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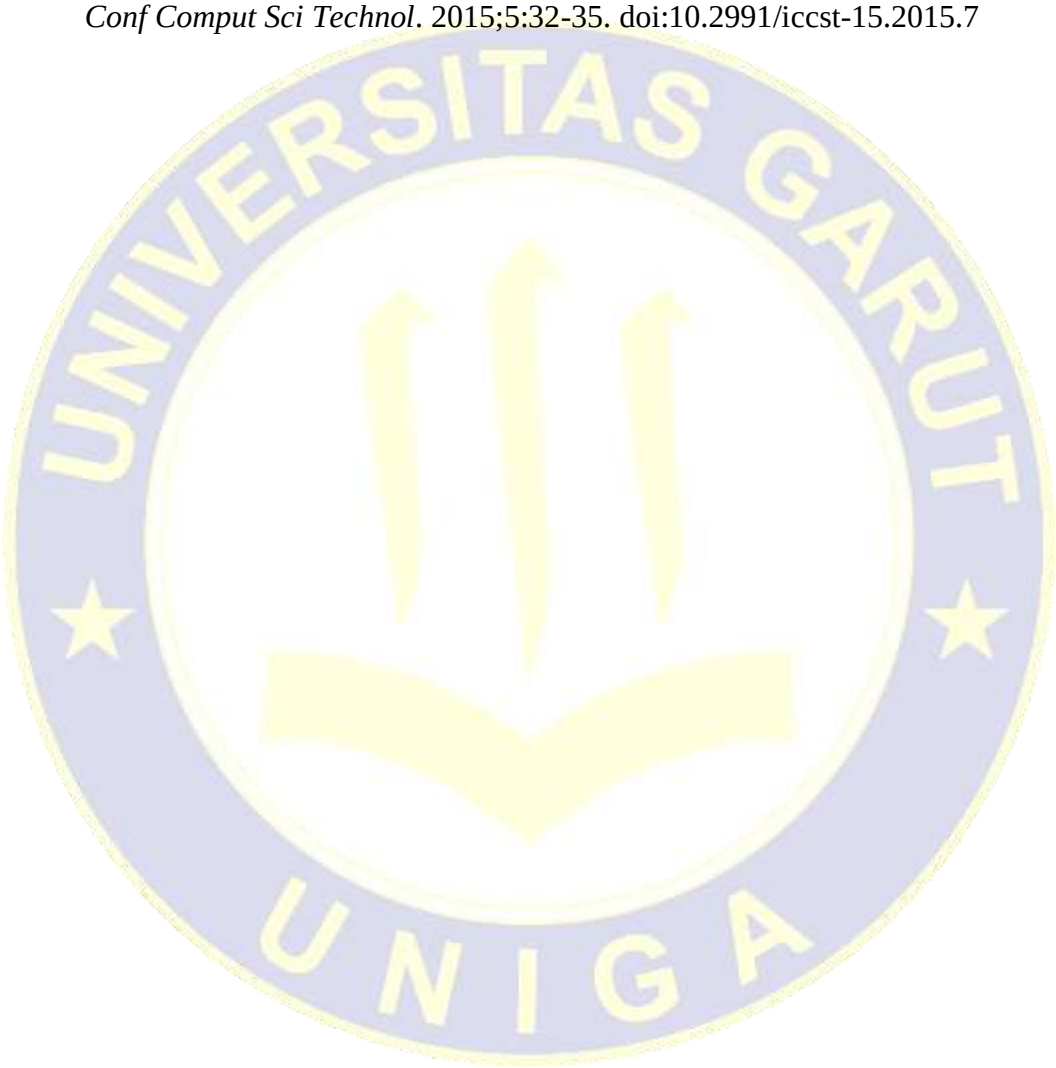
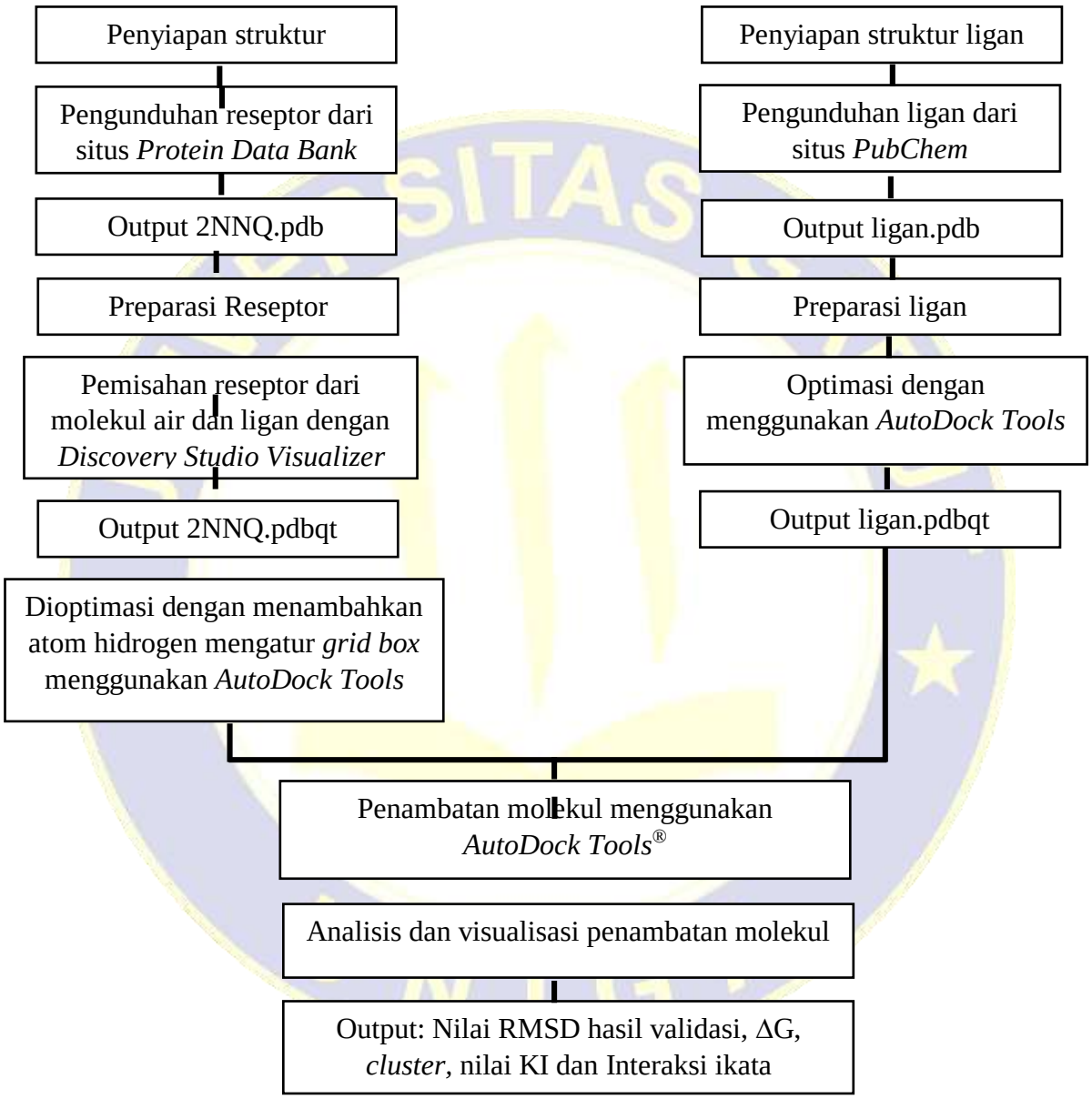


LAMPIRAN 1

ALUR PENELITIAN PENAMBATAN MOLEKUL

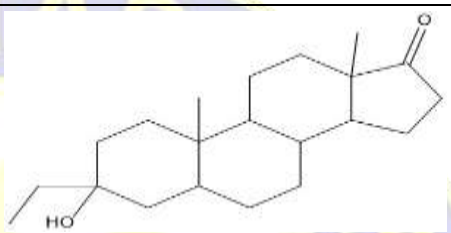
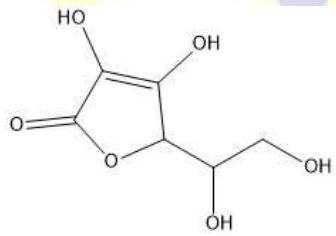
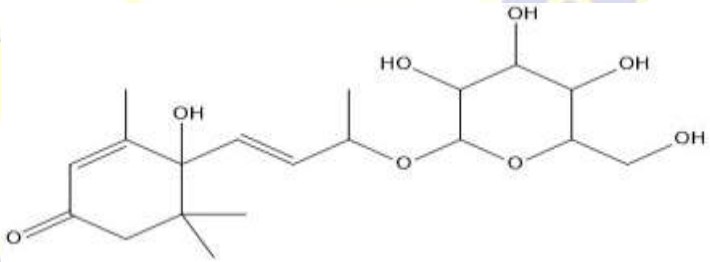
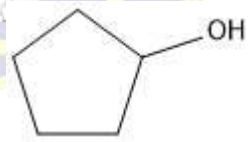


Gambar III.1 Alur penelitian penambatan molekul reseptor 2NNQ

LAMPIRAN 2

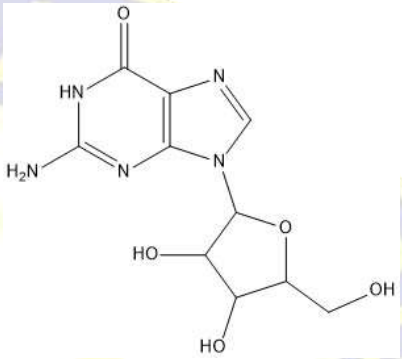
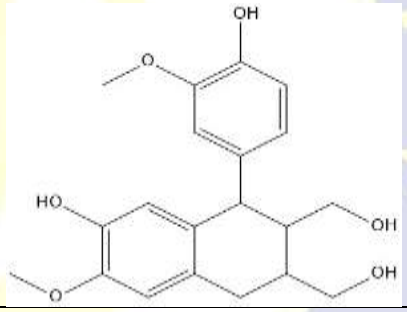
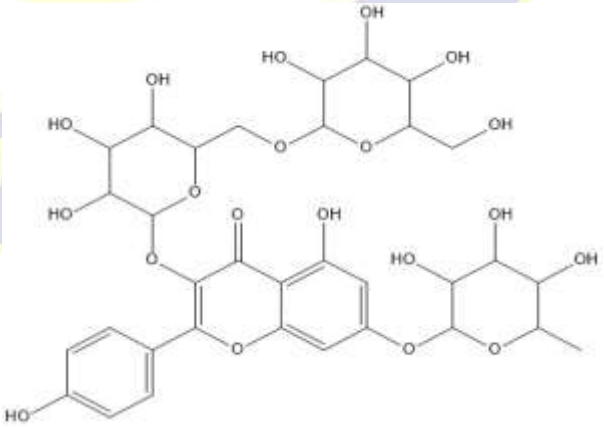
SENYAWA DAUN KATUK (*Sauropus androgynus* L. Merr.)

Tabel V.1
Senyawa Daun katuk (*Sauropus androgynus* L. Merr.)

No	Nama Senyawa	Struktur 2D
1	*Androstan-17-one-3-ethyl-3-hydroxy-5 alpha*	
2	*Ascorbic acid*	
3	*Chorcoinoside C*	
4	*Cyclopentanol*	

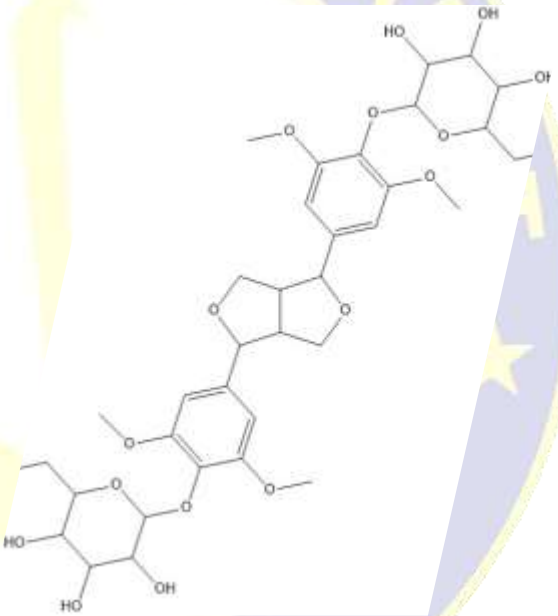
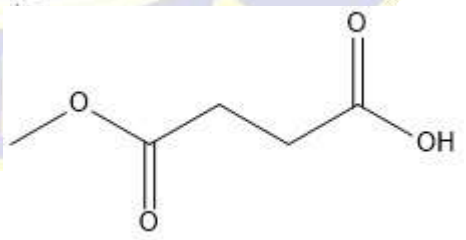
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
5	*Guanosine*	
6	*Isolariciresinol*	
7	*Kaempferol 3 gentiobioside-7 rhamnoside*	

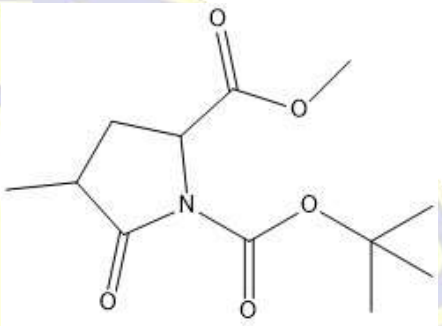
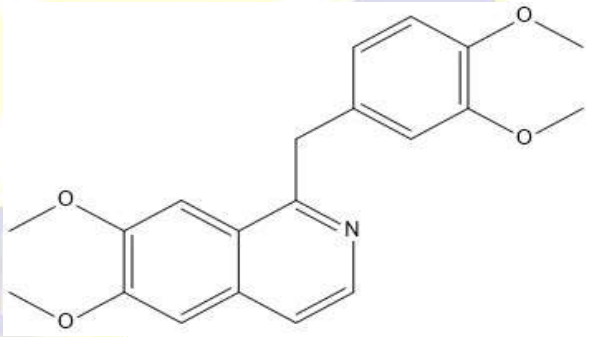
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
8	*9-eicosyne*	
9	*Liriodendrin*	
11	*Monomethyl succinate*	

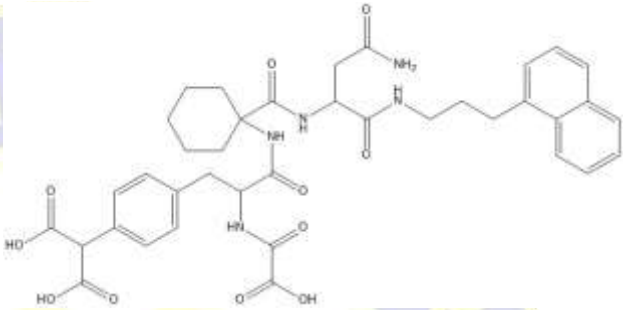
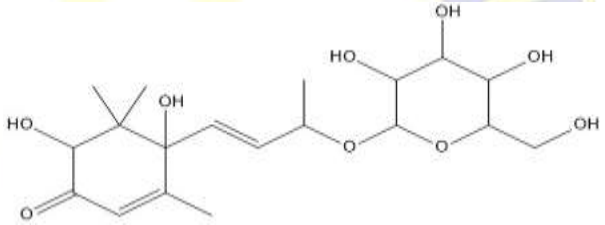
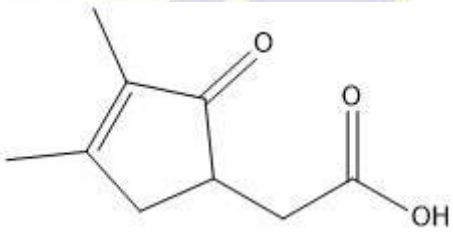
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
10	*Methylpyroglutamate*	
12	*Octadecanoic acid*	
13	*Papaverine*	

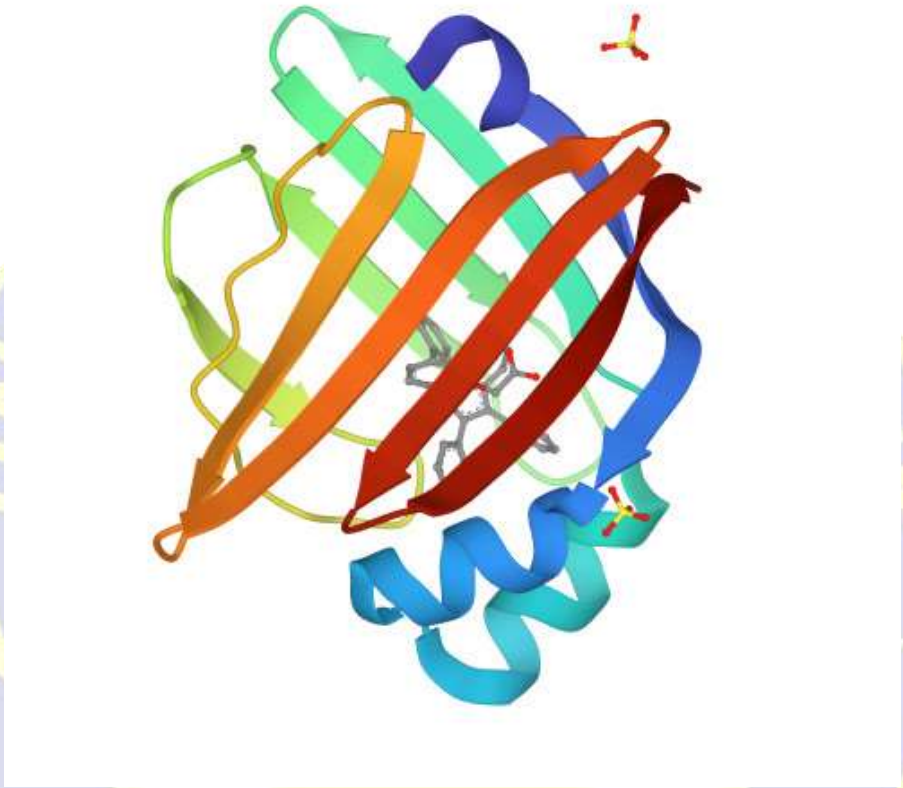
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

No	Nama Senyawa	Struktur 2D
14	*Phenyl malonic acid*	
15	*Sauroposide*	
16	*3,4-dimethyl-2-oxocyclopent-3-enylacetic acid*	
17	*11,14,17-eicosatrienoic acid methyl ester*	

LAMPIRAN 3

STRUKTUR 3D RESEPTOR

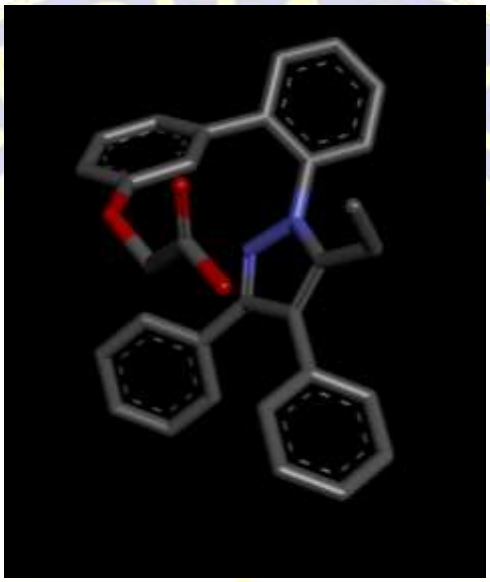


Gambar III.2 Struktur 3D reseptor *Human Adipocyte Fatty Acid Binding Protein* (aFABP)

LAMPIRAN 4

LIGAN ALAMI

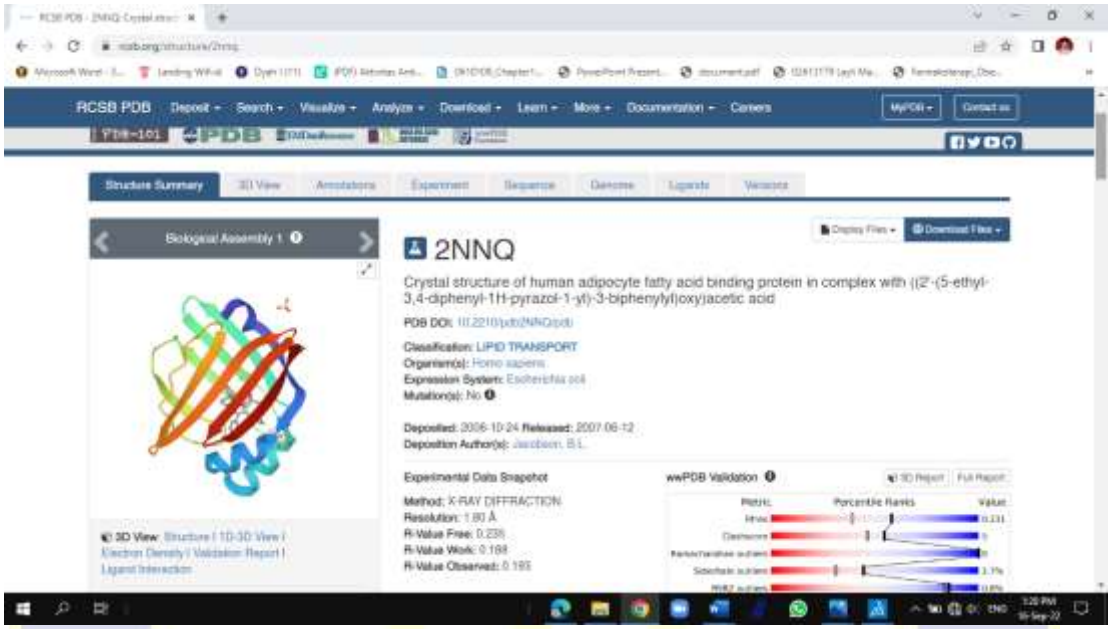
((*2'-(5-ethyl-3,4-diphenyl-1H-pyrazol-1-YL)-3-biphenylyl)oxy)acetic acid*) dari reseptor adipocyte Fatty Acid Binding Protein (aFABP)



Gambar IV.1 Ligan alami aFABP

LAMPIRAN 5

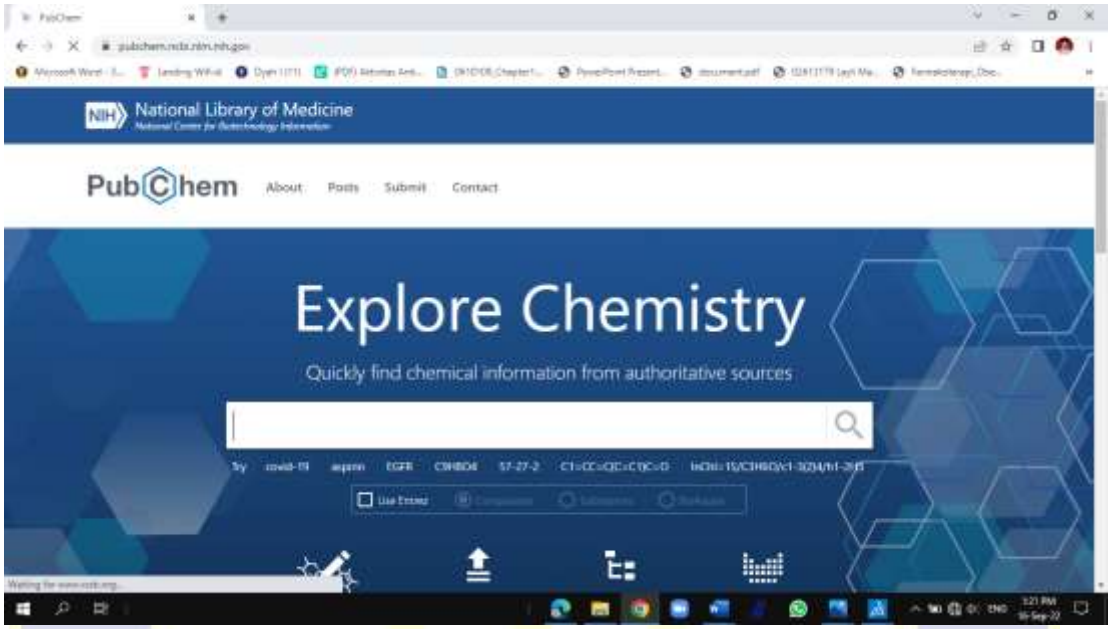
SITUS *PROTEIN DATA BANK*



Gambar IV.2 Situs *Online Protein Data Bank*

LAMPIRAN 6

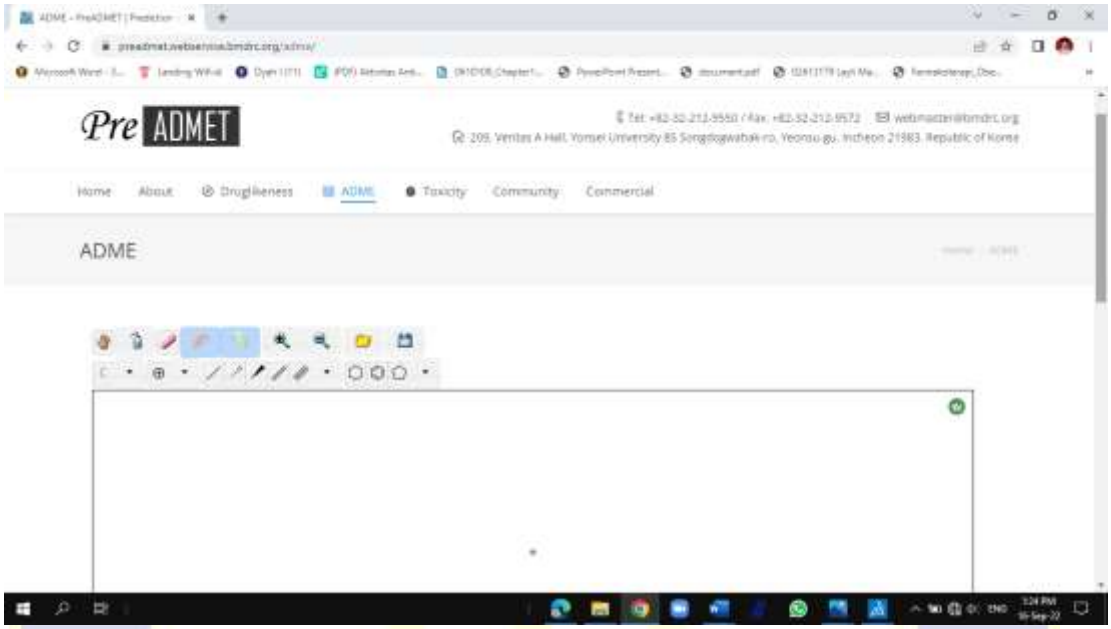
SITUS *PUBCHEM*



Gambar IV.3 Situs *Online PubChem*

LAMPIRAN 7

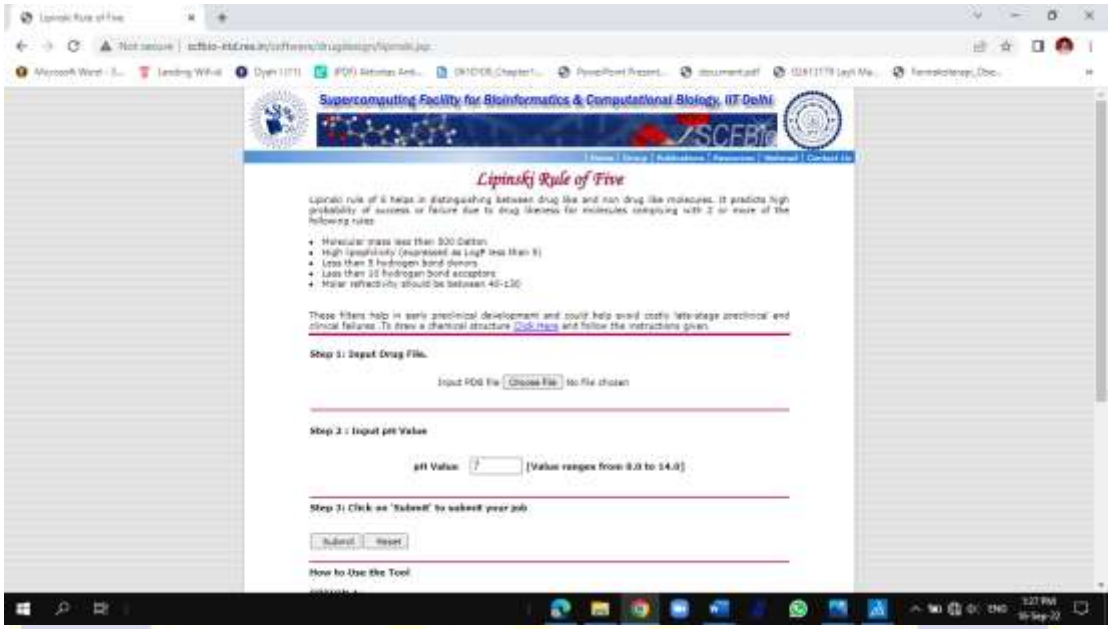
SITUS *Pre-ADMET*



Gambar IV.4 Situs *Online Pre-ADMET*

LAMPIRAN 8

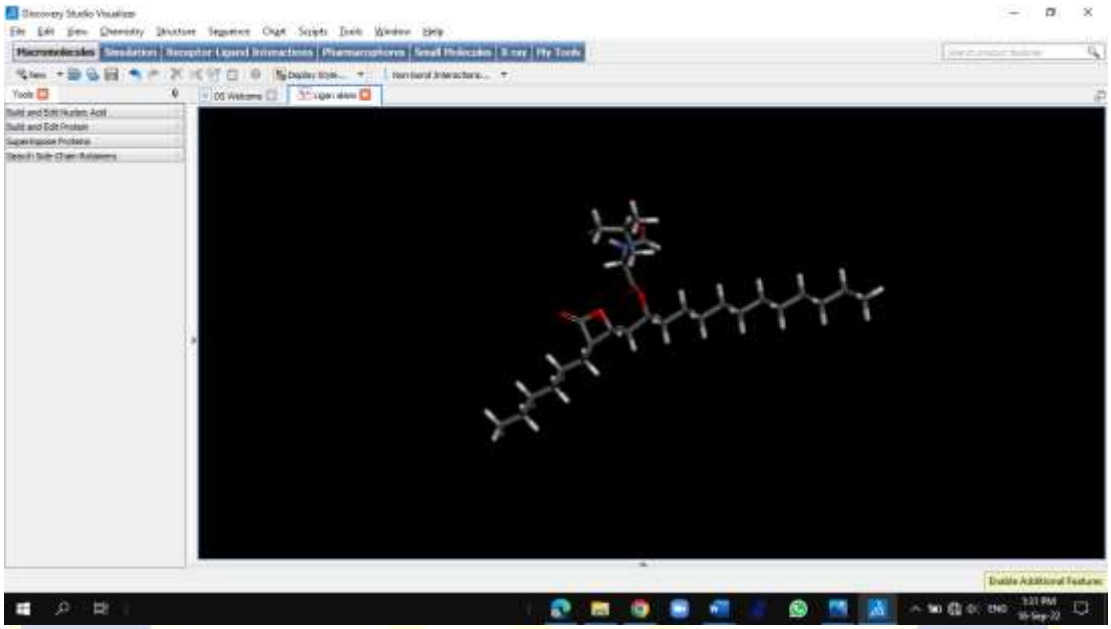
SITUS *LIPINSKI'S RULE OF FIVE*



Gambar IV.5 Situs *Online Lipinski's Rule Of Five*

LAMPIRAN 9

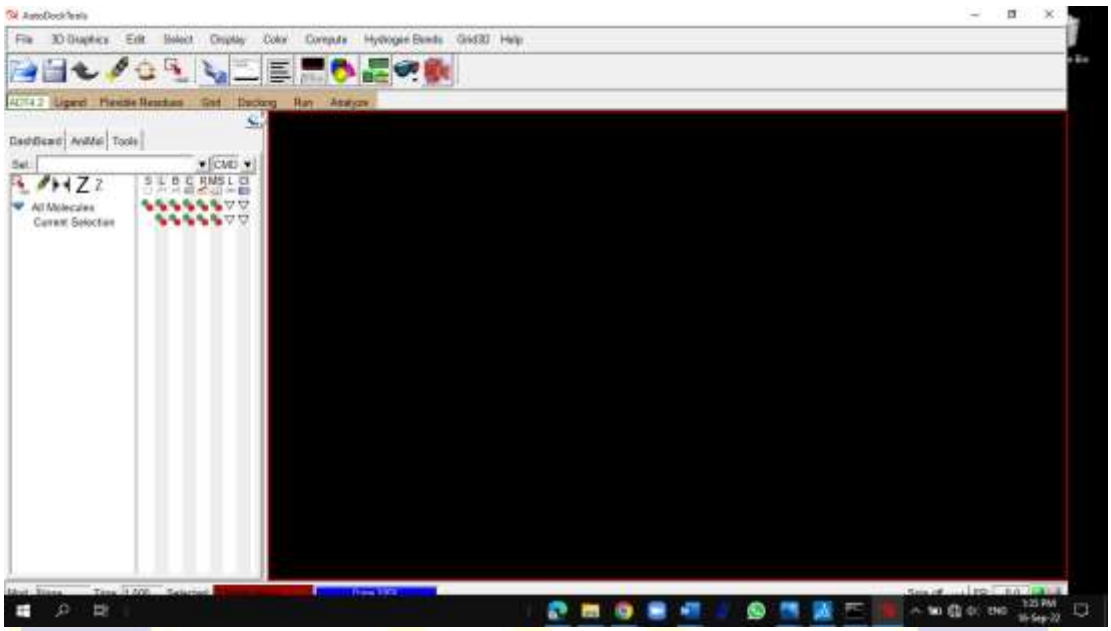
PERANGKAT LUNAK *DISCOVERY STUDIO VISUALIZER*



Gambar IV.6 Perangkat lunak *Discovery Studio Visualizer*

LAMPIRAN 10

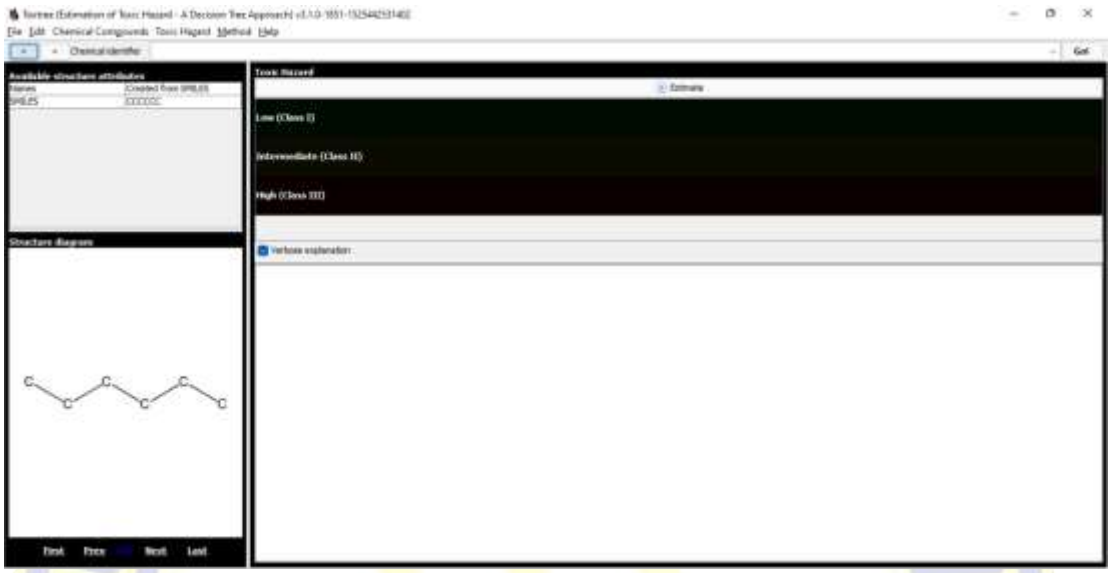
PERANGKAT LUNAK *AUTODOCK TOOLS*



Gambar IV.7 Perangkat lunak *AutoDock Tools*

LAMPIRAN 11

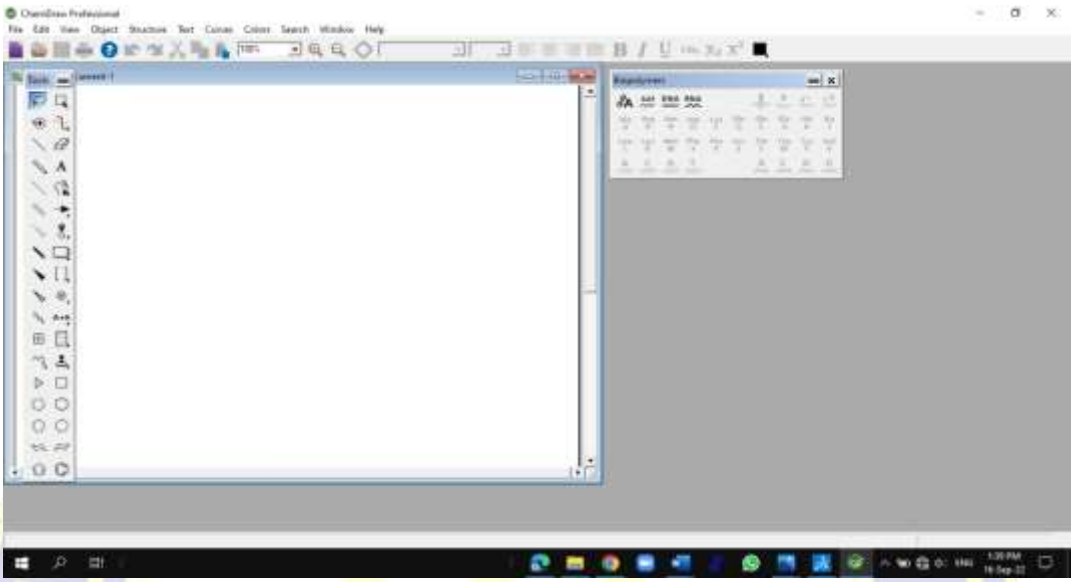
PERANGKAT LUNAK *TOXTREE*



Gambar IV.8 Perangkat lunak *Toxtree*

LAMPIRAN 12

PERANGKAT LUNAK *CHEM DRAW*

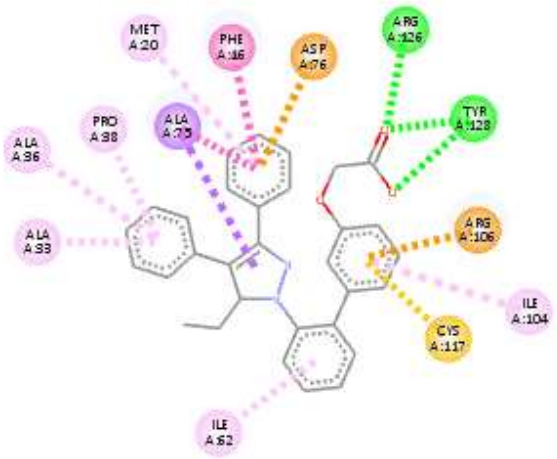


Gambar IV.9 Perangkat lunak *Chem Draw*

LAMPIRAN 13

HASIL VALIDASI

Gambar V.1 Visualisasi tumpang tindih ligan alami dengan ligan hasil *re-docking* dari reseptor *human adipocyte fatty acid binding protein* (aFABP)



Gambar V.2 Visualisasi interaksi residu asam amino ligan alami dengan reseptor *adipocyte Fatty Acid Binding Protein* (aFABP)

LAMPIRAN 13

(LANJUTAN)

Tabel V.2
Grid Box, Nilai RMSD, Nilai ΔG (Energi bebas)

Reseptor	**Grid Box**		**RMSD**	**ΔG (Energi Bebas Gibbs)**	**Konstanta Inhibisi (Ki)**
	Center	**Size**			
Human Adipocyte Fatty Acid Binding Protein (aFABP) Kode 2NNQ	X: 4.687 Y: 7.609 Z: 18.565	X : 24 Y : 26 Z: 24	1.8 Å	-7.17	5.51 uM

LAMPIRAN 14

HASIL PENAMBATAN MOLEKUL

Hasil penambatan molekul senyawa aktif dari daun katuk (*Sauropus androgynus* L Merr) dan identifikasi interaksi hidrogen menggunakan *Discovery Studio Visualizer* terhadap reseptor target *Human Adipocyte Fatty Acid Binding Protein* (aFABP)

Tabel V.3
Hasil Penambatan Molekul

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan	
				Hidrofobik	Hidrogen
1.	*Androstan-17-one-3-ethyl-3-hydroxy-5 alpha*	-8,48	613,32	-	ARG126A TYR128A ASP76A
2.	*Papaverine*	-7,16	5,620	GLU72A ARG78A ASP76A MET20A ALA33A HIS93A PHE57A	ALA75A GLN95A
3.	*Chorcoinoside C*	-6,43	19,41	PHE16A PHE57A ALA33A	ARG126A ARG106A ARG78A TYR128A ASP76A
4.	*Isolariciresinol*	-6,42	19,680	TYR19A ALA75A CYS117A VAL115A	ARG126A ASP76A TYR128A GLN95A

LAMPIRAN 14

(LANJUTAN)

Tabel V.3
Lanjutan

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan	
				Hidrofobik	Hidrogen
5.	*Sauroposide*	-6,36	21,780	-	ARG126A ARG106A ASP76A TYR128A GLN95A
6.	*11,14,17-eicosatrienoic acid methyl ester*	-4,34	659,380	PHE57A PHE16A ALA33A PRO38A CYS117A TYR19A MET20A VAL25A	ARG126A
7.	*Methylpyroglutamate*	-5,43	104,290	ALA33A PRO38A PHE16A	TYR128A ARG126A

LAMPIRAN 14

(LANJUTAN)

Tabel V.3
Lanjutan

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan	
				Hidrofobik	Hidrogen
8.	*Octadecanoic acid*	-5,23	146,310	ILE106A CYS117A TYR19A ALA75A MET20A PHE57A PRO38A PHE16A ALA33A	ARG126A
9.	*3,4-dimethyl-2-oxocyclopent-3-enylacetic acid*	-5,22	149,440	-	ARG126A ARG106A TYR128A
10.	*Guanosine*	-4,74	337,010	ALA75A ALA33A	ASP76A TYR128A
11.	*9-eicosyne*	-5,84	52,380	VAL23A ALA75A ALA33A ALA36A PRO38A ILE104A TYR128A TYR19A	-

LAMPIRAN 14

(LANJUTAN)

Tabel V.3
Lanjutan

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan	
				Hidrofobik	Hidrogen
12.	*Monomethyl succinate*	-4,08	1,010	-	ARG126A ARG106A TYR128A
13.	*Ascorbic acid*	-3,83	1550000	-	TYR19A GLN95A ASP76A
14.	*Cyclopentanol*	-3,54	2540000	CYS117A VAL115A	ARG126A TYR128A
15.	*Phenyl malonic acid*	+0,50	-	ARG78A ILE104A ALA75A PRO38A ALA33A ALA36A SER53A	ASP76A ARG106A ARG126A CYS117A
16.	*Liriodendrin*	+13,73	-	TYR128A THR60A ILE51A ALA75A MET20A TYR19A GUN95A	ARG106A ARG78A CYS117A

LAMPIRAN 14

(LANJUTAN)

Tabel V.3
Lanjutan

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang berikatan	
				Hidrofobik	Hidrogen
17.	*Kaempferol 3-gentiobioside-7-rhamnoside*	+48,28	-	ALA33A MET20A PHE57A CYS117A THR60A SER53A ARG126A	ASP76A ARG106A
18	*Orlistat*	-7,17	5,150	ALA75A MET20A PHE16A ASP76A ARG106A ILE104A CYS117A ILE62A ALA93A ALA96A PRO98A	ARG126A TY128A

LAMPIRAN 15

HASIL PENGUJIAN *PREADMET*

Tabel V.4
Hasil Pengujian *Pre-ADMET*

No.	Ligan	Absorpsi		Distribusi
		$Caco_2$ ($nm.Sec^{-1}$)	HIA (%)	PPB(%)
1.	*Isolariciresinol*	21,09	84,23	85,05
2.	*Guanosine*	9,24	25,89	8,04
3.	*Corchoionoside C*	10,89	46,82	41,86
4.	*Papaverine*	52,34	97,38	88,69
5.	*Sauroposide*	9,18	25,04	35,53
6.	*Ascorbic Acid*	2,48	33,15	5,30
7.	*Liriodendrin*	16,12	10,59	32,35
8.	*Kamferol-3-gentiobioside-7-rhamnoside*	6,79	0,59	25,92
9.	*Monomethyl succinate*	19,63	69,54	80,20
10.	*Phenyl malonic acid*	20,03	40,32	80,28
11.	*Cyclopentanol*	19,68	100	86,46
12.	*Methylpyroglutamate*	22,08	88,62	75,30
13.	*Andostan-17-one-3-ethyl-3-hydroxy-5-alpha*	33,27	95,62	100
14.	*3,4-dimethyl-2-oxocyclopent-3-enylacetic acid*	20,83	89,98	33,83
15.	*Octadecanoic acid*	28,29	98,44	100
16.	*9-eicosyne*	22,51	100	100
17.	*11,14,17-eicosatrienoic acid methyl ester*	48,21	100	100

Keterangan: *In vitro CaCo-2 permeabilitas sel ($nm. Sec^{-1}$) :*
>70 permeabilitas tinggi; 4-70 permeabilitas menengah; <4 permeabilitas rendah
Human Intestinal Absorption (HIA) : 70-100 % penyerapan baik
20-70% penyerapan cukup; 0-20% penyerapan kurang baik
Plasma Protein Binding (PPB): >90% ikatan kuat; <90% ikatan lemah

LAMPIRAN 16

HASIL PENGUJIAN TOKSISITAS

Tabel V.5
Hasil Pengujian Toksisitas

NO.	Senyawa	Crame Ruls	Kroes TTC	Benigne/bosarulebse
1.	*Isolariciresinol*	3	1	8,9
2.	*Guanosine*	3	2	1,9
3.	*Corchoionoside C*	3	2	1,9
4.	*Papaverine*	3	1	8,9
5.	*Sauroposide*	3	2	1,9
6.	*Ascorbic Acid*	3	1	8,9
7.	*Liriodendrin*	3	1	8,9
8.	*Kamferol-3-gentiobioside-7-rhamnoside*	3	1	8,9
9.	*Monomethyl succinate*	1	1	8,9
10.	*Phenyl malonic acid*	3	1	8,9
11.	*Cyclopentanol*	2	1	8,9
12.	*Methylpyroglutamate*	3	1	8,9
13.	*Andostan-17-one-3-ethyl-3-hydroxy-5-alpha*	3	1	8,9
14.	*3,4-dimethyl-2-oxocyclopent-3-enylacetic acid*	2	2	1,9
15.	*Octadecanoic acid*	1	1	8,9
16.	*9-eicosyne*	3	1	8,9
17.	*11,14,17-eicosatrienoic acid methyl ester*	1	1	8,9

Keterangan: *Cramer ruler class 1 : low, class 2 : intermediet, class 3 : high. Benigni/bosa rulebase 2 (structural alert for non genotoxic carcinogenicity), 8 (negative for genotoxic carcinogenity), 9 (negative for non-genotoxic carcinogencity). Kroes TTC decission tree 1 (Subtance would not be expected to be a safety concern)*

LAMPIRAN 17

HASIL PENGUJIAN *LIPINSKI'S RULE OF FIVE*

Tabel V.6
Hasil Pengujian *Lipinski's Rule Of Five*

No.	Ligan	BM	Log P	Ikatan hidrogen		Keterangan
				Donor	Akseptor	
1.	*Isolariciresinol*	360	1,787	4	6	Memenuhi Syarat
2.	*Guanosine*	283	-2,81	6	9	Memenuhi Syarat
3.	*Corchoionoside C*	386	-0,57	5	8	Memenuhi Syarat
4.	*Papaverine*	339	3,859	0	5	Memenuhi Syarat
5.	*Sauroposide*	402	-1,60	6	9	Memenuhi Syarat
6.	*Ascorbic Acid*	176	-1,40	4	6	Memenuhi syarat
7.	*Liriodendrin*	742	-2,69	8	18	Tidak Memenuhi Syarat
8.	*Kamferol-3-gentiobioside-7-rhamnoside*	756	-4,11	12	20	Tidak Memenuhi Syarat
9.	*Monomethyl succinate*	132	0,024	1	4	Memenuhi Syarat
10.	*Phenyl malonic acid*	745	1,132	9	16	Tidak Memenuhi Syarat
11.	*Cyclopentanol*	86	0,921	1	1	Memenuhi Syarat
12.	*Methylpyroglutamate*	257	1,331	0	6	Memenuhi Syarat
13.	*Andostan-17-one-3-ethyl-3-hydroxy-5-alpha*	318	4,739	1	2	Memenuhi Syarat
14.	*3,4-dimethyl-2-oxocyclopent-3-enylacetic acid*	168	1,386	1	3	Memenuhi Syarat
15.	*Octadecanoic acid*	284	6,332	1	2	Memenuhi Syarat
16.	*9-eicosyne*	278	7,271	0	0	Memenuhi Syarat
17.	*11,14,17-eicosatrienoic acid methyl ester*	320	6,529	0	2	Memenuhi Syarat

***Keterangan* :** *BM (Berat molekul) <500 Dalton*

Log P <5

Donor ikatan hidrogen <5

dan Akseptor ikatan hidrogen <10

1. IDENTITAS DIRI

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2. RIWAYAT PENDIDIKAN

Jenjang Pendidikan	Nama Sekolah/ Universitas	Tahun Masuk	Tahun Keluar
SD/ MI	SDN 1 WANARAJA	2006	2012
SMP/ MTs	SMPN 1 WANARAJA	2012	2015
SMA/ SMK/ MA	SMAN 18 GARUT	2015	2018
Perguruan tinggi	UNIVERSITAS GARUT	2018	2022