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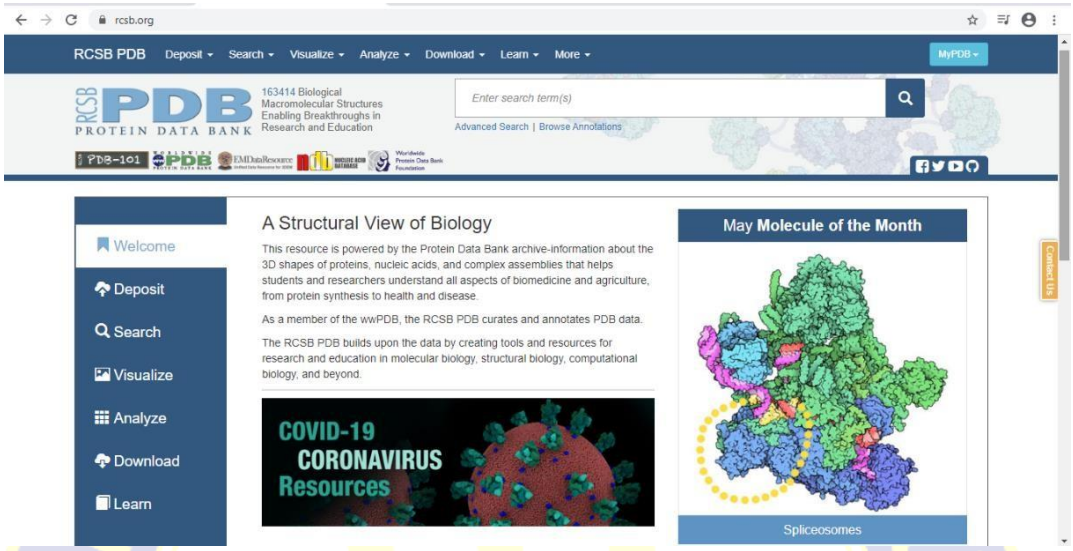
LAMPIRAN 1

ALUR PENELITIAN *SCREENING* FARMAKOFOR DAN PENAMBATAN MOLEKUL

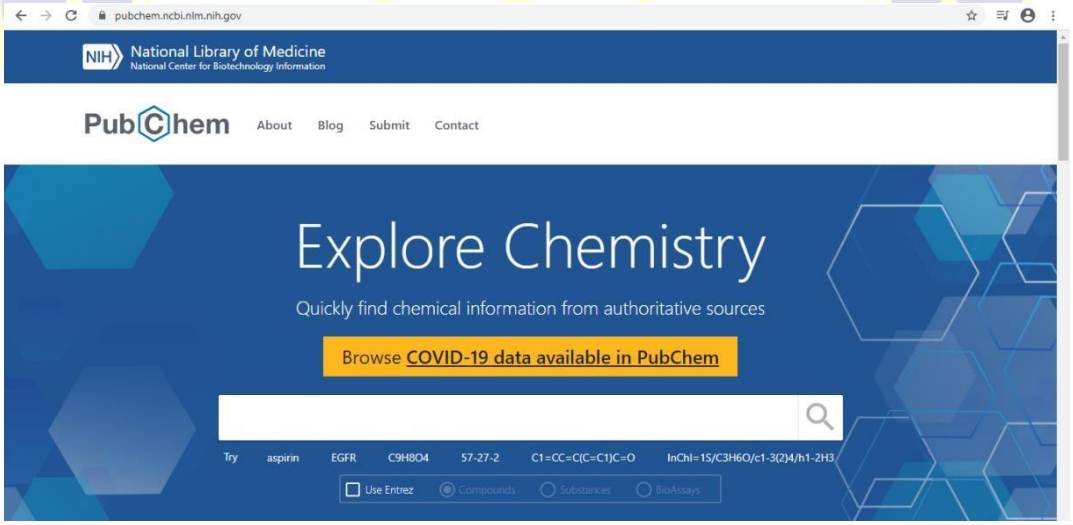
Gambar IV.1 Alur penelitian *screening* farmakofor dan penambatan molekul

LAMPIRAN 2

SITUS DAN APLIKASI



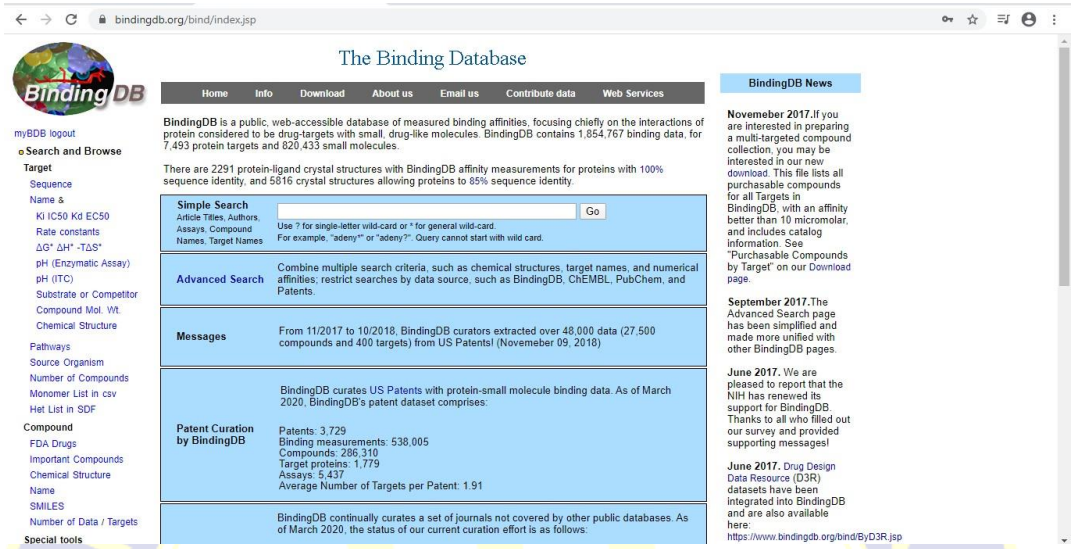
Gambar IV.2 Tampilan situs *Protein Data Bank*



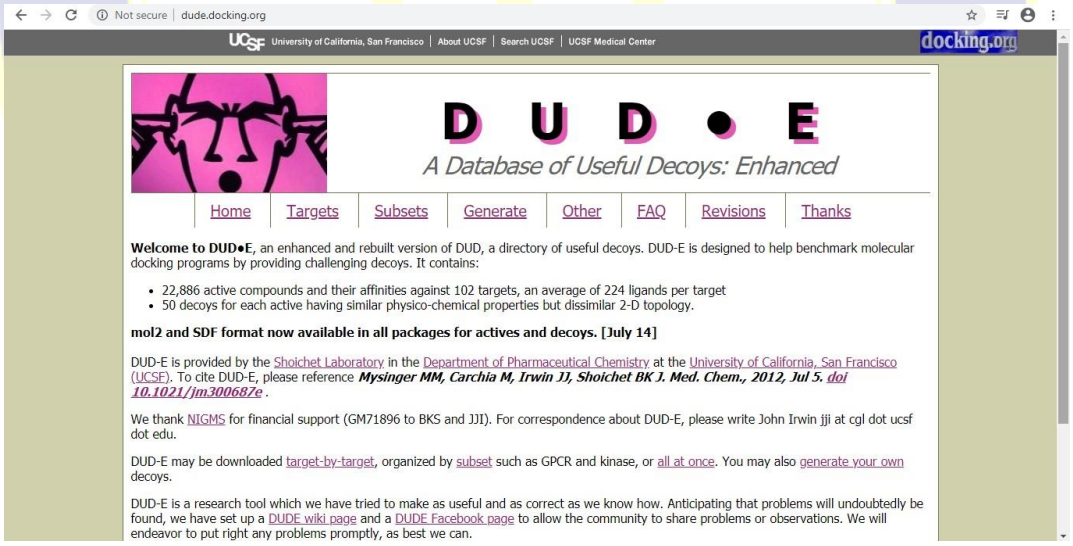
Gambar IV.3 Tampilan situs *PubChem*

LAMPIRAN 2

(LANJUTAN)



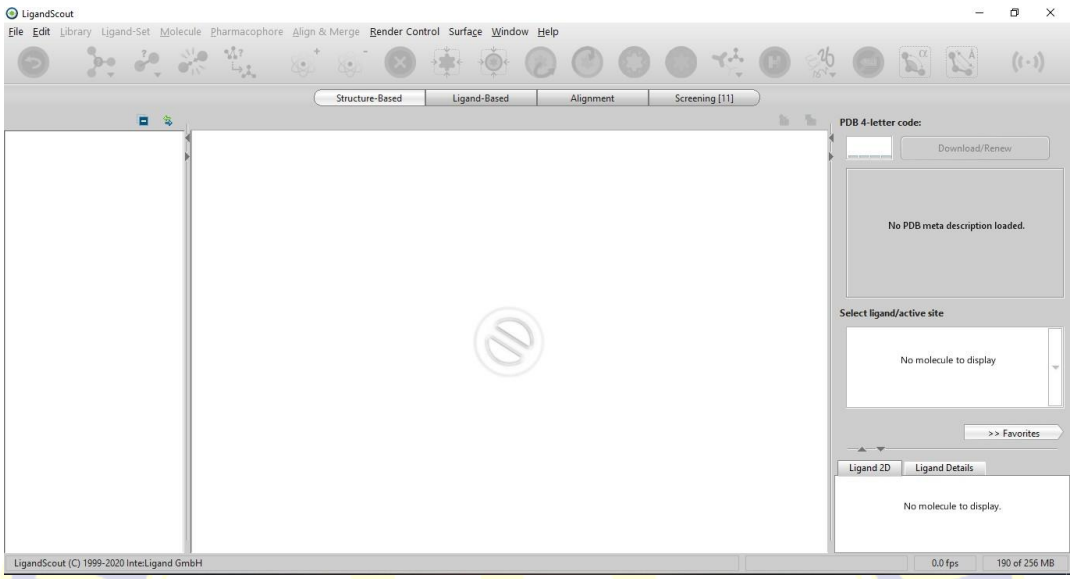
Gambar IV.4 Tampilan situs *Binding Database*



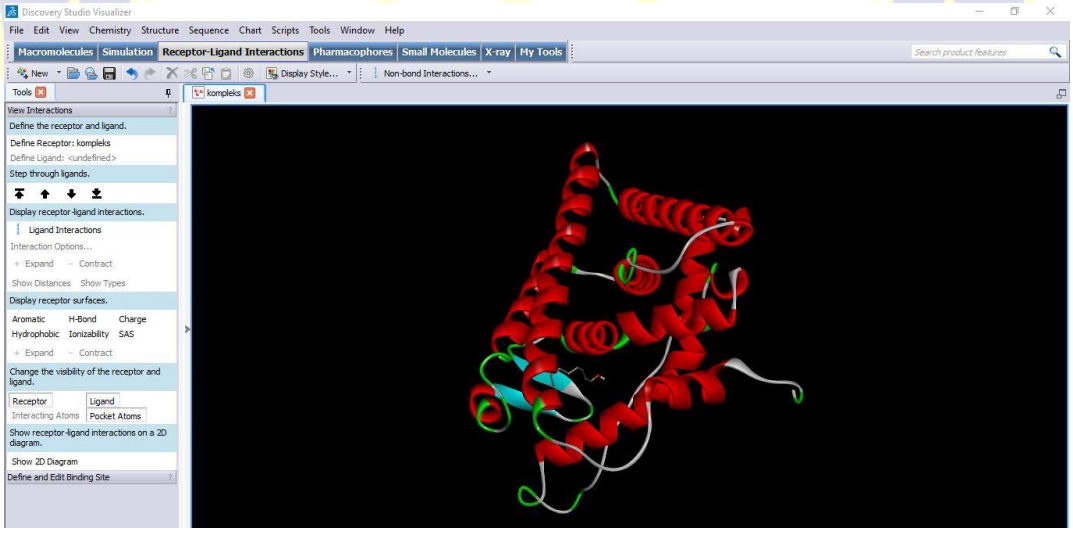
Gambar IV.5 Tampilan situs *DUD-E*

LAMPIRAN 2

(LANJUTAN)



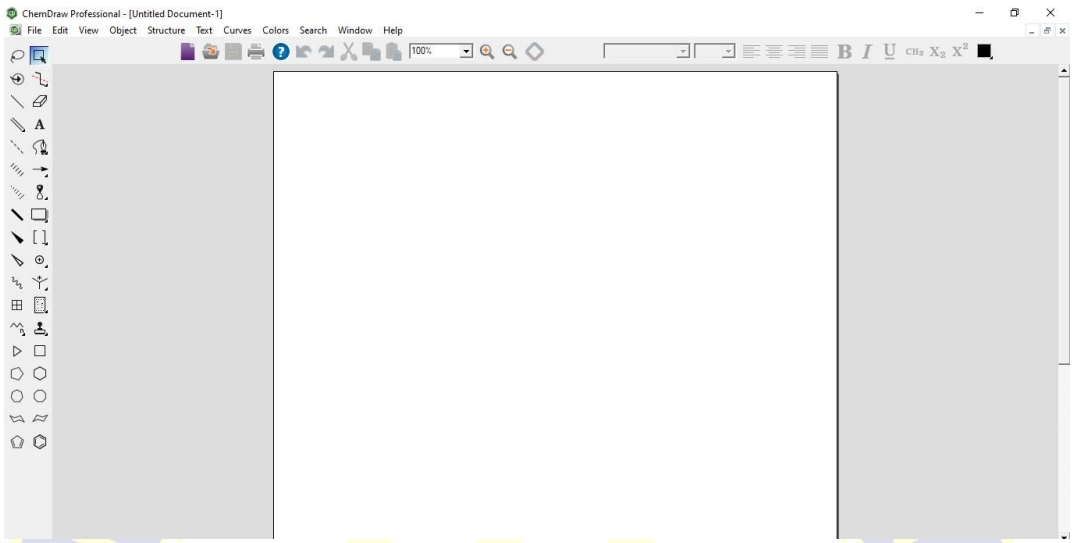
Gambar IV.6 Tampilan aplikasi *LigandScout*®



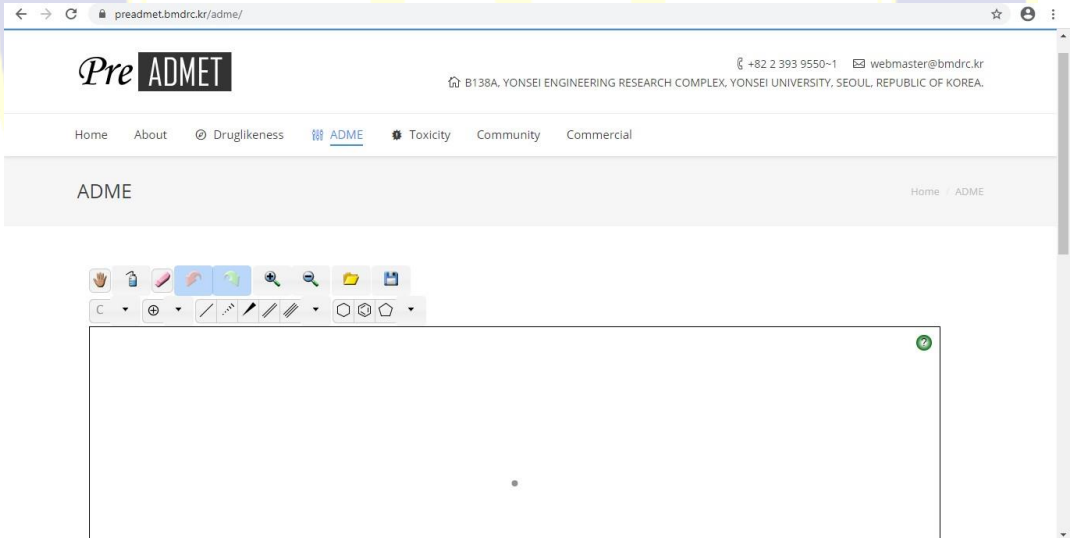
Gambar IV.7 Tampilan aplikasi *Discovery Studio Visualizer*®

LAMPIRAN 2

(LANJUTAN)



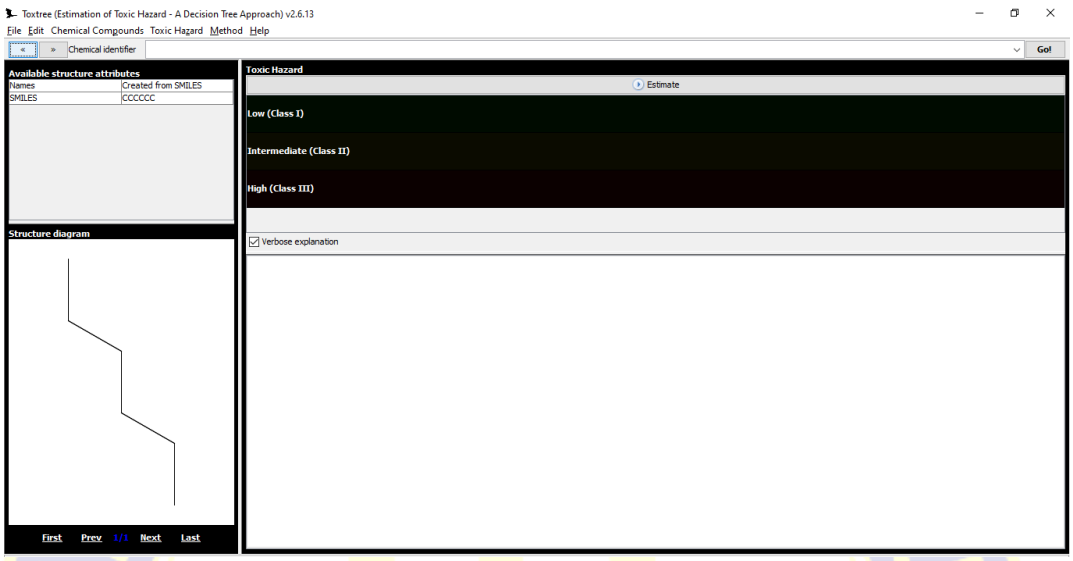
Gambar IV.8 Tampilan aplikasi *ChemDraw Professional 15.0®*



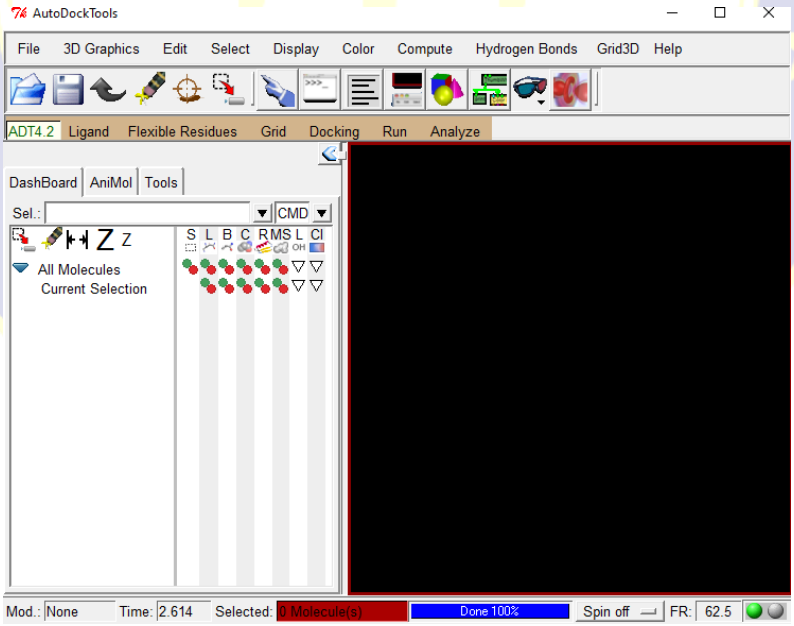
Gambar IV.9 Tampilan situs *PreADMET*

LAMPIRAN 2

(LANJUTAN)



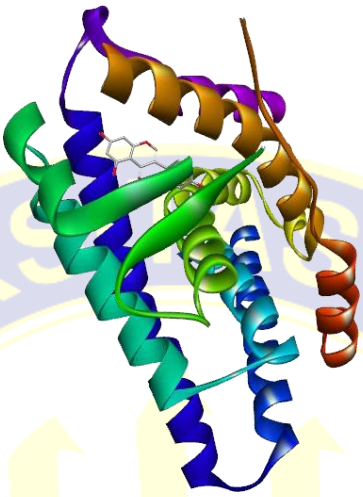
Gambar IV.10 Tampilan aplikasi *Toxtree*®



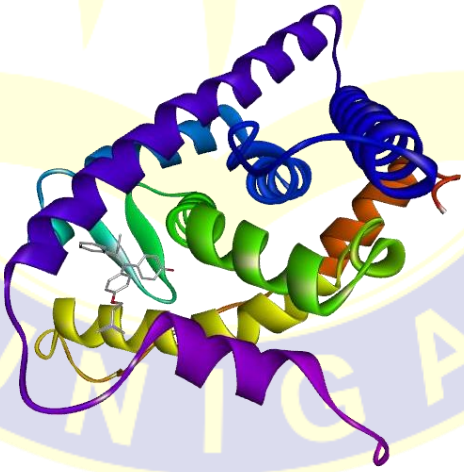
Gambar IV.11 Tampilan aplikasi *AutoDock Tools*®

LAMPIRAN 3

STRUKTUR 3D MAKROMOLEKUL PROTEIN



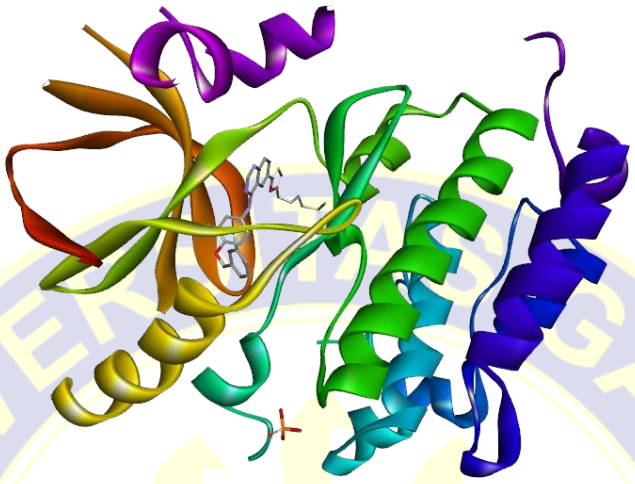
Gambar IV.12 *Estrogen Receptor - Beta* ID 1QKM



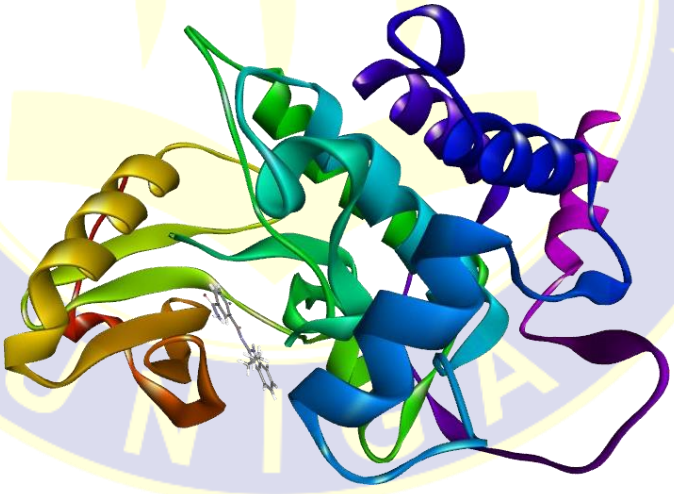
Gambar IV.13 *Estrogen Receptor - Alpha* ID 3ERT

LAMPIRAN 3

(LANJUTAN)



Gambar IV.14 *Epidermal Growth Factor Receptor* ID 1XKK



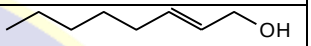
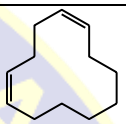
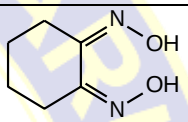
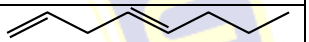
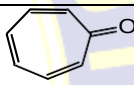
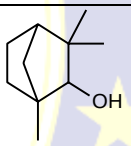
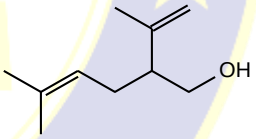
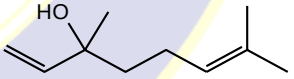
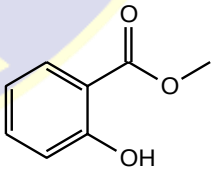
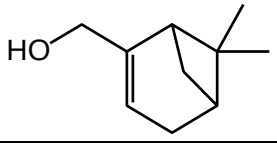
Gambar IV.15 *Mitogen-Activated Protein Kinase Kinase Kinase 7* ID 5V5N

LAMPIRAN 4

STRUKTUR 2D LIGAN UJI

Tabel IV.1

Senyawa Minyak Atsiri Tanaman Jelatang (*Laportea aestuans* (L.) Chew)

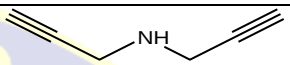
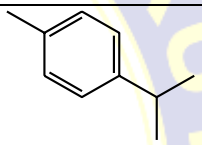
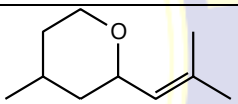
No.	Nama Senyawa	Compound ID	Struktur 2D
1.	*(E)-2-Octen-1-ol*	5318599	
2.	*(E,E)-1,5-Cyclododecadiene*	5364368	
3.	*N-(2-hydroxylminocyclohexylidene) Hydroxylamine*	135492011	
4.	*1,4-Octadiene*	5364369	
5.	*2,4,6-Cycloheptatriene -1-one*	10881	
6.	*1,3,3-trimethylbicyclo[2.2.1] heptan-2-ol*	6997371	
7.	*2-isopropenyl-5-methyl-4 -hexen-1-ol*	94060	
8.	*3,7-dimethylocta-1,6-dien -3-ol*	6549	
9.	*Methyl-2-hydroxybenzoate*	4133	
10.	*(6,6-dimethyl-2-bicyclo[3.1.1] hept-2-enyl)methanol*	10582	

LAMPIRAN 4

(LANJUTAN)

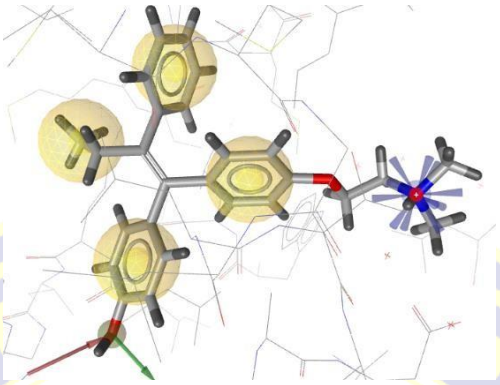
Tabel IV.1

Lanjutan

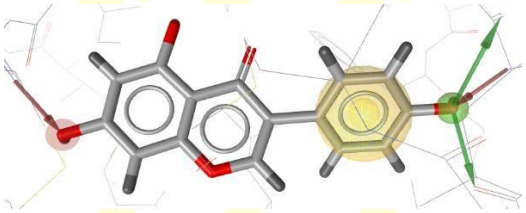
No.	Nama Senyawa	Compound ID	Struktur 2D
11.	*N-2-propynyl-2-propyn-1-amine*	23350	
12.	*Cyclohexa-2,5-diene-1,4-dione*	4650	
13.	*1-methyl-4-(propan-2-yl)benzene*	7463	
14.	*(2S,4S)-4-methyl-2-(2-methylprop-1-enyl)oxane*	1712086	

LAMPIRAN 5

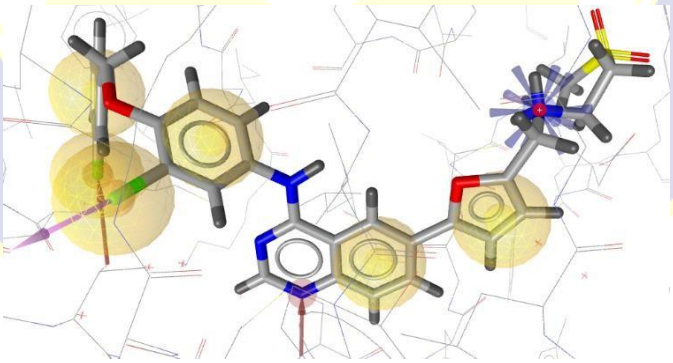
SCREENING FARMAKOFOR



Gambar V.1 Hasil *screening* farmakofor pada *Estrogen Receptor – Alpha*



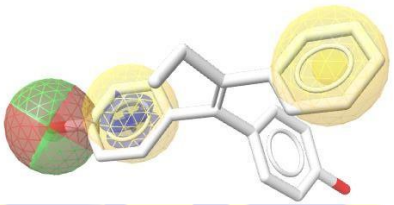
Gambar V.2 Hasil *screening* farmakofor pada *Estrogen Receptor – Beta*



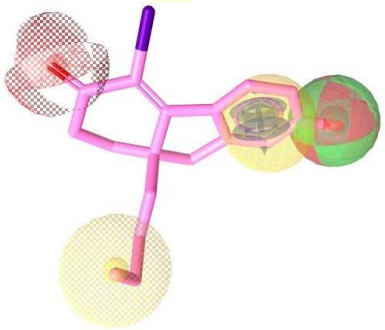
Gambar V.3 Hasil *screening* farmakofor pada *Epidermal Growth Factor Receptor*

LAMPIRAN 5

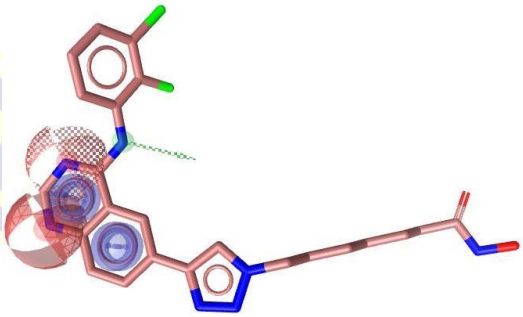
(LANJUTAN)



Gambar V.4 Model 1 farmakofor ligan pada *Estrogen Receptor – Alpha*



Gambar V.5 Model 1 farmakofor ligan pada *Estrogen Receptor – Beta*



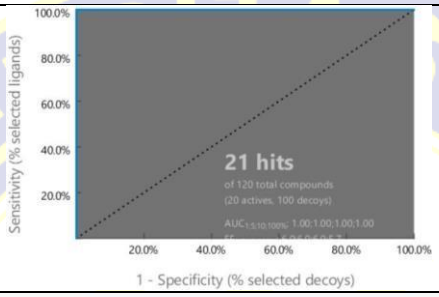
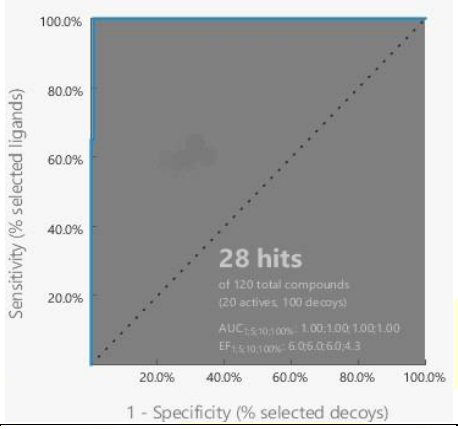
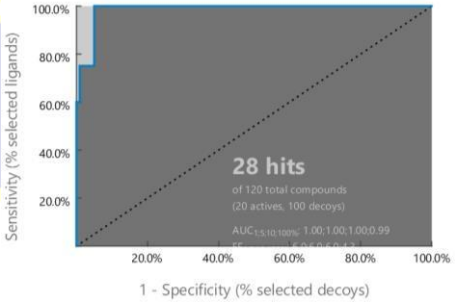
Gambar V.6 Model 1 farmakofor ligan *Epidermal Growth Factor Receptor*

LAMPIRAN 5

(LANJUTAN)

Tabel V.1

Hasil Validasi Model *Pharmacophore*

Reseptor	**ROC *Curve***	**AUC**	**GH *Score***
ER-□		1,00	0,95
ER-□		1,00	0,78
EGFR		0,99	0,72

LAMPIRAN 5

(LANJUTAN)

Tabel V.2

Hasil *Screening* Farmakofor *Estrogen Receptor – Alpha*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	Tamoxifen (ligan pembanding)		-
2.	*Linalool*		44,00
3.	*(E)-2-Octen-1-ol*		43,93
4.	*Lavandulol*		43,78

Tabel V.3

Hasil *Screening* Farmakofor *Estrogen Receptor - Beta*

No.	Nama Senyawa	*Matching Features*	*Fit Score*
1.	Genistein (ligan pembanding)		-
2.	*Methyl salicylate*		45,69
3.	*Fenchol*		38,67
4.	*(E)-2-Octen-1-ol*		38,51
5.	*Lavandulol*		38,04
6.	*Myrtenol*		37,69
7.	*Linalool*		35,21

LAMPIRAN 5

(LANJUTAN)

Tabel V.4

Hasil *Screening* Farmakofor *Epidermal Growth Factor Receptor*

No.	**Nama Senyawa**	***Matching Features***	***Fit Score***
1.	Lapatinib (ligan pembanding)		-
2.	*Methyl salicylate*		35,86
3.	*Nioxime*		33,50

Keterangan :

Warna biru = Cincin aromatik

Warna kuning = Ikatan hidrofobik

Warna merah = Akseptor ikatan hidrogen

Warna hijau = Donor ikatan hidrogen

LAMPIRAN 6

PREDIKSI *DRUG LIKENESS* BERDASARKAN ATURAN *LIPINSKI'S RULE OF FIVE*

Tabel V.5

Prediksi *Drug Likeness* Senyawa Minyak Atsiri Tanaman Jelatang (*Laportea aestuans* (L.) Chew) Berdasarkan Aturan *Lipinski's Rule of Five*

Senyawa	Berat Molekul (gr/mol)	Akseptor ikatan hidrogen	Donor ikatan hidrogen	Log P	Keterangan
(E)-2-Octen-1-ol	128,12	1	5	2,655	Memenuhi syarat
(E,E)-1,5-Cyclododecadiene	164,157	0	0	5,74	Memenuhi syarat
Nioxime	142,074	4	2	0,846	Memenuhi syarat
1,4-Octadiene	110,11	0	0	3,958	Memenuhi syarat
Tropone	106,042	1	0	0,612	Memenuhi syarat
Fenchol	154,136	1	1	3,099	Memenuhi syarat
Lavandulol	154,136	1	1	2,639	Memenuhi syarat
Linalool	154,136	1	1	2,749	Memenuhi syarat
Methyl salicylate	152,047	2	1	2,335	Memenuhi syarat
Myrtenol	152,12	1	1	2,915	Memenuhi syarat
Dipropargylamine	93,058	1	1	0,322	Memenuhi syarat
Benzoquinone	108,021	2	0	0,208	Memenuhi syarat
P-Cymene	134,11	0	0	4,068	Memenuhi syarat

LAMPIRAN 6

(LANJUTAN)

Tabel V.5

Lanjutan

Senyawa	Berat Molekul (gr/mol)	Akseptor ikatan hidrogen	Donor ikatan hidrogen	Log P	Keterangan
Trans-Rose Oxide	154,136	1	0	3,116	Memenuhi syarat

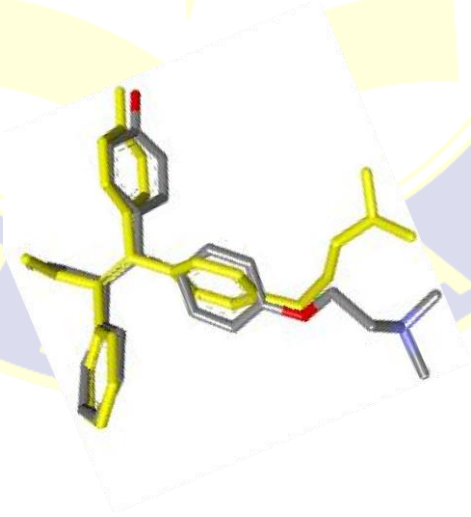
LAMPIRAN 7

VALIDASI METODE

Tabel V.6

Hasil Validasi Metode Penambatan Molekul

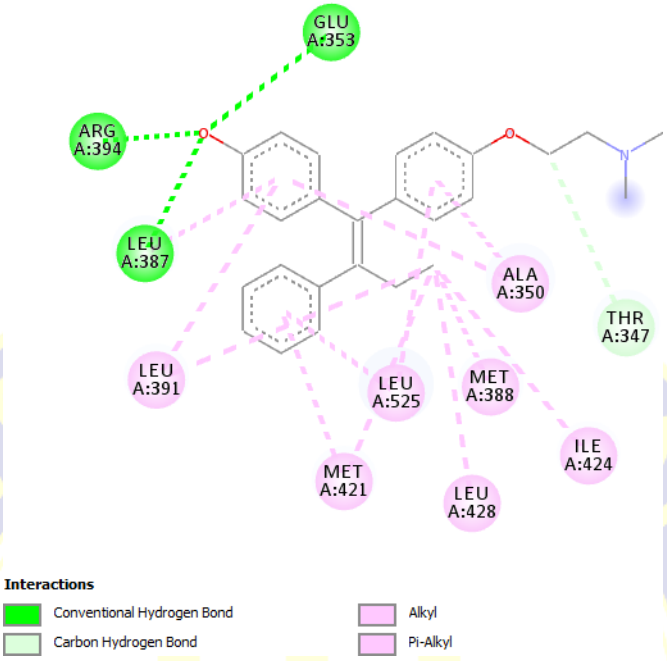
No.	Kode PDB	RMSD	Grid Box
1.	3ERT	1,180 Å	X = 30,282 Y = - 1,913 Z = 24,207
2.	1QKM	1,775 Å	X = 22,333 Y = 8,098 Z = 113,228
3.	1XKK	1,876 Å	X = 18,866 Y = 35,252 Z = 37,650
4.	5V5N	0,829 Å	X = -14,810 Y = -48,790 Z = -16,291



Gambar V.7 Visualisasi tumpang tindih ligan alami 3ERT (merah-abu-biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 7

(LANJUTAN)

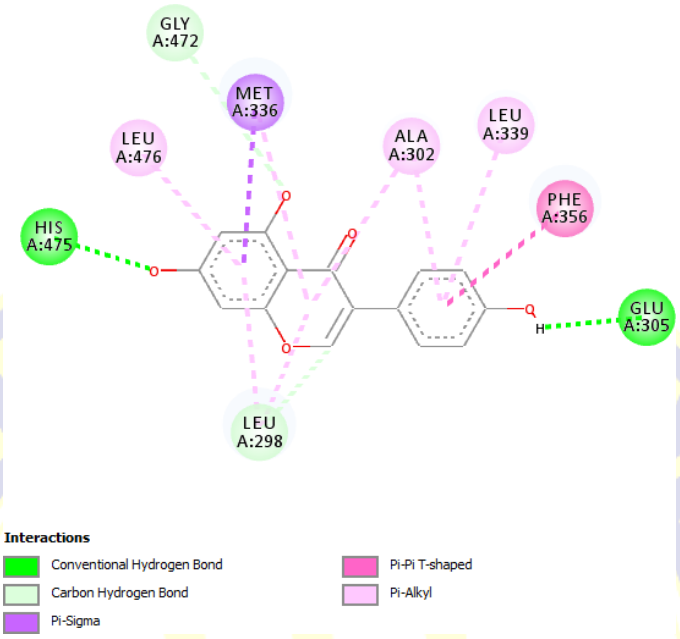


Gambar V.8 Interaksi tamoxifen dengan residu-residu asam amino pada *Estrogen Receptor – Alpha*

Gambar V.9 Visualisasi tumpang tindih ligan alami 1QKM (merah-abu-putih) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 7

(LANJUTAN)

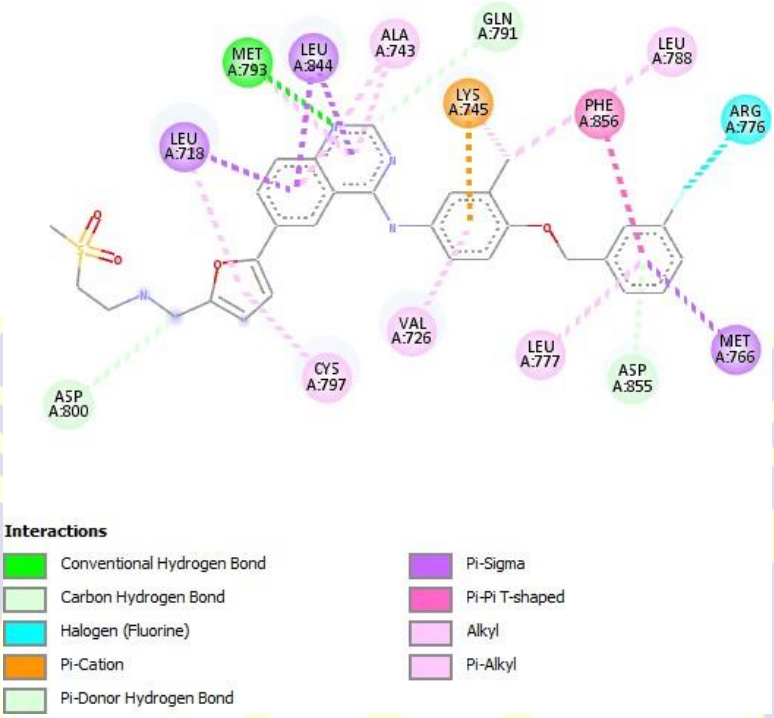


Gambar V.10 Interaksi genistein dengan residu-residu asam amino pada *Estrogen Receptor – Beta*

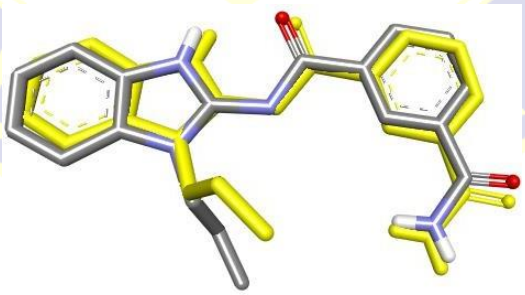
Gambar V.11 Visualisasi tumpang tindih ligan alami 1XKK (merah-abu-biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 7

(LANJUTAN)



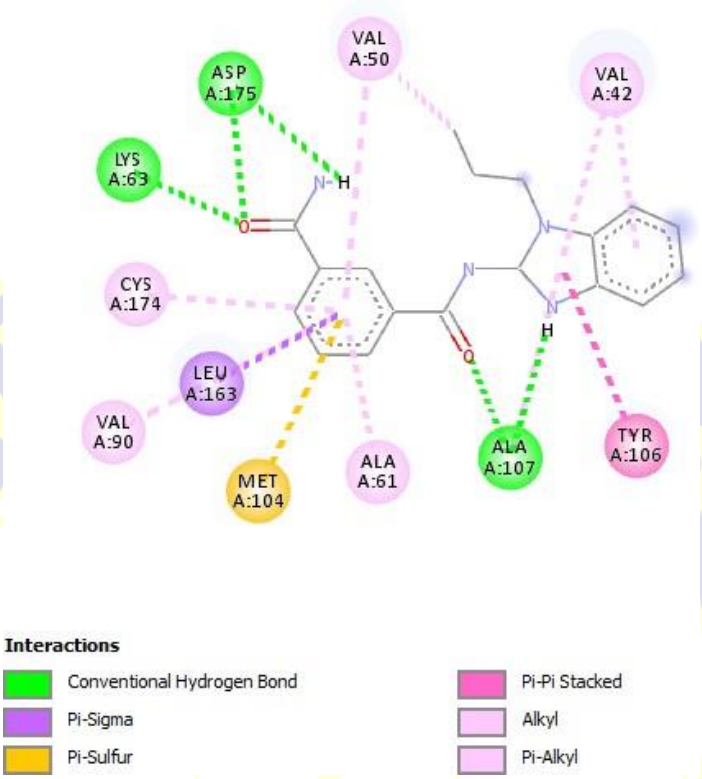
Gambar V.12 Interaksi lapatinib dengan residu-residu asam amino pada *Epidermal Growth Factor Receptor*



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

LAMPIRAN 7

(LANJUTAN)



Gambar V.14 Interaksi takinib dengan residu-residu asam amino pada *Mitogen-Activated Protein Kinase Kinase Kinase 7*

LAMPIRAN 8

PENAMBATAN MOLEKUL LIGAN UJI

Tabel V.7

Hasil Penambatan Molekul Ligan Uji Pada *Estrogen Receptor – Alpha*

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
1.	Tamoxifen (Ligan Pembanding)	-11,65	2,88	MET421A, ILE424A, LEU428A,MET388A, LEU391A, LEU525A, ALA350A,THR347A, GLU353A,ARG394A, LEU387A, LEU387A
2.	*(E)-2-Octen-1-ol*	-4,15	$907{,}21 \times 10^3$	GLU353A,ARG394A, PHE404A, LEU346A, MET421A
3.	*(E,E)-1,5-Cyclododecadiene*	-6,49	$17{,}58 \times 10^3$	LEU391A, LEU387A, LEU346A
4.	*Nioxime*	-5,79	$59{,}63 \times 10^3$	LEU387A, LEU391A, ARG394A, GLU353A
5.	*1,4-Octadiene*	-3,71	$1{,}91 \times 10^6$	MET388A,LEU428A, LEU391A, LEU349A, LEU346A, ALA350A
6.	*Tropone*	-4,56	$453{,}64 \times 10^3$	LEU387A, LEU391A, ARG394A,GLU353A, LEU349A, LEU346A, ALA350A
7.	*Fenchol*	-6,05	$36{,}66 \times 10^3$	MET388A,LEU391A, LEU387A, PHE404A, LEU346A, LEU349A, ALA350A, GLU353A
8.	*Lavandulol*	-5,49	$95{,}05 \times 10^3$	LEU428A,MET388A, LEU391A,GLU353A, PHE404A, LEU349A, LEU346A,ALA350A, MET421A

LAMPIRAN 8

(LANJUTAN)

Tabel V.7

Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
9.	*Linalool*	-5,74	$61,64 \times 10^3$	MET421A, ILE424A, MET388A,LEU428A, LEU391A, LEU387A, PHE404A, LEU346A, ALA350A,LEU349A, GLU353A, ARG394A
10.	*Methyl salicylate*	-5,29	$132,76 \times 10^3$	LEU391A,ALA387A, ARG394A,GLU353A, LEU349A, LEU346A
11.	*Myrtenol*	-6,23	$27,17 \times 10^3$	LEU387A,GLU353A, ARG394A, ALA350, LEU349A, LEU391A, PHE404, LEU346A,
12.	*Dipropargylamine*	-4,46	$540,47 \times 10^3$	GLU353A,ALA350A, LEU346A, LEU349A, PHE404, LEU391A
13.	*Benzoquinone*	-4,18	$860,36 \times 10^3$	LEU387A, LEU391A, ARG394A,GLU353A, LEU349A, LEU346A, ALA350
14.	*P-Cymene*	-4,95	$236,24 \times 10^3$	MET388A,LEU428A, ILE424A, MET421A, LEU391A, LEU387A, LEU349A
15.	*Trans-Rose Oxide*	-5,22	$149,83 \times 10^3$	MET421A, ILE424A, MET388A,LEU428A, LEU391A, LEU387A, ALA350A,LEU346A, LEU349

LAMPIRAN 8

(LANJUTAN)

Tabel V.8

Hasil Penambatan Molekul Ligan Uji Pada *Estrogen Receptor – Beta*

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
1.	Genistein (Ligan Pembanding)	-9,62	88,20	PHE356A, LEU339A, ALA302A,LEU298A, MET336A,GLY472A, LEU476A, LEU298A, HIS475A
2.	*(E)-2-Octen-1-ol*	-4,92	$248{,}18 \times 10^3$	ALA302A, VAL487, LEU476A,GLU305A, ARG346A
3.	*(E,E)-1,5-Cyclododecadiene*	-7,38	$3{,}91 \times 10^3$	PHE356A, LEU298A, ALA302A, LEU339A
4.	*Nioxime*	-6,32	$23{,}42 \times 10^3$	PHE356A, LEU343A, ARG346A,GLU305A, LEU339A
5.	*1,4-Octadiene*	-4,17	$871{,}69 \times 10^3$	LEU301A, PHE356A, LEU343A, LEU339A, ALA302A,MET336A, TRP335A, VAL487A, LEU476A
6.	*Tropone*	-4,80	301×10^3	HIS475A, LEU476A, MET336A
7.	*Fenchol*	-6,44	$18{,}91 \times 10^3$	LEU298A, PHE356A, LEU301A, LEU343A, MET340A,LEU339A, MET336A
8.	*Lavandulol*	-6,11	$33{,}01 \times 10^3$	LEU298A, PHE356A, LEU343A,ARG346A, GLU305A,MET340A, LEU339A,MET336A, ALA302A
9.	*Linalool*	-6,17	$30{,}24 \times 10^3$	PHE356A, LEU380A, MET340A,MET336A, ALA302A,LEU339A, LEU301A, ARG346A

LAMPIRAN 8

(LANJUTAN)

Tabel V.8

Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
10.	*Methyl salicylate*	-4,95	$234,91 \times 10^3$	LEU343A, PHE356A, LEU301A,GLU305A, LEU339A,MET336A, ALA302A, LEU298A
11.	*Myrtenol*	-6,65	$13,32 \times 10^3$	ARG346A,LEU343A, PHE356, LEU298A, ALA302A,MET336A, LEU339A, MET340A
12.	*Dipropargylamine*	-4,89	$259,90 \times 10^3$	LEU298A, PHE356A, LEU301A, PHE356A, LEU343A,MET340A, LEU339A
13.	*Benzoquinone*	-4,39	$608,50 \times 10^3$	MET336A,LEU476A, HIS475A
14.	*P-Cymene*	-5,63	$74,21 \times 10^3$	LEU298A,ALA302A, MET336A,LEU339A, MET340A,LEU343A, PHE356A, LEU301A
15.	*Trans-Rose Oxide*	-5,94	$44,35 \times 10^3$	LEU298A,VAL487A, ALA302A,LEU339A, MET340A,LEU343A, PHE356A, LEU301A

LAMPIRAN 8

(LANJUTAN)

Tabel V.9

Hasil Penambatan Molekul Ligan Uji Pada *Epidermal Growth Factor Receptor*

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
1.	Lapatinib (Ligan Pembanding)	-12,54	0,64373	ASP800A, CYS797A, LEU718A, LEU844A, ALA743A,MET793A, GLN791A,VAL726A, LYS745A, LEU788A, ASP855A, MET766A, LEU777A, PHE856A, ARG776A
2.	*(E)-2-Octen-1-ol*	-4,37	$621,80 \times 10^3$	PHE856A,MET766A, LEU777A, ASP855A
3.	*(E,E)-1,5-Cyclododecadiene*	-7,34	$4,16 \times 10^3$	MET766A, LEU777A
4.	*Nioxime*	-6,46	$18,37 \times 10^3$	ASP837A, ARG841A, PHE723A, GLY724A,
5.	*1,4-Octadiene*	-4,43	$561,92 \times 10^3$	PHE856A,MET766A, LEU788A, LYS745A
6.	*Tropone*	-4,85	277×10^3	PHE856A, CYS775A, MET766A, LEU777A
7.	*Fenchol*	-5,68	$69,03 \times 10^3$	THR854A, CYS775A, LEU858A,MET766A, LEU777A, LEU788A, LYS745A, VAL726A
8.	*Lavandulol*	-5,26	$138,41 \times 10^3$	ASP855A, PHE856A, CYS775A, LEU777A, MET766A,MET788A, LYS745A, VAL726A
9.	*Linalool*	-5,46	$100,31 \times 10^3$	MET766A,PHE856A, CYS775A, LEU777A, ALA743A, LYS745A, VAL726A

LAMPIRAN 8

(LANJUTAN)

Tabel V.9

Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
10.	*Methyl salicylate*	-5,48	$96{,}29 \times 10^3$	LYS745A, LEU858A, ASP855A, PHE856A, MET766A,CYS775A, LEU777A
11.	*Myrtenol*	-5,56	$83{,}95 \times 10^3$	CYS775A,THR854A, MET766A,LEU777A, LEU788A, LYS745A, LEU858A
12.	*Dipropargylamine*	-3,79	$1{,}66 \times 10^6$	ASP855A, THR854A, PHE856A,MET766A, LEU788A, LYS745A
13.	*Benzoquinone*	-4,52	$488{,}95 \times 10^3$	PHE856A, CYS775A, LEU777A, MET766A
14.	*P-Cymene*	-5,69	$67{,}76 \times 10^3$	LEU777A,MET766A, PHE856A, LEU788A, LYS745A
15.	*Trans-Rose Oxide*	-6,29	$24{,}57 \times 10^3$	ASP855A,MET766A, LEU777A, PHE856A, LEU788A, LYS745A

LAMPIRAN 8

(LANJUTAN)

Tabel V.10

Hasil Penambatan Molekul Ligan Uji Pada *Mitogen-Activated Kinase Kinase Kinase 7*

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
1.	Takinib (Ligan Pembanding)	8,86	319,88	LYS63A, ASP175A, CYS174A,MET104A, VAL90A, LEU163A, VAL50A, ALA61A, ALA107A, VAL42A, TYR106A,
2.	*(E)-2-Octen-1-ol*	-4,18	$867{,}01 \times 10^3$	ALA107A,MET104A, ALA61A, LYS63A
3.	*(E,E)-1,5-Cyclododecadiene*	-5,79	$56{,}71 \times 10^3$	CYS174A, LEU163A, ALA61A, VAL50A
4.	*Nioxime*	-4,55	$459{,}08 \times 10^3$	LEU163A,ALA107A, ALA61A, VAL50A
5.	*1,4-Octadiene*	-3,77	$1{,}72 \times 10^6$	LEU163A,ALA107A, TYR106A, ALA61A, LYS63A, LEU102A, MET104A
6.	*Tropone*	-4,21	$817{,}12 \times 10^3$	LYS63A, ASP175A, MET104A,CYS174A, LEU163A, VAL50A
7.	*Fenchol*	-4,98	$224{,}42 \times 10^3$	ALA61A, LEU163A, ALA107A,TYR106A, GLY110A, VAL42A, VAL50
8.	*Lavandulol*	-4,62	$441{,}08 \times 10^3$	VAL50, LYS63A, MET104A, ALA61A, GLU105A,ALA107A, CYS174A, LEU163A
9.	*Linalool*	-4,88	$266{,}29 \times 10^3$	LYS63A, VAL50A, ALA61A, MET104A, ALA107A, LEU163A

LAMPIRAN 8

(LANJUTAN)

Tabel V.10

Lanjutan

No.	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan
10.	*Methyl salicylate*	-4,40	$594{,}99 \times 10^3$	VAL50, MET104A, ALA61A, LEU163A, GLU105A,ALA107A, TYR106A
11.	*Myrtenol*	-5,12	$175{,}76 \times 10^3$	LEU163A,ALA107A, GLU105A,TYR106A, ALA61A, VAL42A, VAL50A
12.	*Dipropargylamine*	-3,76	$1{,}74 \times 10^6$	ALA46A, PRO160A, APS175A, CYS174A, VAL50A, ARG44A
13.	*Benzoquinone*	-3,84	$1{,}54 \times 10^6$	LYS63A, ASP175A, MET104A,CYS174A, LEU163A, VAL50A
14.	*P-Cymene*	-4,52	$483{,}64 \times 10^3$	VAL42A, VAL50A, ALA61A, MET104A, VAL90A, LEU163A, ALA107A, TYR106A
15.	*Trans-Rose Oxide*	-5,28	$135{,}75 \times 10^3$	VAL42A, VAL50A, ALA61A, MET104A, VAL90A, LEU163A, ALA107A, TYR106A

LAMPIRAN 9

PREDIKSI PROFIL ABSORBSI DAN DISTRIBUSI LIGAN DAN SENYAWA MINYAK ATSIRI TANAMAN JELATANG (*Laportea aestuans* (L.) Chew)

Tabel V.11

Hasil Prediksi Profil Absorbsi Dan Distribusi Ligan Dan Senyawa Minyak Atsiri Tanaman Jelatang (*Laportea aestuans* (L.) Chew)

No.	Senyawa	Absorbsi		Distribusi
		HIA (%)	CACO-2 cell (nm sec^{-1})	*Plasma Protein Binding* (%)
1.	Tamoxifen (Ligan pembanding)	97,20[a]	47,73[b]	99,51[a]
2.	Genistein (Ligan pembanding)	88,12[a]	5,74[b]	89,73[b]
3.	Lapatinib (Ligan pembanding)	96,86[a]	17,99[b]	97,56[a]
4.	Takinib (Ligan pembanding)	94,57[a]	21,16[b]	95,33[a]
5.	*(E)-2-Octen-1-ol*	100[a]	1,9078[c]	100[a]
6.	*(E,E)-1,5-Cyclododecadiene*	100[a]	23,39[b]	100[a]
7.	*Nioxime*	77,76[a]	19,21[b]	19,67[b]
8.	*1,4-Octadiene*	100[a]	23,40[b]	100[a]
9.	*Tropone*	100[a]	43,76[b]	91,48[a]
10.	*Fenchol*	100[a]	24,23[b]	100[a]
11.	*Lavandulol*	100[a]	24,62[b]	100[a]
12.	*Linalool*	100[a]	29,35[b]	100[a]
13.	*Methyl salicylate*	88,13[a]	20,13[b]	8,77[b]
14.	*Myrtenol*	100[a]	21,46[b]	35,76[b]
15.	*Dipropargylamine*	100[a]	23,17[b]	82,00[b]
16.	*Benzoquinone*	97,80[a]	17,45[b]	85,19[b]
17.	*P-Cymene*	100[a]	23,43[b]	100[a]
18.	*Trans-Rose Oxide*	100[a]	38,13[b]	100[a]

LAMPIRAN 9

(LANJUTAN)

Tabel V.11

Lanjutan (keterangan tabel)

Keterangan :

% *Human Intestinal Absorbsi* (% HIA) = (a)70-100% *well absorbed*

(b) 20-70% *moderately absorbed*

(c) 0-20% *poorly absorbed*

In Vitro Caco-2 *cell permeability* (nm sec-1) = (a) >70 *higher permeability*

(b) 4-70 *medium permeability*

(c) <4 *low permeability*

Plasma protein binding = (a) >90 *strongly bound*

(b) < 90% *weakly bound*

LAMPIRAN 10

PREDIKSI SIFAT TOKSISITAS LIGAN DAN SENYAWA MINYAK ATSIRI TANAMAN JELATANG (*Laportea aestuans* (L.) Chew)

Tabel V.12

Hasil Prediksi Sifat Toksisitas Ligan dan Senyawa Minyak Atsiri Tanaman Jelatang (*Laportea aestuans* (L.) Chew)

No.	Senyawa	*Crammer Rules*	*Beningni/Bossa Rulebase*	*Kroes TTC*
1.	Tamoxifen (Ligan pembanding)	3	8,9	1
2.	Genistein (Ligan pembanding)	3	1,8,9	2
3.	Lapatinib (Ligan pembanding)	3	2,8	1
4.	Takinib (Ligan pembanding)	3	2,8	1
5.	*(E)-2-Octen-1-ol*	1	2,8	1
6.	*(E,E)-1,5-Cyclododecadiene*	1	2,8	1
7.	*Nioxime*	3	8,9	1
8.	*1,4-Octadiene*	1	8,9	1
9.	*Tropone*	2	1,8,9	2
10.	*Fenchol*	1	8,9	1
11.	*Lavandulol*	1	2,8	1
12.	*Linalool*	3	8,9	1
13.	*Methyl salicylate*	1	8,9	1
14.	*Myrtenol*	1	8,9	1
15.	*Dipropargylamine*	3	8,9	1
16.	*Benzoquinone*	2	1,9	2
17.	*P-Cymene*	1	8,9	1
18.	*Trans-Rose Oxide*	3	8,9	1

LAMPIRAN 10

(LANJUTAN)

Tabel V.12

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/Bossa rulebase = (1) *Structural Alert for genotoxic carcinogenicity.*

(2) *Structural Alert for nongenotoxic carcinogenicity.*

(8) Negative for genotoxic carcinogenicity.

(9) Negative for nongenotoxic carcinogenicity.

Kroes TTC = (1) *Substance would not be expected to be a safety concern.*

(2) *Negligible risk (low probability of life-time cancer risk greater than 1 in 10^6).*

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