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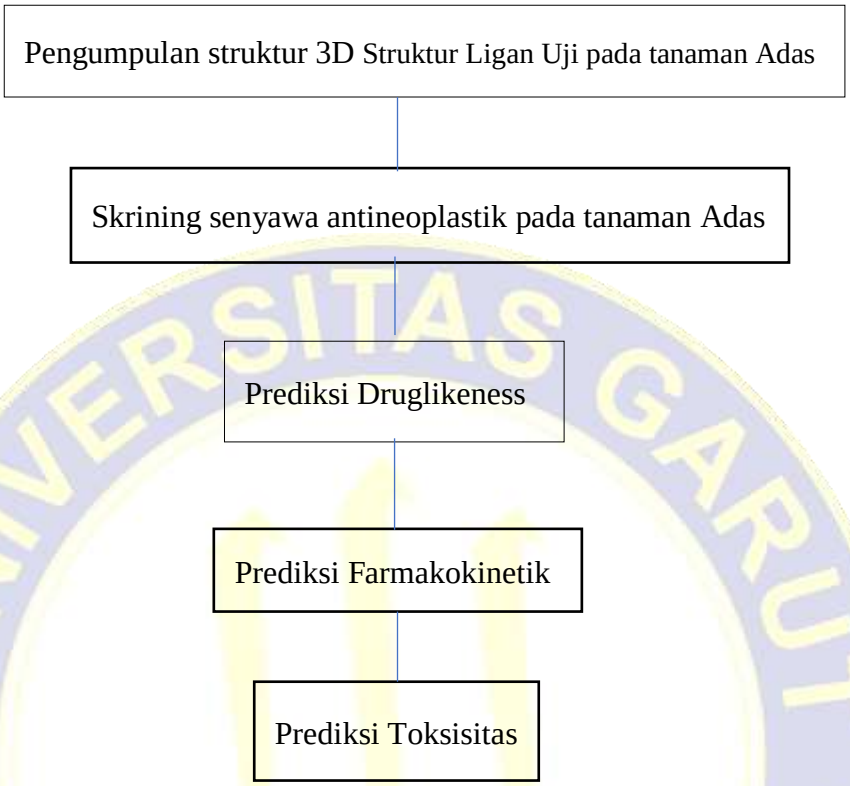
LAMPIRAN I
ALUR PENELITIAN



Gambar VI.1 Alur Penelitian

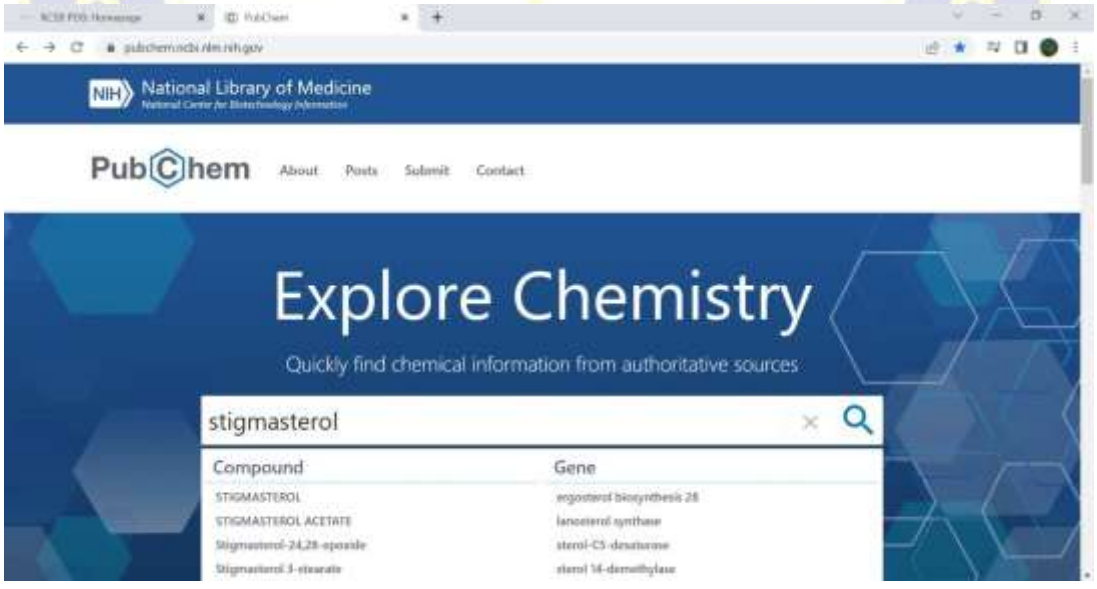
LAMPIRAN I
(LANJUTAN)

Gambar VI.1 Alur Penelitian

LAMPIRAN II

WEBSITE

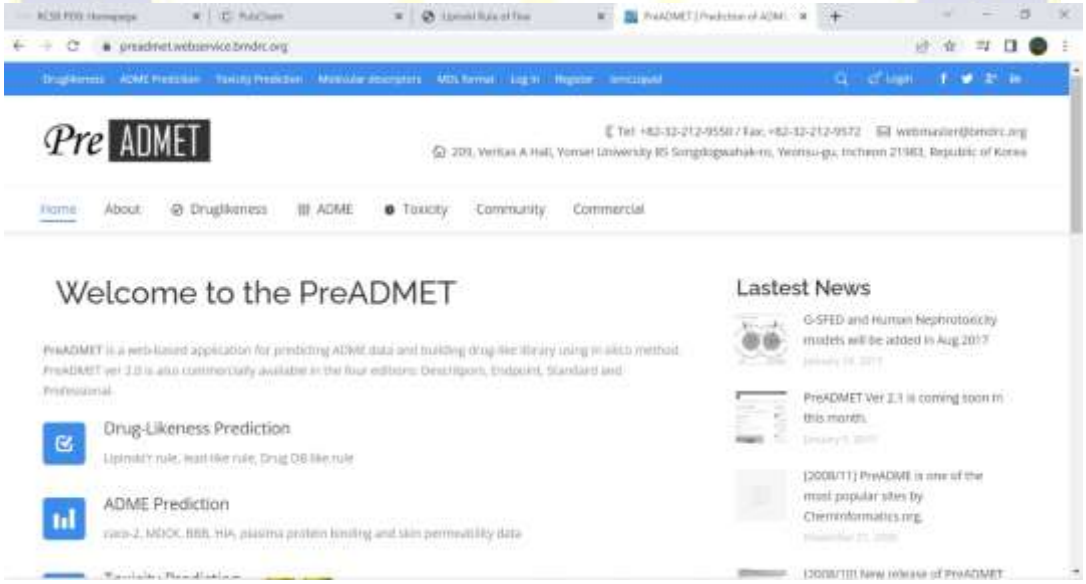
Gambar VI.2 Tampilan Website *Protein Data Bank*



Gambar VI.3 Tampilan Website Pubchem

LAMPIRAN II
(LANJUTAN)

Gambar VI.4 Tampilan Website *Lipinski's Rule of Five*

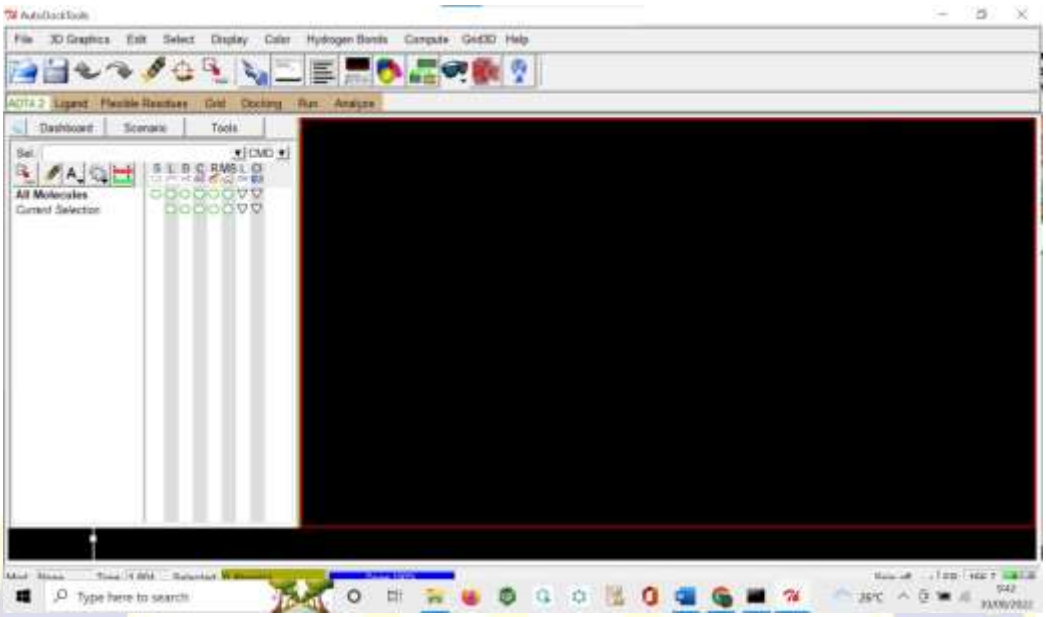


Gambar VI.5 Tampilan Website Pre-ADMET

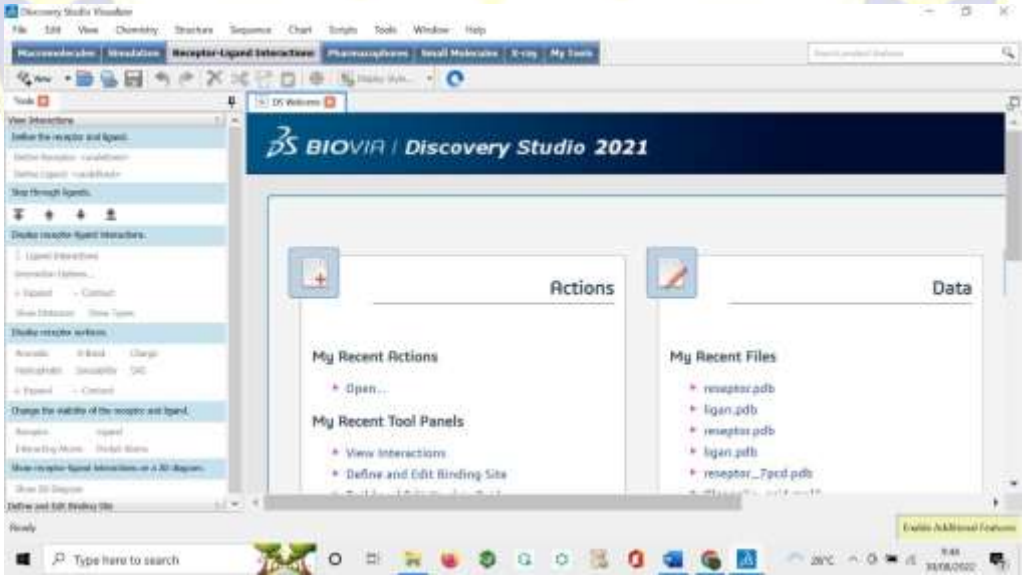
LAMPIRAN II
(LANJUTAN)

Gambar VI.6 Tampilan Website Knapsack

LAMPIRAN III
SOFTWARE

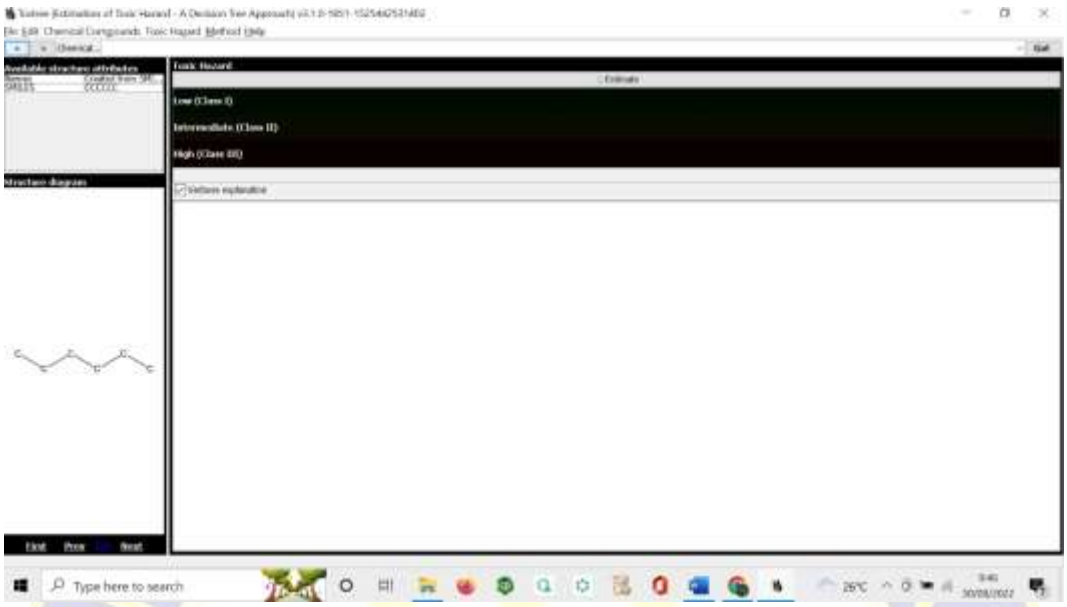


Gambar VI.7 Tampilan Program Autodock Tools®



Gambar VI.8 Tampilan Program Discovery Studio Visualizer®

LAMPIRAN III
(LANJUTAN)



Gambar VI.9 Tampilan Program Toxtree®

Gambar VI.10 Tampilan Program Marvin Sketch®

LAMPIRAN IV
HASIL PENELITIAN

Tabel VI.1
Hasil Prediksi Aktivitas Senyawa pada Tanaman Adas (*Foeniculum vulgare*) menggunakan Website *Way2Drug*

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
1.	Syringin		Yes		0,498	0,014
2.	1,8-cineole		Yes		0,777	0,004
3.	Seselin		Yes		0,173	0,083
4.	beta-Pinene		Yes		0,489	0,014
5.	Camphor		Yes		0,222	0,060
6.	Limonene		Yes		0,536	0,012
7.	3-Carene		Yes		0,194	0,073
8.	beta-Myrcene		Yes		0,677	0,007
9.	alpha-Terpinolene		Yes (sama NSCLC)		0,217	0,062
10.	Umbelliferone		Yes (sama NSCLC & SCLC)		0,240	0,054
11.	Anisaldehyde		Yes (sama NSCLC & SCLC)		0,246	0,052
12.	Gentisic acid		Yes (SCLC)		0,228	0,127
13.	Syringic acid		Yes (sama SCLC)		0,297	0,040

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
14.	(E)-Anethole		Yes (NSCLC)		0,404	0,011
15.	Apiol		Yes		0,430	0,019
16.	Methyl chavicol		Yes (NSCLC)		0,257	0,036
17.	Ferulic acid		Yes (NSCLC)		0,303	0,028
18.	Sinapic acid		Yes		0,349	0,031
19.	Camphene		Yes		0,399	0,023
20.	Fenchone		Yes		0,152	0,098
21.	Linalool		Yes		0,366	0,028
22.	Stigmasterol		Yes		0,167	0,087
23.	Juglanin		Yes		0,417	0,021
24.	Guaijaverin		Yes		0,487	0,014
25.	Miquelianin		Yes		0,411	0,022
26.	Platanoside		Yes		0,460	0,017
27.	(+)-Limonene		Yes		0,531	0,011
28.	beta-Phellandrene		Yes		0,218	0,062
29.	(-)-Fenchone		Yes		0,152	0,098
30.	Germacrene D		Yes		0,243	0,053
31.	Miyabenol C		Yes		0,156	0,089
32.	Oleanolic acid		Yes		0,766	0,005

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
33.	trans-Anethol		Yes (NSCLC)		0,404	0,011
34.	(E)-beta-Ocimene		Yes		0,636	0,008
35.	4-Carene		Yes		0,153	0,098
36.	Cinnamic acid		Yes (NSCLC)		0,248	0,040
37.	Glucosyringic acid		Yes		0,436	0,019
38.	Quinic acid		Yes		0,221	0,060
39.	7alpha-Hydroxycampesterol		Yes		0,228	0,057
40.	Benzaldehyde		Yes		0,168	0,086
41.	cis-Miyabenol C		Yes		0,156	0,095
42.	alpha-Tocotrienol		Yes		0,431	0,019
43.	beta-Tocotrienol		Yes		0,440	0,018
44.	delta-Tocotrienol		Yes		0,461	0,016
45.	gamma-Tocotrienol		Yes		0,394	0,024
46.	1,4-Dimethoxybenzene		Yes (NSCLC)		0,324	0,019
47.	Erythro Anethole glycol		Yes		0,133	0,118
48.	2,6-Dimethyl-2,4,6-octatriene		Yes		0,619	0,008
49.	beta-Terpineol		Yes		0,441	0,018
50.	cis-2,8-Menthadien-1-ol		Yes		0,585	0,009

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
51.	Melatonin		Yes (NSCLC)		0,220	0,058
52.	1-(3-Methoxyphenyl)-1-propanone		Yes (NSCLC)		0,178	0,110
53.	1,6-Hexanediol		Yes (NSCLC)		0,192	0,090
54.	2-Cyclohexen-1-ol		Yes		0,363	0,029
55.	2-Methoxycyclohexanone		Yes		0,160	0,092
56.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-ol		Yes		0,241	0,054
57.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one		Yes		0,140	0,110
58.	Benzothiazole		Yes		0,142	0,108
59.	cis-Limonene oxide		Yes		0,605	0,009
60.	Fenchyl acetate		Yes		0,431	0,019
61.	trans-Limonene oxide		Yes		0,605	0,009
62.	trans-p-2,8-menthadien-1-ol		Yes		0,585	0,009
63.	Acetanisole		Yes (NSCLC)		0,264	0,034
64.	beta-Elemenone		Yes		0,415	0,021

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
65.	2-Deoxy-L-ribono-1,4-lactone		Yes		0,421	0,020
66.	Isopentyl beta-D-glucoside		Yes		0,381	0,026
67.	Syringin methyl ether		Yes		0,451	0,017
68.	Sphalleroside A		Yes		0,410	0,022
69.	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside		Yes		0,151	0,100
71	alpha-Thujene	Yes			0,643	0,036
72	Hexanal	Yes			0,196	0,020
73	(+)-alpha-pinene	Yes			0,072	0,068
74	Palmitic acid	Yes			0,301	0,009
75	Heptan-2-one	Yes			0,339	0,131
76	1-Octanol	Yes			0,281	0,010
77	Falcarindiol	Yes			0,718	0,023
78	(-)-Falcarinol	Yes			0,548	0,057
79	Cathine	Yes			0,118	0,058
80	Folic acid	Yes			0,347	0,127
81	alpha-Terpinene	Yes			0,248	0,187

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
82	gamma-Terpinene	Yes			0,257	0,181
83	m-Cymene	Yes			0,182	0,023
84	Undecan-1-ol	Yes			0,281	0,010
85	Foeniculoside X	Yes			0,494	0,014
86	Sabinene hydrate	Yes			0,292	0,157
87	1,3-Butanediol	Yes			0,259	0,012
88	2-Heptene	Yes			0,257	0,180
89	2-Propyn-1-ol	Yes			0,623	0,040
90	5-Methyl-2-heptanol	Yes			0,135	0,045
91	Anisketone	Yes			0,251	0,185
92	Dicyclopropylcarbinol	Yes			0,111	0,065
93	Fenchyl alcohol	Yes			0,299	0,040
94	Mannoheptulose	Yes			0,380	0,005
95	E-Pinane	Yes			0,108	0,067
96	Tetradecyloxirane	Yes			0,293	0,009
97	3-Deoxy-D-arabinitol	Yes			0,394	0,005
98	2,4,5-Trimethylbenzaldehyde	Yes			0,604	0,044
99	delta-Tocopherol			Yes	-	-
100	beta-Tocophero			Yes	-	-
101	gamma-Tocopherol			yes	-	-

LAMPIRAN IV
(LANJUTAN)

Tabel VI.1
(Lanjutan)

No	Daftar senyawa	Antineoplastic (general)	Antineoplastik (lung cancer)	No antineoplastic	Pa	Pi
102	alpha-Tocopherol			Yes	-	-
103	Isovaleraldehyde			Yes	-	-
104	2-Heptanol			Yes	-	-
105	Allantoic acid			Yes	-	-
106	Isooleic acid			yes	-	-
107	Mephenesin			Yes	-	-

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
Nilai ΔG, Nilai Ki, dan Interaksi Residu Asam Amino Ligan Uji dengan Ligan Alami (*Epidermal Growth Factor Receptor*) Kode PDB 3POZ.

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
1.	Syringin	-5.60	78.58	ARG 841; LEU 844; LEU 718; ASN 842; ASP 855; PHE 856; MET 766; LEU; 777; THR 854; ILE 744; THR 790; ILE 789 ALA 743; LEU 788; LYS 745; VAL 726; CYS 797; GLY 719
2.	1,8-cineole	-6.39	20.73	ARG 776; THR 790; LEU 788; LEU 858; LEU 777; THR 854; CYS 775; ASP 855; MET 766; ILE 853; PHE 856;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
3.	Seselin	-7.68	2.34	LEU 788; GLY 857; LEU 858; MET 766; ASP 855; PHE 856; LEU 777; CYS 775; THR 854; THR 790; VAL 726; ALA 743; ILE 744; LYS 745
4.	beta-Pinene	-6.05	36.47	LEU 858; ASP 855; THR 854; THR 790; LEU 788; CYS 775; LEU 777; ARG 776; PHE 856; MET 766
5.	Camphor	-6.27	25.45	MET 766; ARG 776; LEU 777; THR 790; LEU 788; CYS 775; ILE 853; PHE 856; THR 854; ASP 855
6.	Limonene	-5.79	57.05	VAL 769; CYS 775; LEU 777; ARG 776; PHE 856; THR 790; MET 766; THR 854; LYS 745; LEU 858;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
7.	3-Carene	-5.51	91.50	THR 790; THR 854; LEU 858;PHE 856; LEU 788; MET 766; ASP 855; LEU 777; CYS 775; ARG 776
8.	beta-Myrcene	-5.27	138.16	ARG 776; PHE 856; THR 854; MET 766; ASP 855; LEU 788; LYS 745; LEU 858; CYS 775; THR 790; LEU 777
9.	alpha-Terpinolene	-5.93	45.11	LEU 788; LYS 745; THR 790; ARG 776; CYS 775; PHE 856; MET 766; ASP 855; LEU 777; THR 854
10.	Umbelliferone	-6.68	12.73	LYS 745; ASP 855; THR 790; ARG 776; PHE 856; LEU 777; THR 854; MET 766; LEU 788; CYS 775; LEU 858

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
11.	Anisaldehyde	-4.83	290.42	LEU 788; LYS 745; LEU 777; ASP 855; CYS 775; ILE 853; PHE 856; THR 854; MET 766;THR 790
12.	Gentisic acid	-6.65	13.40	PHE 856; LEU 788; ASP 855; LYS 745; LEU 858; MET 766; THR 854; CYS 775; LEU 777;ARG 776
13.	Syringic acid	-6.59	14.85	LEU 788; THR 790; LYS 745; LEU 777; ARG 776; CYS 775; THR 854; MET 766; PHE 856; LEU 858; ASP 855
14.	(E)-Anethole	-5.42	106.58	PHE 856; MET 766; ASP 855; LEU 777; THR 854; LEU 788; VAL 726; ILE 744; ILE 789; ALA 743; THR 790; LYS 745; CYS 775

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
15.	Apiol	-7.02	7.18	LEU 858; PHE 856; ASP 855; THR 854; CYS 775; MET 766; ARG 776; LEU 777; THR 790; LEU 788; ILE 744; ALA 743; ILE 789; LYS 745
16.	Methyl chavicol	-5.40	109.55	PHE 856; MET 766; ASP 855; THR 854; LEU 777; CYS 775; LEU 788; THR 790; ALA 743; LYS 745; ILE 744; ILE 789; VAL 726
17.	Ferulic acid	-6.76	11.13	THR 854; ASP 855; LEU 777; VAL 726; LYS 745; ILE 744; ALA 743; ILE 789; LEU 788; THR 790; MET 766; LEU 858; PHE 856

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
18.	Camphene	-6.27	25.56	ARG 776; THR 790; THR 854; LEU 788; ASP 855; MET 766; LEU 777; PHE 856; CYS 775
19.	Sinapic acid	-6.46	18.42	ASN 842; LYS 745; LEU 858; ASP 855; LEU 788; VAL 726; THR 854; THR 790; LEU 844; ALA 743; LEU 792; GLN 791; MET 793
20.	Fenchone	-6.90	8.70	ARG 776; PHE 856; LEU 777; MET 766; THR 790; LEU 788; ASP 855; CYS 775; THR 854; ILE 853
21.	Linalool	-5.69	67.10	LEU 858; THR 790; VAL 726; ILE 744; ILE 789; LYS 745; ALA 743; LEU 777; LEU 788; ARG 776; MET 766; CYS 775; PHE 856; ASP 855; THR 854

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
22.	Stigmasterol	-11.93	1.80	ASN 843; LEU 844; MET 766; ARG 776; THR 854; ASP 855; LEU 777; CYS 775; PHE 856; LEU 858; LEU 788; THR 790; ILE 789; LYS 745; VAL 726; ALA 743; CYS 797; ARG 841
23.	Juglanin	-9.18	186.31	PHE 723; ASP 855; THR 854; LYS 745; LEU 858; LEU 788; ILE 789; THR 790; LEU 777; ILE 744; LEU 844; ALA 743; LEU 718; VAL 726; GLY 796; PHE 997; CYS 797; ARG 841; ASN 842
24.	Guaijaverin	-9.40	129.68	ASN 842; ARG 841; CYS 797; LEU 792; MET 793; LEU 1001; GLY 796; PHE 997; LEU 844; ALA 743; VAL 726; LEU 718; THR 790; ILE 789; 777;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
25.	Miquelianin	-9.75	70.91	CYS 775; GLN 791; LEU 792; MET 793; THR 790; ALA 743; LEU 844; THR 854; MET 766; LEU 777; PHE 856; ASP 855; LEU 858; LEU 788; LYS 745; VAL 726; LEU 718; CYS 797; ARG 841; ASN 842
26.	Platanoside	-10.48	20.82	PRO 794; PHE 997; MET 793; GLN 791; CYS 775; ASP 855; THR 854; THR 790; PHE 856; VAL 769; ARG 776; ALA 767; MET 766; LEU 777; LEU 788; LEU 858; LEU 747; ASN 842; ARG 841; LYS 745; PHE 723; ALA 722; GLY 721; SER 720; THR 725; GLY 724; GLY 719; VAL 726; CYS 797; ALA 743; LEU 844; LEU 718; GLY 796; LEU 792; LEU 1001

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
27.	(+)-Limonene	-5.79	57.48	LEU 788; LEU 858; PHE 856; LEU 777; ASP 855; MET 766; CYS 775; THR 854; THR 790; ARG 776
28.	beta-Phellandrene	-6.14	31.75	PHE 856; LEU 858; MET 766; ASP 855; THR 790; ARG 776; LEU 777; CYS 775; THR 854; LEU 788
29.	(-)-Fenchone	-6.77	10.90	CYS 775; THR 790; THR 854; LEU 777; MET 766; LEU 858; LEU 788; ASP 855; PHE 856; ARG 776
30.	Germacrene D	-6.76	11.03	MET 766; ASP 855; PHE 856; ASN 842; THR 854; VAL 726; ALA 743; LYS 745; ILE 744; ILE 789; LEU 788; THR 790; LEU 777; LEU 858

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
31.	Miyabenol C	+16.43		
32.	Oleanolic acid	-9.54	101.96	MET 766; LEU 788; LEU 858; ASP 855; LYS 745; ARG 841; CYS 797; GLY 719; LEU 718; LEU 844; VAL 726; THR 854; THR 790; ASN 842; CYS 775; LEU 777; ALA 743
33.	trans-Anethol	-5.41	107.43	PHE 856; MET 766; ASP 855; LEU 777; THR 854; LEU 788; ILE 744; ILE 789; VAL 726; ALA 743; THR 790; LYS 745; CYS 775
34.	(E)-beta-Ocimene	-5.40	109.63	ILE 789; ILE 744; VAL 726; LYS 745; THR 790; ALA 743; LEU 777; THR 854; ASP 855; LEU 788; MET 766; PHE 856; ARG 776; CYS 775

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
35.	4-Carene	-6.20	28.42	ARG 776; LEU 777; CYS 775; THR 854; PHE 856; ASP 855; LEU 858; LEU 788; THR 790; VAL 769; MET 766
36.	Cinnamic acid	-5.92	45.89	MET 766; ARG 776; PHE 856; CYS 775; ILE 853; THR 854; ASP 855; ILE 744; THR 790; ALA 743; LEU 788; ILE 789; LYS 745; LEU 777
37.	Glucosyringic acid	-4.73	340.82	CYS 797; LYS 745; ASP 855; ASN 842; THR 854; ARG 841; VAL 843; THR 790; VAL 726; LEU 718; GLN 791; ALA 743; LEU 792; LEU 844; MET 793; GLY 796
38.	Quinic acid	-6.46	18.26	THR 790; THR 854; LEU 777; CYS 775; ARG 776; MET 766; PHE 856; GLY 857; LEU 858

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
39.	7alpha-Hydroxycampesterol	-11.05	8.00	ARG 841; ASN 842; LEU 844; THR 854; CYS 775; ASP 855; ARG 776; PHE 856; LEU 777; LEU 788; MET 766; ALA 743; THR 790; VAL 726; ILE 789;
40.	Benzaldehyde	-4.90	257.29	LEU 858; LEU 777; PHE 856; THR 854; MET 766; LEU 788; ASP 855; CYS 775; ARG 776
41.	cis-Miyabenol C	+5.43		
42.	alpha-Tocotrienol	-11.31	5.13	PHE 856; ASP 855; LEU 788; LEU 858; MET 766; THR 854; CYS 797; GLN 791; LEU 792; MET 793; LEU 844; GLY 796; ALA 743; LEU 718; VAL 726; THR 790; LYS 745; CYS 775;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
43.	beta-Tocotrienol	-11.01	8.54	PHE 997; GLY 796; LEU 788; LEU 858; PHE 856; GLY 857; MET 766; ASP 855; THR 854; CYS 775; ARG 776; LEU 777; LYS 745; THR 790; ALA 743; VAL 726; GLY 719; LEU 718; CYA 797; LEU 844; LEU 792; MET 793
44.	delta-Tocotrienol	-10.61	16.75	VAL 769; MET 766; PHE 856; LEU 777; LEU 858; THR 854; ASP 855; LEU 788; LYS 745; ALA 743; LEU 844; GLN 791; MET 793; GLY 796; VAL 726; THR 790; LEU 792; LEU 718; LEU 1001; CYS 775; ARG 776

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
45.	gamma-Tocotrienol	-10.62	16.39	PHE 856; MET 766; LEU 777; THR 854; THR 790; LEU 792; CYS 797; MET 793; LEU 718; ALA 743; LEU 844; GLN 791; GLY 796; VAL 726; LEU 788; LYS 745; ASP 855; LEU 858
46.	1,4-Dimethoxybenzene	-4.75	327.48	PHE 856; LEU 777; MET 766; THR 854; LEU 788; ILE 744; ILE 789; ALA 743; THR 790; LYS 745; ASP 855
47.	Erythro-Anethole glycol	-4.49	510.53	LEU 718; CYS 797; VAL 726; LEU 844; LYS 745; LEU 788; MET 766; PHE 856; LEU 777; ASP 855; THR 854; ALA 743; THR 790; ARG 841; ASN 842

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
48.	2,6-Dimethyl-2,4,6-octatriene	-5.73	62.89	LYS 745; ALA 743; LEU 777; MET 766; THR 854; ASP 855; LEU 788; PHE 856; ARG 776; CYS 775; THR 790; ILE 789
49.	beta-Terpineol	-5.64	73.79	ARG 841; LYS 745; ASN 842; ASP 855; PHE 856; MET 766; VAL 726; LEU 777; ALA 743; THR 854; THR 790; LEU 788; ILE 744; LEU 718; LEU 844; GLY 719; CYS 797
50.	cis-2,8-Menthadien-1-ol	-5.92	45.73	ARG 776; PHE 856; THR 854; LEU 788; LEU 777; MET 766; LEU 858; ASP 855; LYS 745; THR 790; CYS 775
52.	1-(3-Methoxyphenyl)-1-propanone	-6.22	27.71	ILE 853; LEU 858; LYS 745; LEU 788; PHE 856; MET 766; ASP 855; LEU 777; ARG 776; CYS 775; THR 854

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
53.	1,6-Hexanediol	-3.73	1.86	MET 766; PHE 856; LEU 777; LEU 858; LYS 745; LEU 788; ASP 855; CYS 775; VAL 774; ILE 853; THR 854; ARG 776
54.	2-Cyclohexen-1-ol	-4.72	344.85	ARG 776; CYS 775; THR 790; THR 854; LEU 788; PHE 856; ASP 855; LEU 777; MET 766
55.	2-Methoxycyclohexanone	-5.24	143.20	PHE 856; LEU 858; ASP 855; THR 790; MET 766; LEU 777; CYS 775; THR 854; LEU 788; ARG 776
56.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-ol	-6.23	26.94	ARG 776; CYS 775; MET 766; PHE 856; LEU 777; LEU 788; THR 790; THR 854; LYS 745; LEU 858; ASP 855
57.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one	-6.21	27.90	LEU 788; LEU 777; ASP 855; MET 766; PHE 856; ARG 776; CYS 775; THR 854; THR 790;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
58.	Benzothiazole	-5.18	158.28	ARG 776; LEU 777; THR 790; ASP 855; THR 854; MET 766; LEU 788; CYS 775; PHE 856;
59.	cis-Limonene oxide	-5.91	46.61	LEU 788; LYS 745; ASP 855; LEU 777; CYS 775; PHE 856; THR 854; ARG 776; MET 766; THR 790
60.	Fenchyl acetate	-7.29	4.53	ARG 776; MET 766; LEU 858; PHE 856; ASP 855; LEU 788; LEU 777; THR 854; CYS 775; THR 790
61.	trans-Limonene oxide	-6.27	25.30	LEU 788; THR 790; ARG 776; MET 766; CYS 775; PHE 856; THR 854; LEU 777; ASP 855; LYS 745

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
62.	trans-p-2,8-menthadien-1-ol	-6.34	22.57	LYS 745; LEU 858; MET 766; LEU 777; PHE 856; ARG 776; CYS 775; VAL 774; ILE 853; THR 854; THR 790; LEU 788; ASP 855
63.	Acetanisole	-5.57	82.00	PHE 856; THR 790; ALA 743; ILE 744; LEU 788; LYS 745; LEU 777; MET 766; ASP 855; ARG 776; CYS 775; THR 854
64.	beta-Elemenone	-6.47	18.18	ASP 855; THR 854; MET 766; LEU 844; VAL 726; THR 790; ALA 743; LEU 777; ILE 789; LYS 745; LEU 858; LEU 788

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
65.	2-Deoxy-L-ribono-1,4-lactone	-4.99	221.24	VAL 774; CYS 775; ARG 776; VAL 769; LEU 777; MET 766; PHE 856; ASP 855; THR 854; THR 790
66.	Isopentyl-beta-D-glucoside	-5.52	140.59	LEU 844; LYS 745; ASP 855; VAL 726; THR 790; CYS 775; MET 766; LEU 777; ARG 776; PHE 856; LEU 788; ILE 789;
67.	Syringin methyl ether	-5.69	67.14	ARG 841; CYS 797; LEU 718; GLY 719; THR 790; ALA 743; LEU 844; PHE 856; MET 766; CYS 775; LEU 777; ASP 855; VAL 726; LEU 788; THR 854; ASN 842; LYS 745

LAMPIRAN IV
(LANJUTAN)

Tabel VI.2
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
68.	Sphalleroside A	-5.79	56.96	LEU 777; MET 766; LYS 745; PHE 856; ASP 855; ASN 842; ARG 841; LEU 844; THR 854; VAL 726; ALA 743; THR 790; ILE 744; ILE 789; LEU 788
69.	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	-3.5	2.74	GLY 719; LEU 718; THR 854; VAL 726; LEU 844; ASP 855; CYS 797; ASN 842; ARG 841; LYS 745; THR 790; ALA 743; GLN 791; LEU 792; MET 793;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
Nilai ΔG, Nilai Ki, dan Interaksi Residu Asam Amino Ligan Uji dengan Ligan Alami (*Epidermal Growth Factor Receptor*) Kode PDB 3W32

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
1.	Syringin	-4.50	500.49	ARG 841; CYS 797; ASN 842; ASP 855; THR 854; VAL 726; ILE 744; LEU 788; ILE 789; LEU 777; LEU 718; THR 790; ALA 743; LYS 745; LEU 792; MET 793; LEU 844; GLY 719
2.	1,8-cineole	-6.59	14.76	CYS 775; ARG 776; MET 766; THR 790; LEU 788; LEU 777; LEU 858; LYS 745; ASP 855; PHE 856; THR 854
3.	Seselin	-7.73	2.16	VAL 726; ALA 743; LYS 745; LEU 788; GLY 857; LEU 858; MET 766; LEU 777; PHE 856; ASP 855; THR 854;CYS 775; THR790

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
4.	beta-Pinene	-6.04	37.59	LEU 858; THR 854; ASP 855; THR 790; CYS 775; ARG 776; PHE 856; LEU 788; MET 766; LEU 777
5.	Camphor	-5.66	71.42	MET 793; ALA 743; LEU 792; VAL 726; LEU 1001; LEU 718; PHE 997; CYS 797; GLY 796; LEU 844
6.	Limonene	-5.90	47.25	LEU 858; LYS 745; LEU 788; THR 854; THR 790; ARG 776; PHE 856; LEU 777; CYS 775; ASP 855; MET 766
7.	3-Carene	-5.66	70.49	THR 790; THR 854; PHE 856; MET 766; LEU 858; ASP 855; LEU 788; LEU 777; ARG 776; CYS 775

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
8.	beta-Myrcene	-5.26	138.98	LEU 788; LYS 745; LEU 858; LEU 777; ASP 855; PHE 856; THR 854; THR 790; MET 766; ARG 776; CYS 775
9.	alpha-Terpinolene	-6.02	38.89	ASP 855; ARG 776; THR 790; CYS 775; THR 854; PHE 856; LEU 777; LEU 788; MET 766; LYS 745; LEU 858
10.	Umbelliferone	-6.98	7.61	LEU 747; ASP 855; THR 854; ARG 776; CYS 775; PHE 856; LEU 777; LEU 788; MET 766; LEU 858; LYS 745
11.	Anisaldehyde	-5.22	150.29	THR 790; ARG 776; CYS 775; MET 766; LEU 777; THR 854; PHE 856

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
12.	Gentisic acid	-5.54	86.24	THR 790; THR 854; ARG 776; CYS 775; PHE 856; MET 766; LEU 788; LEU 777; LEU 858; LYS 745; ASP 855
13.	Syringic acid	-6.27	25.19	MET 766; LEU 858; PHE 856; ASP 855; LEU 788; LYS 745; THR 854; THR 790; CYS 775; LEU 777; ARG 776
14.	(E)-Anethole	-5.38	114.13	PHE 856; MET 766; ASP 855; THR 790; ALA 743; ILE 744; LYS 745; VAL 726; LEU 777; LEU 788; THR 854
15.	Apiol	-7.10	6.27	ILE 789; LYS 745; LEU 788; LEU 858; MET 766; ASP 855; CYS 775; PHE 856; THR 854; ARG 776; LEU 777

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
16.	Methyl chavicol	-5.45	100.48	PHE 856; MET 766; ASP 855; LEU 777; LEU 788; THR 790; ILE 789; ILE 744; ALA 743; LYS 745; VAL 726; THR 854
17.	Ferulic acid	-6.45	18.61	VAL 726; ALA 743; ILE 744; LYS 745; ILE 789; LEU 788; THR 790; ASP 855; MET 766; LEU 858; CYS 775; PHE 856; ARG 776; THR 854; LEU 777
18.	Camphene	-6.28	24.96	LEU 858; THR 790; LEU 777; CYS 775; MET 766; PHE 856; ARG 776; ASP 855; THR 854; LEU 788

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
19.	Sinapic acid	-5.81	55.26	PHE 997; CYS 797; GLY 796; LEU 792; MET 793; PRO 794; ALA 743; THR 790; GLN 791; LEU 844; VAL 726; THR 854; LYS 745; ASP 855
20.	Fenchone	-6.71	12.11	LEU 777; PHE 856; MET 766; ARG 776; THR 854; CYS 775; ASP 855; THR 790; LEU 788
21.	Linalool	-5.72	63.67	ALA 743; LEU 788; THR 854; ASP 855; LEU 777; CYS 775; PHE 856; ARG 776; MET 766; THR 790; VAL 726; ILE 789; LYS 745

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
22.	Stigmasterol	-12.47	723.47	CYS 797; PHE 997; GLY 796; MET 793; LEU 718; ALA 743; CYS 775; ARG 776; PHE 856; LEU 777; MET 766; LEU 788; LEU 858; ASP 855; LYS 745; THR 790; THR 854; ASN 842; VAL 726; ARG 841; LEU 844; ASP 800
23.	Juglanin	-8.35	755.31	ARG 841; CYS 797; LEU 718; LEU 1001; PHE 997; GLY 796; PRO 794; MET 793; LEU 792; LEU 844; ALA 743; THR 854; THR 790; VAL 726; ILE 789; LEU 788; LEU 777; ASP 855; LYS 745; LEU 858; ASN 842

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
24.	Guaijaverin	-8.66	445.63	ARG 841; CYS 797; MET 793; LEU 792; PRO 794; GLY 796; LEU 1001; PHE 997; LEU 718; ALA 743; VAL 726; LEU 844; THR 790; ILE 744; ILE 789; LEU 777; LEU 788; LYS 745; ASP 855; THR 854; LEU 858; GLY 721; SER 720; ASN 842
25.	Miquelianin	-9.71	76.41	ARG 841; CYS 797; LEU 792; MET 793; GLY 796; PRO 794; PHE 997; LEU 1001; LEU 844; ALA 743; LEU 718; THR 854; VAL 726; THR 790; LEU 788; LEU 777; ILE 789; ASP 855; LYS 745; LEU 858

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
26.	Platanoside	+5.87		
27.	(+)-Limonene	-6.09	34.36	ARG 776; CYS 775; LEU 777; THR 790; THR 854; PHE 856; LEU 788; MET 766; LYS 745; LEU 858; ASP 855
28.	beta-Phellandrene	-6.31	23.81	ASP 855; PHE 856; LEU 858; LEU 777; LEU 788; MET 766; THR 790; ARG 776; CYS 775; THR 854
29.	(-)-Fenchone	-6.72	11.85	CYS 775; THR 790; LEU 788; PHE 856; LEU 777; ASP 855; MET 766; ARG 776; THR 854
30.	Germacrene D	-6.75	11.33	LEU 858; ASP 855; PHE 856; ASN 842; VAL 726; THR 854; LYS 745; ALA 743; ILA 744; LEU 788

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
31.	Miyabenol C	+34.32		
32.	Oleanolic acid	-9.40	127.79	LEU 788; LEU 777; THR 790; ALA 743; VAL 726; LEU 718; GLY 719; ASP 800; ARG 841; CYS 797; LEU 844; GLY 796; ASN 842; THR 854; LYS 745; ASP 855; LEU 858
33.	trans-Anethol	-5.38	113.49	PHE 856; MET 766; ASP 855; THR 790; ILE 744; ALA 743; LYS 745; VAL 726; LEU 777; LEU 788; THR 854
34.	(E)-beta-Ocimene	-5.36	117.83	CYS 775; ARG 776; MET 766; LEU 777; ASP 855; PHE 856; THR 854; LYS 745; LEU 858; LEU 788; ILE 789; ALA 743

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
35.	4-Carene	-6.46	18.55	ARG 776; CYS 775; LEU 788; LYS 745; LEU 858; LEU 777; PHE 856; ASP 855; MET 766; THR 854
36.	Cinnamic acid	-5.75	60.81	PHE 856; CYS 775; ARG 776; THR 854; VAL 726; ALA 743; ILE 744; THR 790; ILE 789; LEU 788; LYS 745; ASP 855; LEU 777
37.	Glucosyringic acid	-5.12	176.15	ARG 841; PHE 997; GLY 796; CYS 797; LEU 718; LEU 1001; LEU 792; MET 793; GLN 791; LEU 844; VAL 726; ALA 743; THR 854; LYS 745; ASP 855; ASN 842; THR 790

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
38.	Quinic acid	-3.88	1.44	LEU 844; LYS 745; VAL 726; ASN 842; THR 854; ASP 855; LEU 777; THR 790; LEU 788
39.	7alpha-Hydroxycampesterol	-12.06	1.44	ASN 842; ARG 841; LEU 844; ASP 800; CYS 797; PHE 997; GLY 796; LEU 718; VAL 726; ALA 743; CYS 775; ASP 855; LYS 745; ARG 776; PHE 856; MET 766; LEU 788; THR 790; LEU 777; THR 854
40.	Benzaldehyde	-4.95	233.71	CYS 775; THR 854; ARG 776; PHE 856; LEU 777; MET 766; LEU 788; LEU 858; ASP 855
41.	cis-Miyabenol C	+1.52		

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
42.	alpha-Tocotrienol	-9.28	157.33	LEU 788; ILE 789; ILE 744; LYS 745; THR 790; ARG 841; LEU 792; GLN 791; LEU 844; MET 793; CYS 797; GLY 796; LEU 1001; LEU 718; PHE 997; ALA 743; ASP 800; VAL 726; ASN 842; ASP 855; LEU 777; THR 854
43.	beta-Tocotrienol	-9.88	57.30	PHE 856; THR 854; LEU 777; ASP 855; MET 766; LEU 788; LEU 858; CYS 797; ARG 841; PHE 997; LEU 718; GLY 796; MET 793; LEU 844; ASN 842; ALA 743; GLN 791; LEU 792; VAL 726; THR 790; LYS 745; CYS 775; ARG 776
44.	delta-Tocotrienol	-8.84	333.27	LEU 1001; GLY 796; MET 793; LEU 792; ASP 855; LEU 858; LYS 745; ILE 744; ILE 789; THR 790; LEU 718; LEU 788; LEU 844; ALA 743; THR 854; VAL 726

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
45.	gamma-Tocotrienol	-8.94	279.66	LEU 858; LEU 788; THR 854; LYS 745; ILE 744; GLY 719; VAL 726; LEU 718; THR 790; ASP 800; PHE 997; CYS 797; LEU 884; ALA 743; LEU 792; MET 793; GLY 796; GLN 791; ASN 842; ASP 855; LEU 777
46.	1,4-Dimethoxybenzene	-4.79	305.90	MET 766; ASP 855; PHE 856; THR 854; LEU 777; LEU 788; ILE 789; ILE 744; ALA 743; THR 790; LYS 745
47.	Erythro-Anethole glycol	-4.76	323.22	LEU 718; LEU 844; ALA 743; THR 854; VAL 726; LEU 788; LEU 858; ASP 855; LYS 745; THR 790; LEU 792; MET 793;

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
48.	2,6-Dimethyl-2,4,6-octatriene	-5.69	67.15	ILE 789; ALA 743; LYS 745; LEU 777; LEU 788; MET 766; ASP 855; PHE 856; CYS 775; ARG 776; THR 854; THR 790; ILE 744; VAL 726
49.	beta-Terpineol	-4.59	433.08	GLY 719; LEU 844; LEU 718; LEU 792; MET 793; ALA 743; LEU 777; ILE 789; LEU 788; THR 790; ILE 744; VAL 726; LYS 745; THR 854; ASP 855; ARG 841; CYS 797; ASN 842
50.	cis-2,8-Menthadien-1-ol	-5.88	48.76	ARG 776; MET 766; PHE 856; LEU 858; ASP 855; LYS 745; LEU 788; THR 854; THR 790; LEU 777; CYS 775

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
51.	Melatonin	-7.32	4.28	THR 854; ASP 855; GLY 996; PHE 856; LEU 792; MET 793; GLN 791; LEU 844; VAL 726; ALA 743; ILE 744; LEU 788; ILE 789; LYS 745; THR 790; LEU 777
52.	1-(3-Methoxyphenyl)-1-propanone	-6.06	35.89	LEU 788; LEU 858; LEU 777; MET 766; ARG 776; PHE 856; THR 854; CYS 775; ASP 855; LYS 745; ALA 743; THR 790; ILE 789; ILE 744
53.	1,6-Hexanediol	-3.62	2.21	LEU 777; CYS 775; ARG 776; MET 766; PHE 856; LEU 788; LEU 858; LYS 745; ASP 855; THR 854; THR 790

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
54.	2-Cyclohexen-1-ol	-4.65	392.51	ARG 776; CYS 775; LEU 777; THR 790; THR 854; ASP 855; MET 766; LEU 788; PHE 856
55.	2-Methoxycyclohexanone	-5.12	176.11	THR 790; LEU 777; LEU 788; CYS 775; THR 854; ARG 776; MET 766; PHE 856; ASP 855
56.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-ol	-6.21	27.88	LEU 858; ASP 855; LYS 745; LEU 788; MET 766; THR 854; LEU 777; CYS 775; ARG 776; THR 790; PHE 856
57.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one	-6.37	21.39	THR 790; THR 854; LEU 777; LEU 788; ASP 855; LYS 745; MET 766; LEU 858; PHE 856; ARG 776; CYS 775

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
58.	Benzothiazole	-5.42	107.01	ASP 855; THR 854; ARG 776; THR 790; CYS 775; LEU 777; LEU 788; MET 766; LEU 858; PHE 856
59.	cis-Limonene oxide	-6.41	20.12	LYS 745; LEU 788; PHE 856; MET 766; THR 790; LEU 777; ARG 776; CYS 775; THR 854; ASP 855; LEU 858
60.	Fenchyl acetate	-7.05	6.74	LEU 858; LYS 745; LEU 788; THR 790; CYS 775; LEU 777; ARG 776; MET 766; PHE 856; ASP 855; THR 854
61.	trans-Limonene oxide	-6.31	23.76	LEU 788; LYS 745; PHE 856; THR 854; ASP 855; MET 766; CYS 775; ARG 776; LEU 777; THR 790

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
62.	trans-p-2,8-menthadien-1-ol	-6.41	19.94	LEU 858; ASP 855; ARG 776; THR 854; CYS 775; PHE 856; MET 766; THR 790; LEU 777; LEU 788; LYS 745
63.	Acetanisole	-5.60	78.16	MET 766; PHE 856; THR 854; CYS 775; ASP 855; THR 790; ILE 789; ILE 744; ALA 743; LYS 745; LEU 777; LEY 788
64.	beta-Elemenone	-6.50	17.14	LEU 844; VAL 726; THR 790; ALA 743; ILE 744; ILE 789; LYS 745; LEU 858; LEU 788; LEU 777; ASP 855; THR 854; ASN 842

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
65.	2-Deoxy-L-ribono-1,4-lactone	-4.55	436.67	ARG 776; CYS 775; LEU 777; ASP 855; MET 766; PHE 856; LEU 858; THR 854; LEU 788; THR 790
66.	Isopentyl-beta-D-glucoside	-4.95	236.27	MET 766; ARG 776; CYS 775; LEU 788; ILE 789; THR 790; ILE 744; ALA 743; LYS 745; VAL 726; LEU 844; THR 854; ASP 855; LEU 777; PHE 856
67.	Syringin methyl ether	-5.58	80.65	CYS 797; LEU 718; GLY 796; LEU 792; ALA 743; THR 790; ILE 744; LEU 777; THR 854; LYS 745; ASP 855; LEU 788; VAL 726; ASN 842; LEU 844; ARG 841

LAMPIRAN IV
(LANJUTAN)

Tabel VI.3
(Lanjutan)

No	Senyawa	ΔG (kkal/mol)	KI (nM)	Residu Asam Amino
68.	Sphalleroside A	-5.52	89.65	LEU 718; PHE 997; LEU 1001; GLY 796; PRO 794; LEU 792; MET 793; CYS 797; LEU 844; ARG 841; THR 854; ASN 842; ASP 855; ALA 743; VAL 726; THR 790; LEU 788; LYS 745
69.	1,2,10-Trihydroxydihydro- trans-linalyl oxide 7-O-beta-D-glucopyranoside	-3.13	5.09	LYS 745; ASP 855; THR 854; THR 790; ALA 743; GLN 791; GLY 796; LEU 792; MET 793; PHE 997; LEU 844; VAL 726; LEU 718; CYS 797; ASN 842; ARG 841

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
Lipinski Rule of Five Ligan Uji

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
1.	Syringin	372	2.083250	5	9	Tidak sesuai syarat
2.	1,8-cineole	154	2.858119	0	1	Sesuai syarat
3.	Seselin	228	2.037670	0	3	Sesuai syarat
4.	beta-Pinene	136	2.467649	0	0	Sesuai syarat
5.	Camphor	152	2.192240	0	1	Sesuai syarat
6.	Limonene	136	2.532510	0	0	Sesuai syarat
7.	3-Carene	136	2.654899	0	0	Sesuai syarat
8.	beta-Myrcene	136	2.664829	0	0	Sesuai syarat
9.	alpha-Terpinolene	136	2.654899	0	0	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
10.	Umbelliferone	162	0.576230	1	3	Sesuai syarat
11.	Anisaldehyde	136	1.502140	0	2	Sesuai syarat
12.	Gentisic acid	154	-0.067150	3	4	Sesuai syarat
13.	Syringic acid	198	0.861640	2	5	Sesuai syarat
14.	(E)-Anethole	148	2.204120	0	1	Sesuai syarat
15.	Apiol	222	2.277110	0	4	Sesuai syarat
16.	Methyl chavicol	148	2.266930	0	1	Sesuai syarat
17.	Ferulic acid	194	0.556120	2	4	Sesuai syarat
18.	Camphene	136	2.786439	0	0	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
19.	Sinapic acid	224	0.781620	2	5	Sesuai syarat
20.	Fenchone	152	2.570120	0	1	Sesuai syarat
21.	Linalool	154	2.611600	1	1	Sesuai syarat
22.	Stigmasterol	412	7.541615	1	1	Tidak sesuai syarat
23.	Juglanin	418	1.136320	6	10	Tidak sesuai syarat
24.	Guaijaverin	434	1.014510	7	11	Tidak sesuai syarat
25.	Miquelianin	478	0.687700	8	13	Tidak sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
26.	Platanoside	724	3.561149	6	14	Tidak sesuai syarat
27.	(+)-Limonene	136	2.532510	0	0	Sesuai syarat
28.	beta-Phellandrene	136	2.543010	0	0	Sesuai syarat
29.	(-)-Fenchone	152	2.263030	0	1	Sesuai syarat
30.	Germacrene D	204	3.838959	0	0	Sesuai syarat
31.	Miyabenol C	680	4.155020	7	9	Tidak sesuai syarat
32.	Oleanolic acid	456	7.015814	2	3	Tidak sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
33.	trans-Anethol	148	2.204120	0	1	Sesuai syarat
34.	(E)-beta-Ocimene	136	2.797719	0	0	Sesuai syarat
35.	4-Carene	136	2.703409	0	0	Sesuai syarat
36.	Cinnamic acid	148	0.744450	1	2	Sesuai syarat
37.	Glucosyringic acid	360	1.330870	5	10	Tidak Sesuai syarat
38.	Quinic acid	192	0.353730	5	6	Sesuai syarat
39.	7alpha-Hydroxycampesterol	416	7.150024	2	2	Tidak sesuai syarat
40.	Benzaldehyde	106	1.390670	0	1	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
41.	cis-Miyabenol C	680	4.155020	7	9	Tidak Sesuai syarat
42.	alpha-Tocotrienol	424	7.014814	1	2	Tidak Sesuai syarat
43.	beta-Tocotrienol	410	6.708523	1	2	Tida sesuai syarat
44.	delta-Tocotrienol	396	6.224242	1	2	Tidak sesuai syarat
45.	gamma-Tocotrienol	410	6.708523	1	2	Tidak sesuai syarat
46.	1,4-Dimethoxybenzene	138	1.676740	0	2	Sesuai syarat
47.	Erythro-Anethole glycol	182	1.781010	2	3	Sesuai Syarat
48.	2,6-Dimethyl 2,4,6-octatriene	136	2.772919	0	0	Sesuai Syarat
49.	beta-Terpineol	154	2.590599	1	1	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
50.	cis-2,8-Menthadien-1-ol	152	2.386600	1	1	Sesuai syarat
51.	Melatonin	232	2.000390	2	2	Sesuai syarat
52.	1-(3-Methoxyphenyl)-1-propanone	164	2.064320	0	2	Sesuai syarat
53.	1,6-Hexanediol	118	1.484140	2	2	Sesuai syarat
54.	2-Cyclohexen-1-ol	98	1.344440	1	1	Sesuai syarat
55.	2-Methoxycyclohexanone	128	1.691930	0	2	Sesuai syarat
56.	2-Methyl-5 (1 -methylethyl)-2-cyclohexen-1-ol	154	2.590600	1	1	Sesuai syarat
57.	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one	152	2.536099	0	1	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
58.	Benzothiazole	135	0.387370	0	0	Sesuai syarat
59.	cis-Limonene oxide	152	2.546599	0	1	Sesuai syarat
60.	Fenchyl acetate	196	3.053399	0	2	Sesuai syarat
61.	trans-Limonene oxide	152	2.546599	0	1	Sesuai syarat
62.	trans-p-2,8-menthadien-1- ol	152	2.386600	1	1	Sesuai syarat
63.	Acetanisole	150	1.720020	0	2	Sesuai syarat
64.	beta-Elemenone	218	3.628049	0	1	Sesuai syarat
65.	2-Deoxy-L-ribono-1,4-lactone	132	0.490250	2	4	Sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.4
(Lanjutan)

No	Senyawa	BM <500 Da	Log P < 5	DIH <5	AIH <5	Kesimpulan
66.	Isopentyl-bet D- glucoside	250	1.995390	4		Tidak sesuai syarat
67.	Syringin methyl ether	386	2.776040	4	9	Tidak sesuai syarat
68.	Sphalleroside A	342	2.126060	5	8	Tidak sesuai syarat
69.	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	382	2.304640	7	10	Tidak sesuai syarat

LAMPIRAN IV
(LANJUTAN)

Tabel VI.5
Tabel ADME *Prediction* Senyawa Uji

No	Senyawa	$CaCO_2$	HIA	PPB
1	Syringin	14.3612	34.837429	34.526515
2	1,8-cineole	21.895	100.000000	100.000000
3	Seselin	32.2667	98.961540	85.700243
4	beta-Pinene	23.4924	100.000000	100.000000
5	Camphor	26.8158	100.000000	100.000000
6	Limonene	26.8158	100.000000	100.000000
7	3-Carene	23.6313	100.000000	100.000000
8	beta-Myrcene	23.6306	100.000000	100.000000
9	alpha-Terpinolene	23.6372	100.000000	93.161811
10	Umbelliferone	19.518	94.174367	42.394871
11	Anisaldehyde	31.3663	100.000000	36.109900
12	Gentisic acid	18.3041	74.750381	69.613276
13	Syringic acid	18.8327	82.027960	69.775772
14	(E)-Anethole	58.0893	100.000000	89.239441
15	Apiol	57.2419	98.888727	88.847870
16	Methyl chavicol	58.0905	100.000000	100.000000
17	Ferulic acid	21.1177	90.603297	50.414225
18	Camphene	23.4938	100.000000	100.000000
19	Sinapic acid	19.854	88.553867	47.507982
20	Fenchone	26.8574	100.000000	100.000000

LAMPIRAN IV
(LANJUTAN)

Tabel VI.5
(Lanjutan)

No	Senyawa	$CaCO_2$	HIA	PPB
21	Linalool	29.355	100.000000	100.000000
22	Stigmasterol	52.3376	100.000000	100.000000
23	Juglanin	7.88817	43.519546	62.738307
24	Guaijaverin	6.60347	22.624249	61.953580
25	Miquelianin	11.5076	7.398706	62.015896
26	Platanoside	15.1515	83.451446	100.000000
27	(+)-Limonene	21.1416	100.000000	100.000000
28	beta-Phellandrene	23.4151	100.000000	91.196226
29	(-)-Fenchone	26.8574	100.000000	100.000000
30	Germacrene D	23.4009	100.000000	100.000000
31	Miyabenol C	13.028	90.272965	100.000000
32	Oleanolic acid	21.8872	95.996305	100.000000
33	trans-Anethol	58.0893	100.000000	89.239441
34	(E)-beta-Ocimene	23.6338	100.000000	100.000000
35	4-Carene	23.4019	100.000000	100.000000
36	Cinnamic acid	21.0342	97.845200	60.852531
37	Glucosyringic acid	17.2014	22.193699	36.691099
38	Quinic acid	8.27242	20.286936	6.595022
39	7alpha-Hydroxycampesterol	34.5829	94.118953	100.000000
40	Benzaldehyde	21.8774	100.000000	4.508017

LAMPIRAN IV
(LANJUTAN)

Tabel VI.5
(Lanjutan)

No	Senyawa	$CaCO_2$	HIA	PPB
41	cis-Miyabenol C	13.028	90.272965	100.000000
42	alpha-Tocotrienol	29.1335	97.915683	100.000000
43	beta-Tocotrienol	27.948	97.907022	100.000000
44	delta-Tocotrienol	26.8337	97.894118	100.000000
45	gamma-Tocotrienol	24.5371	97.180256	100.000000
46	1,4-Dimethoxybenzene	56.8546	100.000000	100.000000
47	Erythro-Anethole glycol	21.765	100.000000	100.000000
48	2,6-Dimethyl-2,4,6-octatriene	23.43	100.000000	98.874999
49	beta-Terpineol	50.8083	100.000000	21.989862
50	cis-2,8-Menthadien-1-ol	50.7099	100.000000	40.475563
51	Melatonin	2.75681	88.229198	47.393021
52	1-(3-Methoxyphenyl)-1-propanone	53.2132	100.000000	100.000000
53	1,6-Hexanediol	20.0344	83.606083	0.000000
54	2-Cyclohexen-1-ol	22.557	100.000000	90.536825
55	2-Methoxycyclohexanone	44.713	100.000000	100.000000
56	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-ol	38.7293	100.000000	99.394792
57	2-Methyl-5-(1-methylethyl)-2-cyclohexen-1-one	47.8983	100.000000	100.000000
58	Benzothiazole	54.9158	98.290171	100.000000

LAMPIRAN IV
(LANJUTAN)

Tabel VI.5
(Lanjutan)

No	Senyawa	$CaCO_2$	HIA	PPB
59	cis-Limonene oxide	53.6813	100.000000	46.627930
60	Fenchyl acetate	37.6774	100.000000	82.919955
61	trans-Limonene oxide	53.6813	100.000000	46.627930
62	trans-p-2,8-menthadien-1-ol	50.7099	100.000000	40.475563
63	Acetanisole	50.5066	100.000000	34.311856
64	beta-Elemenone	52.9102	100.000000	100.000000
65	2-Deoxy-L-ribono-1,4-lactone	11.2418	69.678205	80.476207
66	Isopentyl-beta-D-glucoside	1.71332	47.170571	54.154490
67	Syringin methyl ether	14.6478	66.261349	39.258035
68	Sphalleroside A	9.55127	51.753609	52.668817
69	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-glucopyranoside	8.12074	7.940541	20.732551

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
Tabel Toxicity *Prediction* Senyawa Uji

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
1	Syringin	Tidak Berisiko	-	-	no alert
2	1,8-cineole	Tidak Berisiko	-	-	no alert
3	Seselin	Negligible Risk	Structural alert	-	Structural alert
4	beta-Pinene	Tidak Berisiko	-	-	no alert
5	Camphor	Tidak Berisiko	-	-	no alert
6	Limonene	Tidak Berisiko	-	-	no alert
7	3-Carene	Tidak Berisiko	-	-	no alert
8	beta-Myrcene	Tidak Berisiko	-	-	no alert
9	alpha-Terpinolene	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (AmestTest)
			Genotoksik	Non Genotoksik	
10	Umbelliferone	Negligible Risk	Structural alert	-	Structural alert
11	Anisaldehyde	Negligible Risk	Structural alert	-	Structural alert
12	Gentisic acid	Tidak Berisiko	-	-	no alert
13	Syringic acid	Tidak Berisiko	-	-	no alert
14	(E)-Anethole	Tidak Berisiko	-	-	no alert
15	Apiol	Negligible Risk	Structural alert	Structural alert	Structural alert
16	Methyl chavicol	Negligible Risk	Structural alert	-	Structural alert
17	Ferulic acid	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	KroesTTC	Karsinogenik		Mutagen (AmestTest)
			Genotoksik	Non Genotoksik	
18	Camphene	Tidak Berisiko	-	-	no alert
19	Sinapic acid	Tidak Berisiko	-	-	no alert
20	Fenchone	Tidak Berisiko	-	-	no alert
21	Linalool	Tidak Berisiko	-	-	no alert
22	Stigmasterol	Tidak Berisiko	-	-	no alert
23	Juglanin	Tidak Berisiko	-	-	no alert
24	Guaijaverin	Tidak Berisiko	-	-	Structural alert
25	Miquelianin	Tidak Berisiko	-	-	Structural alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
26	Platanoside	Tidak Berisiko	-	-	no alert
27	(+)-Limonene	Tidak Berisiko	-	-	no alert
28	beta-Phellandrene	Tidak Berisiko	-	-	no alert
29	(-)-Fenchone	Tidak Berisiko	-	-	no alert
30	Germacrene D	Tidak Berisiko	-	-	no alert
31	Miyabenol C	Tidak Berisiko	-	-	no alert
32	Oleanolic acid	Tidak Berisiko	-	-	no alert
33	trans-Anethol	Tidak Berisiko	-	-	no alert
34	(E)-beta-Ocimene	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
35	4-Carene	Tidak Berisiko	-	-	no alert
36	Cinnamic acid	Tidak Berisiko	-	-	no alert
37	Glucosyringic acid	Tidak Berisiko	-	-	no alert
38	Quinic acid	Tidak Berisiko	-	-	no alert
39	7alpha-Hydroxycampesterol	Tidak Berisiko	-	-	no alert
40	Benzaldehyde	Negligible Risk	Structural alert	-	Structural alert
41	cis-Miyabenol C	Tidak Berisiko	-	-	no alert
42	alpha-Tocotrienol	Tidak Berisiko	-	-	no alert
43	beta-Tocotrienol	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
44	delta-Tocotrienol	Tidak Berisiko	-	-	no alert
45	gamma-Tocotrienol	Tidak Berisiko	-	-	no alert
46	1,4-Dimethoxybenzene	Tidak Berisiko	-	-	no alert
47	Erythro-Anethole glycol	Tidak Berisiko	-	-	no alert
48	2,6-Dimethyl-2,4,6-octatriene	Tidak Berisiko	-	-	no alert
49	beta-Terpineol	Tidak Berisiko	-	-	no alert
50	cis-2,8-Menthadien-1-ol	Tidak Berisiko	-	-	no alert
51	Melatonin	Tidak Berisiko	-	-	no alert
52	1-(3-Methoxyphenyl)-1-propanone	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
53	1,6-Hexanediol	Tidak Berisiko	-	-	no alert
54	2-Cyclohexen-1-ol	Tidak Berisiko	-	-	no alert
55	2-Methoxycyclohexanone	Tidak Berisiko	-	-	no alert
56	2-Methyl 5-(1-methyleth yl)-2-cyclohexen-1-ol	Tidak Berisiko	-	-	no alert
57	2-Methyl-5-(1-methyleth yl)-2-cyclohexen-1-one	Negligible Risk	Structural alert	-	Structural alert
58	Benzothiazole	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
59	cis-Limonene oxide	Negligible Risk	Structural alert	-	Structural alert
60	Fenchyl acetate	Tidak Berisiko	-	-	no alert
61	trans-Limonene oxide	Negligible Risk	Structural alert	-	Structural alert
62	trans-p-2,8-menthadien-1-ol	Tidak Berisiko	-	-	no alert
63	Acetanisole	Tidak Berisiko	-	-	no alert
64	beta-Elemenone	Negligible Risk	Structural alert	-	Structural alert
65	2-Deoxy-L-ribono-1,4-lactone	Tidak Berisiko	-	-	no alert
66	Isopentyl-beta-D-glucoside	Tidak Berisiko	-	-	no alert
67	Syringin methyl ether	Tidak Berisiko	-	-	no alert

LAMPIRAN IV
(LANJUTAN)

Tabel VI.6
(Lanjutan)

No	Senyawa	Kroes TTC	Karsinogenik		Mutagen (Amest Test)
			Genotoksik	Non Genotoksik	
68	Sphalleroside A	Negligible Risk	-	-	no alert
69	1,2,10-Trihydroxydihydro-trans- linalyl oxide 7-O-beta-D-glucopyranoside	Tidak Berisiko	-	-	no alert

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