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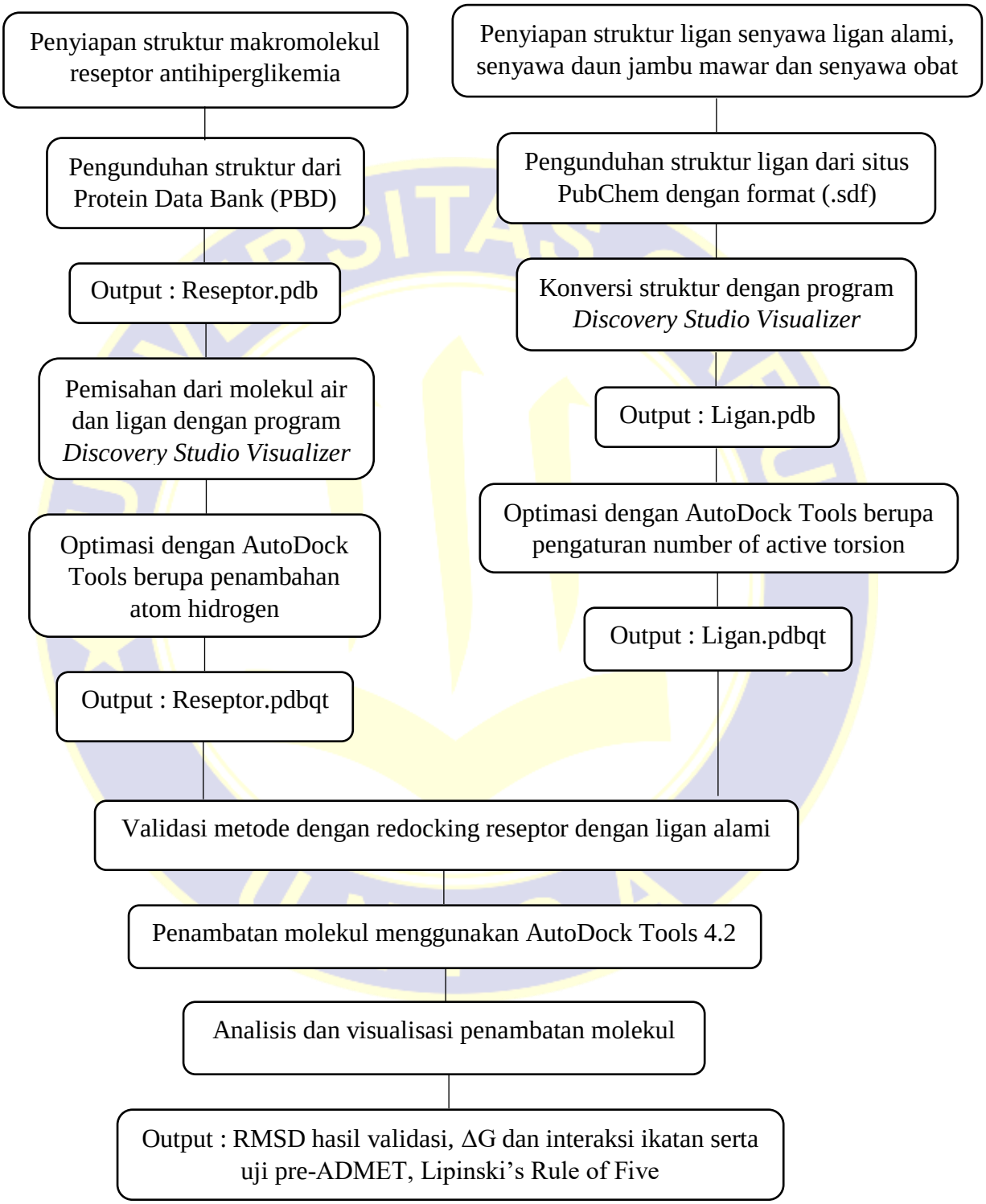
LAMPIRAN 1

ALUR PENELITIAN



Gambar I.1 Alur penelitian

LAMPIRAN 2

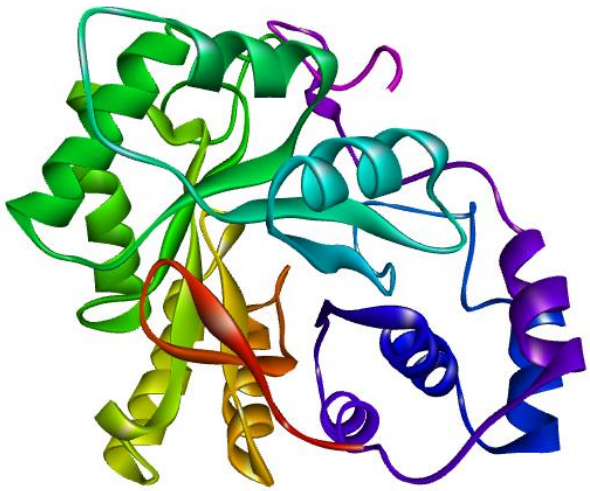
DAUN JAMBU MAWAR

Gambar II.1 Daun jambu mawar

LAMPIRAN 3

STRUKTUR 3D RESEPTOR

Gambar III.1 Reseptor Alpha-Glukosidase



Gambar III.2 Reseptor Aldosa reductase

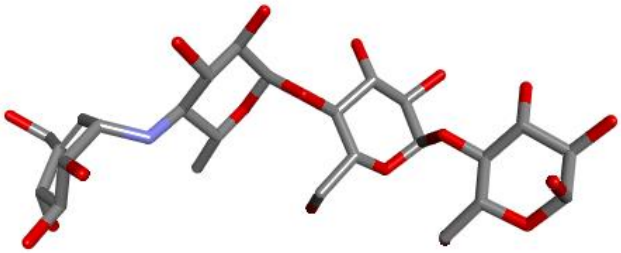
LAMPIRAN 3

(LANJUTAN)

Gambar III.3 Reseptor Dipeptidyl peptidase-IV

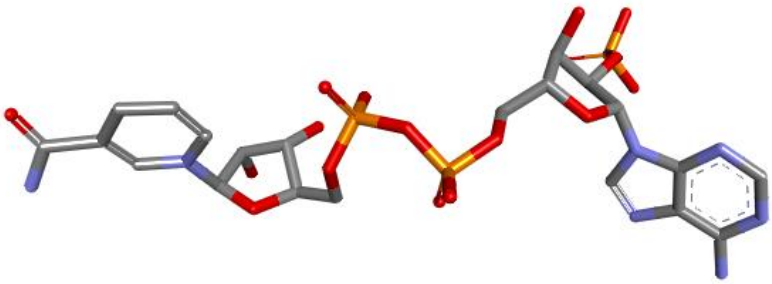
LAMPIRAN 4

LIGAN ALAMI



1,4-DEOXY-4 - ((5-HYDROXYMETHYL-2,3,4-TRIHYDROXYCYCLOHEX-5,6-ENYL) AMINO) FRUCTOSE

Gambar IV.1 Ligan Alami dari Reseptor Alpha-Glukosidase

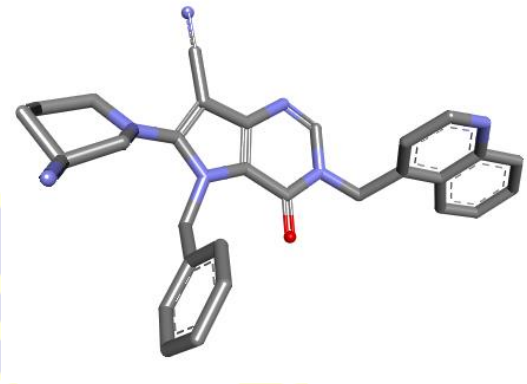


2'-monophosphoadenosine 5'diphosphoribose

Gambar IV.2 Ligan Alami dari Reseptor Aldosa reduktase

LAMPIRAN 4

(LANJUTAN)

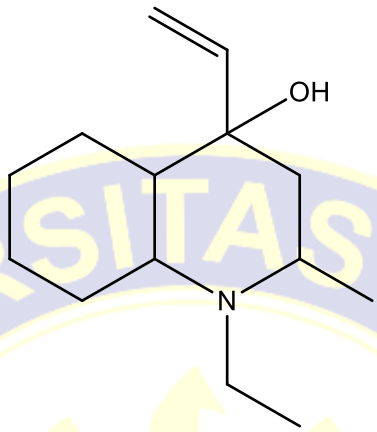


6-[(3s)-3-aminopiperidin-1-yl]-5-benzyl-4-oxo-3-(quinolin-4-ylmethyl)-4,5-dihydro-3h-pyrrolo [3,2-D] pyrimidine-7-carbonitrile

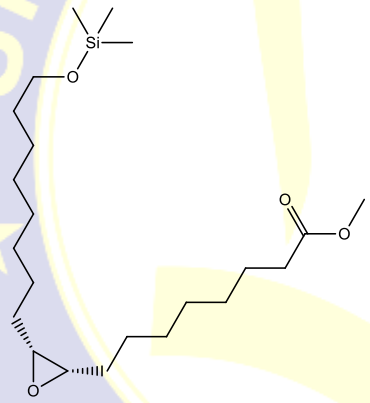
Gambar IV.3 Ligan Alami dari Reseptor Dipeptidyl Peptidase-IV (DPP-IV)

LAMPIRAN 5

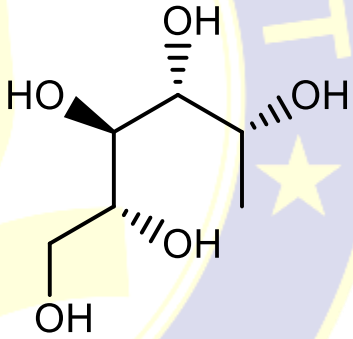
STRUKTUR 2D LIGAN UJI



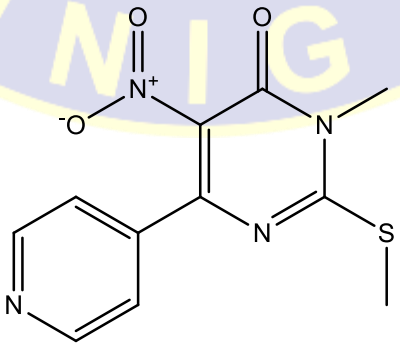
Gambar V.1 4-Quinolinol-4-ethenyl-1-ethyldecahydro-2-methyl



Gambar V.2 Octadecanoic acid



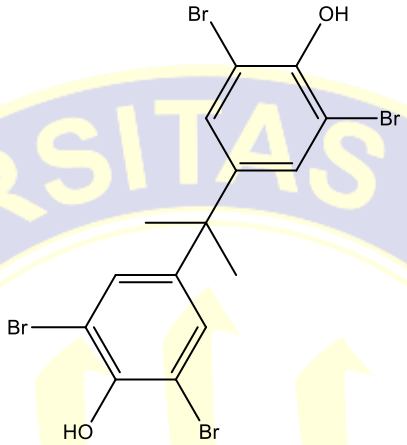
Gambar V.3 1-Deoxy-d-mannitol



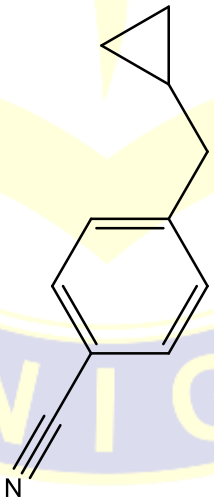
Gambar V.4 3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one

LAMPIRAN 5

(LANJUTAN)



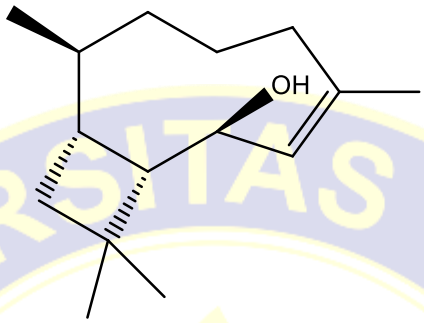
Gambar V.5 2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol



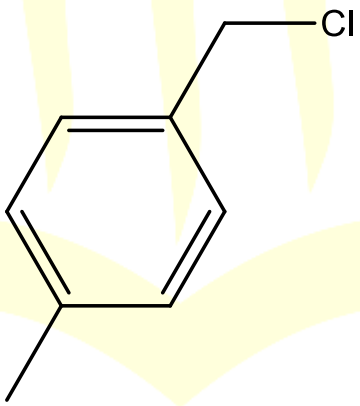
Gambar V.6 4-Cyclopropylmethylbenzonitrile

LAMPIRAN 5

(LANJUTAN)



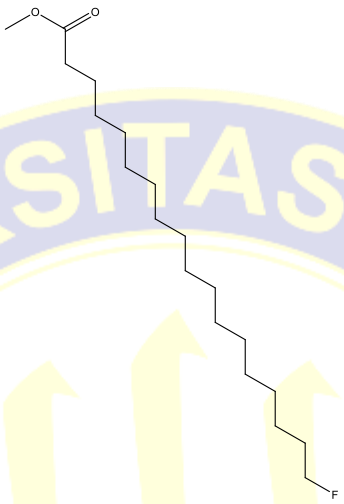
Gambar V.7 Caryophyllen alcohol(3Z)-4,8,11,11-tetramethylbicyclo [7.2.0] undec-3-en-5-ol)



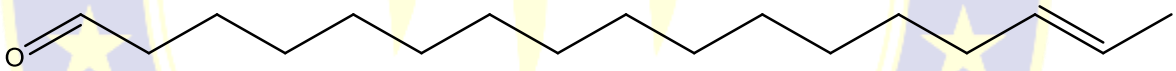
Gambar V.8 4-Methylbenzyl chloride, 1-(Chloromethyl)-4-methylbenzene

LAMPIRAN 5

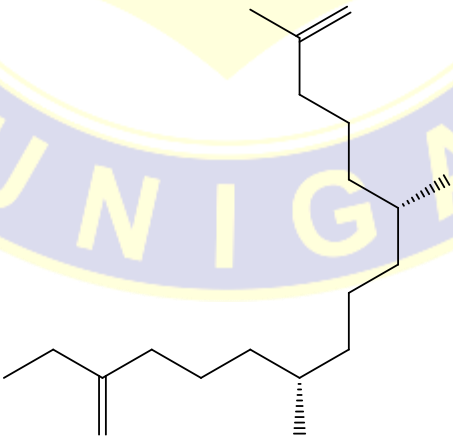
(LANJUTAN)



Gambar V. 9 Methyl 18-fluorooctadecanoate



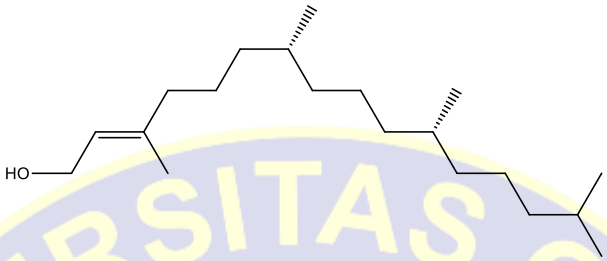
Gambar V. 10 E-15-Heptadecenal



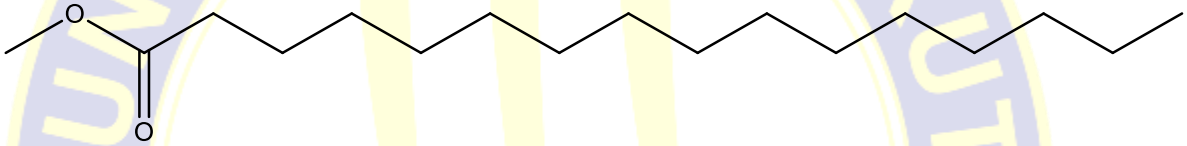
Gambar V. 11 2,6,10-trimethyl, 14-ethylene-14-pentadecne

LAMPIRAN 5

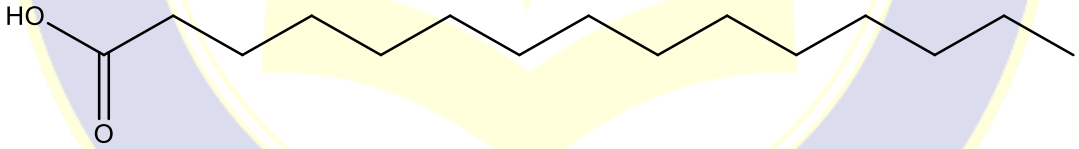
(LANJUTAN)



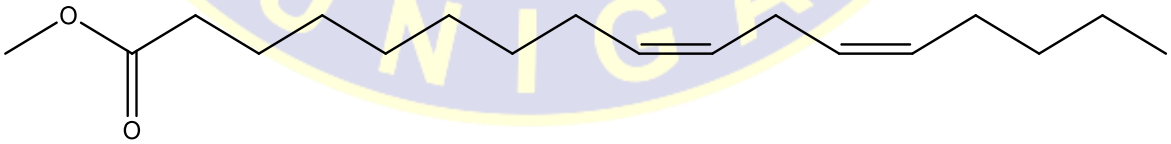
Gambar V. 12 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)



Gambar V. 12 Hexadecano ic acid, methyl ester (palmitic acid



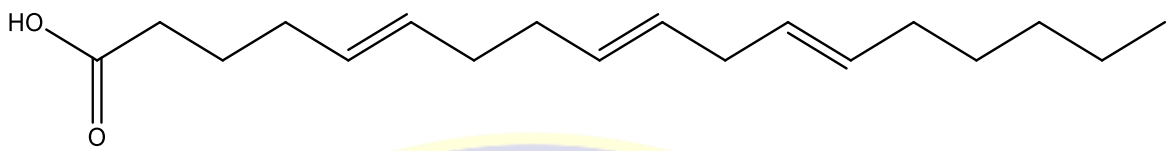
Gambar V.13 pentadecylic acid



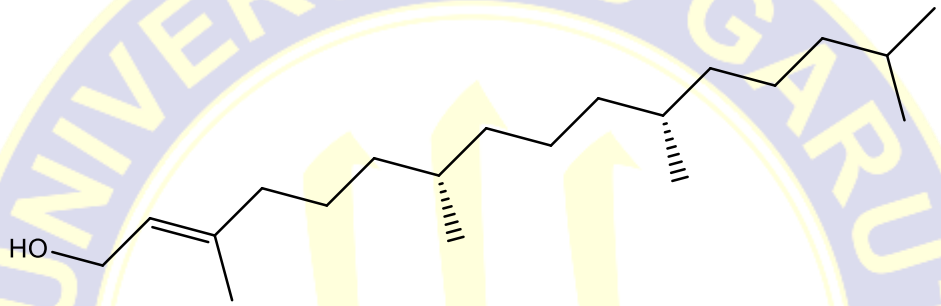
Gambar V.14 Methyl (9Z,12Z)-9,12-heptadecadienoate

LAMPIRAN 5

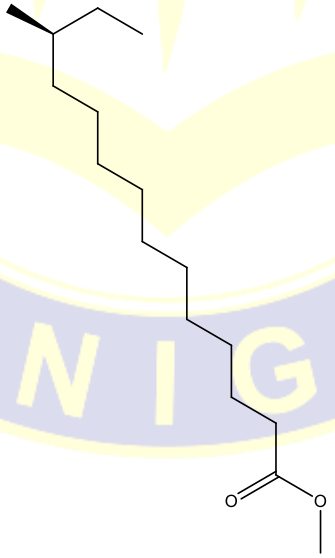
(LANJUTAN)



Gambar V. 15 5,9,12-octadecatrienoic acid



Gambar V.16 3,7,11,15-Tetramethyl-2-hexadecen-1-ol



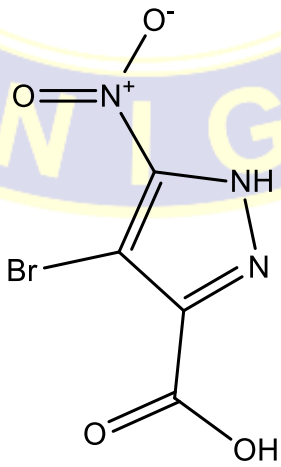
Gambar V. 17 Tetradecanoic acid, 12-methyl-, methyl ester

LAMPIRAN 5

(LANJUTAN)

Gambar V.18 Ethyl (9E,12E)-9,12-octadecadienoate

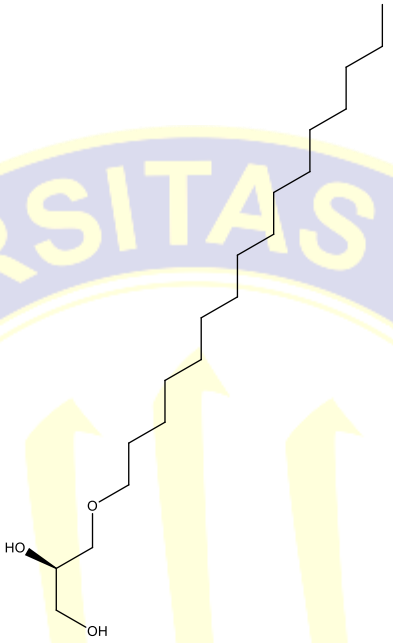
Gambar V. 19 Butyl (9E,12E,15E)-9,12,15-octadecatrienoate



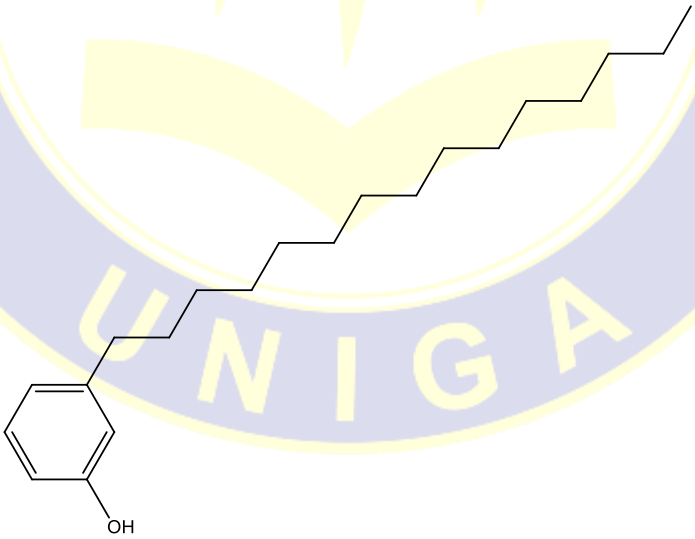
Gambar V. 20 4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid

LAMPIRAN 5

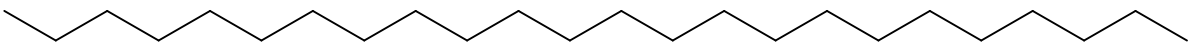
(LANJUTAN)



Gambar V. 21 1-O-hexadecylglycerol – bis-trimethylsi



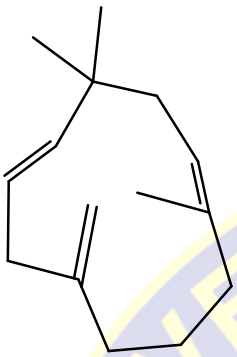
Gambar V. 22 3-Pentadecylphenol



Gambar 23 N-Tetracosane

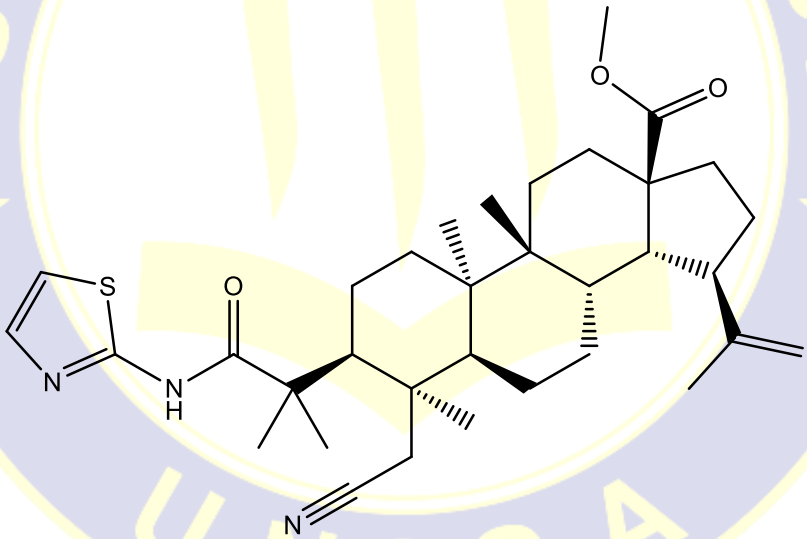
LAMPIRAN 5

(LANJUTAN)



Gambar V. 24 beta.-Humulene

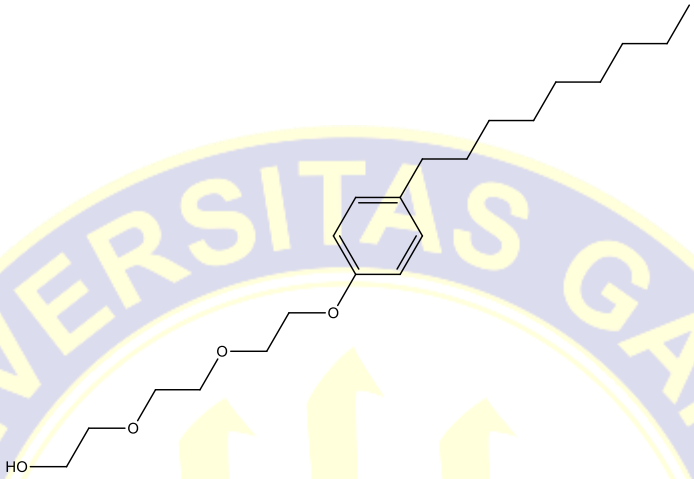
Gambar V. 25 Methyl (Z)-5,11,14,17-eicosatetraenoate



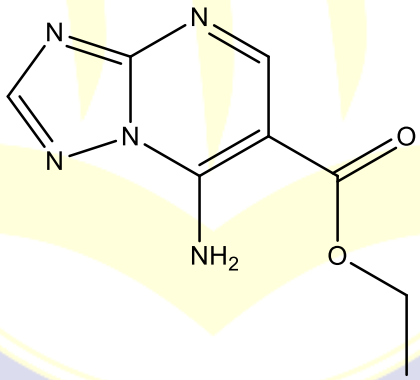
Gambar V. 26 methyl (4R,9R,10R,15R)-4- (cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)

LAMPIRAN 5

(LANJUTAN)



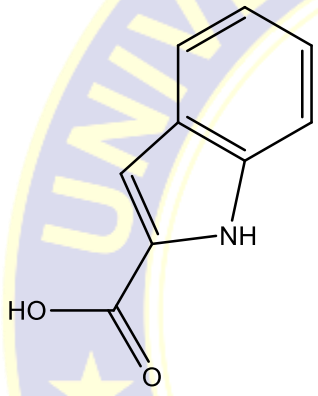
Gambar V. 27 2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol



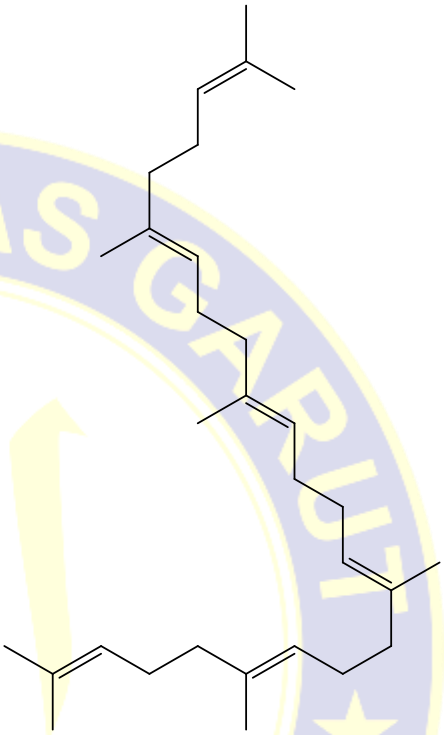
Gambar V. 28 Ethyl 7-amino[1,2,4]triazolo[1,5-a] pyrimidine-6-carboxylate(, 7-amino-, ethyl ester)

LAMPIRAN 5

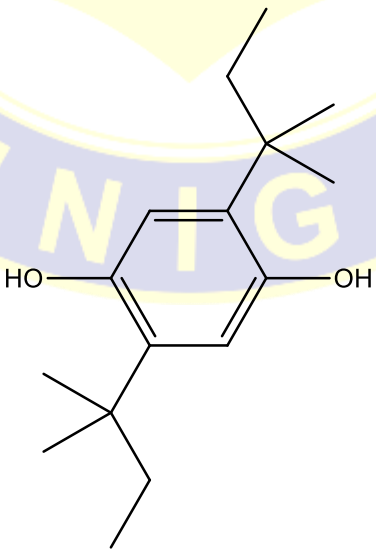
(LANJUTAN)



Gambar V. 29 1H-Indole-2-carboxylic acid



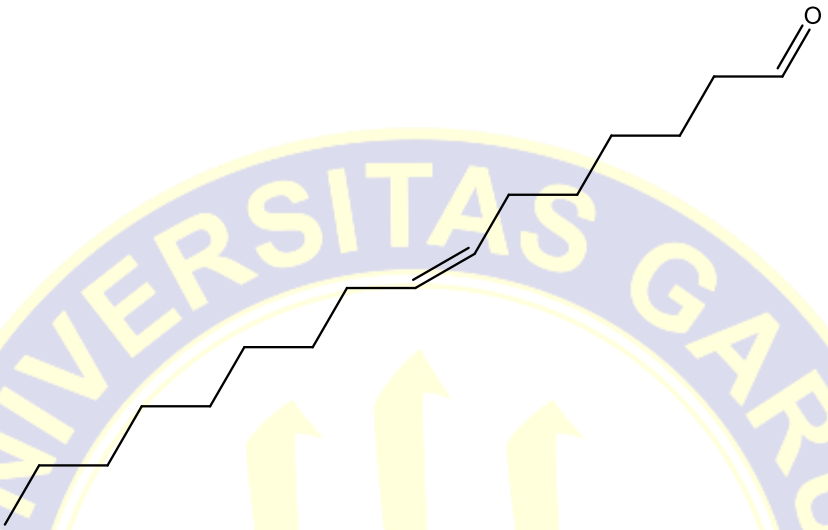
Gambar V. 30 2,6,10,14,18,22-Tetracosahexaene



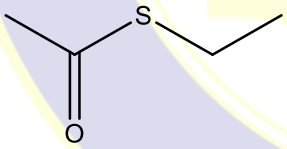
Gambar V.31 2,5-Di-tert-amylhydroquinone(79-74-3;(Santouar A)

LAMPIRAN 5

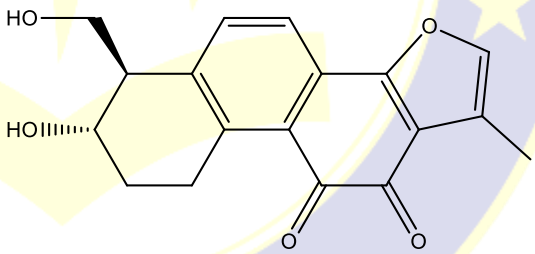
(LANJUTAN)



Gambar V.32 (Z)-7-Hexadecenal



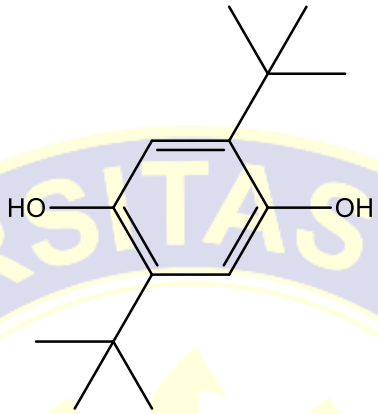
Gambar V. 33 S-Ethyl ethanethioate



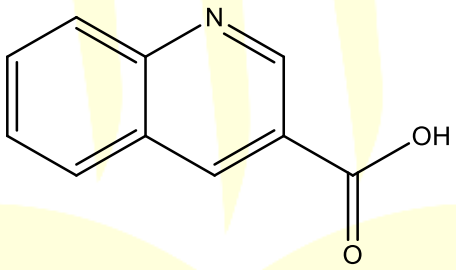
Gambar V. 34 Przewaquinone F; 96839-31-5

LAMPIRAN 5

(LANJUTAN)



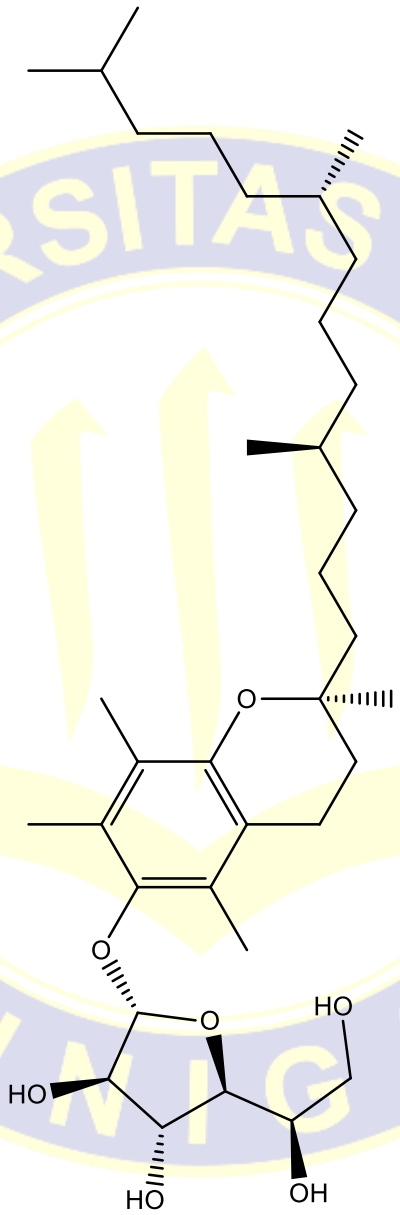
Gambar V. 35 1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)



Gambar V. 36 Quinoline-3-carboxylic acid

LAMPIRAN 5

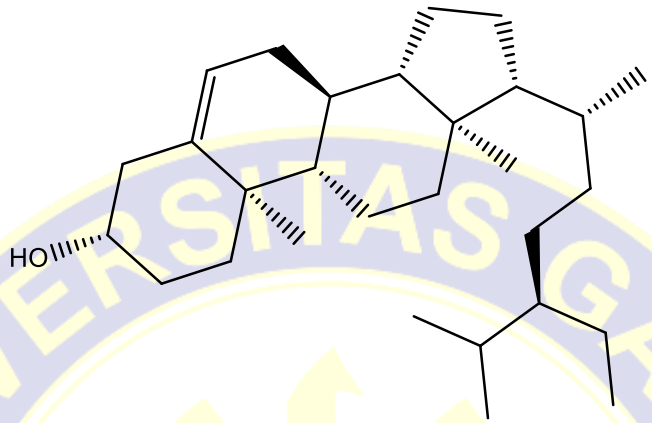
(LANJUTAN)



Gambar V. 37 alpha.-Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)

LAMPIRAN 5

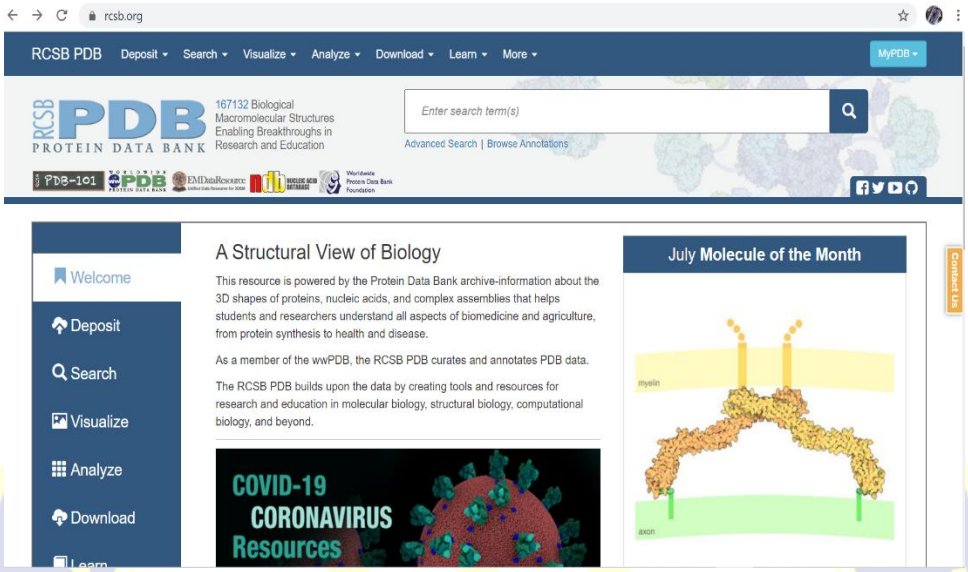
(LANJUTAN)



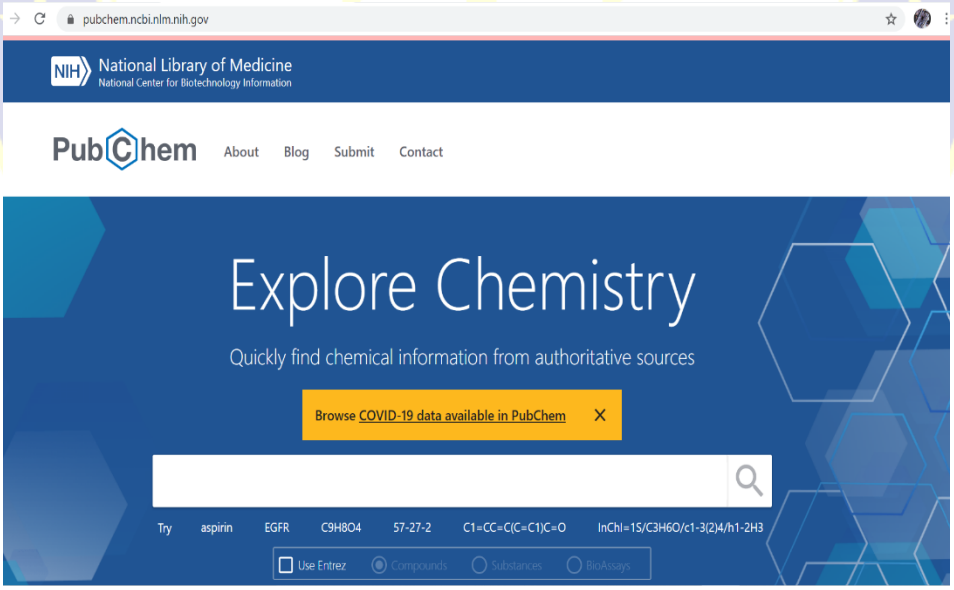
Gambar 38 Stigmast-5-en-3-ol

LAMPIRAN 6

SITUS DAN APLIKASI



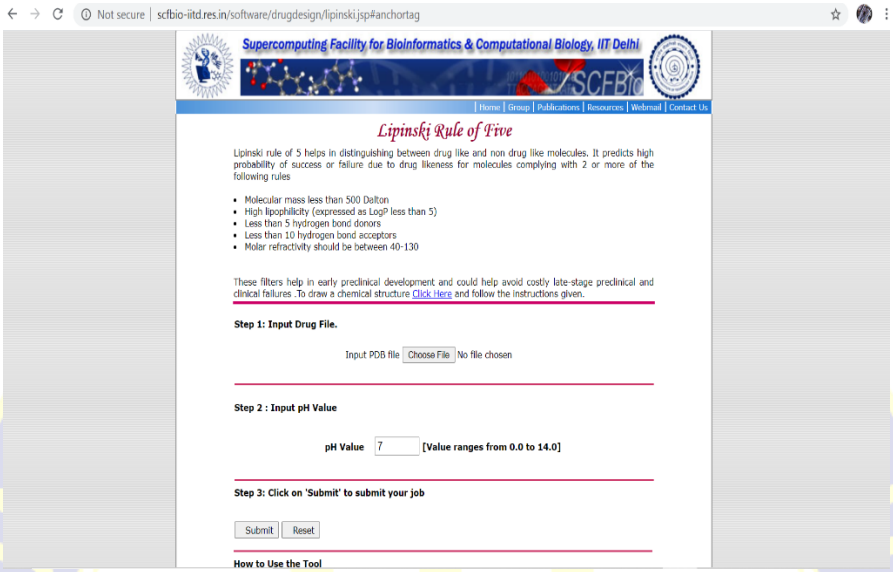
Gambar VI. 1 Tampilan situs *Protein Data Bank* (PDB)



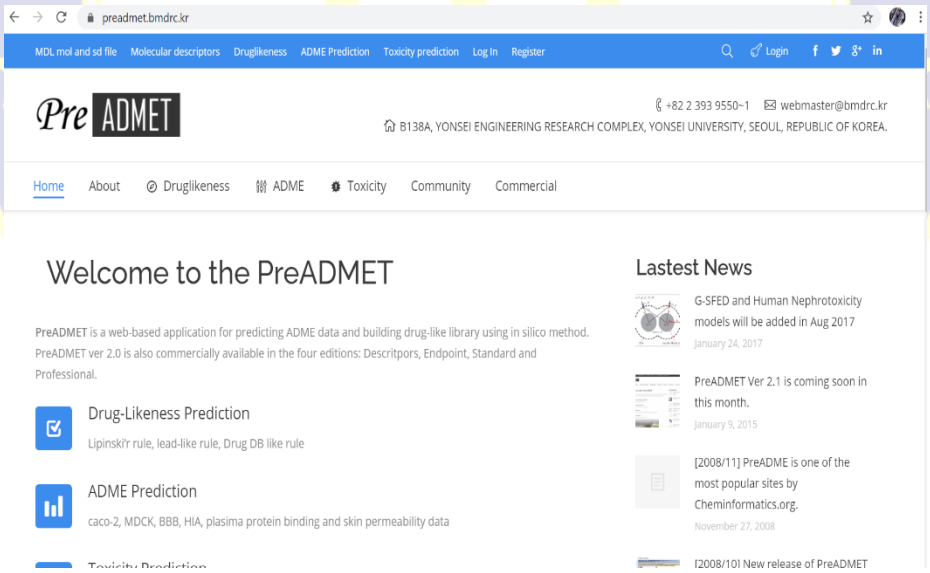
Gambar VI. 2 Tampilan situs *Pubchem*

LAMPIRAN 6

(LANJUTAN)



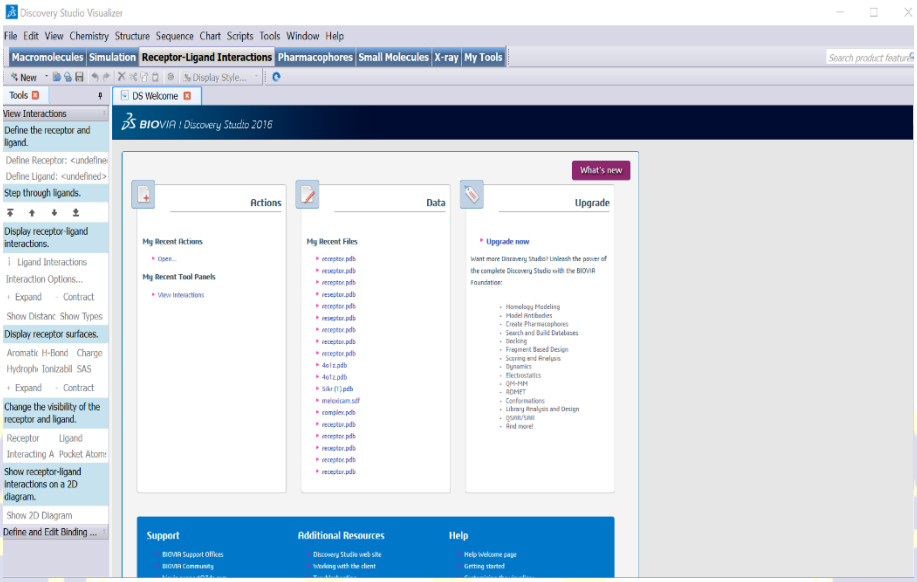
Gambar VI. 3 Tampilan situs *Lipinski's Rule of Five*



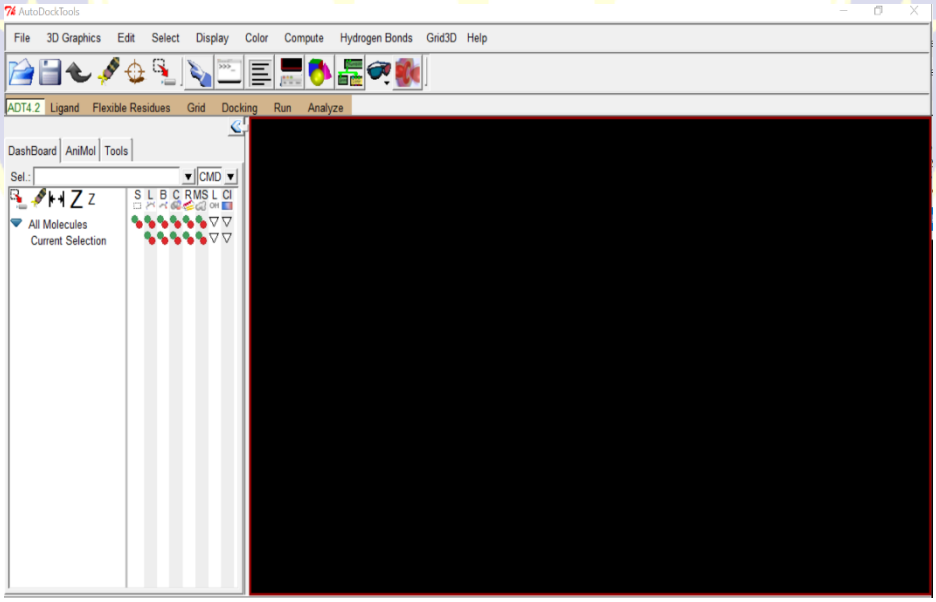
Gambar VI. 4 Tampilan situs Pre*ADMET*

LAMPIRAN 6

(LANJUTAN)



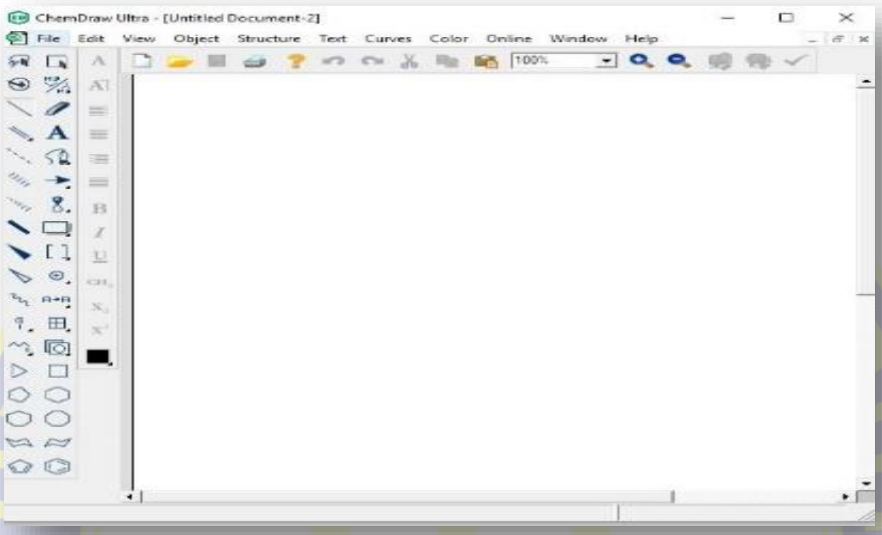
Gambar IV. 5 Tampilan aplikasi *Discovery Studio Visualizer*®



Gambar VI. 6 Tampilan aplikasi *AutoDock Tools*®

LAMPIRAN 6

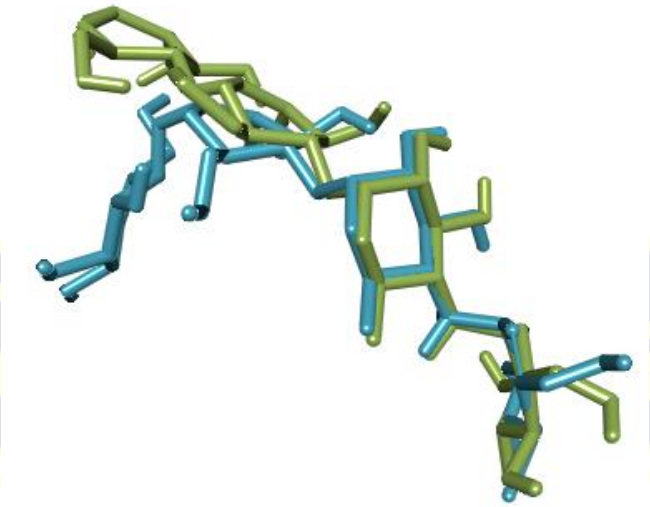
(LANJUTAN)



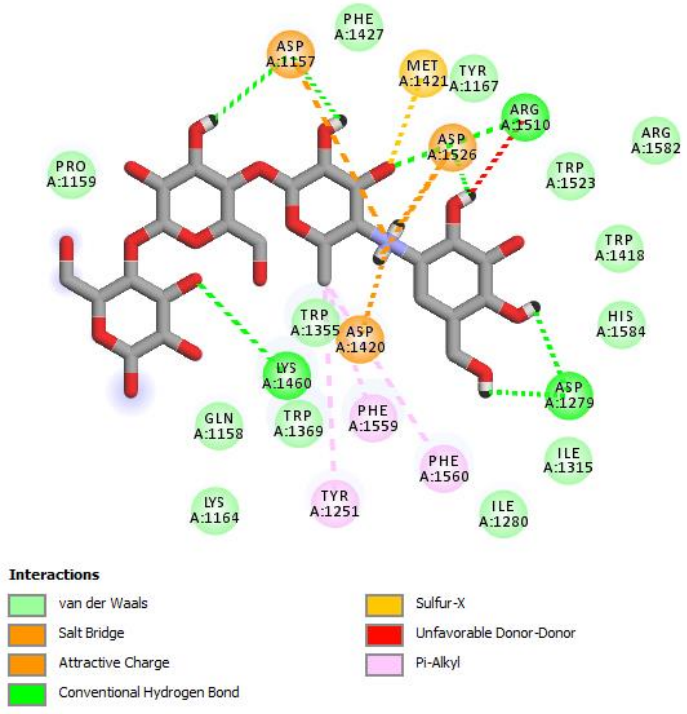
Gambar VI. 7 Tampilan aplikasi *Chemdraw Office®*

LAMPIRAN 7

VALIDASI METODE



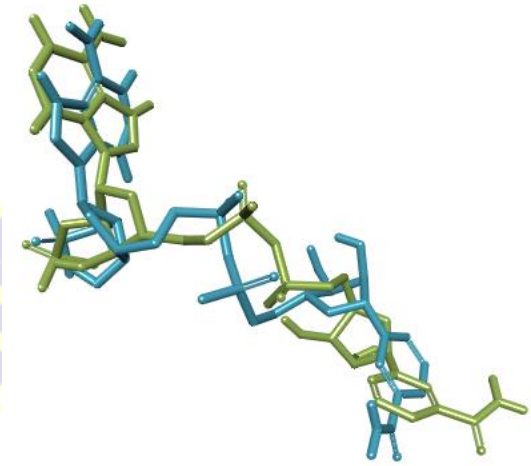
Gambar VII.1 Hasil visualisasi tumpang tindih ligan alami dari Reseptor α-glukosidase dari hasil kristalografi sinar-X (hijau) dengan ligan hasil *redocking* (biru)



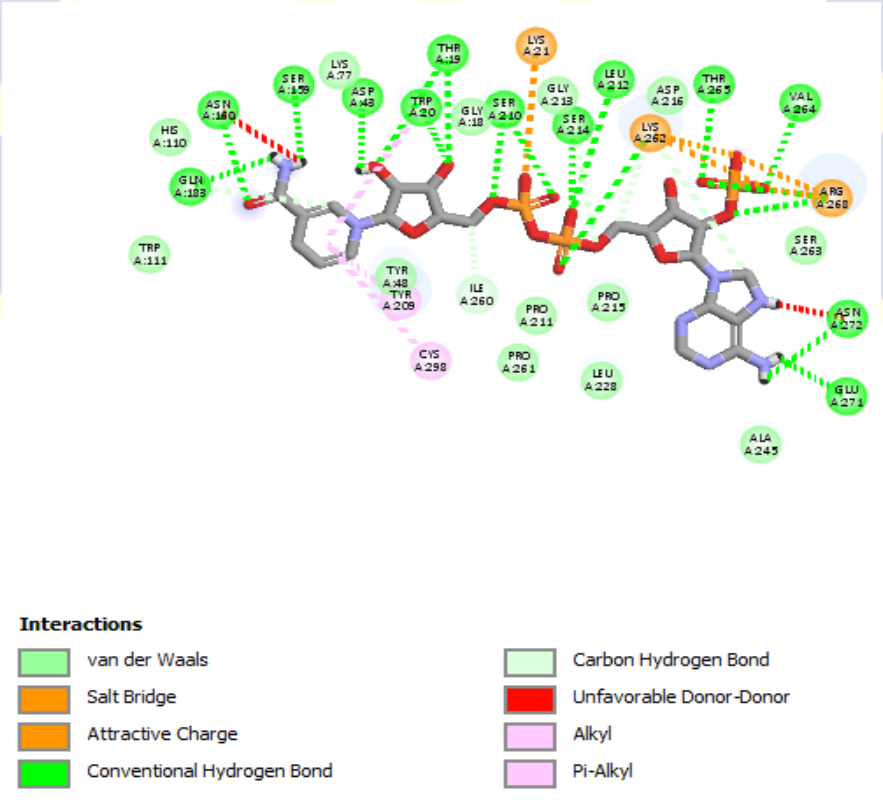
Gambar VII. 2 Hasil visualisasi interaksi ligan alami dengan Reseptor α-glukosidase

LAMPIRAN 7

(LANJUTAN)



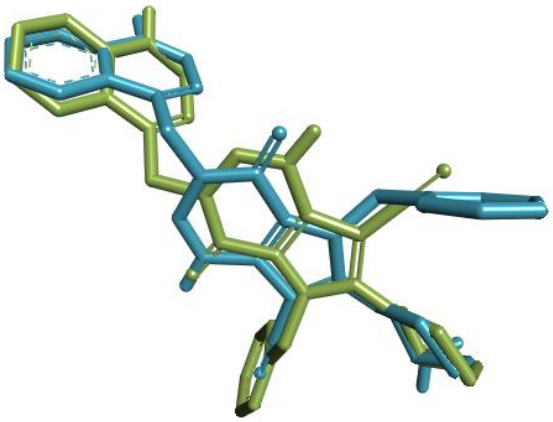
Gambar VII. 3 Hasil visualisasi tumpang tindih ligan alami dari Reseptor Aldosa Reduktase dari hasil kristalografi sinar-X (hijau) dengan ligan hasil redocking (biru)



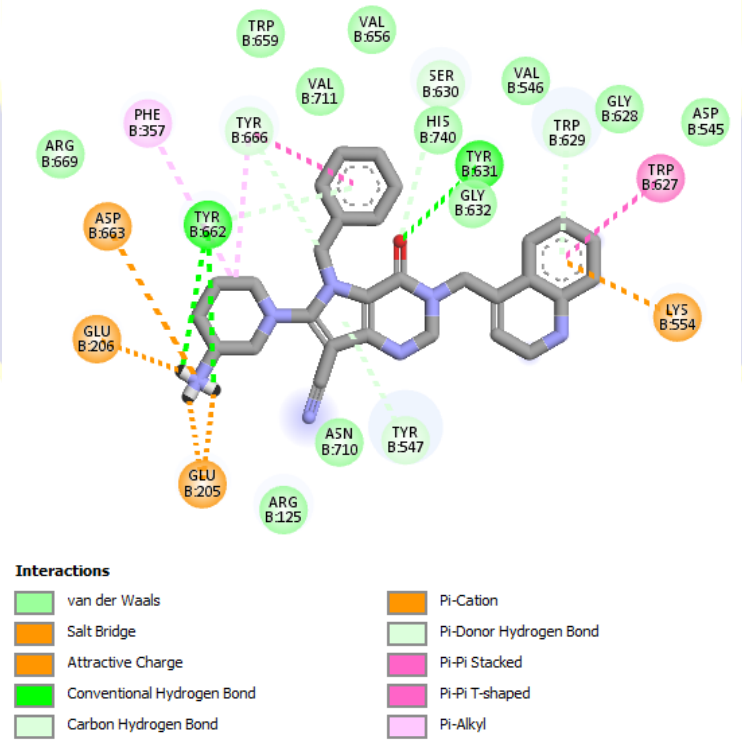
Gambar VII. 4 Hasil visualisasi interaksi ligan alami dengan Reseptor Aldosa Reduktase

LAMPIRAN 7

(LANJUTAN)



Gambar VII. 5 Hasil visualisasi tumpang tindih ligan alami dari Reseptor *Dipeptidyl peptidase*-IV (DPP-4) dari hasil kristalografi sinar-X (hijau) dengan ligan hasil redocking (biru)



Gambar VII. 6 Hasil visualisasi interaksi ligan alami dengan Reseptor *Dipeptidyl peptidase*-IV (DPP-4)

LAMPIRAN 7

(LANJUTAN)

Tabel I.1

Grid Box, *RMSD*, Nilai Ikatan Energi, dan Ligan Alami

Kode Reseptor	Grid Box	RMSD	Ikatan Energi Bebas Ligan Alami
5NN8	X : -31,734 Y : 35,646 Z : 26,388	1,55 Å	-8,78
3BCJ	X : 24,874 Y : 65,708 Z : 81,931	0,69 Å	-15,83
4A5S	X : 19,851 Y : 7,263 Z : 2,542	0,49 Å	-14,93

LAMPIRAN 8

HASIL PENAMBATAN MOLEKUL

Tabel II. 1
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor α-glukosidase

No	Senyawa/Ligan	Ikatan Energi (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (µM)
	Ligan Alami (acarbose)	-8,78	5	ASP1279, ASP1157, ARG1510, LYS1460, ASP1526	0,36874
1.	4-Quinolinol-4-ethenyl-1-ethyldecahydro-2-methyl	-8,28	-	-	0,85231
2.	Glucitol,6-O-nonyl	-4,24	3	LYS1460, ASP1157, ASP1526	782,31
3.	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-6,70	2	ASP1279, ASP1526	12,24
4.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-6,76	1	ASP1526	11,01
5.	4-Cyclopropylmethylbenzonitrile	-5,82	1	ARG1510	54,64
6.	Caryophyllen alcohol(3Z)-4,8,11,11-tetramethylbicyclo [7.2.0] undec-3-en-5-ol)	-7,28	1	ASP1526	4,62
7.	4-Methylbenzyl chloride, 1-(Chloromethyl)-4-methylbenzene	-4,74	-	-	336,46

LAMPIRAN 8
(LANJUTAN)

Tabel II. 1
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor α-glukosidase

8.	Methyl 18-fluorooctadecanoate	-4,57	1	ARG1510	446,78
9.	E-15-Heptadecenal	-5,74	1	LYS1460	62,17
10.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	-6,27	-	-	25,55
11.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)	-6,74	2	ASP1157, LYS1460	11,37
12.	Hexadecano ic acid, methyl ester (palmitic acid)	-5,23	-	-	147,73
13.	pentadecylic acid	-4,66	2	ASP1157, LYS1460	382,72
14.	Methyl (9Z,12Z)-9,12-heptadecadienoate	-5,88	1	LYS1460	48,97
15.	5,9,12-octadecatrienoic acid	-5,67	2	ASP1157, LYS1460	69,33
16.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-6,57	2	ASP1157, LYS1460	15,31
17.	Tetradecanoic acid, 12-methyl-, methyl ester	-5,50	1	LYS1460	93,15
18.	Ethyl (9E,12E)-9,12-octadecadienoate	-5,72	1	LYS1460	64,60
19.	Butyl (9E,12E,15E)-9,12,15-octadecatrienoate	-4,91	1	LYS1460	253,11
20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-2,98	2	ASP1157, LYS1460	6530

LAMPIRAN 8
(LANJUTAN)

Tabel II. 1
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor α-glukosidase

21.	1-O-hexadecylglycerol -bis-trimethylsi	-4,15	1	ASP1157	911,33
22.	3-Pentadecylphenol	-6,53	2	ASP1157, LYS1460	16,41
23.	N-Tetracosane	-5,14	-	-	169,57
24.	beta.-Humulene	-6,95	-	-	8,07
25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	-6,65	1	LYS1460	13,36
26.	methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	-8,38	1	LYS1460	0,72046
27.	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-5,26	1	TRP1369	140,23
28.	Ethyl 7-amino[1,2,4]triazolo [1,5-a] pyrimidine-6-carboxylate(, 7-amino-, ethyl ester)	-6,65	3	ASP1279, ASP1420, ASP1526	13,36
29.	1H-Indole-2-carboxylic acid	-4,12	2	LYS1460, ASP1157	959,06
30.	2,6,10,14,18,22-Tetracosahexaene	-7,21	-	-	5,17
31.	2,5-Di-tert-amylhydroquinone(79-74-3;(Santouar A)	-7,09	1	ASP1526	6,39
32.	(Z)-7-Hexadecenal	-5,43	1	LYS1460	104,44
33.	S-Ethyl ethanethioate	-3,54	-	-	2550
34.	Przewaquinone F; 96839-31-5	-7,37	2	ASP1157, LYS1460	3,96

LAMPIRAN 8
(LANJUTAN)

Tabel II. 1
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor α-glukosidase

35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-6,53	1	ASP1526	16,23
36.	Quinoline-3-carboxylic acid	-4,62	3	ASP1157, LYS1460, ASP1526	410,85
37.	alpha.-Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)	-9,89	1	ASP1279	0,05636
38.	Stigmast-5-en-3-ol	-8,78	1	GLN1158	22,03

LAMPIRAN 8
(LANJUTAN)

Tabel II. 2
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor Aldosa Reduktase

No	Senyawa/Ligan	Ikatan Energi (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (µM)
	Ligan Alami	-15,83	13	THR19, TRP20, ASP43, SER159, ASN160, GLN183, SER210, LEU212, SER214, VAL264, THR265, GLU271, ASN272	0,0000025
	Ponalrestat	-14,28	4	GLN 183, LEU 212, ASP 216, ASN 272	0,20224
1.	4-Quinolinol-4-ethenyl-1-ethyldecahydro-2-methyl	-5,34	1	ARG268	122,15
2.	Glucitol,6-O-nonyl	-7,14	3	LYS21, ASP216, LYS262	5,79
3.	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-6,54	4	LYS262, LYS262, SER263, THR265	15,94
4.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-6,54	2	PRO215, LYS262	16,20

LAMPIRAN 8
(LANJUTAN)

Tabel II. 2
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor Aldosa Reduktase

5.	4-Cyclopropylmethylbenzonitrile	-6,86	2	THR19, TRP20	9,42
6.	Caryophyllen alcohol(3Z)-4,8,11,11-tetramethylbicyclo [7.2.0] undec-3-en-5-ol)	-6,60	1	SER263	14,61
7.	4-Methylbenzyl chloride, 1-(Chloromethyl)-4-methylbenzene	-5,31	-	-	128,58
8.	Methyl 18-fluorooctadecanoate	-7,72	5	LYS262, SER263, VAL264, THR265, ARG268	2,18
9.	E-15-Heptadecenal	-7,93	2	LYS262, VAL264	1,53
10.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	-8,83	-	-	0,33931
11.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)	-9,36	2	SER263, VAL264	0,13776
12.	Hexadecano ic acid, methyl ester (palmitic acid)	-7,96	2	LYS262, VAL264	1,46
13.	pentadecylic acid	-8,32	4	LYS262, SER263, VAL264, ARG268	0,7982

LAMPIRAN 8
(LANJUTAN)

Tabel II. 2
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor Aldosa Reduktase

14.	Methyl (9Z,12Z)-9,12-heptadecadienoate	-8,77	5	LYS262, SER263, VAL264, THR265, ARG268	0,37381
15.	5,9,12-octadecatrienoic acid	-9,88	5	LYS262, SER263, VAL264, THR265, ARG268	0,05725
16.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-9,19	3	SER263, THR265, ARG268	0,18323
17.	Tetradecanoic acid, 12-methyl-, methyl ester	-8,01	4	LYS262, SER263, VAL264, ARG268	1,34
18.	Ethyl (9E,12E)-9,12-octadecadienoate	-8,87	3	SER263, VAL264, ARG268	0,31339
19.	Butyl (9E,12E,15E)-9,12,15-octadecatrienoate	-8,99	2	LYS262, VAL264	0,25507
20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-6,37	7	TRP20, TRP20, LYS21, LEU212, SER214, SER214, ILE263	21,46
21.	1-O-hexadecylglycerol - bis-trimethylsi	-7,83	2	SER263, ARG268	1,82
22.	3-Pentadecylphenol	-9,33	1	SER263	0,14570
23.	N-Tetracosane	-8,01	-	-	1,34
24.	beta.-Humulene	-5,46	-	-	99,23

LAMPIRAN 8
(LANJUTAN)

Tabel II. 2
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor Aldosa Reduktase

25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	-9,49	4	SER263, VAL264, THR265, ARG268	0,11104
26.	methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	-5,97	1	ARG268	42,03
27.	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-7,32	1	ARG268	4,30
28.	Ethyl 7-amino[1,2,4]triazolo [1,5-a] pyrimidine-6-carboxylate(, 7-amino-, ethyl ester)	-6,98	6	SER210, SER214, ASP216, ASP216, ILE260, LYS262	7,68
29.	1H-Indole-2-carboxylic acid	-6,47	2	ILE260, LYS262	18,10
30.	2,6,10,14,18,22-Tetracosahexaene	-9,56	-	-	0,09761
31.	2,5-Di-tert-amylhydroquinone(79-74-3;(Santouar A)	-9,57	3	LYS21, SER214, ILE260	0,09638
32.	(Z)-7-Hexadecenal	-7,64	2	LYS262, VAL264	2,52
33.	S-Ethyl ethanethioate	-4,26	2	LEU212, SER214	756,21
34.	Przewaquinone F; 96839-31-5	-7,27	4	ASP216, ASP216, ASP216, ASP216	4,67

LAMPIRAN 8
(LANJUTAN)

Tabel II. 2
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor Aldosa Reduktase

35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-9,04	3	LYS21, SER214, ILE260	0,23675
36.	Quinoline-3-carboxylic acid	-6,66	3	SER210, LEU212, LYS262	13,03
37.	alpha.-Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)	-12,26	1	GLN183	0,00104
38.	Stigmast-5-en-3-ol	-5,58	1	GLU 271	80,74

LAMPIRAN 8
(LANJUTAN)

Tabel II. 3
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor DPP-IV

No	Senyawa/Ligan	Ikatan Energi (ΔG) kcal/mol	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (μM)
	Ligan Alami	-14,93	2	TYR631, TYR662	0,00001147
	Sitagliptin	-12,56	6	ARG 125, GLU 205, ASP 545, TYR 547, TYR 631, TYR 662	0,61501
1.	4-Quinolinol-4-ethenyl-1-ethyldecahydro-2-methyl	-6,50	1	TYR547	17,26
2.	Glucitol,6-O-nonyl	-4,06	3	TRP629, TYR631, VAL546	1050
3.	3-methyl-2-methylsulfanyl-5-nitro-6-pyridin-4-ylpyrimidin-4-one	-5,96	2	ASP545, TRP629	42,61
4.	2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol	-7,00	2	TRP629, HIS740	7,34
5.	4-Cyclopropylmethylbenzonitrile	-5,62	1	TYR631	76,46
6.	Caryophyllen alcohol(3Z)-4,8,11,11-tetramethylbicyclo [7.2.0] undec-3-en-5-ol)	-6,48	1	VAL546	17,74

LAMPIRAN 8
(LANJUTAN)

Tabel II. 3
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor DPP-IV

7.	4-Methylbenzyl chloride, 1-(Chloromethyl)-4-methylbenzene	-4,29	-	-	717,24
8.	Methyl 18-fluorooctadecanoate	-4,39	1	LYS554	609,03
9.	E-15-Heptadecenal	-5,19	1	TYR752	156,59
10.	2,6,10-trimethyl, 14-ethylene-14-pentadecne	-6,49	-	-	17,62
11.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol (2-Hexadecen-1-ol, 3,7,11,15-tetramethyl)	-5,98	1	ASP545	41,46
12.	Hexadecano ic acid, methyl ester (palmitic acid)	-5,40	2	LYS554, TRP629	110,16
13.	pentadecylic acid	-4,94	1	LYS554	237,37
14.	Methyl (9Z,12Z)-9,12-heptadecadienoate	-6,12	-	-	32,57
15.	5,9,12-octadecatrienoic acid	-4,89	2	ARG125, ARG125	261,14
16.	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	-5,94	1	ASP545	44,25
17.	Tetradecanoic acid, 12-methyl-, methyl ester	-6,01	2	LYS554, TRP629	39,00
18.	Ethyl (9E,12E)-9,12-octadecadienoate	-5,98	1	LYS554	41,08
19.	Butyl (9E,12E,15E)-9,12,15-octadecatrienoate	-6,21	1	TYR631	28,26

LAMPIRAN 8
(LANJUTAN)

Tabel II. 3
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor DPP-IV

20.	4-bromo-5-nitro-1h-pyrazole-3-carboxylic acid	-4,07	4	VAL546, LYS554, TRP629, TYR631	1030
21.	1-O-hexadecylglycerol -bis-trimethylsi	-4,87	3	ASP545, VAL546, TRP629	269,50
22.	3-Pentadecylphenol	-6,43	1	ASP545	19,35
23.	N-Tetracosane	-5,01	-	-	214,16
24.	beta.-Humulene	-6,24	-	-	26,78
25.	Methyl (Z)-5,11,14,17-eicosatetraenoate	-6,00	-	-	40,16
26.	methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	-8,13	-	-	1,10
27	2-[2-[2-(4-nonylphenoxy) ethoxy] ethoxy] ethanol	-5,37	3	ASP545, LYS554, TRP629	116,21
28.	Ethyl 7-amino[1,2,4]triazolo [1,5-a] pyrimidine-6-carboxylate(, 7-amino-, ethyl ester)	-6,75	4	GLU205, TYR547, TYR662, TYR631	11,29
29.	1H-Indole-2-carboxylic acid	-5,21	2	VAL546, TRP629	152,24
30.	2,6,10,14,18,22-Tetracosahexaene	-7,23	-	-	4,98
31.	2,5-Di-tert-amylhydroquinone(79-74-3;(Santouar A)	-6,04	1	TRP629	37,19
32.	(Z)-7-Hexadecenal	-5,39	1	LYS554	112,50
33.	S-Ethyl ethanethioate	-3,37	2	LYS554, TRP629	3360

LAMPIRAN 8
(LANJUTAN)

Tabel II. 3
Nilai Ikatan Energi dari Ligan Alami dan Senyawa Uji Pada Reseptor DPP-IV

34.	Przewaquinone F; 96839-31-5	-8,15	1	ASP545	1,06
35.	1,4-Benzenediol, 2,5-bis (1,1-dimethylethyl)	-5,74	2	VAL546, SER630	62,05
36.	Quinoline-3-carboxylic acid	-4,96	1	TRP629	230,50
37.	alpha.-Tocopherol-.beta.-D-mannoside (2,5,7,8-Tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2H-chromen-6-yl hexofuranoside)	-11,09	1	ASP545	0,00745
38.	Stigmast-5-en-3-ol	-5,47	1	GLU205	97,70

LAMPIRAN 9

HASIL PENGUJIAN *LIPINSKI'S RULE OF FIVE*

Tabel III. 1
Sifat Fisikokimia Senyawa yang Terkandung Didalam Daun Jambu Mawar Berdasarkan Aturan 5 Lipinski

Senyawa Uji	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/Tidak
methyl (4R,9R,10R,15R)-4- (cyanomethyl) -4,9,10-trimethyl-3-[2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	1	6	579	8,03	Tidak memenuhi
alpha.-Tocopherol-.beta.-D-mannoside	5	6	312	-0,05	Memenuhi
Stigmast-5-en-3-ol	1	1	414	8,02	Tidak memenuhi

Keterangan : Donor Ikatan Hidrogen : ≤ 5

Akseptor Ikatan Hidrogen : ≤ 10

Bobot Molekul : ≤ 500 g mol

Log P : ≤ 5

LAMPIRAN 10

HASIL PENGUJIAN *Pre-ADME*

Tabel IV. 1
Uji PreADME (Absorpsi dan Distribusi)

Senyawa/Ligan	Absorpsi		Distribusi
	Caco-2 cell (nm sec-1)	**HIA (%)**	**Protein Plasma Binding (%)**
methyl (4R,9R,10R,15R)-4- (cyanomethyl) -4,9,10-trimethyl-3- [2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	36,87	100,0	100,0
alpha.-Tocopherol-.beta.-D-mannoside	40,11	90,54	94,16
Stigmast-5-en-3-ol	52,53	100,0	100,0

Keterangan : HIA (*Human Intestinal Absorpsi*) = 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*

Plasma Protein Binding = > 90% *strongly bond*
< 90% *weakly bound*

LAMPIRAN 11

UJI TOKSISITAS

Tabel V. 1
Uji Toksisitas

Senyawa/Ligan	Ames Test	Karsinogenik
	Mutagen / Non Mutagen	**(-) / (+)**
methyl (4R,9R,10R,15R)-4-(cyanomethyl) -4,9,10-trimethyl-3- [2-methyl-1-oxo-1-(1,3-thiazol-2-ylamino)	Mutagen	Positif
alpha.-Tocopherol-.beta.-D-mannoside	Non-Mutagen	Negatif
Stigmast-5-en-3-ol	Non-Mutagen	Positif

Riwayat Hidup

Data Pribadi

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