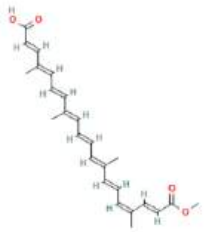
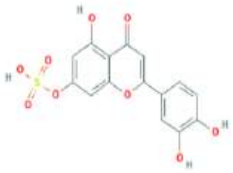
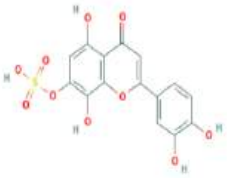
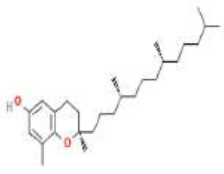
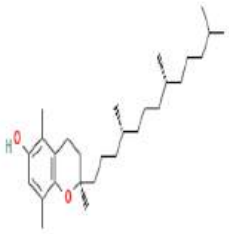
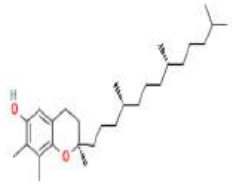
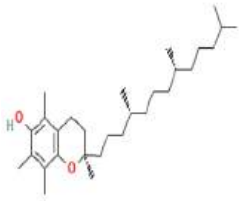
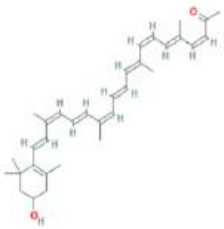
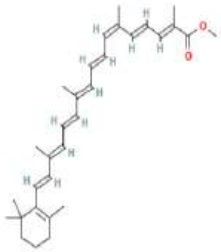
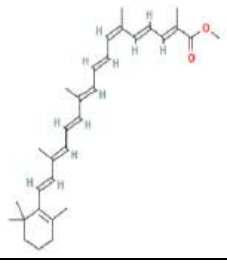
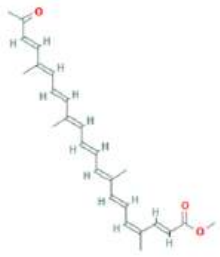
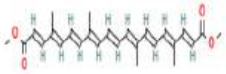
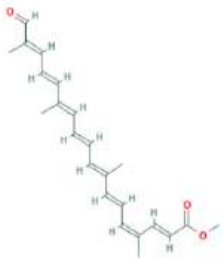
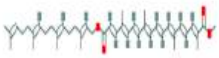
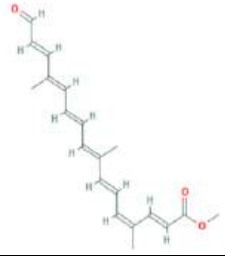
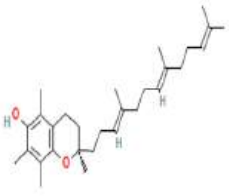
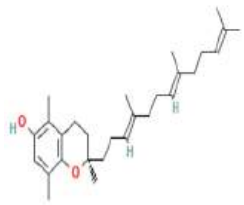
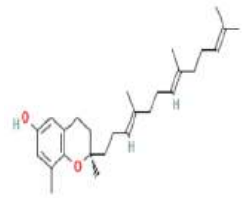
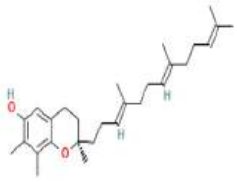
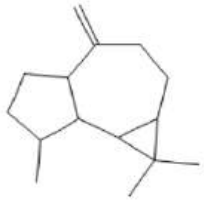
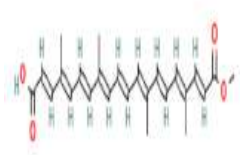
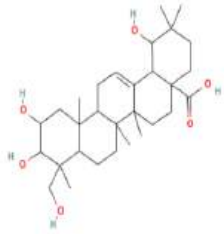
LAMPIRAN

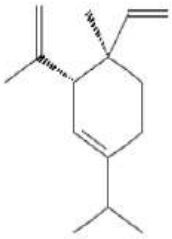
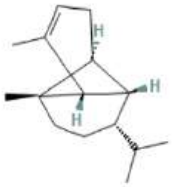
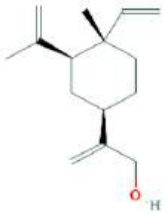
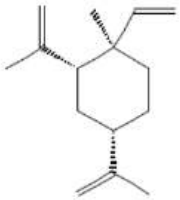
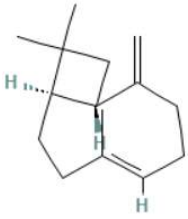
Lampiran 1. Daftar senyawa uji yang digunakan pada penelitian

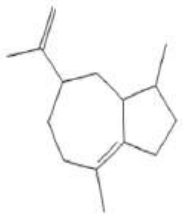
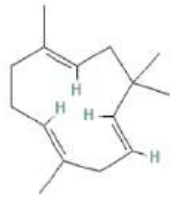
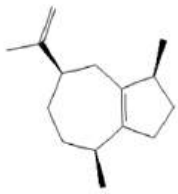
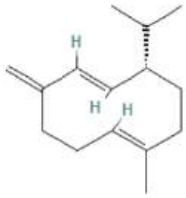
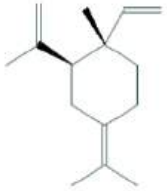
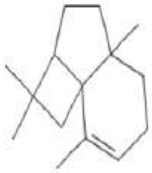
No	Senyawa	Struktur 2D
1.	bixin	
2	Norbixin	
3	Luteolin 7-sulfate	
4	8-Hydroxyluteolin 7-sulfate	
5	delta-Tocopherol	

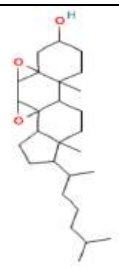
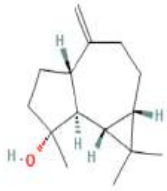
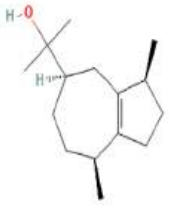
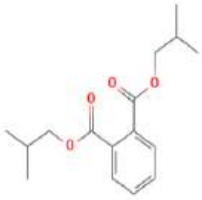
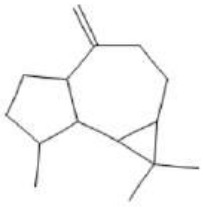
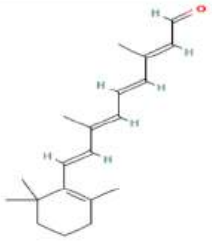
7	beta-Tocopherol	
8	gamma-Tocopherol	
9	alpha-Tocopherol	
10	Methyl apo-6'-lycopenoate	
11	Methyl 8'-apo-beta-carotenoate	
12	Methyl apo-8'-lycopenoate	

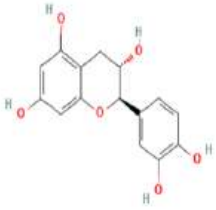
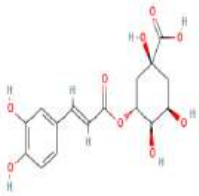
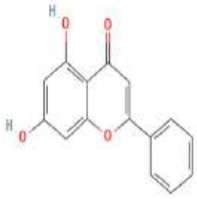
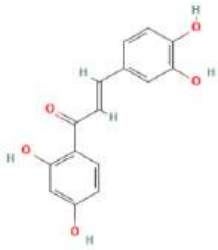
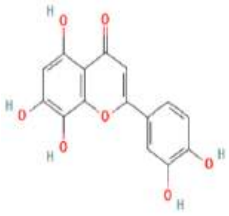
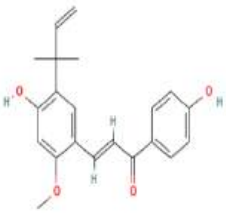
13	Methyl (9Z)-6'-oxo-6,5'-diapocaroten-6-oate	
14	Methyl bixin	
15	Apo-8'-bixinal	
16	6-Geranylgeranyl 8'-methyl 6,8'-diapocarotene-6,8'-dioate	
17	Apo-10'-bixinal	
18	alpha-Tocotrienol	

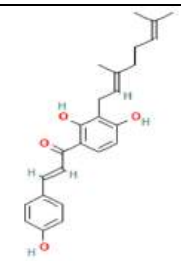
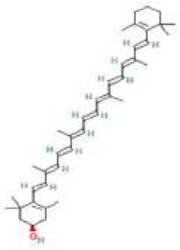
19	beta-Tocotrienol	
20	delta-Tocotrienol	
21	gamma-Tocotrienol	
22	(-)-Aromadendrene	
23	beta-Bixin	
24	Tomentosic acid	

25	Octadecane	
26	Delta-elemene	
27	(-)-.Alpha.-copaene	
28	(-)-Elema-1,3,11(13)-trien-12-ol	
29	.Beta.-elemen	
30	(-)-.Beta.-caryophyllene	

31	alpha-bulnesene	
32	Alpha.-caryophyllene	
33	Alpha-guaiene	
34	(-)-Germacrene d	
35	.Gamma.-elemene	
36	(-)-Alpha-panasinsen	

37	5,6:7,8-Diepoxycholestan-3.beta.-ol	
38	(-)-Spathulenol	
39	(-)-Guaiol	
40	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	
41	Aromadendrene	
42	Retinal	

43	catechin	
44	Chlorogenic acid	
45	Chrysin	
46	Butein	
47	Hypolaetin	
48	Licochalcone A	

49	Xanthoangelol	
50	Cryptoxanthin	
51	Geranylgeraniol	

Lampiran 2. Daftar senyawa uji lipinski of five

No	Kode Senyawa	Mass	Hydrogen Bond Donor	Hydrogen Bond Acceptors	LOGP	Molar Refractivity
1	A 1	394	1	4	4	116
2	A 2	380	2	4	5	115
3	A 3	350	3	8	2	81
4	A 4	366	4	9	2	83
5	A 5	382	5	10	2	84
6	A 6	402	1	2	8	124
7	A 7	416	1	2	8	129
8	A 8	416	1	2	8	128
9	A 9	430	1	2	8	133
10	A 10	350	1	4	5	109
11	A 11	446	0	2	8	143
12	A 12	446	0	2	8	143
13	A 13	392	0	3	6	122
14	A 14	394	1	4	5	117
15	A 15	352	0	3	5	109
16	A 16	640	0	4	1	202
17	A 17	312	0	3	4	95
18	A 18	424	1	2	8	134
19	A 19	410	1	2	8	129
20	A 20	396	1	2	7	124
21	A 21	410	1	2	8	129
22	A 22	204	0	0	4	64
23	A 23	394	1	4	5	119
24	A 24	552	0	0	11	116
25	A 25	254	0	0	7	85
26	A 26	204	0	0	4	68
27	A 27	204	0	0	4	64
28	A 28	220	1	1	3	70
29	A 29	204	0	0	4	68
30	A 30	204	0	0	4	66
31	A 31	204	0	0	4	66
32	A 32	204	0	0	5	68
33	A 33	204	0	0	4	66
34	A 34	204	0	0	4	68
35	A 35	204	0	0	4	68
36	A 36	204	0	0	4	64
37	A 37	338	3	1	5	95
38	A 38	220	1	1	3	65
39	A 39	222	1	1	3	68
40	A 40	278	0	4	3	76
41	A 41	204	0	0	4	64
42	A 42	284	0	1	5	92
43	A 43	290	5	6	1	72
44	A 44	354	6	9	1	82
45	A 45	254	2	4	2	69
46	A 46	272	4	5	2	72
47	A 47	302	5	7	1	74
48	A 48	338	2	4	4	99
49	A 49	392	3	4	5	117
50	A 50	552	1	1	1	182
51	A 51	954	0	0	5	954

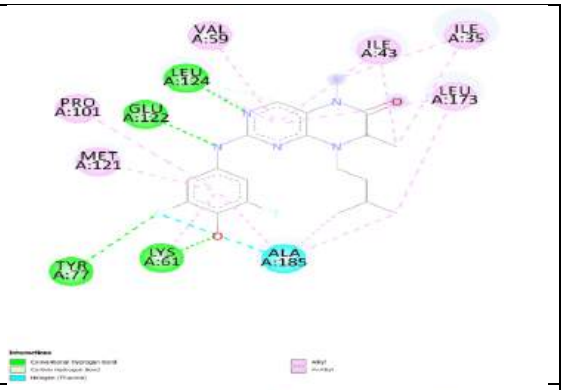
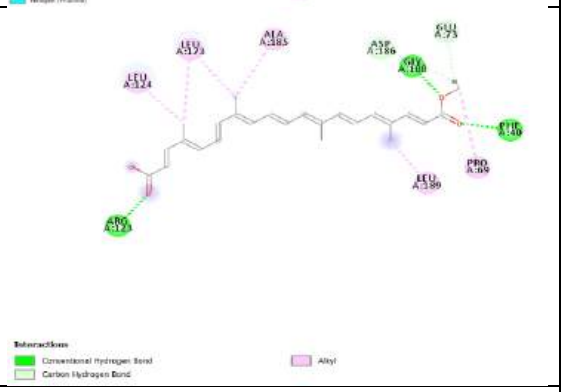
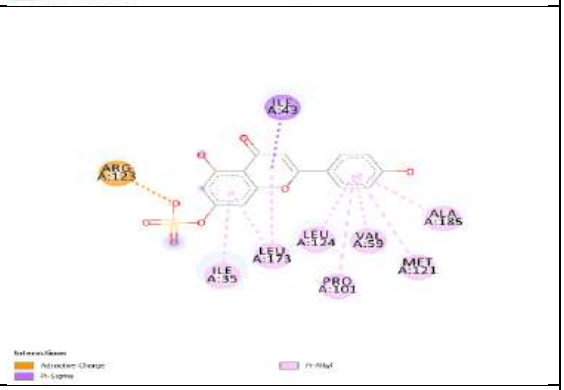
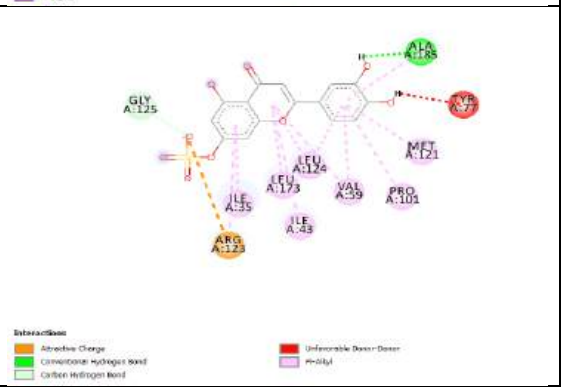
Lampiran 3. Daftar senyawa lolos uji lipinski rule of five

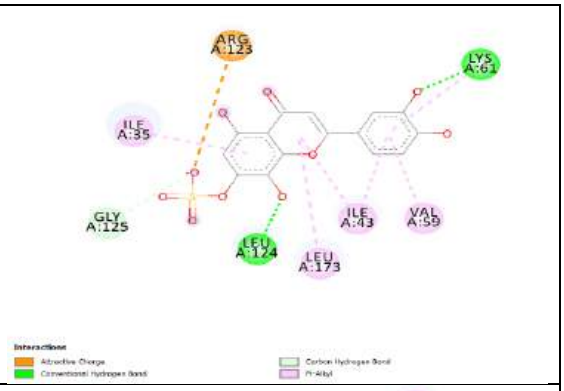
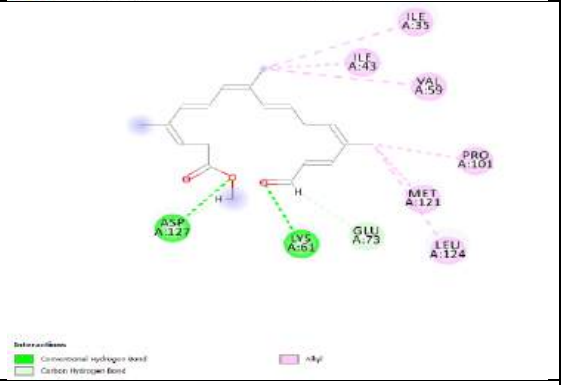
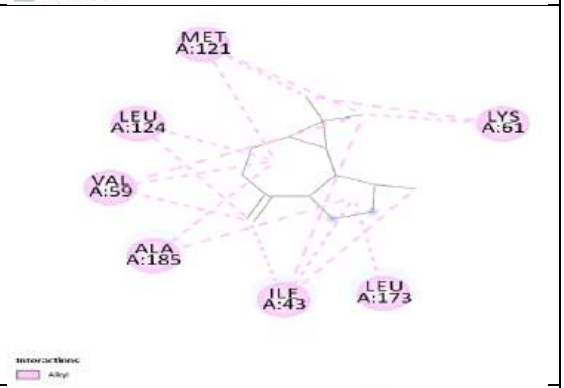
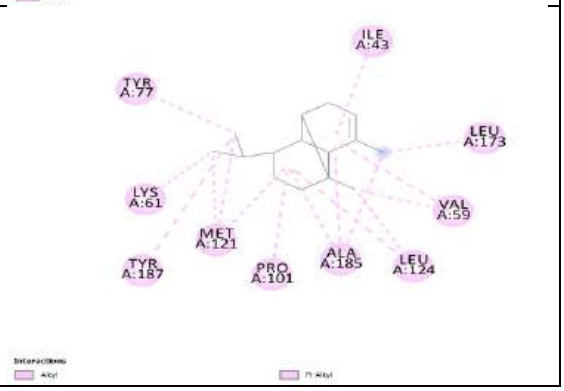
No	kode senyawa	mass	hydrogen bond donor	hydrogen bond acceptors	LOGP	Molar Refractivity
1	A 1	394	1	4	4	116
2	A 2	380	2	4	5	115
3	A 3	350	3	8	2	81
4	A 4	366	4	9	2	83
5	A 5	382	5	10	2	84
6	A 6	402	1	2	8	124
7	A 7	416	1	2	8	129
8	A 8	416	1	2	8	128
9	A 9	430	1	2	8	133
10	A 10	350	1	4	5	109
11	A 11	446	0	2	8	143
12	A 12	446	0	2	8	143
13	A 13	392	0	3	6	122
14	A 14	394	1	4	5	117
15	A 15	352	0	3	5	109
16	A 16	640	0	4	1	202
17	A 17	312	0	3	4	95
18	A 18	424	1	2	8	134
19	A 19	410	1	2	8	129
20	A 20	396	1	2	7	124
21	A 21	410	1	2	8	129
22	A 22	204	0	0	4	64
23	A 23	394	1	4	5	119
24	A 24	552	0	0	11	116
25	A 25	254	0	0	7	85
26	A 26	204	0	0	4	68
27	A 27	204	0	0	4	64
28	A 28	220	1	1	3	70
29	A 29	204	0	0	4	68
30	A 30	204	0	0	4	66
31	A 31	204	0	0	4	66
32	A 32	204	0	0	5	68
33	A 33	204	0	0	4	66
34	A 34	204	0	0	4	68
35	A 35	204	0	0	4	68
36	A 36	204	0	0	4	64
37	A 37	338	3	1	5	95
38	A 38	220	1	1	3	65
39	A 39	222	1	1	3	68
40	A 40	278	0	4	3	76
41	A 41	204	0	0	4	64
42	A 42	284	0	1	5	92
43	A 43	290	5	6	1	72
44	A 44	354	6	9	1	82
45	A 45	254	2	4	2	69
46	A 46	272	4	5	2	72
47	A 47	302	5	7	1	74
48	A 48	338	2	4	4	99
49	A 49	392	3	4	5	117
50	A 50	552	1	1	1	182
51	A 51	954	9	9	5	954

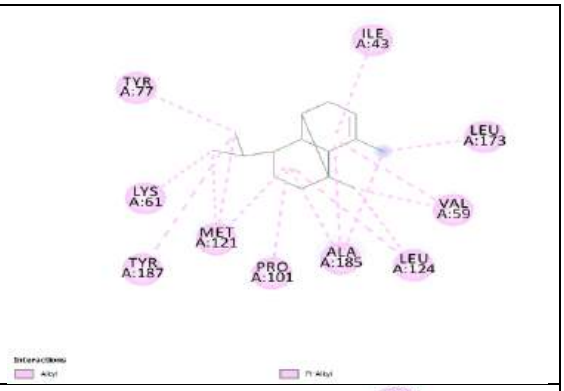
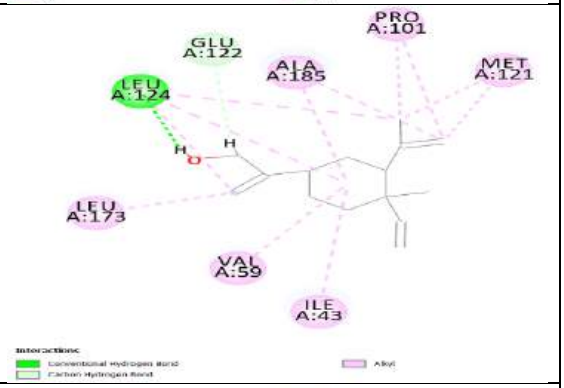
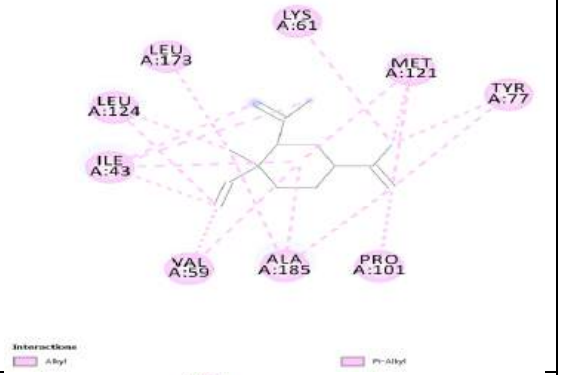
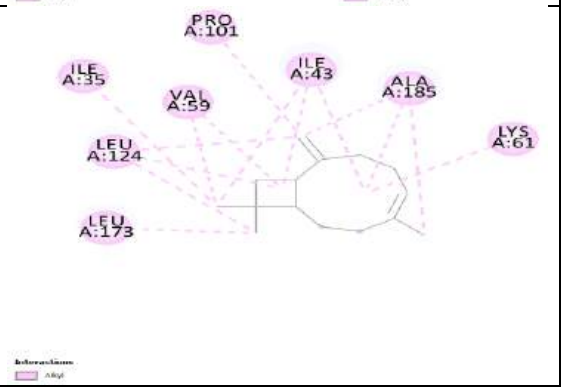
Lampiran 4. Hasil molecular docking

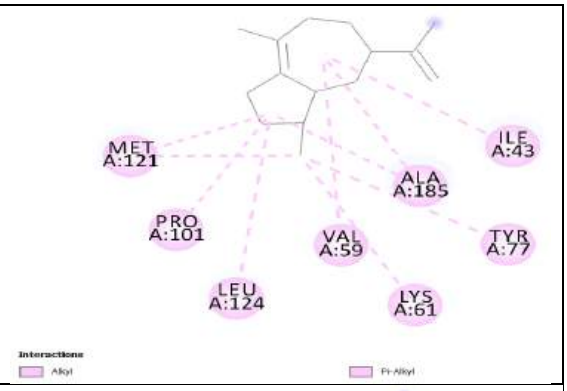
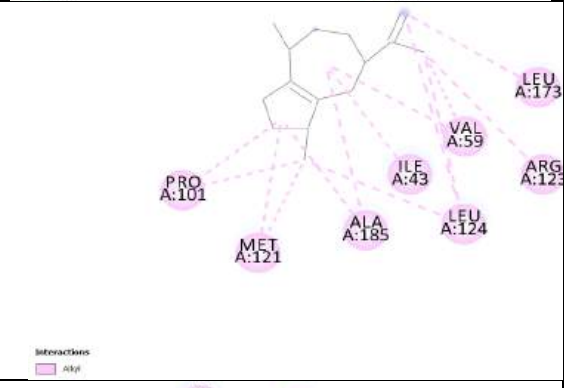
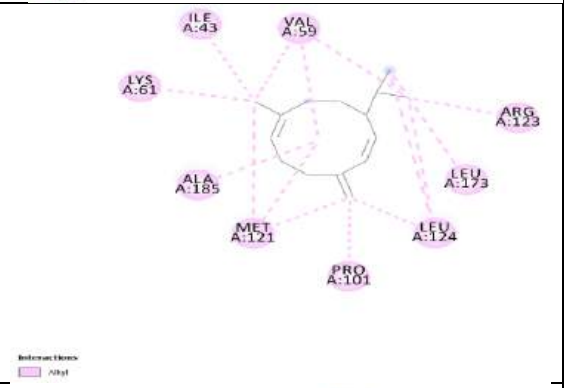
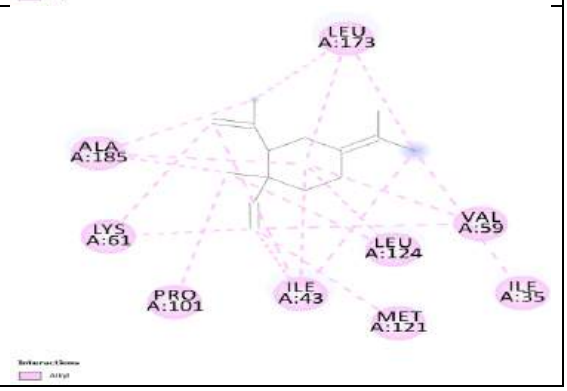
N0	Kode senyawa	Binding Energi	Konstanta Inhibisi
1	5-Fluorourasil	-8.75	0,38 uM
2	A5	-9,98	0,04 uM
3	A4	-9,69	0,07 uM
4	A46	-8,71	0,41 uM
5	A3	-8,65	0,32 uM
6	A43	-8,49	0,60 uM
7	A17	-8,37	0,73 uM
8	A47	-8,36	0,74 uM
9	A45	-7,61	2,63 uM
10	A39	-7,56	2,89 uM
11	A26	-7,01	3,05 um
12	A27	-7,36	4,01 uM
13	A1	-7,36	4,06 uM
14	A22	-7,20	5,25 uM
15	A41	-7,20	5,25 uM
16	A31	-7,17	5,57 uM
17	A34	-7,09	6,31 uM
18	A28	-6,97	7,83 uM
19	A38	-6,92	8,45 uM
20	A30	-6,91	8,64 uM
21	A33	-6,89	8,95 uM
22	A36	-6,74	11,46 uM
23	A29	-6,65	13,28 uM
24	A35	-6,51	16,98 uM
25	A40	-6,49	17,46 uM

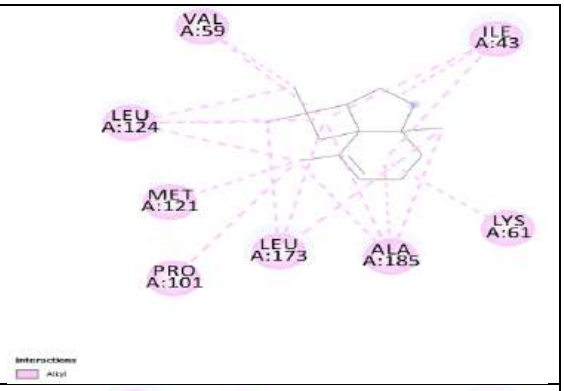
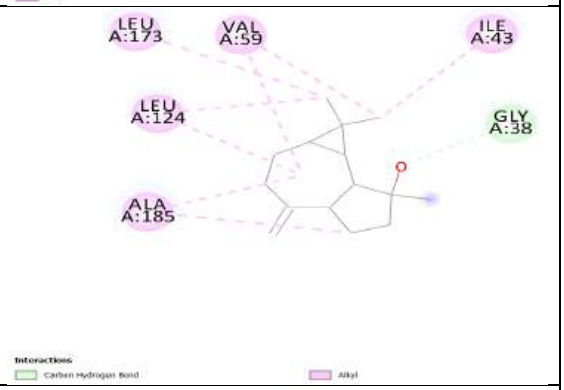
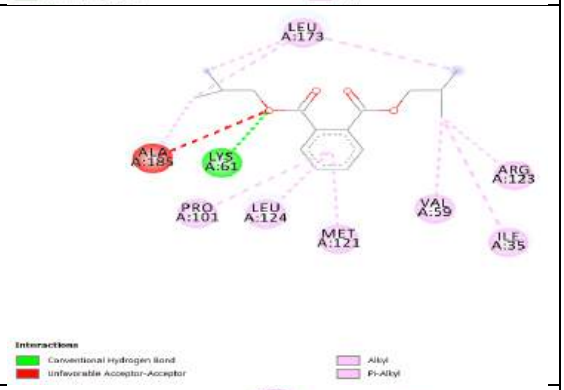
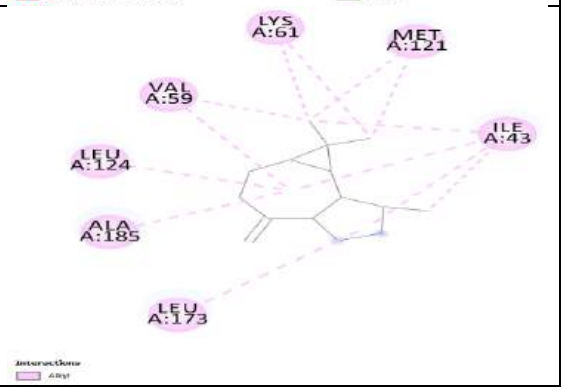
Lampiran 5. Daftar ikatan senyawa uji yang digunakan pada penelitian

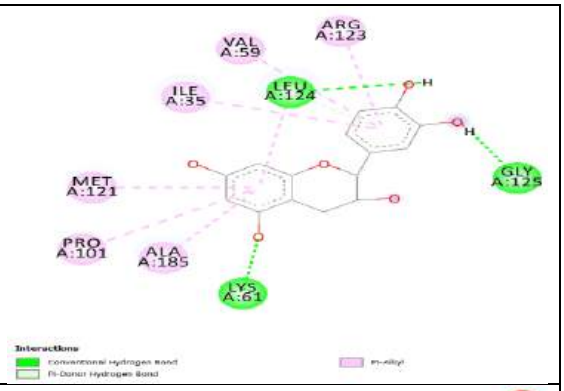
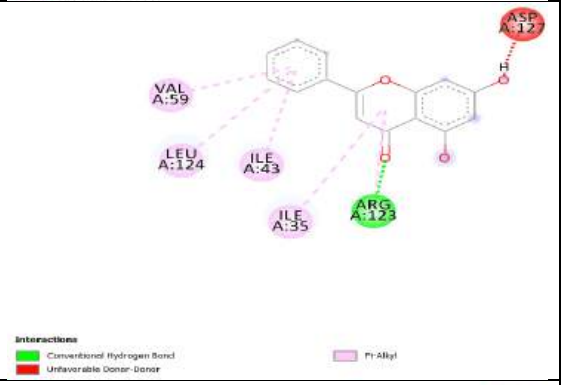
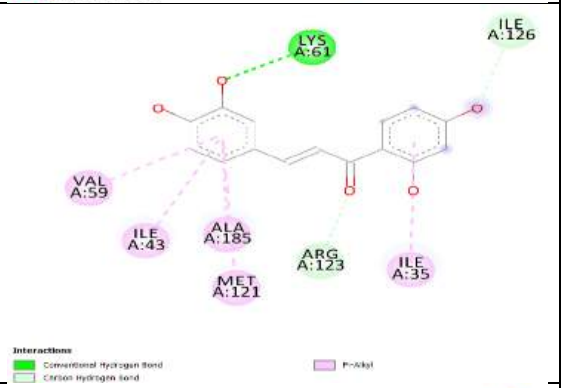
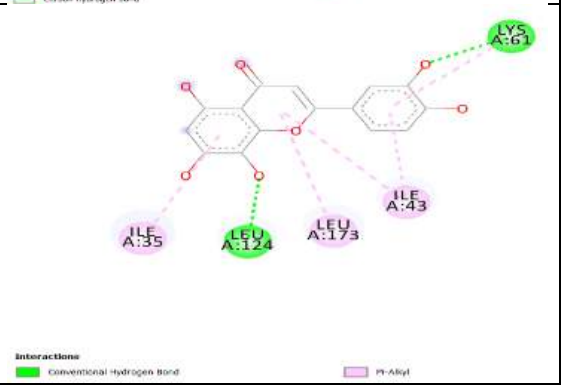
1	**IKATAN HIDROGEN : GLU122,LEU124,LYS61,TYR77 IKATAN HIDROFOBIK : VAL59,ILE43,ILE35,LEU173,PRO101 ,MET121**	
2	**IKATAN HIDROGEN : GLU73,GLY188,ASP186,PHE40,ARG 123 IKATAN HIDROFOBIK :ALA185,LEU173,LEU124,LEU189,P RO69**	
3	**IKATAN HIDROGEN : - IKATAN HIDROFOBIK : ILE43,ILE35,LEU173,LEU124,VAL59, PRO101,MET121,ALA185**	
4	**IKATAN HIDROGEN : ALA185,GLY125 IKATAN HIDROFOBIK :ILE35,LEU173,LEU124,ILE43,VAL5 9,PRO101,MET121**	

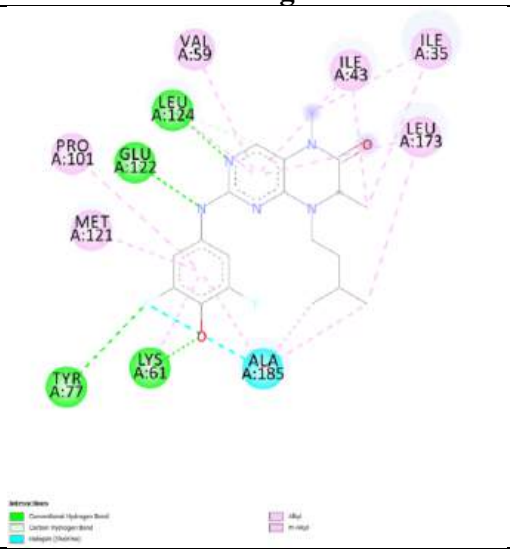
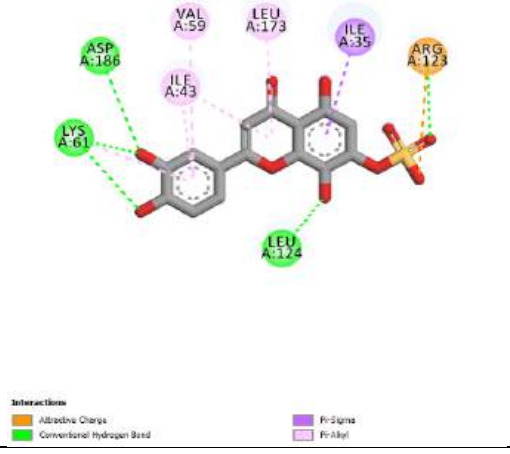
5	**IKATAN HIDROGEN : LYS61,LEU124,GLY125 IKATAN HIDROFOBIK : ILE35,LEU173,ILE43,VAL59**	
6	**IKATAN HIDROGEN : ASP127,LYS61,GLU73 IKATAN HIDROFOBIK : MET121,LEU124,PRO101,VAL59,ILE43,ILE35**	
7	**IKATAN HIDROGEN : - IKATAN HIDROFOBIK :ILE43,LEU173,ALA185,VAL59,LEU124,MET121,LYS61**	
8	**IKATAN HIDROGEN : - IKATAN HIDROFOBIK :TYR77,ILE43,LEU173,VAL59,LEU124,ALA185,PRO101,MET121,TYR187,LYS61**	

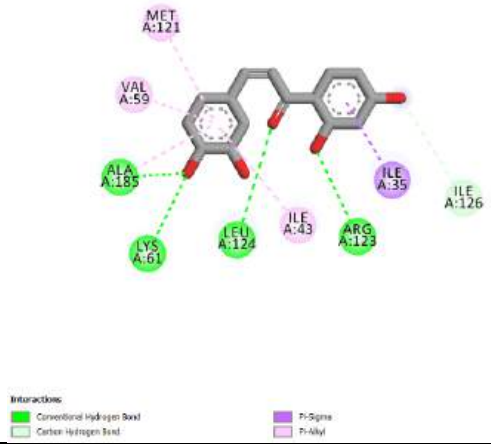
9	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK :TYR77,ILE43,LEU173,VAL59,LEU124,ALA185,PRO101,MET121,TYR187,LYS61**	
10	**IKATAN HIDROGEN : LEU124,GLU122** **IKATAN HIDROFOBIK : LEU173,VAL59,ILE43,ALA185,PRO101,MET121**	
11	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK : PRI101,ALA185,VAL59,ILE43,LEU124,LEU173,LYS61,MET121,TYR77**	
12	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK :LEU173,LEU124,VAL59,ILE35,PRO101,ILE45,ALA185,LYS61**	

13	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK :MET121,PRO101,LEU124,VAL59,LYS61,TYR77,ALA185,ILE43**	
14	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK :PRO101,MET121,ALA185 LEU124,VAL59,LEU173**	
15	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK : VAL59,ILE43,LYS61,ALA185,MET121,PRO101,LEU124,LEU173,ARG123**	
16	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK : ALA,185,LEU173,LYS61,PRO101,ILE43,MET121,LEU124ILE35,VAL59**	

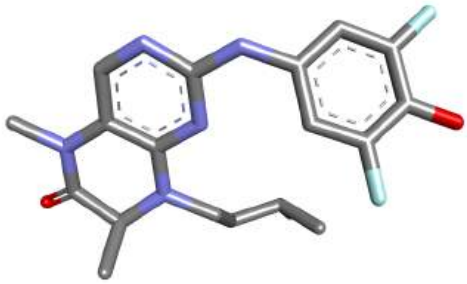
17	**IKATAN HIDROGEN : -** **IKATAN HIDROFOBIK :VAL59,LEU124,MET121,PRO101,LEU173,ALA185,LYS61,ILE43**	
18	**IKATAN HIDROGEN : GLY38** **IKATAN HIDROFOBIK : ILE43,VAL59,LEU173,LEU124,AL185**	
19	**IKATAN HIDROGEN: LYS62** **IKATAN HIDROFOBIK : LEU173,PRO101,LEU124,MET121,VAL59,ILE35,ARG123**	
20	**IKATAN HIDROGEN: -** **IKATAN HIDROFOBIK : LEU173, ALA185,LEU124,VAL59,LYS61,MET121,ILE43**	

21	**IKATAN HIDROGEN : LEU124,GLY125,LYS61 IKATAN HIDROFOBIK : ALA185,PRO101,MET121,ILE35,VAL59,ARG123**	
22	**IKATAN HIDROGEN : ARG123 IKATAN HIDROFOBIK : VAL59,LEU124,ILE43,ILE35**	
23	**IKATAN HIDROGEN : LYS61,ILE126,ARG124 IKATAN HIDROFOBIK : VAL59,ILE43,ALA185,MET121,ILE35**	
24	**IKATAN HIDROGEN : LEU124,LYS61 IKATAN HIDROFOBIK : ILE35,LEU173,ILE43**	

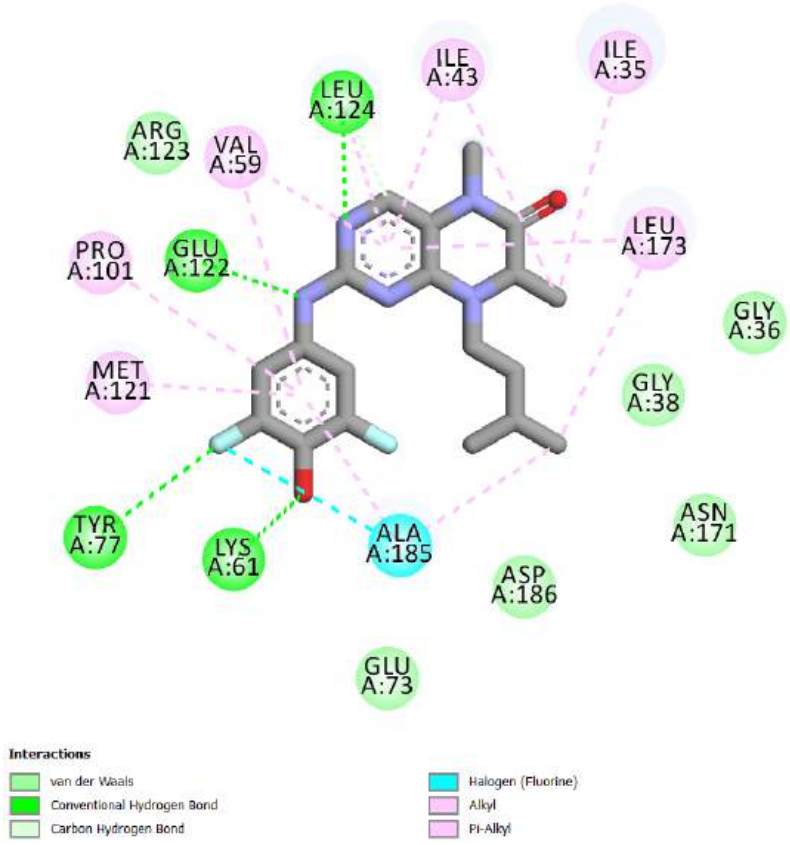
No	Kode senyawa	Visualisai hasill docking
1	5-Fluorourasil	
2	A4	
3	A5	

4	**A46**	 MET A:121 VAL A:59 ALA A:185 LYS A:61 LEU A:124 ILE A:43 ARG A:123 ILE A:35 ILE A:126 Interactions Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Sigma Pi-Alkyl

Lampiran 6. Preotein dan ligan alami

Lampiran 7. Visualisasi ikatan ligan alami

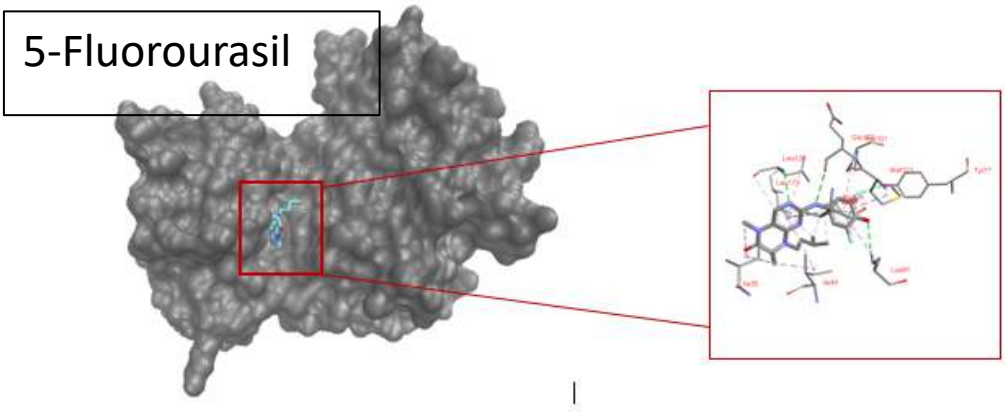


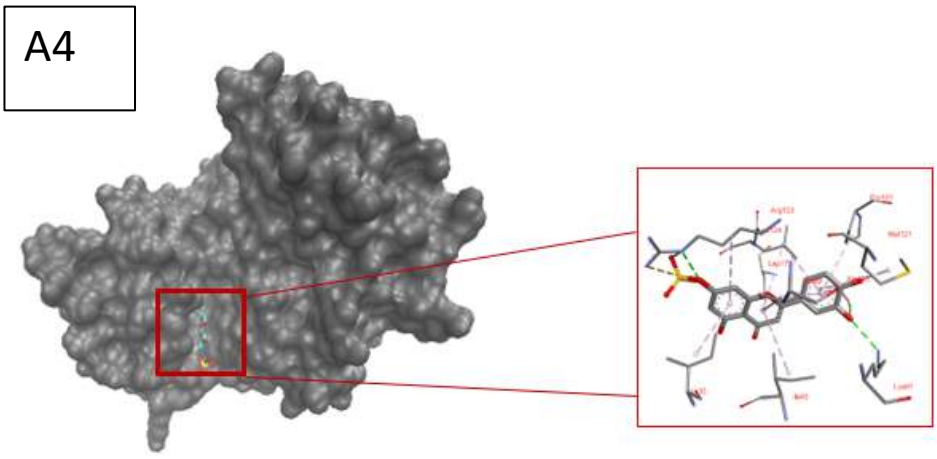
Grid Box			***Grid Spacing***	***Grid Center***		
X	***Y***	***Z***	0.375 Å	***X center***	***Y center***	***Z center***
60	*40*	*40*		*0.539*	*-18.004*	*-13.408*
Number of Runs: 100						
Number of Evals: Medium						
Metode Algoritma: Lamarckian Genetic Algorith						
RMSD: 0.464 A						
Energi Ikatan: -8.86 kcal/mol						
Konstanta Inhibisi: 3.65 uM						

Keterangan :

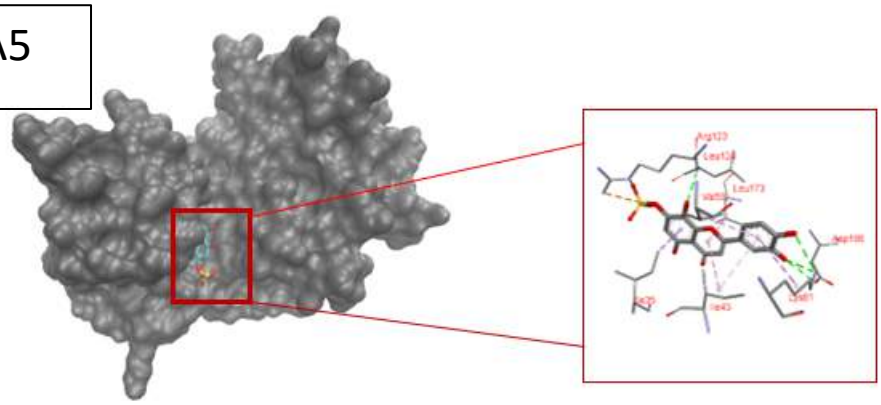
- Warna hijau : ligan alami
- Warna merah : ligan hasil redocking
- RMSD : 0,464 Å

Lampiran 8. VMD senyawa uji terbaik

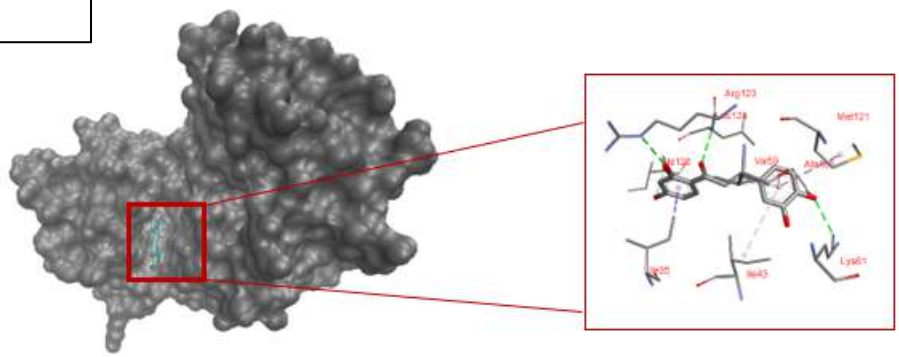


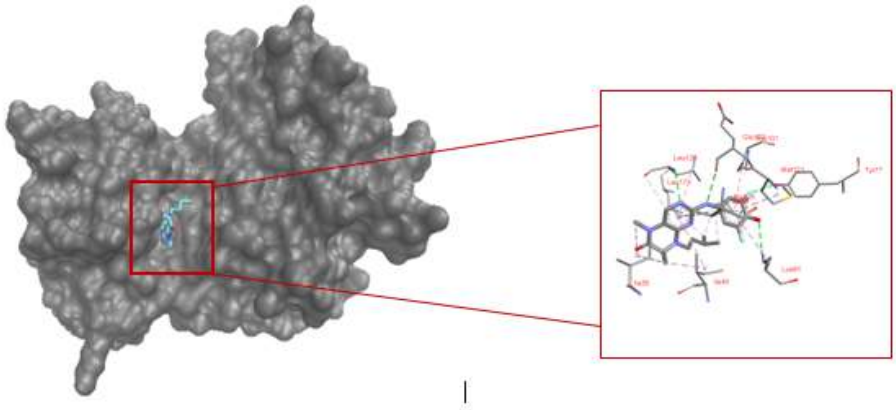


A5

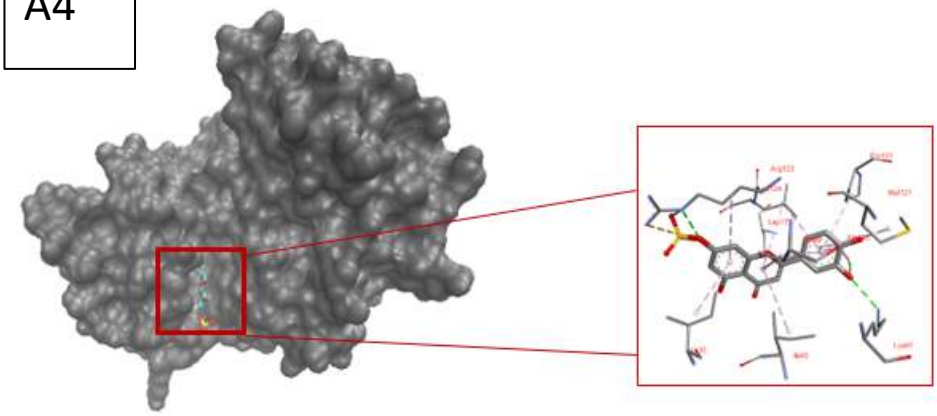


A26

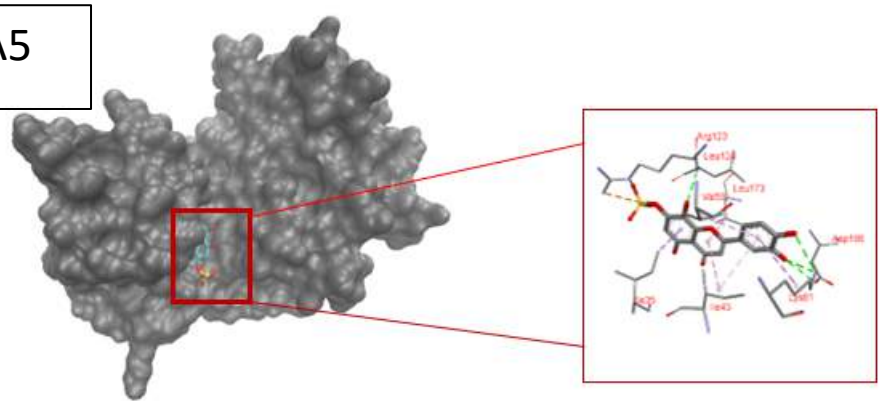




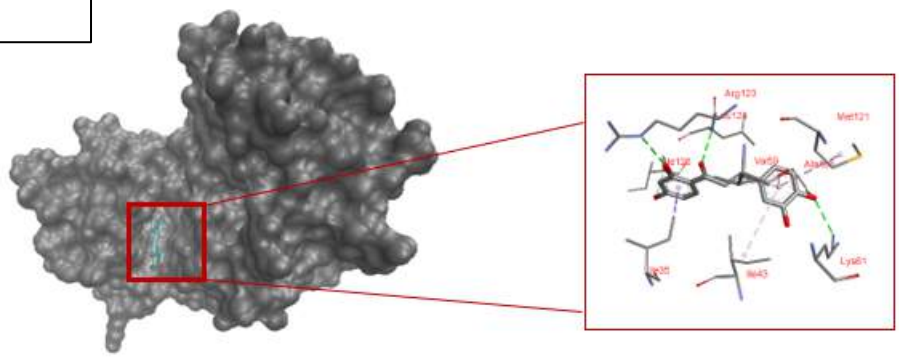
A4



A5

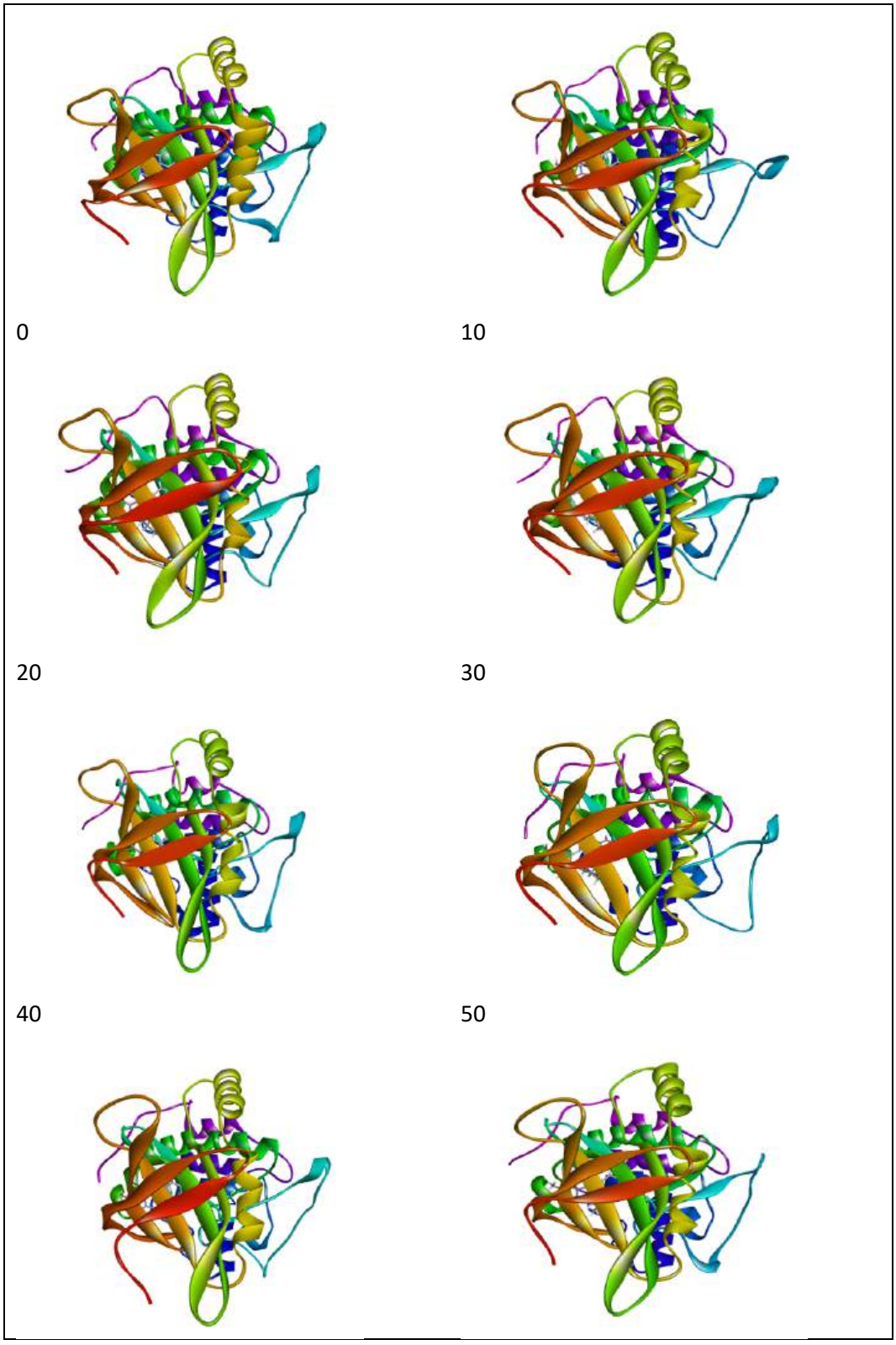


A26



Lampiran 9. Daftar pergerakan simulasi

LIG



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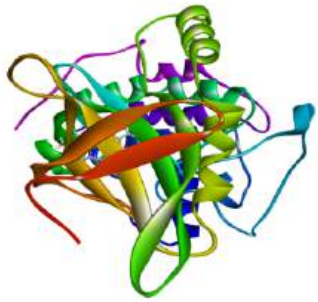

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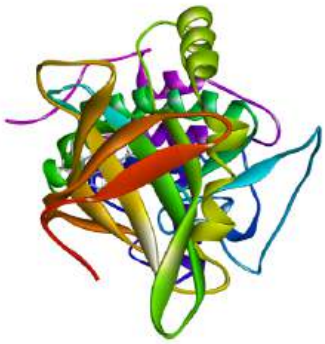

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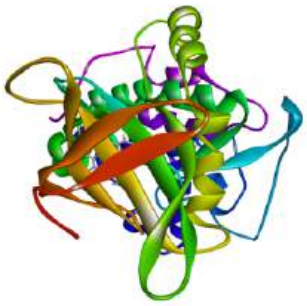


90

100

A4

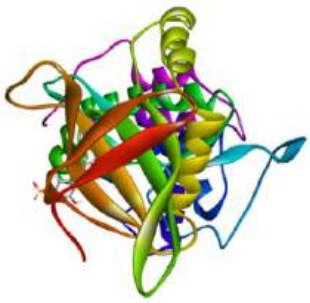
0

10

20

30

40



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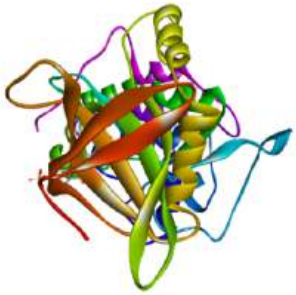

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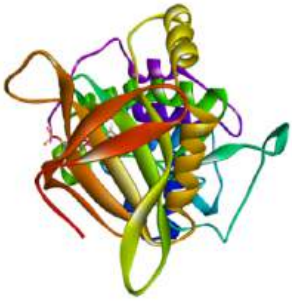

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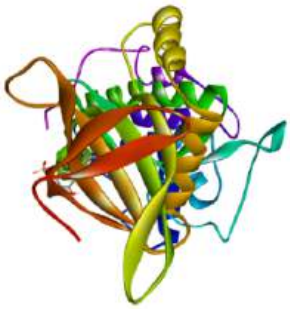

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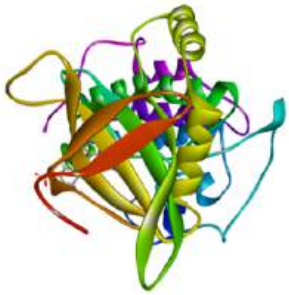

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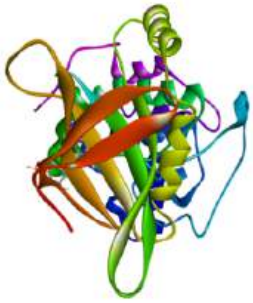

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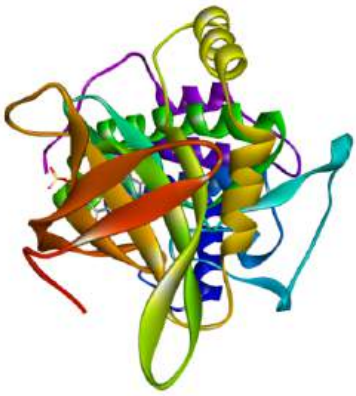

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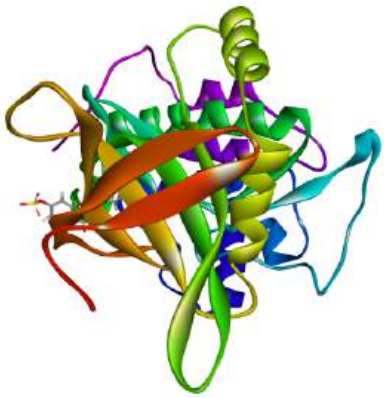

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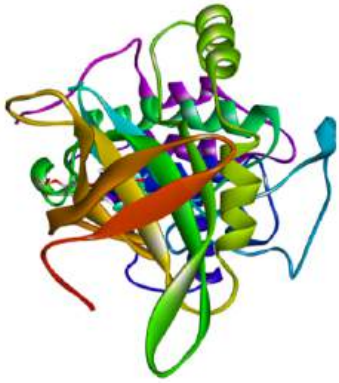

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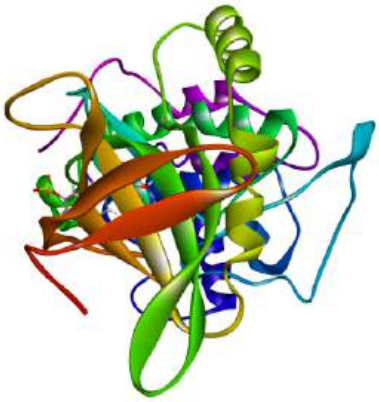

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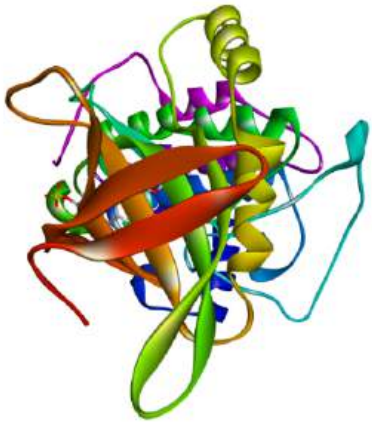

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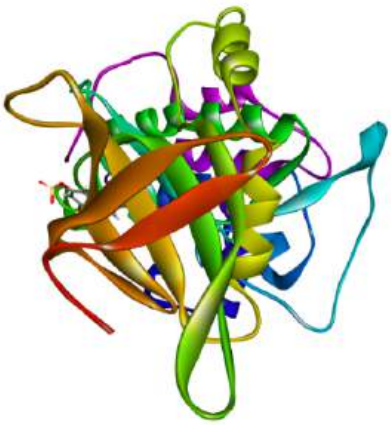

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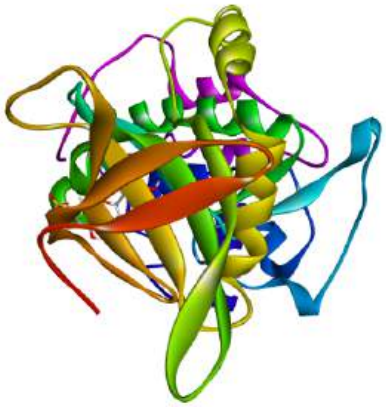

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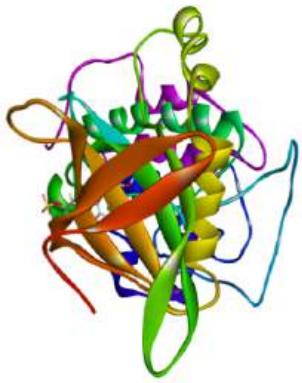

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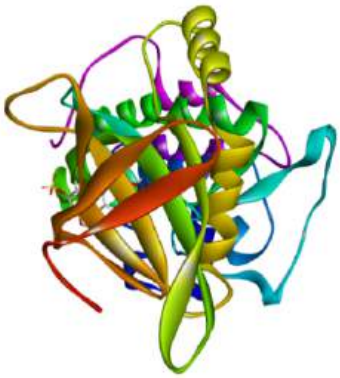

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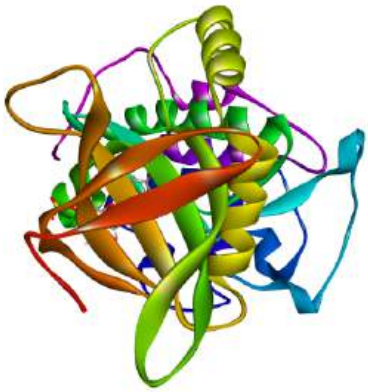

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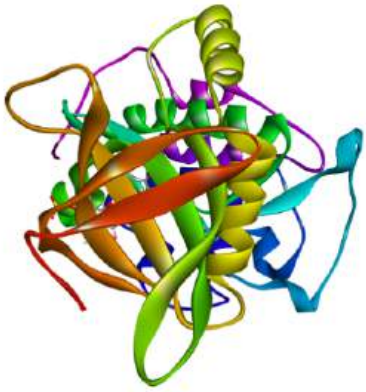

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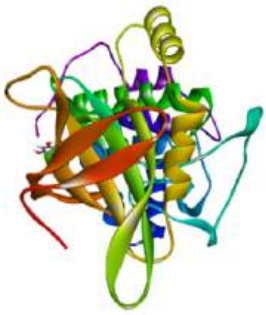

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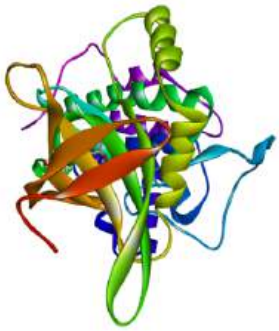

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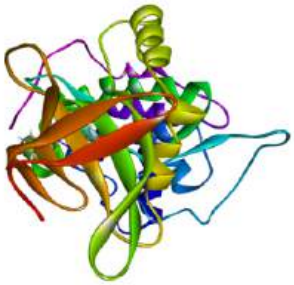

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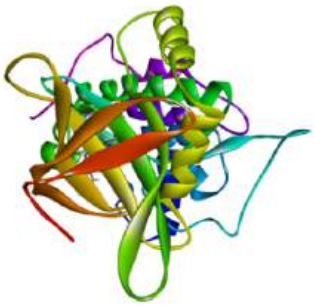

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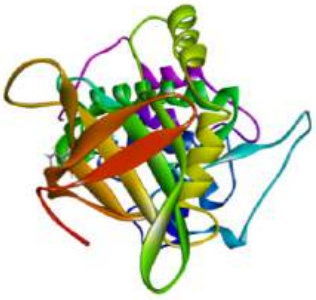

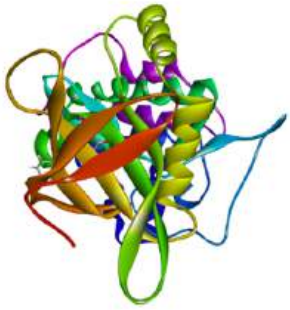

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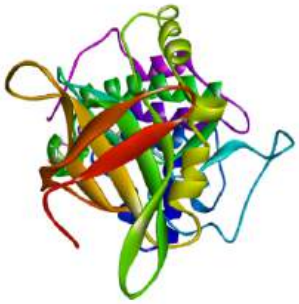

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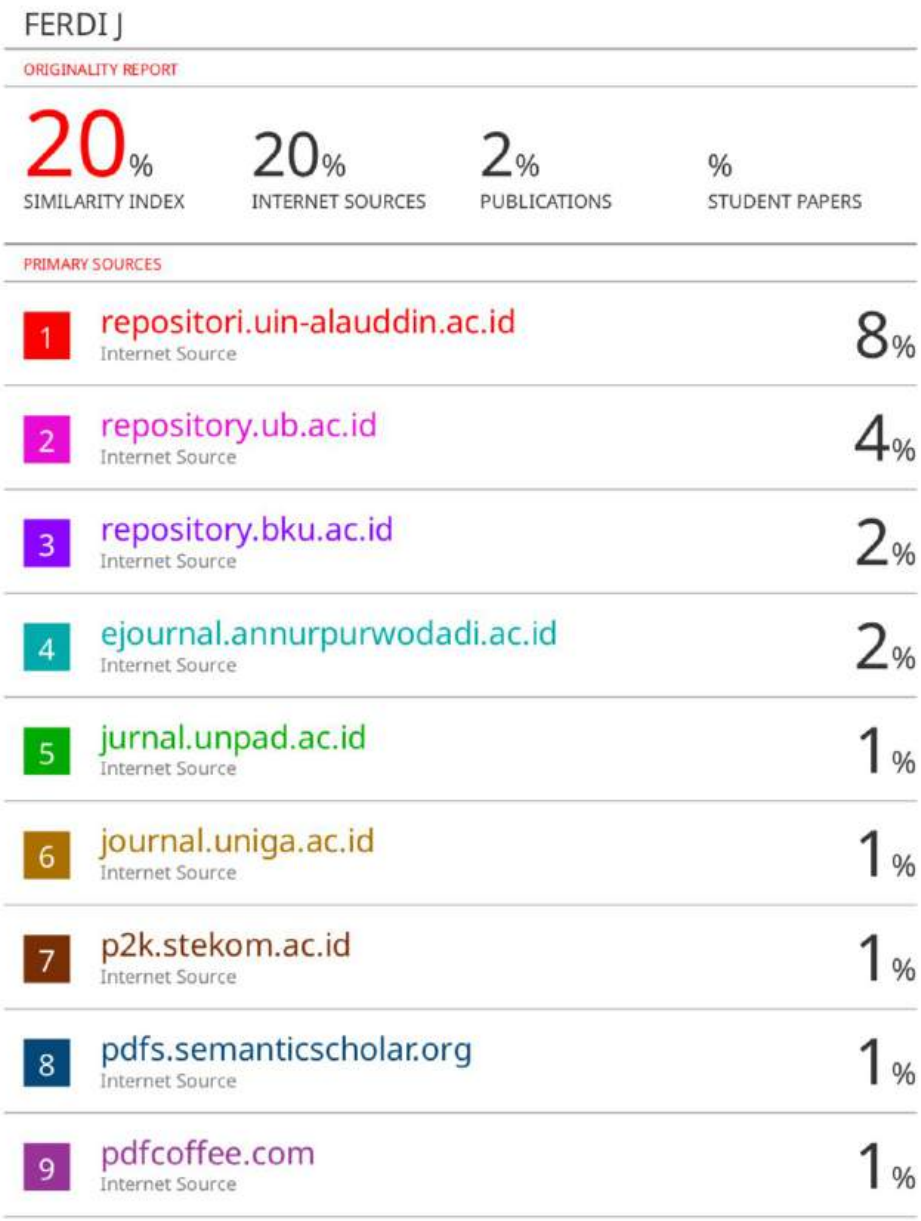
Lampiran 10. Hasil plagiarisme



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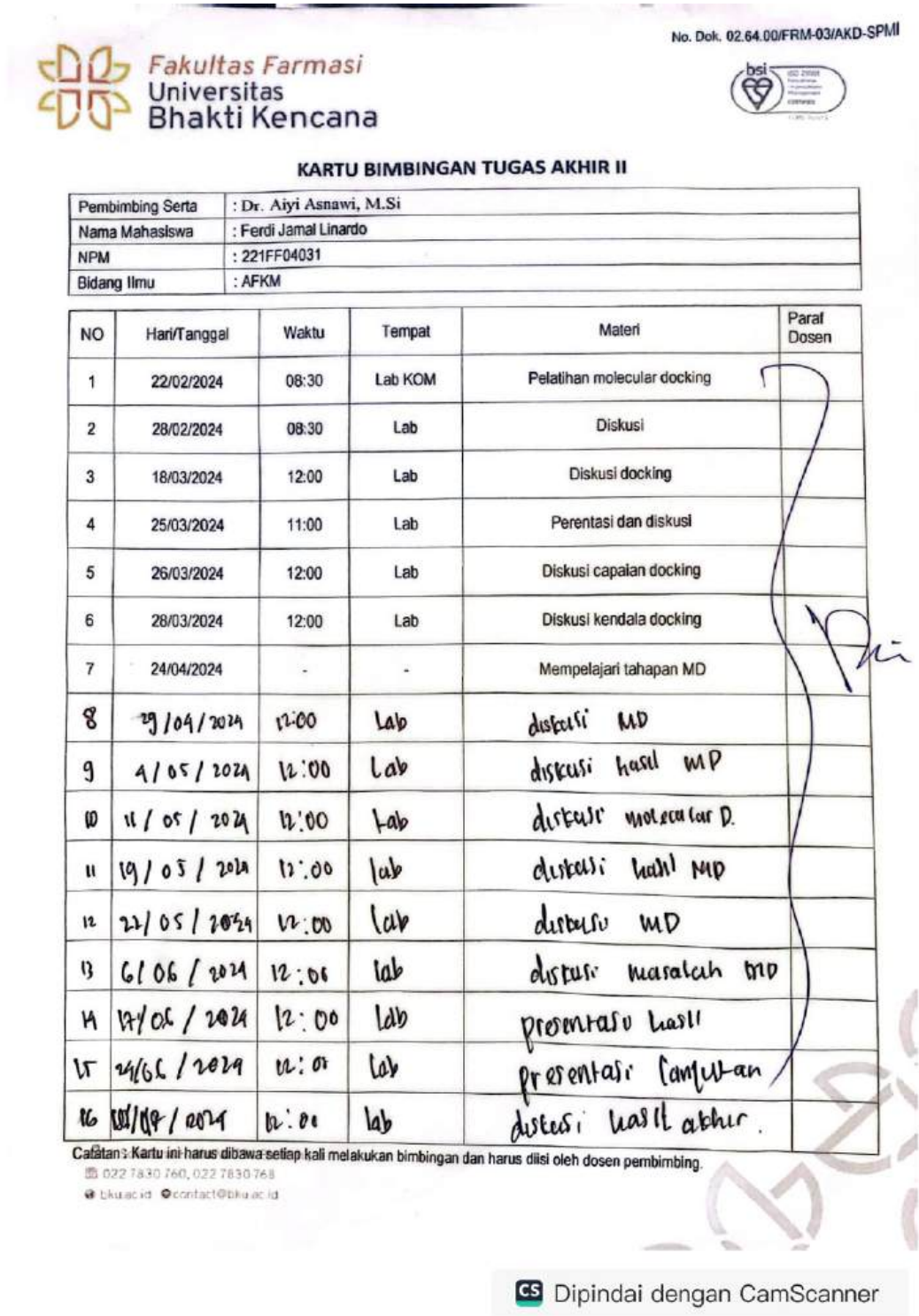

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KARTU BIMBINGAN TUGAS AKHIR II

Pembimbing Serta	: Dr. Aiyi Asnawi, M.Si
Nama Mahasiswa	: Ferdi Jamal Linardo
NPM	: 221FF04031
Bidang Ilmu	: AFKM

NO	Hari/Tanggal	Waktu	Tempat	Materi	Paraf Dosen
1	22/02/2024	08:30	Lab KOM	Pelatihan molecular docking	
2	28/02/2024	08:30	Lab	Diskusi	
3	18/03/2024	12:00	Lab	Diskusi docking	
4	25/03/2024	11:00	Lab	Perentasi dan diskusi	
5	26/03/2024	12:00	Lab	Diskusi capaian docking	
6	28/03/2024	12:00	Lab	Diskusi kendala docking	
7	24/04/2024	-	-	Mempelajari tahapan MD	
8	29/04/2024	12:00	Lab	diskusi MD	
9	9/05/2024	12:00	Lab	diskusi hasil MD	
10	11/05/2024	12:00	Lab	diskusi molecular D.	
11	19/05/2024	12:00	lab	diskusi hasil MD	
12	22/05/2024	12:00	lab	diskusi MD	
13	6/06/2024	12:00	lab	diskusi masalah MD	
14	17/06/2024	12:00	lab	presentasi hasil	
15	24/06/2024	12:00	lab	presentasi capaian	
16	01/07/2024	12:00	lab	diskusi hasil akhir.	

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

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KARTU BIMBINGAN TUGAS AKHIR II

Pembimbing Serta	: Dr. apt. FAUZAN ZEIN MUTTAQIN, M.Si.
Nama Mahasiswa	: FERDI JAMAL LINARDO
NPM	: 221FF04031
Bidang Ilmu	: AFKM

1	15/02/2024	08:00	Lab	pelatihan molecular docking	
2	27/02/2024	08:00	Lab	diskusi	
3	25/03/2024	12:00	Lab	diskusi kemajuan	
4	10/04/2024	12:00	Lab	laporan kemajuan	
5	25/04/2024	12:00	Lab	Laporan kemajuan	
6	15/05/2024	12:00	Lab	Diskusi kemajuan	
7	24/05/2024	12:00	Lab	diskusi hasil MD	
8	10/06/2024	12:00	Lab	diskusi hasil MD.	
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Lampiran 12. Curriculum Vitae

Nama Lengkap	: Ferdi Jamal Linardo
Tempat Tanggal lahir	: JL.P TENDEAN, Liwa, lampung barat
Status	: Belum Menikah
Agama	: Islam
No Hp	: 081222776169
Email	: ferdijamallinardo12@gmail.com

PENDIDIKAN TERAKHIR

2019-2022 D3 FARMASI UNIVERSITAS BHAKTI KENCANA

2022-2024 S1 FARMASI UNIVERSITAS BHAKTI KENCANA

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Bandung, 25 November 2024

Ferdi Jamal Linardo