,874	140,2308
SU27 O13	GLN135 HE22	0,001	2,8793	151,4457
SU27 O13	ARG82 HH21	0,001	2,8846	151,2356
SU27 O13	ARG82 HE	0,001	2,908	155,858
SU27 O13	ARG82 HH11	0,063	2,882	154,8897
SU27 O13	ARG82 HH12	0,669	2,8936	153,0429
SU27 O13	GLN135 HE21	0,808	2,896	156,3536
SU27 O13	ARG82 HH22	21,747	2,8666	153,1714
SU27 O14	GLN135 HE22	0,033	2,8901	155,6376
SU27 O14	THR308 HG1	0,068	2,7895	157,9389
SU27 O14	GLN135 HE21	0,042	2,8776	161,9479
SU27 O14	THR308 H	0,144	2,9357	149,2452
SU27 O14	ARG82 HH21	0,010	2,8641	151,4645
SU27 O14	ARG82 HH22	0,001	2,8745	144,8919
SU27 O14	ARG82 HH11	2,743	2,9008	146,4333
SU27 O14	ARG82 H	0,694	2,961	166,7602
SU27 O15	SER84 HG	0,611	2,8225	153,8654
SU27 O15	SER84 H	0,063	2,9197	150,2804
SU27 O15	THR308 HG1	0,006	2,8705	161,6576

	SU27 O15	ARG82 HH21	4,632	2,8307	141,3387
	SU27 O15	ARG82 HH22	9,139	2,8773	149,4843
	SU27 O15	ARG82 HH12	1,853	2,9264	149,8874
	SU27 O16	SER84 H	0,020	2,9183	155,7685
	SU27 O16	SER84 HG	0,972	2,8238	158,7655
	SU27 O16	THR308 HG1	0,003	2,8657	153,2024
	SU27 O17	TYR230 HH	0,001	2,8629	153,4956
	SU27 O17	SER232 HG	0,001	2,8554	154,5234
	SU27 O17	HIE300 HE2	0,120	2,8983	152,1902
	SU27 O18	SER232 HG	0,116	2,8498	154,6186
	SU27 O18	HIE300 HE2	0,001	2,9358	149,2402
	SU27 O2	SER84 HG	0,021	2,7475	158,9946
	SU27 O4	HIE300 HE2	0,006	2,8717	165,655
	SU27 O5	THR18 HG1	7,532	2,7912	160,305
	SU27 O5	TYR230 HH	0,578	2,8257	160,1585
	SU27 O5	GLN19 HE21	0,385	2,8937	158,3683
	SU27 O5	GLN19 HE22	0,646	2,9173	155,9062
	SU27 O5	TYR15 HH	0,048	2,8898	158,6842
	SU27 O5	HIE300 HE2	0,287	2,9029	160,1566
	SU27 O6	TYR230 HH	0,010	2,8393	158,2737
	SU27 O6	ALA228 H	0,001	2,9167	145,7903
	SU27 O9	THR308 HG1	0,013	2,8135	160,5471
	SU27 O9	GLN135 HE22	0,001	2,8904	148,5779
	SU27 O9	GLN135 HE21	5,271	2,895	151,0038
	SU27 O9	ARG82 H	0,080	2,9139	150,2132
	SU27 O9	SER84 H	1,258	2,8676	146,2811
	THR18 O	SU27 H9	0,187	2,7596	150,5548
	THR18 OG1	SU27 H9	0,013	2,7655	162,2405
	THR308 OG1	SU27 H80	0,037	2,812	149,38
	THR308 OG1	SU27 H78	4,415	2,8092	156,7855
	THR308 OG1	SU27 H77	0,579	2,8986	152,3857
	THR308 OG1	SU27 H12	1,133	2,8117	157,8572
	THR308 OG1	SU27 H11	2,577	2,8038	160,7414
	THR39 OG1	SU27 H82	5,604	2,9422	168,7683
	THR80 O	SU27 H77	2,572	2,792	163,2909
	THR80 O	SU27 H12	0,010	2,8175	151,2822
	TYR230 O	SU27 H81	0,395	2,9088	159,7184
	TYR230 OH	SU27 H9	0,094	2,8506	159,6417
	TYR230 OH	SU27 H81	0,054	2,8591	152,7233
	TYR230 OH	SU27 H10	45,654	2,8809	155,0106
	TYR83 O	SU27 H78	30,474	2,8307	155,8897
	TYR83 O	SU27 H77	0,001	2,8604	142,807
	VAL224 O	SU27 H82	0,037	2,8297	152,907
2V0Z-SU33	ALA136 O	SU33 H75	2,306	2,8786	146,046
	ARG82 O	SU33 H75	0,026	2,8081	156,6266
	ASN43 ND2	SU33 H75	0,022	2,9323	151,7329
	ASP225 OD1	SU33 H74	0,003	2,6956	159,7244
	ASP225 OD1	SU33 H73	1,146	2,7195	162,5001
	ASP225 OD1	SU33 H71	0,144	2,8828	147,2813
	ASP225 OD2	SU33 H74	0,047	2,8124	150,2626

ASP225 OD2	SU33 H73	0,034	2,8119	161,6262
ASP303 O	SU33 H74	0,011	2,7841	160,973
ASP303 O	SU33 H73	0,006	2,818	150,738
ASP303 O	SU33 H72	0,505	2,6491	157,2769
ASP303 OD1	SU33 H74	0,392	2,6945	163,8806
ASP303 OD1	SU33 H73	0,276	2,7213	158,3085
ASP303 OD1	SU33 H72	0,055	2,6881	164,2128
ASP303 OD2	SU33 H74	0,019	2,6868	164,3158
ASP303 OD2	SU33 H73	1,762	2,7105	158,2594
ASP303 OD2	SU33 H72	0,409	2,7002	166,142
ASP38 OD1	SU33 H8	0,163	2,707	162,2659
ASP38 OD1	SU33 H76	0,073	2,7421	164,6004
ASP38 OD1	SU33 H71	0,006	2,7452	162,8705
ASP38 OD2	SU33 H8	0,005	2,7064	163,3737
ASP38 OD2	SU33 H76	0,004	2,758	160,431
ASP38 OD2	SU33 H71	0,001	2,7544	156,8664
ASP38 OD2	SU33 H	0,018	2,7594	162,0063
GLN135 NE2	SU33 H75	0,228	2,8692	151,1998
GLN135 O	SU33 H75	3,62	2,7821	156,88
GLN135 OE1	SU33 H75	1,897	2,7511	161,3595
GLN19 NE2	SU33 H8	0,204	2,8871	156,6063
GLN19 NE2	SU33 H	0,121	2,8693	149,1614
GLN19 OE1	SU33 H8	0,076	2,7675	160,4929
GLN19 OE1	SU33 H	0,013	2,7797	155,9862
GLY227 O	SU33 H8	0,006	2,9813	152,6861
GLY227 O	SU33 H72	0,003	2,8225	157,1152
GLY227 O	SU33 H	0,002	2,7813	155,695
GLY40 O	SU33 H75	12,629	2,8642	151,5957
SER229 OG	SU33 H8	0,003	2,8585	164,3311
SER41 OG	SU33 H8	0,001	2,8906	156,233
SER41 OG	SU33 H75	0,002	2,8473	157,8358
SER42 OG	SU33 H75	0,327	2,8709	157,9934
SER84 OG	SU33 H74	0,079	2,8433	157,6878
SER84 OG	SU33 H71	0,01	2,7805	150,6193
SER84 OG	SU33 H	0,002	2,848	155,2321
SU33 O	SER84 HG	0,121	2,834	159,2342
SU33 O10	ARG82 H	0,023	2,8997	158,146
SU33 O10	ASN43 HD21	5,05	2,8842	157,084
SU33 O10	SER41 HG	52,443	2,8163	161,4924
SU33 O10	GLN135 HE21	1,529	2,8866	160,8782
SU33 O10	ASN43 HD22	7,268	2,8617	146,7737
SU33 O10	ARG82 HH11	0,004	2,8882	151,8333
SU33 O10	GLN135 HE22	0,199	2,8492	149,9974
SU33 O10	SER42 HG	0,02	2,9297	140,2542
SU33 O10	ARG82 HH21	2,644	2,9645	152,316
SU33 O2	THR85 HG1	33,99	2,8539	154,2476

	SU33 O3	GLN19 HE22	0,019	2,9049	159,2561
	SU33 O4	GLN19 HE22	0,007	2,8942	152,4785
	SU33 O4	GLN19 HE21	0,588	2,89	157,1005
	SU33 O4	TYR83 HH	0,014	2,8042	160,5575
	SU33 O4	THR85 HG1	1,301	2,8607	158,6723
	SU33 O4	SER229 HG	3,344	2,6995	153,6009
	SU33 O4	THR85 H	1,618	2,9689	159,8997
	SU33 O4	THR18 HG1	0,196	2,8998	156,3072
	SU33 O4	SER229 H	0,045	2,9717	149,1163
	SU33 O5	TYR83 HH	20,869	2,8441	159,0163
	SU33 O5	GLN19 HE22	2,752	2,894	152,46
	SU33 O5	GLN19 HE21	2,181	2,8885	155,5299
	SU33 O5	SER41 HG	0,006	2,8429	150,8585
	SU33 O5	THR85 HG1	3,168	2,801	157,1076
	SU33 O6	THR85 HG1	17,164	2,8655	161,6031
	SU33 O6	GLN19 HE21	0,228	2,9125	152,7141
	SU33 O6	SER41 HG	0,238	2,8332	154,0683
	SU33 O6	GLN19 HE22	0,901	2,8963	151,4896
	SU33 O6	SER84 H	0,001	2,9185	157,4322
	SU33 O6	TYR83 HH	0,162	2,8191	162,0362
	SU33 O7	SER84 HG	0,01	2,9748	160,3301
	SU33 O8	SER232 HG	10,423	2,8548	158,9822
	SU33 O8	ALA228 H	18,247	2,9123	157,7913
	SU33 O9	SER84 HG	0,003	2,834	157,7516
	THR18 O	SU33 H8	0,004	2,7217	161,9975
	THR18 O	SU33 H	0,062	2,7675	154,6926
	THR18 OG1	SU33 H8	0,032	2,7327	159,3813
	THR85 OG1	SU33 H8	0,03	2,7246	151,4885
	THR85 OG1	SU33 H71	1,005	2,8106	159,553
	THR85 OG1	SU33 H	0,104	2,8025	162,522
	TYR83 OH	SU33 H8	0,006	2,8453	160,2278
	TYR83 OH	SU33 H	0,074	2,9008	151,5592
2V0Z-SU42	ARG82 N	SU42 H13	0,019	2,9744	138,208
	ARG82 NE	SU42 H81	0,024	2,9619	138,473
	ARG82 NH1	SU42 H81	0,018	2,8687	163,0409
	ARG82 O	SU42 H13	0,002	2,7119	159,6466
	ARG82 O	SU42 H79	0,002	2,7518	156,3479
	ARG82 O	SU42 H80	0,232	2,7639	153,2123
	ARG82 O	SU42 H82	0,002	2,8194	158,8144
	ASP225 OD1	SU42 H11	10,537	2,7221	163,9589
	ASP225 OD1	SU42 H12	0,004	2,799	152,6557
	ASP225 OD1	SU42 H81	0,002	2,7565	160,6301
	ASP225 OD1	SU42 H82	0,224	2,6926	162,646
	ASP225 OD1	SU42 H83	0,167	2,6962	156,045
	ASP225 OD1	SU42 H84	0,018	2,7159	160,7154
	ASP225 OD2	SU42 H11	0,009	2,77	160,2998

ASP225 OD2	SU42 H12	0,001	2,7407	156,0527
ASP225 OD2	SU42 H81	6,01	2,8658	145,3383
ASP225 OD2	SU42 H83	1,462	2,6984	158,419
ASP225 OD2	SU42 H84	0,016	2,6561	165,4258
ASP38 OD1	SU42 H11	0,006	2,7025	162,3868
ASP38 OD1	SU42 H83	0,01	2,6656	162,8611
ASP38 OD1	SU42 H84	0,001	2,6689	164,4529
ASP38 OD2	SU42 H11	0,001	2,7267	160,4467
ASP38 OD2	SU42 H13	0,006	2,7328	151,6583
ASP38 OD2	SU42 H83	0,006	2,7291	157,024
ASP38 OD2	SU42 H84	0,04	2,6959	154,2171
GLN135 NE2	SU42 H13	0,007	2,8775	154,3154
GLN135 O	SU42 H13	0,003	2,8554	159,0238
GLN135 O	SU42 H79	0,002	2,7427	159,2385
GLN135 OE1	SU42 H12	0,001	2,7827	149,6749
GLN135 OE1	SU42 H13	0,079	2,7579	159,8025
GLN135 OE1	SU42 H79	0,076	2,7943	168,4943
GLY227 O	SU42 H	0,031	2,7789	162,1786
GLY40 O	SU42 H11	0,012	2,9117	138,9629
GLY40 O	SU42 H12	0,005	2,8016	158,3697
GLY40 O	SU42 H13	0,002	2,8506	156,7409
GLY40 O	SU42 H79	2,4	2,7922	149,9623
HIE300 ND1	SU42 H8	0,639	2,8991	158,2782
HIE300 ND1	SU42 H9	0,116	2,9203	135,6286
HIE300 NE2	SU42 H10	0,012	2,825	145,9011
PHE252 O	SU42 H10	0,002	2,8323	135,2172
PHE252 O	SU42 H9	0,443	2,8134	152,1948
SER229 OG	SU42 H	0,078	2,8682	149,0129
SER232 OG	SU42 H82	0,006	2,8713	143,023
SER84 O	SU42 H8	0,003	2,7928	159,476
SER84 OG	SU42 H	0,954	2,8678	150,2743
SER84 OG	SU42 H11	0,39	2,8118	156,4561
SER84 OG	SU42 H8	0,279	2,8001	160,0246
SER84 OG	SU42 H9	0,007	2,8499	155,2362
SU42 O	SER84 HG	0,004	2,8206	156,1419
SU42 O1	SER84 HG	0,312	2,9306	144,5143
SU42 O10	GLN135 HE22	0,092	2,9132	151,6362
SU42 O10	THR308 HG1	0,001	2,857	158,9845
SU42 O10	THR39 HG1	0,372	2,8393	149,2825
SU42 O11	ARG82 HE	0,024	2,9277	146,1947
SU42 O11	ARG82 HH21	0,02	2,89	148,2201
SU42 O11	GLN135 HE22	0,008	2,8938	147,6271
SU42 O12	THR308 HG1	0,27	2,8128	157,6919
SU42 O13	ARG82 H	0,04	2,8997	151,5084
SU42 O13	GLN135 HE21	0,033	2,893	154,9874
SU42 O13	GLN135 HE22	0,105	2,8993	158,4695

SU42 O13	TYR83 HH	0,001	2,9491	157,6447
SU42 O14	ARG82 H	0,002	2,9101	155,9056
SU42 O14	GLN135 HE21	15,584	2,8915	151,8213
SU42 O14	GLN135 HE22	67,499	2,8971	146,6099
SU42 O14	THR308 HG1	10,372	2,8599	152,6164
SU42 O15	ARG82 H	2,074	2,8916	155,41
SU42 O15	ARG82 HE	2,385	2,8872	152,5687
SU42 O15	ARG82 HH11	26,668	2,9492	149,8847
SU42 O15	ARG82 HH21	2,326	2,8972	150,8466
SU42 O15	THR308 HG1	1,244	2,835	159,2526
SU42 O16	ARG82 HE	0,005	2,9032	154,7105
SU42 O16	ARG82 HH11	62,999	2,8609	151,174
SU42 O16	ARG82 HH12	0,094	2,9455	136,2871
SU42 O16	ARG82 HH21	0,001	2,8894	152,4931
SU42 O16	ARG82 HH22	0,025	2,8304	148,1937
SU42 O16	THR308 HG1	52,705	2,7861	159,7669
SU42 O17	ARG82 HE	0,001	2,9808	165,9268
SU42 O17	ARG82 HH11	0,001	2,8931	143,9926
SU42 O17	ARG82 HH21	0,597	2,9174	149,674
SU42 O17	SER232 HG	2,998	2,9237	147,4204
SU42 O17	SER84 H	5,612	2,8845	149,5581
SU42 O18	ALA228 H	0,031	2,875	145,5198
SU42 O18	GLY40 H	0,04	2,8994	145,7332
SU42 O19	SER41 H	0,001	2,9333	140,7491
SU42 O19	SER41 HG	0,072	2,88	173,6253
SU42 O19	THR39 HG1	0,744	2,7939	156,2312
SU42 O2	SER84 H	0,005	2,9183	157,2291
SU42 O2	SER84 HG	1,416	2,7519	160,6361
SU42 O2	THR85 H	0,34	2,8998	152,1083
SU42 O2	THR85 HG1	0,001	2,8733	147,2799
SU42 O3	HIE300 HE2	0,05	2,8821	150,7163
SU42 O3	SER229 H	1,877	2,919	154,6626
SU42 O3	SER229 HG	0,007	2,9166	176,5944
SU42 O3	THR85 HG1	0,041	2,8143	147,6053
SU42 O3	TYR230 HH	0,024	2,8245	157,395
SU42 O4	HIE300 HE2	7,288	2,9656	157,5301
SU42 O4	SER84 H	0,001	2,8825	151,9844
SU42 O4	SER84 HG	56,278	2,7793	159,3549
SU42 O5	SER84 HG	0,003	2,8231	159,7245
SU42 O5	THR85 HG1	0,047	2,835	152,8027
SU42 O6	HIE300 HE2	0,954	2,8897	152,9284
SU42 O6	SER84 HG	0,017	2,8475	159,5951
SU42 O6	TYR230 HH	7,58	2,8767	172,8419
SU42 O7	SER84 HG	0,463	2,8084	161,7323
SU42 O8	SER84 H	0,108	2,9142	148,4092
THR308 OG1	SU42 H12	0,001	2,8395	157,2299

	THR308 OG1	SU42 H79	1,342	2,8641	155,4653
	THR308 OG1	SU42 H80	10,365	2,8155	159,6502
	THR308 OG1	SU42 H81	0,002	2,9454	165,8219
	THR39 OG1	SU42 H12	0,538	2,8451	154,8239
	THR39 OG1	SU42 H84	0,001	2,9751	157,4671
	THR85 OG1	SU42 H	0,001	2,8388	147,7513
	THR85 OG1	SU42 H9	0,001	2,8313	156,4019
	TYR230 OH	SU42 H	0,383	2,8509	156,6922
	TYR230 OH	SU42 H10	0,25	2,7756	168,826
	TYR83 OH	SU42 H13	0,109	2,9599	142,0948
	TYR83 OH	SU42 H79	0,021	2,879	157,0623
	VAL224 O	SU42 H12	1,675	2,7399	164,3091
2V0Z-SU52	ARG82 NE	SU52 H	10,906	2,9559	147,1653
	ARG82 NH1	SU52 H	0,477	2,9341	155,1183
	ARG82 NH2	SU52 H	0,367	2,9105	154,5307
	ARG82 O	SU52 H	0,249	2,7837	160,1687
	ASP303 O	SU52 H	0,059	2,7948	164,7951
	ASP38 OD1	SU52 H	0,027	2,5098	167,7716
	ASP38 OD2	SU52 H	0,004	2,7683	160,8006
	GLN135 O	SU52 H	0,003	2,7722	159,7948
	GLN135 OE1	SU52 H	0,010	2,8148	157,607
	PRO306 O	SU52 H	0,003	2,8033	155,2594
	SER41 OG	SU52 H	0,025	2,8447	148,9038
	SU52 O	TYR83 HH	0,045	2,8094	161,703
	SU52 O	ARG82 HH11	0,013	2,8725	152,2531
	SU52 O	ARG82 HE	0,202	2,8978	153,9702
	SU52 O	ARG82 HH21	13,768	2,8812	153,9944
	SU52 O	ARG82 HH12	0,001	2,8768	151,9767
	SU52 O	ARG82 HH22	0,007	2,9061	151,5953
	SU52 O	SER41 HG	0,059	2,9571	139,2352
	SU52 O	GLN135 HE21	0,004	2,959	146,1206
	THR308 OG1	SU52 H	0,005	2,9081	172,9241
	TYR83 OH	SU52 H	0,001	2,8349	148,7094

Lampiran 11 Surat Pernyataan Bebas Plagiasi

SURAT PERNYATAAN

Yang bertanda tangan di bawah ini,

Nama : Pebi Pebrianti

N P M : 11181035

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Bandung , Agustus 2022

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(Pebi Pebrianti)

NPM 11181035

Lampiran 12 Surat Penyataan Persetujuan Untuk Publikasi Online

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N P M : 11181035

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NPM 11181035

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