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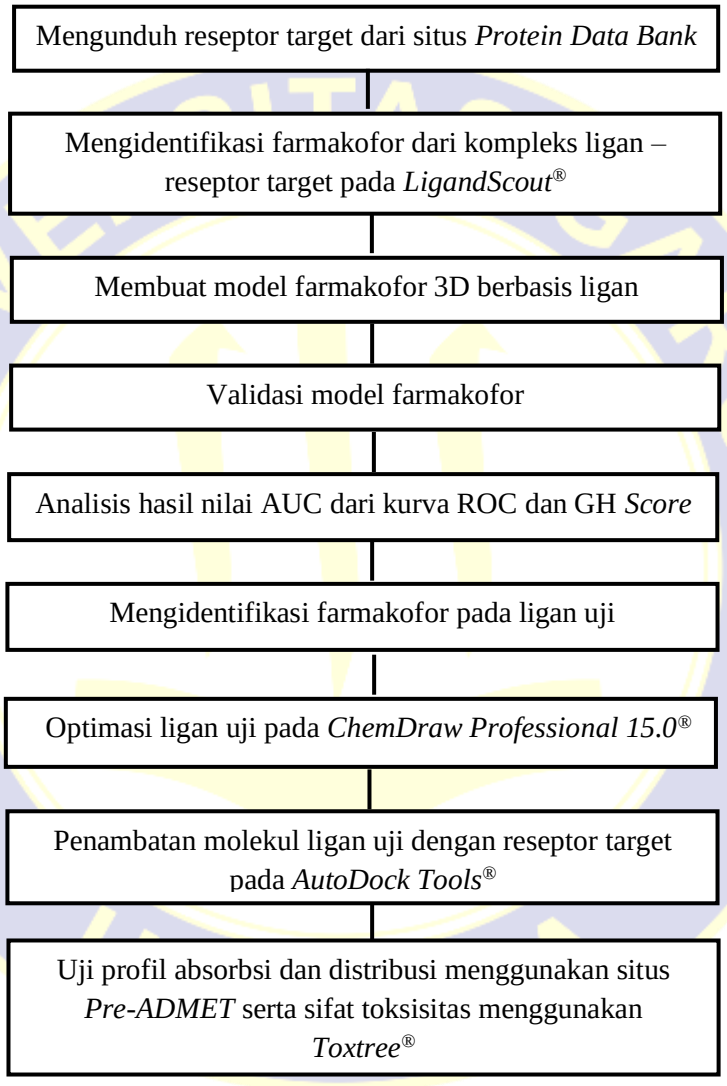
LAMPIRAN 1

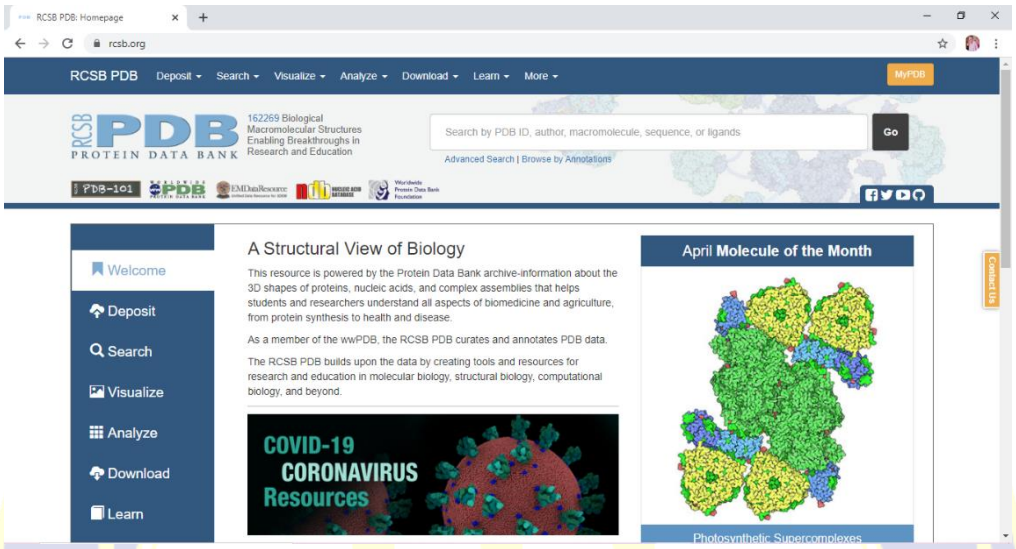
ALUR PENELITIAN *SCREENING* FARMAKOFOR DAN PENAMBATAN MOLEKUL



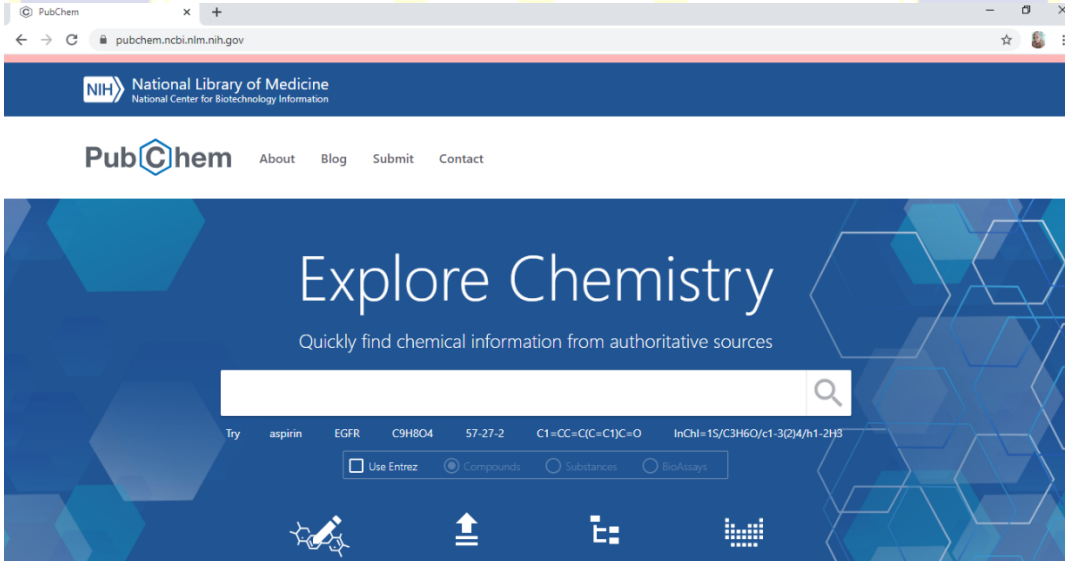
Gambar IV.1 Alur penelitian *screening* farmakofor dan penambatan molekul

LAMPIRAN 2

SITUS DAN APLIKASI



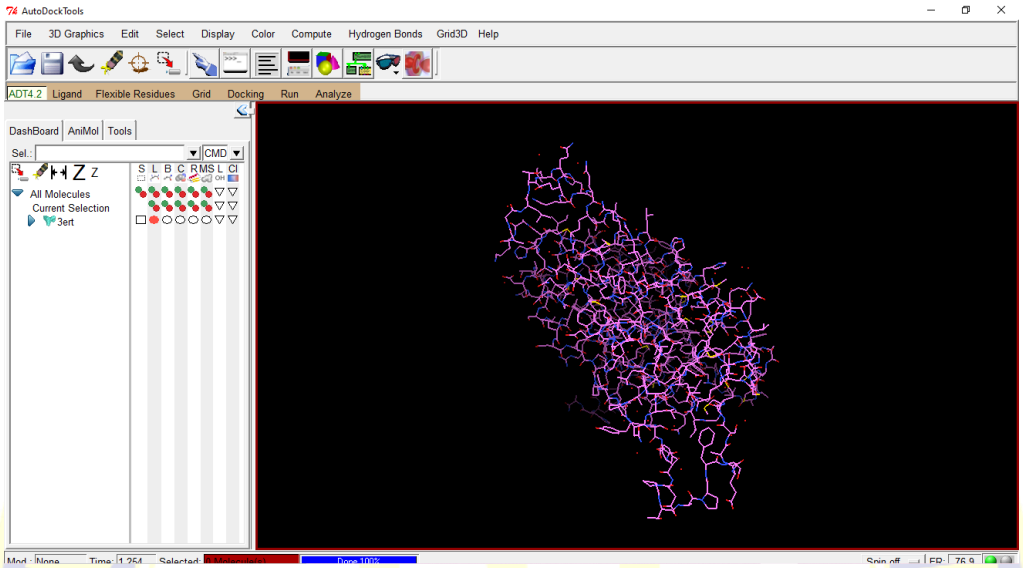
Gambar IV.2 Tampilan *situs protein data bank*



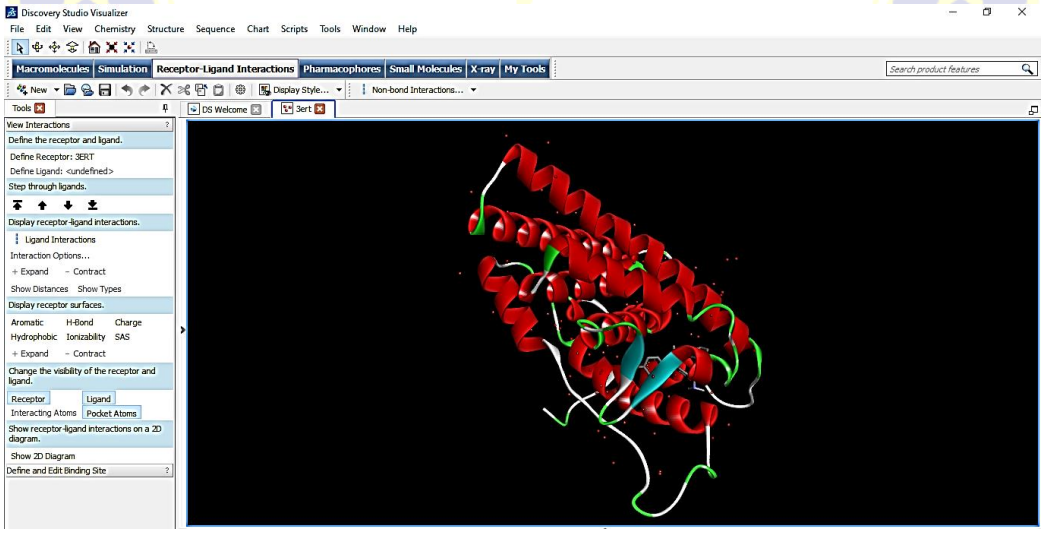
Gambar IV.3 Tampilan situs *pubChem*

LAMPIRAN 2

(LANJUTAN)



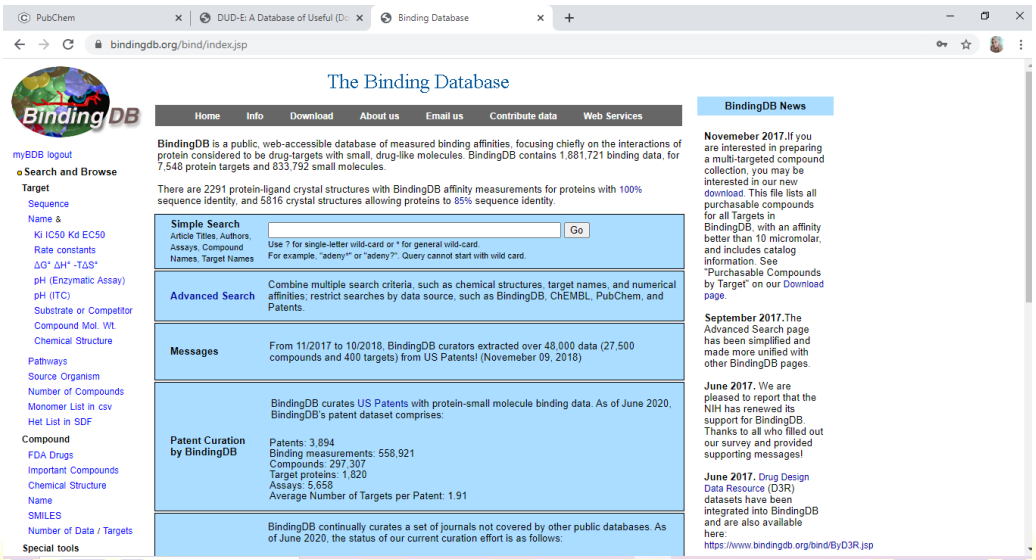
Gambar IV.4 Tampilan program *autodock tools*®



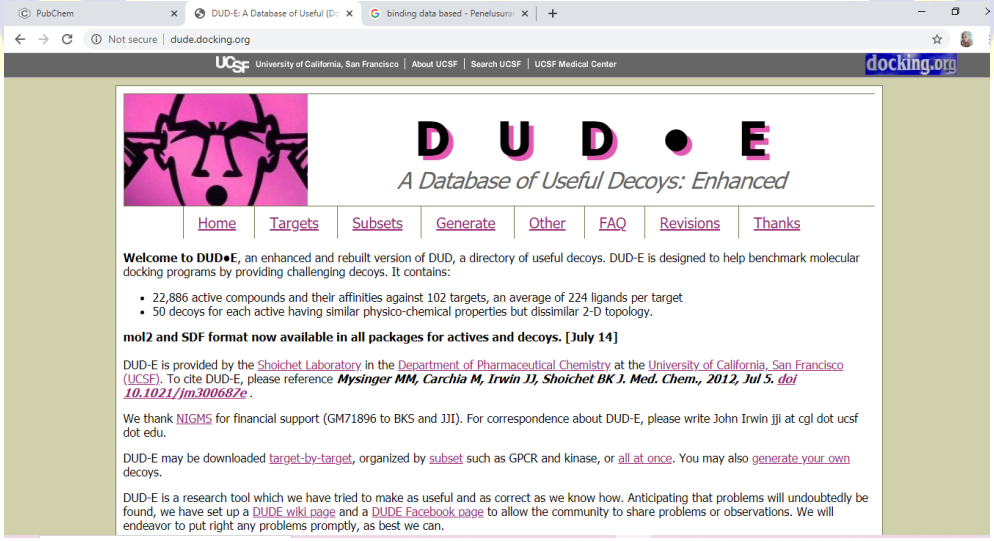
Gambar IV.5 Tampilan program *discovery studio visualizer*®

LAMPIRAN 2

(LANJUTAN)



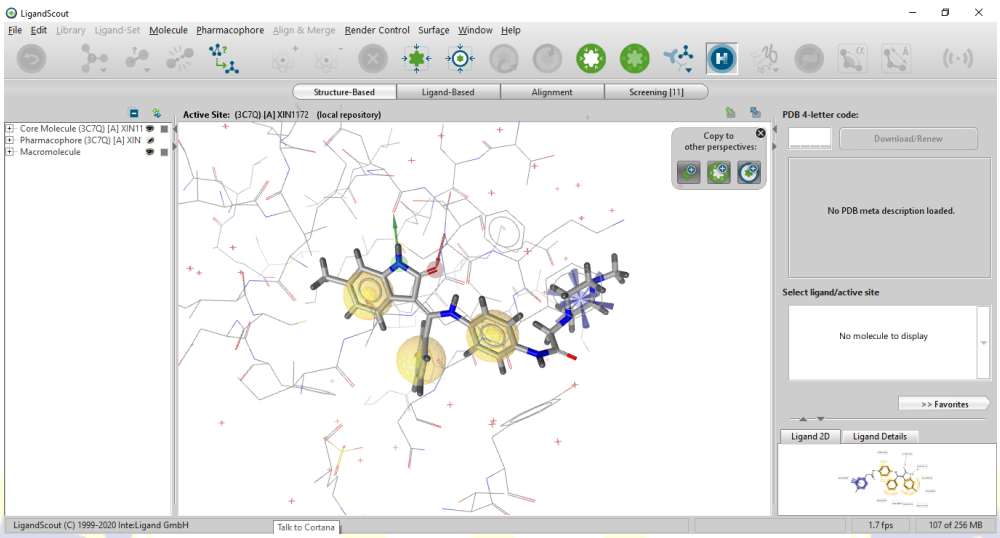
Gambar IV.6 Tampilan situs *binding database*



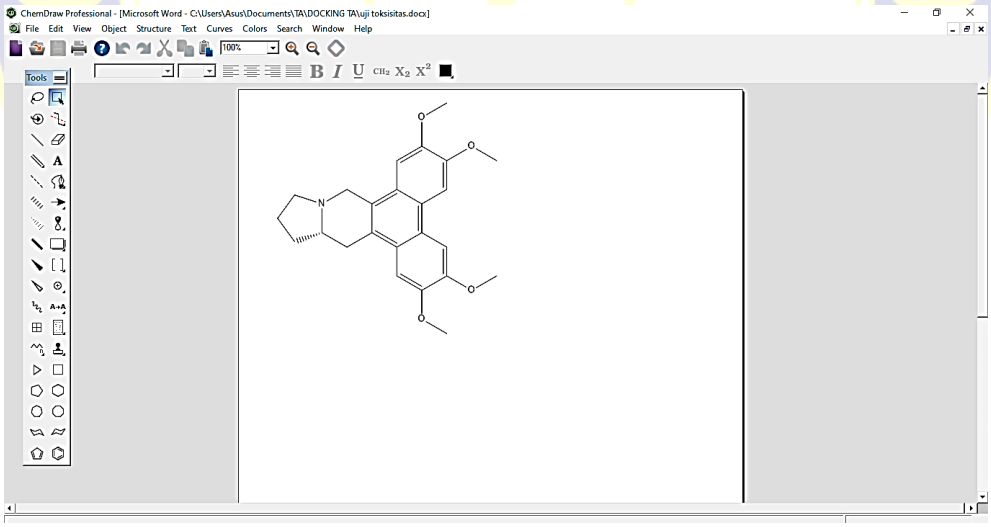
Gambar IV.7 Tampilan situs *DUD-E*

LAMPIRAN 2

(LANJUTAN)



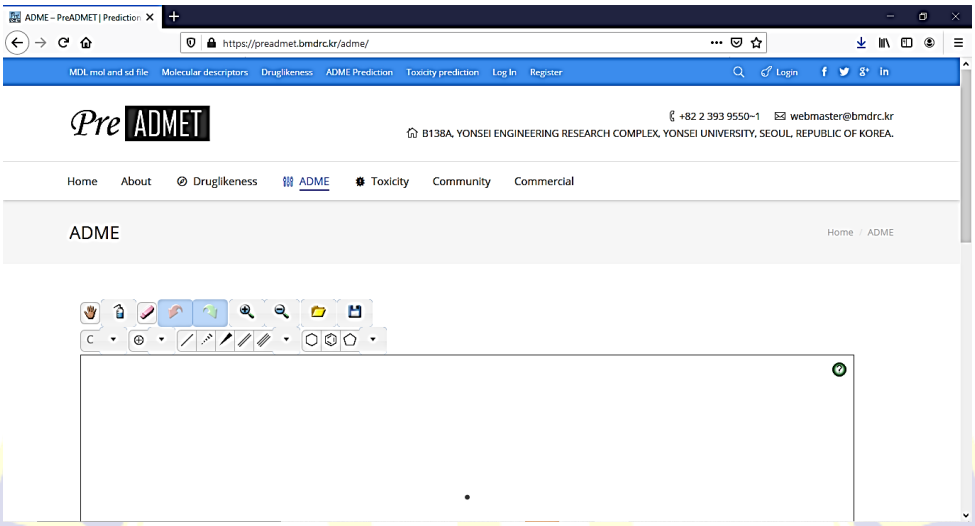
Gambar IV.8 Tampilan program *ligandscout*®



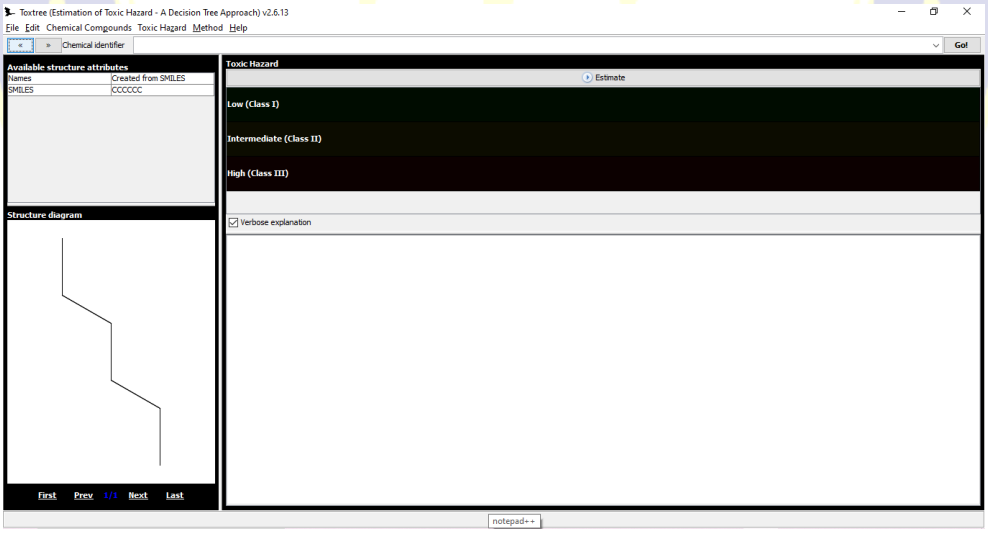
Gambar IV.9 Tampilan program *chem draw professional 15.0*®

LAMPIRAN 2

(LANJUTAN)



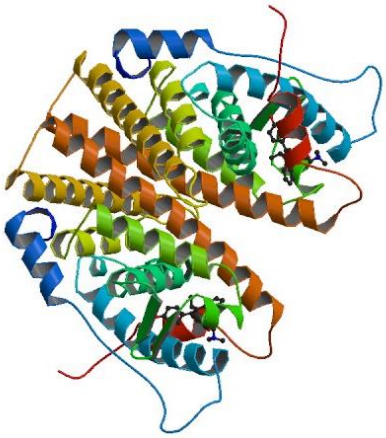
Gambar IV.10 Tampilan situs *pre-ADMET*



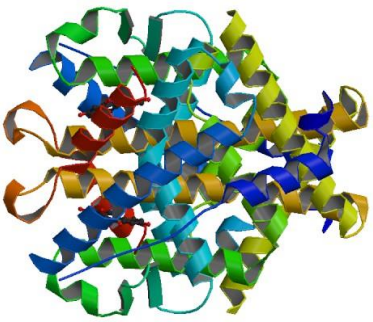
Gambar IV.11 Tampilan program *toxtree*®

LAMPIRAN 3

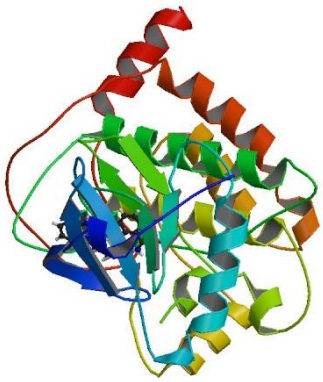
STRUKTUR 3D RESEPTOR



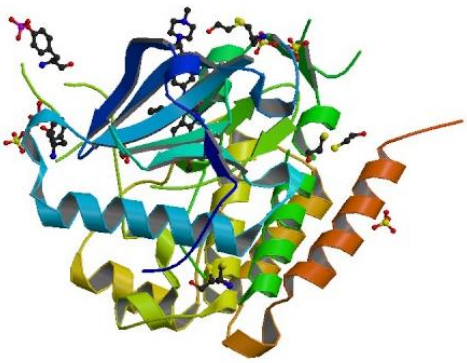
a. *Estrogen receptor alpha* (kode 3ERT)



b. *Estrogen receptor beta* (kode 1QKM)



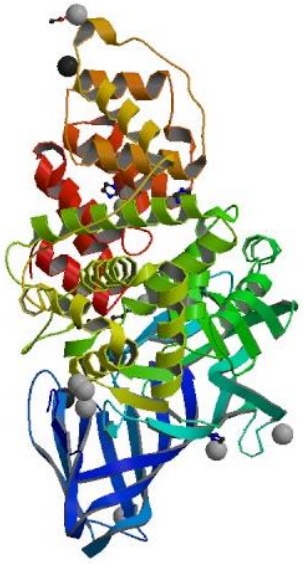
c. *Mitogen-activated protein kinase kinase kinase 7 (MAP3K7)* (kode 5V5N)



d. Reseptor *vascular endothelia growth factor* kinase (kode 3C7Q)

LAMPIRAN 3

(LANJUTAN)



e. Reseptor leukotriene A4 hydrolase (kode 3u9w)

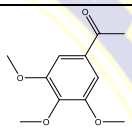
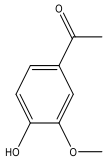
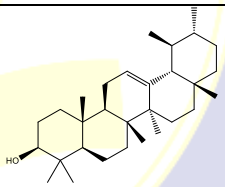
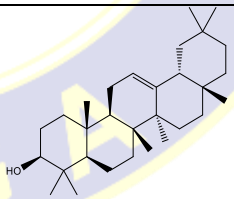
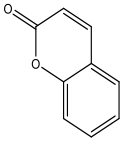
Gambar IV.12 Struktur 3D reseptor

LAMPIRAN 4

STRUKTUR 2D SENYAWA UJI

Tabel IV.1

Senyawa Daun Awar-awar (*Ficus septica* Burm. L)

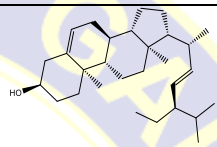
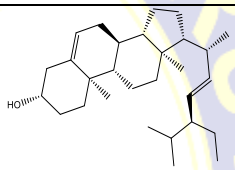
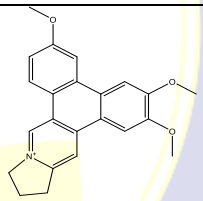
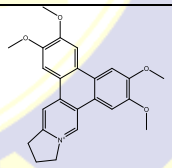
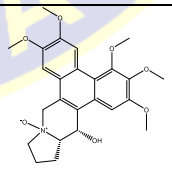
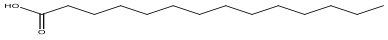
No.	Nama Senyawa	Struktur 2D
1.	1-triacontanol (ID 68972)	
2.	3',4',5'-Trimethoxyacetophenone (ID 14345)	
3.	4-hidroxy-3-methoxy-acetophenone (ID 2214)	
4.	Alfa-Amyrin (ID 73170)	
5.	Beta-Amyrin (ID 73145)	
6.	Coumarin (ID 323)	

LAMPIRAN 4

(LANJUTAN)

Tabel IV.1

(lanjutan)

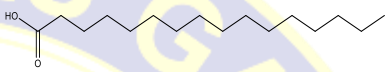
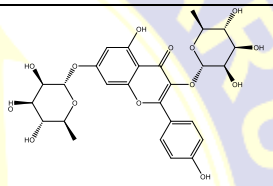
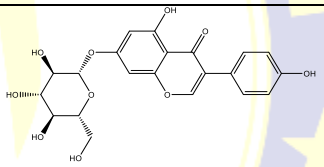
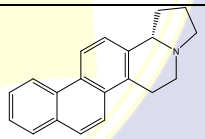
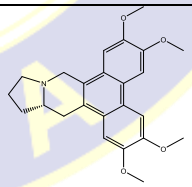
No.	Nama Senyawa	Struktur 2D
7.	Beta-Stigmasterol (ID 91692579)	
8.	Stigmasterol (ID 5280794)	
9.	Dehydroantofine (ID 14489153)	
10.	Dehydrotylophorine (ID 11583623)	
11.	Ficuseptine A (ID 10411696)	
12	Myristic Acid (ID 11005)	

LAMPIRAN 4

(LANJUTAN)

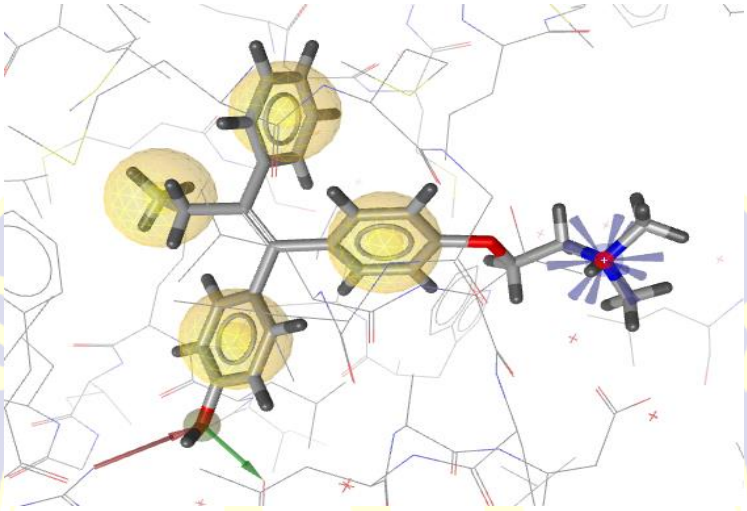
Tabel IV.1

(lanjutan)

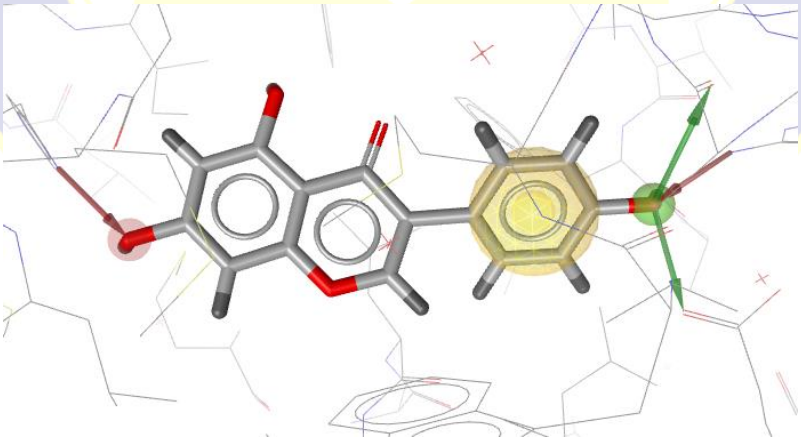
No.	Nama Senyawa	Struktur 2D
13.	Palmitic Acid (ID 985)	
14.	Kaempferitrin (ID 5486199)	
15.	Genistein (ID 5281377)	
16	Phenanthroindolizidine (ID 129650425)	
17.	Tylophorine (ID 92114)	

LAMPIRAN 5

SCREENING FARMAKOFOR



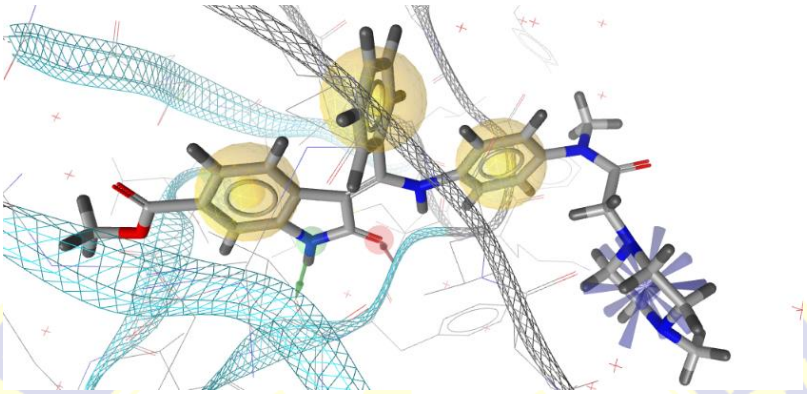
Gambar V.1 Hasil *screening* farmakofor pada *estrogen receptor – alfa*



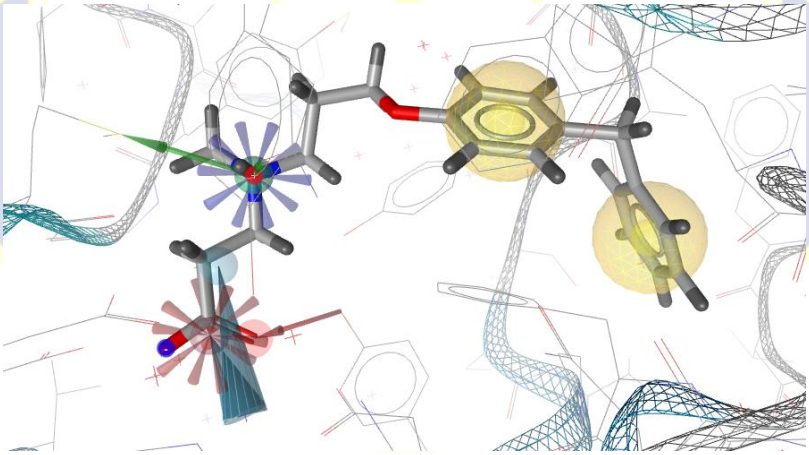
Gambar V.2 Hasil *screening* farmakofor pada *estrogen receptor - beta*

LAMPIRAN 5

(LANJUTAN)



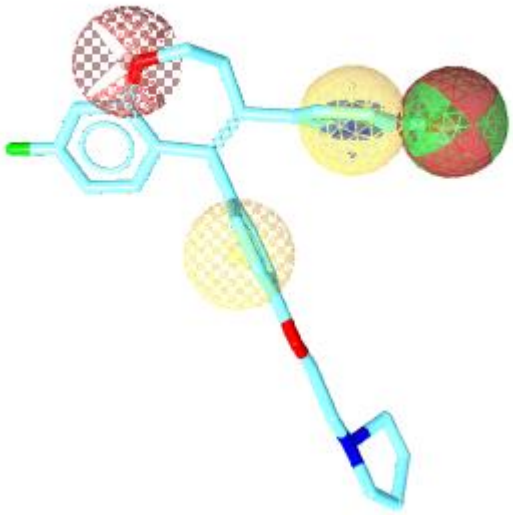
Gambar V.3 Hasil *screening* farmakofor pada reseptor *vascular endothelia growth factor receptor-2 kinase* (VEGFR-2 *kinase*)



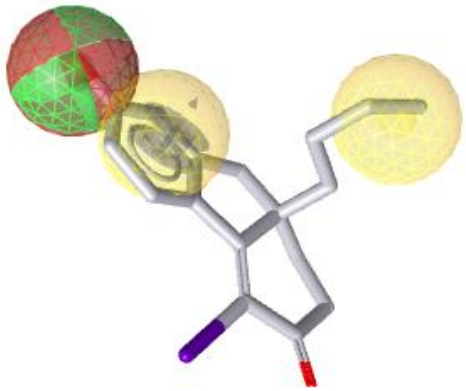
Gambar V.4 Hasil *screening* farmakofor pada reseptor *leukotriene A4 hydrolase*

LAMPIRAN 5

(LANJUTAN)



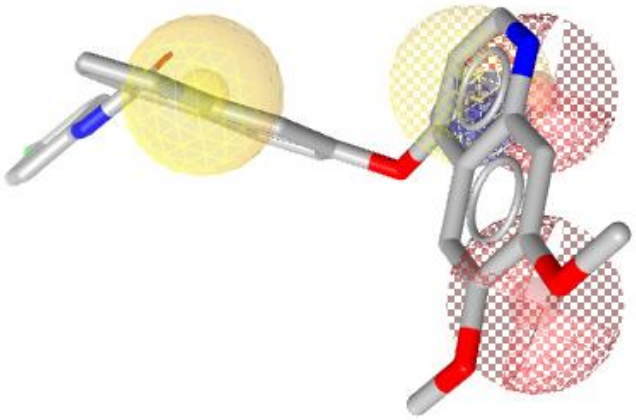
Gambar V.5 Model 1 farmakofor ligan *estrogen receptor - alfa*



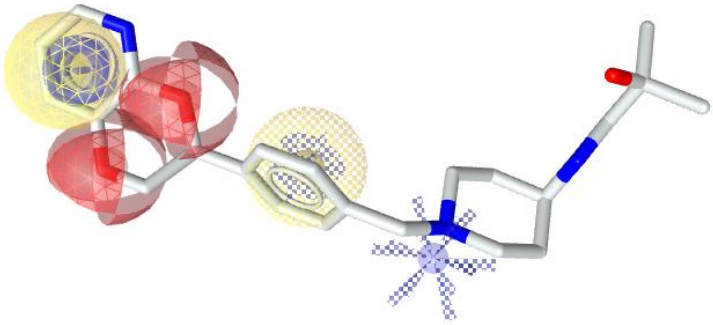
Gambar V.6 Model 1 farmakofor ligan *estrogen receptor - beta*

LAMPIRAN 5

(LANJUTAN)



Gambar V.7 Model 1 farmakofor ligan reseptor *vascular endothelia growth factor* (VEGFR) kinase



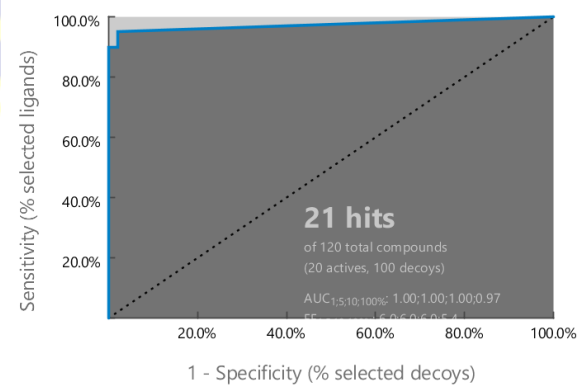
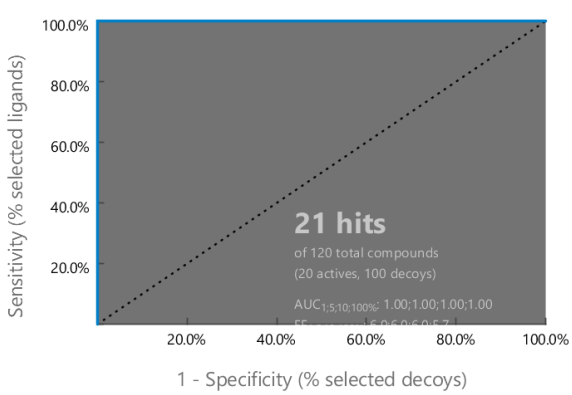
Gambar V.8 Model 1 farmakofor ligan reseptor *leukotriene A4 hydrolase*

LAMPIRAN 5

(LANJUTAN)

Tabel V.1

Hasil Validasi Model *Pharmacophore*

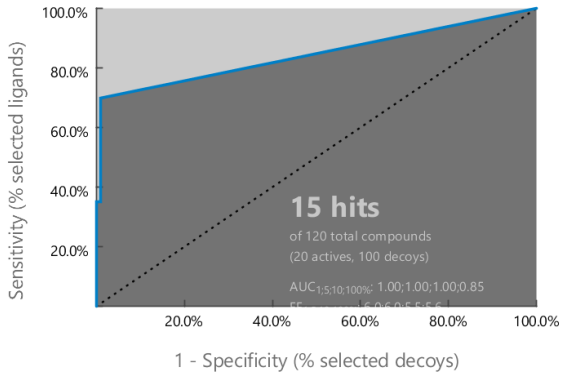
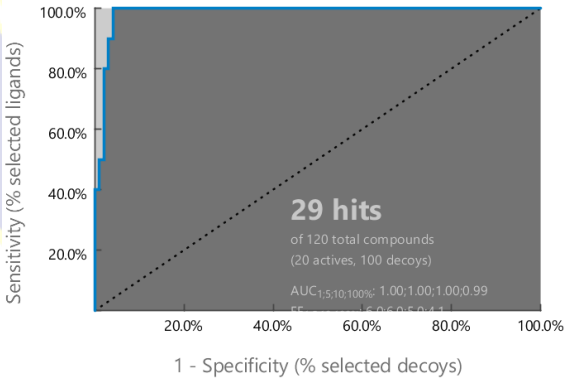
Reseptor	ROC *Curve*	AUC	GH *Score*
ER-α		0,97	0,90
ER-β		1,00	0,95

LAMPIRAN 5

(LANJUTAN)

Tabel V.1

(lanjutan)

Reseptor	ROC *Curve*	AUC	GH *Score*
VEGFR-2 Kinase		0,85	0,87
LTA4H		0,99	0,70

LAMPIRAN 5

(LANJUTAN)

Tabel V.2

Hasil *Screening* Farmakofor *Estrogen Receptor – Alfa*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	Tamoxifen (Ligan Pembanding)		-
2.	Genistein		48,82
3.	4-hydroxy-3-methoxyaceptophenone		47,05

Tabel V.3

Hasil *Screening* Farmakofor *Estrogen Receptor – Beta*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	Genistein (Ligan Pembanding)		-
2.	Beta- Amyrin		47,57
3.	Kaempferitrin		45,35

LAMPIRAN 5

(LANJUTAN)

Tabel V.4

Hasil *Screening* Farmakofor *Vascular Endothelia Growth Factor Receptor-2 kinase*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	BIBF 1120 (ligan pembanding)		-
2.	4-hydroxy-3-methoxyaceptophenone		42,33
3.	Genistein		35,18

Tabel V.5

Hasil *Screening* Farmakofor Reseptor *Leukotriene A4 hydrolase*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	sc57461a (Ligan Alami)		-
2.	Bestatin (Ligan Pembanding)		35,12
3.	4-hydroxy-3-methoxyaceptophenone		37,87

Keterangan :

Warna biru = Cincin aromatic

Warna kuning = Ikatan hidrofobik

Warna merah = Akseptor ikatan hydrogen

Warna hijau = Donor ikatan hydrogen

LAMPIRAN 6

HASIL PREDIKSI *DRUG LIKENESS* MENURUT ATURAN *LIPINSKI'S RULE OF FIVE*

Tabel V.6

Hasil Prediksi *Drug Likeness* Senyawa Daun Awar-awar (*Ficus septica* Burm. L) menurut aturan *Lipinski's Rule of Five*

No	Ligan	BM	Log P	Ikatan Hidrogen		Memenuhi syarat/tidak
				D	A	
1	1-triacontanol	438	14,58	1	1	Memenuhi syarat
2	3,4,5-trimethoxyacetophenone	210	1,08	0	4	Memenuhi syarat
3	4-hydroxy-3-methoxyacetophenone	166	1,28	3	1	Memenuhi syarat
4	α-Amyrin	426	10,66	1	1	Memenuhi syarat
5	β-Amyrin	426	10,66	1	1	Memenuhi syarat
6	β-Stigmasterol	412	9,96	1	1	Memenuhi syarat
7	Coumarin	146	1,41	0	1	Memenuhi syarat
8	Dehydroantofine	360	0,55	0	3	Memenuhi syarat
9	Deydrotylophorine	350	0,18	0	4	Memenuhi syarat
10	Ficuseptine A	455	3,24	1	7	Memenuhi syarat
11	Genistein	432	0,91	6	10	Memenuhi syarat
12	Kaempferitrin	578	-0,15	0	4	Memenuhi syarat
13	Myristic acid	220	6,15	1	1	Memenuhi syarat
14	Palmitic acid	256	7,21	1	1	Memenuhi syarat
15	Phenanthroindolizidine	273	4,96	0	1	Memenuhi syarat

LAMPIRAN 6

(LANJUTAN)

Tabel V.6

(lanjutan)

No	Ligan	BM	Log P	Ikatan Hidrogen		Memenuhi syarat/tidak
				D	A	
16	Sigmasterol	413	9,96	1	1	Memenuhi syarat
17	Tylophorine	393	4,21	0	5	Memenuhi syarat

Keterangan: BM (Berat molekul) <500 Dalton**,** Log P <5, Donor ikatan hidrogen <5 dan Akseptor ikatan hidrogen <10.

LAMPIRAN 7

VALIDASI METODE PENAMBATAN MOLEKUL

Tabel V.7

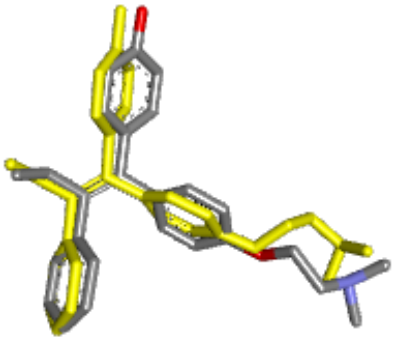
Hasil Validasi Metode Penambatan Molekul

No.	Reseptor	RMSD	Grid Box
1.	ER-α (3ERT)	1,162 Å	X : 30,282 Y : -1,913 Z : 24,207
2.	ER-β (1QKM)	0,481 Å	X : 28, 438 Y : 8,003 Z : 113,539
3.	MAP3K7/TAK1 (5V5N)	0,842 Å	X : -14,81 Y : -48,766 Z : -16,291
4.	VEGFR-2 kinase (3C7Q)	0,977 Å	X : 20,187 Y : 67,208 Z : 29,806
5.	Leukotrien A4 Hidrolase (3U9W)	1,180 Å	X : 29,679 Y : 1,546 Z: 1,893

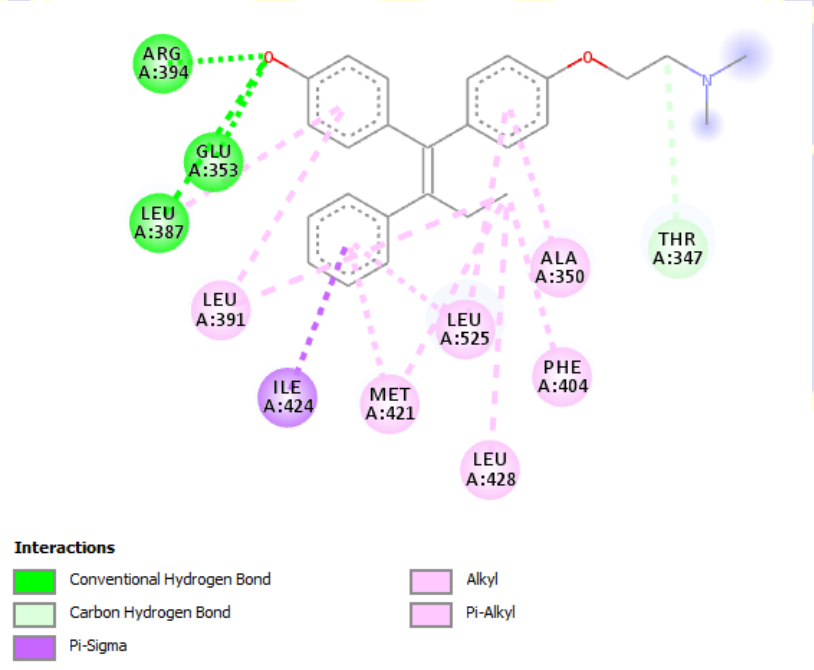
Keterangan: Nilai RMSD < 2 Å

LAMPIRAN 7

(LANJUTAN)



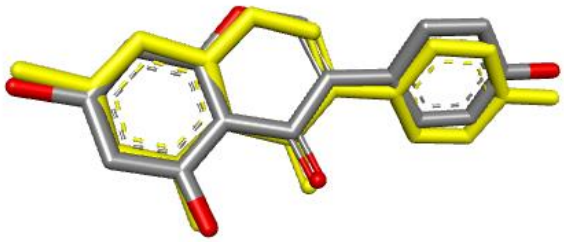
Gambar V.9 Visualisasi tumpang tindih ligan alami 3ERT (merah-abu-biru) dengan ligan hasil *redocking* (kuning)



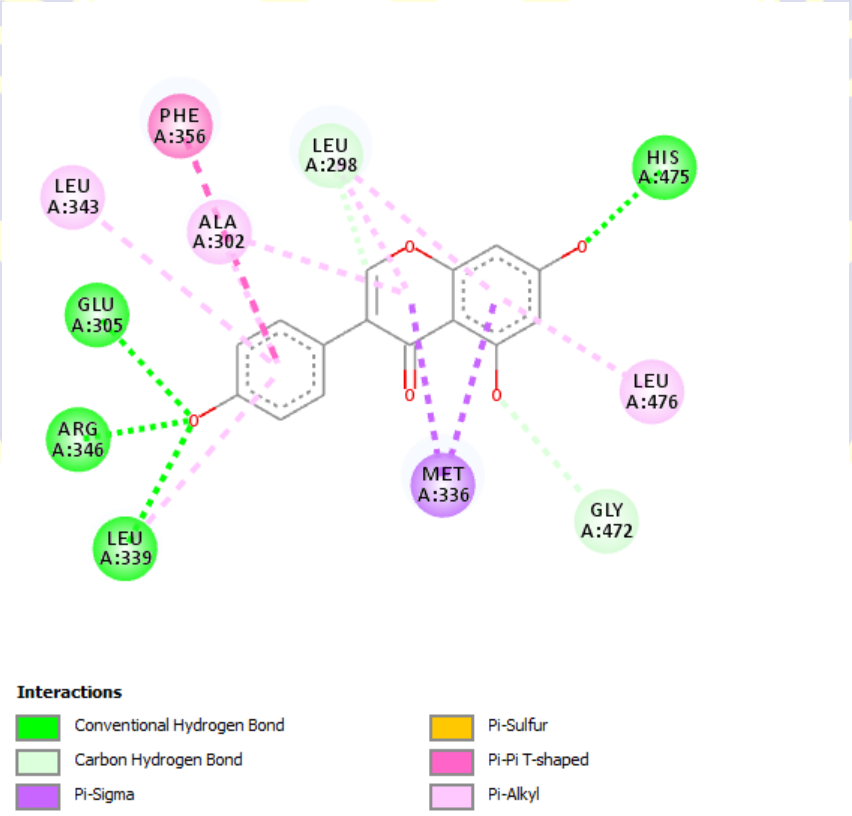
Gambar V.10 Interaksi ligan alami dengan residu-residu asam amino pada *estrogen receptor – alfa*

LAMPIRAN 7

(LANJUTAN)



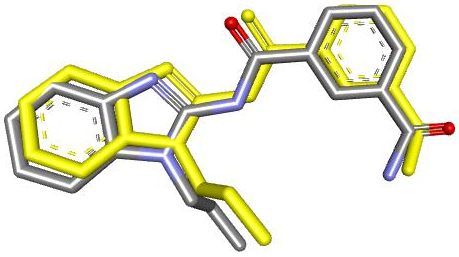
Gambar V.11 Visualisasi tumpang tindih ligan alami 1QKM (merah-abu) dengan ligan hasil *redocking* (kuning)



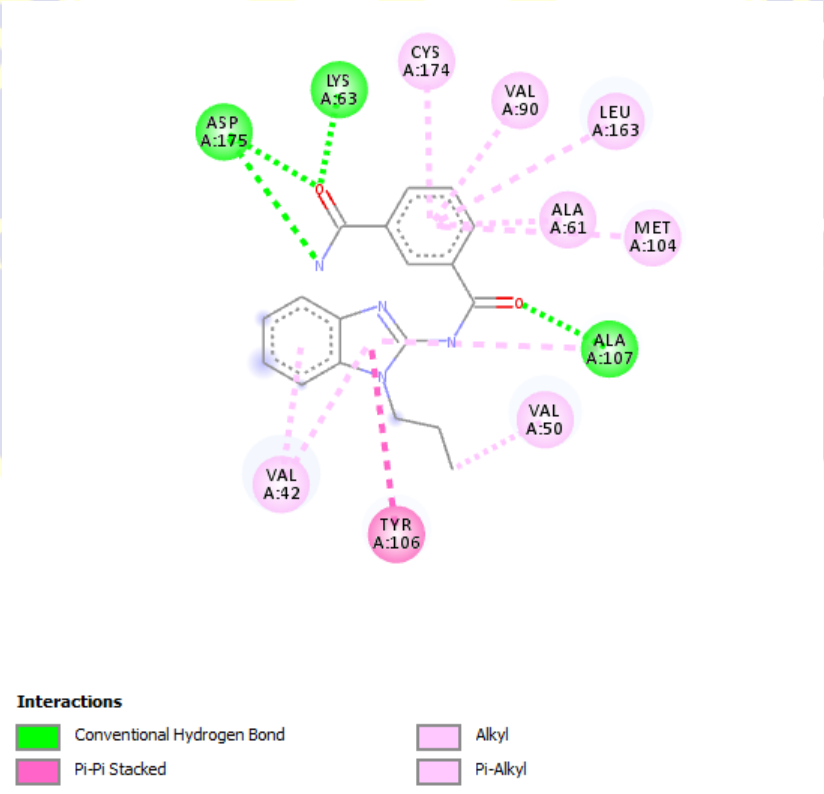
Gambar V.12 Interaksi ligan alami dengan residu-residu asam amino pada *estrogen receptor - beta*

LAMPIRAN 7

(LANJUTAN)



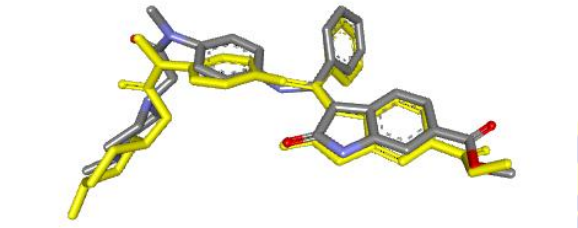
Gambar V.13 Visualisasi tumpang tindih ligan alami 5V5N (merah-abu-biru) dengan ligan hasil *redocking* (kuning)



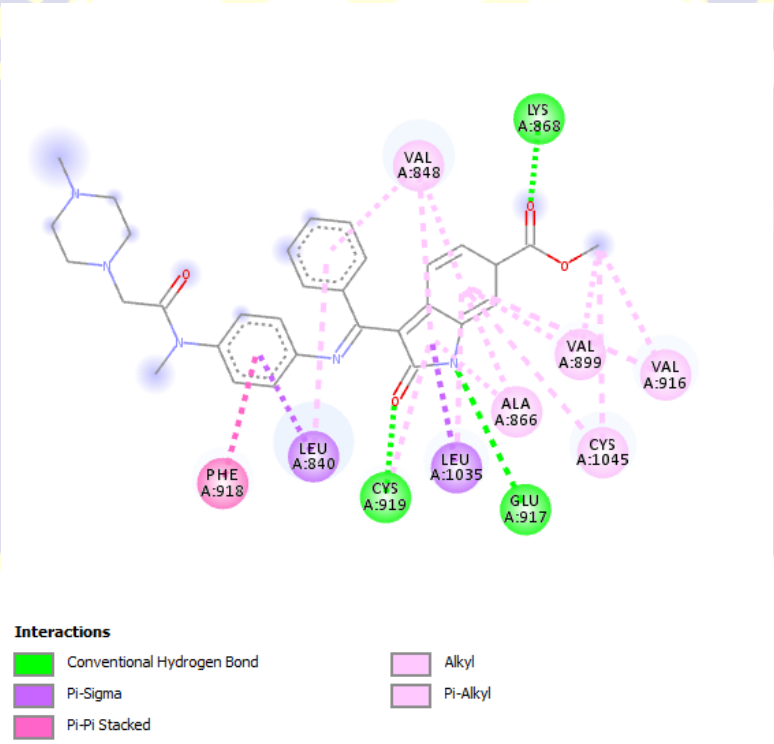
Gambar V.14 Interaksi ligan alami dengan residu-residu asam amino pada *mitogen-activated protein kinase kinase 7*

LAMPIRAN 7

(LANJUTAN)



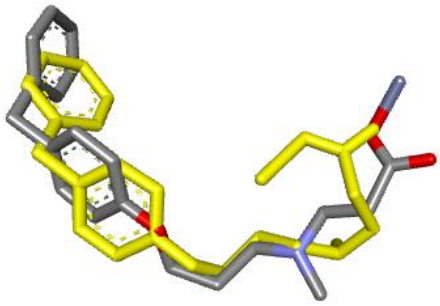
Gambar V.15 Visualisasi tumpang tindih ligan alami 3C7Q (merah-abu-biru) dengan ligan hasil *redocking* (kuning)



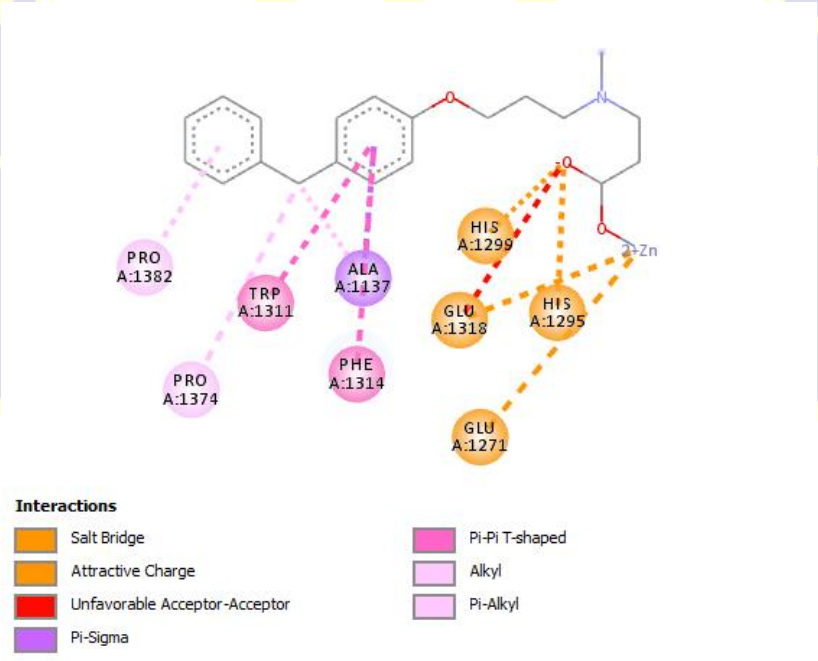
Gambar V.16 Interaksi ligan alami dengan residu-residu asam amino pada *vascular endothelia growth factor* (VEGFR) kinase

LAMPIRAN 7

(LANJUTAN)



Gambar V.17 Visualisasi tumpang tindih ligan alami 3U9W (merah-abu-biru) dengan ligan hasil *redocking* (kuningp)



Gambar V.18 Interaksi ligan alami dengan residu-residu asam amino pada *leukotriene A4 hydrolase*

LAMPIRAN 8

HASIL PENAMBATAN MOLEKUL

Tabel V.8

Hasil Penambatan Molekul Senyawa Uji pada *Estrogen Receptor - Alfa*

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
1.	**Tamoxifen (Pembanding)**	**-11,71**	**2,60**	**ARG 394A, GLU 353A, LEU 387A, THR 347A**	**LEU391A, LEU438A, PHE404A, ILE 424A, ALA 350A, LEU 525A, MET 421A**
2.	1-triacontanol	-6,70	12,22 x 10^3	GLU 353A, LEU 387A	ALA 350A, LEU 354A, TRP 383A, LEU 387A
3.	3,4,5-trimethoxyacetophenone	-4,93	241,36 x 10^3	THR 347A, HIS 524A	MET 343A, LEU 346A, MET 421A
4.	4-hydroxy-3-methoxyacetophenone	-5,23	147,26 x10^3	GLU 353A, ARG 394A, LEU 346A	LEU 391A, LEU 387A
5.	α-Amyrin	-7,30	4,47 x 10^3	LEU 384A, LEU 346A, MET 343A, TRP 383A	LEU 525A, MET 528A, TRP 383A, LEU 525A, ALA 350A
6.	β-Amyrin	-8,34	765,70	LEU 428A, LEU 391A, MET 388A, LEU 384A, TRP 383A	LEU 346A, MET 343A, LEU 525A, ALA 350A
7.	β-Stigmasterol	-10,96	9,23	LEU 349A, PHE 404A, ALA 350A, LEU 346A, LEU 387A, LEU 391A	TRP 383A, LEU 387A, LEU 525A, MET 343A
8.	Coumarin	-5,51	91,76 x 10^3	ARG 394A	LEU 387A, LEU 391A, LEU 346A, MET 388A, MET 421A

LAMPIRAN 8

(LANJUTAN)

Tabel V.8

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
9.	Dehydroantofine	-9,34	141,94	GLY 521A, ASP 351A	LEU 525A, MET 343A, ALA 350A, LEU 349A, LEU 391A, PHE 404A, LEU 346A
10.	Deydrotylophorine	-7,62	2,61 x 10^3	GLU 353A, LEU 346A, ASP 351A	LEU 525A, ALA 350A, LEU 346A, MET 343A, ILE 424A, MET 421A, HIS 524A
11.	Ficuseptine A	-7,86	1,74 x 10^3	THR 347A, MET 343A, ALA 350A, ASP 351A	LEU 525A, ALA 350A, THR 347A,
12.	Genistein	-7,19	5,34 x 10^3	ARG 346A, GLU 305A, LEU 387A, LEU 346A, THR 347A	ALA 350A, LEU 525A, LEU 346A
13.	Kaempferitrin	-9,43	123,08	GLU 419A, LEU 346A, ASP 351A	LEU 525A, LEU 346A, LEU 387A, ALA 350A
14.	Myristic acid	-4,80	301,56 x 10^3	PHE 404A	ALA 350A, LEU 346A
15.	Palmitic acid	-5,16	165,57 x 10^3	THR 347A	MET 421A, LEU 346A
16.	Phenanthroindolizidine	-9,71	76,48	LEU 387A	MET 388A, LEU 391A, PHE 404A, LEU 346A, MET 421A, ILE 424A, LEU 525A, LEU 384A

LAMPIRAN 8

(LANJUTAN)

Tabel V.8

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
17.	Sigmasterol	-11,74	2,48	ASP 351A	LEU 349A, MET 343A, LEU 391A, LEU 525A, PHE 404A, MET 421A, LEU 346A, LEU 384A, LEU 387A, ALA 350A
18.	Tylophorine	-8,47	622,77	ASP 351A, GLU 353A	MET 421A, ILE 424A, HIS 524A, LEU 525A, MET 343A, LEU 346A, ALA 350A

LAMPIRAN 8

(LANJUTAN)

Tabel V.9

Hasil Penambatan Molekul Senyawa Uji pada *Estrogen Receptor – Beta*

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
1.	**Genistein (Pembanding)**	**-10,25**	**30,60**	**GLU 305A, ARG 346A, LEU 339A, HIS 475A, GLY 472A, LEU 298A**	**LEU 476A, MET 336, ALA 302A, LEU 343A, PHE 356A**
2.	1-triacontanol	-2,93	7,15 x 10^6	-	ALA 302A, LEU 339A, LEU 301A
3.	3,4,5-trimethoxyacetophenone	-6,11	33,09 x 10^3	HIS 475A	LEU 476A, LEU 298A, MET 3336A
4.	4-hydroxy-3-methoxyacetophenone	-5,71	65,34 x 10^3	GLU 305A, ARG 346A, LEU 298A	LEU 343A, MET 340A, LEU 399A, PHE 356A
5.	α-Amyrin	+20,13	-	GLY 472A	MET 295A, LEU 476A, ILE 373A, HIS 475A, ILE 376A, LEU 298A, PHE 356A, MET 336A, MET 340A, LEU 339A
6.	β-Amyrin	+17,62	-	GLY 472A	LEU 476A, HIS 475A, MET 295A, ILE 373A, LEU 298A, MET 336A, MET 340A, LEU 339A, LEU 343A, PHE 356A
7.	β-Stigmasterol	-10,12	37,97	MET 479A, LEU 476A, MET 295A, ILE 376A, ILE 373A	MET 340A, MET 336A, ALA 302A, LEU 343A, PHE 356A
8.	Coumarin	-5,95	43,70 x 10^3	ARG 346A	LEU 343A, PHE 356A

LAMPIRAN 8

(LANJUTAN)

Tabel V.9

(Lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
9.	Dehydroantofine	-9,08	221,62	ILE 373A	LEU 476A, ALA 302A, LEU 298A, ILE 376A, MET 340A, PHE 356A, LEU 339A, LEU 343A, MET 336
10.	Deydrotylophorine	-5,55	85,16 x 10^3	-	MET 336A, ALA 302A, LEU 476A, LEU 298A, PHE 336A, ALA 302A, LEU 339A, MET 340A, PHE 356A, LEU 343A, ILE 376A
11.	Ficuseptine A	-3,83	1,55 x 10^6	MET 336A, ILE 373A, LEU 339A, GLY 472A	ILE 376A, MET 340A, ALA 302A, LEU 476A
12.	Genistein	+2,17	-	GLY 472A, ARG 346A, GLU 305A	LEU 298A, LEU 380A, ALA 302A, LEU 343A
13.	Kaempferitrin	+11,67	-	ILE 373A, GLY 472A, GLU 305A	HIS 475A, ILE 376A, LEU 298A, LEU 380A, ALA 302A, LEU 343A
14.	Myristic acid	-6,10	34,01 x 10^3	ARG 346A, GLU 305A	ILE 376A
15.	Palmitic acid	-6,38	20,97 x 10^3	HIS 475A, GLY 472A	ALA 302A, LEU 298A
16.	Phenanthroindolizidine	-11,28	5,43	-	LEU 343A, PHE 356A, LEU 298A, LEU 301A, ALA 302A, LEU 476A, MET 336A, LEU 339A, MET 340A

LAMPIRAN 8

(LANJUTAN)

Tabel V.9

(Lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
17.	Sigmasterol	-8,11	1,13 x 10^3	LEU 339A	VAL 484A, MET 479A, LEU 476A, HIS 475A, MET 295A, ILE 373A, LEU 298A, PHE 356A, MET 340A, LEU 380A, LEU 343A, LEU 339A, MET 336A
18.	Tylophorine	-5,82	54,52 x 10^3	ILE 373A	LEU 298A, LEU 476A, MET 336A, ALA 302A, MET 340A, LEU 339A

LAMPIRAN 18

(LANJUTAN)

Tabel V.10

Hasil Penambatan Molekul Senyawa Uji pada *Mitogen-Activated Protein Kinase Kinase Kinase 7*

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
1.	**Takinib (Pembanding)**	**-8,05**	**1,26 x 10^3**	**ASP 175A, LYS 63A, ALA 107A**	**TYR 106A, VAL 42A, VAL 90A, ALA 107A, LEU 163A, CYA 174A, MET 104A**
2.	1-triacontanol	-3,76	1,75 x 10^6	GLU 108A, TRY 106A	-
3.	3,4,5-trimethoxyacetophenone	-4,85	278,97 x 10^3	ALA 107A	ALA 61A, CYS 174A, LEU 163A
4.	4-hydroxy-3-methoxyacetophenone	-4,87	270,98 x 10^3	ALA 107A, ASP 175A	VAL 50A, VAL 90A, LEU 163A, MET 104A, CYS 174A
5.	α-Amyrin	-9,58	94,26	-	MET 104A, LYS 63A, VAL 50A, ALA 61A, CYS 174A, LEU 163A, VAL 42A, PRO 160A
6.	β-Amyrin	-9,65	85,86	-	VAL 42A, VAL 50A, LEU 163A, ALA 107A, MET 104A, LYS 63A, LYS 174A, PRO160A
7.	β-Stigmasterol	-9,57	95,89	-	VAL 42A, VAL 50A, LEU 163A, ALA 61A, MET 104A, LYS63A, VAL 90A, ALA 107A
8.	Coumarin	-5,33	122,97 x 10^3	ASP 175A, LYS 63A	MET 104A, VAL 50A, ALA 61A, ALA 107A, LEU 163A, VAL 90A, CYS 174A

LAMPIRAN 8

(LANJUTAN)

Tabel V.10

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
9.	Dehydroantofine	-8,57	522,21	LYS 63A, ARG 44A, GLU 77A	VAL 50A, CYS 174A, LEU 163A, ALA 107A, TYR 106A
10.	Deydrotylophorine	-8,53	563,39	LYS 63A, GLU 77A, GLU 105A, GLY 110A, ASN 161A, ASP 175A	PRO 160A, CYS 174A, LEU 163A, VAL 50A, LEU 163A, ALA 107A
11.	Ficuseptine A	-8,59	501,44	TRY 106A, ASP 175A, PRO 160A, GLY 110A	VAL 42A, VAL 50A, LEU 163A, ALA 107A, TYR 106A
12.	Genistein	-7,86	1,74 x 10^3	GLU 105A, ALA 107A	ALA 61A, LEU 163A, VAL 42A, VAL 50A, TYR 106A, VAL 90A,
13.	Kaempferitrin	-6,82	10,04 x 10^3	MET 104A, ARG 44A,	VAL 42A, LEU 163A, VAL 50A, CYS 174A, LYS 63A, MET 104A
14.	Myristic acid	-4,11	967,06 x 10^3	MET 104A, ASP 175A, LYS 63A	LEU 163A, ALA 61A, ALA 107A
15.	Palmitic acid	-4,61	417,48 x 10^3	ALA 107A, GLU 105A	ALA 61A, MET 104A, VAL 50A
16.	Phenanthroindolizidine	-7,91	1,61 x 10^3	ALA 107A	VAL 42A, TYR 106A, ALA 107A, VAL 90A, MET 104A, VAL 50A, LEU 163A, ALA 161A

LAMPIRAN 8

(LANJUTAN)

Tabel V.10

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
17.	Sigmasterol	-9,68	80,50	-	ALA 107A, ALA 61A, TYR 106A, LEU 163A, VAL 50A, CYS 174A, LYS 63A, MET 104A, VAL 90A
18.	Tylophorine	-8,77	371,85	LYS 63A, GLU 77A, PRO 160A	TYR 106A, VAL 42A, VAL 50A, CYS 174A, LEU 163A, GLY 45A

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(LANJUTAN)

Tabel V.11

Hasil Penambatan Molekul Senyawa Uji pada Reseptor *Vascular Endothelia Growth Factor Receptor-2 kinase* (VEGFR-2 *kinase*)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
1.	**BIBF 1120 (Pembanding)**	**-10,54**	**18,76**	**LYS 868A, CYS 919A, LEU 840A, GLU 917A**	**PHE 918A, ALA 866A, VAL 848A, VAL 899A, CYS 1045A, VAL 916A**
2.	1-triacontanol	-2,85	8,21 x 10^6	ARG 1032A	VAL 848A, VAL 866A, VAL 916A
3.	3,4,5-trimethoxyacetophenone	-4,61	415,95 x 10^3	CYS 919A, PHE 918A, LYS 920A, GLY 922A	CYS 919A, LEU 840A
4.	4-hydroxy-3-methoxyacetophenone	-4,30	701,96 x 10^3	GLU 917A, CYS 919A,	VAL 848A, LEU 1035A, LEU 840A
5.	α-Amyrin	-8,93	286,83	-	VAL 848A, LEU 840A, ALA 866A, VAL 916A, VAL 899A, LEU 1035A, PHE 918A, CYS 919A
6.	β-Amyrin	-8,77	375,03	-	ARG 1032A, LEU 1035A, VAL 916A, ALA 866A, CYS 919A, VAL 848A, LEU 840A
7.	β-Stigmasterol	-10,89	10,42 x 10^3	-	PHE 918A, LEU 840A, ALA 848A, LEU 1035A, CYS 1045A, PHE 1047A, LYS 868A
8.	Coumarin	-5,27	137,98 x 10^3	-	LEU 840A, ALA 866A, LEU 1035

LAMPIRAN 8

(LANJUTAN)

Tabel V.11

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
9.	Dehydroantofine	-7,92	1,56 x 10^3	ASN 923A, CYS 920A	LEU 840A, ALA 866A, LEU 1035A, VAL 848A, CYS 1045A, VAL 916A
10.	Deydrotylophorine	-7,96	1,46 x 10^3	ASN 923A, ARG 1032A	LEU 1035A, ALA 866A, LEU 840A, PHE 918A
11.	Ficuseptine A	-7,80	1,90 x 10^3	CYS 919A, LYS 920A, PHE 921A, ARG 1032A	LEU 840A
12.	Genistein	-7,46	3,42 x 10^3	LYS 920A, CYS 919A, LYS 868A, PHE 1047A	LEU 1035A, LEU 840A, ALA 866A, VAL 848A
13.	Kaempferitrin	-7,20	5,26 x 10^3	GLU 917A, ASN 923A,	LYS 838A, LEU 840A, ALA 866A, LEU 1035A
14.	Myristic acid	-4,68	369,26 x 10^3	LYS 868A, CYS 1045A, PHE 1047A,	VAL 899A, VAL 916A, VAL 848A
15.	Palmitic acid	-4,74	337,53 x 10^3	ASN 923A	VAL 848A
16.	Phenanthroindolizidine	-7,61	2,62 x 10^3	-	VAL 916A, VAL 899A, CYS 1045A, VAL 848A, LEU 1035A , ALA 866A, CYS 919A, LEU 840A

LAMPIRAN 8

(LANJUTAN)

Tabel V.11

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
17.	Sigmasterol	-10,93	9,67	CYS 919A	PHE 1047A, CYS 1045A, VAL 848A, LEU 840A
18.	Tylophorine	-7,47	3,35 x 10^3	CYS 919A, ARG 1032A, GLU 917A	VAL 848A, PHE 1047A, LEU 840A, CYS 1045A, LEU 1035A

LAMPIRAN 8

(LANJUTAN)

Tabel V.12

Hasil Penambatan Molekul Senyawa Uji pada Reseptor *Leukotriene A4 hydrolase*

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
1.	**sc5746A (Ligan Alami)**	**-12,7**	**0,49183**	-	**TRP 1311A, PRO 1374A, ALA 1137A, PHE 1314A, PRO 1382A, GLU 1271A, GLU 1318A**
2.	**Bestatin (Ligan Pembanding)**	**-10,02**	**45,41**	**PRO 1374A, ASP 1375A, GLN 1136A, TRP 1311A, TYR 1267A**	**ALA 1377A, VAL 1367A, PRO 1382A, MET 1270A**
3.	1-triacontanol	+2,89	-	GLY 1269A,	PHE 1314A, VAL 1367A
4.	3,4,5-trimethoxyacetophenone	-5,61		TYR 1378A, ALA 1137A, ASP 1375A	TYR 1267A, PHE 1314A, ALA 1137A
5.	4-hydroxy-3-methoxyacetophenone	-5,60	77,65 x 10^6	LEU 1365A, ASP 312A	PRO 1382A, VAL 1367A
6.	α-Amyrin	+9A,18	-	TRP 1311A	LEU 1369A, ALA 1137A, PRO 1374A, PHE 1314A, TYR1378A, TYR 1383A, TYR 1267A, MET 1270A
7.	β-Amyrin	+43,66	-	TRP 1311A	ALA 1137A, LEU 1369A, PRO 1374A, PHE 1314A, TYR1378A, TYR 1267A, MET 1270A

LAMPIRAN 8

(LANJUTAN)

Tabel V.12

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
8.	β-Stigmasterol	-9,20	181,34	GLU 1271A, HIS 1299A, HIS 1295A, ALA 1377A, LEU 1379A, TRP 1311A	ALA 1137A, PHE 1314A, TYR 1378A, TYR 1267A, MET 1270A
9.	Coumarin	-6,27	25,15 x 10^6	PHE 1314A, TRP 1315A	ALA 1377A, VAL 1367A, PRO 1382A, PHE 1314A
10.	Dehydroantofine	-1,63	64,06 x 10^9	PRO 1374A, ASP 1373A,	MET 1270A, TYR 1267A, TYR 1378A, ALA 1137A, PHE 1314A, PRO 1374A, ASP 1375A
11.	Deydrotylophorine	+3,14	-	GLN 1136A, GLY 1269A, TRP 1311A, PRO 1374A, GLU 1271A	ALA 1137A, TYR 1267A, TYR 1378A, LEU 1602A, MET 1564A
12.	Ficuseptine A	+0,21	-	GLN 1136A, GLU 1271A, TRP 1311A, TRP1267A, PRO 1374A	ALA 1137A, TYR 1378A, TYR 1267A
13.	Genistein	-10,95	9,38	GLY 1269A, TRP 1311A, ALA 1137A	TYR 1378A, TYR 1267A, MET 1270A, TRP 1311A, PRO 11374A

LAMPIRAN 8

(LANJUTAN)

Tabel V.12

(lanjutan)

No.	Nama Senyawa	ΔG kkal/ mol	KI (nM)	Interaksi Residu Asam Amino	
				Ikatan Hidrogen	Ikatan Hidrofobik
14.	Kaempferitrin	+10,37	-	GLN 1134A, MET 1270A, GLU 1271A, GLU 1296A, HIS 1295A, GLN 1136A, ASP 1375A, PRO 1374A	TRY 1267A, TYR 1378A, ALA 1137A, PHE 1374A, VAL 1367A, LEU 1369A, TYR 1383A, GLU 1318A
15.	Myristic acid	-5,68	68,89 x 10^3	TRP 1311A	TYR 1378A, TYR 1267A, MET 1270A
16.	Palmitic acid	-7,10	6,24 x 10^6	GLN 1134A, GLN 1136A	VAL 1367A, PRO 1382A
17.	Phenanthroindolizidine	-10,21	32,71	TRY 1267A	VAL 1367A, LEU 1369A, ALA 1137A, PHE 1314A, TYR 1378A, TYR 1267A
18.	Sigmasterol	-9,99	47,20	GLU 1296A, LEU 1369A	PRO 1374A, TRP 1311A, ALA 1137A, PHE 1314A, TYR 1378A, TYR 1267A, PRO 1382A, MET 1270A
19.	Tylophorine	-0,05	924,15 x 10^9	GLN 1136A, GLU 1271A, PRO 1374A, TRP 1311A	PHE 1314A, ALA 1137A, TYR 1378A, TYR 1267A, LEU 1602A

LAMPIRAN 9

HASIL PREDIKSI PROFIL ABSORBSI DAN PROFIL DISTRIBUSI DARI SENYAWA DAUN AWAR-AWAR (*Ficus septica* Burm. L)

Tabel V.13

Hasil Prediksi Profil Absorbsi dan Profil Distribusi dari Senyawa Daun Awar-awar (*Ficus septica* Burm. L)

No	Nama Ligan	Absorbsi		Distribusi
		CaCo-2 (nm. Sec-1)	HIA (%)	PBB (%)
1.	1-triacontanol	51,34	100,00	100,00
2.	3,4,5-trimethoxyacetophenone	53,72	97,51	81,41
3.	4-hydroxy-3-methoxyacetophenone	18,06	93,54	73,51
4.	α-Amyrin	45,28	100,00	100,00
5.	β-Amyrin	46,75	100,00	100,00
6.	β-Stigmasterol	52,34	100,00	100,00
7.	Coumarin	32,12	100,00	43,40
8.	Dehydroantofine	49,21	96,87	44,63
9.	Deydrotylophorine	57,57	98,35	49,96
10.	Ficuseptine A	41,73	97,35	45,92
11.	Genistein	8,20	42,26	39,71
12.	Kaempferitrin	5,18	13,77	42,73
13.	Myristic acid	24,07	97,85	100,00

LAMPIRAN 9

(LANJUTAN)

Tabel V.13

(lanjutan)

No	Nama Ligan	Absorbsi		Distribusi
		CaCo-2 (nm. Sec-1)	HIA (%)	PBB (%)
14.	Palmitic acid	26,07	98,30	100,00
15.	Phenanthroindolizidine	34,48	100,00	83,18
16.	Stigmasterol	52,34	100,00	100,00
17.	Tylophorine	57,47	98,11	74,48

Keterangan:

In Vitro CaCo-2 cell permeability (nm. Sec^{-1}): >70 higher permeability; 4-70 medium permeability; <4 low permeability

% Human Intestinal Absorption (%HIA): 70-100% well absorbed, 20-70% moderately absorbed; 0-20% poorly absorbed

% Plasma Protein Binding: >90% strongly bound; <90% weakly bound

LAMPIRAN 10

HASIL PREDIKSI TOKSISITAS SENYAWA DAUN AWAR-AWAR (*Ficus septica* Burm. L)

Tabel V.14

Hasil Prediksi Toksisitas Senyawa Daun Awar-awar (*Ficus septica* Burm. L)

No	Nama Ligan	Cramer rules	Benigni/bosa rulebase	Kroes TTC decision tree
1.	1-triacontanol	1	8,9	1
2.	3,4,5-trimethoxyacetophenone	1	8,9	1
3.	4-hydroxy-3-methoxyacetophenone	1	8,9	1
4.	α-Amyrin	1	8,9	1
5.	β-Amyrin	1	8,9	1
6.	β-Stigmasterol	2	8,9	1
7.	Coumarin	3	8,9	1
8.	Dehydroantofine	3	8,9	1
9.	Deydrotylophorine	3	8,9	1
10.	Ficuseptine A	3	8,9	1
11.	Genistein	3	8,9	1
12.	Kaempferitrin	3	8,9	1
13.	Myristic acid	1	8,9	1
14.	Palmitic acid	1	8,9	1
15.	Phenanthroindolizidine	3	8,9	1
16.	Stigmasterol	2	8,9	1
17.	Tylophorine	3	8,9	1

LAMPIRAN 10

(LANJUTAN)

Tabel V.14

(lanjutan keterangan tabel)

Keterangan:

Cramer rules:

1. *Substances with sample chemical structures and fix which efficient modes of metabolism exist, suggesting a low order of oral toxicity*
2. *Substances which possess structures that are less innocuous than class I substances, but do not contain structural features suggestive of toxicity like those substances in class III*
3. *Substances with chemical structures that permit no strong unitial presumption of safety or may even suggest significant toxicity ir have reactive functional groups*

Benigni/bose rulebase:

8. *Negative for genotoxic carcinogenity*
9. *Negative for non-genotoxic carcinogencity*

Kroes TTC decision tree:

1. *Subtance would not be expected to be a safety concern*

DATA PRIBADI

NAMA : FUJI AYU NOVIARTIKA

Tempat/Tanggal lahir : Indramayu, 10 November 1996

Jenis Kelamin : Perempuan

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Warga Negara : Indonesia

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PENDIDIKAN

Formal

SDN karanganyar III, indramayu 2003-2009

SMP Negeri I Losarang, Indramayu 2009-2012

SMK Farmasi Indramayu, Indramayu 2012-2015

Universitas Garut Prodi S1 Farmasi, Garut 2016-2020

Non Formal

PKL RSUD Bhayangkara Indramayu

PKL Puskesmas Lohbener, Indramayu

PENGALAMAN ORGANISASI

SEKOLAH MENENGAH PERTAMA (SMP)

- Praja Muda Karana (PRAMUKA) (Non Formal)
- Pasukan Pengibar Bendera (PASKIBRA) (Non Formal)

SEKOLAH MENENGAH KEJURUAN (SMK)

- Palang Merah Remaja (PMR) (Non Formal)

UNIVERSITAS

- Lembaga Dakwah Kampus (LDK) (Formal)
  - Sebagai Anggota 2016-1017
  - Sebagai Bendahara 2017-2018

PENGALAMAN KERJA

- Klinik Heri Kandanghaur, Indrmayu (2015 – 2016)