

LAMPIRAN

Lampiran 1. Nama senyawa dan kode SMILE

No.	Nama Senyawa	Kode SMILE
1.	4-Hydroxybenzaldehyde	<chem>C1=CC(=CC=C1C=O)O</chem>
2.	4-Hydroxybenzoic acid	<chem>C1=CC(=CC=C1C(=O)O)O</chem>
3.	Gallic Acid	<chem>C1=C(C=C(C(=C1O)O)O)C(=O)O</chem>
4.	Formaldehyde	<chem>C=O</chem>
5.	Lovenox	<chem>CC(=O)NC1C(C(C(OC1O)COS(=O)(=O)O)OC2C(C(C(C(O2)C(=O)O)OC3C(C(C(C(O3)CO)OC4C(C(C(C(O4)C(=O)O)O)O)OS(=O)(=O)O)OS(=O)(=O)O)NS(=O)(=O)O)OS(=O)(=O)O)O</chem>
6.	9,12,15-Octadecatrienoic acid	<chem>CCC=CCC=CCC=CCCCCCCCC(=O)O</chem>
7.	Palmitic Acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
8.	Phenol	<chem>C1=CC=C(C=C1)O</chem>
9.	2,4,6-Tribromophenol	<chem>C1=C(C=C(C(=C1Br)O)Br)Br</chem>
10.	Cholesterol	<chem>C[C@H](CCCC(C)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>
11.	Tyrosine	<chem>C1=CC(=CC=C1C[C@@H](C(=O)O)N)O</chem>
12.	Phenylalanine	<chem>C1=CC=C(C=C1)C[C@@H](C(=O)O)N</chem>
13.	2-Bromophenol	<chem>C1=CC=C(C(=C1)O)Br</chem>
14.	4-Bromophenol	<chem>C1=CC(=CC=C1O)Br</chem>
15.	Behenic Acid	<chem>CCCCCCCCCCCCCCCCCCCCC(=O)O</chem>
16.	Lignoceric Acid	<chem>CCCCCCCCCCCCCCCCCCCCCCCCC(=O)O</chem>
17.	Ursolic Acid	<chem>C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C(=O)O</chem>
18.	Hordenine	<chem>CN(C)CCC1=CC=C(C=C1)O</chem>
19.	3,5-Dibromo-4-hydroxybenzoic acid	<chem>C1=C(C=C(C(=C1Br)O)Br)C(=O)O</chem>
20.	Cycloartenol	<chem>C[C@H](CCC=C(C)C)[C@H]1CC[C@@]2([C@@]1(CC[C@]34[C@H]2CC[C@@H]5[C@]3(C4)CC[C@@H](C5(C)C)O)C)C</chem>
21.	24-Methylenecholesterol	<chem>C[C@H](CCC(=C)C(C)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>
22.	24-Methylenecycloartanol	<chem>C[C@H](CCC(=C)C(C)C)[C@H]1CC[C@@]2([C@@]1(CC[C@]34[C@H]2CC[C@@H]5[C@]3(C4)CC[C@@H](C5(C)C)O)C)C</chem>
23.	Terphenyllin	<chem>COC1=C(C(=C(C(=C1)C2=CC=C(C(=C2)O)OC)O)C3=CC=C(C(=C3)O</chem>
24.	Ponasterone A	<chem>CC(C)CC[C@H]([C@@](C)([C@H]1CC[C@@]2([C@@]1(CC[C@H]3C2=CC(=O)[C@H]4[C@@]3(C[C@@H]([C@@H](C4)O)O)C)O)O)O</chem>
25.	6,9,12,15-Octadecatetraenoic	<chem>CCC=CCC=CCC=CCC=CCCCC(=O)O</chem>

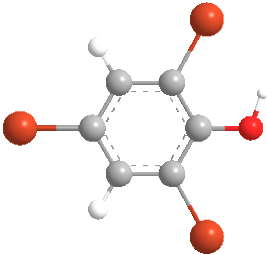
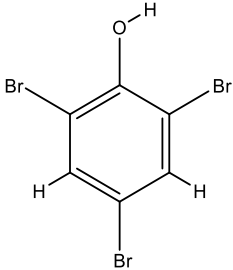
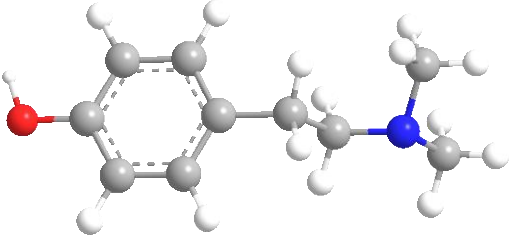
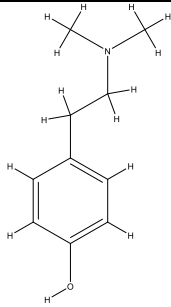
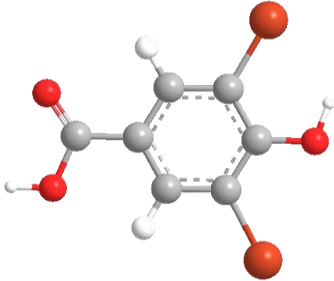
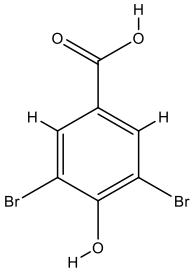
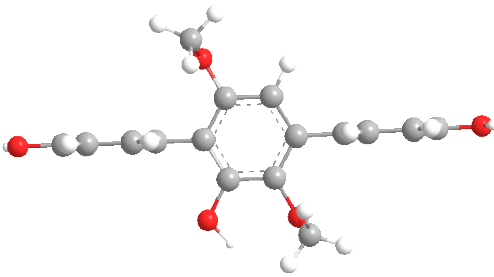
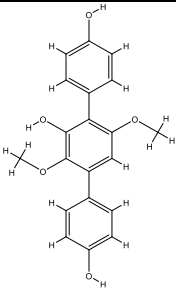
	acid	
26.	Pterosin C	<chem>C[C@H]1[C@@H](C2=C(C1=O)C(=C(C(=C2)C)CCO)C)O</chem>
27.	3-Hydroxyterphenyllin	<chem>COC1=C(C(=C(C(=C1)C2=CC=C(C(=C2)O)OC)O)C3=CC(=C(C(=C3)O)O</chem>
28.	Beta-Sitosterol	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C(C)C</chem>
29.	Lupeol	<chem>CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)C)O)C)C</chem>
30.	Clionasterol	<chem>CC[C@@H](CC[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(C)C</chem>
31.	4-hydroxy-9-(hydroxymethyl)-6-methyl-3-methylidene-4,5,9a,9b-tetrahydro-3aH-azuleno[4,5-b]furan-2,7-dione	<chem>CC1=C2C(C3C(C(C1)O)C(=C)C(=O)O3)C(=CC2=O)CO</chem>
32.	Isoquercetin	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C(=C3O2)O)O)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O</chem>
33.	Linolenic Acid	<chem>CC/C=C\C/C=C\C/C=C\C\CCCCCCCC(=O)O</chem>
34.	Isofucosterol	<chem>C/C=C(/CC[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)\C(C)C</chem>
35.	Brassicasterol	<chem>C[C@H](/C=C/[C@H](C)C(C)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>
36.	Fucosterol	<chem>C/C=C\CC[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)/C(C)C</chem>
37.	Poriferasterol	<chem>CC[C@@H](/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(C)C</chem>
38.	Isogentisin	<chem>COC1=CC2=C(C=C1)OC3=CC(=CC(=C3C2=O)O)O</chem>
39.	22,23-Dihydrobrassicasterol	<chem>C[C@H](CC[C@H](C)C(C)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>
40.	Clerosterol	<chem>CC[C@@H](CC[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(=C)C</chem>
41.	(4Z,7Z,10Z,13Z)-hexadeca-4,7,10,13-tetraenoic acid	<chem>CC/C=C\C/C=C\C/C=C\C/C=C\C\CCCC(=O)O</chem>
42.	Stearidonic Acid	<chem>CC/C=C\C/C=C\C/C=C\C/C=C\C\CCCCC(=O)O</chem>
43.	(4E,8E,11E,15E)-octadeca-4,8,11,15-tetraenoic acid	<chem>CC/C=C/CC/C=C/C/C=C/C/CC/C=C/CCCC(=O)O</chem>

	yl]pentacyclo[9.7.0.01,3.03,8.01 2,16]octadecan-6-ol	
60.	(1S,3aS,4R,8R,8aS)-1,4- dimethyl-8-propan-2-yl- 3a,5,6,7,8,8a-hexahydro-1H- azulen-4-ol	<chem>C[C@H]1C=C[C@H]2[C@@H]1[C@H](CCC[C@@]2(C)O) (C)C</chem>
61.	[(1S,3aS,4R,8S,8aR)-8-ethyl- 1,4-dimethyl-3a,5,6,7,8,8a- hexahydro-1H-azulen-4- yl]methanol	<chem>CC[C@H]1CCC[C@@]([C@@H]2[C@H]1[C@H](C=C2)C) (C)CO</chem>
62.	[(1S,3aS,4R,8S,8aR)-8-ethyl- 1,4-dimethyl-3a,5,6,7,8,8a- hexahydro-1H-azulen-4- yl]methyl acetate	<chem>CC[C@H]1CCC[C@@]([C@@H]2[C@H]1[C@H](C=C2)C) (C)COC(=O)C</chem>
63.	Prenylterphenyllin A	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C(C(=C2OC)O)C3=CC (=C(C=C3)O)O)OC)O)C</chem>
64.	4"-Dehydro-3- hydroxyterphenyllin	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C3C4=CC(=C(C=C4O C3=C2OC)OC)OC)OC)O)C</chem>
65.	Prenylcandidusin B	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C3C4=CC(=C(C=C4O C3=C2OC)OC)OC)OC)O)C</chem>
66.	Prenylterphenyllin C	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C3C4=CC(=C(C=C4O C3=C2OC)O)O)OC)O)C</chem>
67.	Prenylcandidusin A	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C3C4=CC(=C(C=C4O C3=C2OC)O)O)OC)O)C</chem>
68.	Prenylcandidusin C	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C3C4=CC(=C(C=C4O C3=C2OC)OC)O)OC)O)C</chem>
69.	Prenylterphenyllin B	<chem>CC(=CCC1=C(C=CC(=C1)C2=CC(=C(C(=C2OC)O)C3=CC =C(C=C3)O)OC)O)C</chem>
70.	(2S,3S)-sulfated pterodin C	<chem>C[C@H]1[C@@H](C2=C(C1=O)C(=C(C(=C2)C)CCOS(=O) (=O)O)C)O</chem>
71.	Candidusin C	<chem>COC1=CC=C(C=C1)C2=CC(=C3C4=CC(=C(C=C4OC3=C2 OC)O)O)OC</chem>
72.	11R-hydroxy12E-octadecenoic acid	<chem>CCCCC/C=C/[C@@H](CCCCCCCCCCC(=O)O)O</chem>
73.	Hexacos-10-ene	<chem>CCCCCCCCCCCCCCCC=CCCCCCCCCCC</chem>
74.	4"-Deoxyterphenyllin	<chem>COC1=C(C(=C(C(=C1)C2=CC=CC=C2)OC)O)C3=CC=C(C =C3)O</chem>
75.	(2R)-pterodin P	<chem>C[C@@H]1CC2=CC(=C(C(=C2C1=O)C)CCO)CO</chem>
76.	Hexadeca-4,7,10,13-tetraenoic acid	<chem>CCC=CCC=CCC=CCC=CCCC(=O)O</chem>
77.	11-Oxoctadec-12-enoic acid	<chem>CCCCC=CC(=O)CCCCCCCCCCC(=O)O</chem>
78.	(4aS,5R,6R,8aR)-6-hydroxy- 1,1,4a,6-tetramethyl-5-[(3S)-3- methylpent-4-enyl]-3,4,5,7,8,8a- hexahydronaphthalen-2-one	<chem>C[C@@H](CC[C@@H]1[C@]2(CCC(=O)C([C@@H]2CC[C@@]1(C)O)(C)C)C=C</chem>

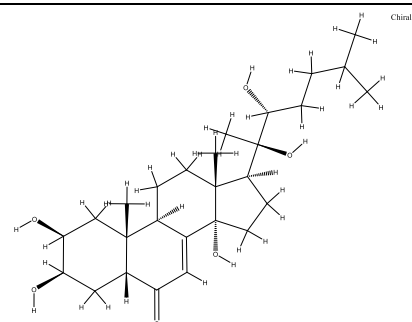
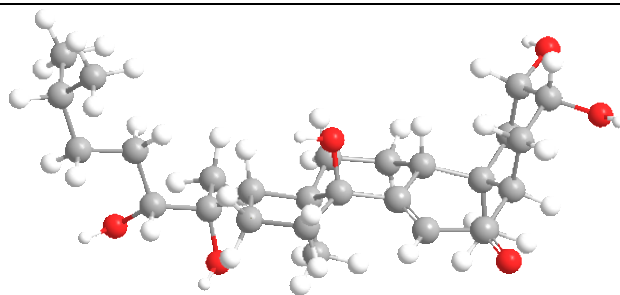
79.	(e)-6-Heptacosen-5-one	<chem>CCCCCCCCCCCCCCCCCCCC/C=C/C(=O)CCCC</chem>
80.	(z)-10-Hexacosene	<chem>CCCCCCCCCCCCCCCC/C=C\CCCCCCCC</chem>
81.	(3S,8S,9S,10R,13R,14S,17R)-17-((R,Z)-5-isopropylhept-5-en-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol	<chem>C/C=C(/CC[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)\C(C)C</chem>
82.	(1S,2R,4aS,8aS)-2,5,5,8a-tetramethyl-1-[(3S)-3-methylpent-4-enyl]-3,4,4a,6,7,8-hexahydronaphthalene-1,2-diol	<chem>C[C@@H](CC[C@@]1([C@]2(CCCC([C@@H]2CC[C@@]1(C)O)(C)C)O)C=C</chem>
83.	(1S,2R,4aS,8aR)-2,5,5,8a-tetramethyl-1-(3-methylidenepent-4-enyl)-1,2,3,4,4a,6,7,8-octahydronaphthalene	<chem>C[C@@H]1CC[C@@H]2[C@@]([C@H]1CCC(=C)C=C)(CCC2(C)C)C</chem>
84.	(1S,4S)-3,4,5,5-tetramethyl-4-(3-methylbutyl)cyclohex-2-en-1-ol	<chem>CC1=C[C@H](CC([C@]1(C)CCC(C)C)(C)C)O</chem>
85.	(6S)-1,5,5,6-tetramethyl-6-(3-methylbutyl)cyclohexene	<chem>CC1=CCCC([C@]1(C)CCC(C)C)(C)C</chem>
86.	Heptacos-6-en-5-one	<chem>CCCCCCCCCCCCCCCCCCCC=CC(=O)CCCC</chem>
87.	(5R)-octadec-6-en-5-ol	<chem>CCCCCCCCCCCC=C[C@@H](CCCC)O</chem>
88.	(1R,4R)-2,5,5-trimethyl-4-(4-methylpent-3-enyl)cyclohex-2-en-1-ol	<chem>CC1=C[C@H](C(C[C@H]1O)(C)C)CCC=C(C)C</chem>
89.	(4R)-3,4,5,5-tetramethyl-4-(3-oxopentyl)cyclohex-2-en-1-one	<chem>CCC(=O)CC[C@]1(C(=CC(=O)CC1(C)C)C)C</chem>
90.	(2R,4aR,5S,6R,8aR)-1,1,4a,6-tetramethyl-5-(3-methylidenepent-4-enyl)-2,3,4,5,6,7,8,8a-octahydronaphthalen-2-ol	<chem>C[C@@H]1CC[C@@H]2[C@@]([C@H]1CCC(=C)C=C)(C[C@H](C2(C)C)O)C</chem>
91.	(3S,8R,9R,10R,13R,14R,17R)-10,13-dimethyl-17-[(E,2R)-5-propan-2-ylhept-5-en-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	<chem>C[C@@H]1CC[C@@H]2[C@@]([C@H]1CCC(=C)C=C)(C[C@H](C2(C)C)O)C</chem>
92.	(1R,2R,4aR,6S,8aS)-2,5,5,8a-tetramethyl-1-[(3S)-3-methylpent-4-enyl]-3,4,4a,6,7,8-hexahydro-1H-naphthalene-2,6-diol	<chem>C[C@@H](CC[C@@H]1[C@]2(CC[C@@H](C([C@@H]2CC[C@@]1(C)O)(C)C)O)C=C</chem>

93.	(4aR,5S,6R,8aR)-1,1,4a,6-tetramethyl-5-(3-methylidenepent-4-enyl)-4,5,6,7,8,8a-hexahydro-3H-naphthalen-2-one	<chem>C[C@@H]1CC[C@@H]2[C@@]([C@H]1CCC(=C)C=C)(C</chem> <chem>CC(=O)C2(C)C</chem>
94.	N-[(2R,3S,4R,5R)-1,3,4,5-tetrahydroxyoctadecan-2-yl]hexadecanamide	<chem>CCCCCCCCCCCCCCCC(=O)N[C@H](CO)[C@@H]([C@</chem> <chem>@H]([C@@H](CCCCCCCCCCCCC)O)O)O</chem>
95.	(6S)-6-hydroxyoct-7-enoic acid	<chem>C=C[C@H](CCCCC(=O)O)O</chem>
96.	(E,5R)-octadec-6-en-5-ol	<chem>CCCCCCCCCCC/C=C/[C@@H](CCCC)O</chem>

Lampiran 2. Struktur senyawa 2D dan 3D ligan metabolit sekunder *Ulva lactuca*

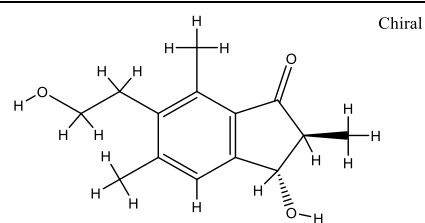
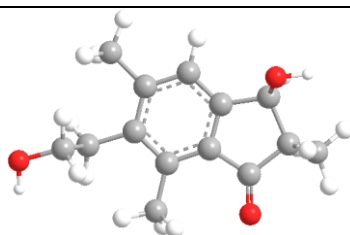
Kode Ligan	CHEMDRAW 3D	CHEMDRAW 2D
S9		
	2,4,6-Tribromophenol	
S18		
	Hordenine	
S19		
	3,5-Dibromo-4-hydroxybenzoic acid	
S23		
	Terphenyllin	

S24



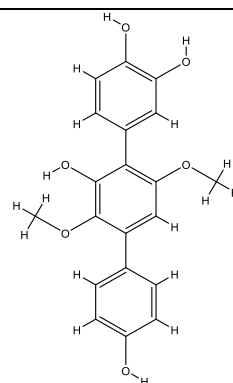
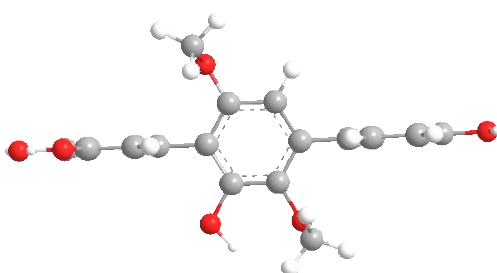
Ponasterone A

S26



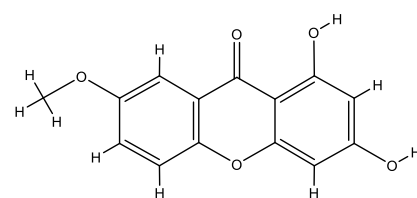
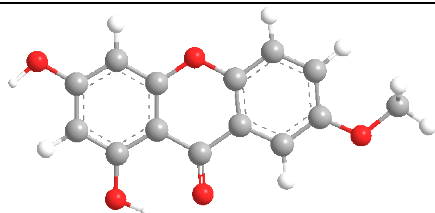
Pterodin C

S27



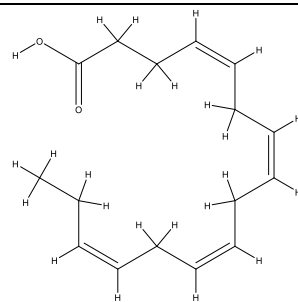
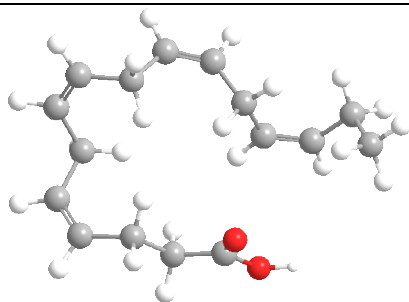
3-Hydroxyterphenyllin

S38



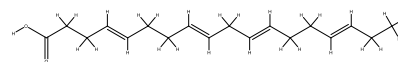
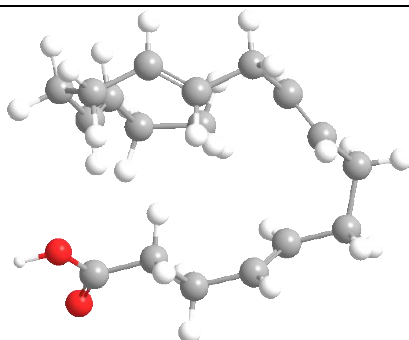
Isogentisin

S41



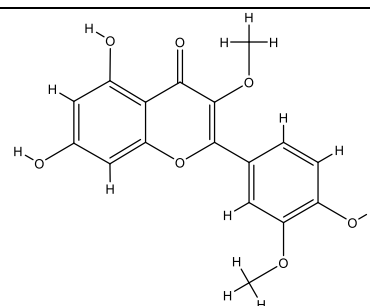
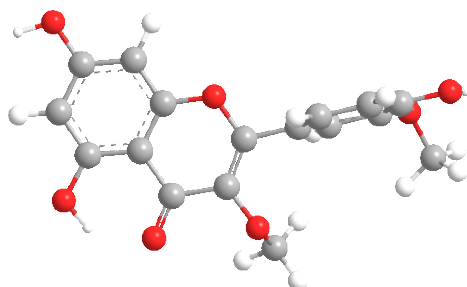
(4Z,7Z,10Z,13Z)-hexadeca-4,7,10,13-tetraenoic acid

S43



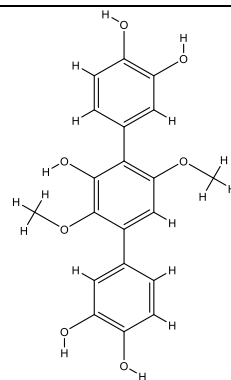
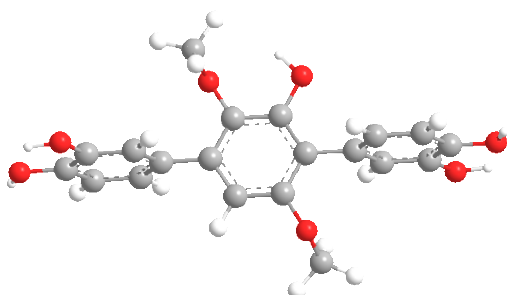
(4E,8E,11E,15E)-octadeca-4,8,11,15-tetraenoic acid

S44



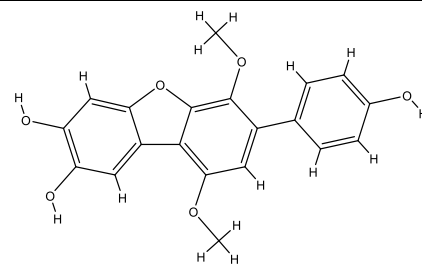
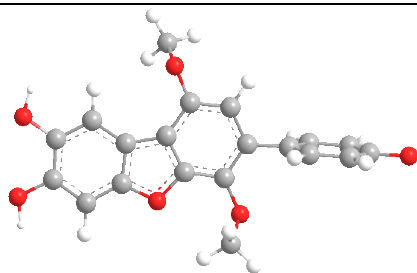
Quercetin 3,3'-dimethyl ether

S50



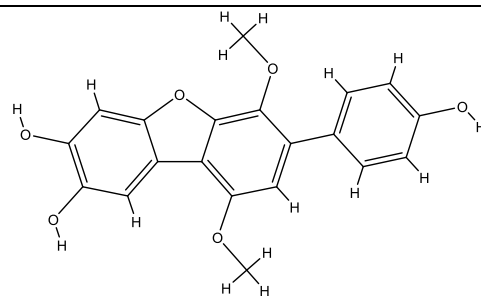
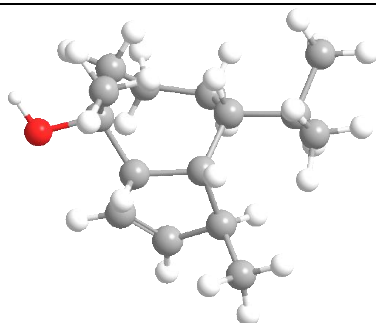
3,3''-Dihydroxyterphenyllin

S56

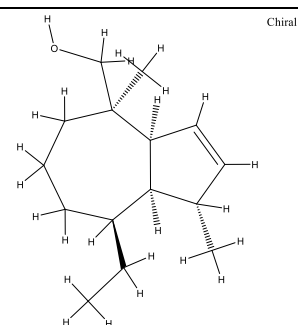
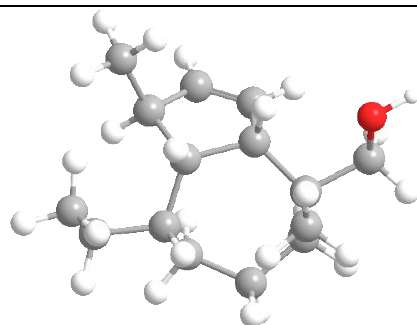


Candidusin A

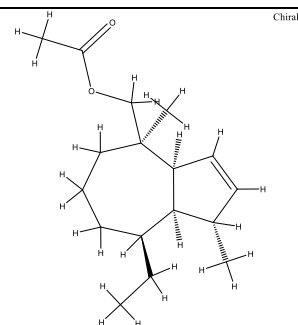
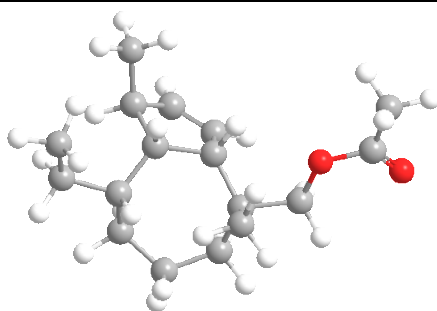
S60

 $(1S,3aS,4R,8R,8aS)$ -1,4-dimethyl-8-propan-2-yl-3a,5,6,7,8,8a-hexahydro-1H-azulen-4-ol

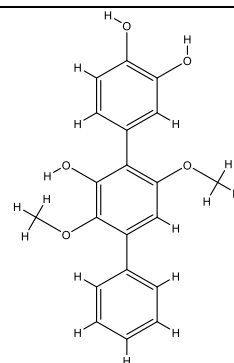
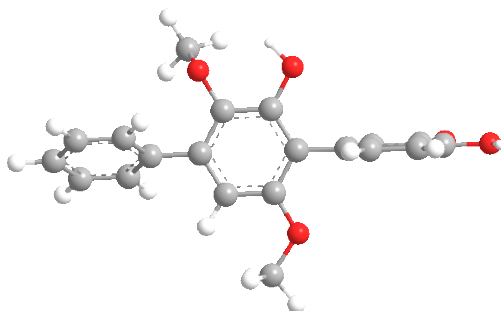
S61

 $[(1S,3aS,4R,8S,8aR)$ -8-ethyl-1,4-dimethyl-3a,5,6,7,8,8a-hexahydro-1H-azulen-4-yl]methanol

S62

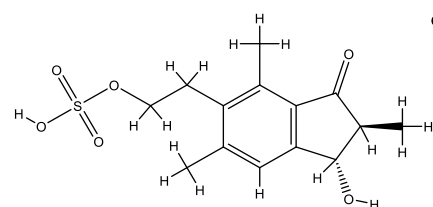
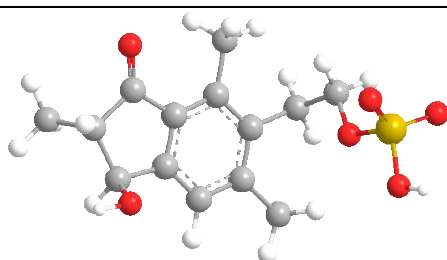
 $[(1S,3aS,4R,8S,8aR)$ -8-ethyl-1,4-dimethyl-3a,5,6,7,8,8a-hexahydro-1H-azulen-4-yl]methyl acetate

S64



4''-Dehydro-3-hydroxyterphenyllin

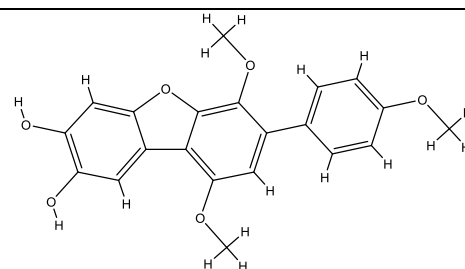
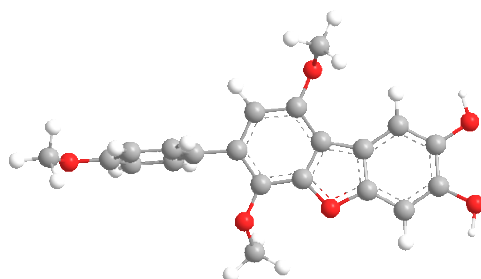
S70



Chiral

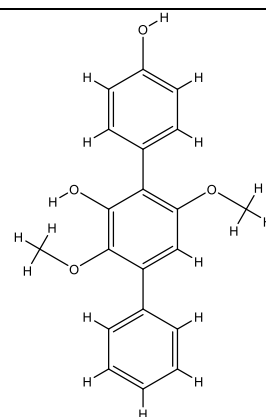
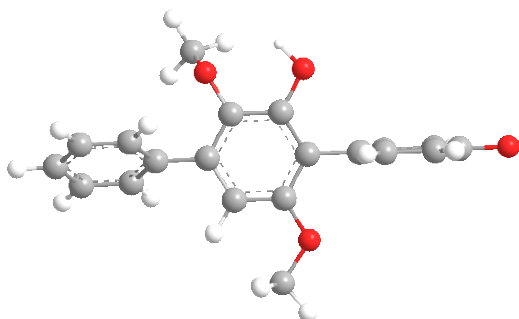
(2S,3S)-sulfated pterodin C

S71



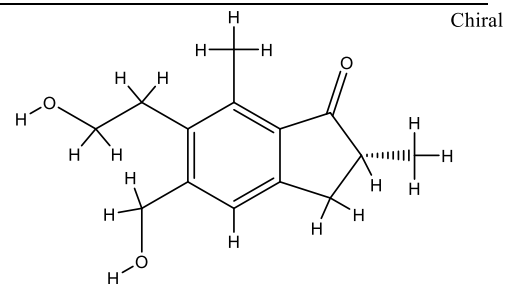
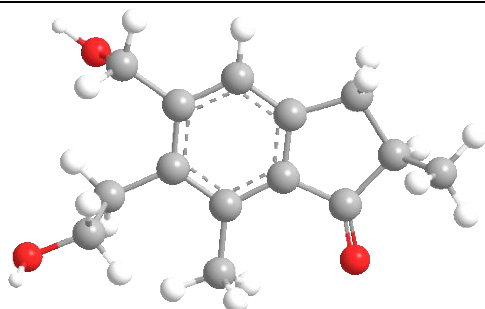
Candidusin C

S74



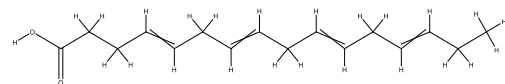
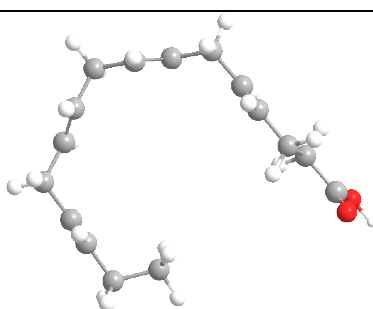
4''-Deoxyterphenyllin

S75



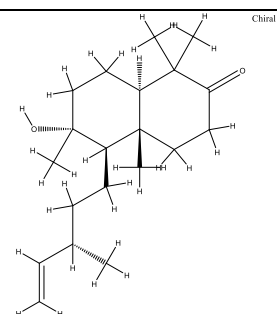
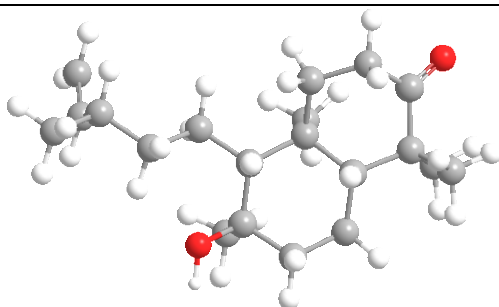
(2R)-pterosin P

S76



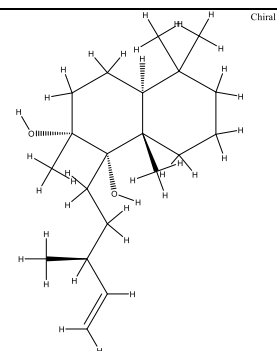
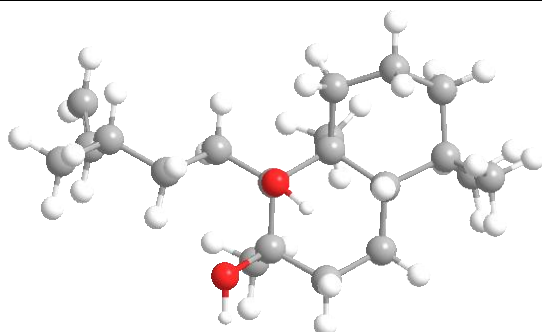
Hexadeca-4,7,10,13-tetraenoic acid

S78



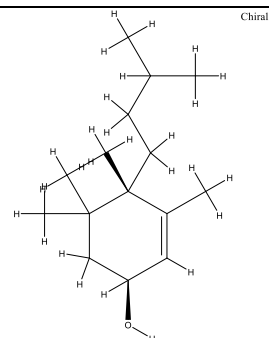
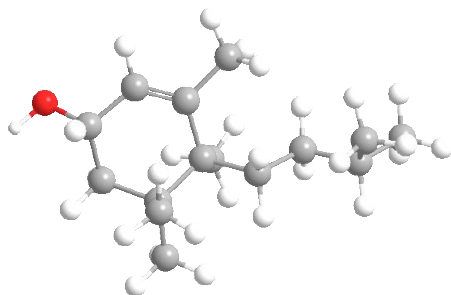
(4aS,5R,6R,8aR)-6-hydroxy-1,1,4a,6-tetramethyl-5-[(3S)-3-methylpent-4-enyl]-3,4,5,7,8,8a-hexahydronaphthalen-2-one

S82



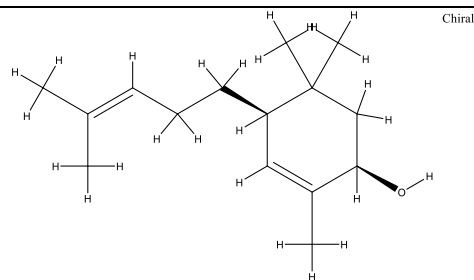
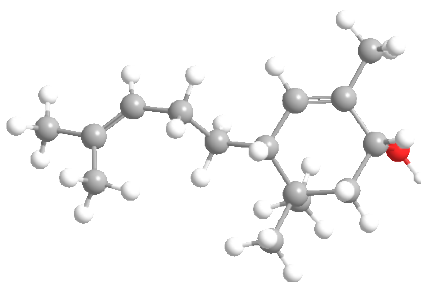
(1S,2R,4aS,8aS)-2,5,5,8a-tetramethyl-1-[(3S)-3-methylpent-4-enyl]-3,4,4a,6,7,8-hexahydronaphthalene-1,2-diol

S84



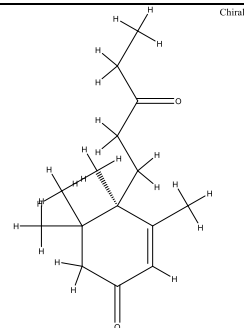
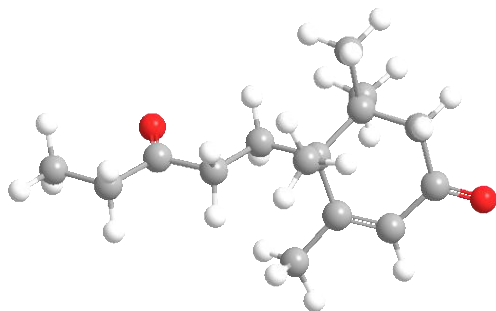
(1S,4S)-3,4,5,5-tetramethyl-4-(3-methylbutyl)cyclohex-2-en-1-ol

S88



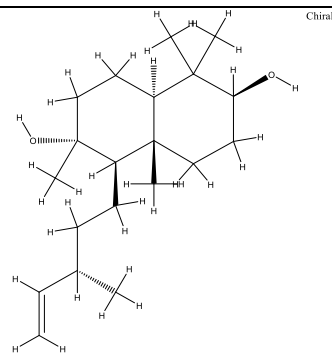
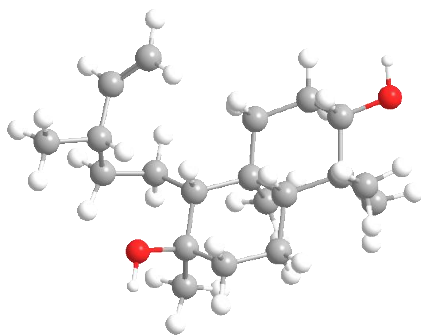
(1R,4R)-2,5,5-trimethyl-4-(4-methylpent-3-enyl)cyclohex-2-en-1-ol

S89



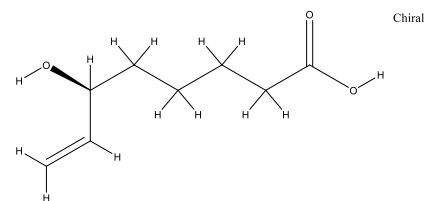
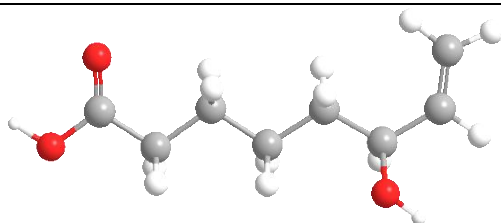
(4R)-3,4,5,5-tetramethyl-4-(3-oxopentyl)cyclohex-2-en-1-one

S92



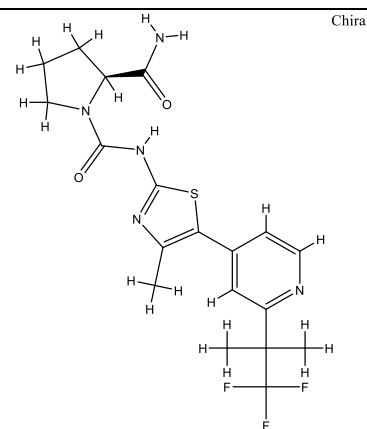
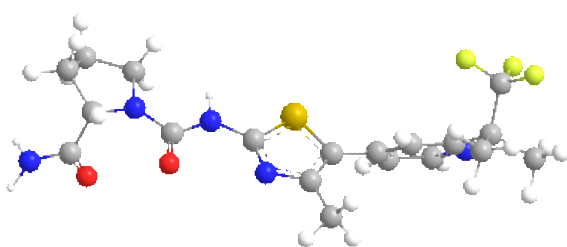
(1R,2R,4aR,6S,8aS)-2,5,5,8a-tetramethyl-1-[(3S)-3-methylpent-4-enyl]-3,4,4a,6,7,8-hexahydro-1H-naphthalene-2,6-diol

S95



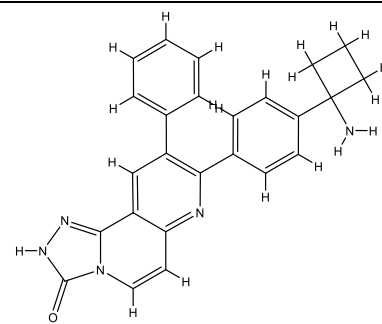
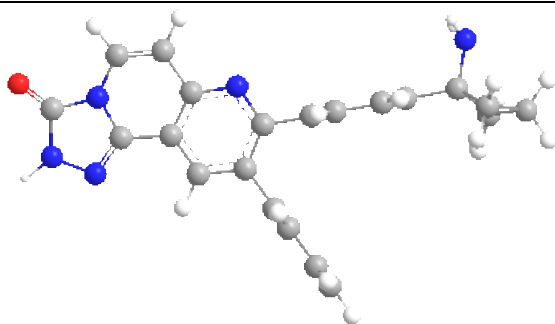
(6S)-6-hydroxyoct-7-enoic acid

PB1



Alpelisib

PB2

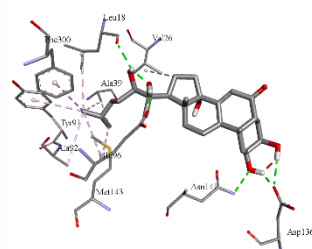
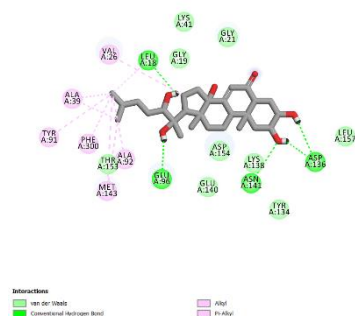


MK-2206

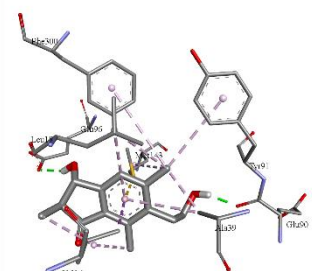
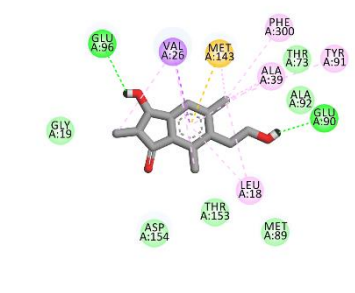
Lampiran 3. Visualisasi hasil penambatan molekul ligan uji dan ligan pembeding

Kode Ligan	Visualisasi Hasil Penambatan Molekul
S9	
S18	
S19	
S23	

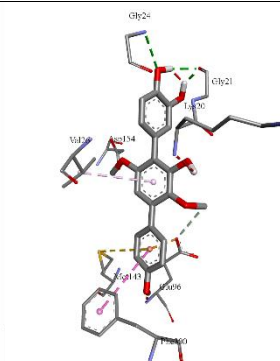
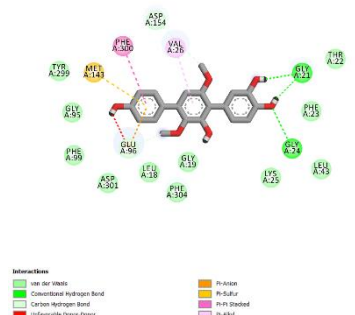
S24



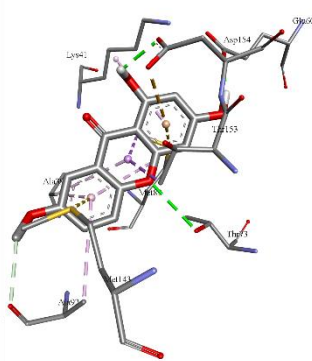
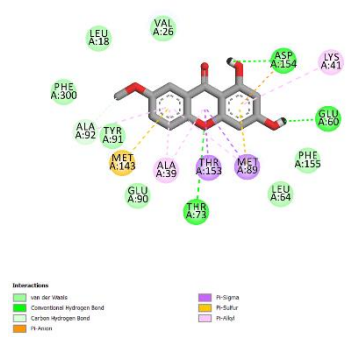
S26



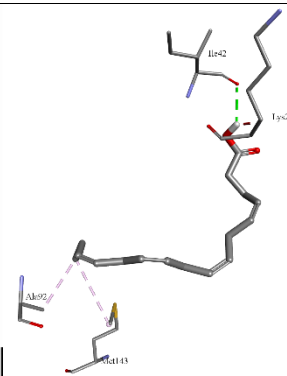
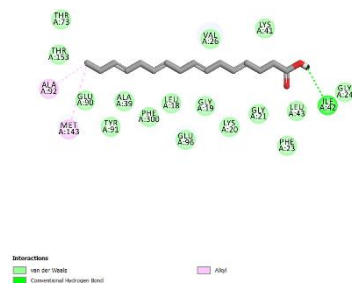
S27



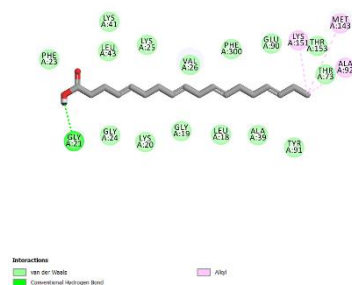
S38



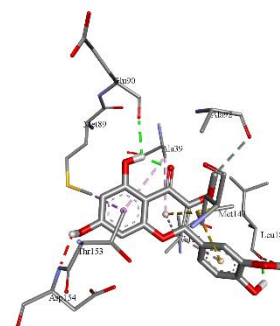
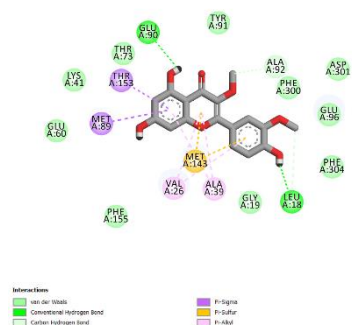
S41



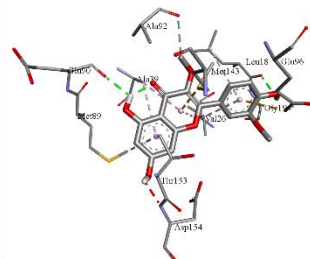
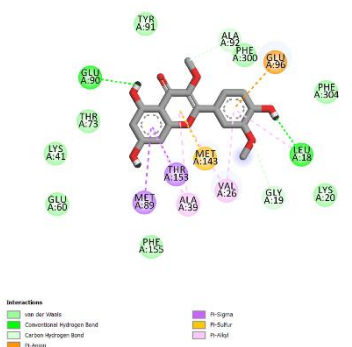
S43



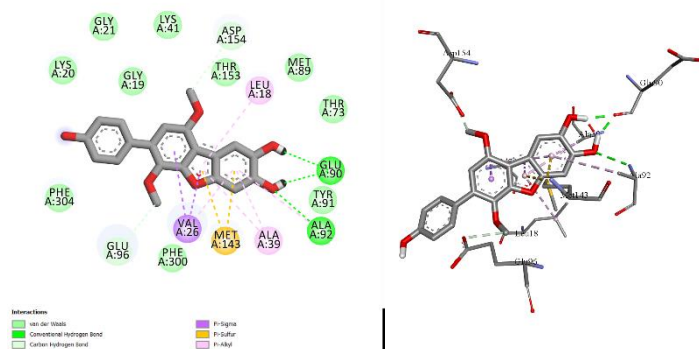
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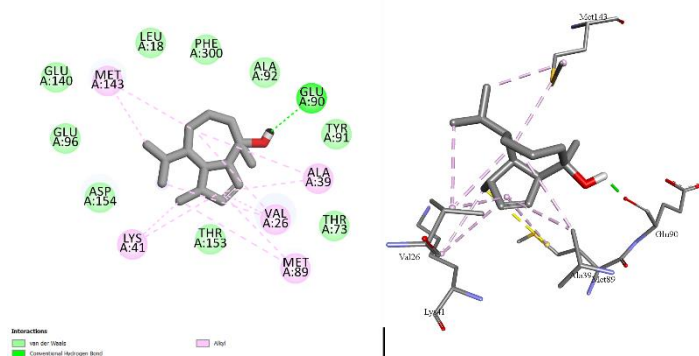
S50



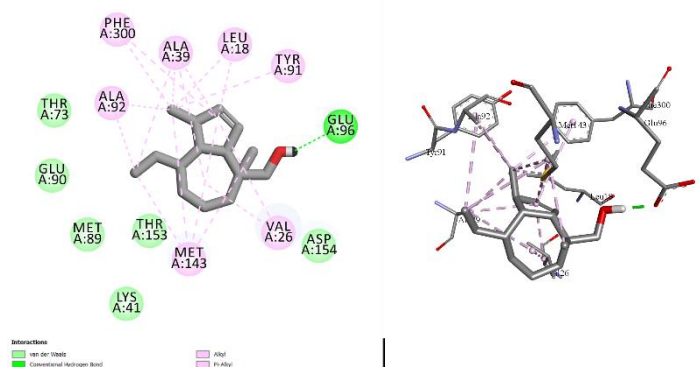
S56



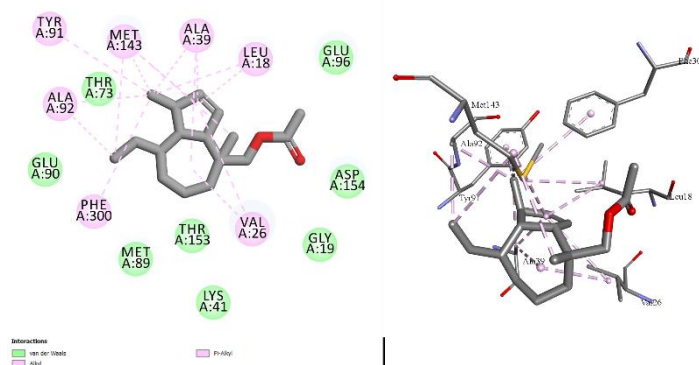
S60



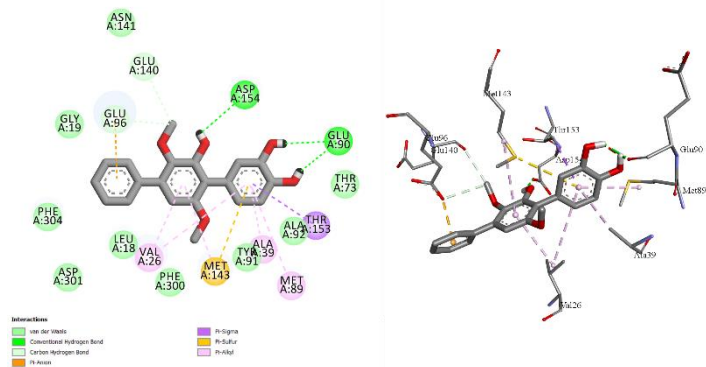
S61



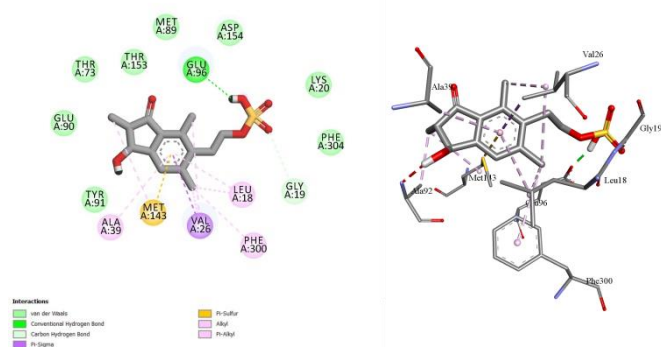
S62



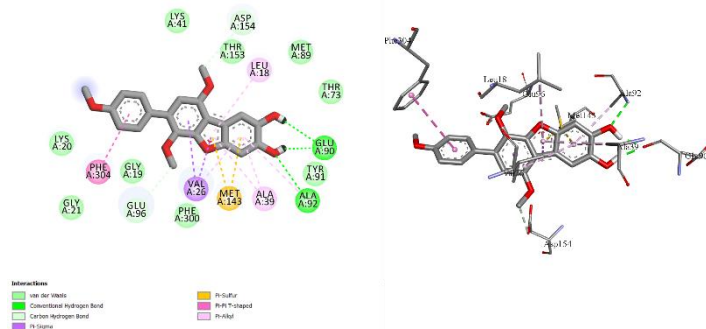
S64



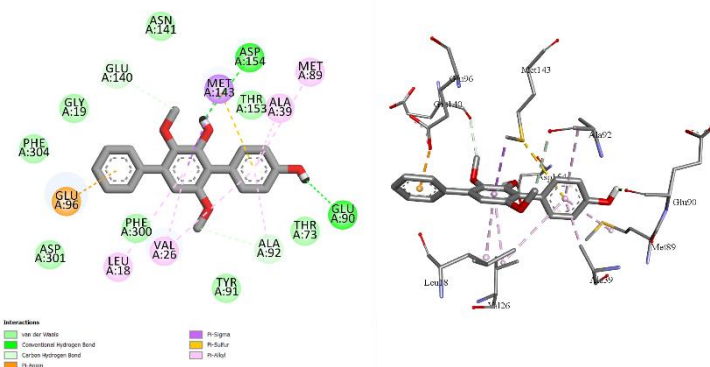
S70



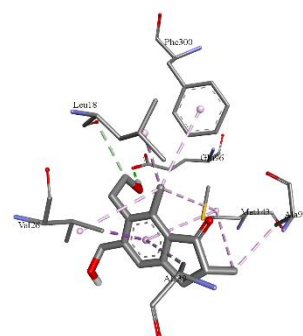
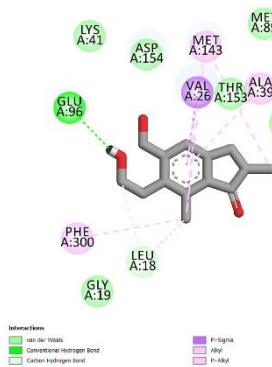
S71



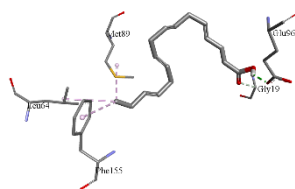
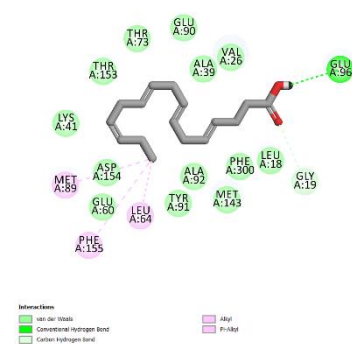
S74



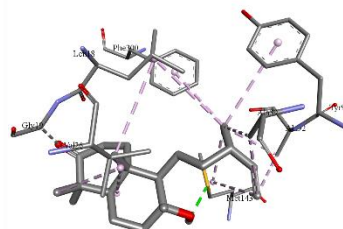
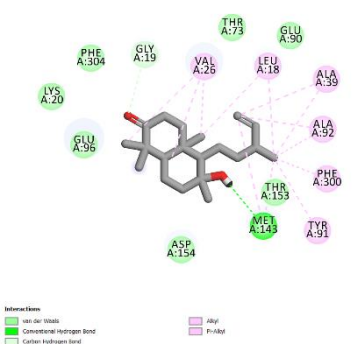
S75



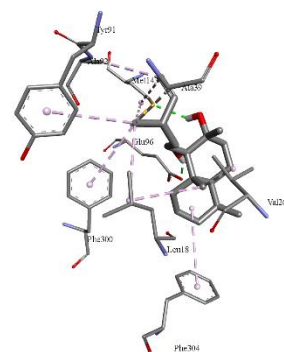
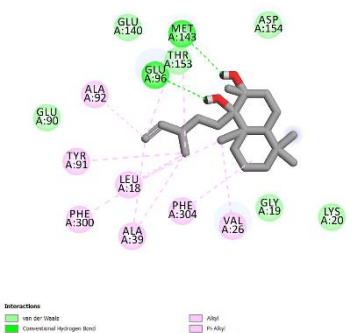
S76



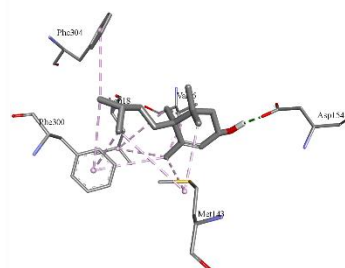
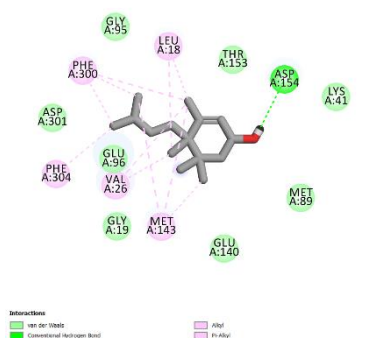
S78



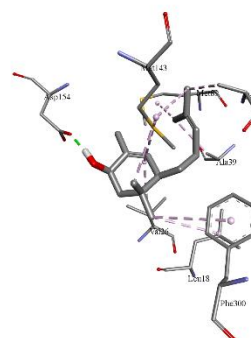
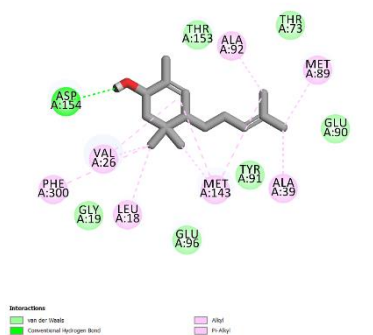
S82



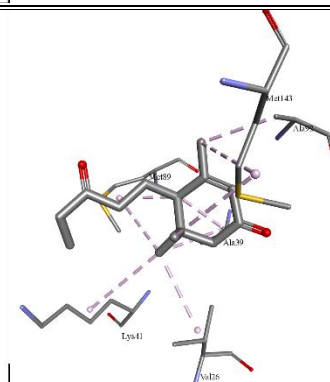
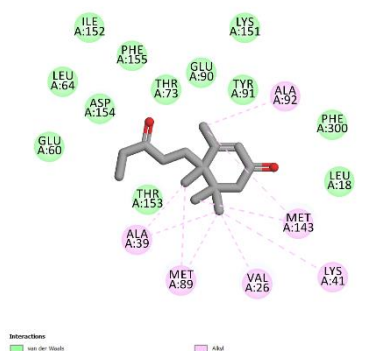
S84



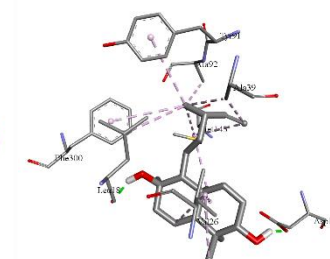
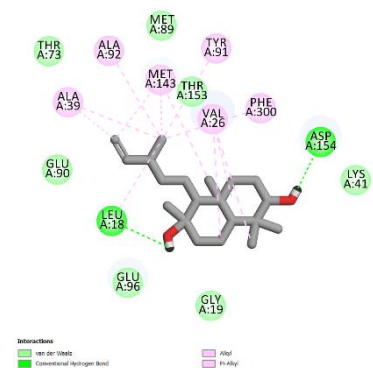
S88



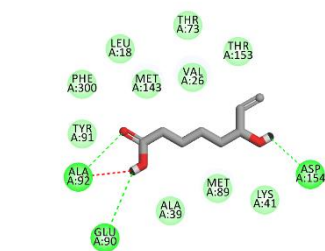
S89



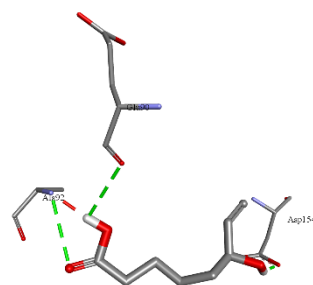
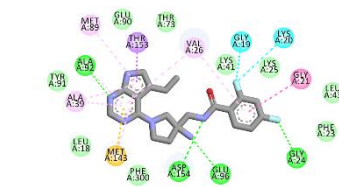
S92



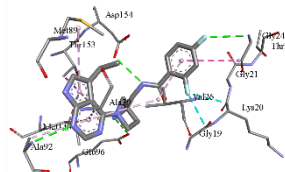
S95



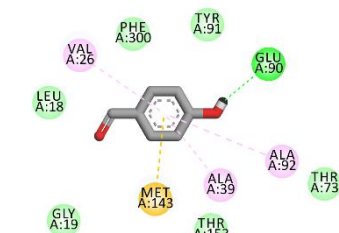
Interaktionen
van der Waals
Conventional hydrogen bond
Unconventional hydrogen bond

Ligan
Alami
WFE

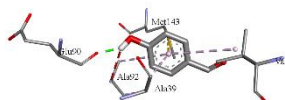
Interaktionen
van der Waals
Conventional hydrogen bond
Hydrogen (blue)
Pi-Pi
Pi-Sigma
Pi-Sulfur
Pi-Allyl



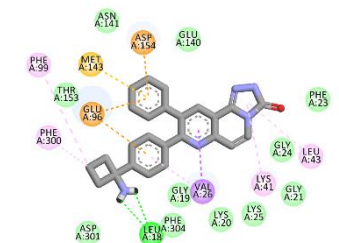
PB1



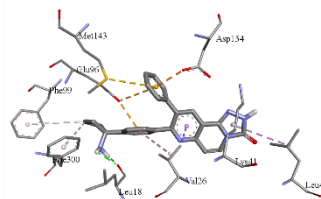
Interaktionen
van der Waals
Conventional hydrogen bond
Pi-Sulfur
Pi-Allyl



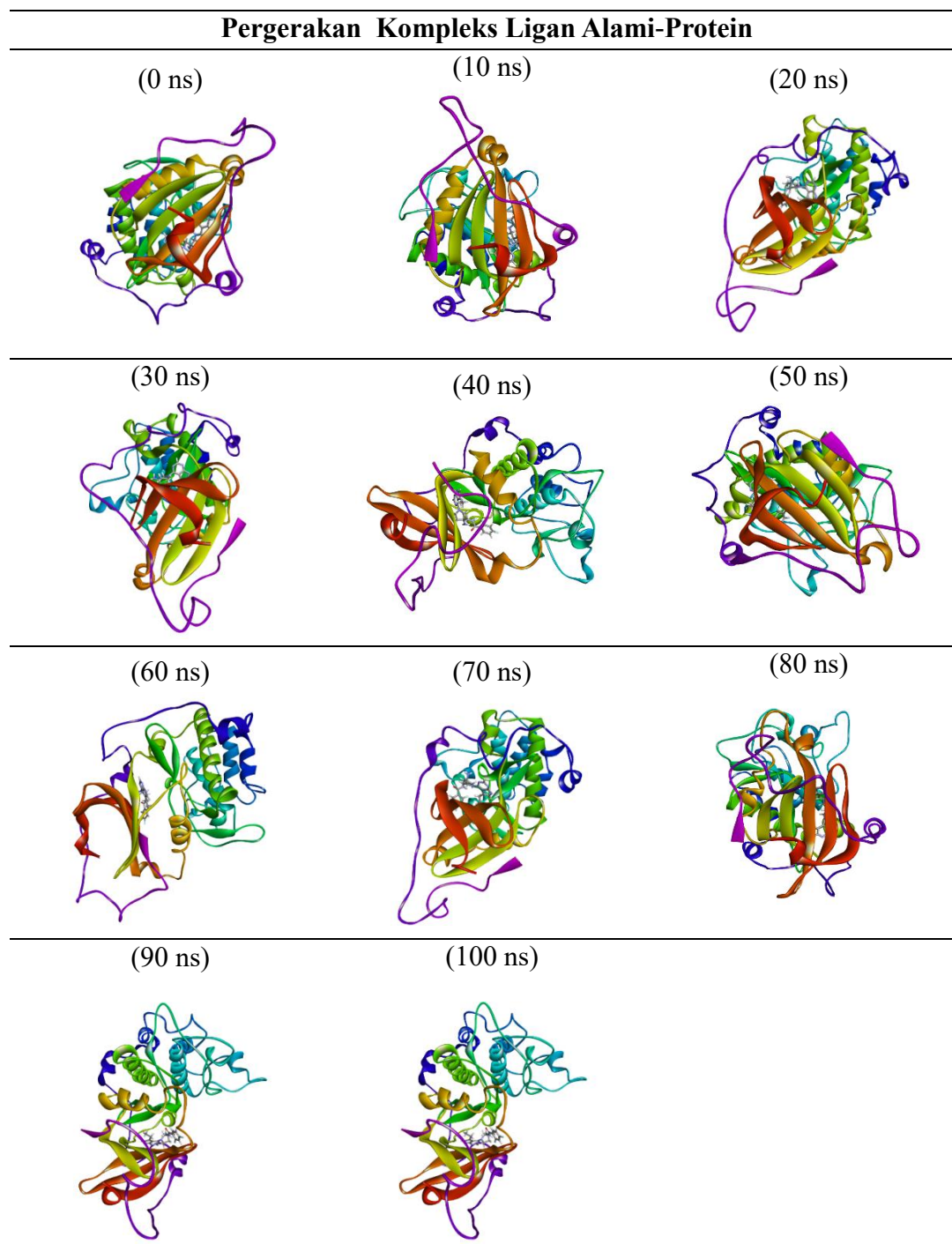
PB2



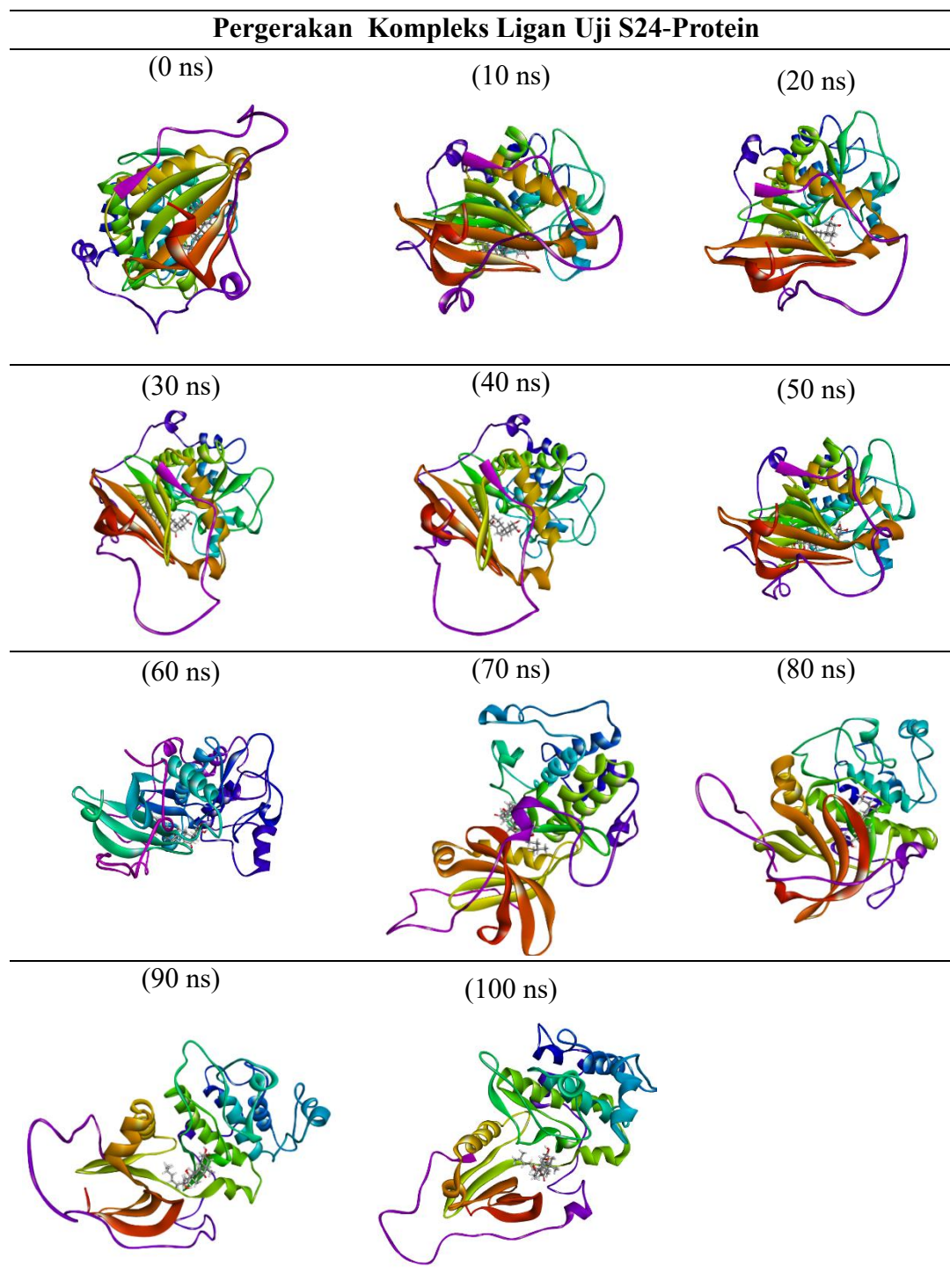
Interaktionen
van der Waals
Conventional hydrogen bond
Pi-Pi
Pi-Sigma
Pi-Sulfur
Pi-Allyl



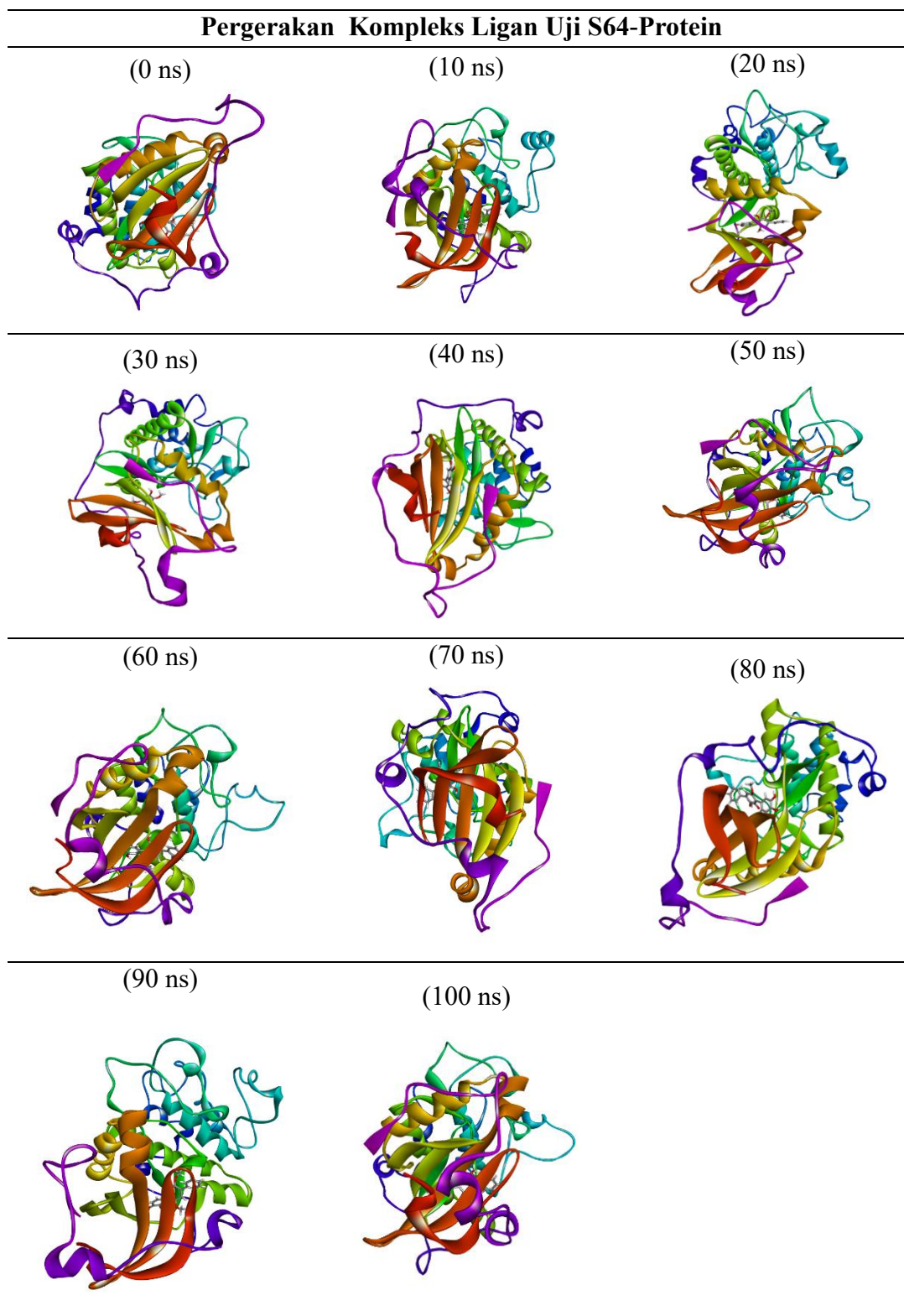
Lampiran 4. Analisis pergerakan kompleks ligan alami-protein per-ns hasil simulasi dinamika molekuler



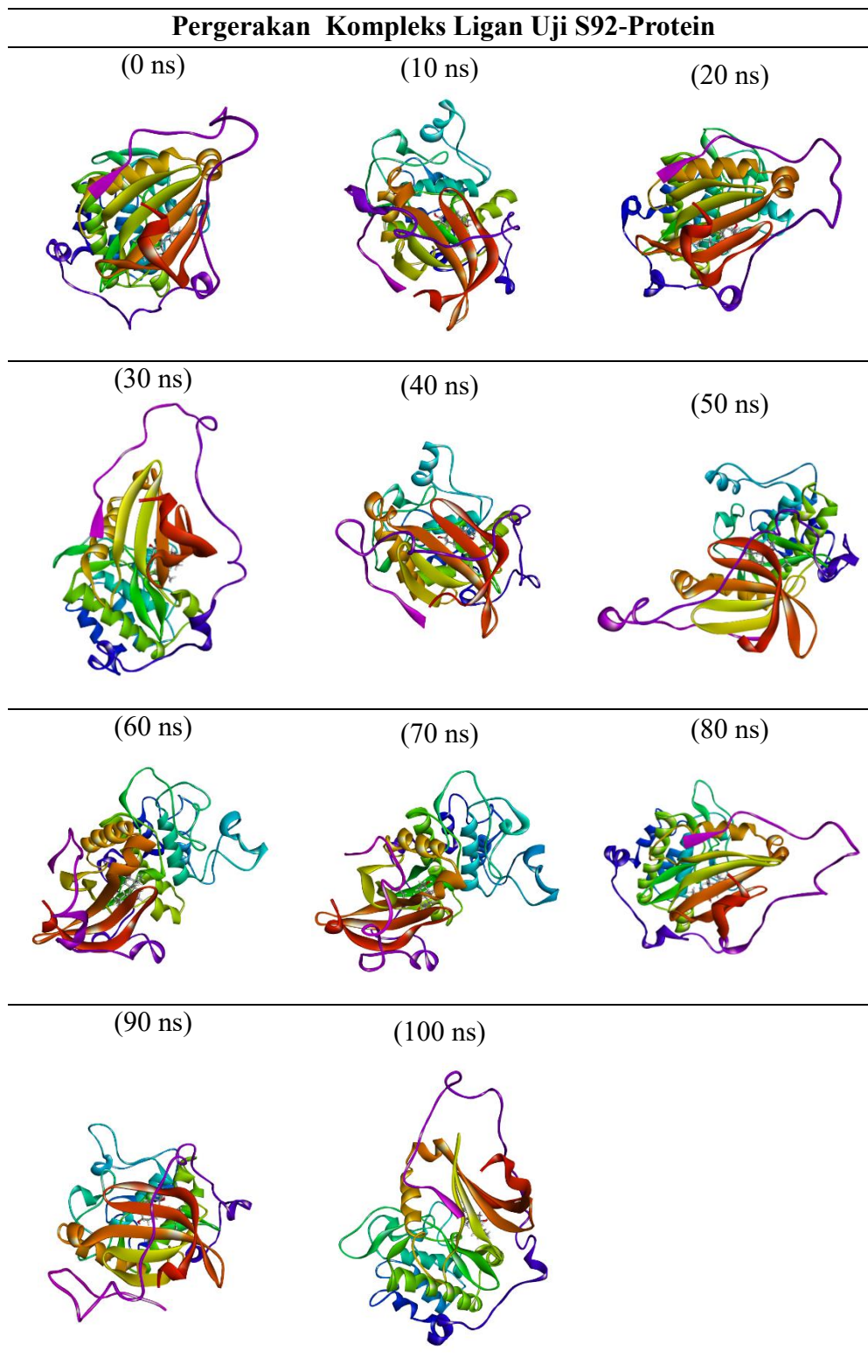
Lampiran 5. Analisis pergerakan kompleks ligan uji S24-protein per-ns hasil simulasi dinamika molekuler



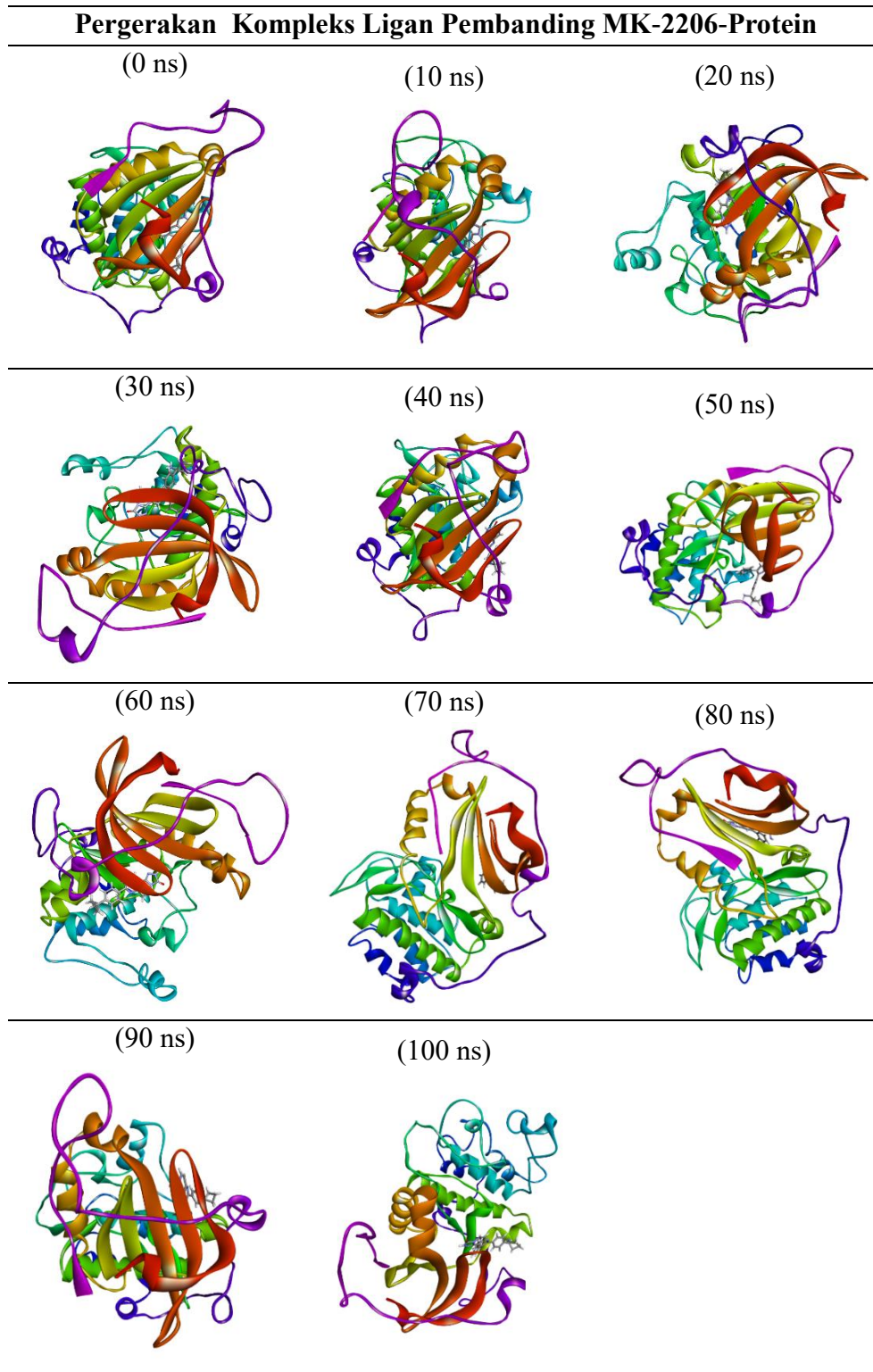
Lampiran 6. Analisis pergerakan kompleks ligan uji S64-protein per-ns hasil simulasi dinamika molekuler



Lampiran 7. Analisis pergerakan kompleks ligan uji S92-protein per-ns hasil simulasi dinamika molekuler



Lampiran 8. Analisis pergerakan kompleks ligan pembinding MK-2206-protein per-ns hasil simulasi dinamika molekuler



Lampiran 9. Bukti cek plagiarisme

Turnitin

ORIGINALITY REPORT

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SIMILARITY INDEX	INTERNET SOURCES	PUBLICATIONS	STUDENT PAPERS
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6	Submitted to Notre Dame of Marbel University Student Paper	<1 %	
Submitted to University of Surrey			

Lampiran 10. Bimbingan tugas akhir

No	Tanggal	Dosen Pembimbing	Topik	Disetujui	Aksi
1	25 April 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	kemajuan hasil	✓	 
1	4 Maret 2025	Dr Aiyi Asnawi, M.Si	Network Farmakologi	✓	 
2	5 Mei 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	kemajuan hasil	✓	 
2	11 Mei 2025	Dr Aiyi Asnawi, M.Si	Preparasi dan Validasi	✓	 
3	5 Mei 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	Progres kemauan TA	✓	 
3	18 Maret 2025	Dr Aiyi Asnawi, M.Si	Simulasi Docking	✓	 
4	16 Mei 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	Diskusi hasil ligan uji	✓	 
4	17 April 2025	Dr Aiyi Asnawi, M.Si	hasil docking	✓	 
5	21 Mei 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	Diskusi swissmodel	✓	 
5	30 April 2025	Dr Aiyi Asnawi, M.Si	Revisi Skripsi	✓	 
6	12 Maret 2025	Dr Aiyi Asnawi, M.Si	Diskusi Docking dan Visualisasi	✓	 
6	22 Mei 2025	Dr.apr. Deden Indra Dinata, S.Si., M.Si.	Diskusi Pembahasan	✓	 
7	7 April 2025	Dr Aiyi Asnawi, M.Si	Presentasi Docking dan	✓	 

Lampiran 11. Curriculum Vitae



Ayatullah Malik Al-Akbar

freshgraduate

DATA DIRI

Tempat / Tanggal Lahir
Bagansiapiapi, 7 September 2001

Jenis Kelamin
Laki-Laki

Status
Belum menikah

Kewarganegaraan
Indonesia

KONTAK

☎ 0822-6848-9445

✉ ayatullahmalik@gmail.com

📍 Jl. Tamtama, Kota Pekanbaru, RIAU

SOSIAL MEDIA

@ohmynangg

TENTANG SAYA

Calon Apoteker lulusan S1 Farmasi dengan pengalaman magang komprehensif di apotek, rumah sakit, dan industri. Terampil dalam pelayanan resep, manajemen sediaan farmasi, dan administrasi, serta berkomitmen tinggi pada ketepatan dan keamanan terapi untuk pasien.

PENDIDIKAN

PSPA Sekolah Tinggi Ilmu Farmasi Riau	2025
S1 Farmasi Bhakti Kencana University (IPK 3,26)	2023 - 2025
D3 Sekolah Tinggi Ilmu Farmasi Riau	2019 - 2022
SMA IT Imam Asy-Syafii 2 Pekanbaru	2016 - 2019
SMP Swasta Wahidin Bagansiapiapi	2013 - 2016
SD Negeri 6 Bagansiapiapi	2007 - 2013

PENGALAMAN KERJA

SRI TANJUNG TRADITIONAL CARE – Magang
Apr 2022

- Mengamati proses produksi sediaan kosmetik tradisional
- Membantu dalam pengelolaan dan penyimpanan bahan baku

CV. HERBA UTAMA – Magang
Mar 2022 – Apr 2022

- Terlibat dalam produksi sediaan herbal
- Mendukung pengelolaan gudang dan penyimpanan bahan

RS AWAL BROS A. YANI – Magang
Feb 2022 – Mar 2022

- Melakukan praktik sebagai tenaga teknis kefarmasian
- Membantu pengelolaan dan pemusnahan sediaan farmasi

APOTEK KIMIA FARMA – Magang
Jan 2022 – Feb 2022

- Melayani pelanggan dalam pembelian obat dan produk farmasi
- Mengelola stok obat serta dokumentasi administrasi apotek

KEMAMPUAN

Hard Skills

- Pelayanan Resep & Konseling
- Manajemen Stok & Administrasi
- Pelayanan Informasi Obat (PIO)
- Sistem POS Farmasi & Microsoft Office

Soft Skills

- Komunikasi & Pelayanan Pasien
- Kerja Sama Tim
- Adaptif & Manajemen Waktu