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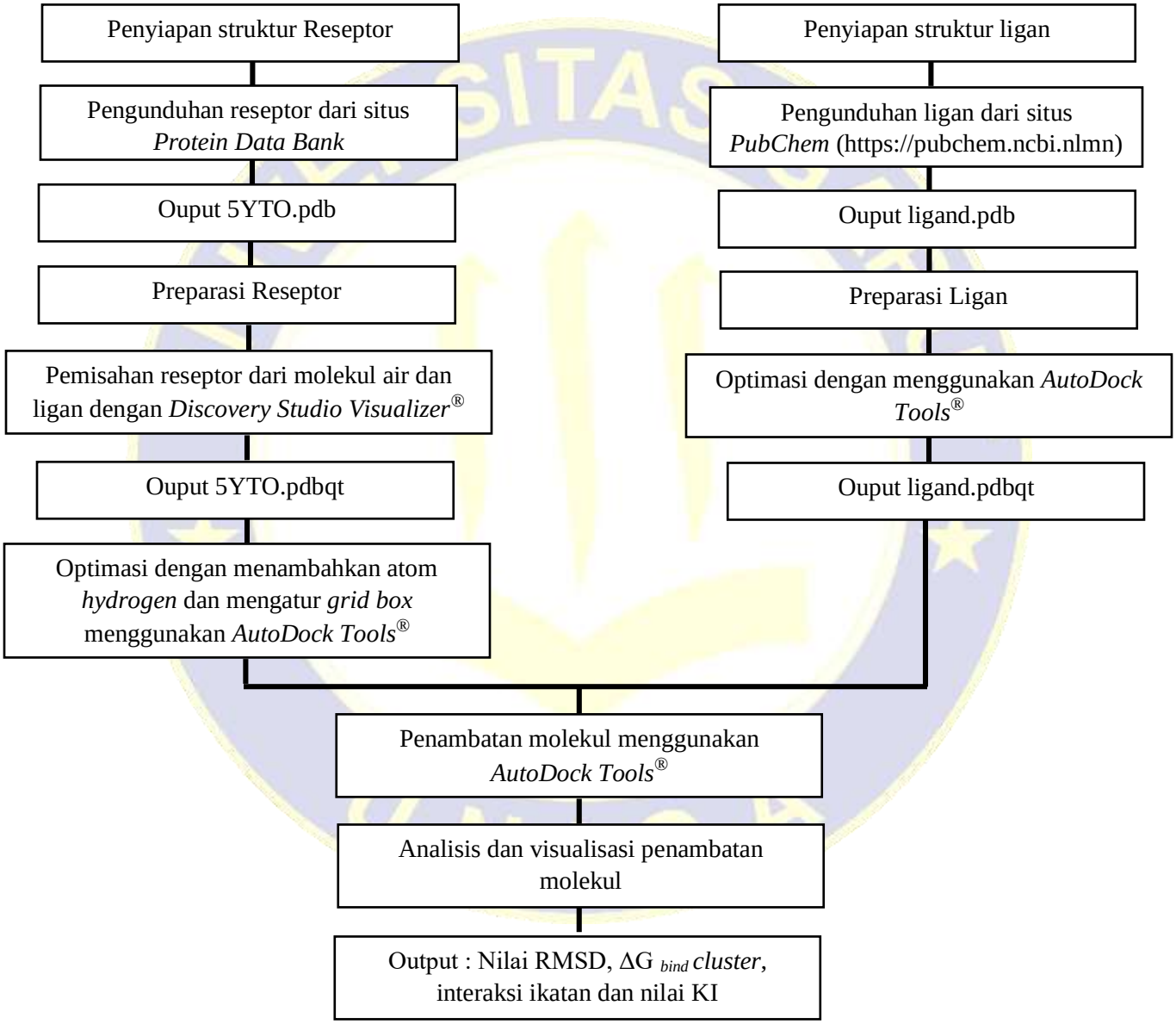
LAMPIRAN 1

ALUR PENELITIAN PENAMBATAN MOLEKUL

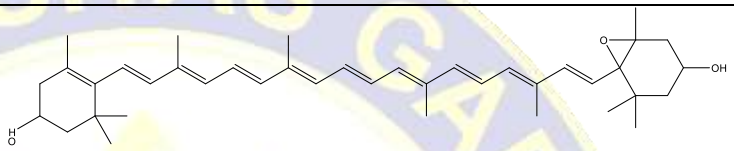
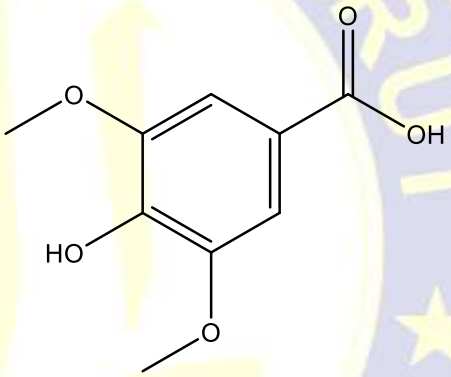
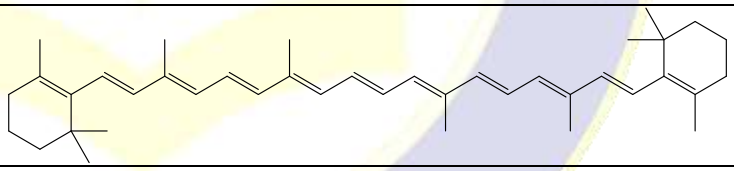
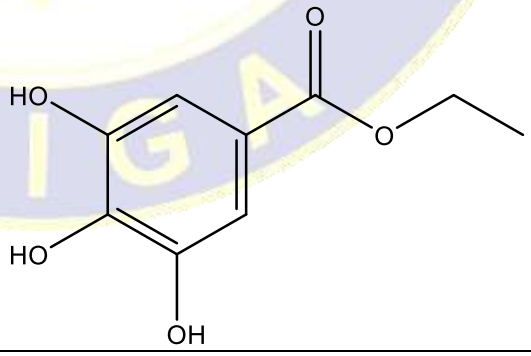


Gambar III.1 Alur penelitian penambatan molekul reseptor 5YTO

LAMPIRAN 2

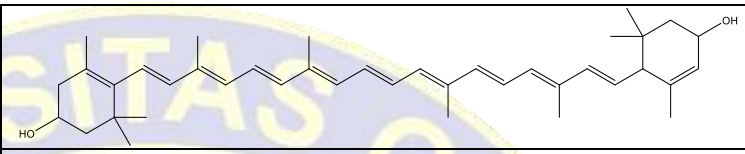
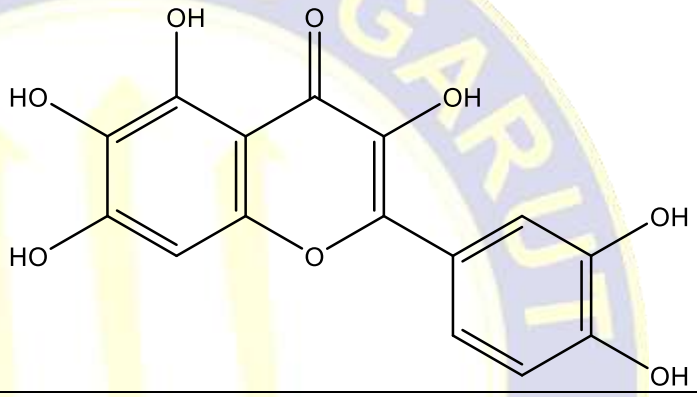
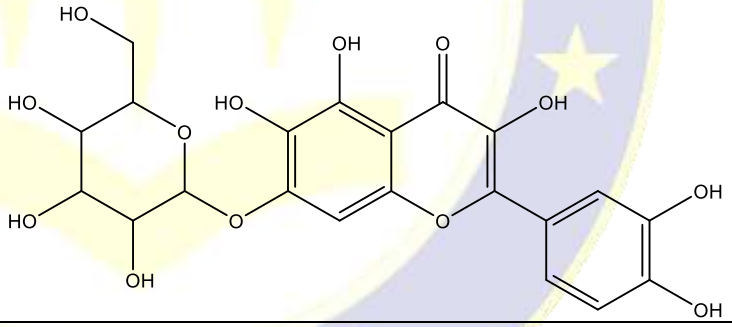
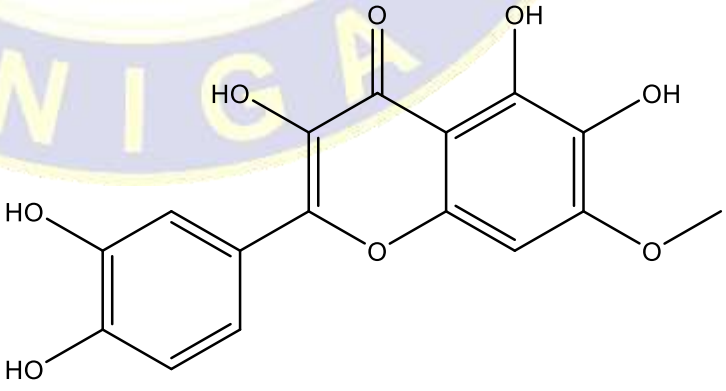
SENYAWA BUNGA KENIKIR (*Tagetes erecta* L*)*

Tabel V. 1
Senyawa Bunga Kenikir (*Tagetes erecta* L)

No	Nama Senyawa	Struktur 2D
1	Antraxantin	
2	Asam syringic	
3	β- karoten	
4	Etil galat	

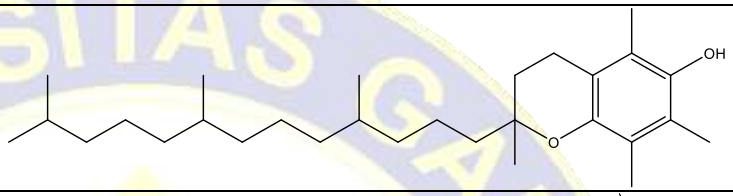
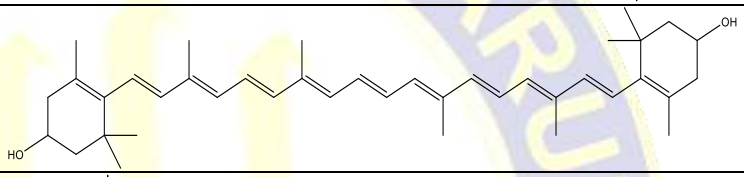
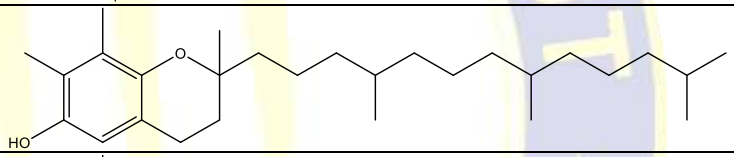
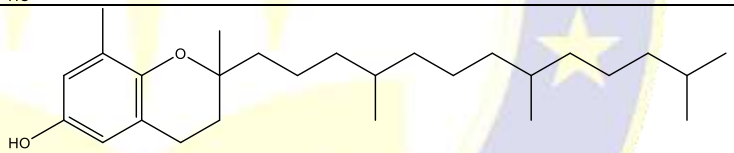
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

5	Lutein	
6	Kuarsetagetin	
7	Kuarsetagetin-7 metil eter	
8	Kuarsetagetin-7-O-glukosida	

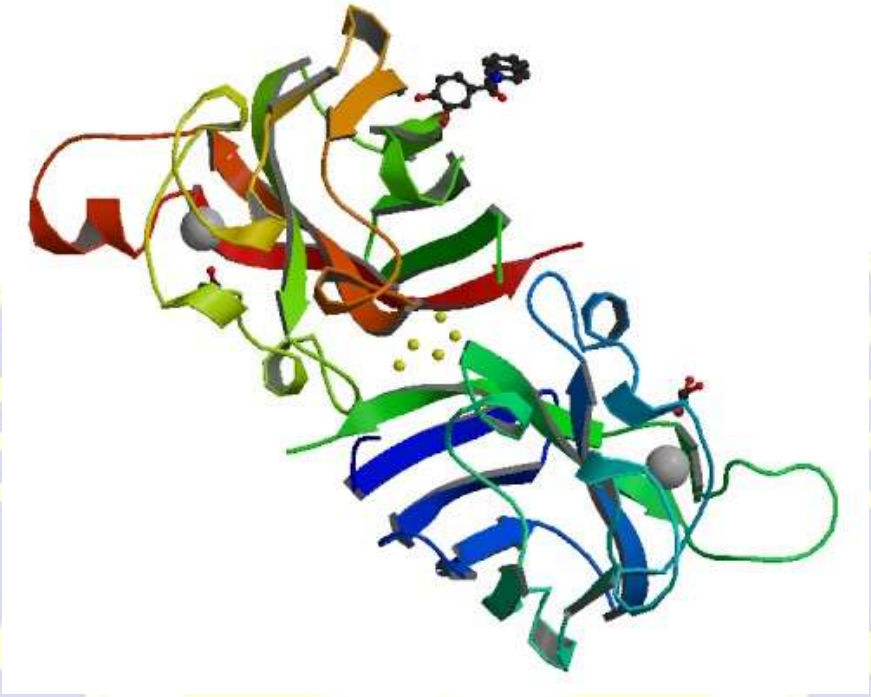
LAMPIRAN 2
(LANJUTAN)

Tabel V.1
Lanjutan

9	Tokoferol	
10	Zeaxantin	
11	γ-tokoferol	
12	δ-tokoferol	

LAMPIRAN 3

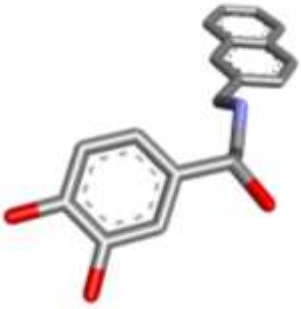
RESEPTOR SUPEROXIDE DISMUTASE I (SOD1)



Gambar III.2 Struktur 3D reseptor

LAMPIRAN 4

LIGAN ALAMI



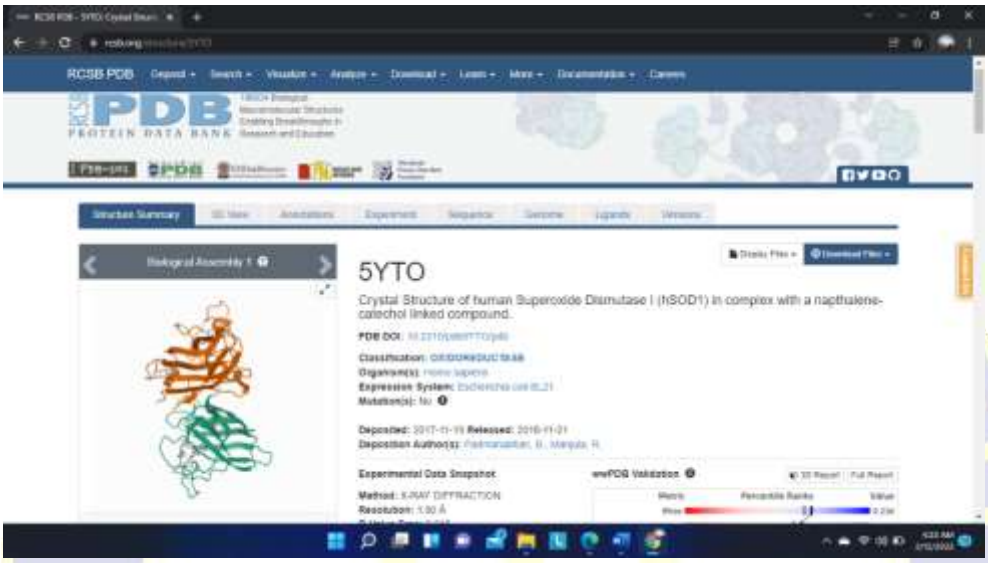
SOD1 inhibitor

Ligan alami (*napthalene-catechol*) dari reseptor superoxide dismutase 1 (SOD1)

Gambar IV. 1 Ligan alami

LAMPIRAN 5

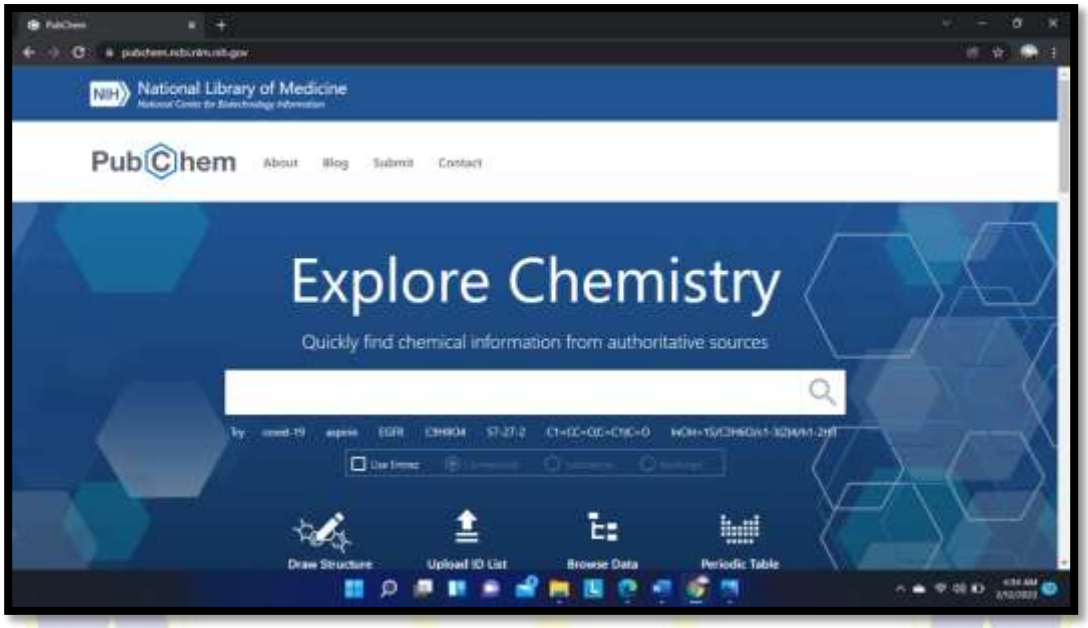
SITUS PDB (PROTEIN DATA BANK)



Gambar IV. 2 Situs online PDB *(Protein Data Bank)*

LAMPIRAN 6

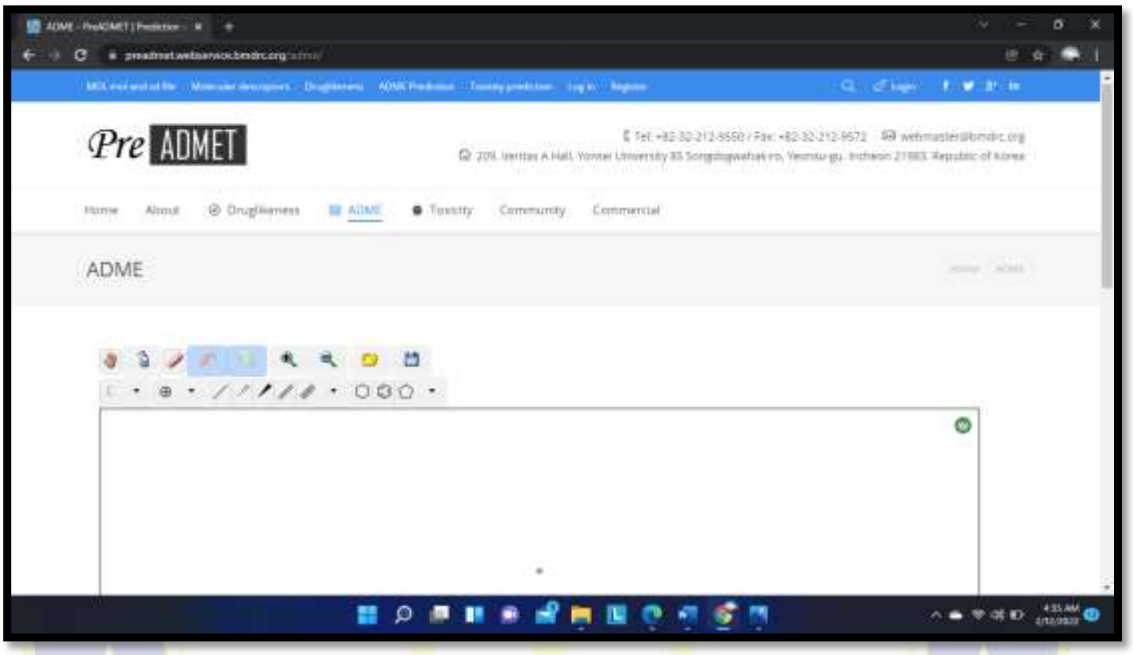
SITUS PubChem



Gambar IV. 3 Situs Online PubChem

LAMPIRAN 7

SITUS Pre-ADMET



Gambar IV. 4 Situs Online Pre-ADMET

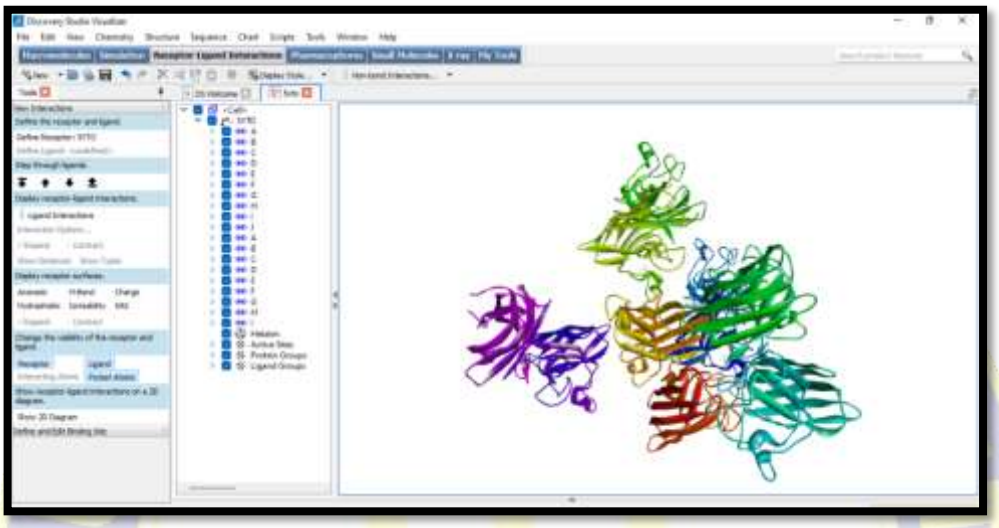
LAMPIRAN 8

SITUS *Lipinski Rule Of Five*

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

LAMPIRAN 9

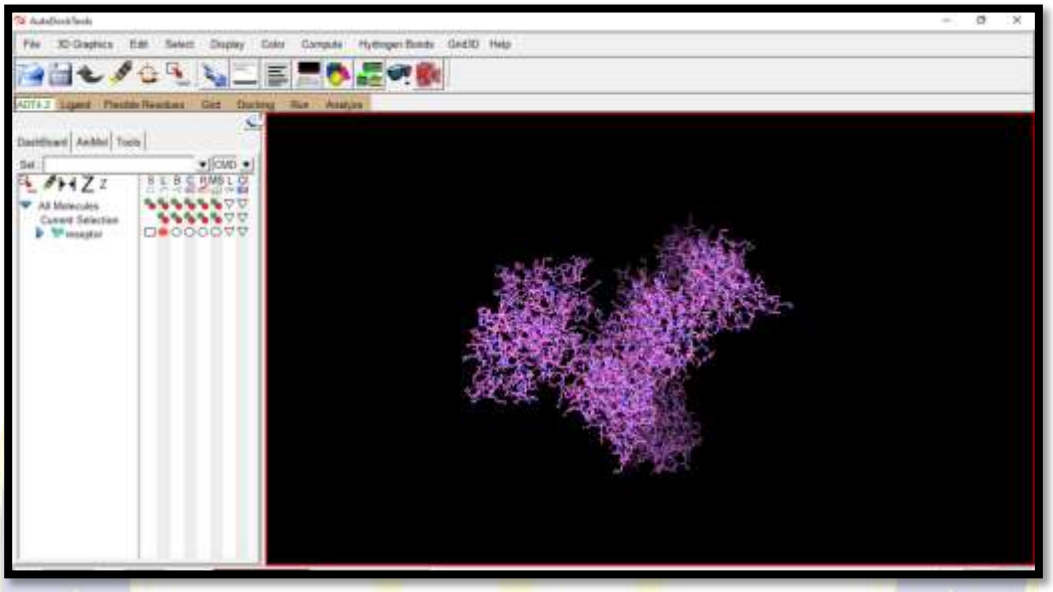
PERANGKAT LUNAK *DISCOVERY STUDIO VISUALIZER*



Gambar IV. 6 Perangkat lunak discovery studio visualizer

LAMPIRAN 10

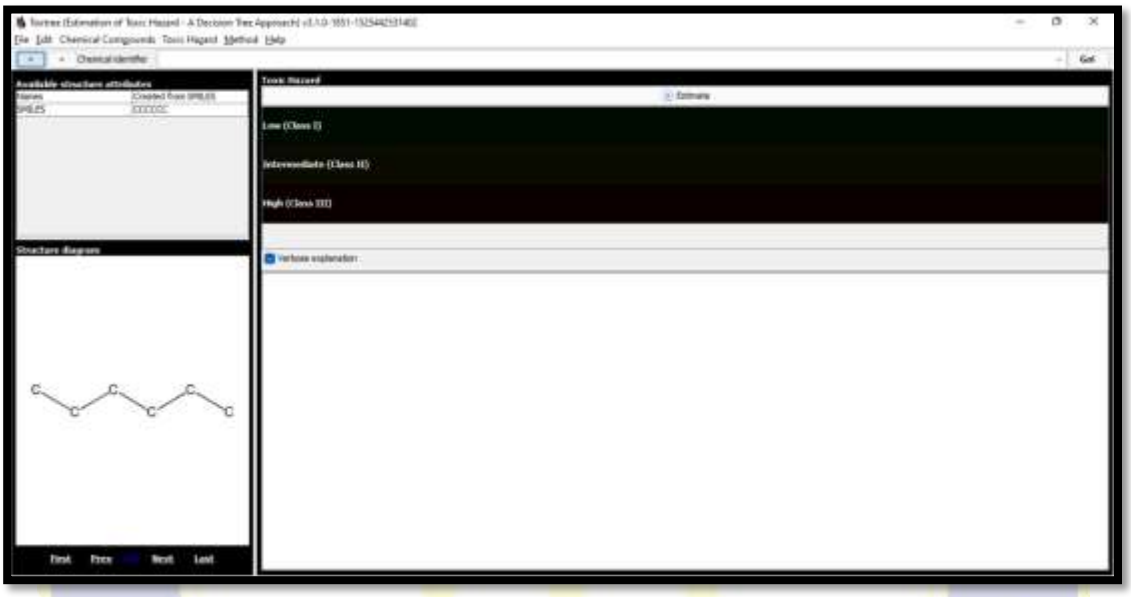
PERANGKAT LUNAK *AUTODOCK TOOLS*



Gambar IV. 7 Perangkat lunak autodock tools

LAMPIRAN 11

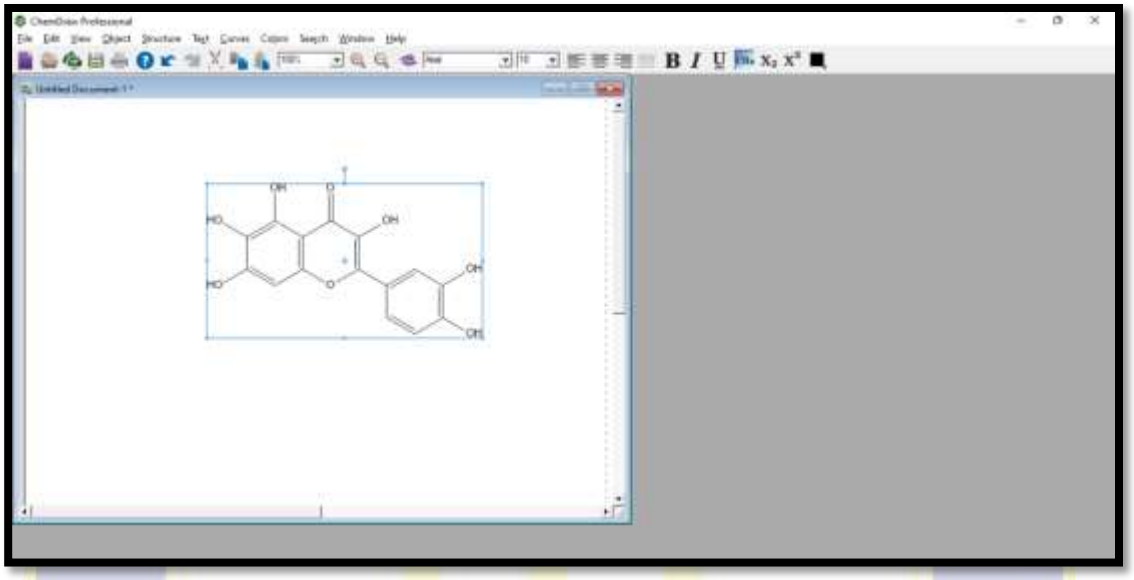
PERANGKAT LUNAK *TOXTREE*



Gambar IV. 8 Perangkat lunak *toxtree*

LAMPIRAN 12

PERANGKAT LUNAK *CHEMDRAW*



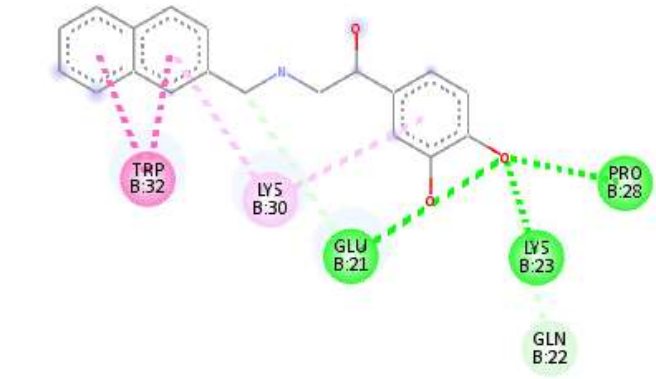
Gambar IV. 9 Perangkat lunak *chemdraw*

LAMPIRAN 13

HASIL VALIDASI

Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor *superoxide dismutase 1* (SOD1)

Gambar V. 1 Hasil validasi



Visualisasi interaksi residu asam amino ligan alami dengan reseptor *superoxide dismutase 1* (SOD1)

Gambar V. 2 Hasil visualisasi interaksi residu asam amino

LAMPIRAN 13
(LANJUTAN)

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

Reseptor	Grid Box		RMSD	ΔG (Energi Bebas)	Konstanta Inhibisi (Ki)
	Center	Size			
Superoxide dismutase 1 (SOD1) Kode 5YTO	X: 70.465 Y: 75.837 Z: -12.275	X : 24 Y : 16 Z: 34	1.424 Å	-7,76	2,05

LAMPIRAN 14

HASIL PENAMBATAN MOLEKUL

Hasil penambatan senyawa aktif dari bunga kenikir (*Tagetes erecta* L.) dan identifikasi interaksi hidrogen menggunakan Discovery Studio Visualizer terhadap reseptor target Superoxide dismutase 1 (SOD1) kode 5YTO

Tabel V. 3
Hasil Penambatan Molekul

No.	Ligan	ΔG (kkal/mol)	KI (nM)	Residu asam amino yang beriakatan	
				Hidrofobik	Hidrogen
1.	Antrhraxantin	+3,23	-	TRP92B LYS23B	-
2.	Asam syringic	-2,47	15,46	LYS30B GLU21B PRO28B GLU100B LYS23B	PRO28B GLU21B
3.	Beta karoten	+2,29	-	LYS90B	-
4.	Etil galat	-3,47	2,85	GLU21B GLN22B LYS30B LYS23B	PRO28B GLU100B
5.	Lutein	+3,08	-	LYS23B VAL29B PRO28B	SER105B SER25B
6.	Kuarsetagetin	-3,93	1,31	LYS30B	PRO28B
7.	Kuarsetagetin-7 - metil	-4,11	977,81	LYS30B	PRO28B

LAMPIRAN 14
(LANJUTAN)

Tabel V.3
Lanjutan

8.	Kuarsetagetin7-O-Glukosida	-3,39	3.30	LYS30B TRP32B	GLU132C GLU21B SER98H PRO28B
9.	Tokoferol	-3,44	3.00	TRP32H TRP32B LYS30B LYS23B	-
10.	Zeaxantin	+3,08	-	LYS90B TRP92B	-
11.	γ-tokoferol	-5,83	53,45	LYS23B LYS30B TRPB32B TRP32H	PRO28B
12.	δ-tokoferol	-5,46	99,43	LYS23B TRP32B TRP32H	GLU100B
13.	Asam Askorbat	-3,29	77,75	-	LYS23B PRO28B GLU21B

LAMPIRAN 15

HASIL PENGUJIAN PREADMET

Tabel V. 4
Hasil Pengujian Pre-ADMET

No.	Ligan	Absorpsi		Distribusi
		$Caco_2$ ($nm.Sec^{-1}$)	HIA (%)	PPB(%)
1.	Antraxantin	54,90	95,90	93,94
2.	Asam sringyic	18,83	82,02	69,77
3.	Beta karoten	23,22	100	100
4.	Etil Galat	0,18	72,04	96,03
5.	Kuarsetagetin	0,99	40,94	98,33
6.	Kuarsetagetin-7 Metil eter	2,19	60,33	86,21
7.	Kuarsetagetin-7-O-Glukosida	4,03	5,28	62,83
8.	Lutein	54.92	95.52	100
9.	Tokoferol	47.19	98.81	100
10.	Zeaxantin	54.90	95.52	98.68
11.	γ-tokoferol	27.93	97.80	100
12.	δ-tokoferol	26.82	97.77	100

Keterangan: *in vitro CaCo-2 cell permeability (nm. Sec^{-1}): >70 higher permeability, 4-70 medium permeability, <4 low permeability; % human intestinal absorption (%HIA): 700-100% well absorbed, 20-70% moderately absorbed, 0-20% poorly absorbed; %plasma protein binding: >90% strongly bound, <90% weakly bound.*

LAMPIRAN 16

HASIL PENGUJIAN TOKSISITAS

Tabel V. 5
Hasil Pengujian Toksisitas

NO.	Senyawa	Crame Ruls	Kroes TTC	Benigne/bosarulebse
1.	Antraxantin	3	2	1,9
2.	Asam Syringic	1	1	8,9
3.	Beta caroten	2	1	8,9
4.	Etil galat	1	1	8,9
5.	Lutein	2	1	8,9
6.	Kuarsetagetin	3	1	8,9
7.	Kuarsetagetin-7 metil eter	3	1	8,9
8.	Kuarsetagetin-7-O-glukosida	3	1	8,9
9.	Tokoferol	3	1	8,9
10.	Zaexantin	2	1	8,9
11.	γ-tokoferol	2	1	8,9
12.	δ-tokoferol	2	1	8,9

Keterangan: *Cramer ruler class 1 : low, class 2 : intermediet, class 3 : high. Benigni/bosa rulebase 1 (structural alert for 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), 2 (Negligible risk (low probability of a life time cancer risk greater than 1 in 10^6))*

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.	Antraxantin	584	9,7586	2	3	Tidak Memenuhi Syarat
2.	Asam Syringic	198	1,1076	2	5	Memenuhi Syarat
3.	β- karoten	536	12,605	0	0	Tidak Memenuhi Syarat
4.	Etil Galat	198	0,980	3	5	Memenuhi Syarat
5.	Lutein	568	10,433	2	2	Tidak Memenuhi Syarat
6.	Kuarsetagetin	0	0	0	0	Memenuhi Syarat
7.	Kuarsetagetin 7-metil eter	332	2,0195	5	8	Memenuhi syarat
8.	Kuarsetagetin 7-O-glukosida	480	-0.8104	9	13	Tidak Memenuhi Syarat
9.	Tokoferol	472	9.0599	0	3	Memenuhi Syarat
10.	zeaxantin	568	10.547	2	2	Tidak Memenuhi Syarat
11.	γ-tokoferol	416	8,531	1	2	Memenuhi Syarat
12.	δ-tokoferol	402	8,223	1	2	Memenuhi Syarat

Keterangan: *BM (Berat molekul) <500 Dalton,*
Log P <5,
Donor ikatan hidrogen <5
dan Akseptor ikatan hidrogen <10.

DAFTAR RIWAYAT HIDUP

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Non Formal

PKL Rumah Sakit Umum Daerah Subang

PKL Apotek Naga Malim Subang

PKL Apotek Garut