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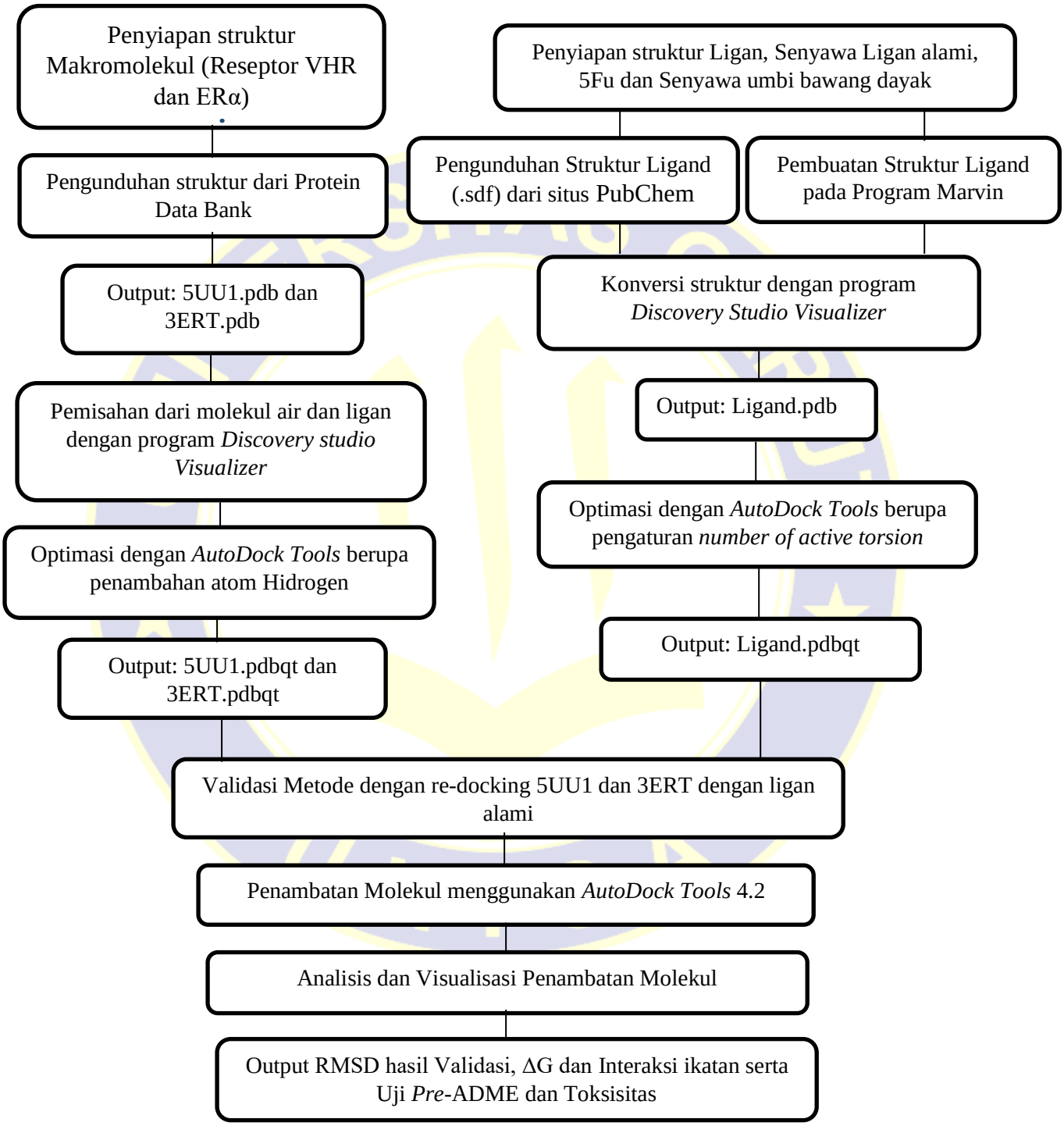
LAMPIRAN 1

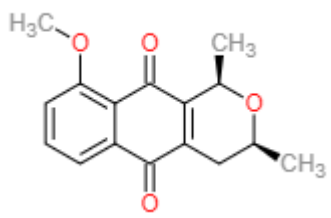
ALUR PENELITIAN



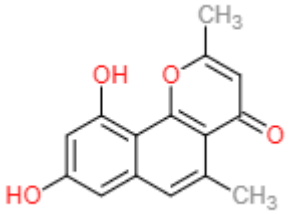
Gambar V.1 Alur penelitian

LAMPIRAN 2

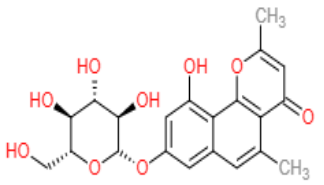
SENYAWA UMBI BAWANG DAYAK



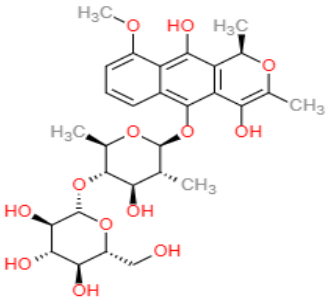
Eleutherine



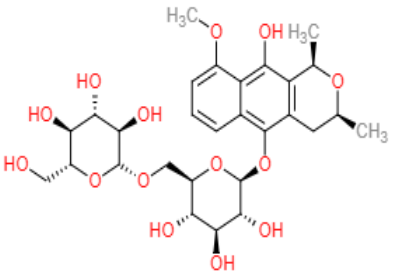
Eleutherinol



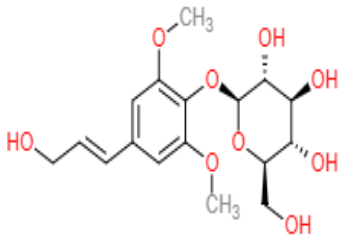
Eleutherinoside A



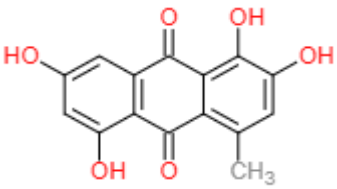
Eleutherinoside B



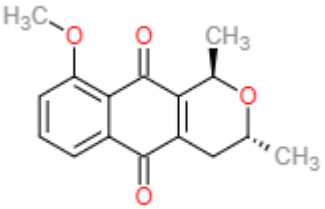
Eleuthoside C



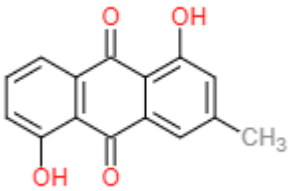
Eleuthoside B



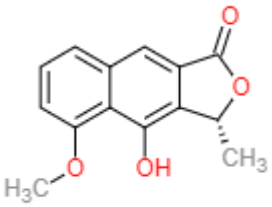
Erytrolaccine



Isoeleutherine



Ziganein



Eleutherol

Gambar V.2 Struktur 2D senyawa umbi bawang dayak (*Eleutherine Palmifolia* (L) Merr.)

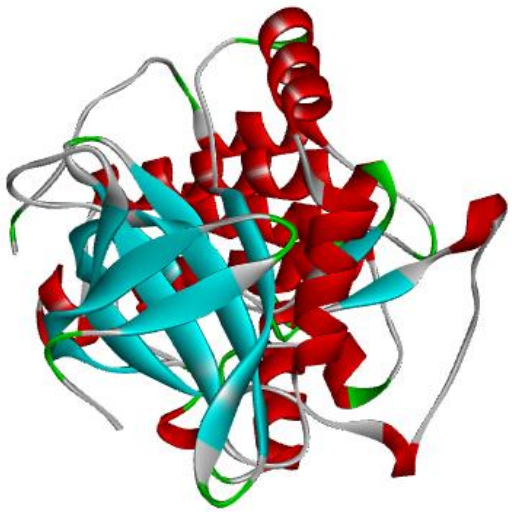
LAMPIRAN 3

SITUS *PROTEIN DATA BANK*

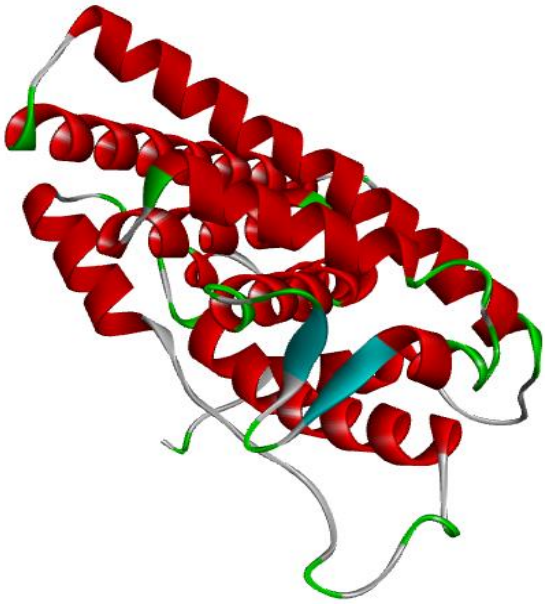
Gambar V.3 Program *protein data bank*

LAMPIRAN 4

STRUKTUR 3D RESEPTOR



Gambar V.4 Struktur 3D reseptor vaccinia h-1 related phospatase (VHR)

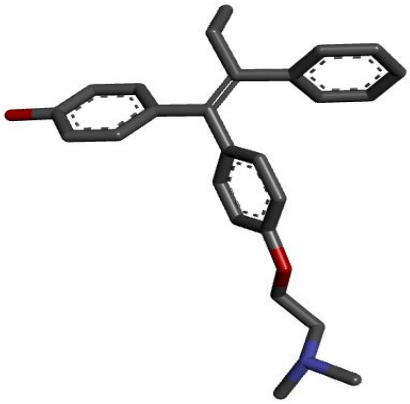


Gambar V.5 Struktur 3D reseptor estrogen alfa (ERα)

LAMPIRAN 5

LIGAN ALAMI

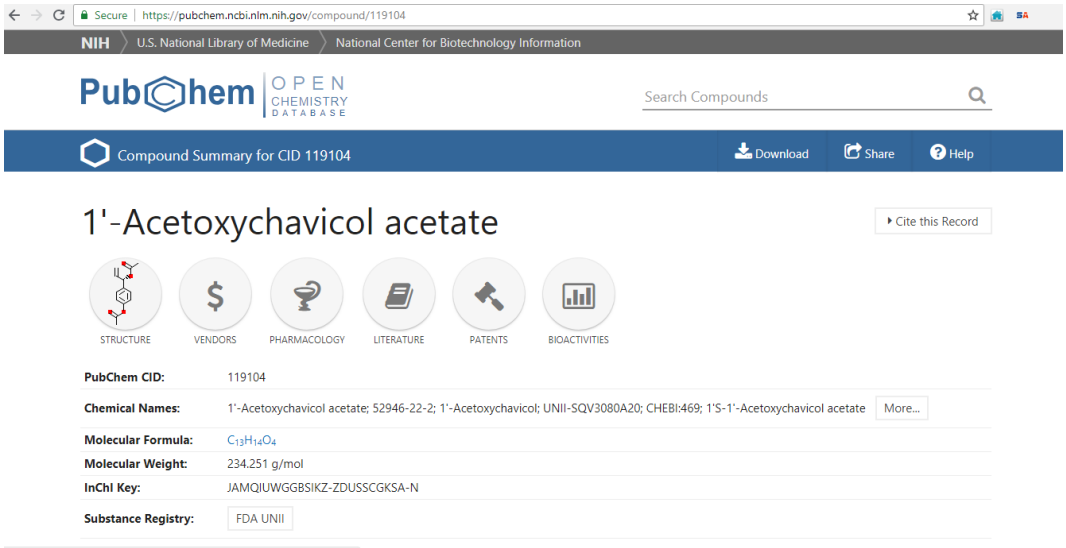
Gambar V.6 Ligan alami dari reseptor 5UU1



Gambar V.7 Ligan alami dari reseptor 3ERT

LAMPIRAN 6

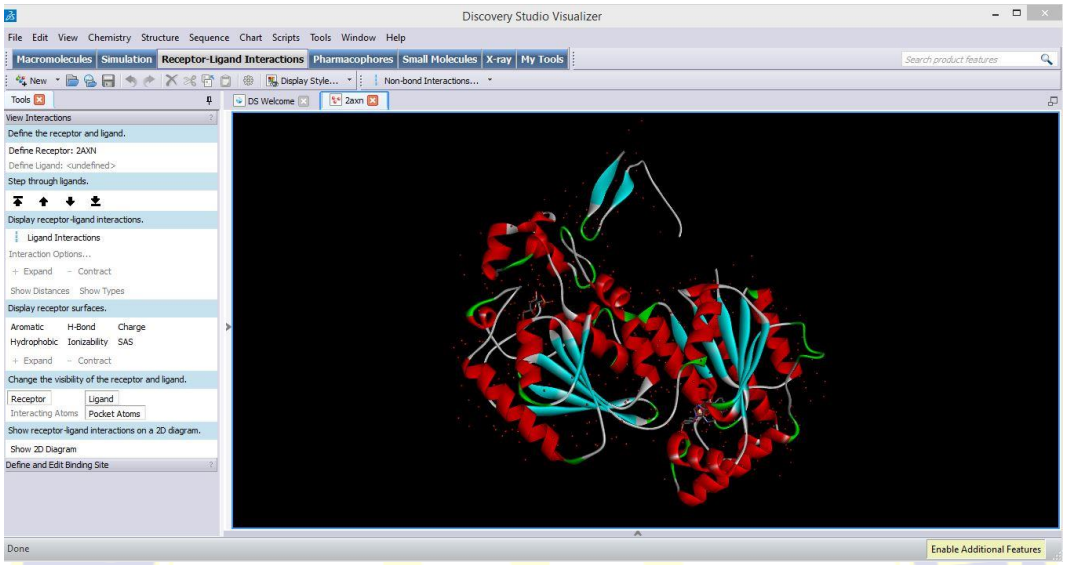
SITUS PUBCHEM



Gambar V.8 Situs pubchem

LAMPIRAN 7

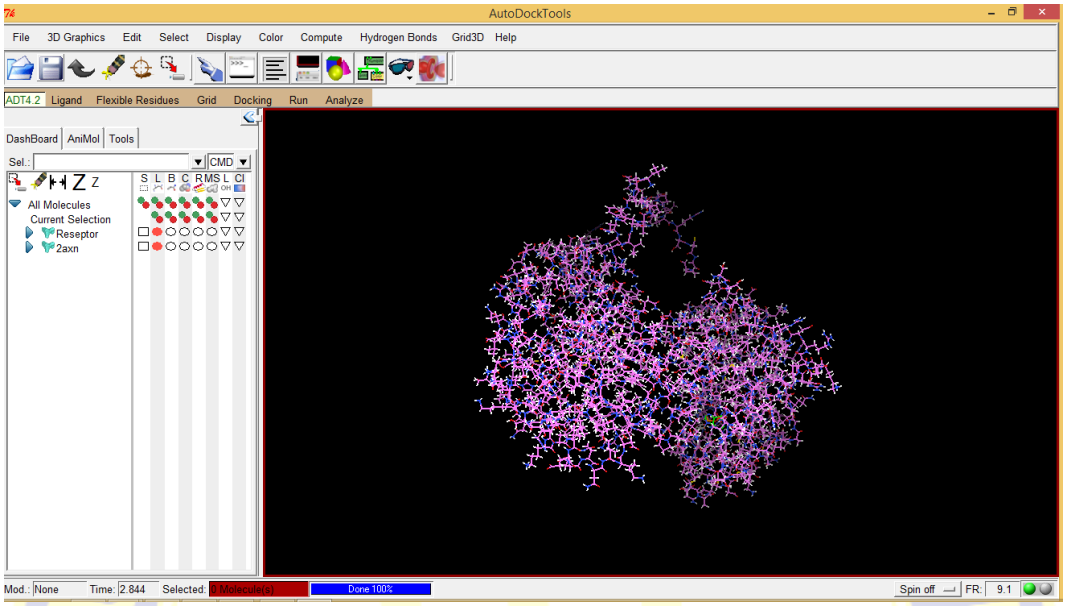
PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER



Gambar V.9 Tampilan program discovery studio visualizer

LAMPIRAN 8

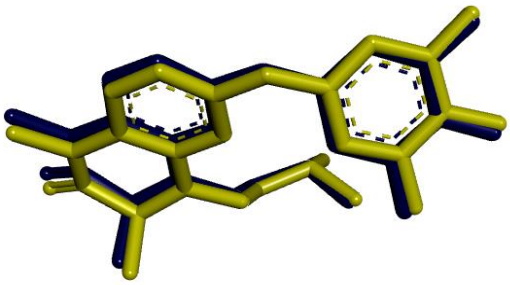
PERANGKAT LUNAK AUTODOCK TOOLS



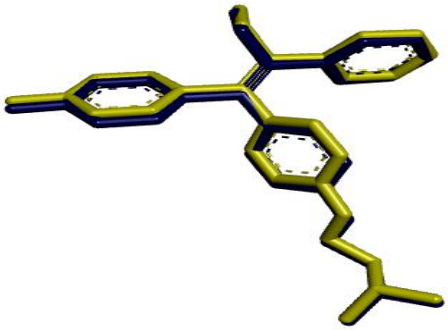
Gambar V.10 Tampilan program autodock tools

LAMPIRAN 9

VALIDASI METODE



Gambar V.11 Visualisasi tumpang tindih ligan alami 5UU1 (Biru) dengan ligan hasil *redocking* (kuning)



Gambar V.12 Visualisasi tumpang tindih ligan alami 3ERT (Biru) dengan ligan hasil *redocking* (kuning)

Tabel V.1
Grid Box, RMSD, Nilai Ikatan Energi, Ligan Alami, dan 5Fluorourasil

Kode PDB	***Grid Box***	**RMSD**	**Ikatan Energi 5 Fluorourasil**	**Ikatan Energi Ligan Alami (kkal/mol)**
5UU1	X : 0,539 Y : -18,004 Z : -13,408	0,282Å	-3,91	-8,79
3ERT	X : 30,282 Y : -1,913 Z : 24,207	0,435Å	-4,20	-10,64

LAMPIRAN 10

SIFAT FISIKOKIMIA 5 LIPINSKI

Tabel V.2

Sifat Fisikokimia Senyawa Umbi Bawang Dayak Berdasarkan Aturan 5 Lipinski

No.	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Refractory Molar	Ket
1	Eleutherine	272	2,33	0	4	72,37	Memenuhi
2	Eleutherinol	256	3,03	2	4	70,73	Memenuhi
3	Eleutherinoside A	418	0,51	4	9	103,46	Memenuhi
4	Eleutherinoside B	612	-1,10	9	15	143,91	Tidak memenuhi
5	Eleutherol	244	2,78	1	4	65,99	Memenuhi
6	Eleuthoside B	568	-1,91	7	14	131,35	Tidak memenuhi
7	Eleuthoside C	598	-1,42	8	14	141,85	Tidak memenuhi
8	Erytrolaccine	286	1,59	4	6	71,14	Memenuhi
9	Isoeleutherine	272	2,33	0	4	72,37	Memenuhi
10	Ziganein	254	2,18	2	4	67,82	Memenuhi

Syarat : 1. BM <500 mg/mol
2. Log P <5
3. Donor Hidrogen <5
4. Akseptor Hidrogen <10
5. *Molar Refrectory* antara 40-130

LAMPIRAN 11

HASIL PENAMBATAN MOLEKUL

Tabel V.3

Hasil Penambatan Molekuler Senyawa Umbi Bawang Dayak (5UU1)

No.	Ligan	ΔG (kkal/mol)	Konstanta inhibisi (nM)
1	Ligan alami	-8,79	357,99
2	5 Fluorourasil	-3,91	-1,360
3	Eleutherine	-7,93	1,55
4	Eleutherinol	-7,10	6,29
5	Eleutherinoside A	-9,55	99,41
6	Eleutherinoside B	-6,67	12,87
7	Eleutherol	-6,42	19,71
8	Eleuthoside B	-8,80	355,69
9	Eleuthoside C	-8,57	522,60
10	Erytrolaccin	-7,70	2,27
11	Isoeleutherine	-7,60	2,67
12	Ziganein	-7,93	1,53

LAMPIRAN 11
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Umbi Bawang Dayak (3ERT)

No.	Ligan	ΔG (kkal/mol)	Konstanta inhibisi (nM)
1	Ligan alami	-10,64	15,97
2	5 Fluorourasil	-4,20	833,28
3	Eleutherine	-7,44	3,53
4	Eleutherinol	-7,49	1,38
5	Eleutherinoside A	-7,63	2,57
6	Eleutherinoside B	-7,19	5,41
7	Eleutherol	-6,82	21,56
8	Eleuthoside B	-8,49	596,68
9	Eleuthoside C	-6,82	10,06
10	Erytrolaccin	-7,22	5,14
11	Isoeleutherine	-7,23	5,04
12	Ziganein	-6,66	13,15

LAMPIRAN 12

INTERAKSI IKATAN HIDROGEN DAN RESIDU ASAM AMINO

Tabel V.5

Hasil Analisis Ikatan Hidrogen dan Residu Asam Amino yang Terlibat (5UU1)

No.	Senyawa	Jumlah ikatan hydrogen	Residu asam amino
1	Liganalami	3 (GLU122, LEU124, LYS61)	GLU122, LEU124, LYS61, PRO101, LEU173, MET121, ALA185, VAL59, ILE35, ILE43
2	5 Fluorourasil	3 (GLU122, LEU124, ALA185)	GLU122, LEU124, ALA185, PRO101, VAL59
3	Eleutherine	1 (LYS61)	LYS61, GLY38, TYR77, MET121, ILE43, VAL59, LEU124, LEU173
4	Eleutherinol	2 (LYS61, LEU124)	LYS61, LEU124, LEU173, VAL59, ILE43, ALA185, MET121
5	Eleutherinoside A	5 (LYS61, LEU124, GLU122, ILE35, ASP127)	LYS61, LEU124, GLU122, ILE35, ASP127, GLY125, ILE43, VAL59, LEU173, PRO101, MET121, ALA185

LAMPIRAN 12
(LANJUTAN)

6	Eleutherinoside B	4 (ASN171, ALA170, SER37, LEU124)	ASN171, ALA170, SER37, LEU124, ALA185, GLY38, VAL59, ILE43, ILE35, LEU173
7	Eleutherol	2 (ALA185, LEU124)	ALA185, LEU124, ARG123, ASP186, ILE43, LEU173, PRO101, MET121, VAL59
8	Eleuthoside B	4 (LEU124, ALA170, ASP124, GLY125)	LEU124, ALA170, ASP127, GLY125, SER37, ASP186, ALA185, LYS61, MET121, VAL59, ILE35, ILE43
9	Eleuthoside C	5 (GLU122, ALA185, GLY125, SER37, ALA170)	GLU122, ALA185, GLY125, SER37, ALA170, ILE35, ALE43, VAL59, ILE126
10	Erytrolaccine	3 (ALA185, GLU122, LEU124)	ALA185, GLU122, LEU124, ILE35, ARG123, VAL59, ILE43, LEU173
11	Isoeleutherine	1 (LYS61)	LYS61, LEU173, VAL59, LEU124, ILE43, MET121
12	Ziganein	2 (ALA185, LEU124)	ALA185, LEU124, MET121, PRO101, ILE35, ILE43

LAMPIRAN 12
(LANJUTAN)

Tabel V.6

Hasil Analisis Ikatan Hidrogendan Residu Asam Amino yang Terlibat (3ERT)

No.	Senyawa	Jumlah ikatan hydrogen	Residu asam amino
1	Ligan alami	2 (GLU353, ARG394)	GLU353, ARG394, ILE424, MET421, LEU525, ASP351, LEU346, MET343, LEU387, LEU391, ALA350
2	5 Fluorourasil	2 (ARG412, MET421)	ARG412, MET421, PHE425, LYS416, ASP426
3	Eleutherine	-	MET288, LEU391, LEU387, LEU346, MET343, LEU525, HIS 524, MET421
4	Eleutherinol	3 (ARG394, GLU353, LEU346)	ARG394, GLU353, LEU346, MET343, MET388, LEU428, MET421, ILE424,LEU387, ALA350
5	Eleutherinoside A	3 (GLU353, LEU346, THR347)	GLU353, LEU346, THR347, ALA350, TRP383, MET528, MET343, LEU525

LAMPIRAN 12
(LANJUTAN)

6	Eleutherinoside B	4 (LEU387, MET343, THR347, ASP351)	LEU387, MET343, THR347, ASP351, ILE424, LEU428, LEU391, MET421, GLU355
7	Eleutherol	1 (ARG394)	ARG394, LEU428, MET388, LEU391, MET421, LEU346, LEU349
8	Eleuthoside B	3 (ASP351, THR347,GLU353)	ASP351, THR347, GLU353,MET343,LEU387, LEU384,MET421,ALA350
9	Eleuthoside C	3 (THR347, ASP351, LEU384)	THR347, ASP351, LEU387, MET343, ILE424, LEU428, LEU384, ALA350, GLU353, MET388
10	Erytrolaccin	3 (ARG394, GLU353, THR347)	ARG394, GLU353, THR347, ALA350, LEU525, LEU428, MET388, LEU391, LEU387
11	Isoeleutherine	-	LEU387, MET388, LEU391, GLU353, LEU346, MET343, LEU525, HIS524,MET421
12	Ziganein	1 (LEU346)	LEU346, LEU525, MET343, MET421, HIS524, LEU349

LAMPIRAN 13

UJI PREADME

Tabel V.7

Uji PreADME (Absorpsi dan Distribusi) Senyawa Umbi Bawang Dayak dan Obat Pembanding

No	Senyawa	Caco-2 (nm.sec^{-1})	HIA (%)	*Protein Plasma Binding (%)*
1	Ligan alami (7DZ)	31,99	97,61	86,31
2	Ligan alami (4-hydroxytamoxifen)	26,30	93,56	64,42
3	5 Fluorourasil	31,56	96,55	73,55
4	Eleutherine	31,31	98,22	85,69
5	Eleutherinol	21, 30	93,03	95,80
6	Eleutherinoside A	11,77	74,29	66,28
7	Eleutherinoside B	8,42	70,79	32,34
8	Eleutherol	8,48	95,51	86,01
9	Eleuthoside B	15,72	74,29	36,78
10	Eleuthoside C	9,51	76,39	30,95
11	Erytrolaccine	20,81	75,72	98,62
12	Isoeleutherine	31,31	98,22	85,69
13	Ziganein	20,93	92,59	96,84

Keterangan :
%HIA = 70-100% well absorbed, 20-70% moderately absorbed, 0-20% poorly absorbed.
In Vitro caco-2 cell permeability = > 70 higher permeability, 4-70 medium permeability, < 4 low permeability.
% PPB = 90% strongly bond, < 90% weakly bond.

LAMPIRAN 14

UJI TOKSISITAS

Tabel V.8
Uji Toksisitas Senyawa Umbi Bawang Dayak dan Obat Pembanding

No	Senyawa Ligan	Kroes TTC decision tree
1	Ligan alami (7DZ)	1
2	Ligan alami (4-hidroxytamoxifen)	2
3	5 Fluorourasil	2
4	Eleutherine	2
5	Eleutherinol	2
6	Eleutherinoside A	1
7	Eleutherinoside B	1
8	Eleutherol	1
9	Eleuthoside B	1
10	Eleuthoside C	1
11	Erytrolaccin	2
12	Isoeleutherine	2
13	Ziganein	2

Kroes TTC decision tree :

1 = Substance would not be expected to be a safety concern

2 = Negligible risk (low probability of a life-time cancer risk greater than in 10^6)

3 = Risk assesment requires compound-specific toxicity data