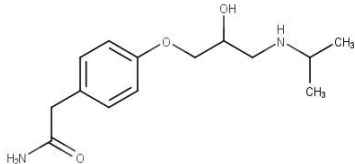
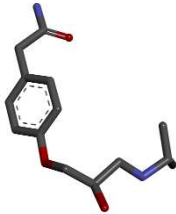
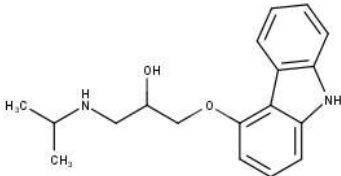
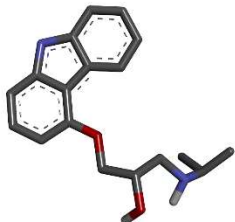
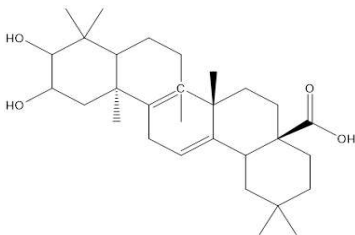
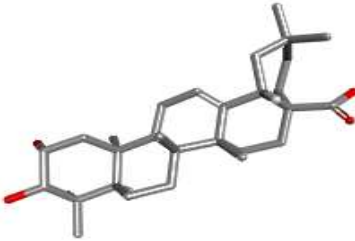
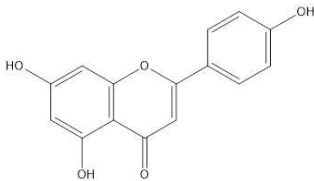
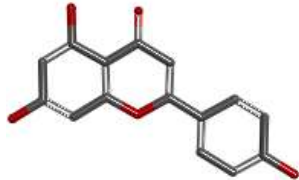
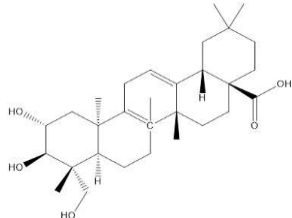
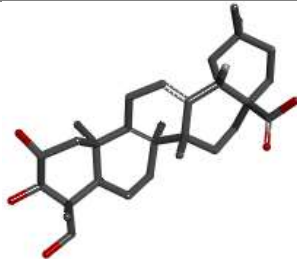
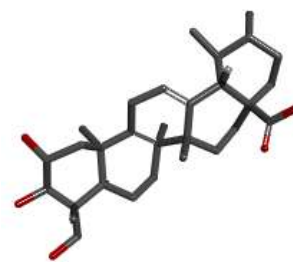
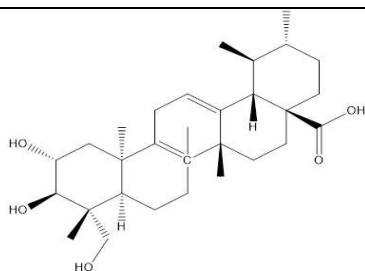


LAMPIRAN

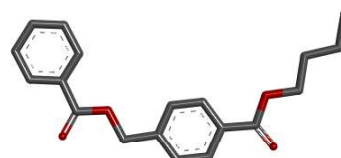
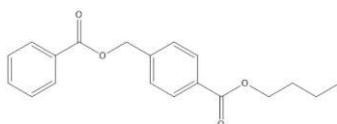
Lampiran 1 Struktur ligan pembanding, ligan kristalografi sinar-X dan ligan uji

Kode ligan	Nama Senyawa	Struktur 2D	Struktur 3D
-	Atenolol		
NL	Carazolol		
L1	3-Epimasclinic Acid		
L2	Apigenin		
L3	Arjunolic acid		

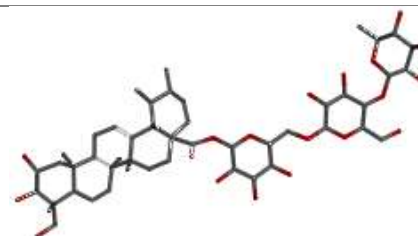
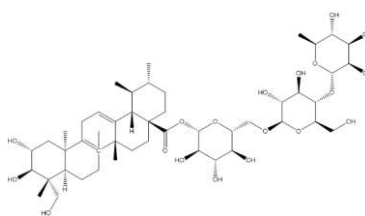
L4 Asiatic acid



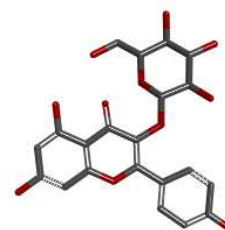
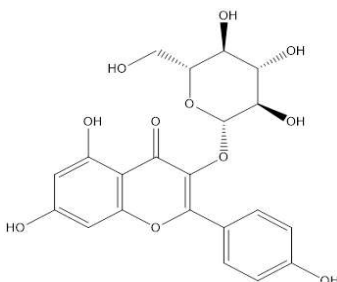
L5 Asiaticin



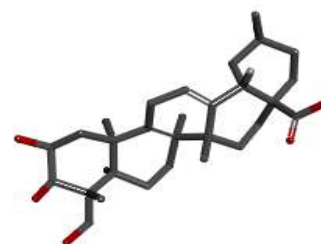
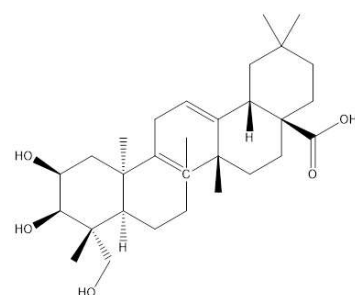
L6 Asiaticoside



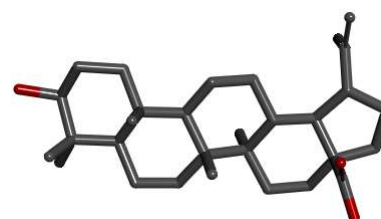
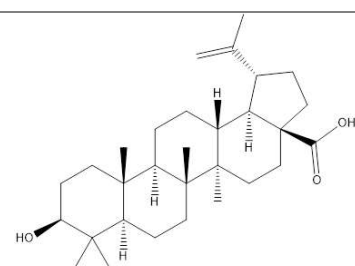
L7 Astragalin

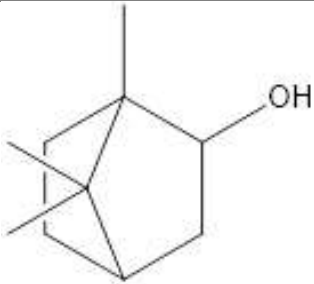
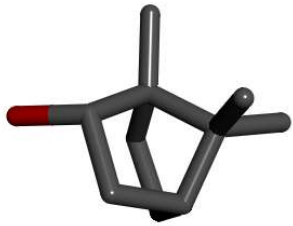
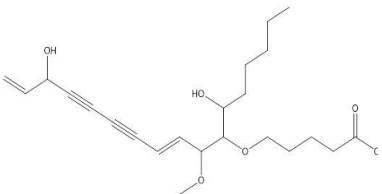
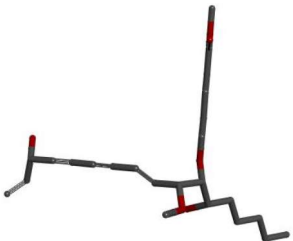
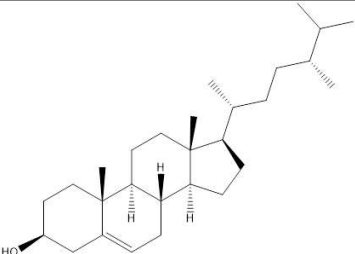
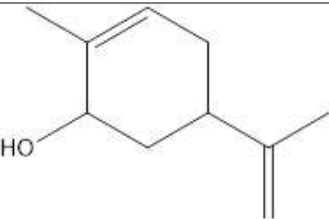
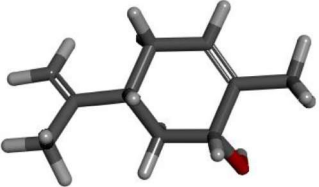
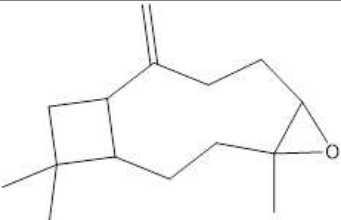
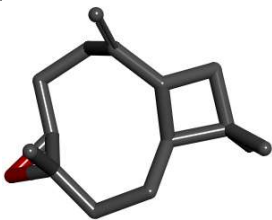
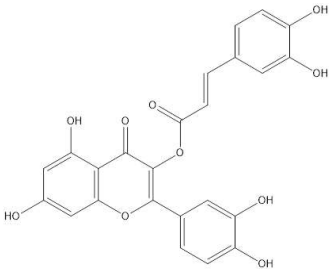
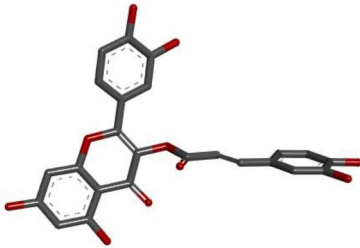


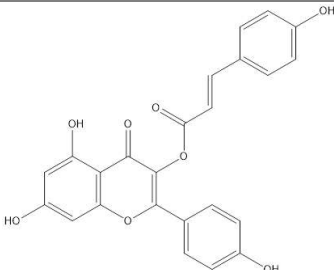
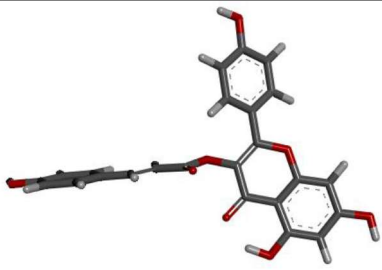
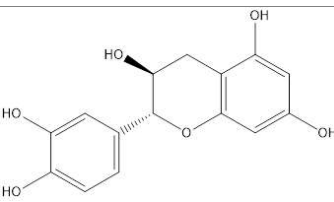
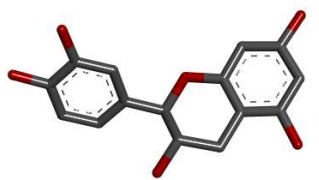
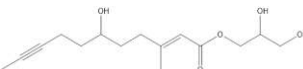
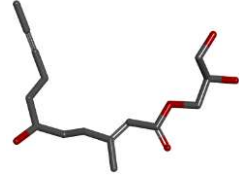
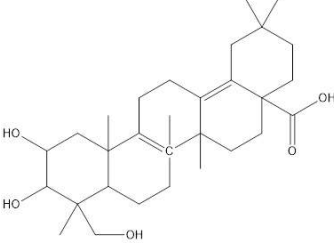
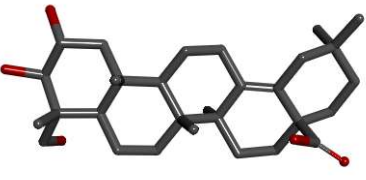
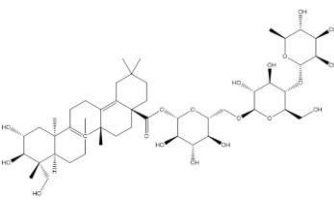
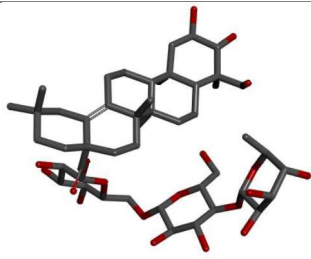
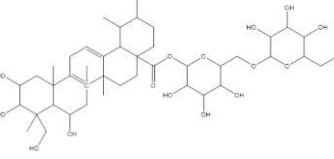
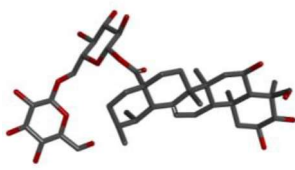
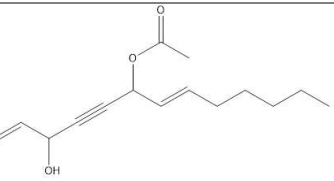
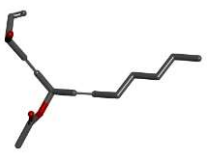
L8 Bayogenin

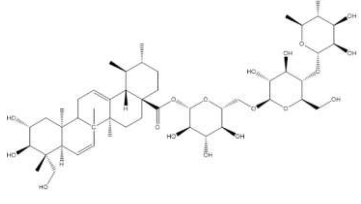
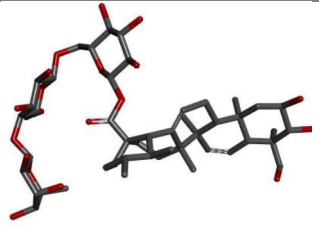
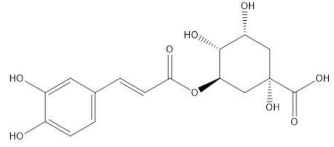
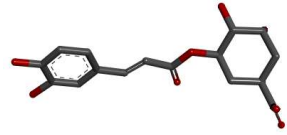
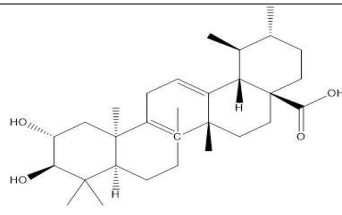
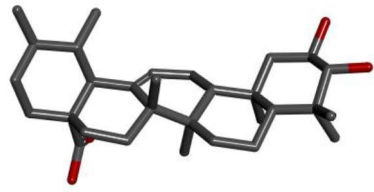
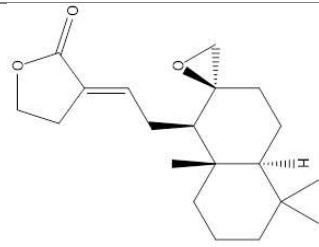
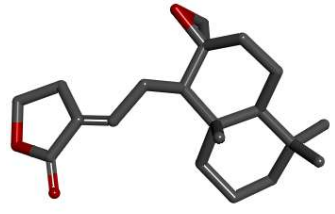
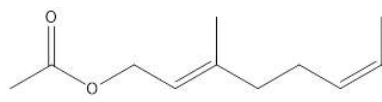
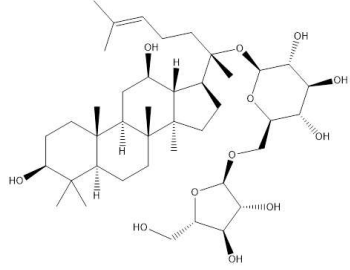
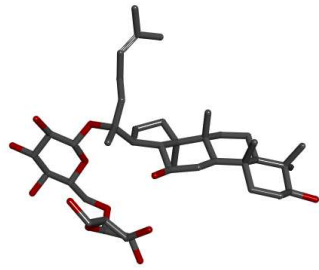
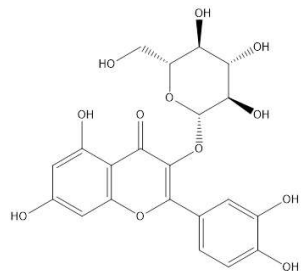
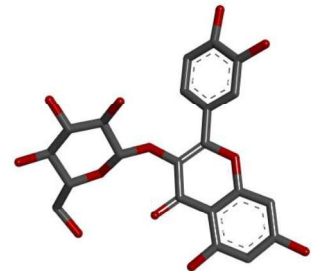
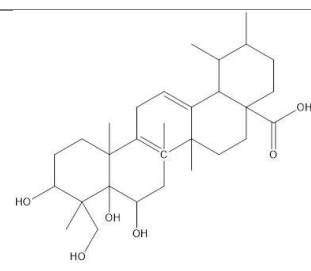
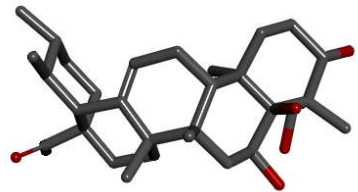


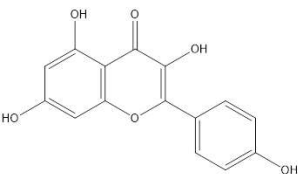
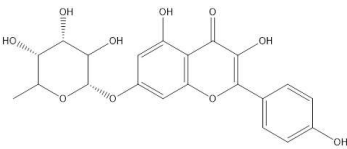
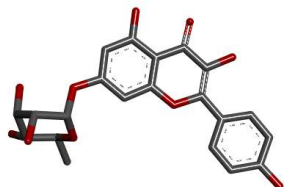
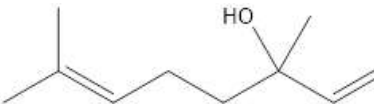
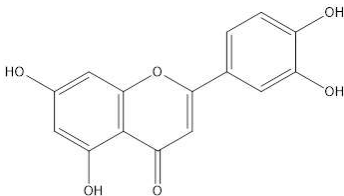
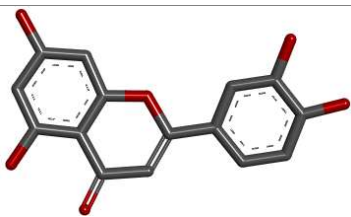
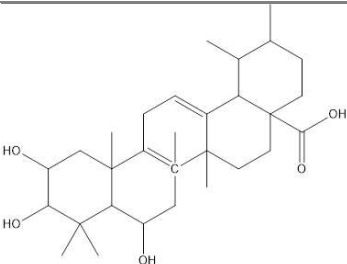
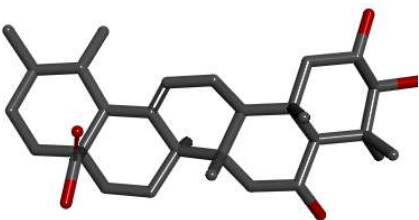
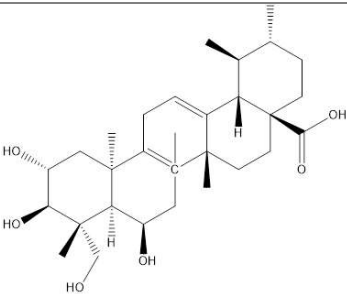
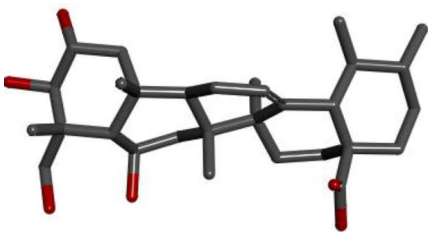
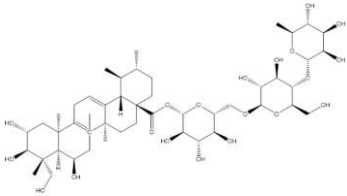
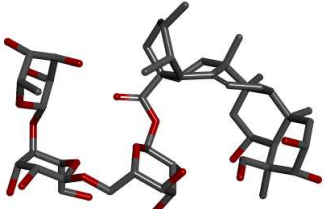
L9 Betulinic acid

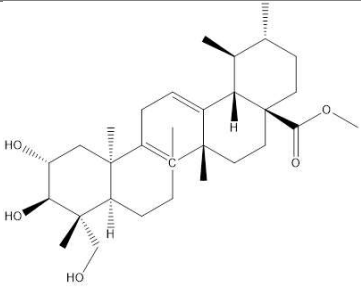
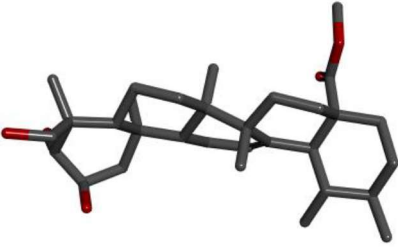
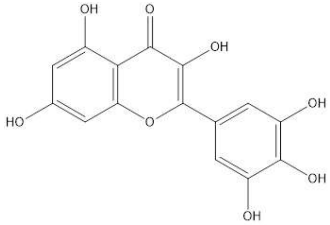
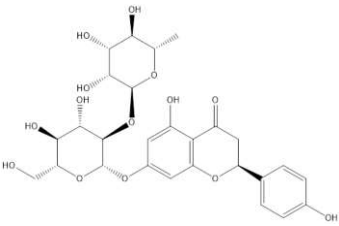
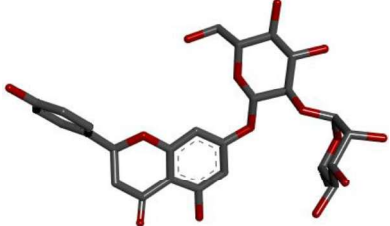
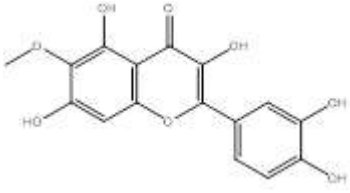
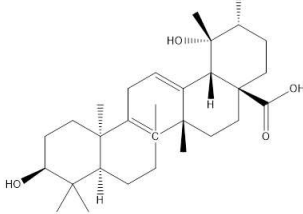
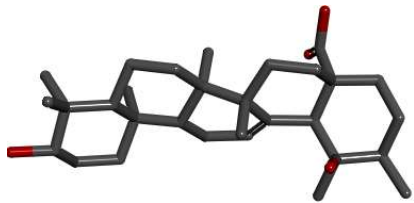
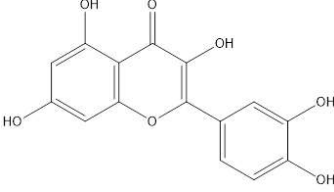
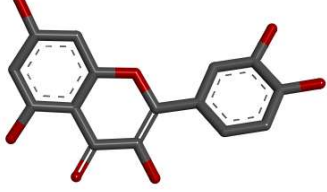
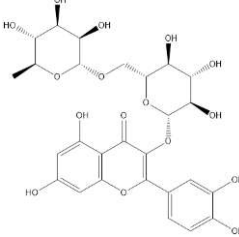
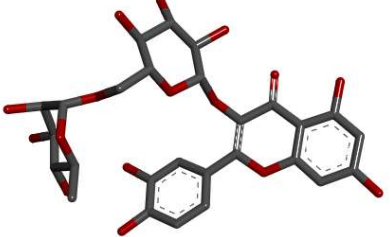


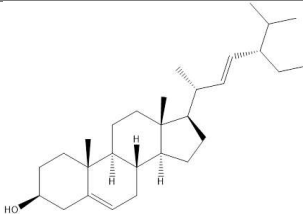
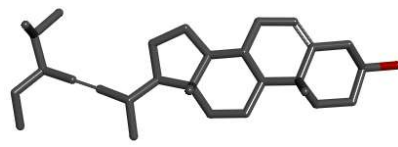
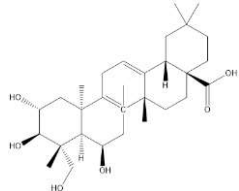
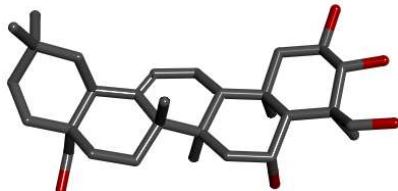
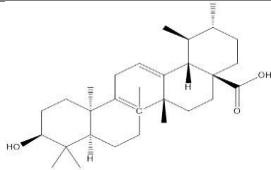
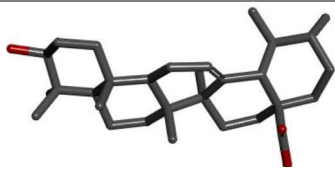
L10	Borneol		
L11	Cadiyenol		
L12	Campesterol		
L13	Carveol		
L14	Caryophyllene Epoxide		
L15	Castillicetin		

L16	Castilliferol		
L17	Catechin		
L18	Cenetellicin		
L19	Centellasapogenol A		
L20	Centellasapogenin A		
L21	Centellasapogenin B		
L22	Centellin		

L23	Centelloside E		
L24	Chlorogenic acid		
L25	Corosolic Acid		
L26	Galanolacto ne		
L27	Geranyl Acetate		
L28	Ginsenoside MC		
L29	Isoquercitrin		
L30	Isothankunic Acid		

L31	Kaempferol		
L32	Kaempferol-7-ramnosida		
L33	Linalool		
L34	Luteolin		
L35	Madasiatic Acid		
L36	Madecassic Acid		
L37	Madecassoside		

L38	Methyl Asiate		
L39	Myricetin		
L40	Naringin		
L41	Patuletin		
L42	Pomolic Acid		
L43	Quercetin		
L44	Rutin		

L45	Stigmasterol	 <chem>CC(C)/C=C/[C@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>	
L46	Terminolic Acid	 <chem>CC1(C)CC[C@H]2[C@@H](C(=O)O)CC[C@H]3[C@H]2CC[C@@H](C)[C@H]1C[C@H]3O</chem>	
L47	Ursolic Acid	 <chem>CC1(C)CC[C@H]2[C@@H](C(=O)O)CC[C@H]3[C@H]2CC[C@@H](C)[C@H]1C[C@H]3O</chem>	

Lampiran 2 Hasil optimasi ligan pembanding dan ligan uji

Kode Ligan	HOMO (kkal/mol)	LUMO (kkal/mol)	Selisih energi (kkal/mol)	Energi Total (amu)
Atenolol	-0,300	0,148	0,448	-876,080
L1	-0,221	-0,010	0,211	-1472,594
L2	-0,225	-0,076	0,149	-953,472
L3	-0,226	-0,012	0,214	-1547,779
L4	-0,221	-0,002	0,219	-1547,760
L5	-0,256	-0,058	0,198	-1036,719
L6	-0,217	-0,008	0,209	-3304,200
L7	-0,232	-0,088	0,144	-1639,195
L8	-0,223	-0,010	0,213	-1547,775
L9	-0,233	-0,014	0,219	-1397,388
L10	-0,252	-0,057	0,194	-466,995
L11	-0,220	-0,048	0,172	-1386,995
L12	-0,228	0,028	0,256	-1170,826
L13	-0,234	0,028	0,262	-390,581
L14	-0,237	0,014	0,252	-465,768
L15	-0,238	0,011	0,250	-661,021
L16	-0,217	-0,077	0,140	-1675,901
L17	-0,221	-0,074	0,147	-1525,535
L18	-0,203	0,005	0,208	-1031,032
L2	-0,249	-0,051	0,197	-961,801
L19	-0,219	-0,010	0,210	-1547,774
L20	-0,212	-0,007	0,205	-3304,215
L21	-0,225	-0,021	0,204	-2844,026
L22	-0,255	0,013	0,268	-810,186
L23	-0,0225	-0,0192	0,003	-3302,980
L24	-0,223	-0,075	0,148	-1297,149
L25	-0,22556	-0,0106	0,215	-1472,591
L26	-0,25587	-0,4680	0,212	-1005,532
L27	-0,22914	-0,0035	0,233	-619,587
L28	-0,21345	0,0277	0,241	-2506,363

L29	-0,23062	-0,0882	0,142	-1714,387
L30	-0,21807	0,01157	0,230	-1614,575
L31	-0,21765	-0,07391	0,144	-1028,648
L32	-0,21635	-0,08421	0,132	-1564,031
L33	-0,22824	0,00893	0,237	-466,969
L34	-0,21908	-0,06134	0,158	-1028,636
L35	-0,22846	-0,01470	0,214	-1547,769
L36	-0,229	-0,013	0,216	-1622,948
L37	-0,222	-0,012	0,210	-3379,355
L38	-0,219	-0,001	0,218	-1587,055
L39	-0,220	-0,077	0,143	-1179,024
L40	-0,227	-0,057	0,170	-2100,547
L41	-0,210	-0,081	0,128	-1218,341
L42	-0,220	-0,013	0,207	-1472,583
L43	-0,217	-0,076	0,141	-1103,841
L44	-0,208	-0,069	0,139	-2249,742
L45	-0,228	0,026	0,254	-1208,906
L46	-0,228	-0,012	0,216	-1622,954
L47	-0,223	-0,009	0,214	-1397,397

Lampiran 3 Interaksi ligan uji dengan residu asam amino

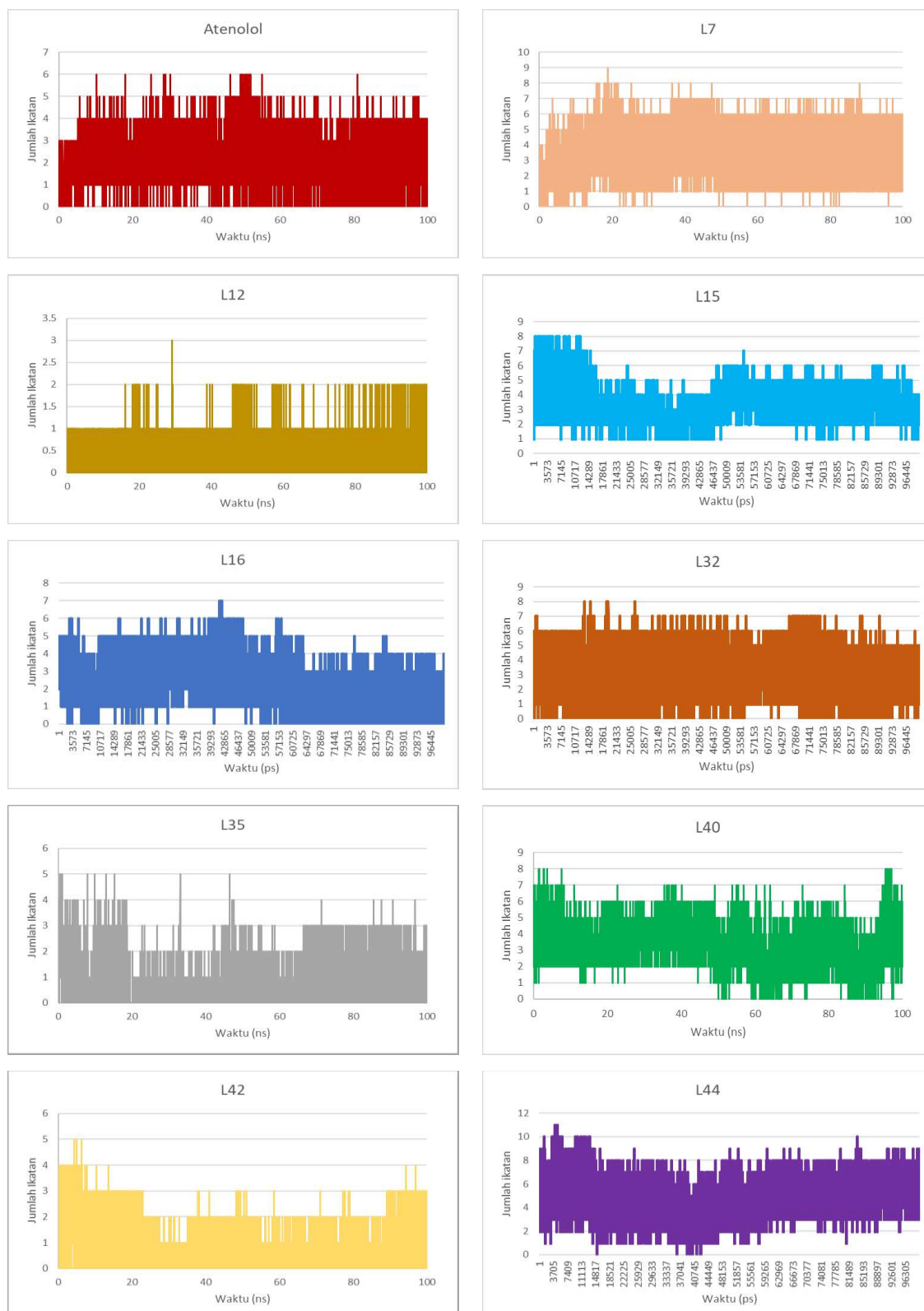
Kode ligan	Residu asam amino
Atenolol	TRP1134, ASP1138 , VAL1139, PHE1218, TYR1224, TYR1367
L1	ASP1138 , CYS1216
L2	ASP1138 , VAL1142, PHE1218, THR1220, PHE1340, ASN1344, LYS1347
L3	ASP1138 , CYS1216
L4	ASP1138 , CYS1216
L5	ASP1138 , VAL1142, PHE1218, THR1220, ARG1222, ALA1225, ASN1344, LYS1347, ALA1348,
L6	GLY1115, TRP1134, VAL1139, PHE1218, THR1220, ALA1225, SER1228 , SER1229, PHE1341 , ASN1344, LYS1347, ASP1356
L7	THR1135, ASP1138 , VAL1139, PHE1218, SER1228 , PHE1340, PHE1341 , LYS1347, PHE1359, ASN1363
L8	ASP1138 , CYS1216, PHE1218
L9	ILE1118, TRP1134, CYS1216, TRP1364
L10	ILE1118, TRP1134, TRP1364, TYR1367
L11	ILE1118, VAL1119, ASP1138 , VAL1142, PHE1218, THR1220, PHE1233, PHE1340, PHE1341 , VAL1360, TRP1364
L12	ILE1118, TRP1134, VAL1139, PHE1218, PHE1340
L13	PHE1218, TYR1224, ASN1344
L14	ILE1118, VAL1360, TRP1364
L15	ILE1118, VAL1360, TRP1364, PHE1218, THR1220, TYR1224,

	ALA1225, SER1228 , PHE1340, ASN1344, VAL1360, ASN1363 , TRP1364, TYR1367
L16	GLY1115, ILE1118, ASP1138 , VAL1139, VAL1142, PHE1218, THR1220, PHE1340, ASN1344, LYS1347
L17	VAL1139, PHE1218, THR1220, ALA1225, SER1228 , PHE1341
L18	VAL1139, VAL1142, PHE1218, THR1220, TYR1224, SER1228 , PHE1341 , ASN1344, LYS1347
L19	ALA1225, SER1228 , ASN1344, TYR1367
L20	VAL1139, THR1143, CYS1216, PHE1218, THR1220, SER1228 , ASN1344, LYS1347, ASN1363 , TRP1364
L21	GLY1115, ASP1217, PHE1218, THR1220, ALA1225, SER1228 , ASN1344, LYS1347, TRP1364
L22	TRP1134, VAL1139, PHE1218, THR1220, ALA1225, PHE1340, ASN1344, LYS1347
L23	GLY1115, ASP1138 , VAL1142, PHE1218, THR1220, ALA1225, SER1229, TRP1337, PHE1340, ASN1344, LYS1347
L24	ASP1138 , PHE1218, TYR1224, SER1228 , SER1229, ASN1344, ASN1363
L25	ASP1138 , CYS1216
L26	ASP1138 , CYS1216, TRP1364

L27	ALA1225, SER1228 , SER1229, ASN1344, LYS1347, ALA1348
L28	PHE1218, THR1220, SER1228 , SER1232, ASN1344, LYS1347, ASN1363
L29	THR1135, ASP1138 , VAL1142 PHE1218, THR1220, TYR1224, ALA1225, SER1228 , SER1229, PHE1340, ASN1344, ASN1363 , TYR1367
L30	ASP1138 , PHE1218, SER1228 , TYR1367
L31	ASP1138 , VAL1142, PHE1218, THR1220, PHE1340, ASN1344, LYS1347
L32	CYS1216, ASP1217, PHE1218, ASN1344, LYS1347, PHE1359
L33	PHE1218, THR1220, TYR1224, ALA1225, LYS1347
L34	ASP1138 , VAL1142, PHE1218, THR1220, PHE1340, ASN1344, LYS1347, TYR1367
L35	GLY1115, ASP1217, TRP1364
L36	ASP1138 , ASP1217, PHE1218
L37	ASP1138 , ASP1217, PHE1218, THR1220, ASN1344, LYS1347, ARG1351, ASP1356, VAL1360, ASN1363
L38	PHE1218, ASN1363
L39	VAL1139, PHE1218, THR1220, ALA1225, SER1228 , SER1229, SER1232, PHE1341
L40	TRP1134, THR1135, ASP1138 , CYS1216, ASP1217, PHE1218,

	THR1220, SER1228 , ASN1344, LYS1347, PHE1359, TYR1367
L41	VAL1139, VAL1142, PHE1340
L42	CYS1216, PHE1218
L43	ASP1138 , VAL1142, PHE1218, THR1220, PHE1340, ASN1344, LYS1347, TYR1367
L44	THR1135, ASP1138 , VAL1139, VAL1142, PHE1218, SER1228 , PHE1341 , ASN1344, PHE1359, VAL1360, ASN1363
L45	ILE1118, VAL1139, VAL1142, PHE1218, PHE1340
L46	CYS1216, PHE1218
L47	CYS1216

Lampiran 4 Jumlah ikatan hidrogen selama 100 ns



Lampiran 5 Hasil Turnitin

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Lampiran 6 Surat Pernyataan Bebas Plagiasi

SURAT PERNYATAAN

Yang bertanda tangan di bawah ini,

Nama : Delfritama Ibadillah

N P M : 11181153

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

**Studi Penambatan Molekul dan Dinamika Molekul Senyawa dari Pegagan
(*Centella asiatica*) terhadap Reseptor $\beta 1$ Adrenergik sebagai Antihipertensi**

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

Bandung, 26 Juli 2022

Yang membuat pernyataan,



Delfritama Ibadillah

NPM 11181153

Lampiran 7 Surat Persetujuan untuk dipublikasikan di media on line

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Yang bertanda tangan di bawah ini,

Nama : Delfritama Ibadillah

N P M : 11181153

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

**Studi Penambatan Molekul dan Dinamika Molekul Senyawa dari Pegagan
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Yang membuat pernyataan,



Delfritama Ibadillah

NPM 11181153