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LAMPIRAN 1

SENYAWA FLAVONOID DAN SUMBERNYA

Tabel VII.1
Daftar senyawa flavonoid dan sumbernya

No.	Flavonoid	Sumber Tanaman
Flavon		
1	Apigenin	<i>Petroselinum</i>
2	Baicalein	<i>Scutellaria</i>
3	Chrysin	<i>Populus</i>
4	Luteolin	<i>Robinia</i>
5	Scutelarein	<i>Scutellaria</i>
6	Hispidulin	<i>Ambrosia</i>
7	Chrysoeriol	<i>Reseda</i>
8	Triectin	<i>Eriodictyon</i>
9	Tangeretin	<i>Diosma</i>
10	Wogonin	<i>Lathyrus</i>
11	Rhoifolin	<i>Triticum</i>
12	Diosmetin	Daun Peterseli
13	Acacetin	<i>Tetracera indica</i>
14	Tricin	Jeruk Nipis
Flavonol		
15	Galangin	<i>Alpinia</i>
16	Fisetin	<i>Rhus</i>
17	Kaemferol	<i>Delphinium</i>
18	Kaemferide	<i>Alpinia</i>
19	Robinetin	<i>Robina</i>
20	Herbasetin	<i>Gossypium</i>
21	Quercetin	<i>Quercus</i>
22	Ramnetin	<i>Rhamnus</i>
23	Isoramnetin	<i>Cheiranthus</i>
24	Myrcetin	<i>Myrica</i>
25	Querstagenin	<i>Tagetes</i>
26	Gossypetin	<i>Gossypium</i>

**LAMPIRAN 1
(LANJUTAN)**

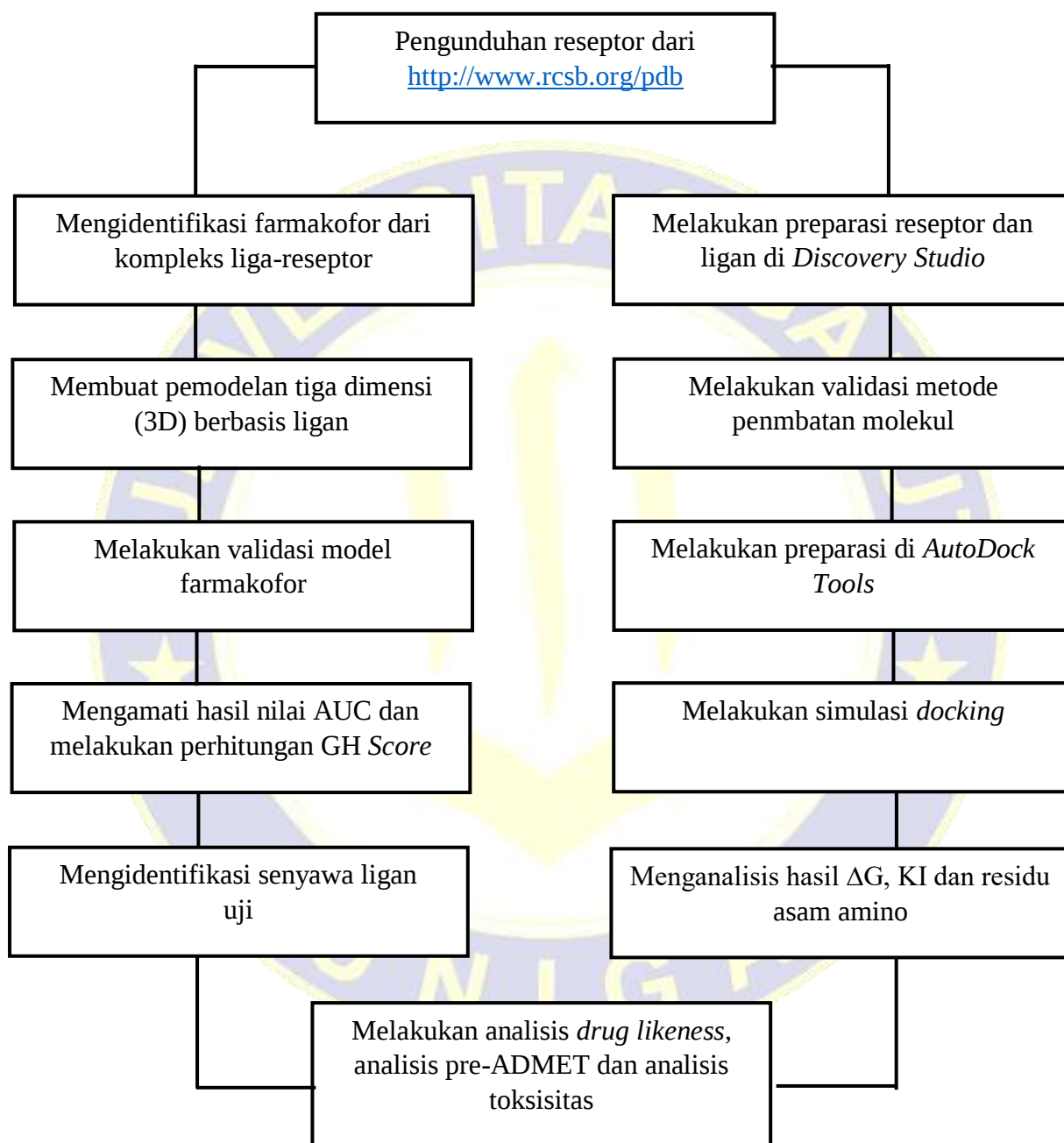
No.	Flavonoid	Sumber Tanaman
27	Isoquercetin	Apel, teh, tomat, anggur merah, cerry, bawang, brokoli, buah, peel, letus, gandum, asam citrus, manga
28	Ramnazin	
29	Rutin	
30	Morin	
31	Pachypodol	
Isoflavon		
32	Daidzein	<i>Pueraira</i>
33	Formononetin	<i>Ononis</i>
34	Genistein	<i>Genista</i>
35	Biokanin A	<i>Cicer</i>
36	Orobol	<i>Orobus</i>
37	Tactorigenin	<i>Iris</i>
38	Baptigenin	<i>Baptisia</i>
Flavanon		
39	Pinocembrin	<i>Pinus</i>
40	Liquiritigenin	<i>Glycyrrhi</i>
41	Narigenin	<i>za Prumus</i>
42	Sakuanetin	<i>Prunus</i>
43	Eriodictyol	<i>Eridictyon</i>
44	Hesperetin	<i>Prunus</i>
45	Homeridictyol	Jeruk Bali
46	Parietin	
47	Epigallocatechin	<i>Camellia sinensis</i>
48	Catechin	
49	Naringin	Jeruk Bali
Dehidroflavonol		
50	Pinobaskin	<i>Pinus</i>
51	Aromadendrin	<i>Eucalyptus</i>
52	Fustin	<i>Rhus</i>
53	Taksifolin	<i>Pseudotsuga</i>
Biflavonoid		
54	Agathisflavone	<i>Agathis</i>
55	Cupresuflavone	<i>Cupressus</i>
56	Ginkgetin	<i>Cupressus</i>
57	Siadopitisin	<i>Ginkgo</i>

**LAMPIRAN 1
(LANJUTAN)**

No	Flavonoid	Sumber Tanaman
58	Robustaflavone	<i>Ginkgo</i>
59	Hinokiflavone	<i>Agathis</i>
60	Ochnaflavone	<i>Cupressus</i>
61	Amentoflavone	<i>Ochna</i>
Khalkon		
62	Isoquiritigenin	<i>Acacia</i>
63	Khalkonarigenin	<i>Salix</i>
64	Butein	<i>Acicia</i>
65	Okanin	<i>Acicia</i>
66	Phloretin	Tomat, Strawberry
67	Phlorizin	
Auron		
68	Sulfuretin	<i>Bidens</i>
69	Aureusidin	<i>Antirrhinum</i>
70	Maritimetin	<i>Bidens</i>
71	Leptosidin	<i>Coreopsis</i>
Antosianidin		
72	Apigenidin	<i>Rechsteineria</i>
73	Luctolinnidin	<i>Rechsteineria</i>
74	Pelargonidin	<i>Pelargonium</i>
75	Cyanidin	<i>Centaurea</i>
76	Peonidin	<i>Paeonia</i>
77	Delpinidin	<i>Delphinium</i>
78	Petunidin	<i>Petunia</i>
79	Malvinidin	<i>Malva</i>
80	Rosinidin	Kacang

LAMPIRAN 2

ALUR PENELITIAN SKKRINING FARMAKOFOR DAN PENAMBATAN MOLEKUL



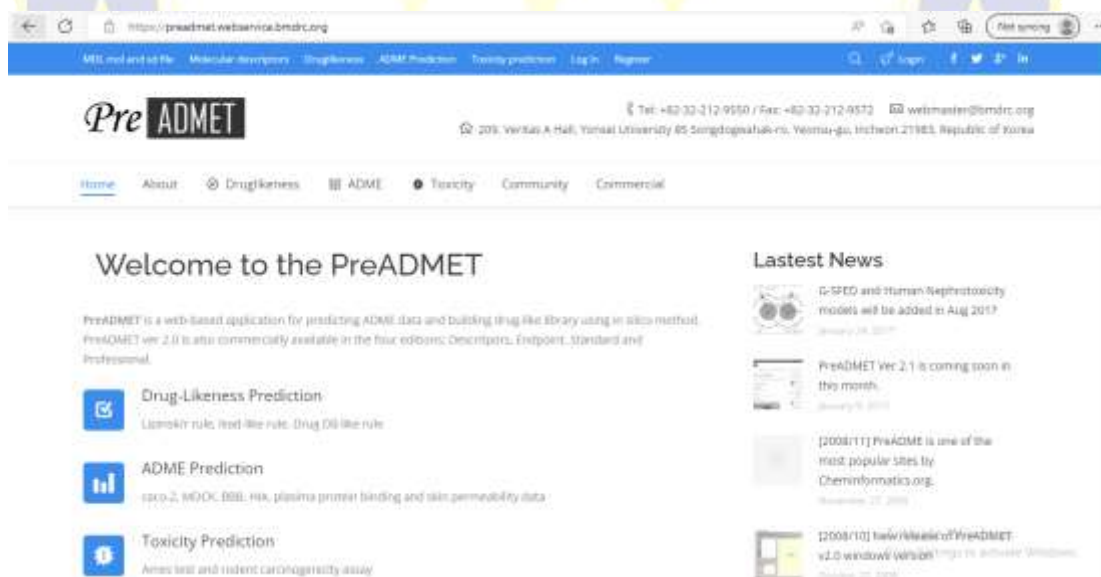
Gambar VII. 1 Alur Penelitian Skrinig Farmakofor dan Penambatan Molekul

LAMPIRAN 3

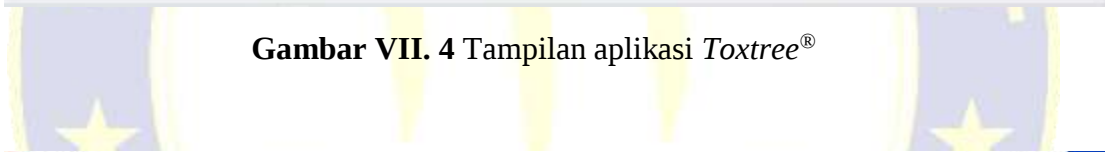
SITUS DAN APLIKASI



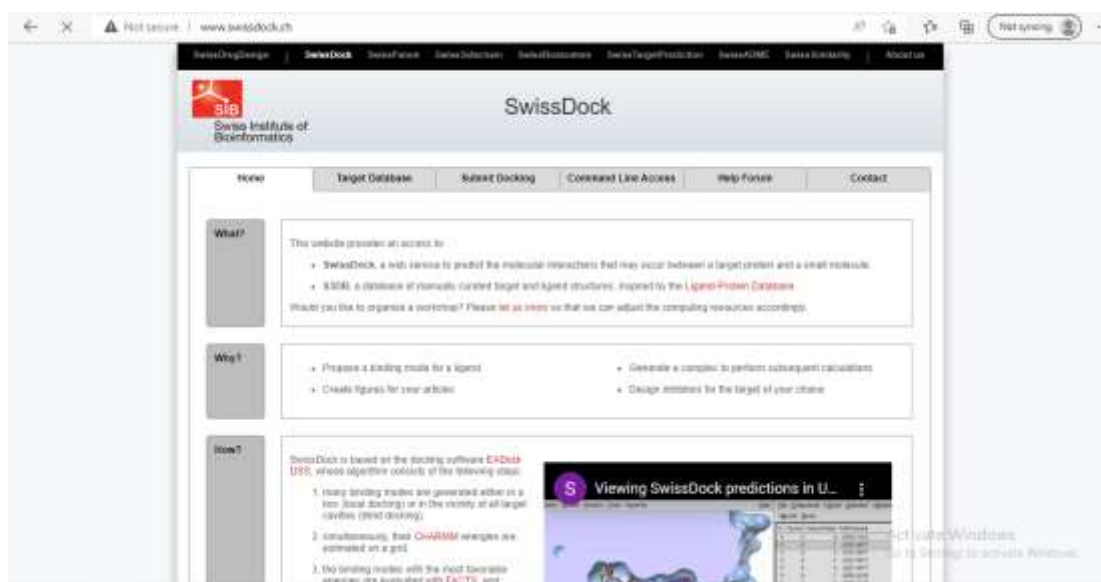
Gambar VII. 2 Tampilan situs online *Lipins'ki Rule of Five*



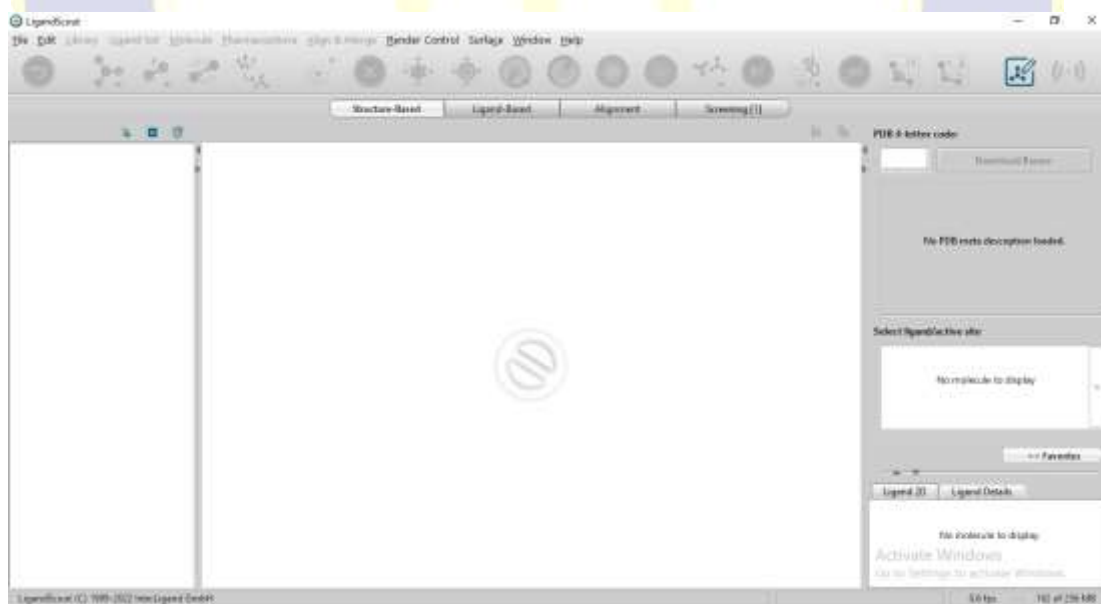
Gambar VII. 3 Tampilan situs online *Pre ADMET*



LAMPIRAN 3 (LANJUTAN)



Gambar VII. 6 Tampilan situs *online* SwissDock



Gambar VII. 7 Tampilan aplikasi *LigandScout* 4.4.5

LAMPIRAN 3 (LANJUTAN)

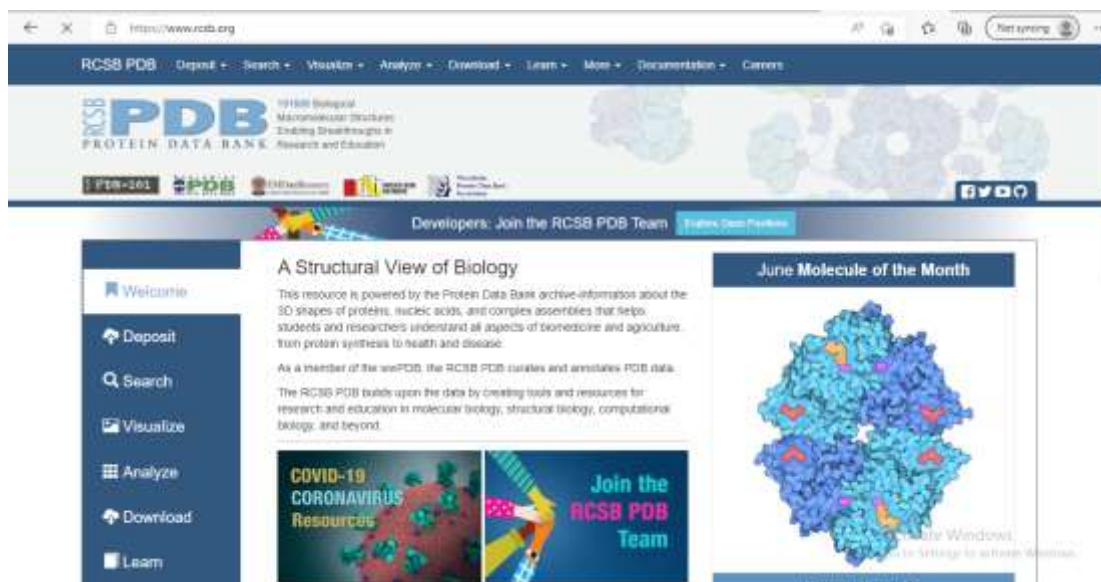


Gambar VII. 8 Tampilan situs online DUD-E



Gambar VII. 9 Tampilan situs online The Binding Data Base

LAMPIRAN 3 (LANJUTAN)

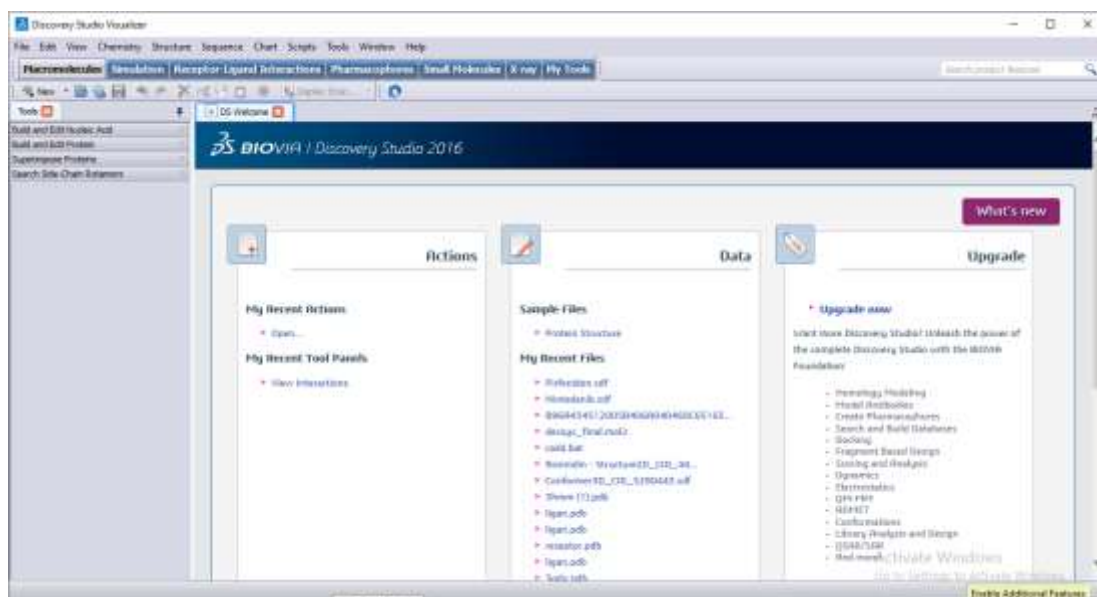


Gambar VII. 9 Tampilan situs online Protein Data Bank

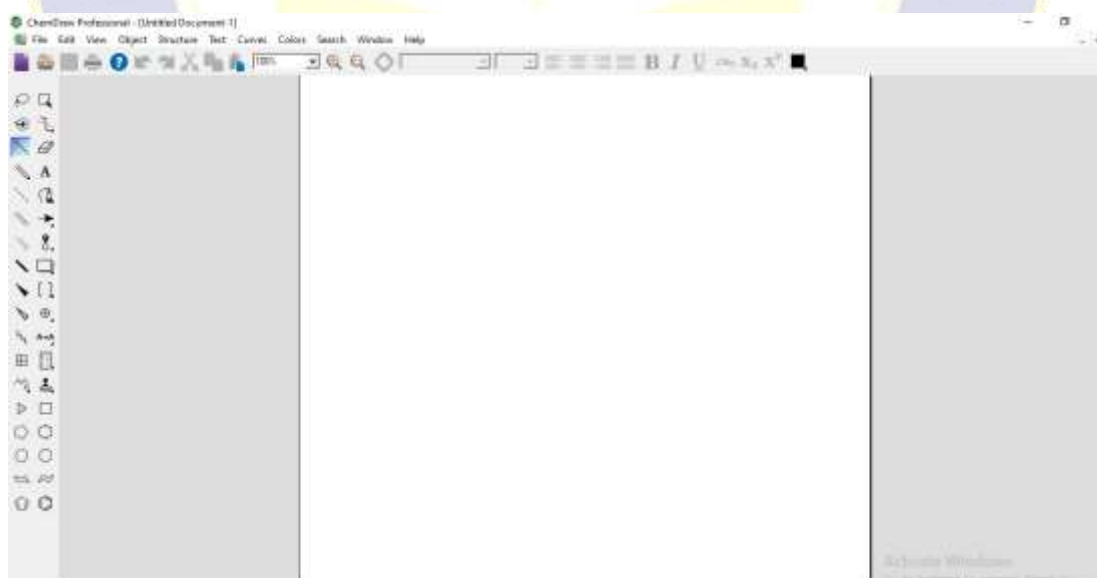


Gambar VII. 15 Tampilan situs online PubChem

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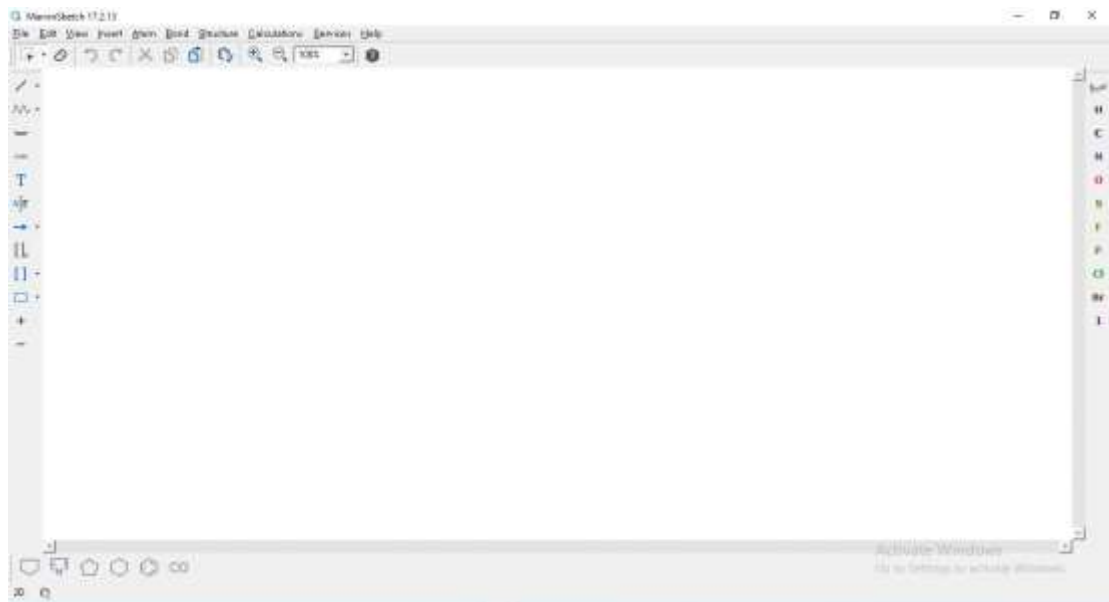


Gambar VII. 10 Tampilan aplikasi *Discovery Studio Visualizer*[®]

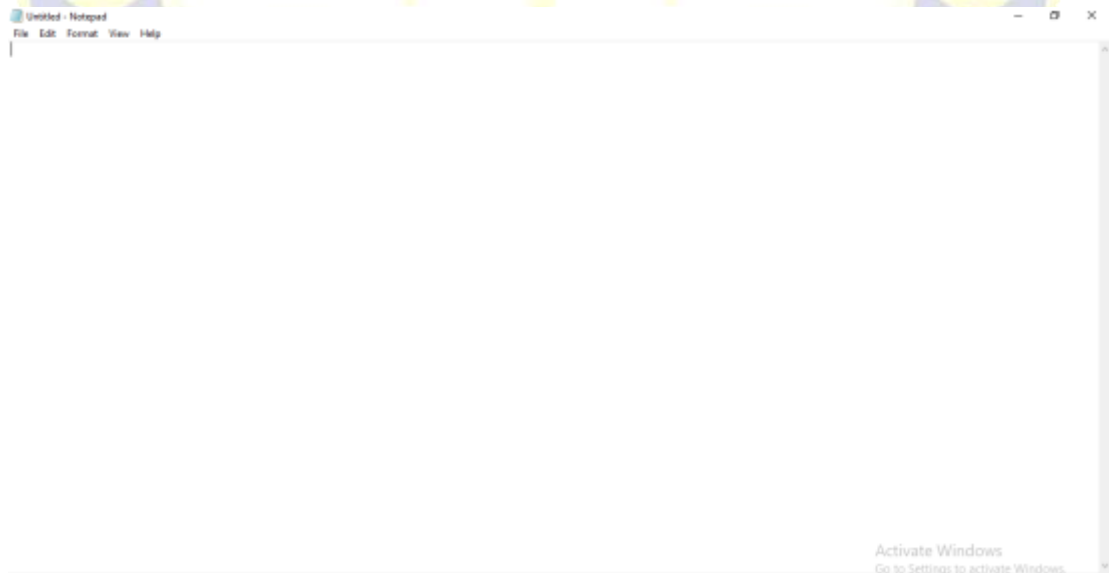


Gambar VII. 11 Tampilan aplikasi *ChemDraw Professional 15.0*

LAMPIRAN 3 (LANJUTAN)



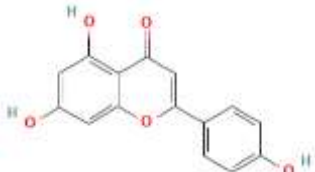
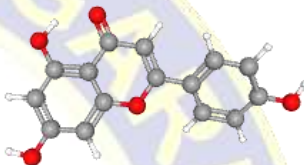
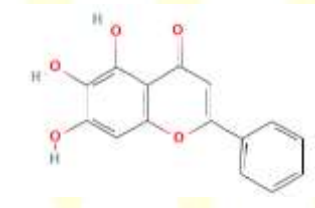
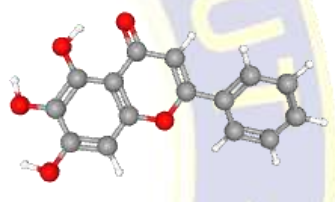
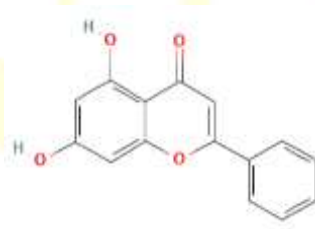
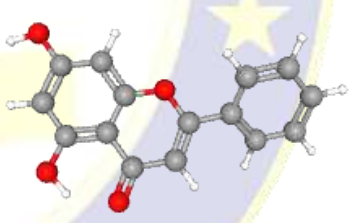
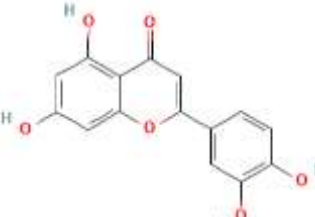
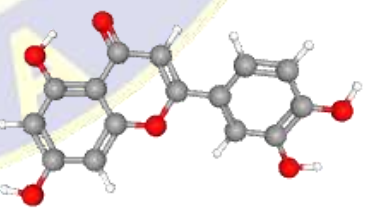
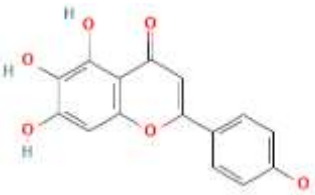
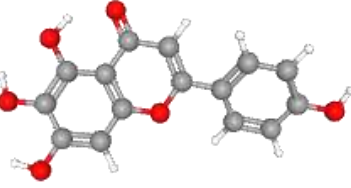
Gambar VII. 12 Tampilan aplikasi *MarvinSketch 17.2.13*



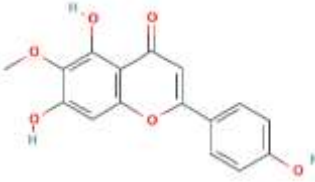
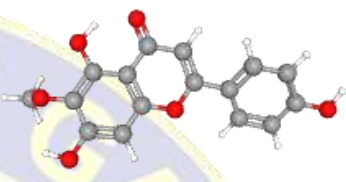
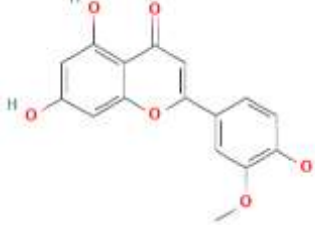
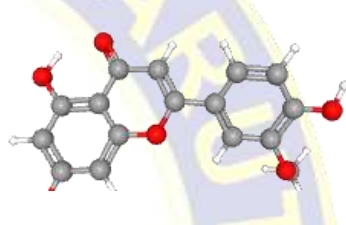
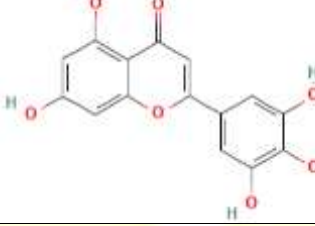
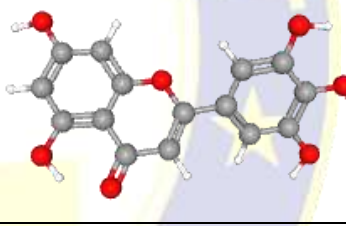
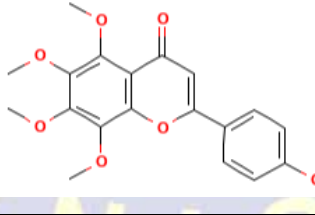
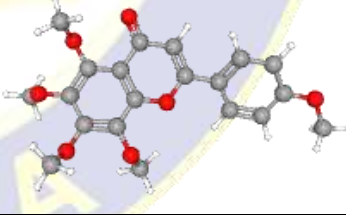
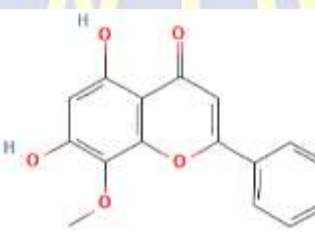
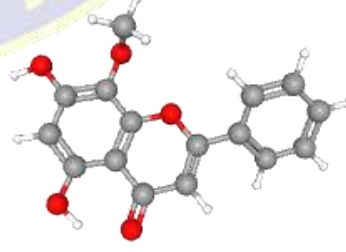
Gambar VII. 13 Tampilan aplikasi *NotePad®*

LAMPIRAN 4
STRUKTUR SENYAWA FLAVONOID

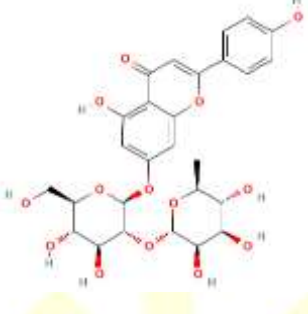
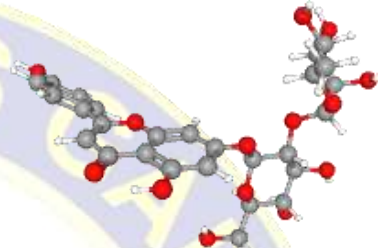
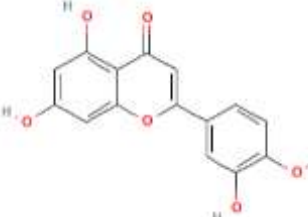
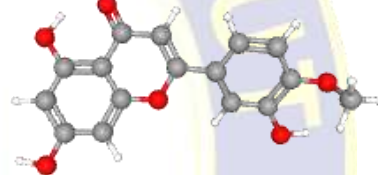
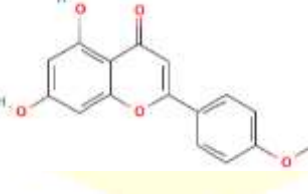
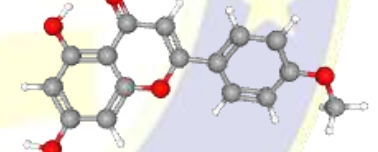
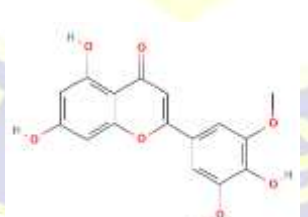
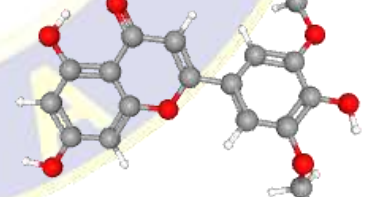
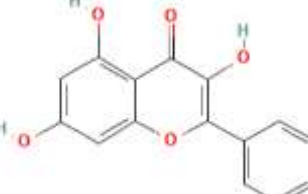
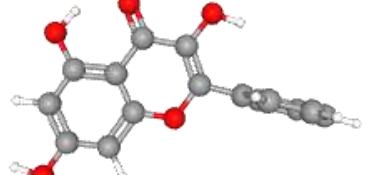
Tabel VII.2
Struktur 2D dan 3D senyawa flavonoid

No	Senyawa	Struktur 2D	Struktur 3D
Flavon			
1	Apigenin		
2	Baicalein		
3	Chrysin		
4	Luteolin		
5	Scutelarein		

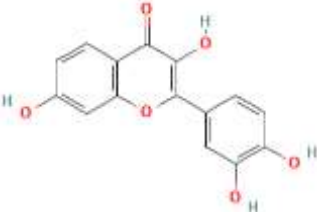
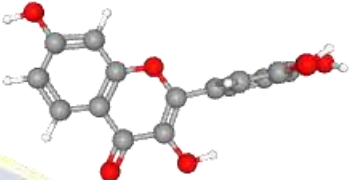
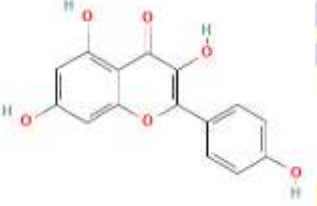
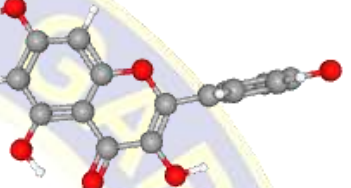
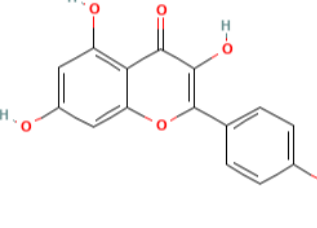
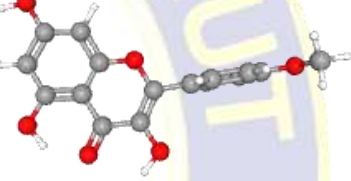
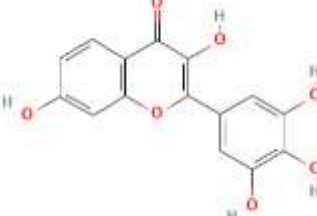
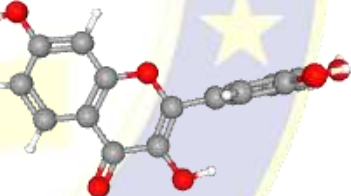
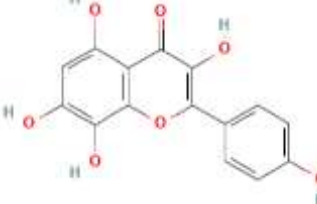
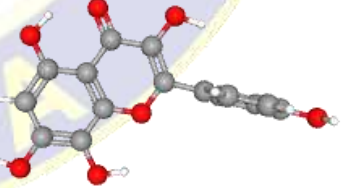
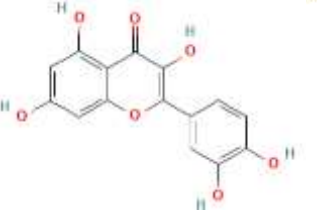
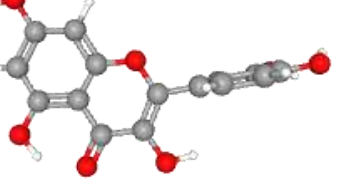
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
6	Hispidulin		
7	Chryseriol		
8	Tricetin		
9	Tangeretin		
10	Wogonin		

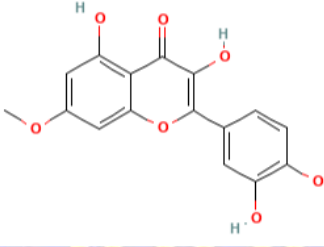
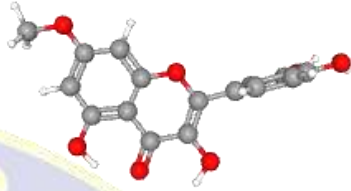
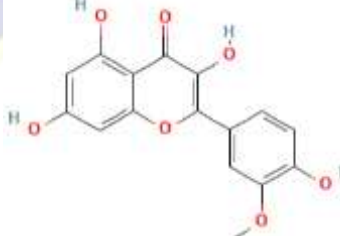
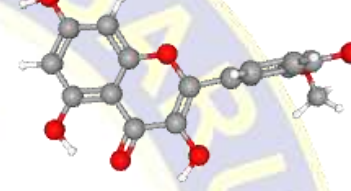
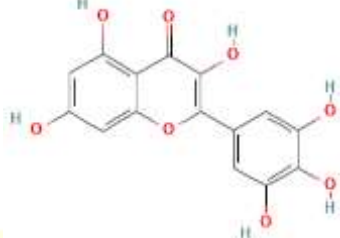
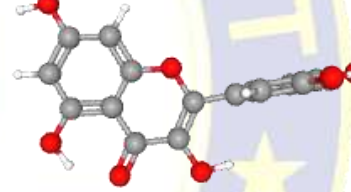
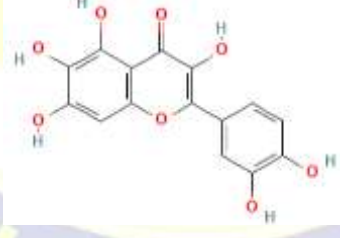
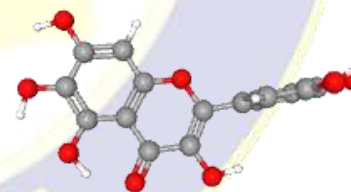
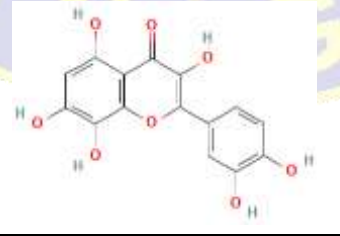
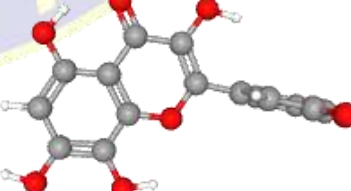
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
11	Rhoifolin		
12	Diosmetin		
13	Acacetin		
14	Tricin		
Flavonol			
15	Galangin		

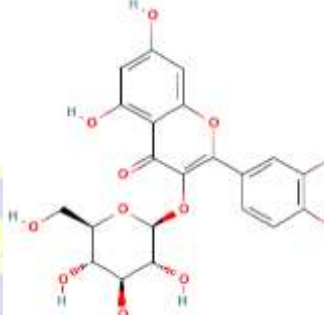
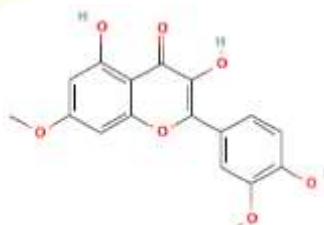
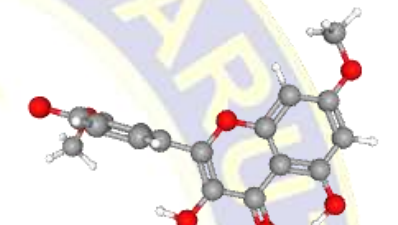
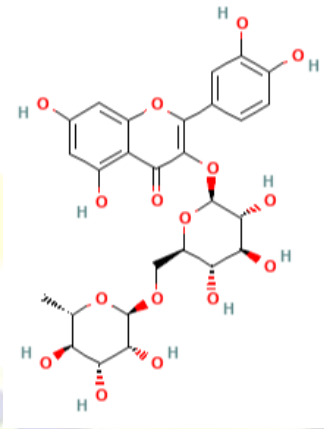
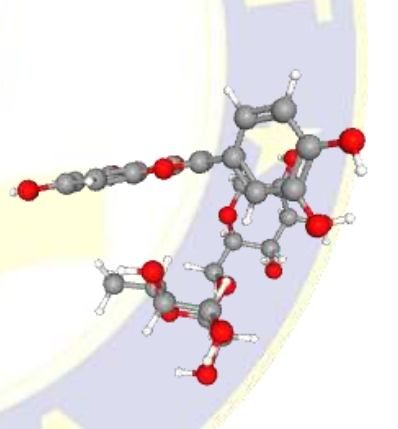
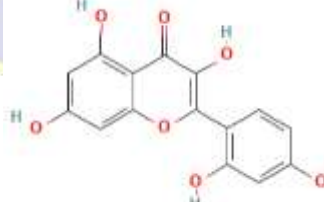
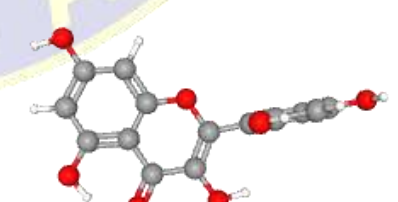
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
16	Fisetin		
17	Kaemferol		
18	Kaemferide		
19	Robinetin		
20	Herbasetin		
21	Quercetin		

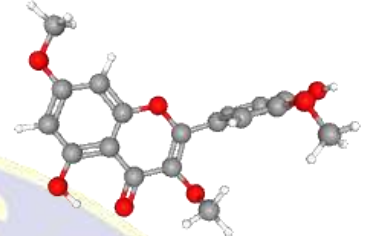
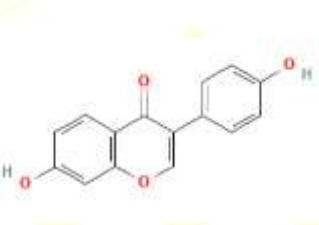
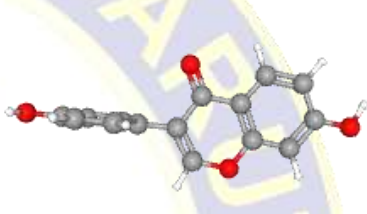
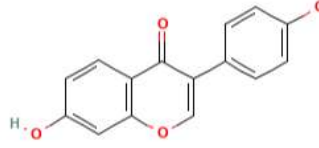
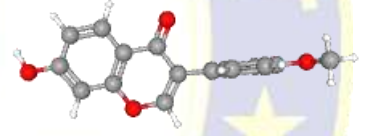
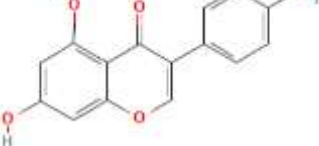
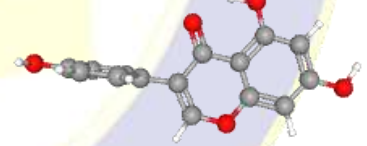
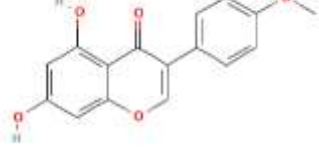
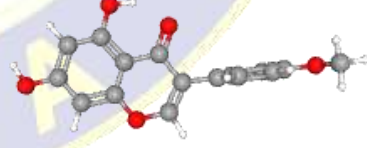
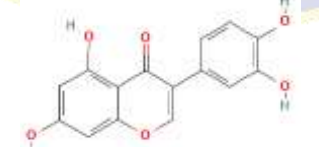
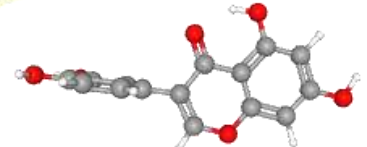
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
22	Ramnetin		
23	Isoramnetin		
24	Myricetin		
25	Querstagenin		
26	Gossypetin		

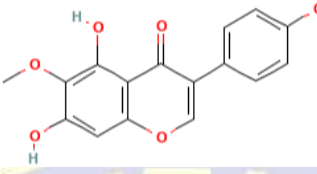
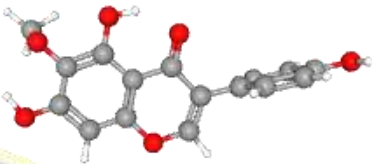
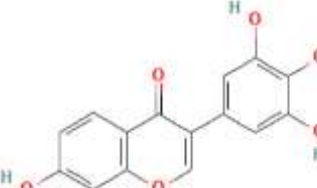
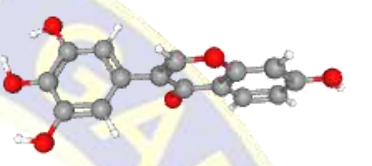
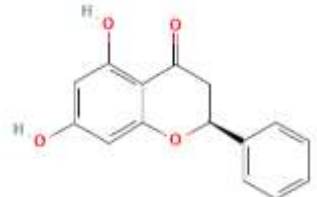
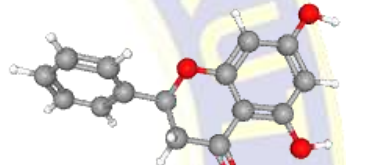
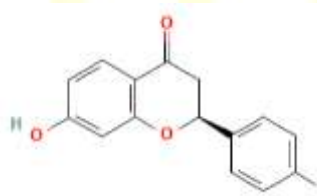
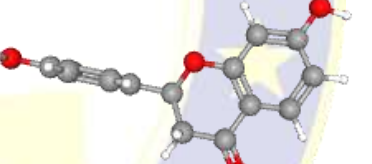
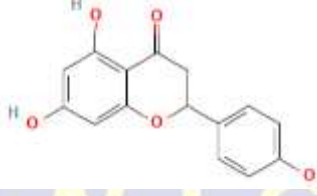
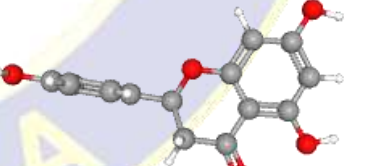
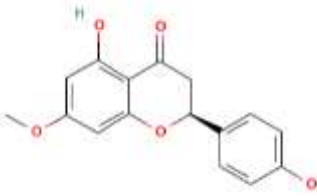
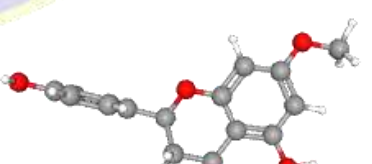
LAMPIRAN 4 (LANJUTAN)

No	Senyawa	Struktur 2D	Struktur 3D
27	Isoquercetin		
28	Ramnazin		
29	Rutin		
30	Morin		

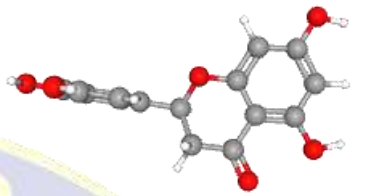
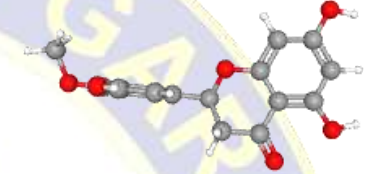
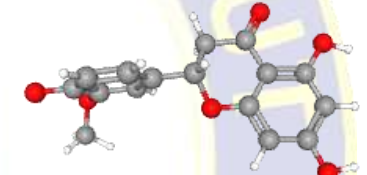
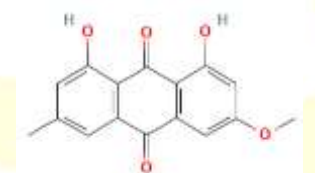
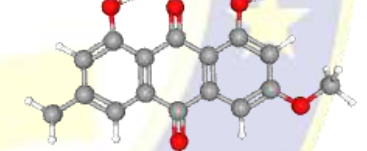
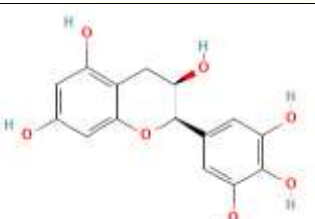
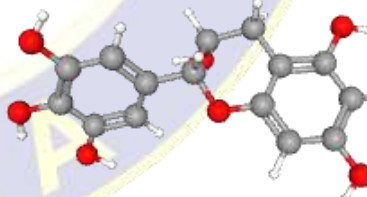
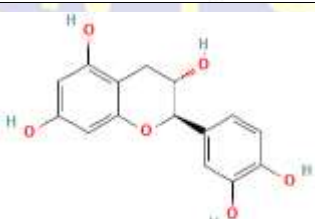
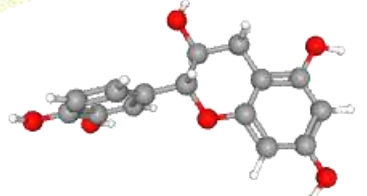
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
31	Pachypodol		
Isoflavone			
32	Daidzein		
33	Formononetin		
34	Genistein		
35	Biokanin A		
36	Orobol		

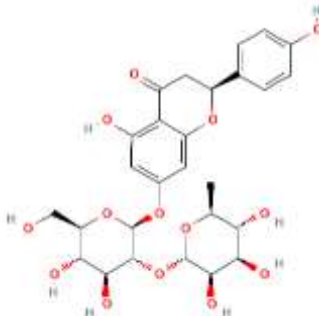
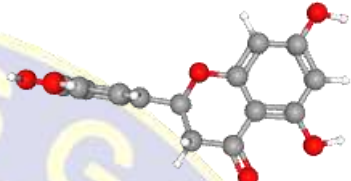
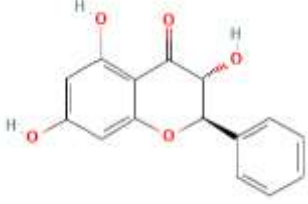
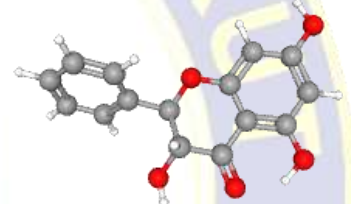
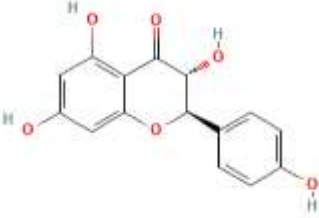
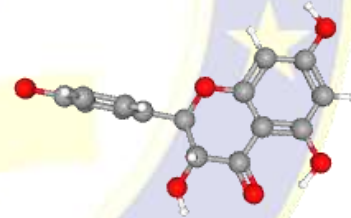
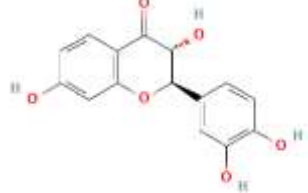
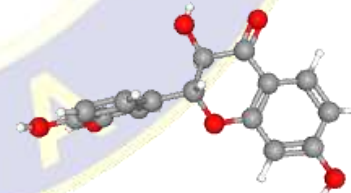
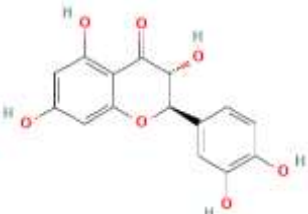
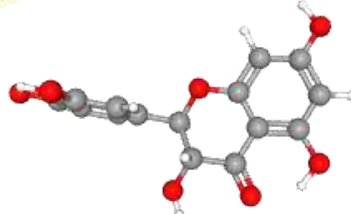
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
37	Tectorigenin		
38	Baptigenin		
Flavanon			
39	Pinocembrin		
40	Liquiritigenin		
41	Narigenin		
42	Sakuranetin		

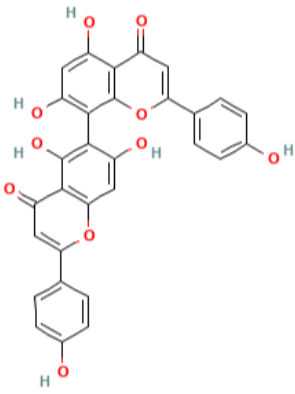
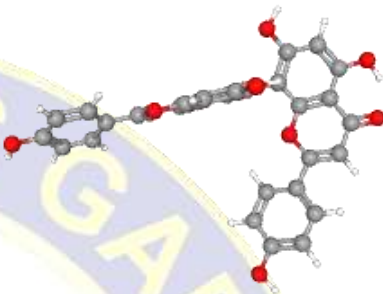
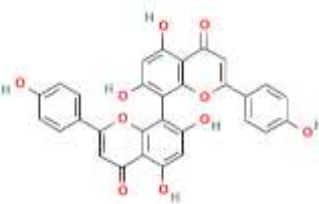
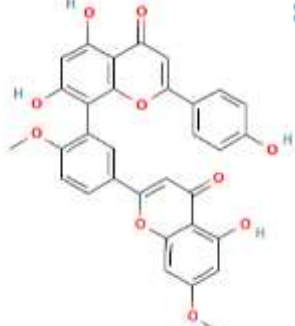
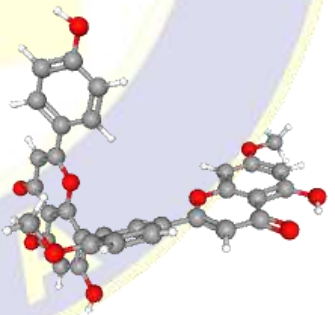
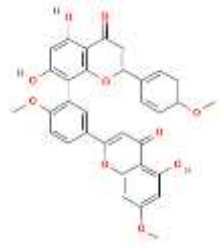
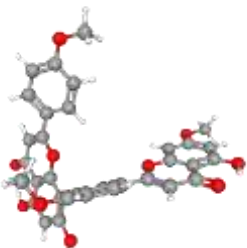
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
43	Eriodictyol		
44	Hesperetin		
45	Homoeriodictyol		
46	Parietin		
47	Epigallocatechin		
48	Catechin		

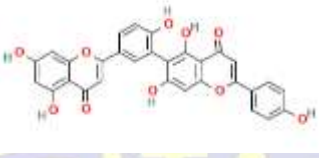
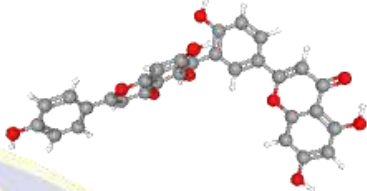
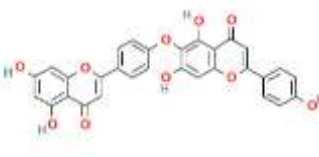
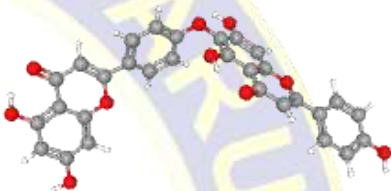
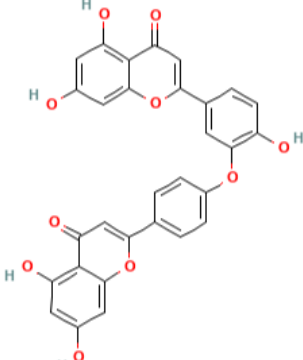
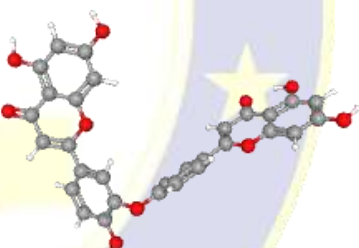
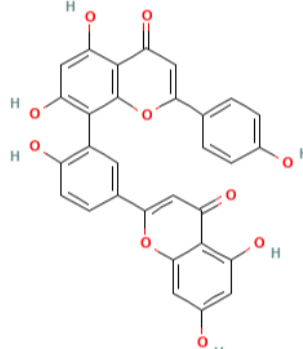
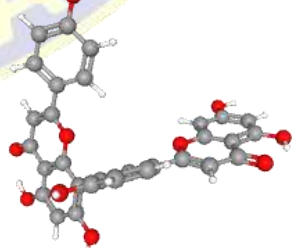
LAMPIRAN 4 (LANJUTAN)

No	Senyawa	Struktur 2D	Struktur 3D
49	Naringin		
Dehidroflavone			
50	Pinobanskin		
51	Aromadendrin		
52	Fustin		
53	Taksifolin		

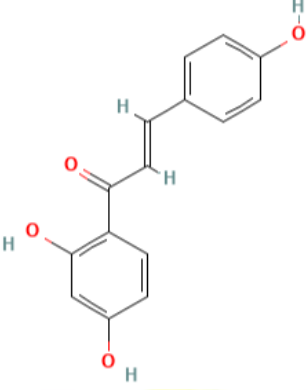
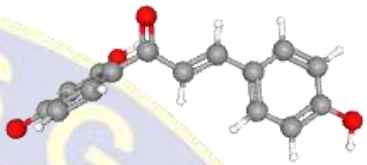
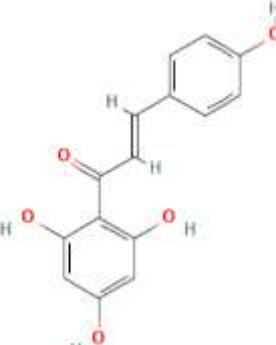
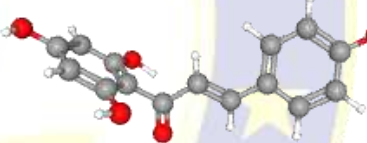
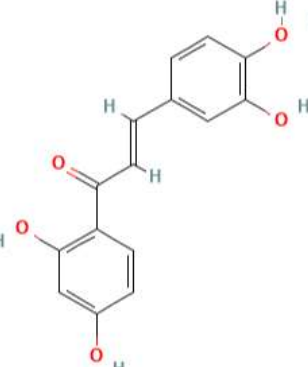
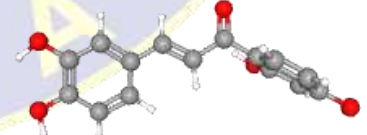
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
BiFlvonoid			
54	Agathisflavone		
55	Cupressuflavone		
56	Ginkgetin		
57	Sciadopitisin		

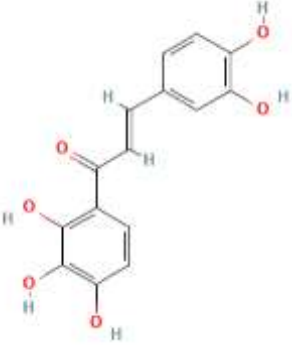
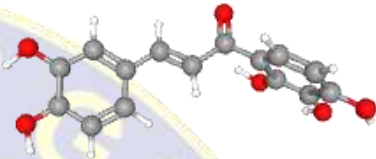
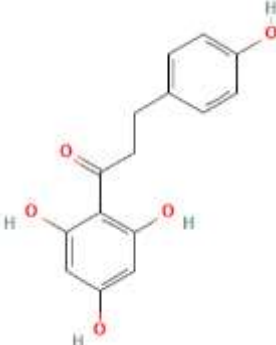
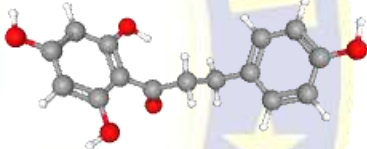
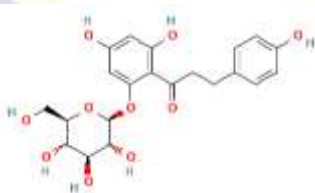
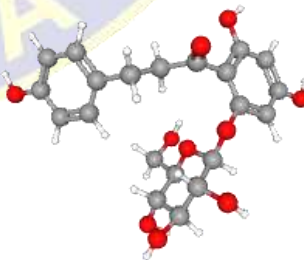
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
58	Robustaflavone		
59	Hinokiflavone		
60	Ochnaflavone		
61	Amentoflavone		

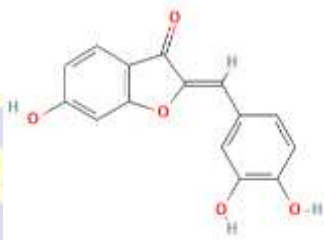
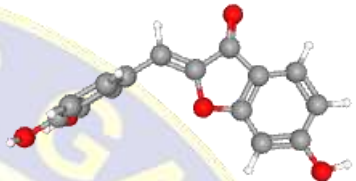
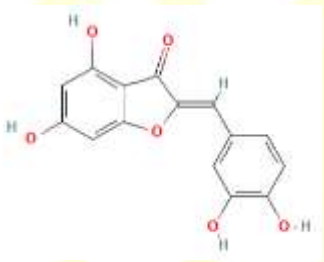
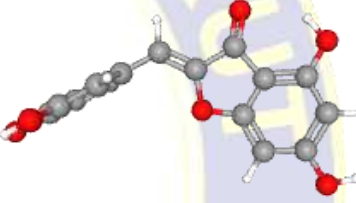
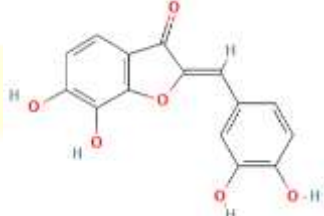
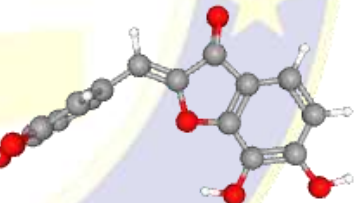
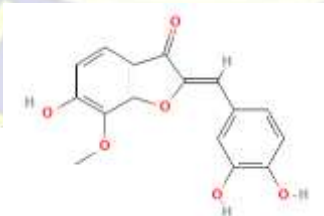
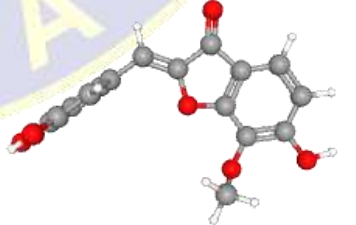
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
62	Isoliquiritigenin		
63	Kalkonaringenin		
64	Butein		

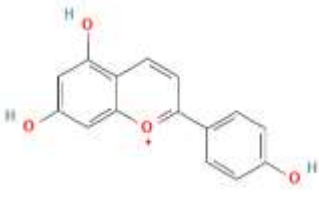
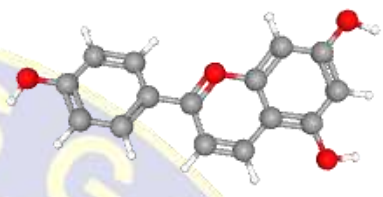
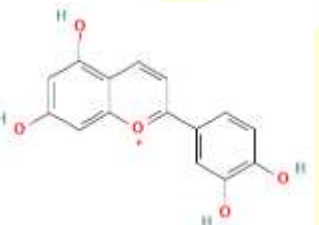
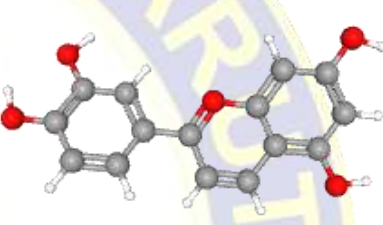
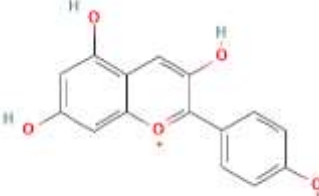
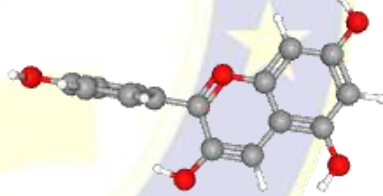
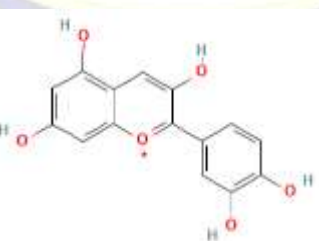
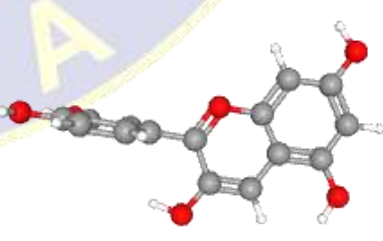
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
65	Okanin		
66	Phloretin		
67	Phlorizin		

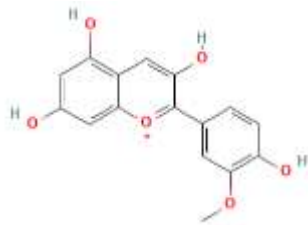
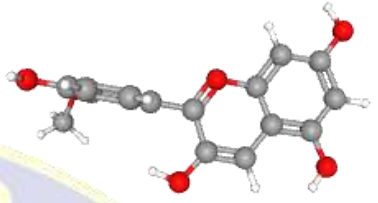
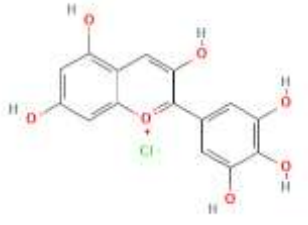
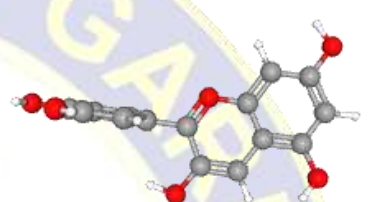
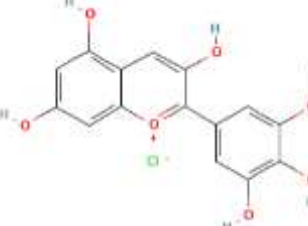
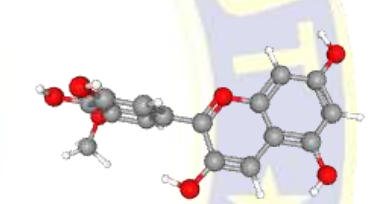
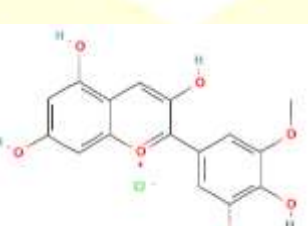
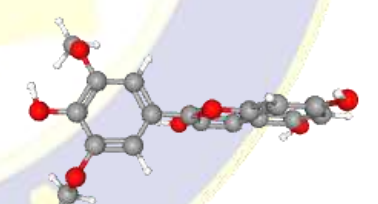
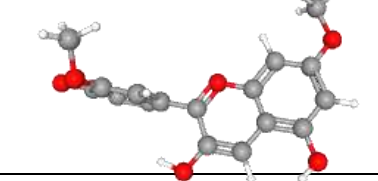
**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
Auron			
68	Sulfuretin		
69	Aureusidin		
70	Maritimetin		
71	Leptosidin		

**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
Antosianidin			
72	Apigenidin		
73	Luteolinidin		
74	Pelargonidin		
75	Cyanidin		

**LAMPIRAN 4
(LANJUTAN)**

No	Senyawa	Struktur 2D	Struktur 3D
76	Peonidin		
77	Delpinidin		
78	Petunidin		
79	Malvinidin		
80	Rosinidin		

LAMPIRAN 5
HASIL PENELITIAN PREDIKSI *DRUGLIKENESS*

Tabel VII.3

Hasil Penelitian Prediksi *Druglikeness* Menggunakan Situs *Online Lipin'ski Rule Of Five*

No	Ligan	BM (Da)	Log P	Donor Ikatan H	Akseptor Ikatan H	Keterangan
1	Pirfenidone (ligan pembanding)	185	1.81	0	1	Memenuhi
2	Nintedanib (ligan pembanding)	539	3.55	2	4	Tidak memenuhi
3	Apigenin	270	0.95	3	5	Memenuhi
4	Baicalein	270	1.42	3	5	Memenuhi
5	Chrysin	254	1.54	2	4	Memenuhi
6	Luteolin	286	0.83	4	6	Memenuhi
7	Scutelarein	286	0.83	4	6	Memenuhi
8	Hispidulin	300	1.32	3	5	Memenuhi
9	Chryseriol	300	1.35	3	6	Memenuhi
10	Tricetin	302	0.53	5	7	Memenuhi
11	Tangeretin	372	3.16	0	7	Memenuhi
12	Wogonin	284	1.91	2	5	Memenuhi
13	Rhoifolin	578	2.41	8	14	Tidak memenuhi
14	Diosmetin	300	1.35	3	6	Memenuhi
15	Acacetin	284	1.65	2	5	Memenuhi
16	Tricin	330	1.58	3	7	Memenuhi
17	Galangin	270	1.23	3	5	Memenuhi
18	Fisetin	286	0.82	4	6	Memenuhi
19	Kaemferol	286	0.64	4	6	Memenuhi
20	Kaemferide	300	1.34	3	6	Memenuhi
21	Robinetin	302	0.52	5	7	Memenuhi
22	Herbasetin	302	0.52	5	7	Memenuhi
23	Quercetin	302	0.52	5	7	Memenuhi
24	Ramnetin	316	1.22	4	7	Memenuhi
25	Isoramnetin	316	1.04	4	7	Memenuhi

**LAMPIRAN 5
(LAJUTAN)**

No	Ligan	BM (Da)	Log P	Donor Ikatan H	Akseptor Ikatan H	Keterangan
26	Myricetin	318	0.22	6	8	Tidak memenuhi
27	Querstagenin	318	0.40	6	8	Tidak memenuhi
28	Gossypetin	318	0.40	6	8	Tidak memenuhi
29	Isoquercetin	464	1.03	8	12	Tidak memenuhi
30	Ramnazin	330	1.75	3	7	Memenuhi
31	Rutin	610	1.83	10	16	Tidak memenuhi
32	Morin	302	0.34	5	7	Memenuhi
33	Pachypodol	344	2.24	2	7	Memenuhi
34	Daidzein	254	1.24	2	4	Memenuhi
35	Formononetin	268	1.94	1	4	Memenuhi
36	Genistein	270	0.94	3	5	Memenuhi
37	Biokanin A	284	1.64	2	5	Memenuhi
38	Orobol	286	0.82	4	6	Memenuhi
39	Tectorigenin	300	1.31	3	6	Memenuhi
40	Baptigenin	286	0.82	4	6	Memenuhi
41	Pinocembrin	256	1.76	2	4	Memenuhi
42	Liquiritigenin	256	1.47	2	4	Memenuhi
43	Narigenin	272	1.17	3	5	Memenuhi
44	Sakuranetin	286	1.87	2	5	Memenuhi
45	Eriodictyol	288	1.04	4	6	Memenuhi
46	Hesperetin	302	1.57	3	6	Memenuhi
47	Homeriodictyol	302	1.57	3	6	Memenuhi
48	Parietin	284	1.81	2	5	Memenuhi
49	Epigallocatechin	306	0.79	6	7	Tidak memenuhi
50	Catechin	290	1.09	5	6	Memenuhi
51	Naringin	500	2.63	8	14	Tidak memenuhi
52	Pinobanskin	272	1.46	3	5	Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

No	Ligan	BM (Da)	Log P	Donor Ikatan H	Akseptor Ikatan H	Keterangan
53	Aromadendrin	288	0.87	4	6	Memenuhi
54	Fustin	288	1.04	4	6	Memenuhi
55	Taksifolin	304	0.74	5	7	Memenuhi
56	Agathisflavone	538	2.35	4	10	Tidak memenuhi
57	Cupresuflavone	538	2.34	4	10	Tidak memenuhi
58	Ginkgetin	566	3.34	4	10	Tidak memenuhi
59	Siadopitisin	580	3.87	3	10	Tidak memenuhi
60	Robustaflavone	538	2.18	5	10	Tidak memenuhi
61	Hinokiflavone	638	2.19	5	10	Tidak memenuhi
62	Ochnaflavone	538	2.18	5	10	Tidak memenuhi
63	Amentoflavone	538	2.15	6	10	Tidak memenuhi
64	Isoliquiritigenin	256	1.32	3	4	Memenuhi
65	Khalkonarigenin	272	1.01	4	5	Memenuhi
66	Butein	272	1.19	4	5	Memenuhi
67	Okanin	288	1.07	5	6	Memenuhi
68	Phloretin	274	1.22	4	5	Memenuhi
69	Phlorizin	436	1.72	7	10	Tidak memenuhi
70	Sulfuretin	270	1.17	3	5	Memenuhi
71	Aureusidin	286	0.65	4	6	Memenuhi
72	Maritimetin	286	1.05	4	6	Memenuhi
73	Leptosidin	300	1.53	3	6	Memenuhi
74	Apigenidin	290	2.68	3	4	Memenuhi
75	Luteolinnidin	271	1.07	4	5	Memenuhi
76	Pelargonidin	271	0.88	4	5	Memenuhi
77	Cyanidin	287	0.76	5	6	Memenuhi
78	Peonidin	301	1.29	4	6	Memenuhi
79	Delpinidin	338.5	1.14	6	7	Memenuhi
80	Peutinidin	301	0.99	5	7	Memenuhi

**LAMPIRAN 5
(LANJUTAN)**

No	Ligan	BM (Da)	Log P	Donor Ikatan H	Akseptor Ikatan H	Keterangan
81	Malvinidin	366.5	2.19	4	7	Memenuhi
82	Rosidinin	315	1.99	3	6	Memenuhi



LAMPIRAN 6
HASIL PENELITIAN PREDIKSI FARMAKOKINETIKA

Tabel VII.4

Hasil penelitian prediksi farmakokinetika menggunakan situs *online Pre-ADMET*

No	Ligan	Absorbsi		Distribusi
		HIA (%)	Caco-2 (nm sec)	Protein Plasma Binding (%)
1	Pirfenidone (ligan pembanding)	100****	47.57**	80.34*
2	Nintedanib (ligan pembanding)	94.74***	35.64**	83.29*
3	Apigenin	88.12****	10.54**	97.25**
4	Baicalein	32.42**	11.55**	75.69*
5	Chrysin	92.64****	2.47*	95.09**
6	Luteolin	79.42****	4.53**	99.71**
7	Scutelarein	79.41****	4.53**	100**
8	Hispidulin	88.18****	5.46**	91.55**
9	Chryseriol	89.01****	4.20**	84.85*
10	Tricetin	63.47**	1.48*	100**
11	Tangeretin	98.88****	53.60**	87.17*
12	Wogonin	93.03****	4.28**	90.44**
13	Rhoifolin	13.77*	7.90**	54.68*
14	Diosmetin	88.18****	7.02**	90.16**
15	Acacetin	93.04****	12.79**	90.91**
16	Tricin	87.82****	3.00*	87.07*
17	Galangin	93.04****	1.62*	84.72*
18	Fisetin	79.43****	9.57**	88.74*
19	Kaemferol	79.43****	9.57**	89.60*
20	Kaemferide	88.12****	9.33**	83.99*
21	Robinetin	63.47**	3.40*	92.63**
22	Herbasetin	63.47**	5.32**	93.07**
23	Quercetin	63.48**	3.41*	93.23**
24	Ramnetin	78.34****	4.93**	85.34*
25	Isoramnetin	76.16****	4.92**	85.01*
26	Myricetin	40.96**	0.99*	96.78**
27	Querstagenin	40.94**	0.99*	98.33**
28	Gossypetin	40.95**	5.20**	96.48**
29	Isoquercetin	11.77*	9.43**	59.15**

**LAMPIRAN 6
(LANJUTAN)**

No	Ligan	Absorbsi		Distribusi
		HIA (%)	Caco-2 (nm sec)	<i>Protein Plasma Binding (%)</i>
30	Ramnazin	87.82***	5.09**	81.21*
31	Rutin	2.86*	7.91**	43.89*
32	Morin	63.49**	17.10**	91.62**
33	Pachypodol	93.45***	4.38**	79.88*
34	Daidzein	92.64***	7.72**	88.70*
35	Formononetin	95.55***	7.60**	85.08*
36	Genistein	88.12***	5.74**	89.73*
37	Biokanin A	93.04***	3.40*	85.00*
38	Orobol	79.42***	11.29**	90.31**
39	Tectorigenin	76.52***	1.44*	91.29**
40	Baptigenin	79.41***	1.56*	90.35**
41	Pinocembrin	92.35***	2.47*	98.45**
42	Liquiritigenin	92.35***	17.64**	97.98**
43	Narigenin	87.31***	10.52**	100**
44	Sakuranetin	92.75***	12.82**	95.21**
45	Eriodictyol	77.43***	4.53**	100**
46	Hesperetin	87.19***	7.00**	96.79**
47	Homeriodictyol	87.19***	5.16**	98.05**
48	Parietin	94.04***	20.74**	95.21**
49	Epigallocatechin	45.95**	0.37*	100**
50	Catechin	66.70**	0.65*	100**
51	Naringin	11.74*	7.89**	51.06*
52	Pinobanskin	87.60***	3.69*	89.64*
53	Aromadendrin	77.83***	9.56**	89.67*
54	Fustin	77.82***	9.56**	88.03*
55	Taksifolin	60.16**	3.42*	95.16**
56	Agathisflavone	81.19***	11.09**	100**
57	Cupresuflavone	40.95**	5.20**	96.48**
58	Ginkgetin	91.40***	11.98**	95.55**
59	Siadopitisin	94.05***	13.68**	90.51**
60	Robustaflavone	81.19***	12.04**	100**
61	Hinokiflavone	86.95***	4.34**	100**
62	Ochnaflavone	86.95***	6.77**	100**
63	Amentoflavone	81.19***	12.87**	100**
64	Isoliquiritigenin	88.30***	20.15**	98.25**

**LAMPIRAN 6
(LANJUTAN)**

No	Ligan	Absorbsi		Distribusi
		HIA (%)	Caco-2 (nm sec)	<i>Protein Plasma Binding (%)</i>
65	Khalkonarigenin	80.61***	18.10**	100**
66	Butein	80.60***	18.10**	99.72**
67	Okanin	66.57**	14.31**	100**
68	Phloretin	78.98***	18.10**	100**
69	Phlorizin	26.79**	9.61**	75.47*
70	Sulfuretin	89.54***	13.36**	100**
71	Aureusidin	82.57***	8.15**	100**
72	Maritimetin	82.56***	8.14**	100**
73	Leptosidin	89.05***	18.74**	94.12**
74	Apigenidin	(-)	(-)	(-)
75	Luteolinnidin	83.57***	0.68*	100**
76	Pelargonidin	83.58***	1.29*	100**
77	Cyanidin	72.50***	0.65*	100**
78	Peonidin	83.43***	1.65*	100**
79	Delpinidin	65.42**	19.47**	88.41*
80	Peutinidin	71.31***	0.96*	100**
81	Malvinidin	86.81***	20.87**	75.24*
82	Rosidinin	90.13***	2.12*	87.78*

HIA (%) :

*** : > 70 (terserap baik)

** : 20 - 70 (terserap cukup)

* : < 20 (kurang terserap)

Protein Plasma Binding (%):

** : > 90 (terikat kuat)

* : < 90 (terikat lemah)

CaCo-2 Cell (nm sec) :

*** : > 70 (permeabilitas tinggi)

** : 4-70 (permeabilitas sedang)

* : < 4 (permeabilitas rendah)

LAMPIRAN 7
HASIL PENELITIAN PREDIKSI TOKSISITAS

Tabel VII.5
 Hasil Penelitian Prediksi Toksisitas Menggunakan Situs Aplikasi *Toxree*[®]

No	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
1	Pirfenidone (ligan pembanding)	(-)	(-)	(-)	Tidak Berisiko
2	Nintedanib (ligan pembanding)	(-)	(-)	(-)	Tidak Berisiko
3	Apigenin	(-)	(-)	(-)	Tidak Berisiko
4	Baicalein	(-)	(-)	(-)	Tidak Berisiko
5	Chrysin	(-)	(-)	(-)	Tidak Berisiko
6	Luteolin	(-)	(-)	(-)	Tidak Berisiko
7	Scutelarein	(-)	(-)	(-)	Tidak Berisiko
8	Hispidulin	(-)	(-)	(-)	Tidak Berisiko
9	Chryseriol	(-)	(-)	(-)	Tidak Berisiko
10	Tricetin	(-)	(-)	(-)	Tidak Berisiko
11	Tangeretin	(-)	(-)	(-)	Tidak Berisiko
12	Wogonin	(-)	(-)	(-)	Tidak Berisiko
13	Rhoifolin	(-)	(-)	(-)	Tidak Berisiko
14	Diosmetin	(-)	(-)	(-)	Tidak Berisiko
15	Acacetin	(-)	(-)	(-)	Tidak berisiko
16	Tricin	(-)	(-)	(-)	Tidak Berisiko
17	Galangin	(-)	(-)	(-)	Tidak Berisiko

**LAMPIRAN 7
(LANJUTAN)**

No	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
18	Fisetin	(-)	(-)	(-)	Tidak Berisiko
19	Kaemferol	(-)	(-)	(-)	Tidak Berisiko
20	Kaemferide	(-)	(-)	(-)	Tidak Berisiko
21	Robinetin	(-)	(-)	(-)	Tidak Berisiko
22	Herbasetin	(-)	(-)	(-)	Tidak Berisiko
23	Quercetin	(+)	(-)	(-)	Tidak Berisiko
24	Ramnetin	(+)	(-)	(-)	Tidak Berisiko
25	Isoramnetin	(+)	(-)	(-)	Tidak Berisiko
26	Myricetin	(+)	(-)	(-)	Tidak Berisiko
27	Querstagenin	(+)	(-)	(-)	Tidak Berisiko
28	Gossypetin	(+)	(-)	(-)	Tidak Berisiko
29	Isoquercetin	(+)	(-)	(-)	Tidak Berisiko
30	Ramnazin	(+)	(-)	(-)	Tidak Berisiko
31	Rutin	(+)	(-)	(-)	Tidak Berisiko
32	Morin	(-)	(-)	(-)	Tidak Berisiko
33	Pachypodol	(+)	(-)	(-)	Tidak Berisiko
34	Daidzein	(-)	(-)	(-)	Tidak Berisiko
35	Formononetin	(-)	(-)	(-)	Tidak Berisiko
36	Genistein	(-)	(-)	(-)	Tidak Berisiko

**LAMPIRAN 7
(LAJUTAN)**

No	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
37	Biokanin A	(-)	(-)	(-)	Tidak Berisiko
38	Orobol	(-)	(-)	(-)	Tidak Berisiko
39	Tectorigenin	(-)	(-)	(-)	Tidak Berisiko
40	Baptigenin	(-)	(-)	(-)	Tidak Berisiko
41	Pinocembrin	(-)	(-)	(-)	Tidak Berisiko
42	Liquiritigenin	(-)	(-)	(-)	Tidak Berisiko
43	Narigenin	(-)	(-)	(-)	Tidak Berisiko
44	Sakuranetin	(-)	(-)	(-)	Tidak Berisiko
45	Eriodictyol	(-)	(-)	(-)	Tidak Berisiko
46	Hesperetin	(-)	(-)	(-)	Tidak Berisiko
47	Homeriodictyol	(-)	(-)	(-)	Tidak Berisiko
48	Parietin	(+)	(+)	(-)	Berisiko Rendah
49	Epigallocatechin	(-)	(-)	(-)	Tidak Berisiko
50	Catechin	(-)	(-)	(-)	Tidak Berisiko
51	Naringin	(-)	(-)	(-)	Tidak Berisiko
52	Pinobanskin	(-)	(-)	(-)	Tidak Berisiko
53	Aromadendrin	(-)	(-)	(-)	Tidak Berisiko
54	Fustin	(-)	(-)	(-)	Tidak Berisiko

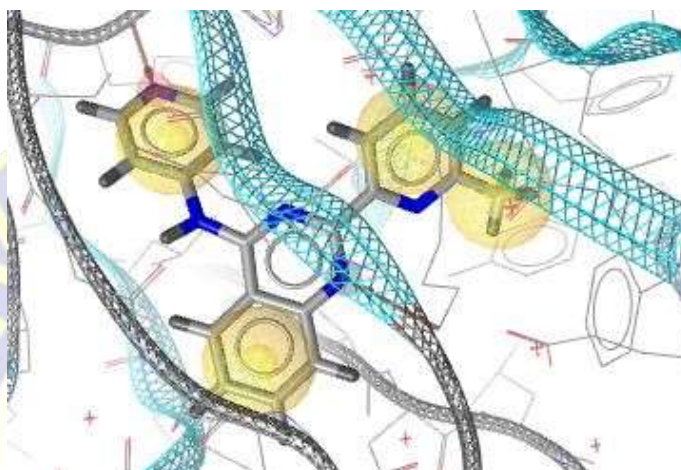
**LAMPIRAN 7
(LANJUTAN)**

No	Ligan	Mutagen (Ames Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
55	Taksifolin	(-)	(-)	(-)	Tidak Berisiko
56	Agathisflavone	(-)	(-)	(+)	Tidak Berisiko
57	Cupresuflavone	(-)	(-)	(+)	Tidak Berisiko
58	Ginkgetin	(-)	(-)	(+)	Tidak Berisiko
59	Siadopitisin	(-)	(-)	(+)	Tidak Berisiko
60	Robustaflavone	(-)	(-)	(+)	Tidak Berisiko
61	Hinokiflavone	(-)	(-)	(-)	Tidak Berisiko
62	Ochnaflavone	(-)	(-)	(-)	Tidak Berisiko
63	Amentoflavone	(-)	(-)	(+)	Tidak Berisiko
64	Isoliquiritigenin	(+)	(+)	(-)	Berisiko Rendah
65	Khalkonarigenin	(+)	(+)	(-)	Berisiko Rendah
66	Butein	(-)	(+)	(-)	Berisiko Rendah
67	Okanin	(+)	(+)	(-)	Berisiko Rendah
68	Phloretin	(-)	(-)	(-)	Tidak Berisiko
69	Phlorizin	(-)	(-)	(-)	Tidak Berisiko
70	Sulfuretin	(-)	(-)	(-)	Tidak Berisiko
71	Aureusidin	(-)	(-)	(-)	Tidak Berisiko
72	Maritimetin	(-)	(-)	(-)	Tidak Berisiko

**LAMPIRAN 7
(LANJUTAN)**

No	Ligan	Mutagen (Amest Test)	Karsinogenik		Kroes TTC
			Genotoxic	Non Genotoxic	
73	Leptosidin	(-)	(-)	(-)	Tidak Berisiko
74	Apigenidin	(-)	(-)	(-)	Tidak Berisiko
75	Luteolinnidin	(-)	(-)	(-)	Tidak Berisiko
76	Pelargonidin	(-)	(-)	(-)	Tidak Berisiko
77	Cyanidin	(-)	(-)	(-)	Tidak Berisiko
78	Peonidin	(-)	(-)	(-)	Tidak Berisiko
79	Delpinidin	(-)	(-)	(-)	Tidak Berisiko
80	Peutinidin	(-)	(-)	(-)	Tidak Berisiko
81	Malvinidin	(-)	(-)	(-)	Tidak Berisiko
82	Rosidinin	(-)	(-)	(-)	Tidak Berisiko

LAMPIRAN 8
HASIL PENELITIAN *SCREENING* FARMAKOFOR



Gambar VII.14 Visualisasi *Native Ligand*



Gambar VII.15 Model 1 farmakofor ligan TGF- β 1

No	Nama Senyawa	Matching Features	Fit Score
1	2-(5-chloro-2-fluorophenyl)-N-(pyridine-4-yl)pteridine-4-amine (Ligan Pembanding)		71.02
2	Kalkonaringenin		70.95
3	Liquiritigenin		48.70
4	Fustin		48.36
5	Isoliquiritigenin		46.86

LAMPIRAN 8 (LANJUTAN)

Keterangan :

Warna biru = cincin aromatik

Warna kuning = ikatan hidrofobik

Warna merah = akseptor ikatan hidrogen

Warna hijau = donor ikatan hidrogen



LAMPIRAN 9
HASIL PENELITIAN SIMULASI PENAMBATAN MOLEKUL

Tabel VII.8

Hasil Penambatan Senyawa Flavonoid Terhadap Reseptor TGF-Beta Tipe 1 PDB 3HMM

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidorgen	Ikatan Lainnya
1	<i>Native Ligan</i>	-9.83	62.00	Ser80, Asp81 Lys32, dan His83	Asn138, Ala30, Ala150, Leu78, Val19, Tyr49, Phe62, dan Leu140
2	<i>2-(5-chloro-2-fluorophenyl)-N-(pyridine-4-yl)pteridine-4-amine (ligan pembanding)</i>	-10.12	38.37	Lys32, Ser80, Asp81, dan His83	Tyr49, Phe62, Val19, Leu78, Ala30, Ala150, dan Leu140,
3	Apigenin	-7.53	3.04	Asp151, Tyr49, Glu45, Ser80, Lys137, Ala30, dan Ser87	Ala150, Val19, Leu60, Leu140, dan Lys32
4	Baicalein	-7.41	3.71	Asp151, Glu45, dan Ser80	Ala30, Ala150, Val19, Leu140, Leu60, Ile11, dan Lys32
5	Chrysin	-7.67	2.40	Asp151, Glu45, Ser80, Ala30, dan Tyr49	Ala150, Lys32, Leu140, dan Leu60

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidorgen	Ikatan Lainnya
6	Luteolin	-7.37	3.95	Asp151, Tyr49, Glu45, Ser80, Lys137, Ala30, dan Ser87	Ala150, Lys32, Leu140, Val19 dan Leu60
7	Scutelarein	-7.23	4.99	Asp51, Tyr49, Glu45, Ser80, Lys137, dan Ala30	Ala150, Val19, Leu60, Leu140, dan Lys32
8	Hispidulin	-7.09	6.31	Asp151, Glu45, Tyr49, Lys137, Ser80, dan Ala30	Ala150, Leu60, Val19, dan Lys32
9	Chryseriol	-5.67	69.49	Lys137 dan Glu45	Lys32, Val19, Leu60, dan Leu140
10	Tricetin	-7.30	4.45	Asp151, Lys137, Tyr49, Glu45, dan Ala30	Lys32, Leu60, dan Ser80
11	Tangeretin	-2.64	11.62	-	Lys32, Val19, Ala150, Leu60, Leu140, dan Lys137
12	Wogonin	-7.21	5.15	Asp151, Glu45, Tyr49, dan Ala30	Ala150, Val19, Leu60, Leu140, Lys32, dan Ser80

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidorgen	Ikatan Lainnya
13	Rhoifolin	+202.80	-	Gly86 dan Tyr49	Ala30, Ala150, Glu45, Gly14, Val79, Ser80, Lys13, Leu60, dan Leu140
14	Diosmetin	-7.78	2.00	Asp151, Glu45, Tyr49, dan His83	Ala30, Ala150, Val19, Leu60, Leu140, dan Lys32
15	Acacetin	-6.99	7.55	Asp151, Tyr49, Glu45, Ser80, dan Ala30	Ala150, Val19, Leu60, dan Lys32
16	Tricin	-6.73	11.60	Asp151, Tyr49, Glu45, Ser80, Lys137, Ala30, dan Asn138	Ala150, Lys32, Val19, dan Leu140
17	Galangin	-7.13	5.91	Lys32, Ser80, dan His83	Ala30, Val19, Leu78, Leu 60, dan Leu140
18	Fisetin	-7.94	1.51	Asp151, Glu45, dan His83	Ala30 Ala150, Leu60, Leu140, Val19, Ile11, dan Lys32
19	Kaemferol	-6.25	26.40	Asp151, Tyr49, Glu45, Ser80, Lys137, dan Ala30	Ala150, Val19, Leu140, Leu60, dan Lys32

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidorgen	Ikatan Lainnya
20	Kaemferide	-6.01	39.34	Lys32, Lys137, dan Gly86	Ala150, Val19, Leu60, dan Leu140
21	Robinetin	-7.67	2.38	Asp151, Glu45, dan His83	Ala30, Ala150, Ile11, Leu60, Leu140, Lys32, dan Val19
22	Herbasetin	-6.19	28.92	Glu45, Lys32, dan Lys137	Ala30, Ala150, Ser80, Val19, dan Leu60
23	Quercetin	-6.35	22.09	His83 dan Ala30	Lys32, Leu60, Leu140, Val19, dan Ser80
24	Ramnetin	-6.43	19.49	Ala30, Lys32, His83, dan Gly86	Leu60, Leu140, Val19, dan Ser80
25	Isoramnetin	-6.23	26.96	Glu45, Ser80, Lys32, dan Lys137	Ala30, Ala150, Val19, Leu60
26	Myricetin	-6.08	35.06	Glu45, Ser80, Lys32, dan Ala30	Ala150, Val19, Leu60, dan Leu140
27	Quercetagenin	-6.56	15.63	Asp151, Tyr49, Glu45, Ser80, Lys137, dan Ala30	Ala150, Val19, Leu140, Leu60, dan Lys32

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidorgen	Ikatan Lainnya
28	Gossypetin	-6.30	24.26	Glu45, Ser80, Lys137, Ala30, dan Ser87	Ala150, Lys32, Val19, Leu60, dan Leu140
29	Isoquercetin	+5.88	-	Tyr49, Ser80, Lys32, dan Ala30	Ala150, Val19, Leu140, Leu60, Lys13, dan His83
30	Rhamnazin	-6.46	18.33	Lys32, Lys137, His83, dan Ser80	Ala150, Val19, Leu60, dan Leu140
31	Rutin	+29.17	-	Ser80, Lys13, dan Lys137	Leu60, Leu140, Ala150, Lys32, Ala30, Asn138, dan Val19
32	Morin	-6.23	27.09	Asp151, Tyr49, Glu45, Ser80, Lys137 dan Ala30	Ala150, Val19, Leu140, Leu60, dan Lys32
33	Pachypodol	-6.83	9.82	Glu45, His83, Ala30, Ser80, dan Leu78	Leu140, Leu60, Val19, dan Ala150
34	Daidzein	-7.20	5.28	Asp151, Tyr49, Val79, Lys137, Ser80,	Lys32, Ala150, Leu78, Leu60

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
35	Formononetin	-6.92	8.42	Asp151, Tyr49, Val79, dan Ser80	Ala150, Val19, Lys32, Leu78, dan Leu60
36	Genistein	-7.11	6.17	Asp151, Tyr49, Glu45, dan Lys137	Val19, Leu78, Leu60, dan Lys32
37	Biokanin A	-6.86	9.83	Asp151, Tyr49, Glu45, Lys32, Lys13, dan Ser80	Ala30, Ala150, Val19, Leu78, dan Leu60
38	Orobol	-7.41	3.68	Asp151, Tyr49, Glu45, Lys137, dan Ser80	Val19, Ala150, Leu78, Leu140, Leu60, dan Lys32
39	Tectorigenin	-6.76	11.11	Ala30, Glu45, Lys32, dan Lys137	Val19, Leu60, dan Ser80
40	Baptigenin	-7.06	6.71	Glu45, Lys32, Lys137, dan Ala30	Ala150, Val19, Leu60, dan Ser80
41	Pinocembrin	-7.31	4.41	Asp151, Tyr49, Glu45, Ser80, dan Ala30	Ala150, Lys32, Val19, Leu60, dan Leu140

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
42	Liquiritigenin	-7.32	4.28	Asp151, Tyr49, Ser80, Lys137, dan Ala30	Ala150, Lys32, Val19, Leu140, dan Leu60
43	Naringenin	-7.42	3.67	Asp151, Tyr49, Glu45, Ser80, Ser87, Lys137, dan Ala30	Ala150, Val19, Lys32, Leu140, dan Leu60
44	Sakuranetin	-7.38	3.90	Asp151, Glu45, Tyr49, Ser80, His83, dan Lys32	Leu60, Leu140, Val19, Ala150, dan Ala30
45	Eriodictyol	-7.29	3.24	Asp151, Tyr49, Glu45, Ser80, Ala30, dan Lys137	Lys32, Val19, dan Leu60
46	Hesperetin	-6.09	34.57	Glu45, Lys13, Lys32, Ser80, dan Gly14	Ala30, Ala150, Leu60, Leu78, dan Val19
47	Homoeriodictyol	-7.32	4.29	Asp151, Tyr49, Glu45, Lys137, Ser80, Ser87, dan Ala30	Ala150, Lys32, Val19, Leu140, dan Leu60

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Higrogen	Ikatan Lainnya
48	Parietin	-7.48	3.30	Asp151, Glu45, dan Ser80	Ala30, Ala150, Val19, Leu140, Leu60, dan Lys32
49	Epigallocatechin	-6.30	24.12	Ser87, Glu45, Lys137, dan Ala30	Ala150, Val19, Lys32, Leu78, Leu60, Leu140, dan Ser80
50	Catechin	-6.69	12.46	Glu45, Ser80, Ser87, Lys137, dan Ala30	Ala150, Val19, Lys32, Leu78, Leu60, dan Leu140
51	Naringin	+144.91	-	Tyr49, Tyr82, Lys32, His83, dan Gly86	Leu140, Val19, Lys13, Gly14, Asp151, Glu45, Leu60, Ser80, dan Ala30
52	Pinobanskin	7.15	5.72	Asp151, Tyr49, Glu45, Ala30,	Lys32, Val19, Leu60, Ser80
53	Aromadendrin	-7.22	5.06	Asp151, Tyr49, Glu45, Ser80, Lys137, dan Ala30	Ala150, Lys32, Val19, Leu10, dan Leu60

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
54	Fustin	-7.23	5.02	Ala30, Ser80, Asp151, Tyr49, dan Lys137	Lys32, Val19, dan Leu60
55	Taxifolin	-7.38	3.92	Asp151, Tyr49, Glu45, Ser80, Lys137, dan Ala30	Ala150, Val19, Lys32, Leu140, dan Leu60
56	Agathisflavone	+3.53	-	His83 dan Tyr49	Ala150, Leu60, Asp151, Glu45, Ala30, Lys32, Lys137, Val79, dan Ser80
57	Cupresuflavone	+60.72	-	His83 dan Gly14	Leu140, Val19, Ala30, Ala150, Asp151, Lys32, Glu45, Leu60, dan Ile11
58	Ginkgetin	+4.88	-	-	Tyr49, Leu140, Asp151, Asn138, Trp20, Ala30, Ala150, Lys137, Val19, Val31, Val79, Leu60,

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
59	Siadopitisin	+6.74	-	Tyr49	Glu45, Leu60, Ile11, Asp151, Asn138, Trp20, Ala30, Ala150, Val19, Val31, Val79, Ser80, dan Lys137
60	Robustaflavone	+7.77	-	Glu45, dan Trp20	Ala150, Leu60, Val30, Val31, Val79, Asp151, Tyr49, Lys137, dan Ser80
61	Hinokiflavone	+8.98	-	Asp90, Lys32, dan Gly14	Leu60, Glu45, Ala30, Ala150, Asp151, Asn138, Lys137, Val79, Val91, Ser80
62	Ochnaflavone	+4.79	-	-	Lys32, Leu60, Leu78, Leu140, Ile11, Lys137, Glu45, Phe62, Ala30, Ser80, His83, dan Val79

**LAMPIRAN 9
(LANJUTAN)**

No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
63	Amentoflavone	+1.37	-	Trp20	Ile11, Asp151, Tyr49, Asn138, Ala30, Ala150, Leu60, Val19, Val31, Val79, Lys137, dan Ser80
64	Isoliquiritigenin	-7.11	6.10	Ser80, Asp151, Tyr49, Glu45, Lys137, dan Ala30	Ala150, Lys32, dan Leu60
65	Kalkonarigenin	-6.68	12.75	Asp151, Tyr49, Lys137, Glu45, dan Ala30	Ala150, Lys32, Leu60, dan Ser80
66	Butein	-	-	-	-
67	Okanin	-6.02	38.80	Gly14, Asp151, Tyr49, Lys13, Lys137, Ser80, dan Ala30	Ala150, Lys32, dan Leu60
68	Phloretin	-6.76	2.37	Asp151, Glu45, dan Lys32	His83, Ala30, Ala150, Leu60, Leu140, dan Val19
69	Phlorizin	-4.73	338.40	Asp151, Tyr49, Glu45, His 83, dan Ser80	Ala30, Ala150, Val19, Leu140, Lys32

**LAMPIRAN 9
(LANJUTAN)**

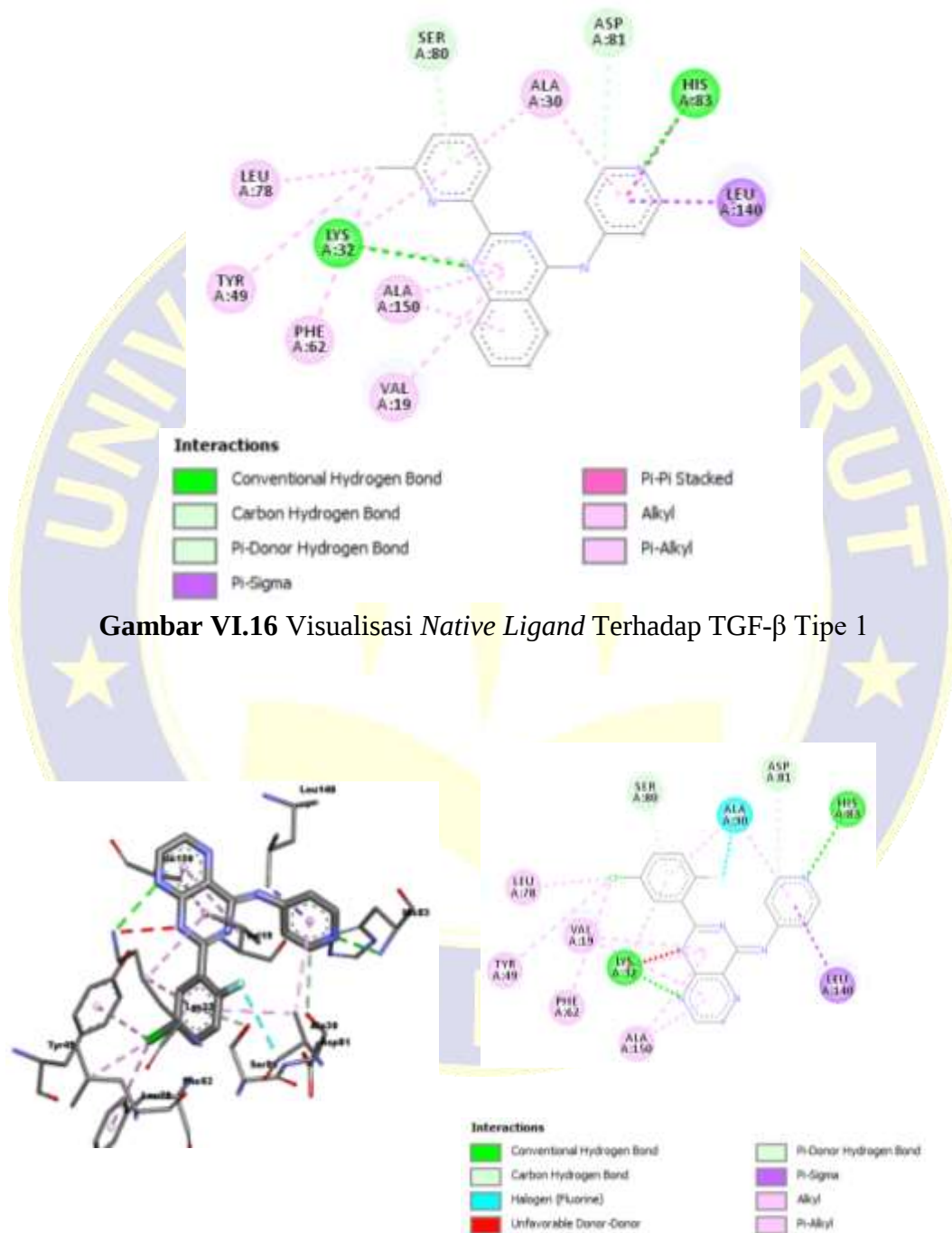
No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
70	Sulfuretin	-7.41	3.71	Asp151, Tyr49, Lys32, dan Ala30	Ala150, Leu140, Leu60, Ser80, dan Lys32
71	Aureusidin	-6.81	10.10	Asp151, Glu45, dan Lys137	Ala30, Ala150, Val19, Leu60, dan Lys32
72	Maritimetin	+6.61	-	Lys137, His83, dan Asn138	Leu60, Leu140, Ala30, Ala150, Tyr82, dan Lys32
73	Leptosidin	-7.16	5.66	Asn151, Lys137, dan Ser80	Ala150, Leu78, Val19, Leu60, dan Lys32
74	Apigenidin	-7.02	7.13	Glu45, Lys137, dan Ala30	Ala150, Lys32, Val19, Leu78, Leu60, Leu140, dan Ser80
75	Luteolinidin	-7.08	6.48	Glu45, Ser80, Lys137, Ala30	Ala150, Val19, Leu140, Leu60, Lys32
76	Pelargonidin	-6.90	8.73	Glu45, Lys137, dan Ala30	Ala150, Lys32, Val19, Leu60, Leu140, dan Ser80
77	Cyanidin	-6.66	13.05	Glu45, Ser80, Lys137, dan Ala30	Ala150, Lys32, Val19, Leu60, dan Leu140

**LAMPIRAN 9
(LANJUTAN)**

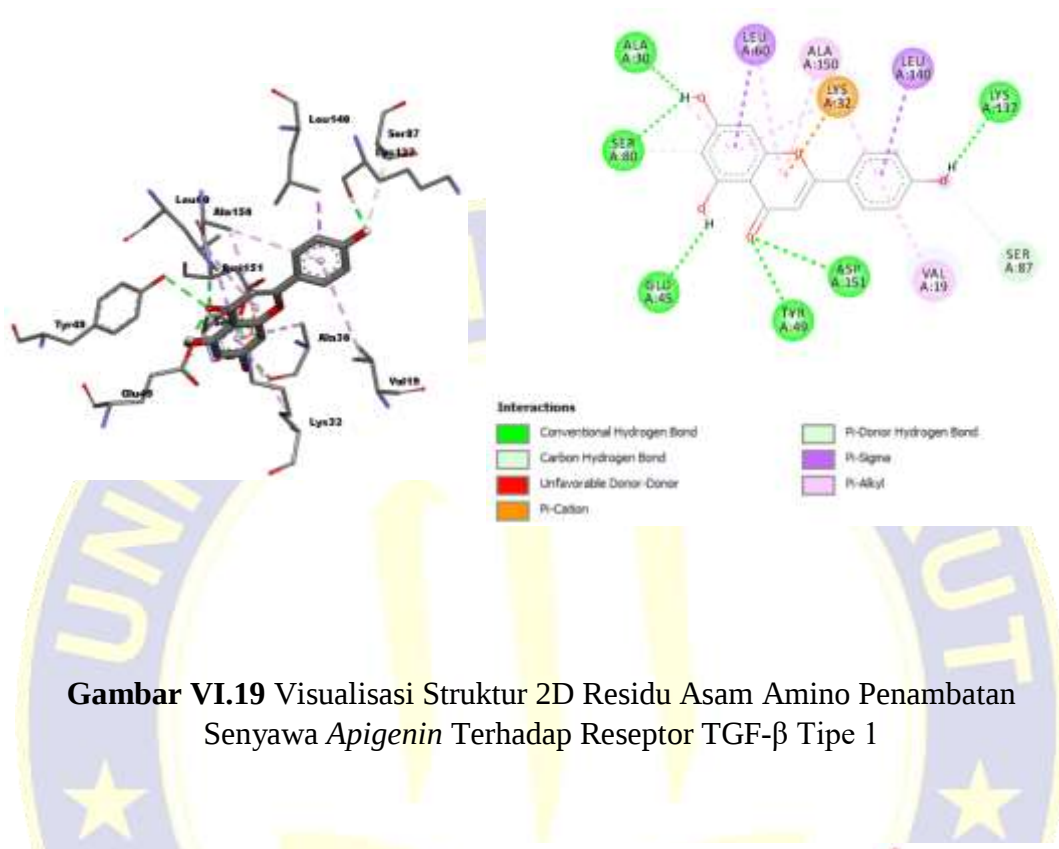
No	Ligan	ΔG (kkal/mol)	Ki (nM)	Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Lainnya
78	Peonidin	-6.25	26.37	Tyr49, Lys13, dan Ala30	Ala150, Val19, Leu60, Lys32, dan Ser80
79	Delpinidin	-	-	-	
80	Petunidin	-8.02	1.32	Asp151, Glu45, His83, Leu78, dan Ala30	Ala150, Val19, Leu60, Leu140, dan Lys32
81	Malvinidin	-	-	-	
82	Rosidinin	-6.41	20.16	Glu45, Lys137, dan Ser80	Val19, Leu78, Leu60, Ala150, dan Lys32

LAMPIRAN 10

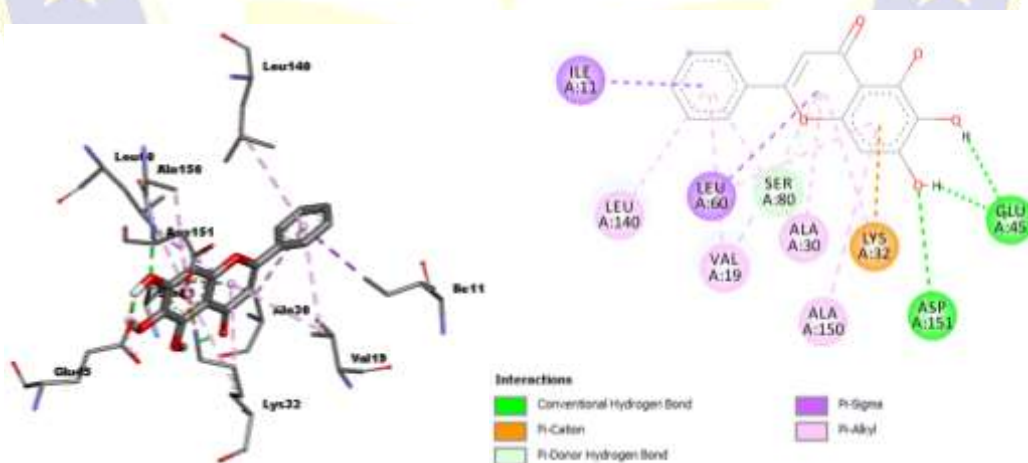
VISUALISASI HASIL PENAMBATAN MOLEKUL



LAMPIRAN 10 (LANJUTAN)

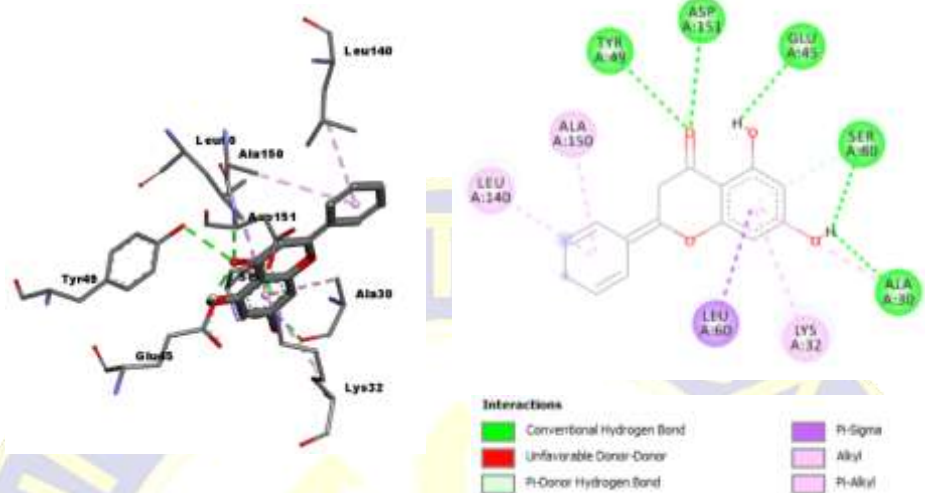


Gambar VI.19 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Apigenin* Terhadap Reseptor TGF- β Tipe 1

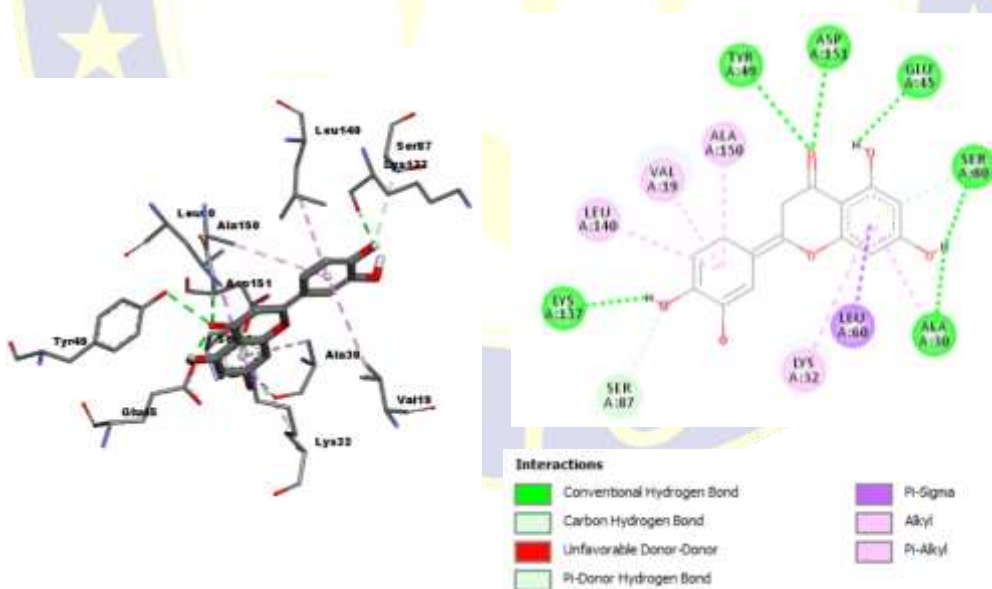


Gambar VI.20 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Baicalein* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

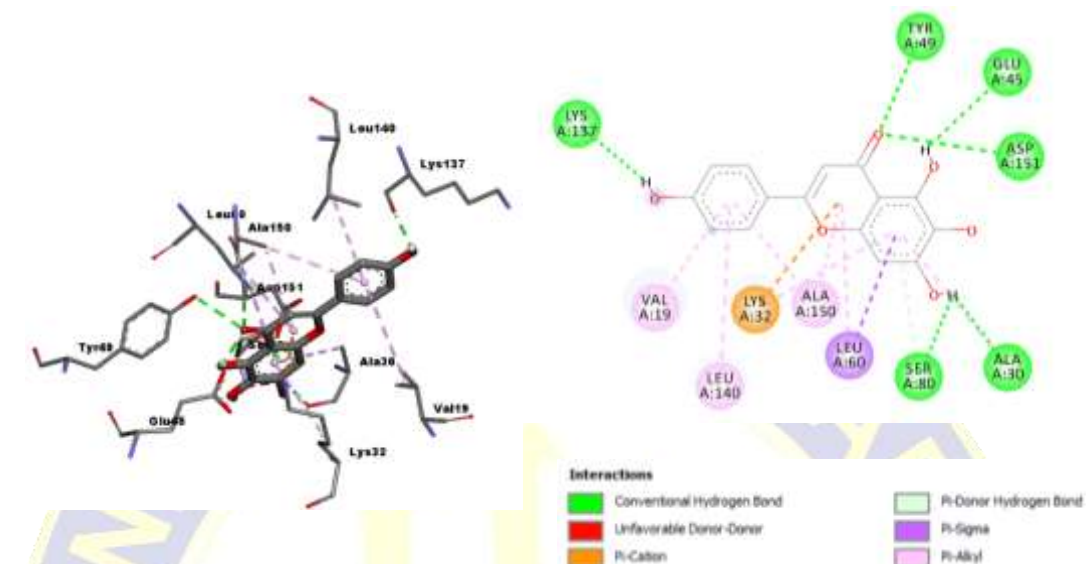


Gambar VI.21 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Chrysin* Terhadap Reseptor TGF- β Tipe 1

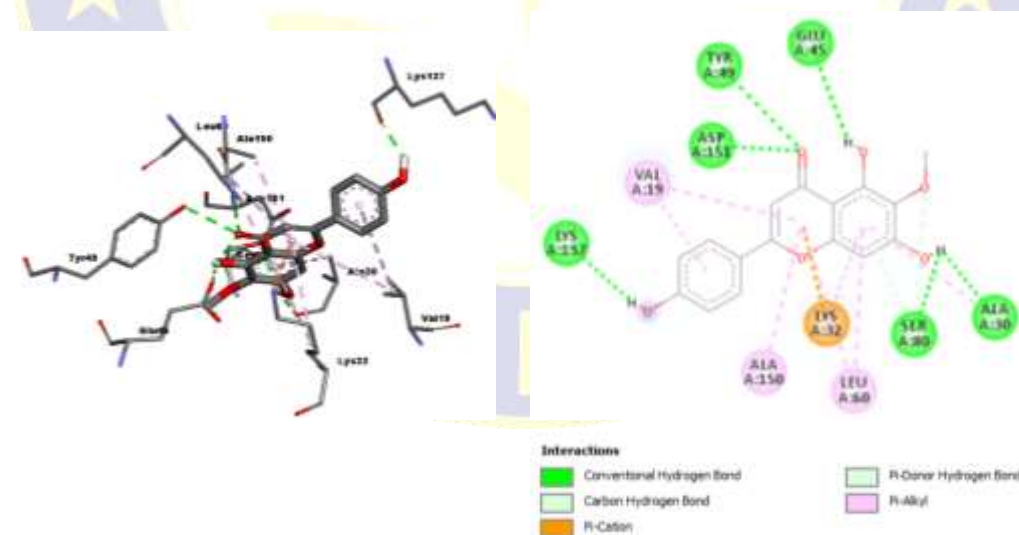


Gambar VI.22 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Luteolin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

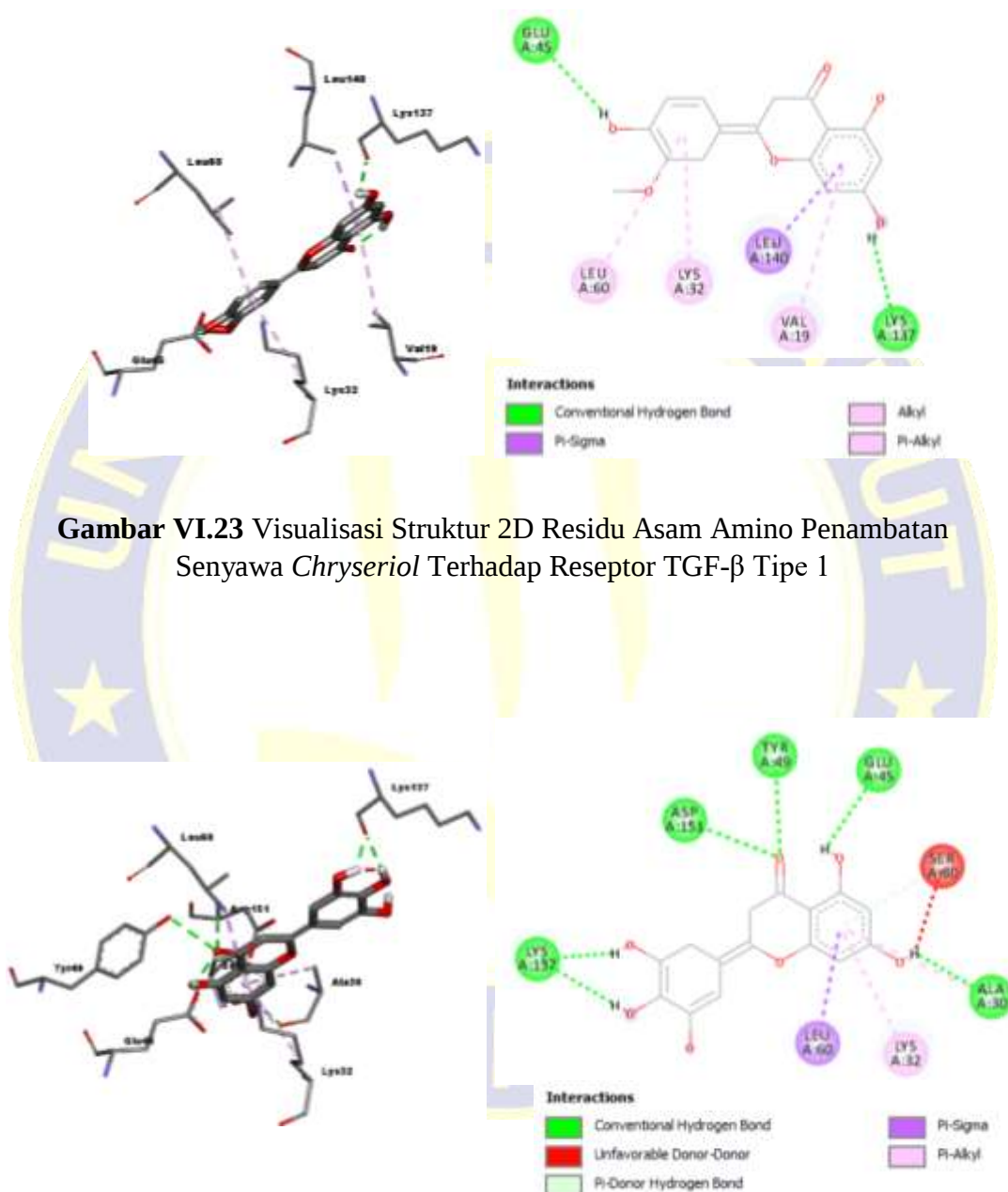


Gambar VI.21 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Scutellarein* Terhadap Reseptor TGF- β Tipe 1

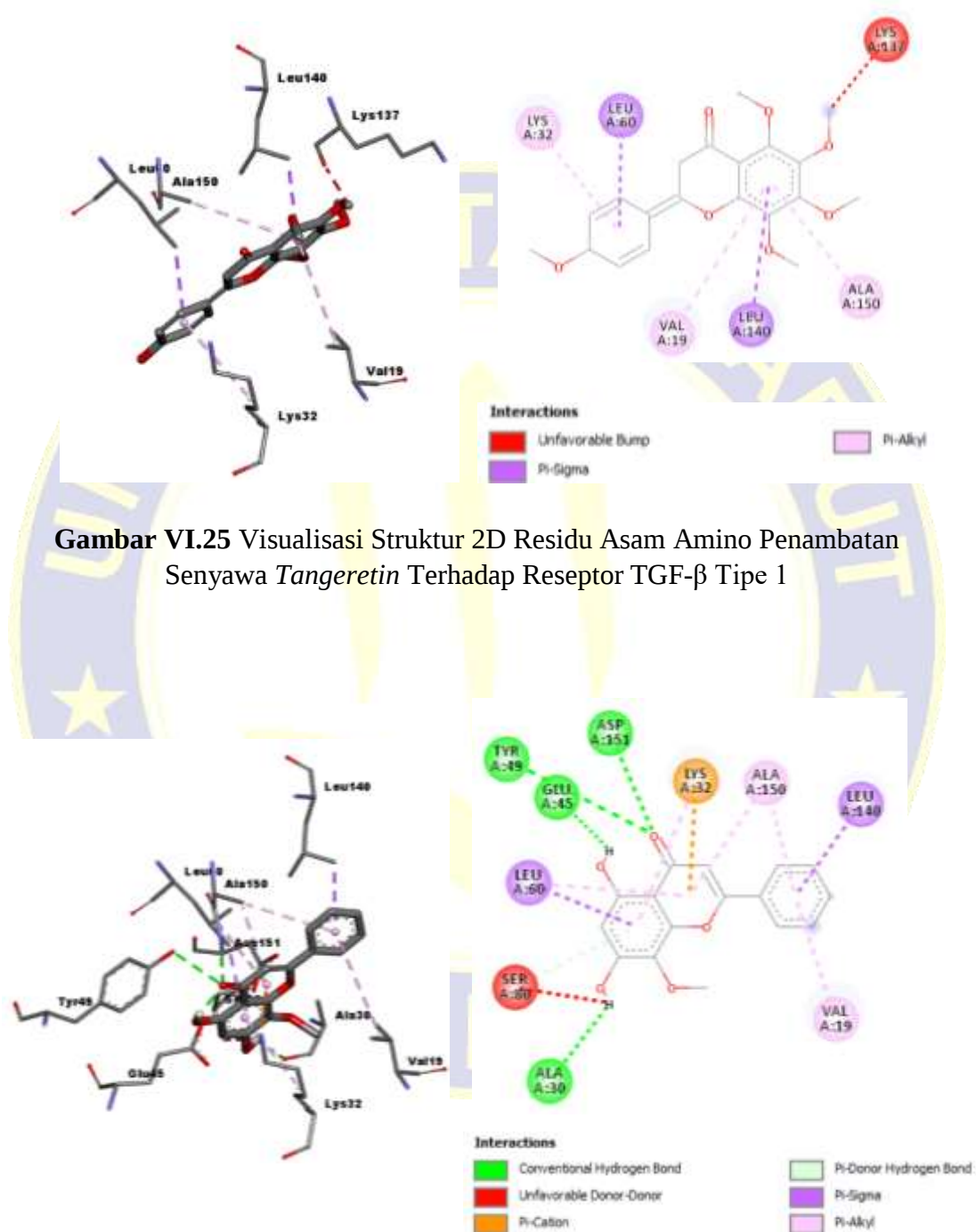


Gambar VI.22 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Hispidulin* Terhadap Reseptor TGF- β Tipe 1

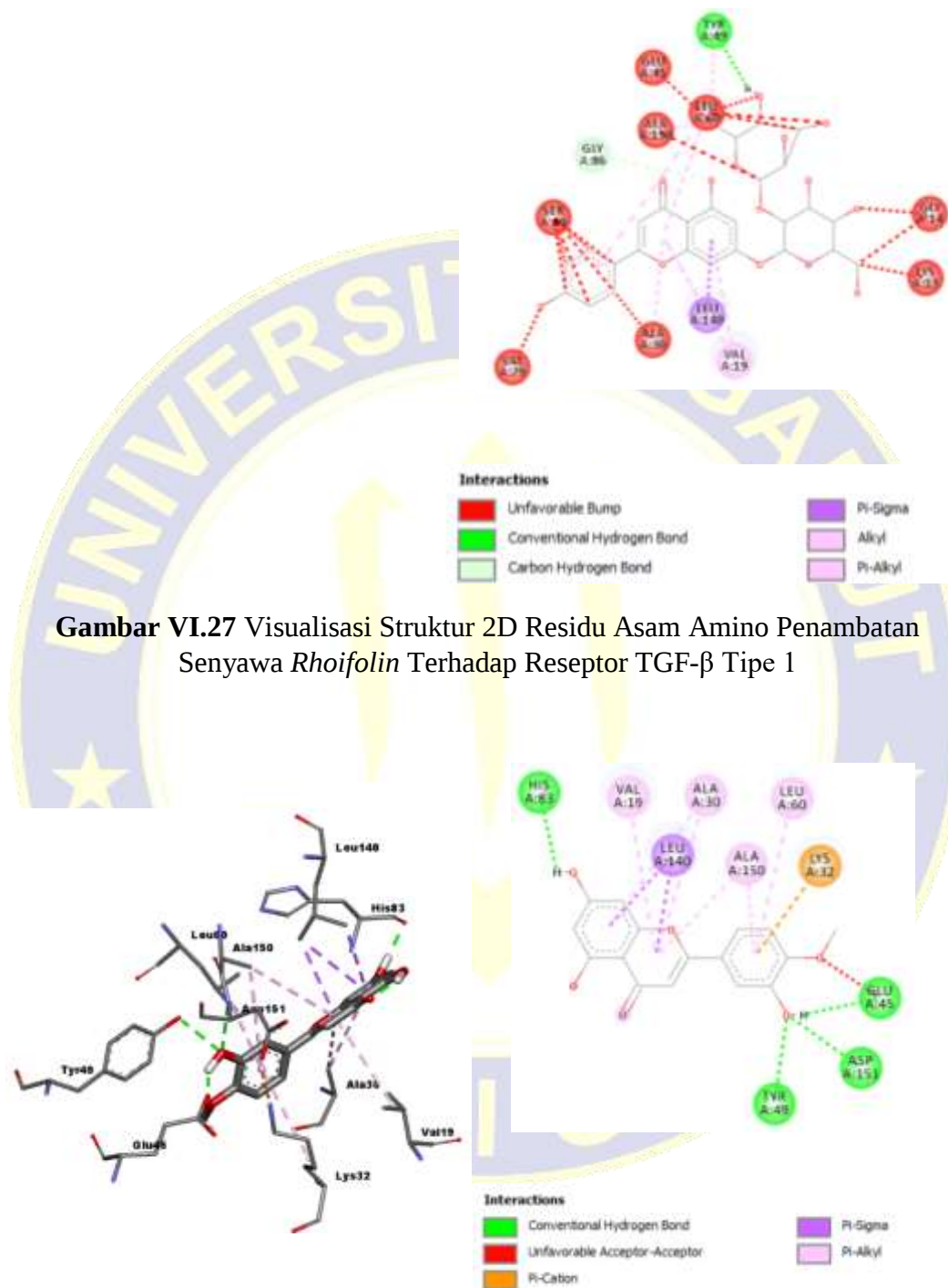
LAMPIRAN 10 (LANJUTAN)



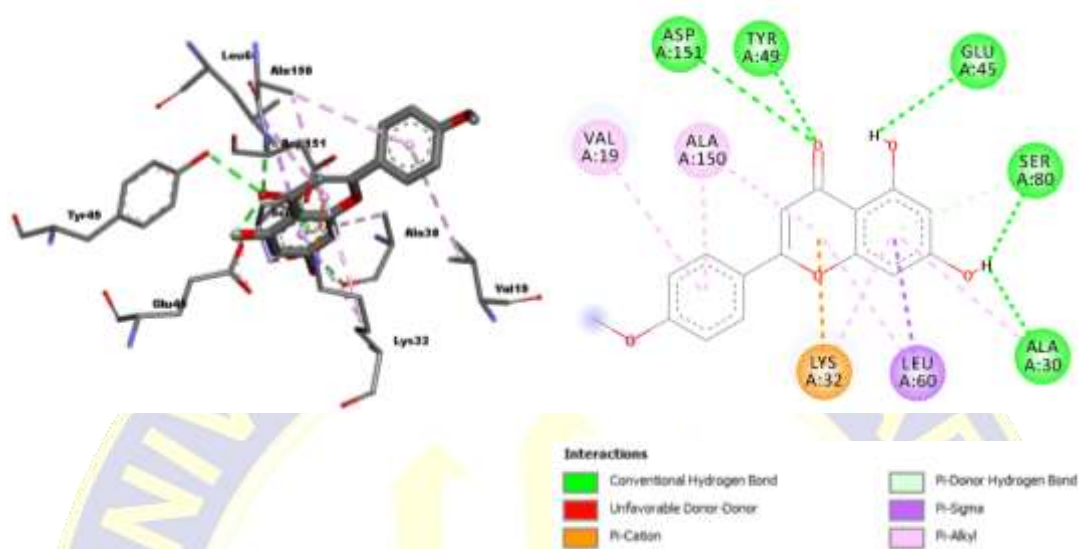
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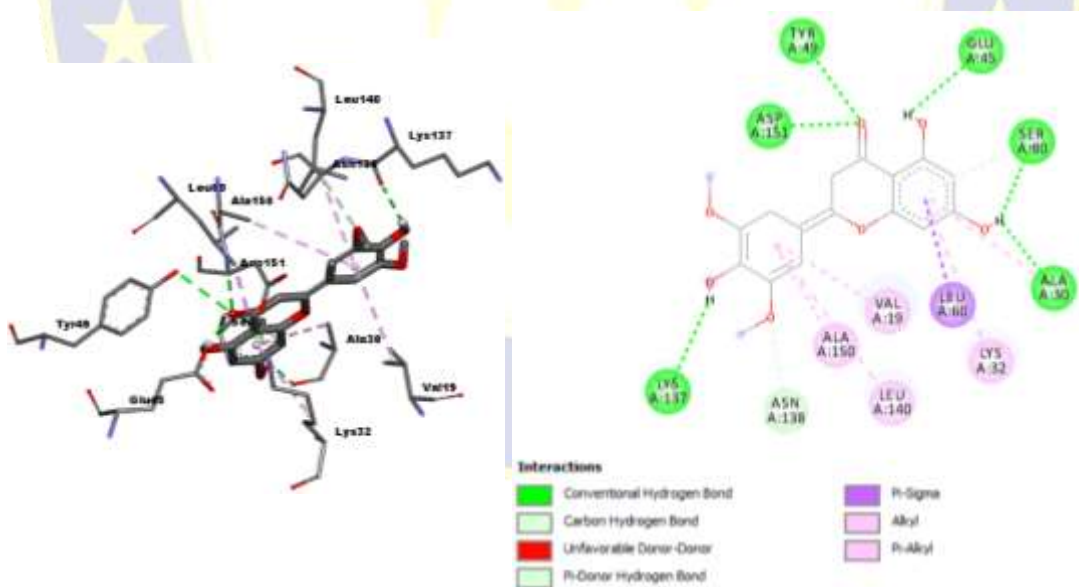
LAMPIRAN 10 (LANJUTAN)



LAMPIRAN 10 (LANJUTAN)

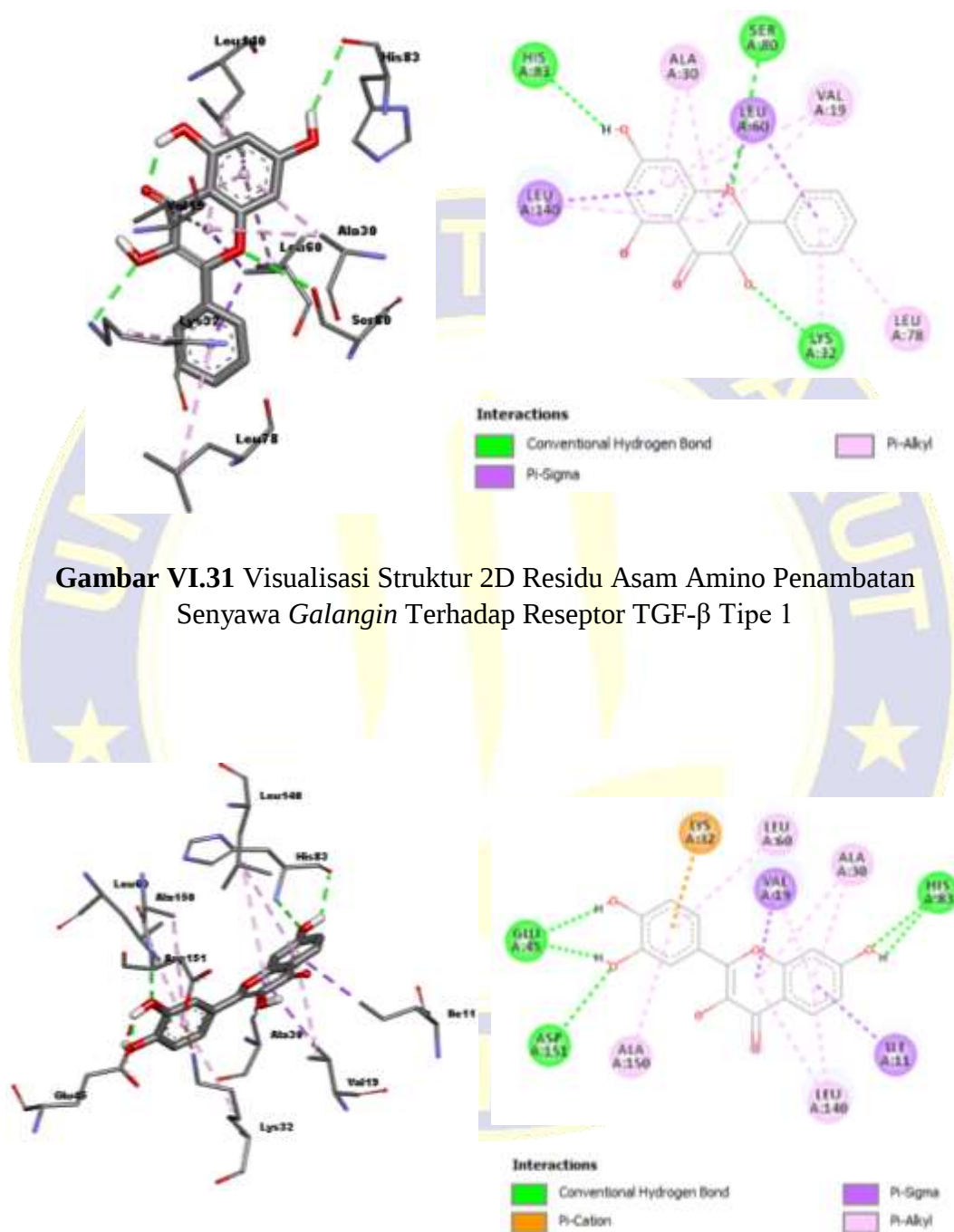


Gambar VI.29 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Acacetin* Terhadap Reseptor TGF- β Tipe 1

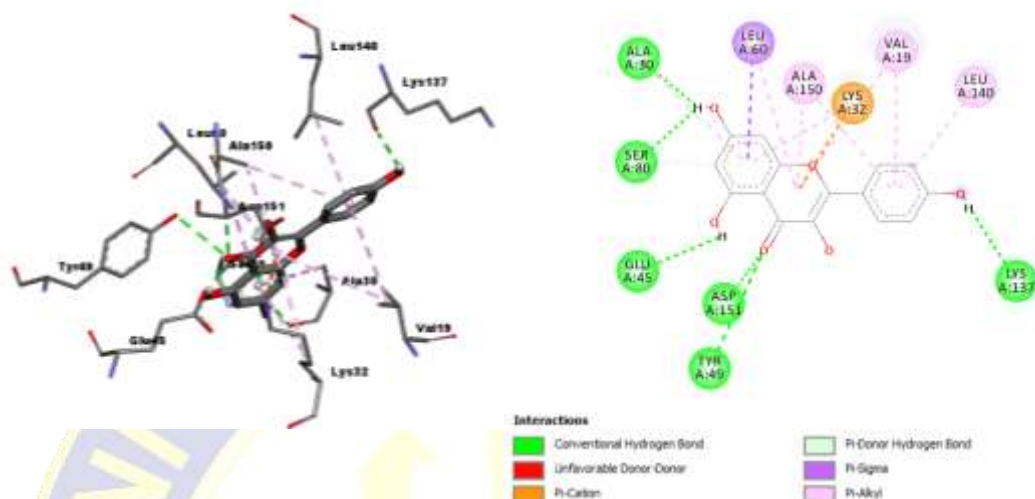


Gambar VI.30 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Tricin* Terhadap Reseptor TGF- β Tipe 1

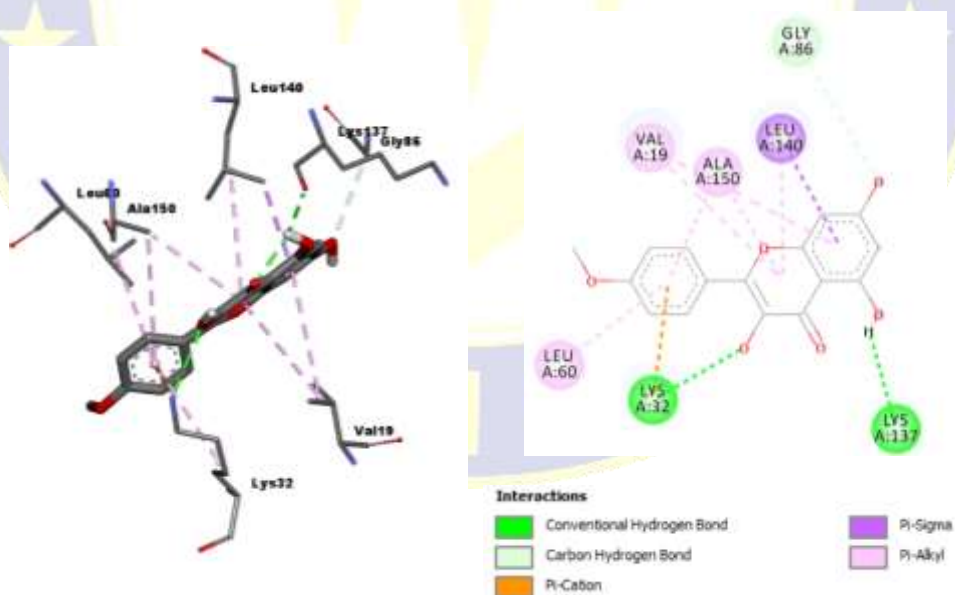
LAMPIRAN 10 (LANJUTAN)



LAMPIRAN 10 (LANJUTAN)

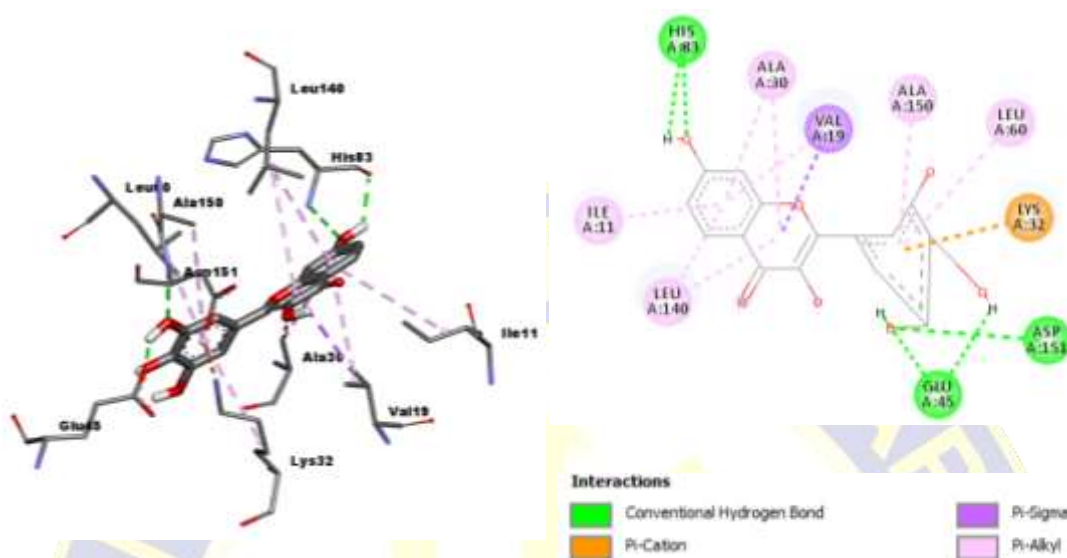


Gambar VI.33 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Kaempferol* Terhadap Reseptor TGF- β Tipe 1

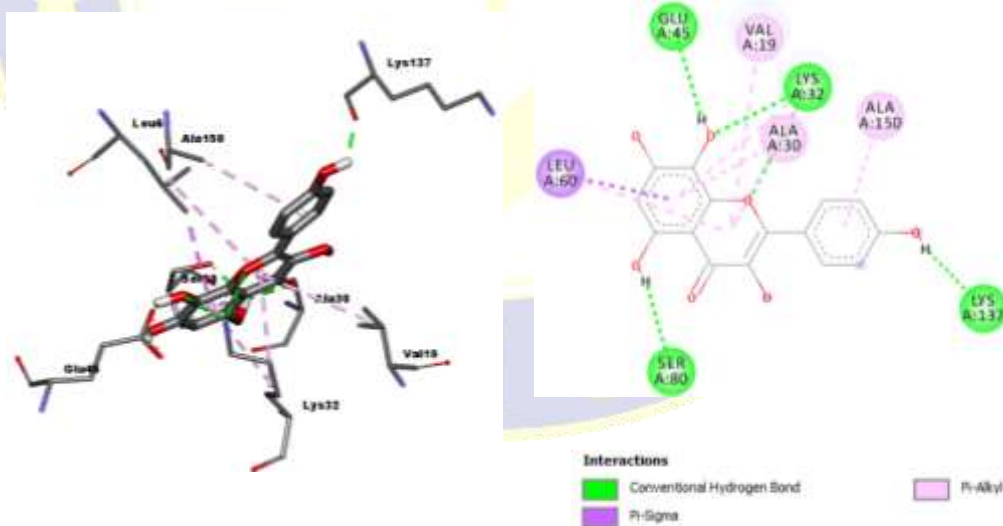


Gambar VI.34 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Kaempferide* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

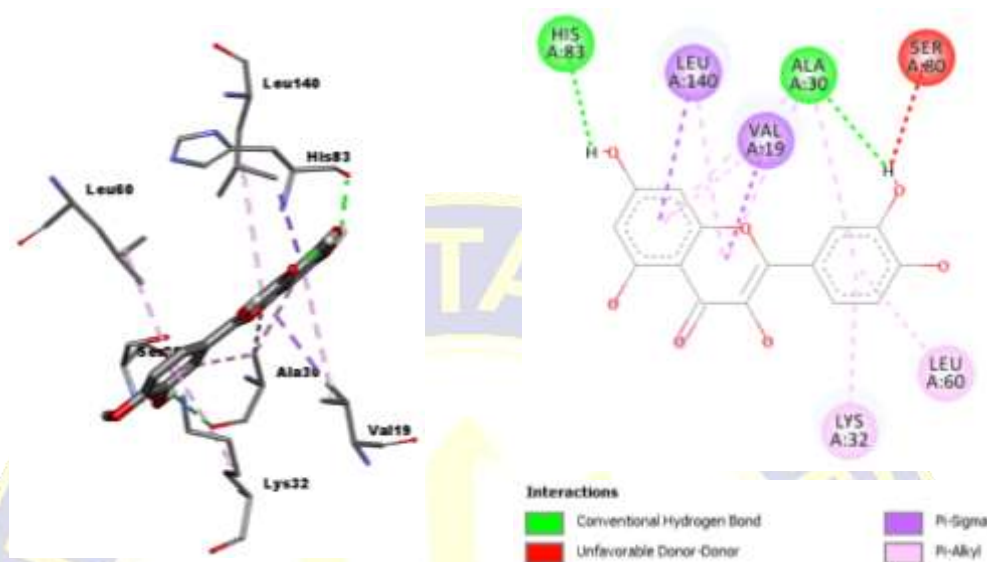


Gambar VI.35 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Robinetin* Terhadap Reseptor TGF- β Tipe 1

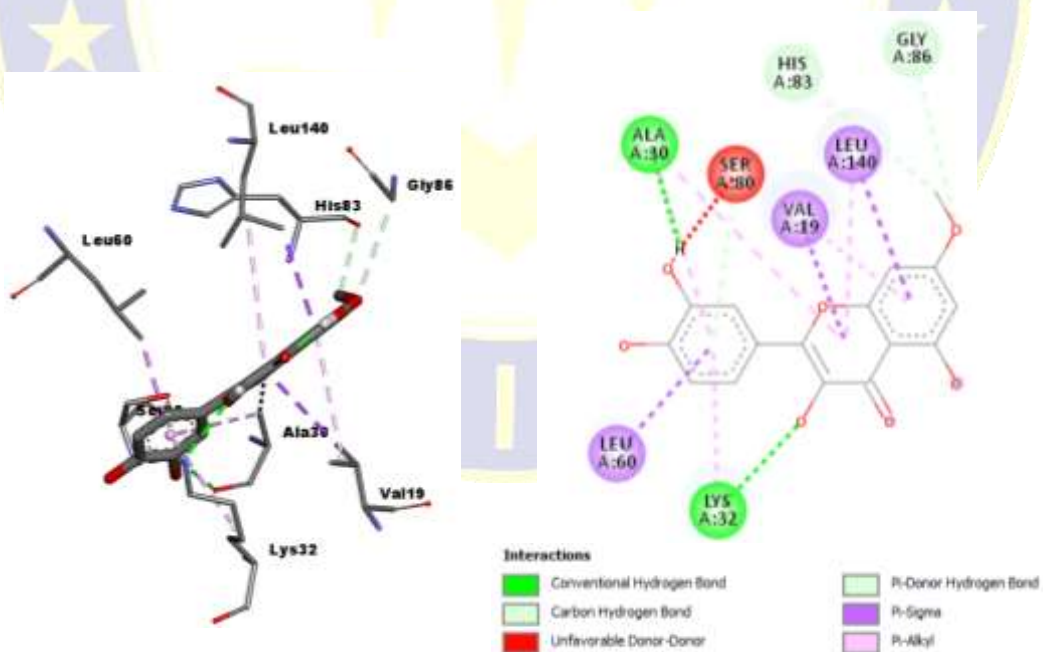


Gambar VI.36 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Herbacetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

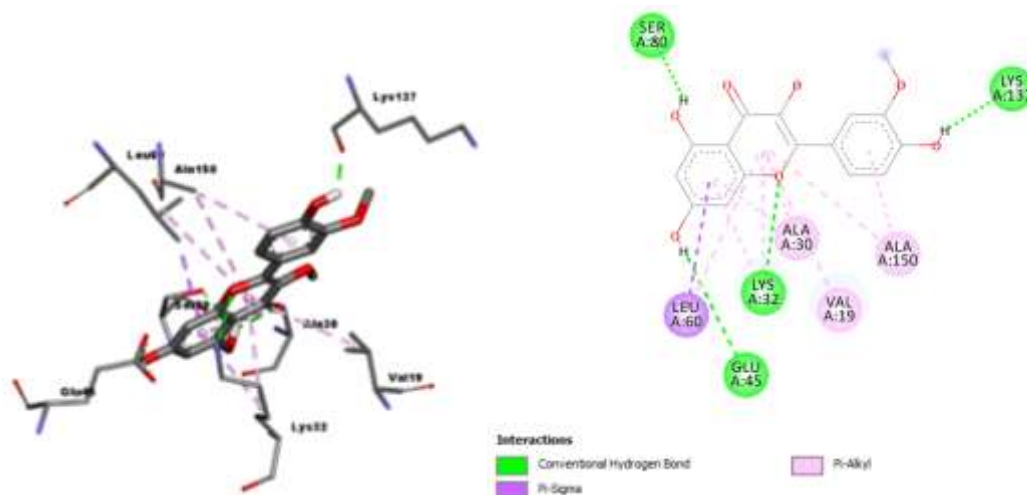


Gambar VI.37 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Quersetin* Terhadap Reseptor TGF- β Tipe 1

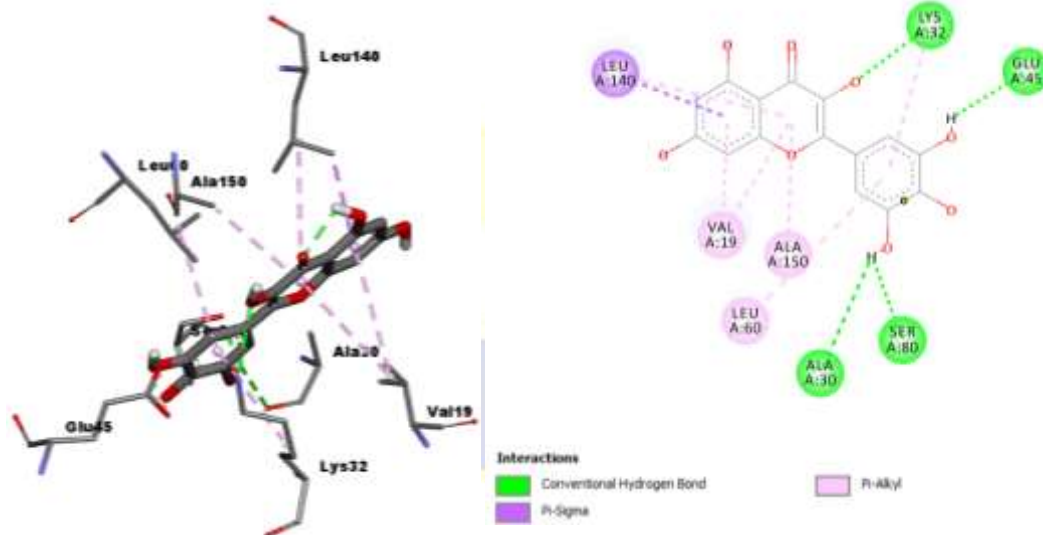


Gambar VI.38 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Rhamnetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

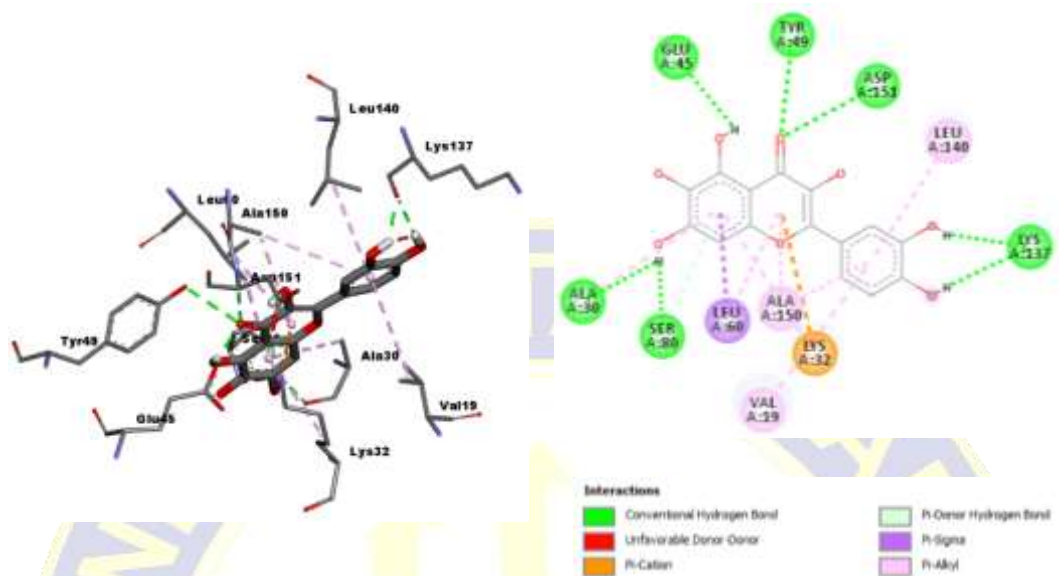


Gambar VI.39 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Isorhamnetin* Terhadap Reseptor TGF- β Tipe 1

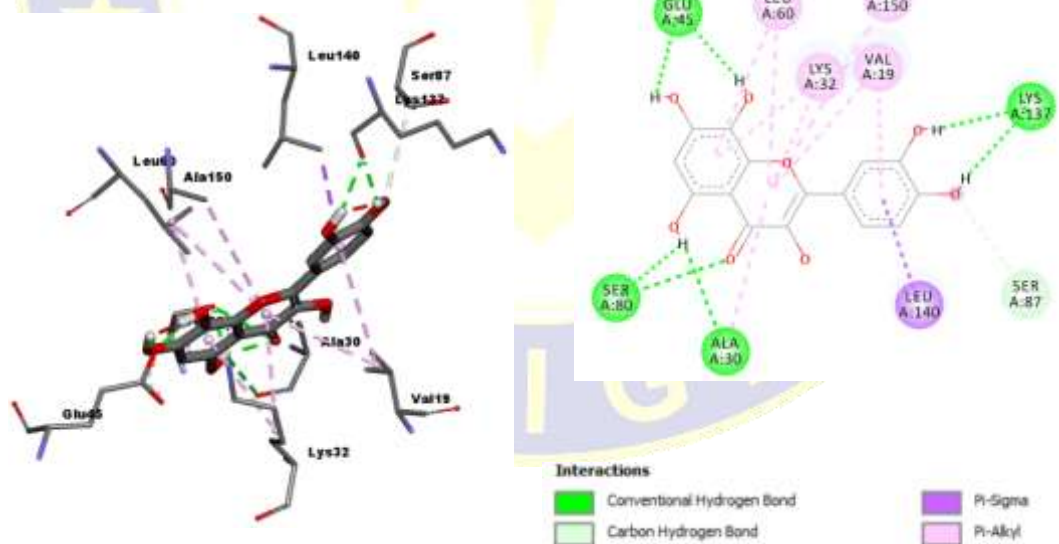


Gambar VI.40 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Myricetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

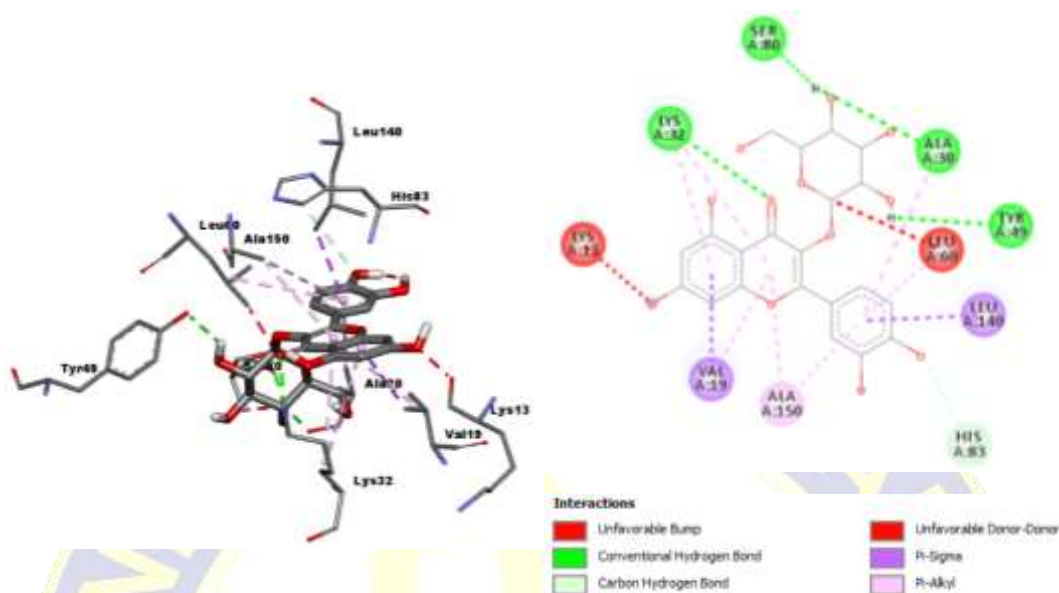


Gambar VI.41 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Quercetagenin* Terhadap Reseptor TGF- β Tipe 1

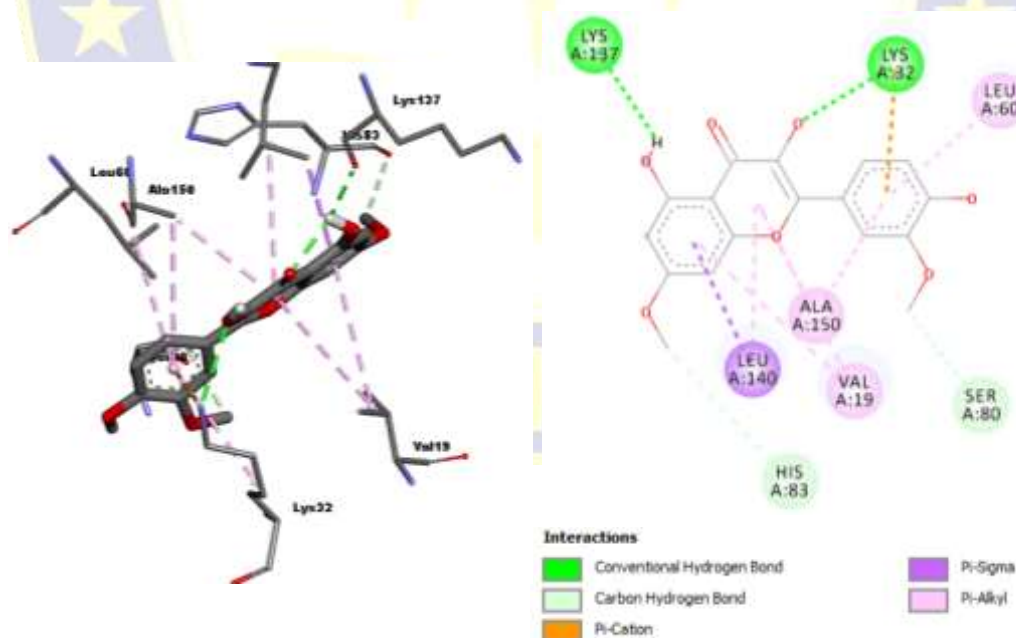


Gambar VI.42 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Gossypetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

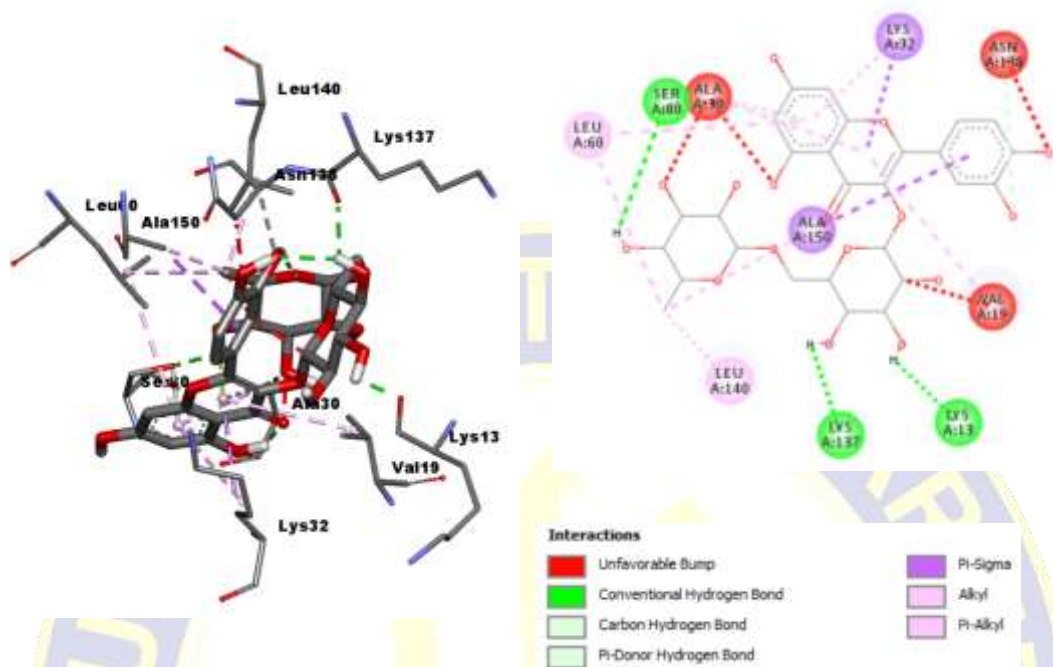


Gambar VI.43 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Isoquercetin* Terhadap Reseptor TGF- β Tipe 1

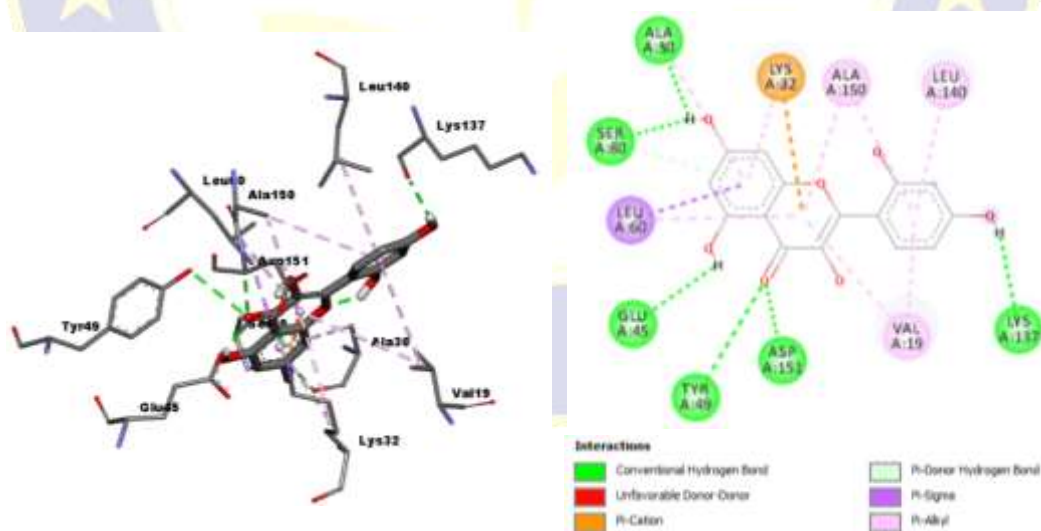


Gambar VI.44 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Rhamnazin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

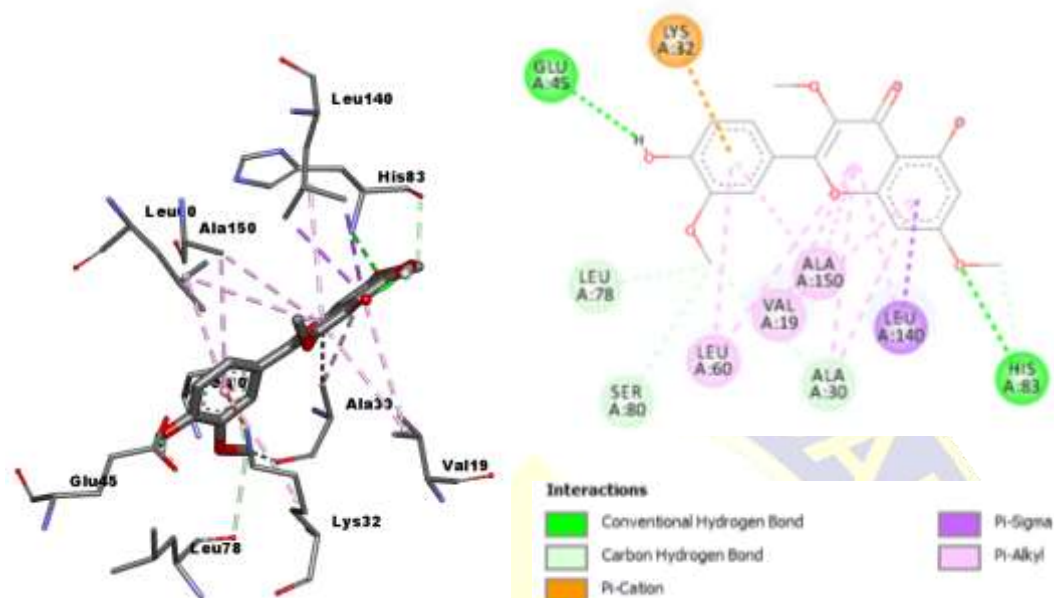


Gambar VI.45 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Rutin* Terhadap Reseptor TGF- β Tipe 1

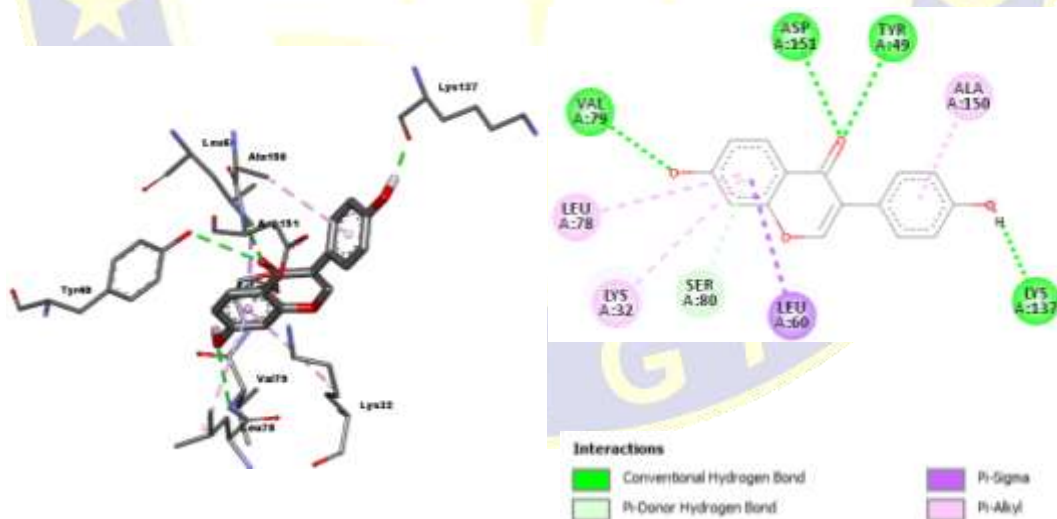


Gambar VI.46 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Morin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

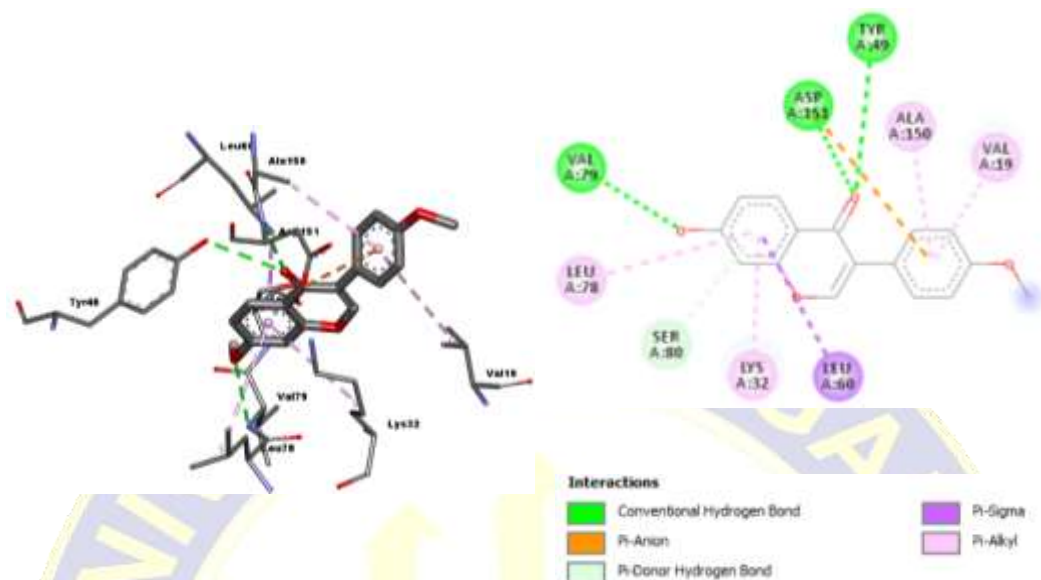


Gambar VI.47 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Pachypodol* Terhadap Reseptor TGF- β Tipe 1

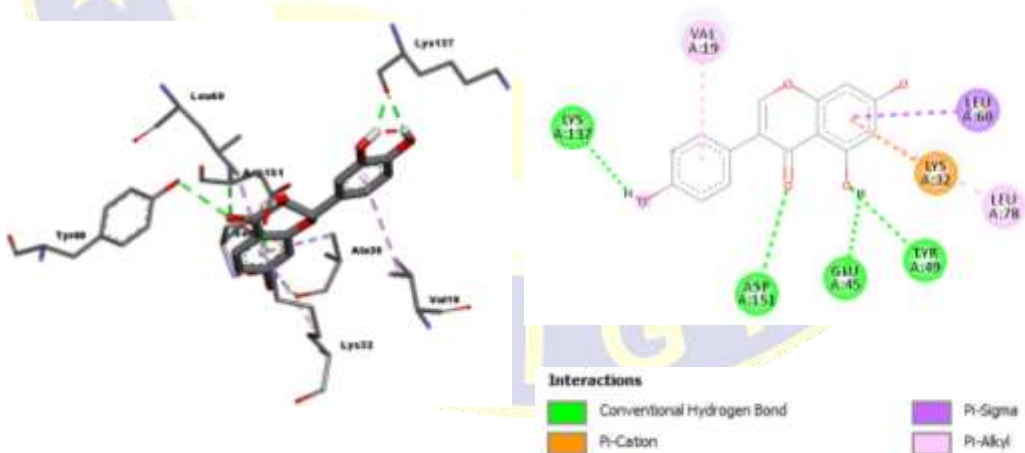


Gambar VI.48 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Daidzein* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)



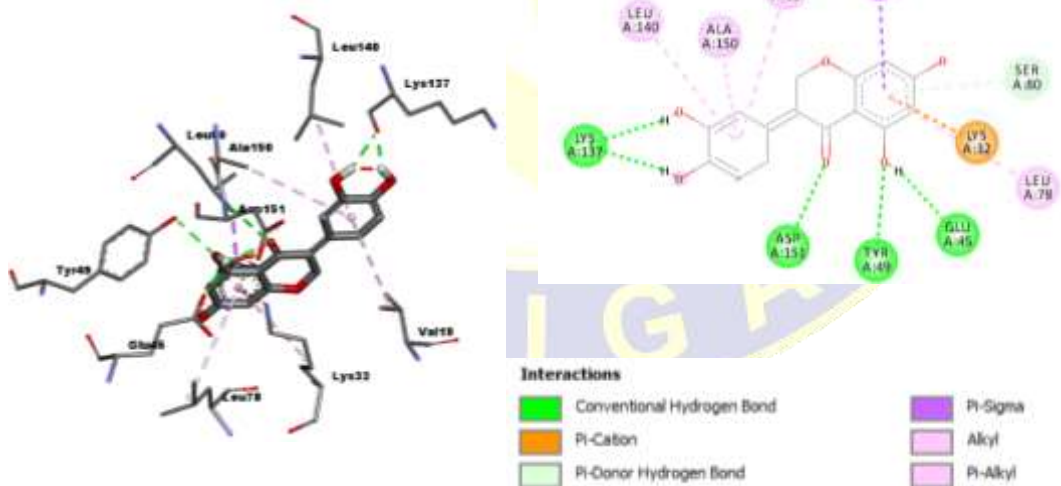
Gambar VI.49 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Formononetin* Terhadap Reseptor TGF- β Tipe 1



Gambar VI.50 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Genistein* Terhadap Reseptor TGF- β Tipe 1

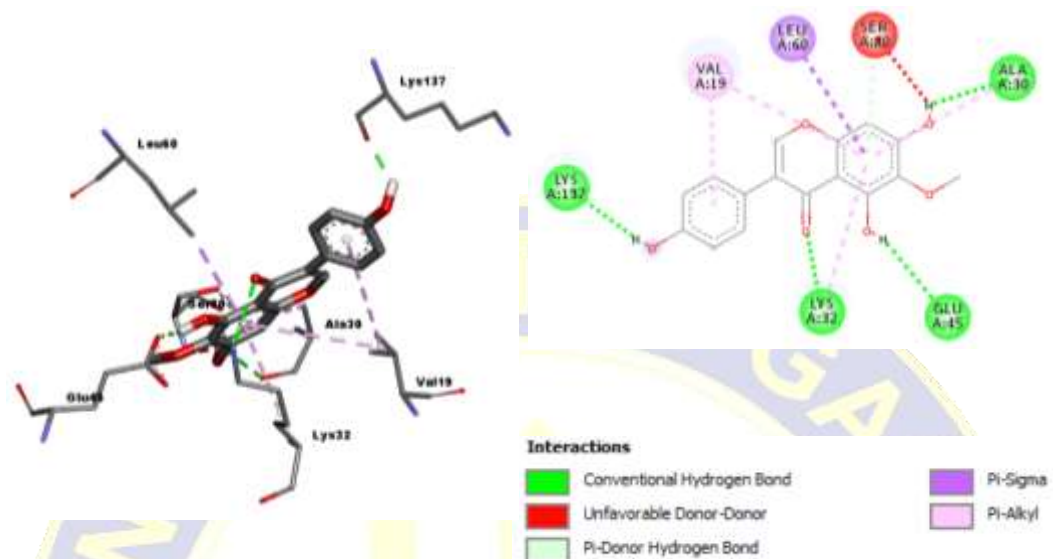
LAMPIRAN 10 (LANJUTAN)

Gambar VI.51 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Biochanin A* Terhadap Reseptor TGF- β Tipe 1

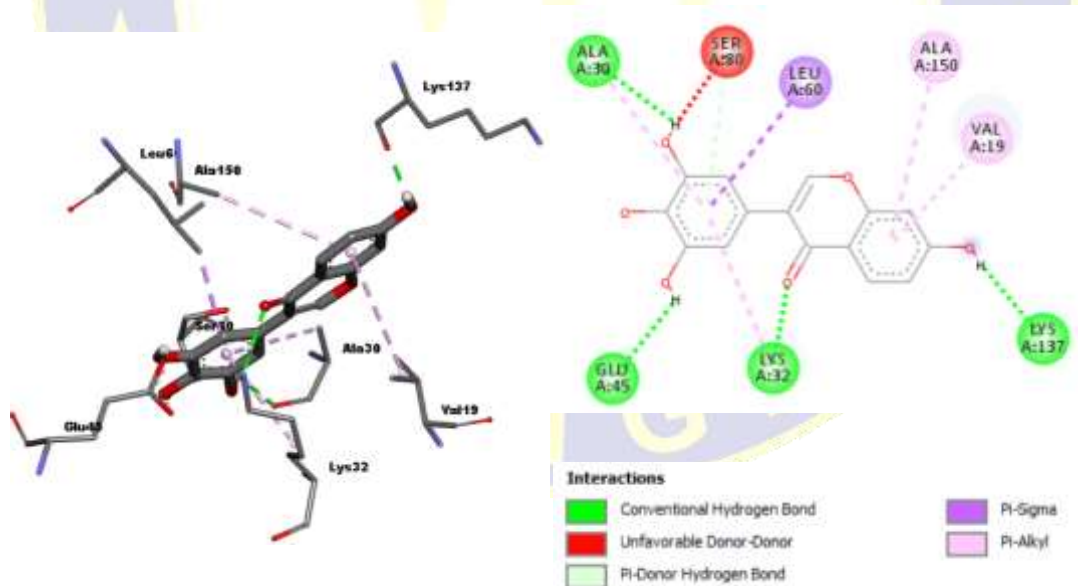


Gambar VI.52 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Orobol* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

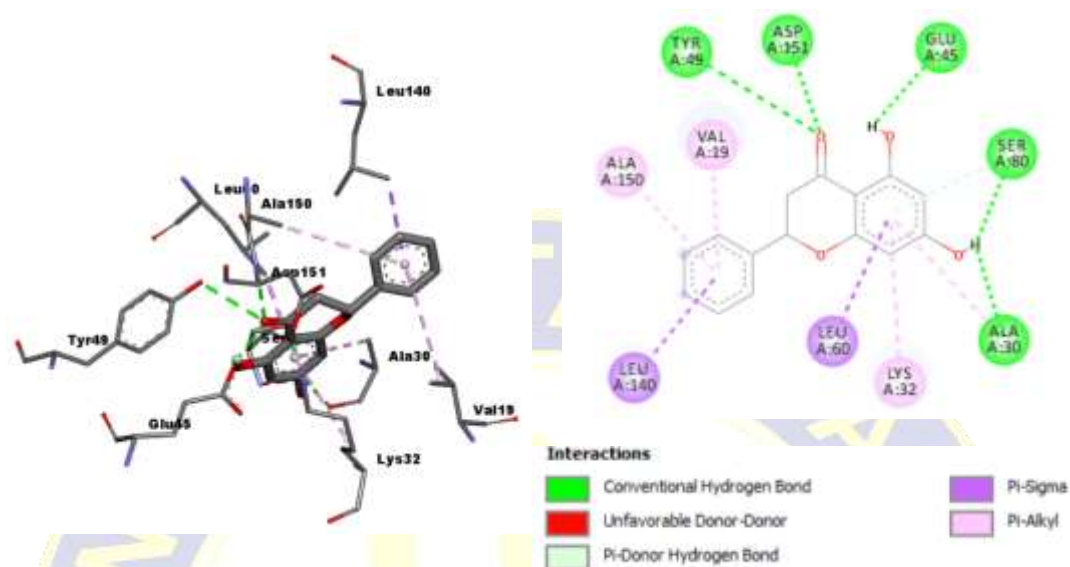


Gambar VI.53 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Tectorigenin* Terhadap Reseptor TGF- β Tipe 1

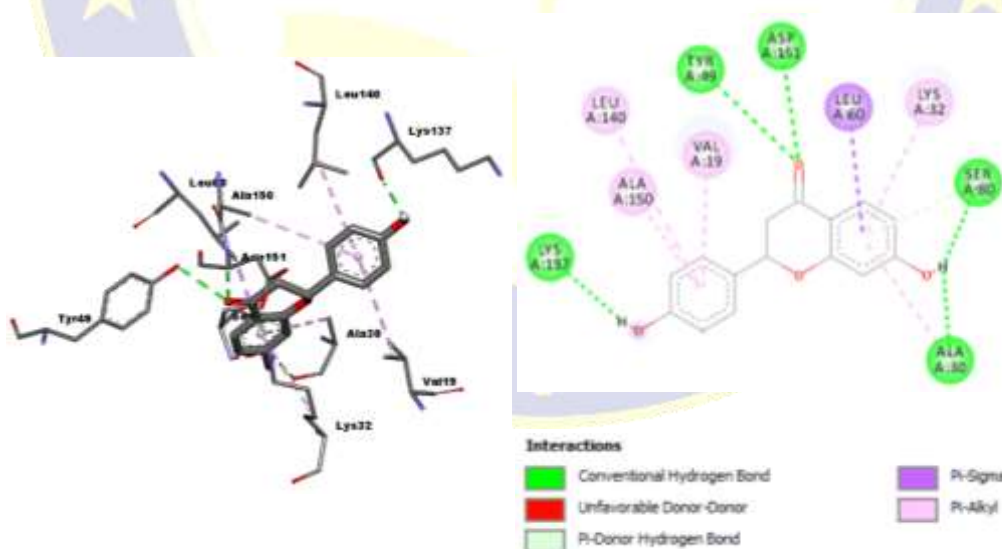


Gambar VI.54 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Baptigenin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

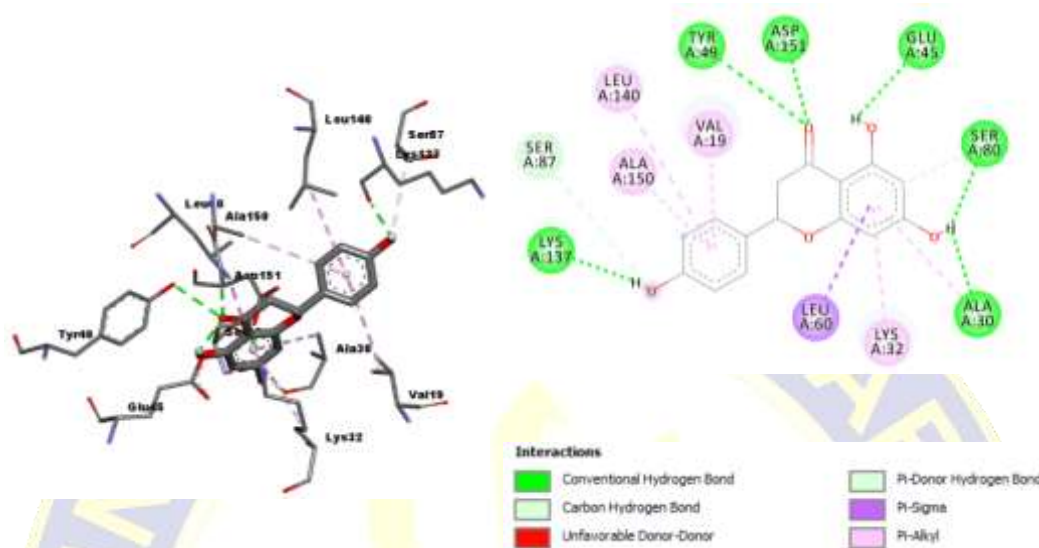


Gambar VI.55 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Pinocembrin* Terhadap Reseptor TGF- β Tipe 1

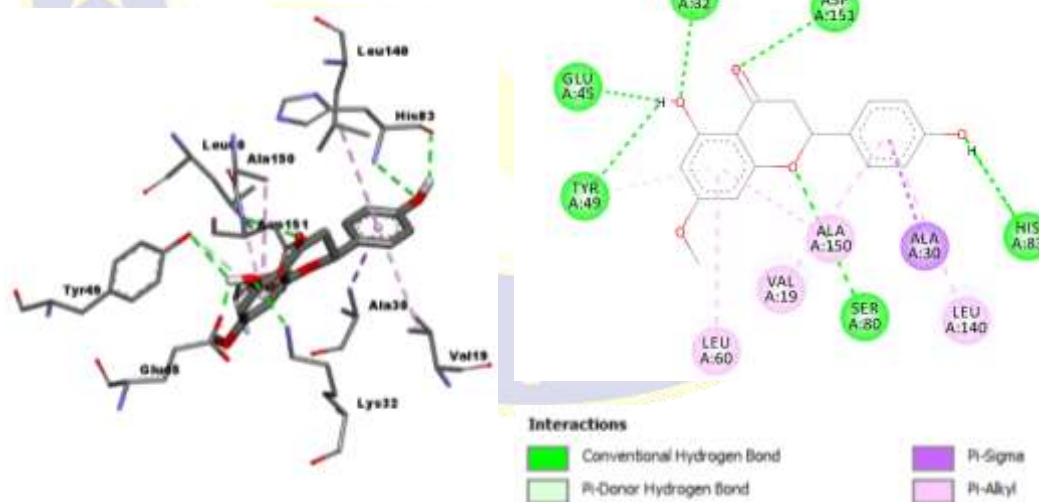


Gambar VI.56 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Liquiritigenin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

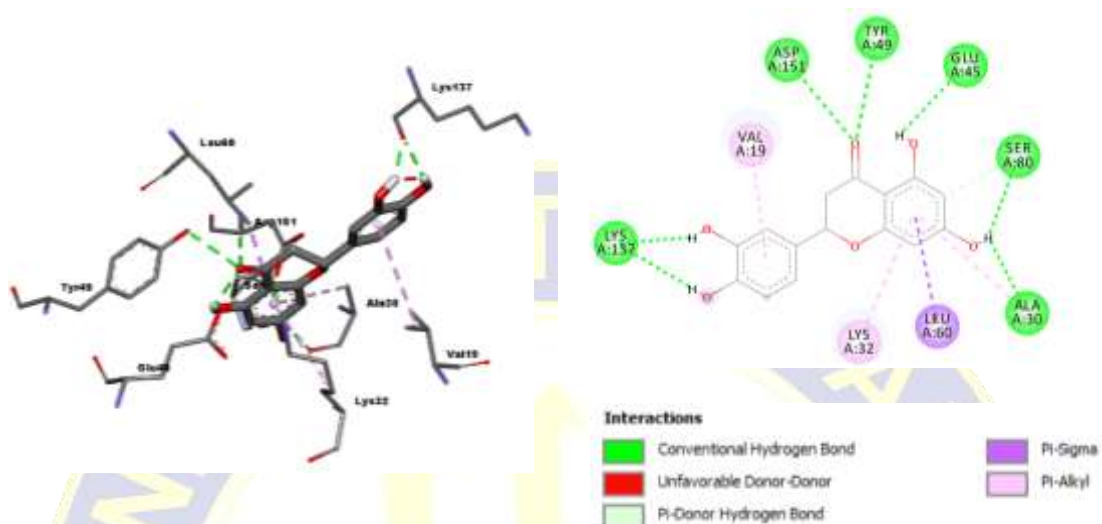


Gambar VI.57 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Naringenin* Terhadap Reseptor TGF-β Tipe 1

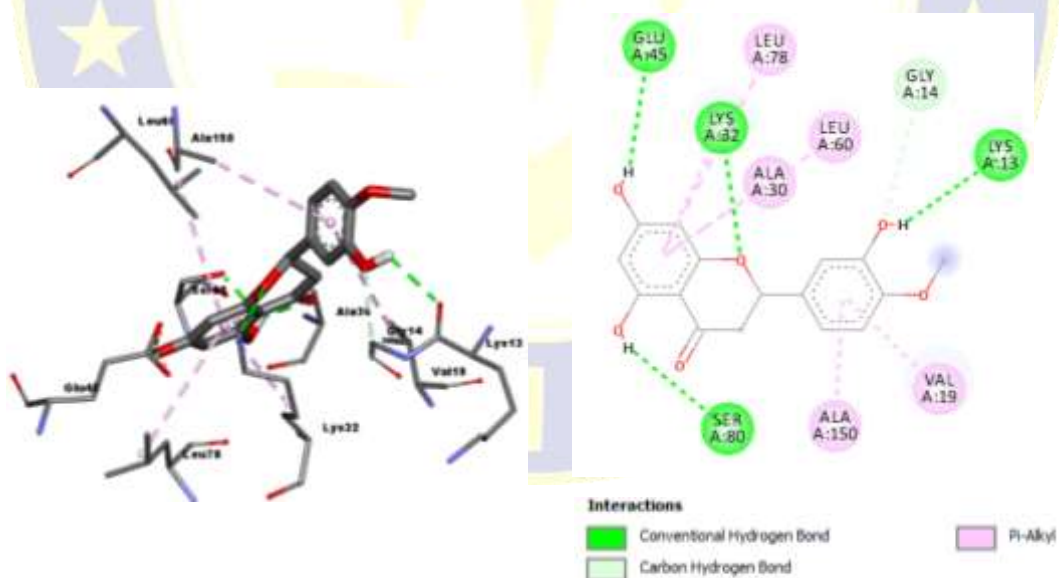


Gambar VI.58 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Sakuranetin* Terhadap Reseptor TGF-β Tipe 1

LAMPIRAN 10 (LANJUTAN)

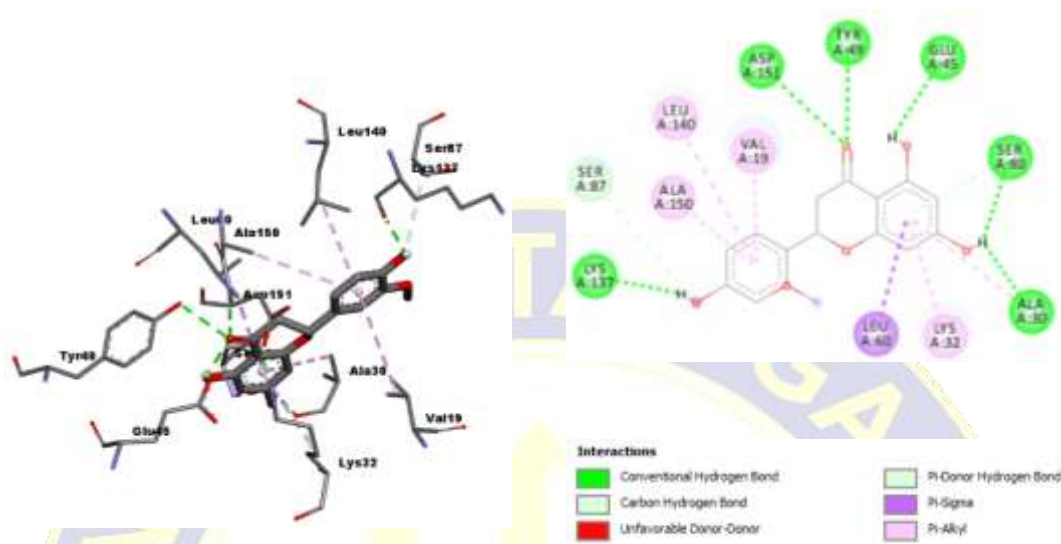


Gambar VI.59 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Eriodictyol* Terhadap Reseptor TGF- β Tipe 1

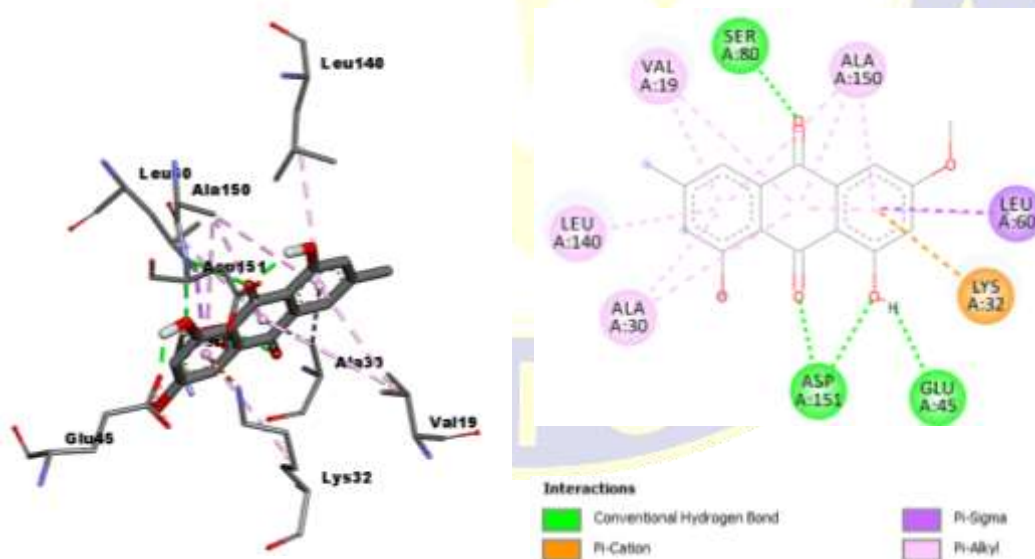


Gambar VI.60 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Hesperetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

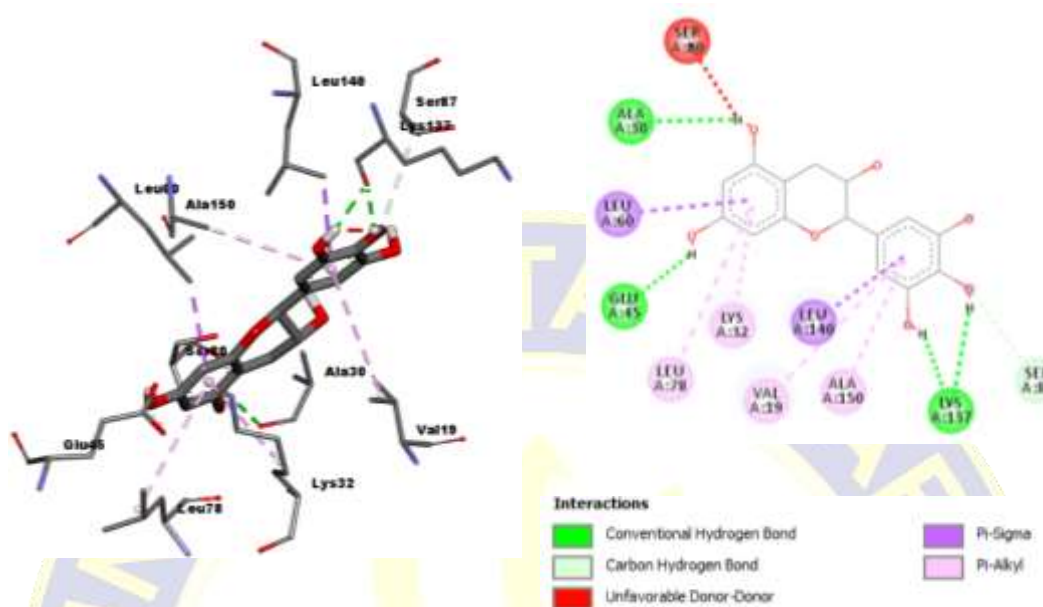


Gambar VI.61 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Homoeriodictyol* Terhadap Reseptor TGF- β Tipe 1

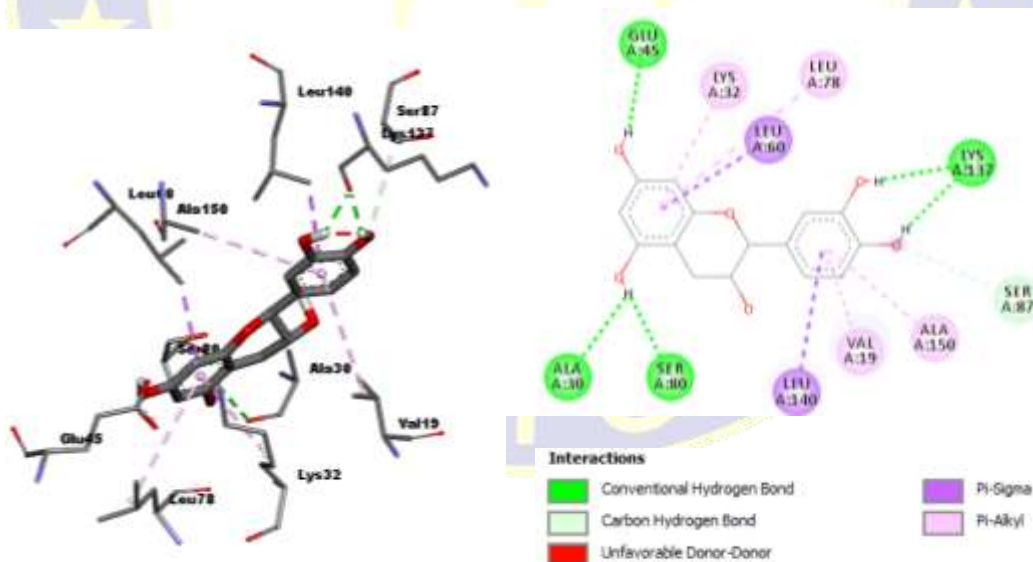


Gambar VI.62 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Parietin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

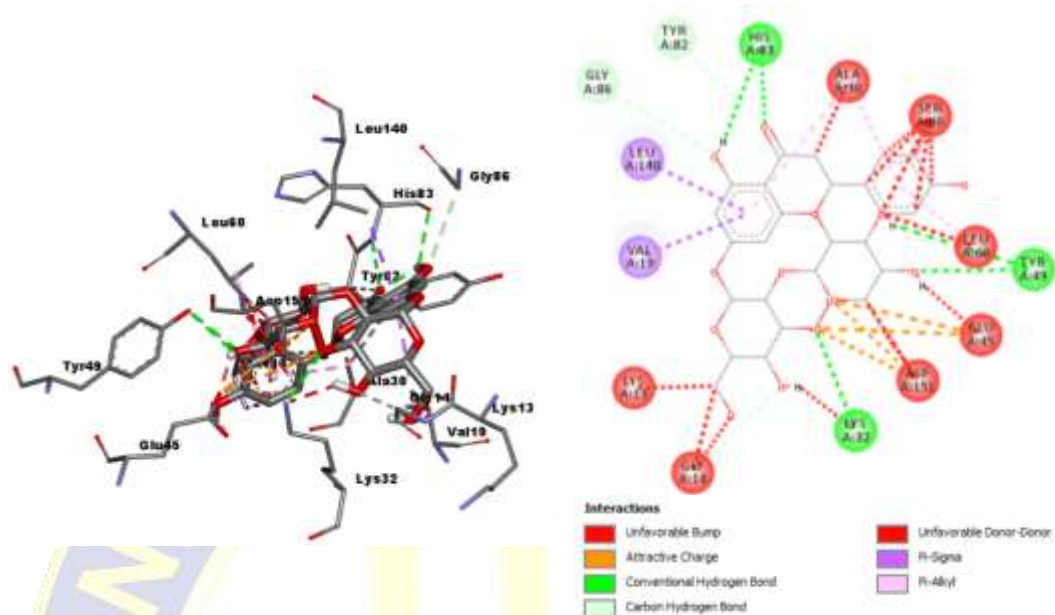


Gambar VI.63 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Epigallocatechin* Terhadap Reseptor TGF- β Tipe 1

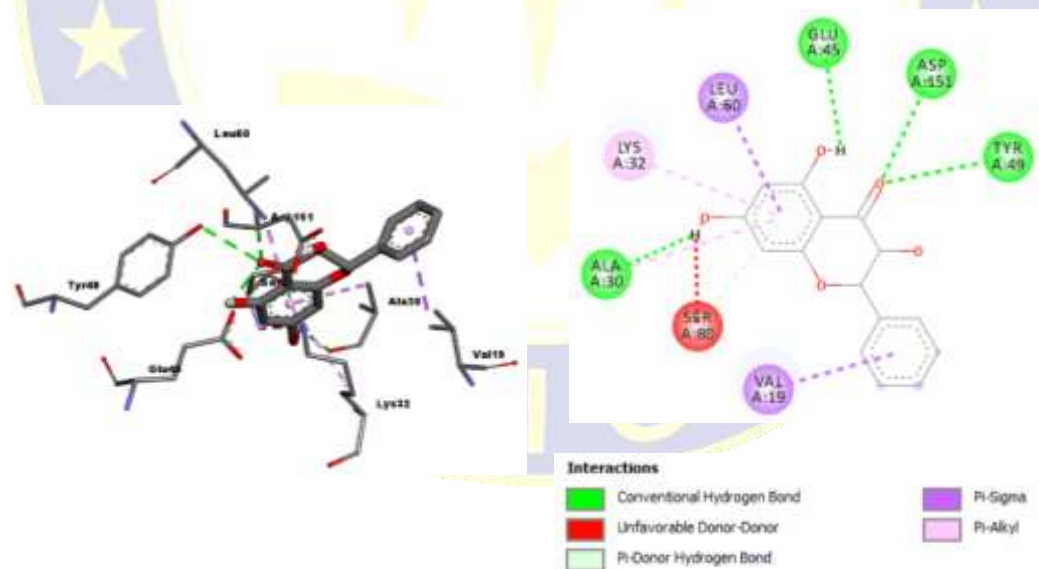


Gambar VI.64 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Catechin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

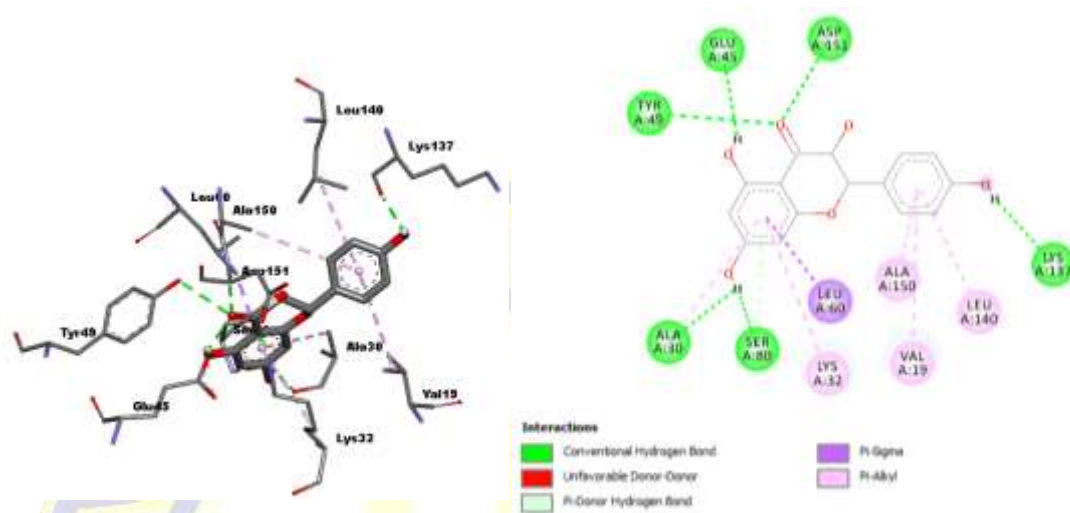


Gambar VI.65 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Naringin* Terhadap Reseptor TGF- β Tipe 1

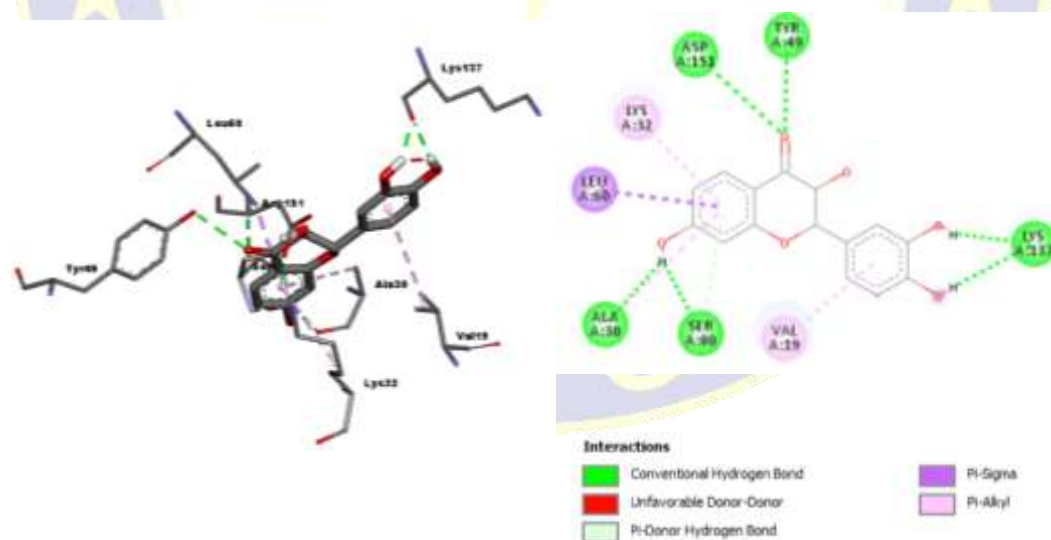


Gambar VI.66 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Pinobanksin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

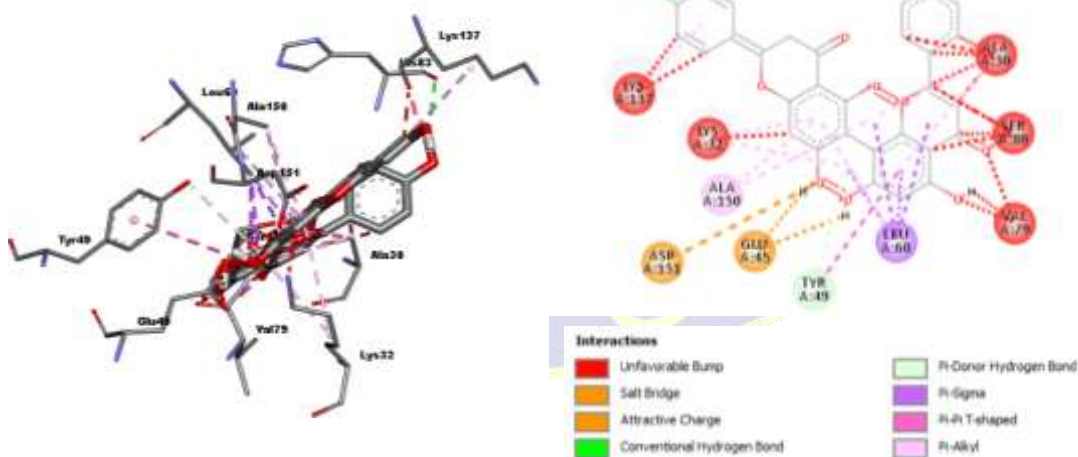
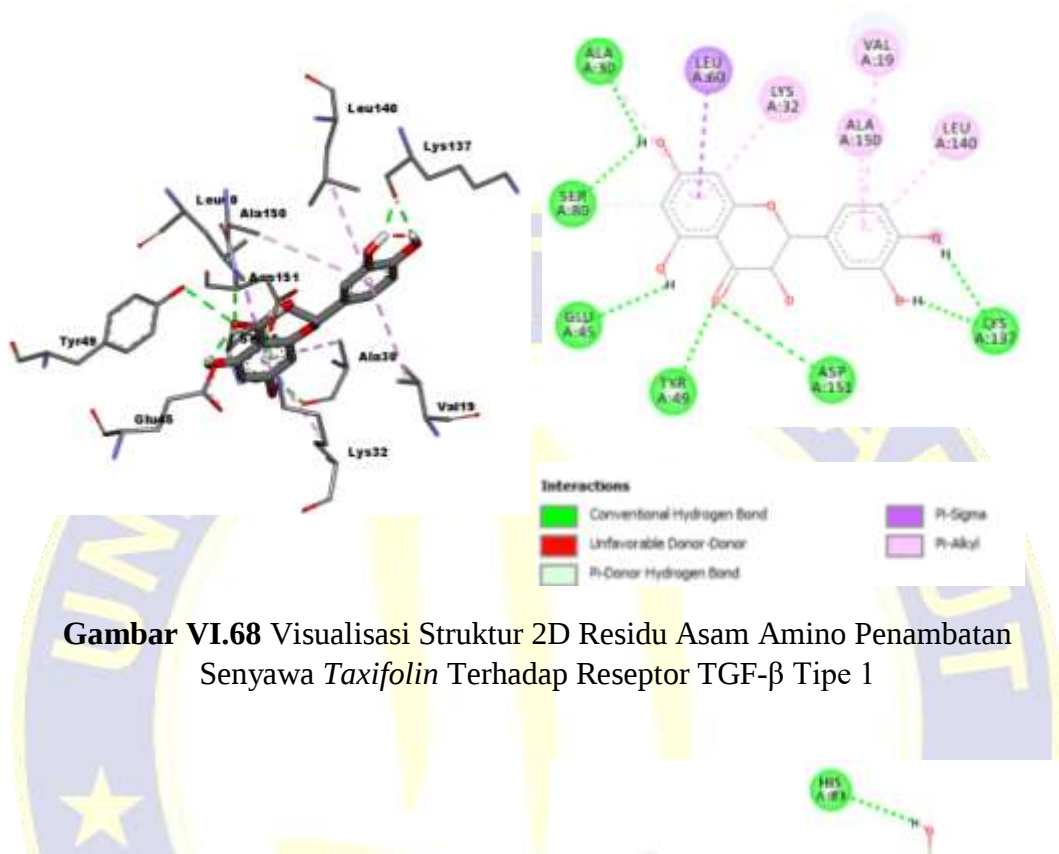


Gambar VI.67 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Aromadendrin* Terhadap Reseptor TGF- β Tipe 1

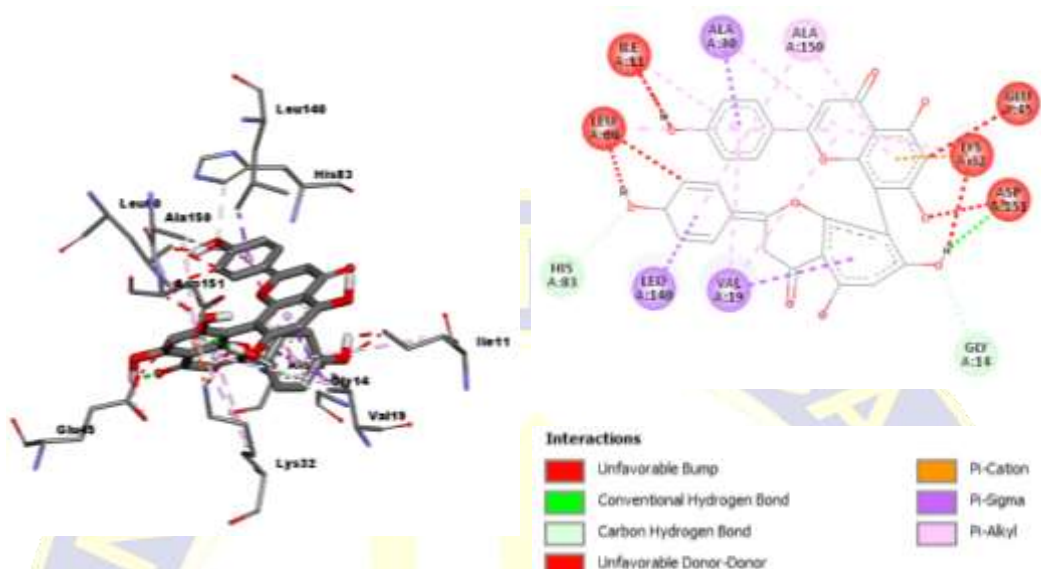


Gambar VI.68 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Fustin* Terhadap Reseptor TGF- β Ti

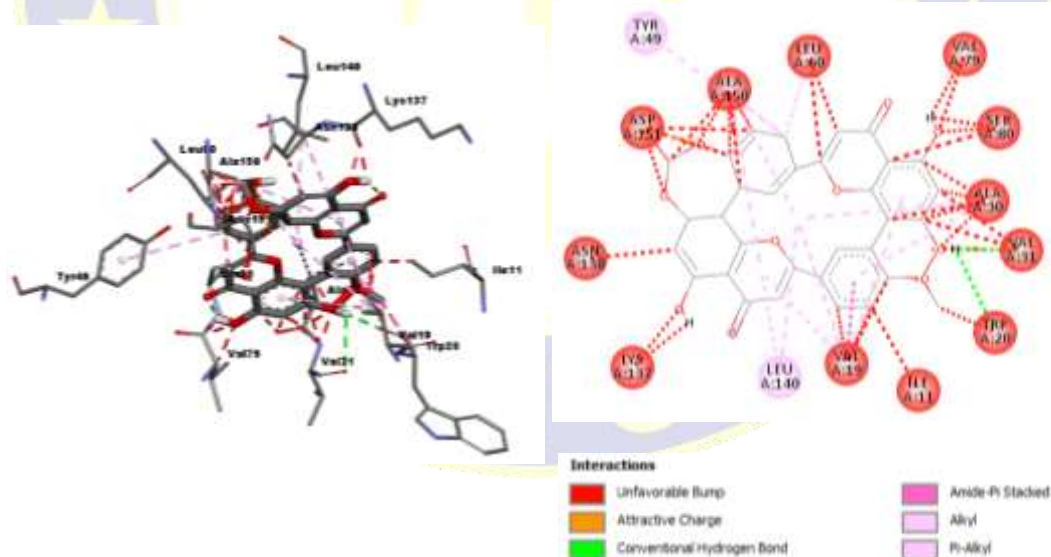
LAMPIRAN 10 (LANJUTAN)



LAMPIRAN 10 (LANJUTAN)

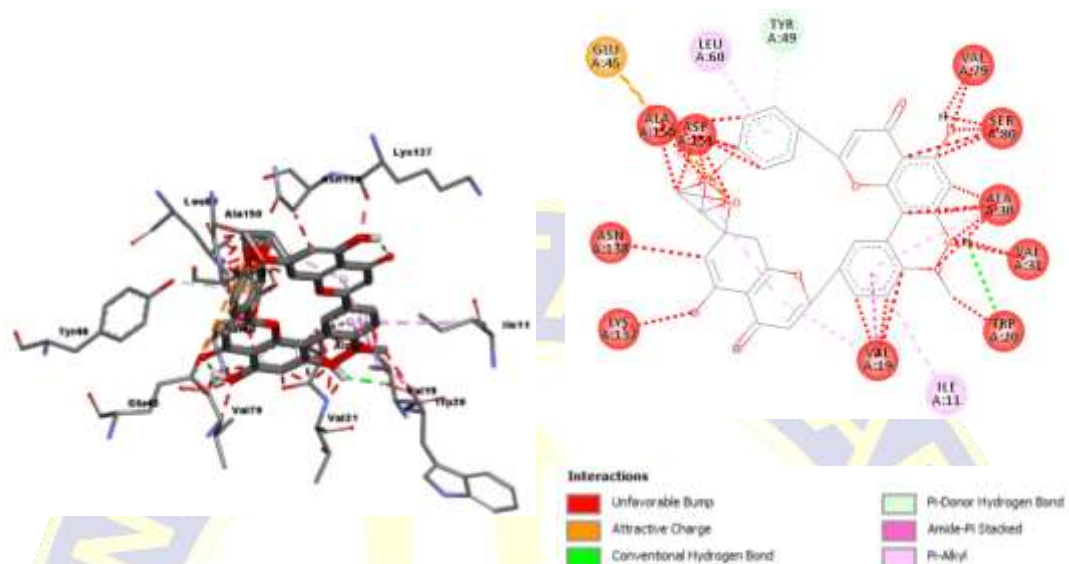


Gambar VI.71 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Cupressuflavone* Terhadap Reseptor TGF- β Tipe 1

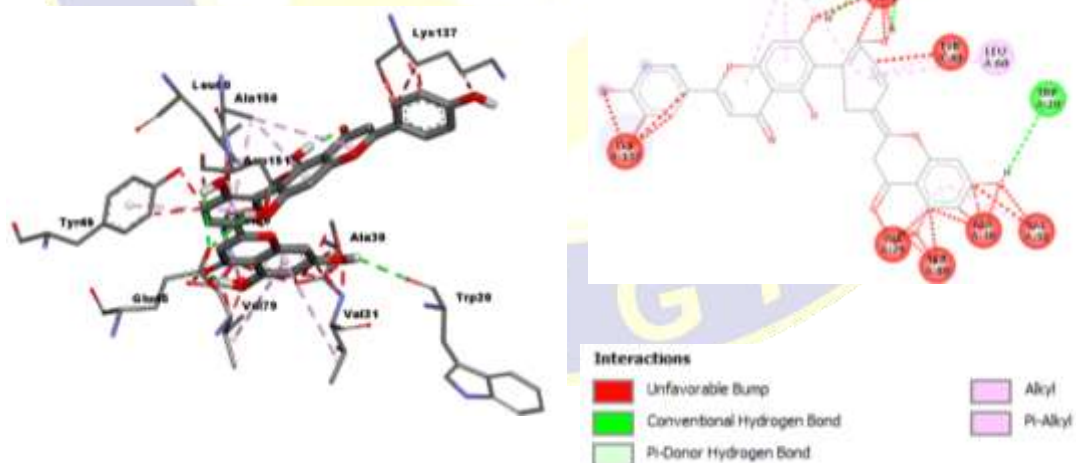


Gambar VI.72 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Ginkgetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

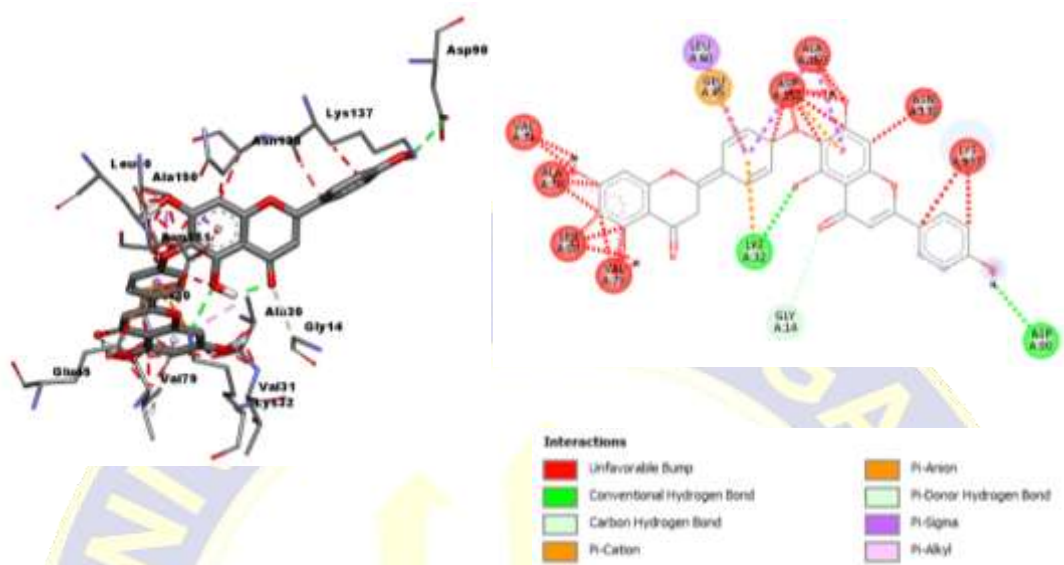


Gambar VI.73 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Syadopitysin* Terhadap Reseptor TGF- β Tipe 1

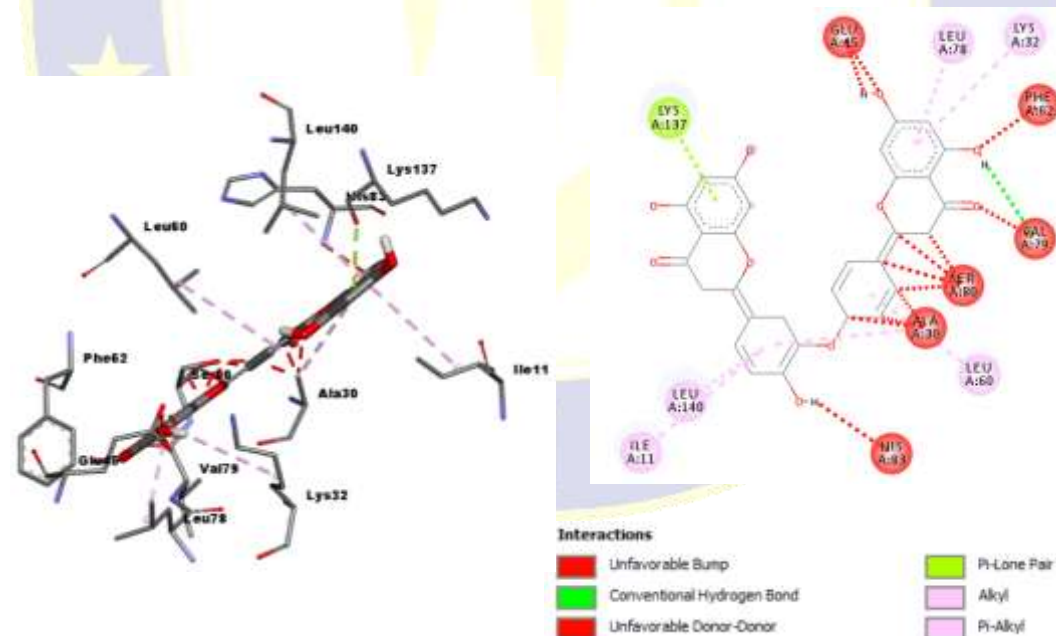


Gambar VI.74 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Robustaflavone* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

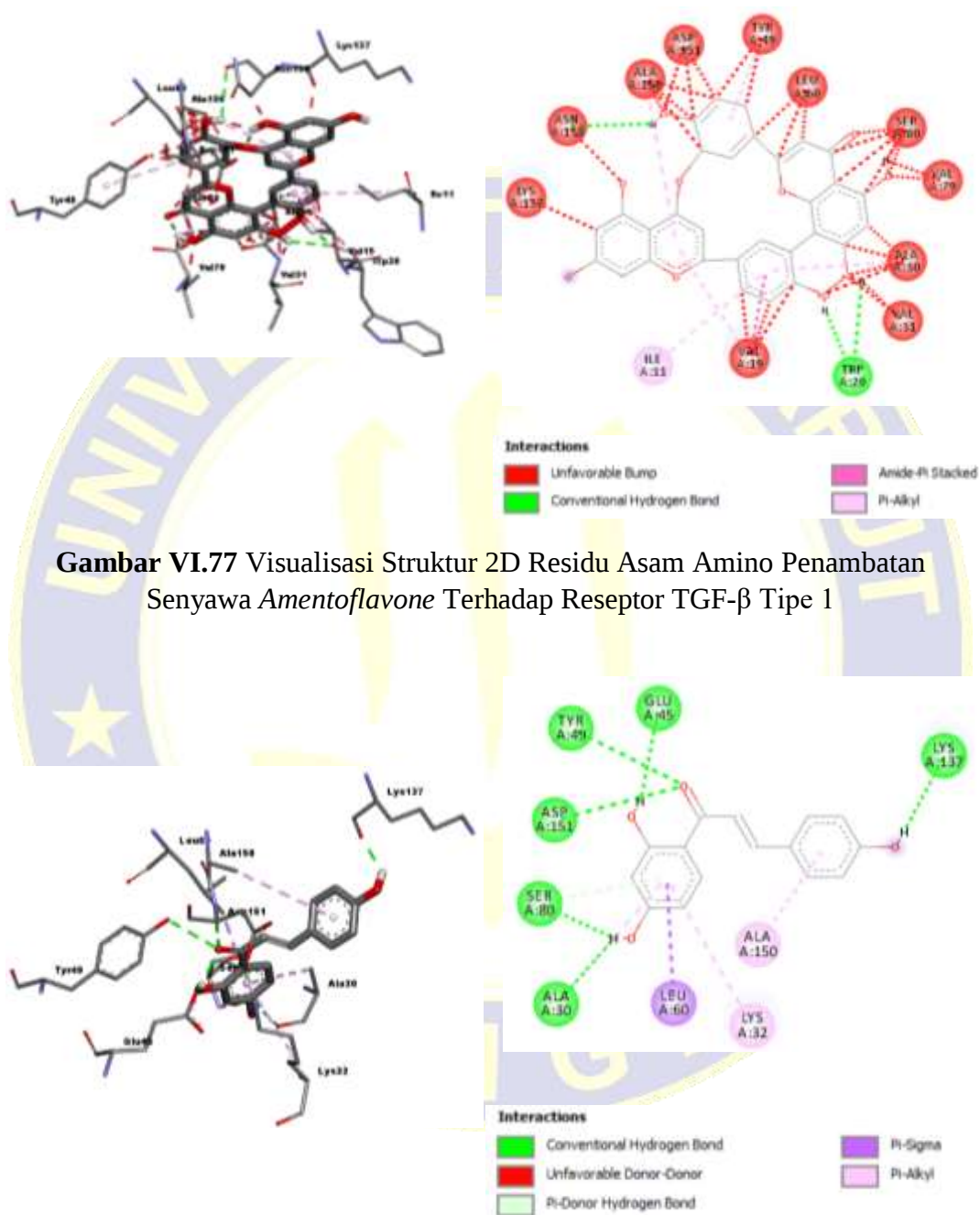


Gambar VI.75 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Hinokiflavone* Terhadap Reseptor TGF- β Tipe 1

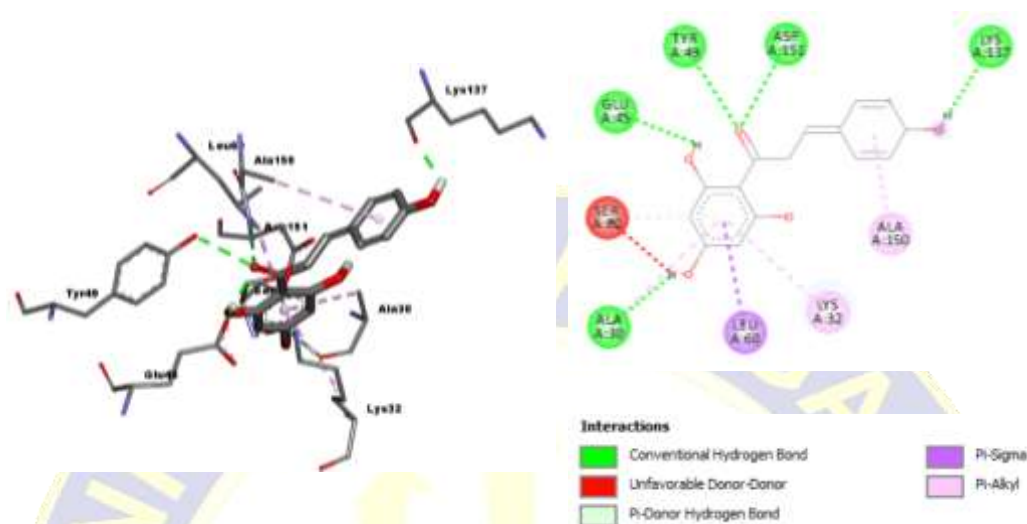


Gambar VI.76 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Ochnaflavone* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

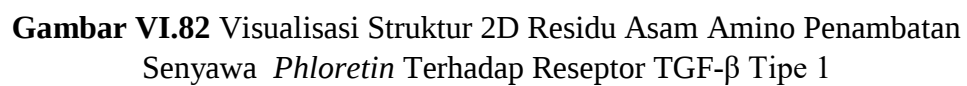
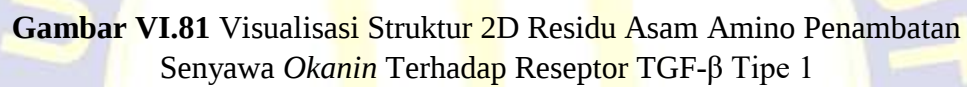


LAMPIRAN 10 (LANJUTAN)

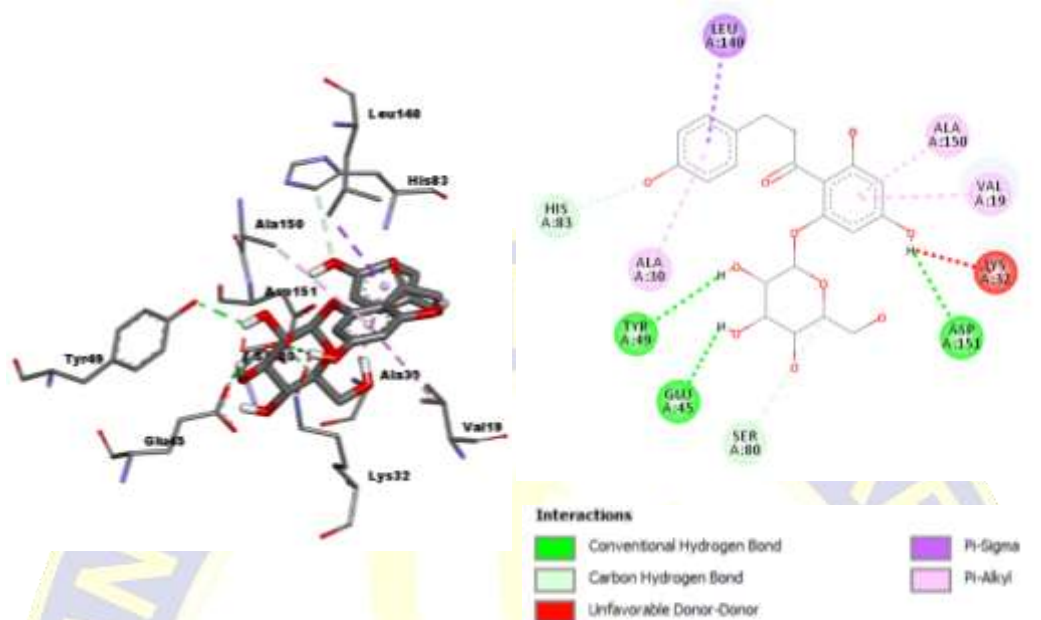


Gambar VI.79 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Kalkonaringenin* Terhadap Reseptor TGF- β Tipe 1

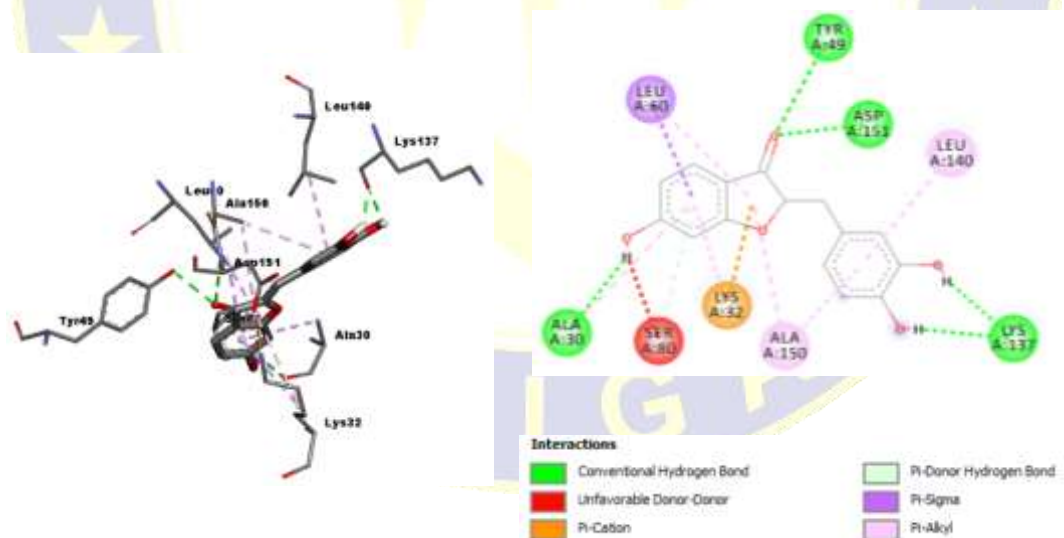
Gambar VI.80 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Butein* Terhadap Reseptor TGF- β Tipe 1



LAMPIRAN 10 (LANJUTAN)

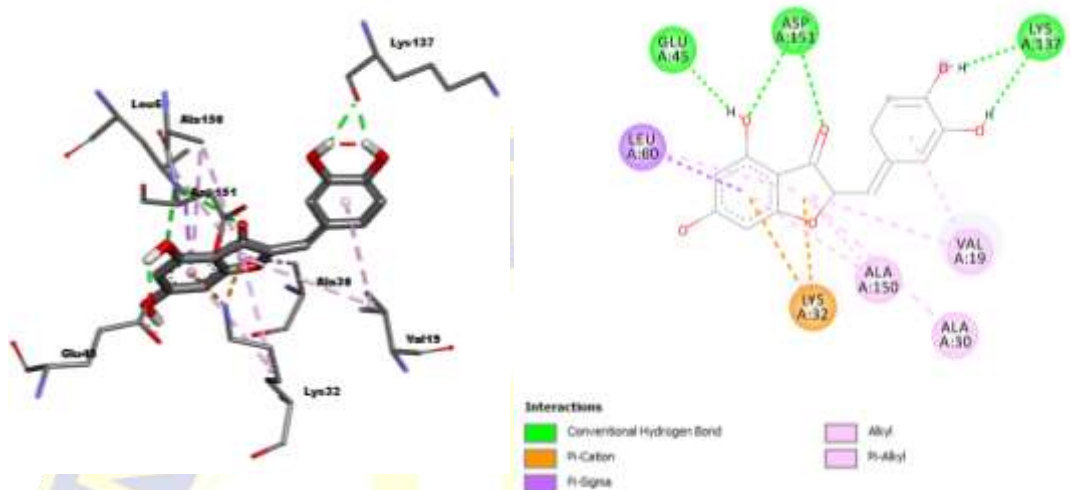


Gambar VI.83 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Phlorizin* Terhadap Reseptor TGF- β Tipe 1

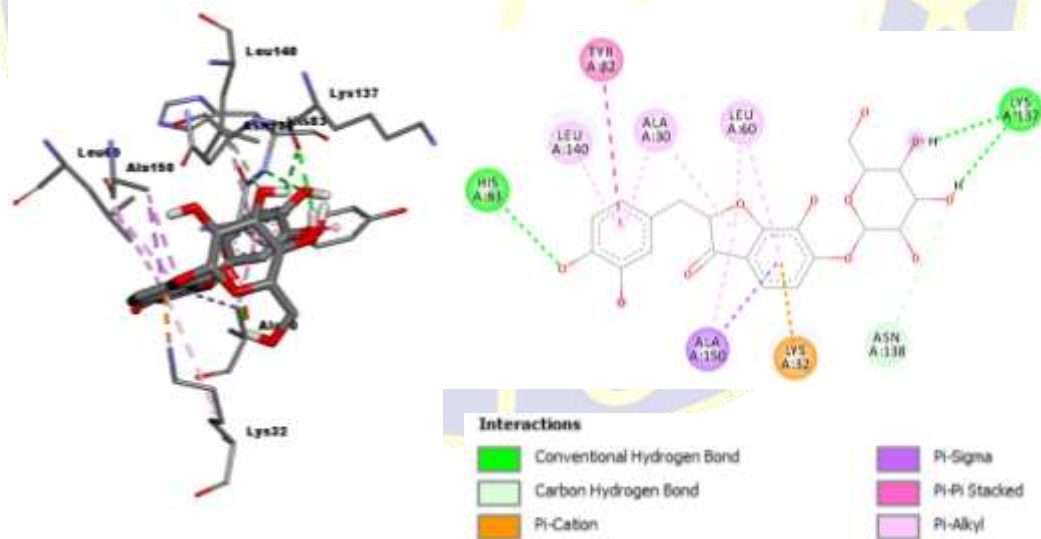


Gambar VI.84 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Sulfuretin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

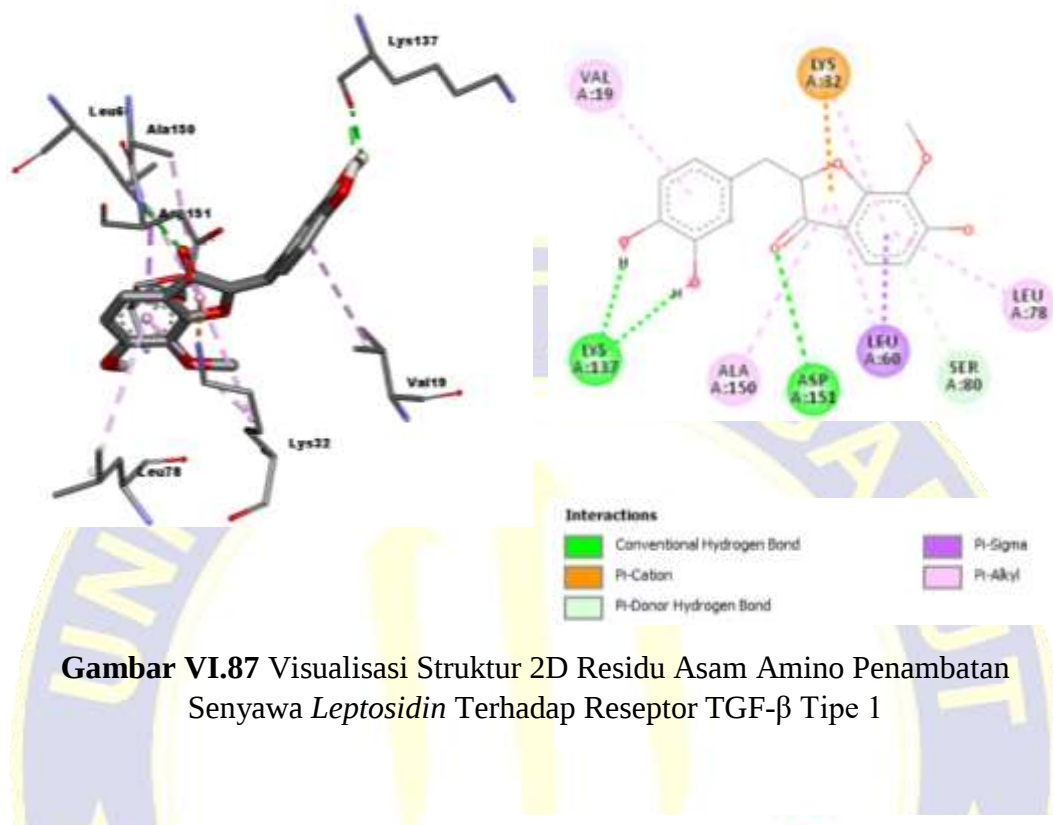


Gambar VI.85 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Aureusidin* Terhadap Reseptor TGF- β Tipe 1

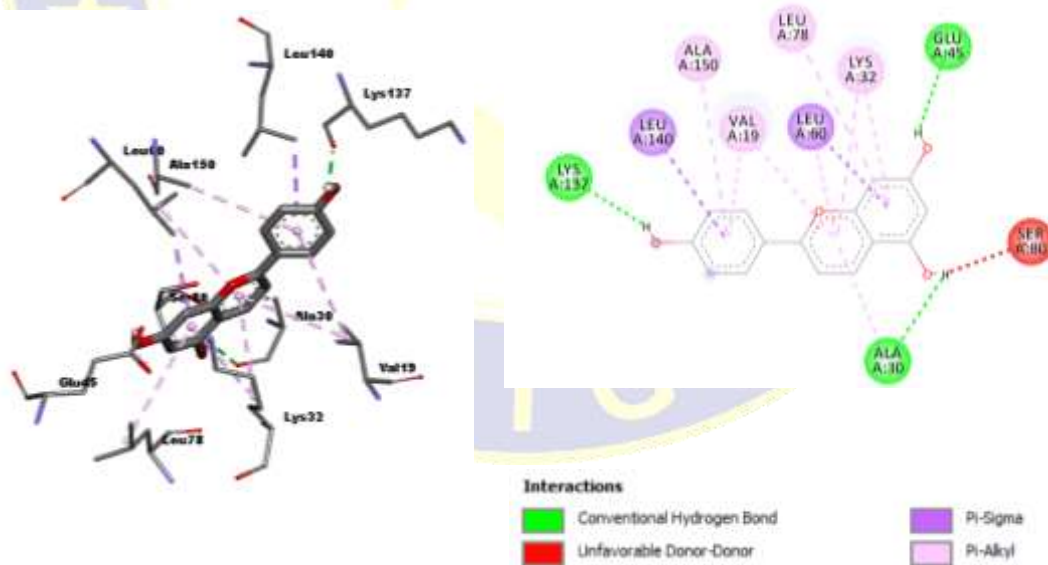


Gambar VI.86 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Maritimetin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

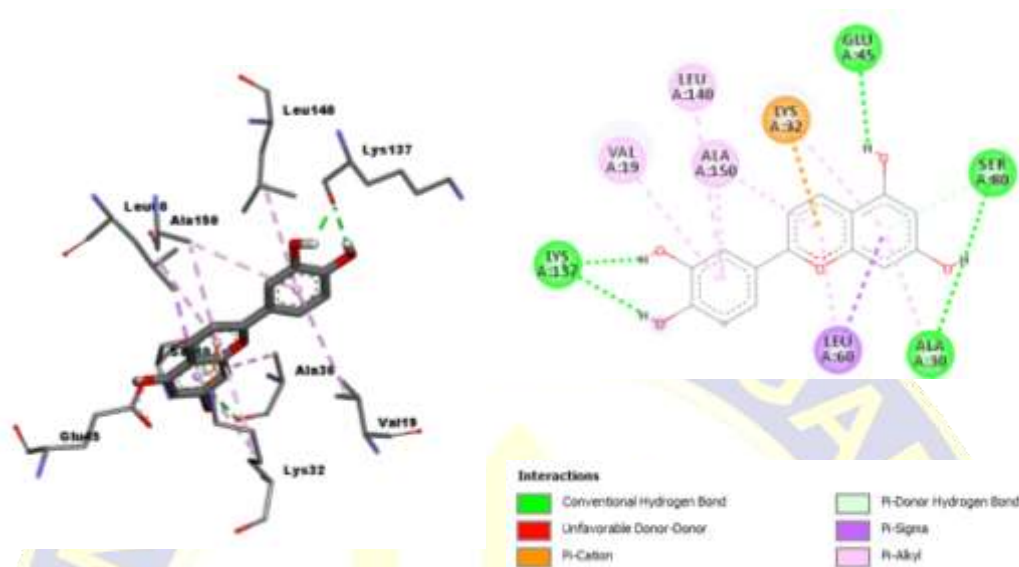


Gambar VI.87 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Leptosidin* Terhadap Reseptor TGF- β Tipe 1

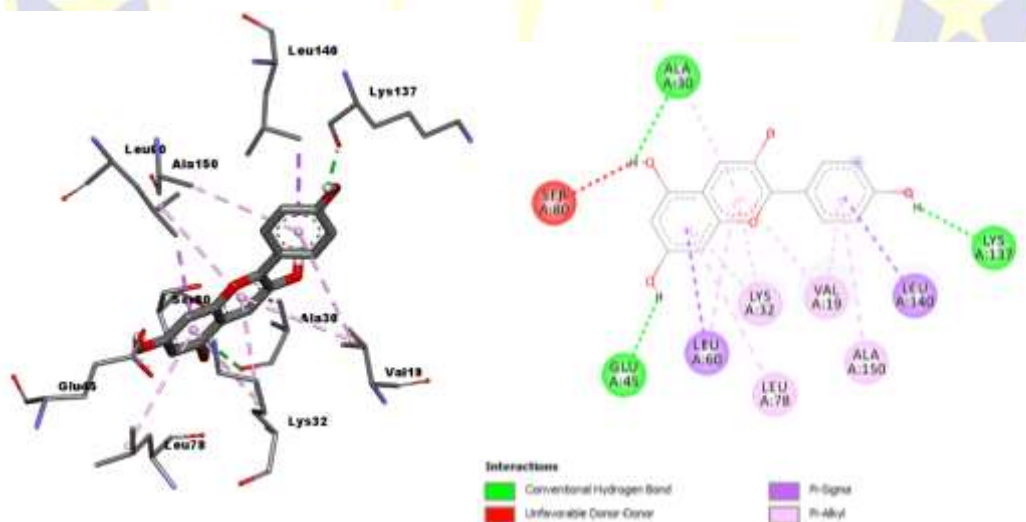


Gambar VI.88 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Apigenidin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

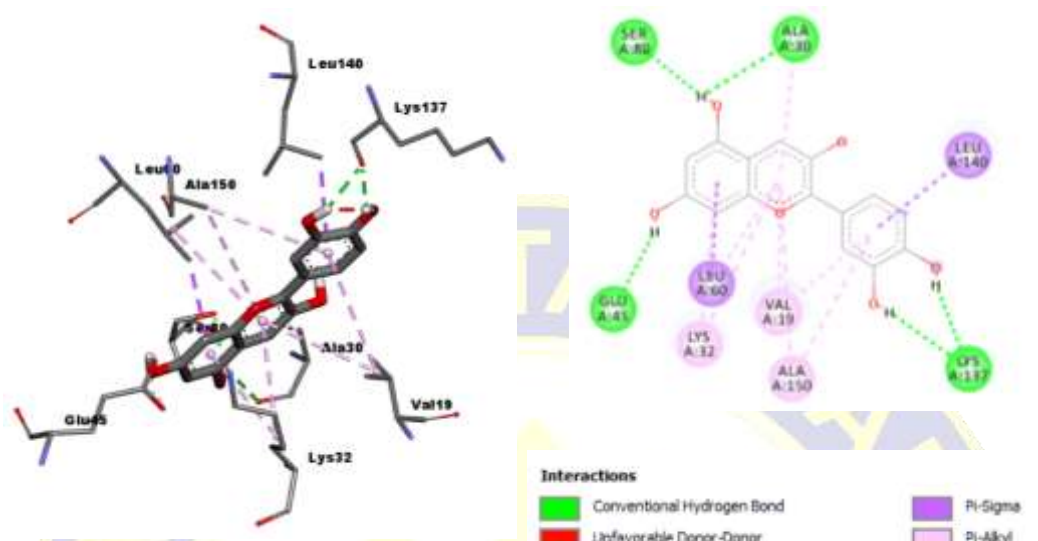


Gambar VI.89 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Luteolinidin* Terhadap Reseptor TGF- β Tipe 1

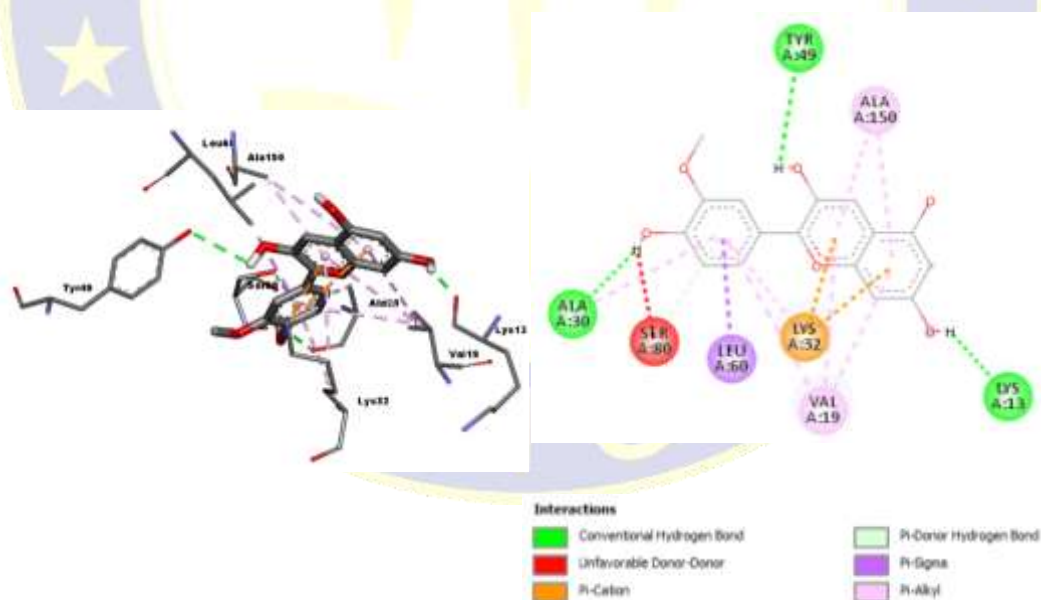


Gambar VI.90 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Pelargonidin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)

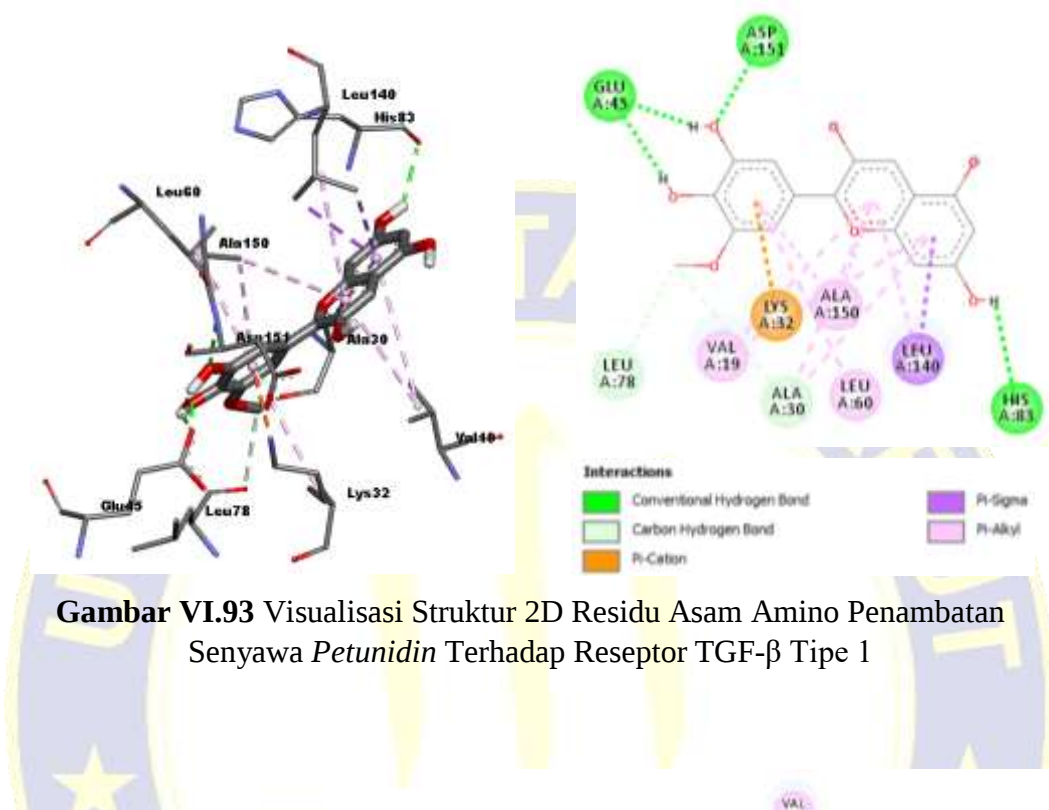


Gambar VI.91 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Cyanidin* Terhadap Reseptor TGF- β Tipe 1

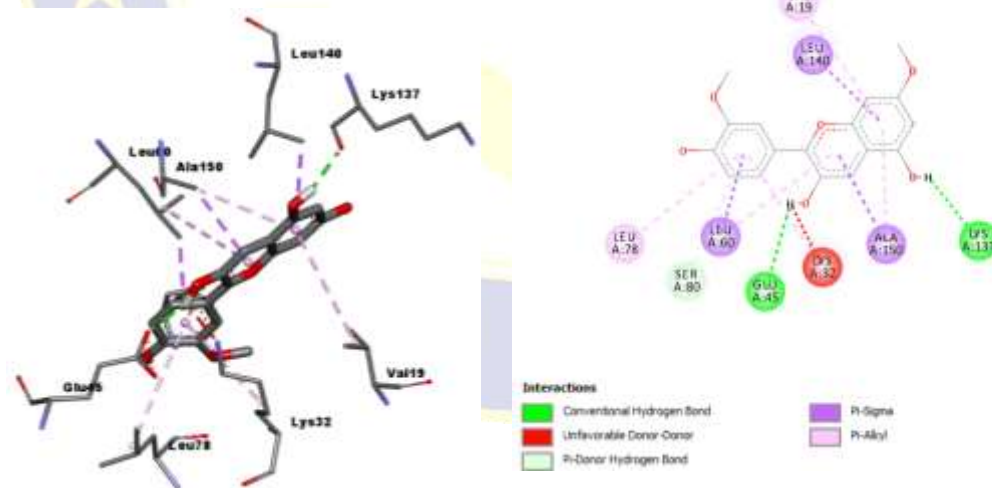


Gambar VI.92 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Peonidin* Terhadap Reseptor TGF- β Tipe 1

LAMPIRAN 10 (LANJUTAN)



Gambar VI.93 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Petunidin* Terhadap Reseptor TGF-β Tipe 1



Gambar VI.94 Visualisasi Struktur 2D Residu Asam Amino Penambatan Senyawa *Rosinidin* Terhadap Reseptor TGF-β Tipe 1

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