LAMPIRAN-LAMPIRAN

LAMPIRAN I

SINTESIS SENYAWA KOMPLEKS *BIS-(1-(4-HEPTYLBENZOIL)-3-METHYLTHIOUREA) COBALT (III)*

Hasil *Refluks*

Proses penguapan

Penimbangan hasil sintesis

Perhitungan Stoikiometri

$2C_{16}H_{23}OSN_2 + (CO(BF_4))_2.6H_2O \longrightarrow CO(C_{16}H_{23}OSN_2)_2 + 6H_2O + 2BF_4$

m	0,25 mmol	0,125 mmol		-	-	-
b	0,125 mmol	0,125 mmol		0,125mmol	0,75mmol	0,25 mmol
s	0,125 mmol	-		0,125 mmol	0,75 mmol	0,25 mmol

$C_{16}H_{23}OSN$ = mmol x massa molar

= 0,25 x 294.464

= 73.61 mg

$(CO(BF_4))_2.6H_2O$ = mmol x massa molar

= 0,125 x 340,63

= 42,57 mg

$CO(C_{16}H_{23}OSN_2)_2$ = mmol x massa molar

= 0,125 x 641.813

= 80,22 mg

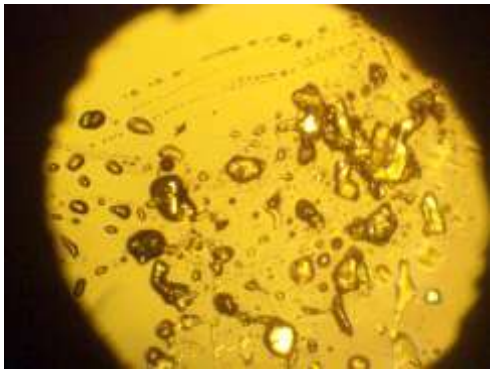
$$\%recovery = \frac{Bobot\ Sintesis}{Bobot\ Teori} x100\%$$

$$\%recovery = \frac{67}{80,22} x100\%$$

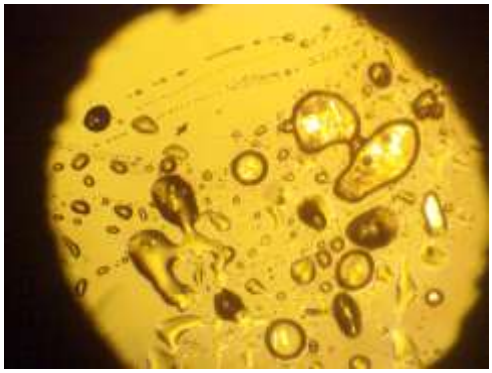
$$\%recovery = 83,52\ \%$$

LAMPIRAN II

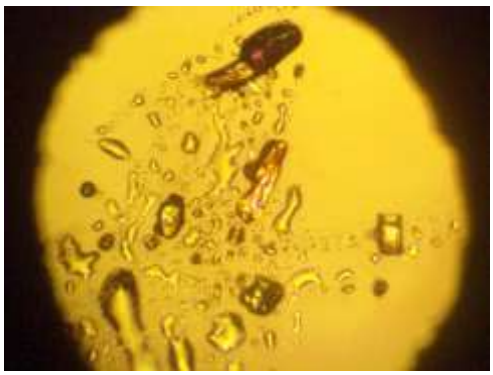
UJI KEMURNIAN



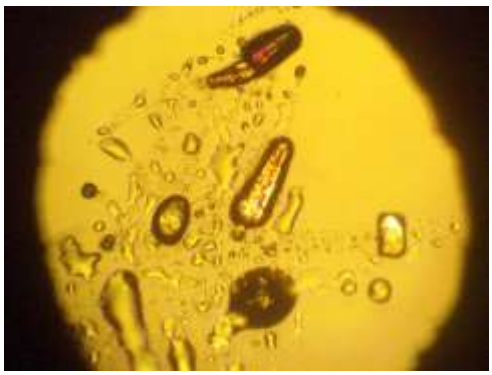
Senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea* sebelum melebur



Senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea* setelah melebur



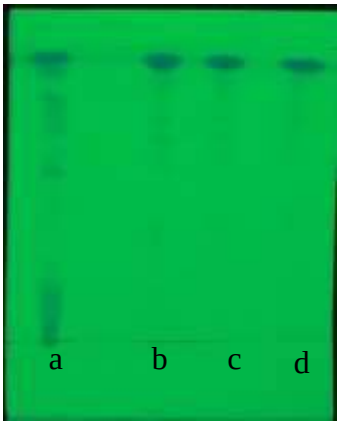
Senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)* sebelum melebur



Senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)* setelah melebur

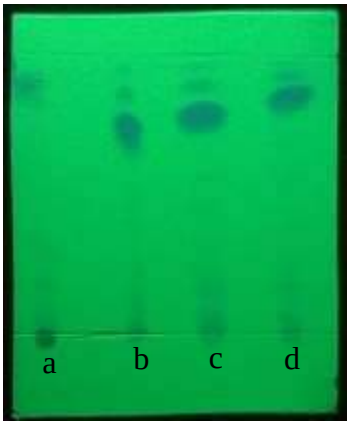
LAMPIRAN III

KROMATOGRAFI LAPIS TIPIS



Kloroform : etil asetat

9 : 2



Kloroform : n-heksan

7 : 3

Perhitungan nilai Rf :

1. Eluen kloroform : etil asetat (9:2)

   Panjang jarak eluen : 3,8

   Panjang jarak senyawa a (pembanding) : 3,6

   Panjang jarak senyawa b (senyawa kompleks) : 3,4

   Panjang jarak senyawa c (senyawa kompleks) : 3,4

   Panjang jarak senyawa d (senyawa kompleks) : 3,4

   Nilai Rf :

   a. $Rf = \frac{\text{Jarak zat terlarut}}{\text{jarak eluen}}$

      $Rf = \frac{3,6}{3,8} = 0,94$

   b. $Rf = \frac{\text{Jarak zat terlarut}}{\text{jarak eluen}}$

      $Rf = \frac{3,4}{3,8} = 0,89$

   c. $Rf = \frac{\text{Jarak zat terlarut}}{\text{jarak eluen}}$

      $Rf = \frac{3,4}{3,8} = 0,89$

d. $Rf = \frac{\text{Jarak zat terlarut}}{\text{jarak eluen}}$

$Rf = \frac{3,4}{3,8} = 0,89$

2. Eluen kloroform : n-heksan (7:3)

Panjang jarak eluen : 3,6

Panjang jarak senyawa a (pembanding) : 3,1

Panjang jarak senyawa b (senyawa kompleks) : 2,6

Panjang jarak senyawa c (senyawa kompleks) : 2,7

Panjang jarak senyawa d (senyawa kompleks) : 3

Nilai Rf :

a. $Rf = \frac{\text{jarak zat terlarut}}{\text{jarak eluen}}$

$Rf = \frac{3,1}{3,6} = 0,86$

b. $Rf = \frac{\text{jarak zat terlarut}}{\text{jarak eluen}}$

$Rf = \frac{2,6}{3,6} = 0,72$

c. $Rf = \frac{\text{jarak zat terlarut}}{\text{jarak eluen}}$

$Rf = \frac{2,7}{3,6} = 0,75$

d. $Rf = \frac{\text{jarak zat terlarut}}{\text{jarak eluen}}$

$Rf = \frac{3}{3,6} = 0,85$

LAMPIRAN IV

SPEKTROFOTOMETRI UV-VIS

1. Perhitungan Nilai Absorptivitas Molar

Hukum Lambert-Beer:

$$A = Ɛ.b.C$$

Keterangan :

A : absorbansi

Ɛ : absorptivitas molar (L mol^{-1} cm^{-1})

b : jarak yang ditempuh (cm)

C : konsentrasi (mol L^{-1})

- Perhitungan Konsentrasi

a. $Co(BF_4)_2.6H_2O$)

$$M = \frac{g}{Mr} \; x \; \frac{1000}{Ml}$$

$$M = \frac{0,002}{340,63} \; x \; \frac{1000}{10}$$

$$M = \frac{2}{3406,3}$$

M = 0,00058

b. *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

$$M = \frac{g}{Mr} \; x \; \frac{1000}{Ml}$$

$$M = \frac{0,0021}{641.813} \; x \; \frac{1000}{10}$$

$$M = \frac{2,1}{6418,13}$$

M = 0,00032

c. *1-(4-hepthylbenzoyl)-3-methylthiourea*

$$M = \frac{g}{Mr} \; x \; \frac{1000}{Ml}$$

$$M = \frac{0.002}{294.464} \; x \; \frac{1000}{10}$$

$$M = \frac{2}{2944.64}$$

M = 0.00067

d. Perhitungan Nilai Absoptivitas Molar

a. $Co(BF_4)_2.6H_2O$)

A = Ɛ.b.C

0,132 = Ɛ.1. 0,00058

0,132 = Ɛ. 0,00058

$Ɛ = \frac{0,132}{0,00058}$

Ɛ = 227,58 L mol^{-1} cm^{-1}

b. *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

A = Ɛ.b.C

2,717 = Ɛ.1. 0,00032

2,717 = Ɛ.0,00032

$Ɛ = \frac{2,717}{0,00032}$

Ɛ = 7991.17 L mol^{-1} cm^{-1}

c. *1-(4-hepthylbenzoyl)-3-methylthiourea*

A = Ɛ.b.C

2,834 = Ɛ.1. 0.00067

2,834 = Ɛ.0.00067

$Ɛ = \frac{2,834}{0,00067}$

Ɛ = 4229,85

2. Perhitungan Energi Pembelahan Kompleks

Dengan mengetahui panjang gelombang maksimum spectra kompleks dapat dihitung besarnya energi transisi (10 Dq) dengan rumus:

$$\Delta_o = \frac{(hc\ No)}{\lambda}$$

Keterangan:

Δ_o : selisih energi orbitas d (J mol^{-1})

h : konstanta planck (6,626 x 10^{-34})

c : kecepatan cahaya (2,998 x 10^8 ms^{-1})

N_o : bilangan Avogadro (6,023 x 10^{23} mol^{-1})

λ : panjang gelombang yang diserap (nm)

a. $Co(BF_4)_2.6H_2O$)

$\Delta_o = \frac{(hc\ No)}{\lambda}$

$\Delta_o = \frac{\left(6{,}626x10^{-34}.2{,}998x10^{8}.6{,}023x10^{23}\right)}{327}$

$\Delta_o = \frac{0{,}119645}{327}$

Δ_o = 0,0003658868501 J.mol^{-1}

10 Dq = 365,886 KJ.mol^{-1}

b. *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

$\Delta_o = \frac{(hc\ No)}{\lambda}$

$\Delta_o = \frac{\left(6{,}626x10^{-34}.2{,}998x10^{8}.6{,}023x10^{23}\right)}{282{,}6}$

$\Delta_o = \frac{0{,}119645}{282{,}6}$

Δ_o = 0,0004233722576 J.mol^{-1}

10 Dq = 423,372 KJ.mol^{-1}

c. *1-(4-hepthylbenzoyl)-3-methylthiourea*

$\Delta_o = \frac{(hc\ No)}{\lambda}$

$\Delta_o = \frac{\left(6{,}626x10^{-34}.2{,}998x10^{8}.6{,}023x10^{23}\right)}{295{,}2}$

$\Delta_o = \frac{0{,}119645}{295{,}2}$

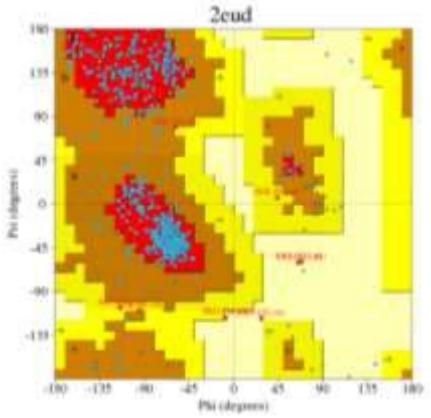
Δ_o = 0,0004053015

10 Dq = 405,3015

LAMPIRAN V

ANALISIS RESEPTOR

Proses pengunduhan Ramachandran plot PDB 2EUD melalui *website* https://www.ebi.ac.uk/pdbsum/



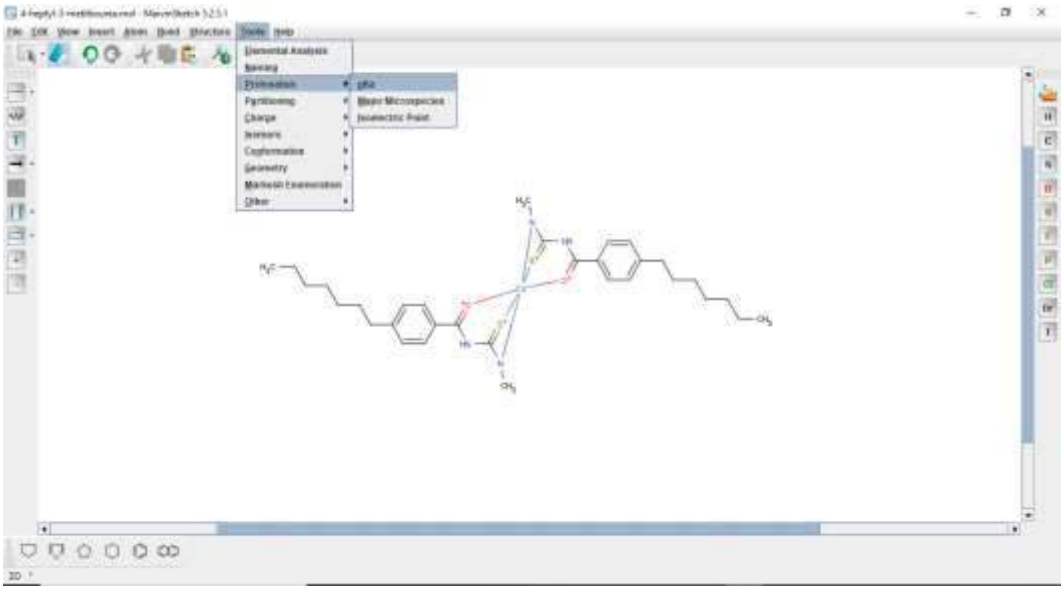
1. Ramachandran Plot statistics

		No. of residues	%-tage
Most favoured regions	[A,B,L]	509	89.8%*
Additional allowed regions	[a,b,l,p]	57	9.9%
Generously allowed regions	[~a,~b,~l,~p]	4	0.7%
Disallowed regions	[XX]	3	0.5%*
Non-glycine and non-proline residues		573	100.0%
End-residues (excl. Gly and Pro)		4	
Glycine residues		42	
Proline residues		29	
Total number of residues		648	

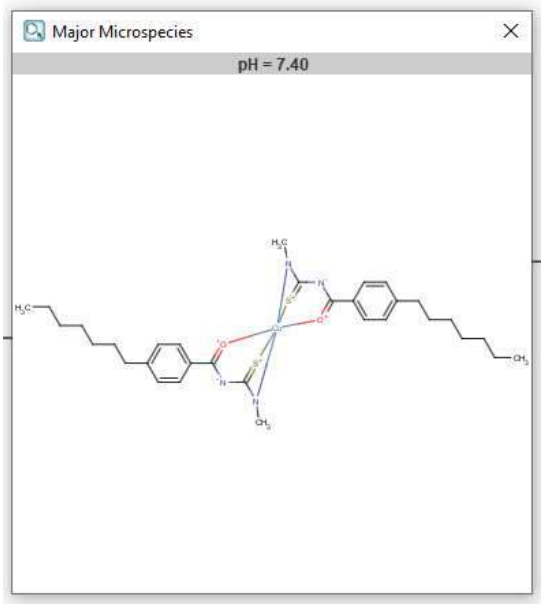
Ramachandran plot Reseptor 2EUD

LAMPIRAN VI

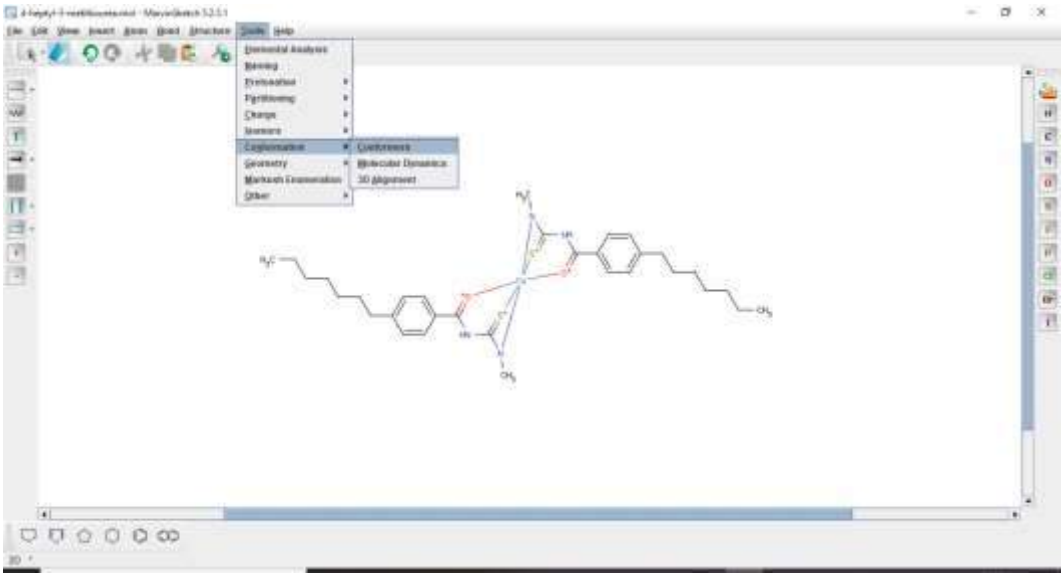
PREPARASI LIGAN



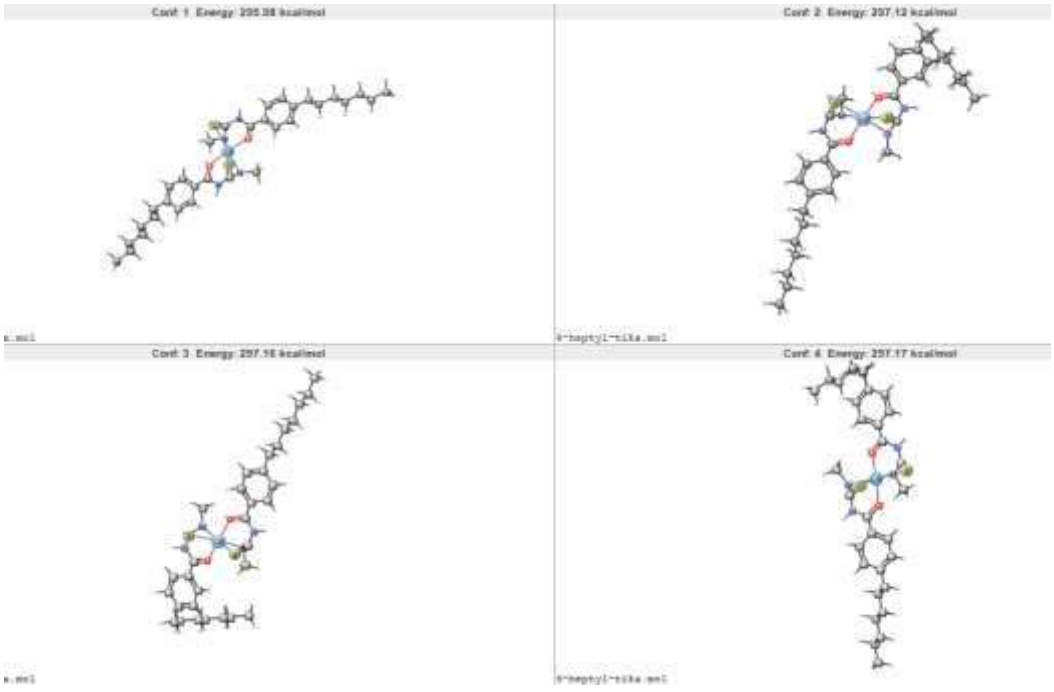
Ligan diprotonasi di menggunakan *software MarvinSketch 5.2.5.1*

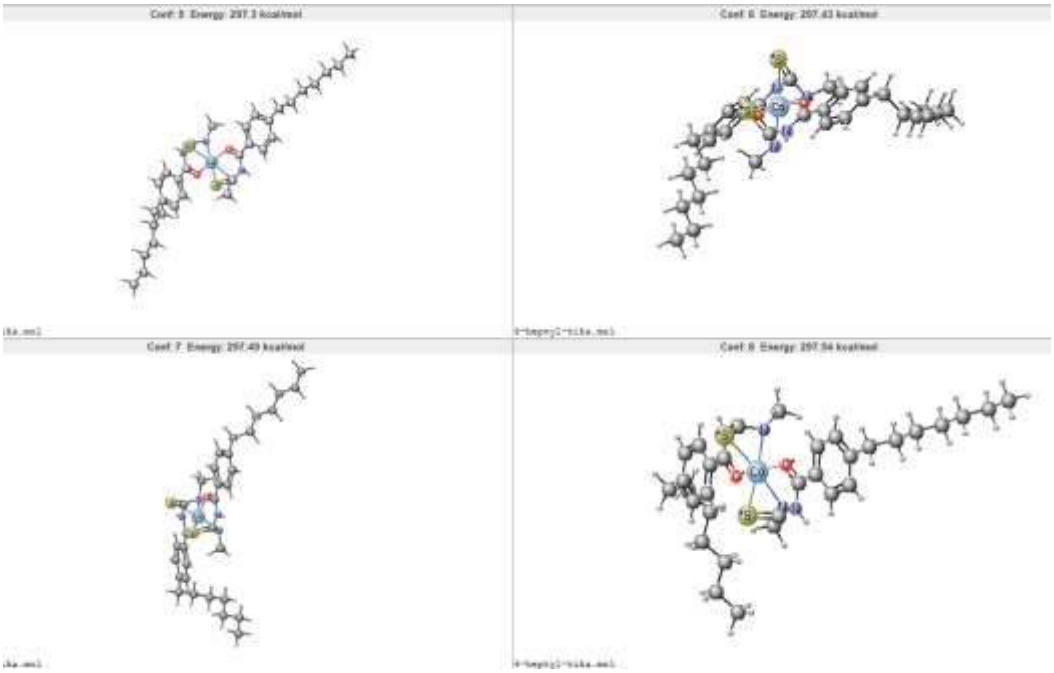


Ligan hasil protonasi



Tahapan ligan dilakukan konformasi



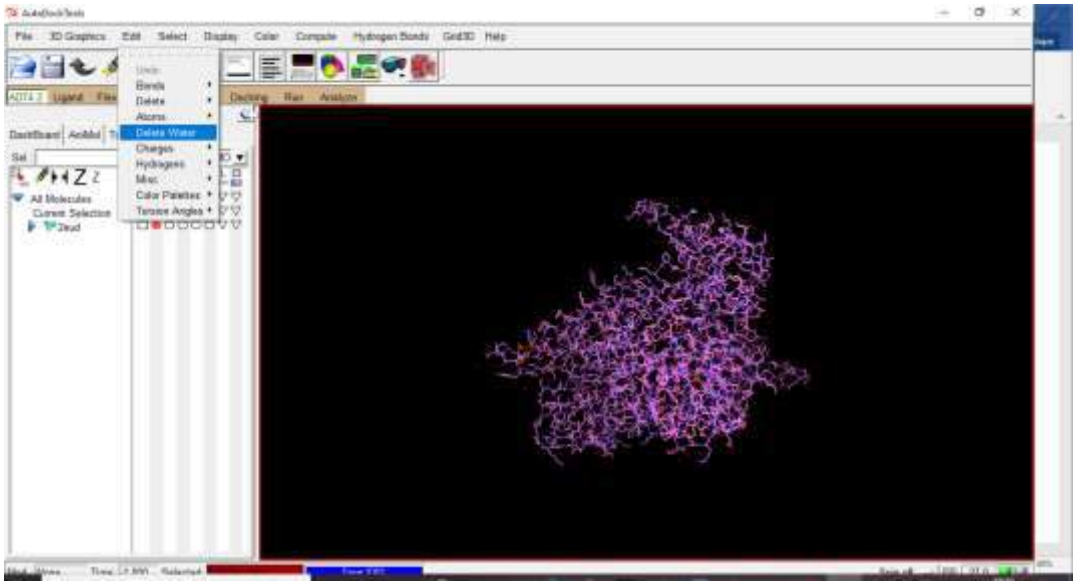


Ligan hasil konformasi

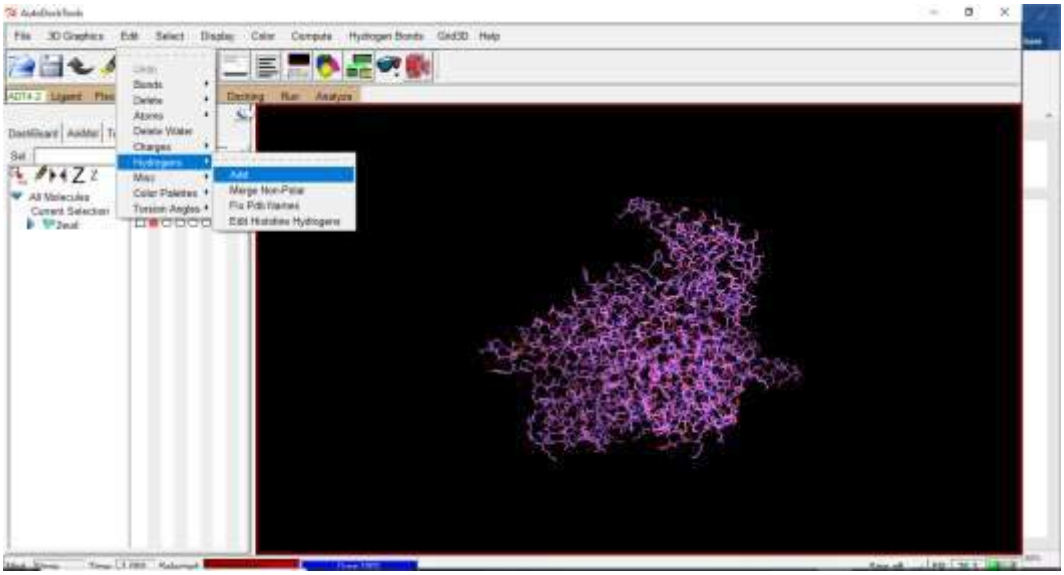
LAMPIRAN VII

PREPARASI RESEPTOR

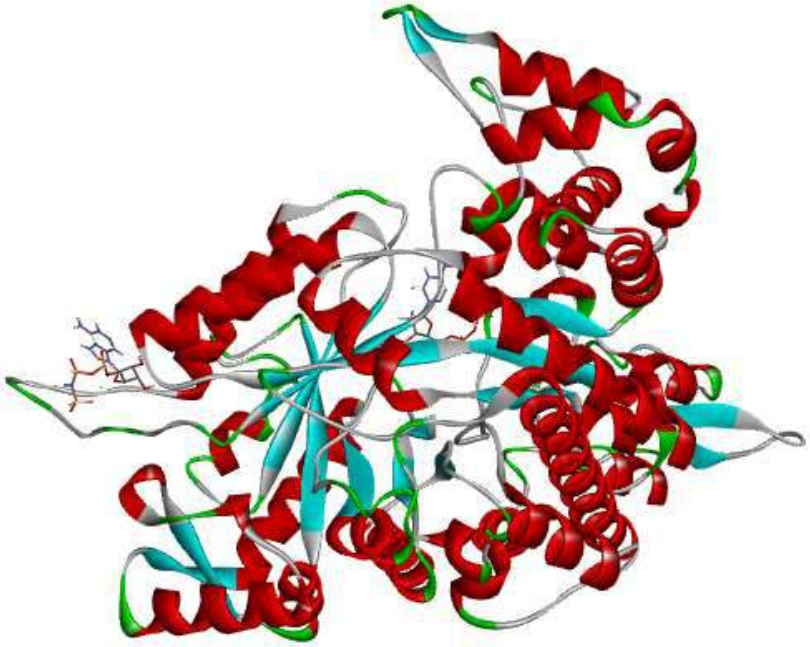
Pengunduhan reseptor 2EUD melalui *website* https://rscb.org/2eud



Proses penghilangan molekul air



Proses penambahan molekul hydrogen



Reseptor 2EUD dalam bentuk 3D

LAMPIRAN VIII

VALIDASI METODE *DOCKING*

RMSD TABLE

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	89	-17.57	0.00	1.77	RANKING
1	2	68	-17.51	1.46	2.09	RANKING
1	3	28	-17.49	1.40	1.89	RANKING
1	4	73	-17.46	0.46	1.68	RANKING
1	5	42	-17.41	1.48	1.89	RANKING
1	6	81	-17.36	1.51	1.93	RANKING
1	7	53	-17.34	1.42	1.90	RANKING
1	8	51	-17.33	1.12	1.81	RANKING
1	9	43	-17.31	1.42	1.88	RANKING
1	10	1	-17.31	1.35	1.87	RANKING
1	11	13	-17.30	1.37	1.84	RANKING
1	12	71	-17.29	0.24	1.71	RANKING
1	13	77	-17.28	0.42	1.72	RANKING
1	14	70	-17.27	0.68	1.75	RANKING
1	15	74	-17.26	1.44	1.88	RANKING
1	16	29	-17.24	0.85	1.70	RANKING
1	17	99	-17.22	0.63	1.68	RANKING
1	18	34	-17.22	0.76	1.70	RANKING
1	19	23	-17.21	1.45	1.89	RANKING
1	20	37	-17.20	1.63	1.96	RANKING
1	21	47	-17.18	0.79	1.77	RANKING
1	22	76	-17.18	1.39	1.91	RANKING
1	23	59	-17.18	1.72	1.95	RANKING
1	24	46	-17.15	0.59	1.73	RANKING
1	25	93	-17.15	0.64	1.77	RANKING
1	26	7	-17.13	0.50	1.75	RANKING
1	27	38	-17.12	0.79	1.76	RANKING
1	28	82	-17.11	1.31	1.93	RANKING
1	29	55	-17.08	1.24	1.92	RANKING

1	30	65	-17.08	1.22	1.90	RANKING
1	31	3	-17.04	0.55	1.73	RANKING
1	32	60	-17.03	0.64	1.72	RANKING
1	33	5	-17.02	1.02	1.92	RANKING
1	34	49	-16.96	1.59	1.90	RANKING
1	35	31	-16.93	1.70	1.87	RANKING
1	36	95	-16.92	1.28	1.94	RANKING
1	37	19	-16.89	1.38	1.74	RANKING
1	38	32	-16.86	0.82	1.65	RANKING
1	39	24	-16.81	1.42	1.95	RANKING
1	40	86	-16.79	1.41	1.78	RANKING
1	41	56	-16.75	1.33	1.61	RANKING
1	42	15	-16.75	1.53	1.86	RANKING
1	43	90	-16.75	1.37	1.62	RANKING
1	44	79	-16.69	1.52	1.82	RANKING
1	45	66	-16.60	0.96	1.63	RANKING
1	46	57	-16.58	1.30	1.86	RANKING
1	47	16	-16.55	1.32	1.70	RANKING
1	48	21	-16.46	1.49	1.81	RANKING
1	49	22	-16.38	1.29	1.79	RANKING
1	50	41	-16.26	1.94	1.93	RANKING
1	51	88	-16.21	0.76	1.68	RANKING
1	52	26	-16.16	1.75	2.03	RANKING
1	53	4	-16.06	0.91	1.69	RANKING
1	54	78	-15.15	1.98	1.97	RANKING
2	1	84	-17.19	0.00	3.87	RANKING
2	2	100	-17.08	0.71	3.81	RANKING
2	3	17	-16.88	0.70	3.84	RANKING
2	4	64	-16.88	0.68	3.94	RANKING
2	5	14	-16.37	0.90	3.91	RANKING
3	1	11	-16.95	0.00	4.88	RANKING
3	2	80	-16.47	0.95	4.97	RANKING
3	3	97	-16.35	0.70	4.84	RANKING
3	4	30	-16.30	1.70	5.57	RANKING
3	5	20	-16.19	1.07	4.91	RANKING
3	6	92	-16.18	0.68	4.83	RANKING
3	7	96	-16.08	0.61	4.86	RANKING
3	8	52	-16.07	1.35	4.43	RANKING

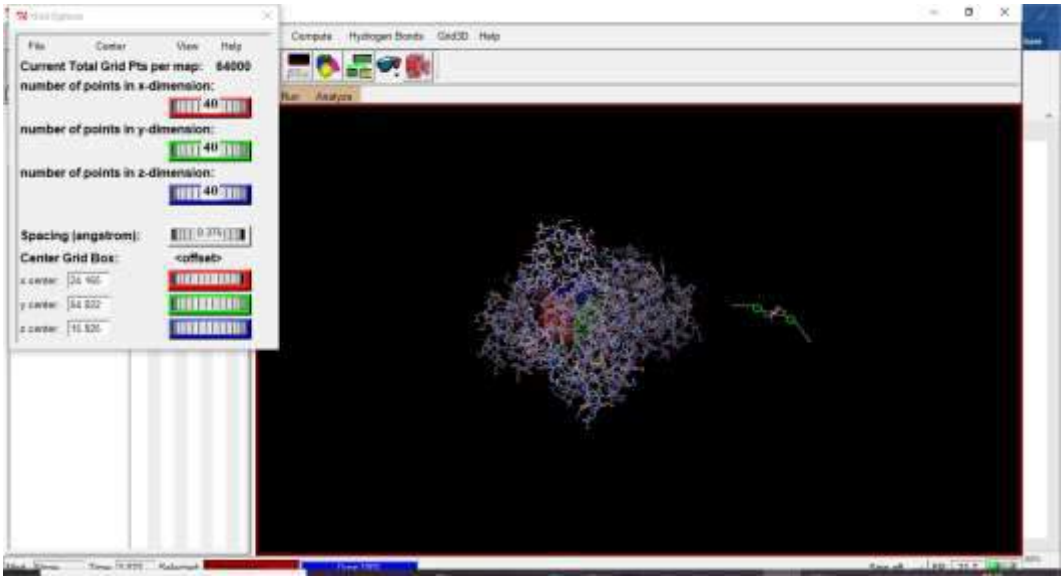
3	8	52	-16.07	1.35	4.43	RANKING
3	9	45	-15.99	1.53	4.99	RANKING
3	10	27	-15.97	1.03	4.95	RANKING
3	11	12	-15.85	1.65	4.96	RANKING
3	12	83	-15.83	1.36	4.63	RANKING
3	13	18	-15.69	1.93	4.15	RANKING
3	14	54	-15.68	1.49	4.30	RANKING
3	15	33	-15.42	1.16	4.64	RANKING
3	16	61	-15.30	1.69	4.34	RANKING
3	17	87	-15.05	1.53	4.72	RANKING
3	18	69	-15.05	1.42	4.45	RANKING
3	19	2	-14.91	1.53	4.70	RANKING
3	20	75	-13.94	1.72	4.83	RANKING
4	1	40	-16.94	0.00	5.05	RANKING
5	1	58	-16.43	0.00	2.28	RANKING
5	2	72	-16.42	1.21	2.47	RANKING
5	3	9	-16.35	1.23	2.27	RANKING
5	4	44	-16.17	1.82	2.38	RANKING
5	5	8	-16.06	1.24	2.03	RANKING
5	6	35	-16.05	1.49	2.03	RANKING
5	7	6	-16.01	1.68	2.82	RANKING
5	8	50	-15.92	0.66	2.30	RANKING
5	9	67	-15.91	1.25	2.37	RANKING
5	10	63	-15.86	1.58	1.87	RANKING
5	11	91	-15.75	1.78	2.33	RANKING
5	12	98	-15.74	1.57	2.52	RANKING
5	13	85	-15.22	1.72	2.22	RANKING
5	14	39	-15.17	1.86	2.57	RANKING
6	1	36	-15.95	0.00	4.41	RANKING
6	2	10	-15.36	1.06	4.18	RANKING
6	3	25	-15.17	1.06	4.17	RANKING
7	1	94	-15.67	0.00	4.13	RANKING
8	1	48	-15.64	0.00	3.99	RANKING
9	1	62	-14.36	0.00	5.60	RANKING

Perolehan nilai *Binding affinity* dan RMSD (*Root Mean Square Deviation*) ligan alami

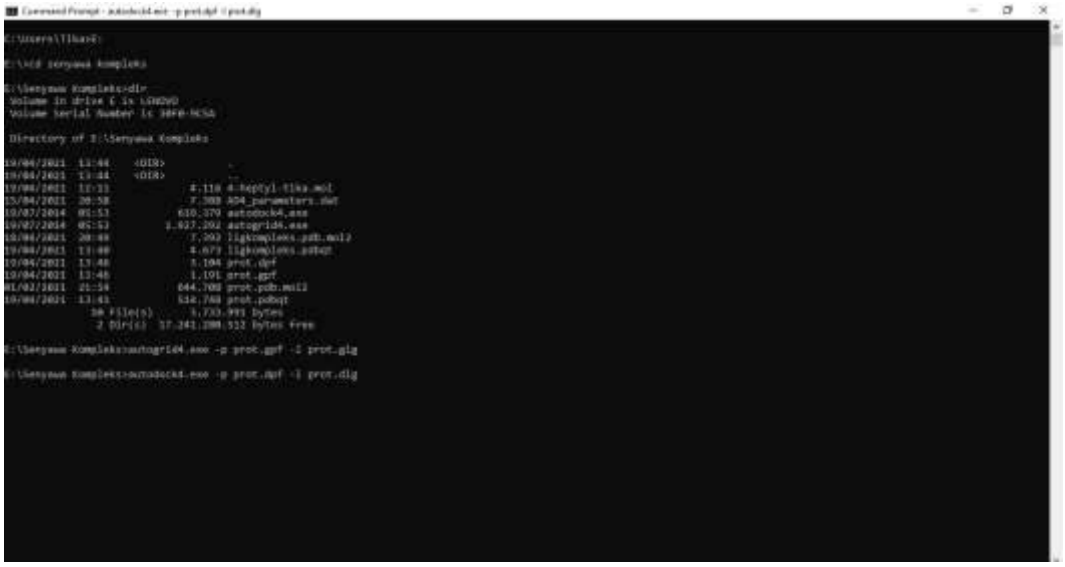
```
MODEL        89
USER    Run = 89
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 54
USER
USER    RMSD from reference structure       = 1.772 A
USER
USER    Estimated Free Energy of Binding    =  -17.57 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  131.88 fM (femtomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -19.66 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -16.83 kcal/mol
USER        Electrostatic Energy            =   -2.83 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.27 kcal/mol
USER    (3) Torsional Free Energy           =   +2.09 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.27 kcal/mol
```

LAMPIRAN IX

DOCKING UJI TERHADAP RESEPTOR TARGET



Pengaturan *grid box center* untuk proses *docking*



Proses *docking* menggunakan *software Command Prompt*

CLUSTERING HISTOGRAM

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-11.79	99	-10.91	49	##
2	-11.35	90	-10.54	7	#######
3	-11.17	46	-10.28	19	###################
4	-11.00	10	-10.14	2	##
5	-10.83	12	-10.83	1	#
6	-10.63	35	-9.97	6	######
7	-10.48	39	-9.89	3	###
8	-10.44	65	-10.44	1	#
9	-10.43	23	-10.02	2	##
10	-10.29	62	-10.29	1	#
11	-10.21	70	-10.21	1	#
12	-10.21	8	-9.83	4	####
13	-9.69	54	-9.57	2	##
14	-9.48	41	-9.48	1	#
15	-9.43	32	-9.43	1	#

Perolehan nilai *Binding Affinity* senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*

```
    LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
    ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       99
USER    Run = 99
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 49
USER
USER    RMSD from reference structure       = 55.447 A
USER
USER    Estimated Free Energy of Binding    =  -11.79 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    2.26 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -15.08 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -15.06 kcal/mol
USER        Electrostatic Energy            =   -0.01 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.61 kcal/mol
USER    (3) Torsional Free Energy           =   +3.28 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.61 kcal/mol
USER
```

Perolehan nilai *Konstanta Inhibition* (Ki) senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*

```
    CLUSTERING HISTOGRAM
    ____________________

_____|____________|_____|____________|_____|_____________________________________________________________
     |            |     |            |     |
Clus | Lowest     | Run | Mean       | Num | Histogram
-ter | Binding    |     | Binding    | in  |
Rank | Energy     |     | Energy     | Clus|    5    10   15   20   25   30   35
_____|____________|_____|____________|_____|____:____|____:____|____:____|____:____|____:____|____:____|____:____
   1 |      -9.05 |  66 |      -4.00 |  79 |#################################################################################
   2 |      +0.56 |  35 |      +5.16 |  14 |##############
   3 |     +31.52 |  63 |     +35.09 |   5 |#####
   4 |     +32.91 |  77 |     +32.99 |   2 |##
_____|____________|_____|____________|_____|_____________________________________________________________
```

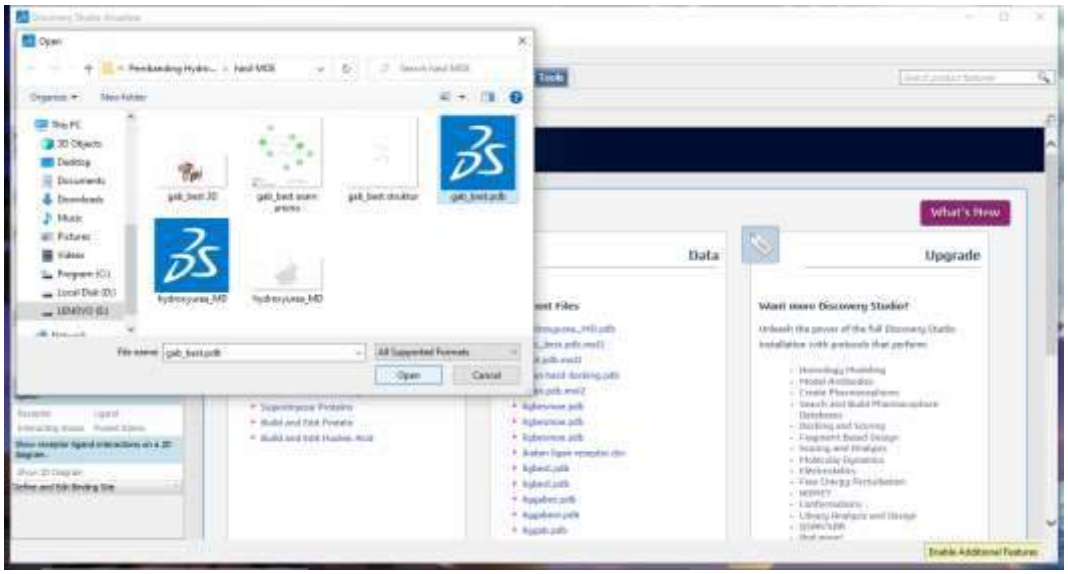
Perolehan nilai *Binding Affinity* senyawa *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

```
    LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
    ___________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       66
USER    Run = 66
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 79
USER
USER    RMSD from reference structure       = 57.720 A
USER
USER    Estimated Free Energy of Binding    =   -9.05 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  233.76 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -12.34 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -12.24 kcal/mol
USER        Electrostatic Energy            =   -0.09 kcal/mol
USER    (2) Final Total Internal Energy     =   +1.39 kcal/mol
USER    (3) Torsional Free Energy           =   +3.29 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   +1.39 kcal/mol
USER
```

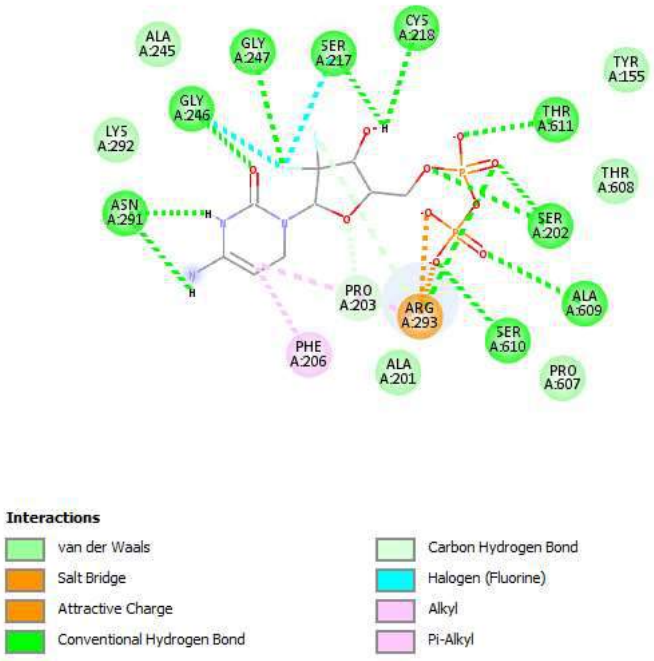
Perolehan nilai *Konstanta Inhibition* (Ki) senyawa *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

LAMPIRAN X

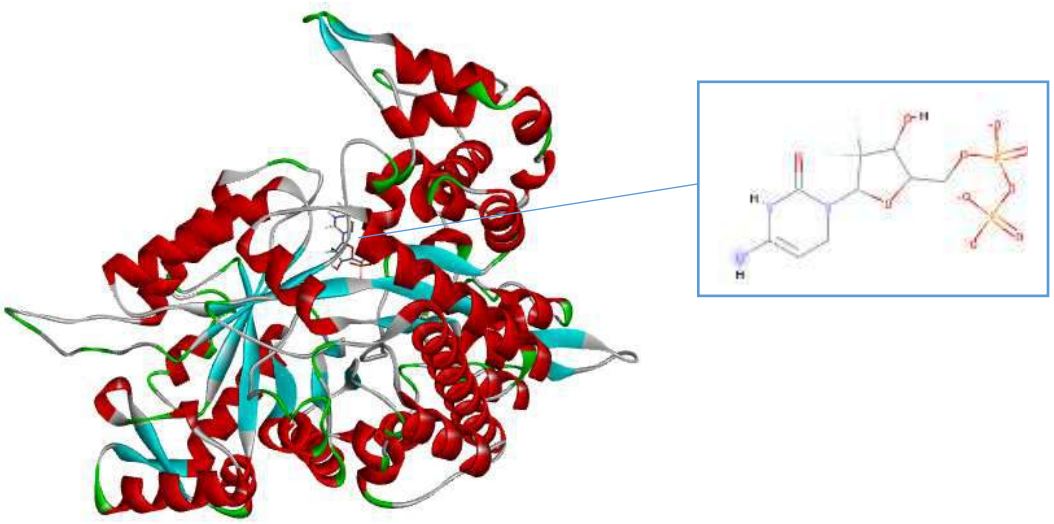
VISUALISASI HASIL *DOCKING*



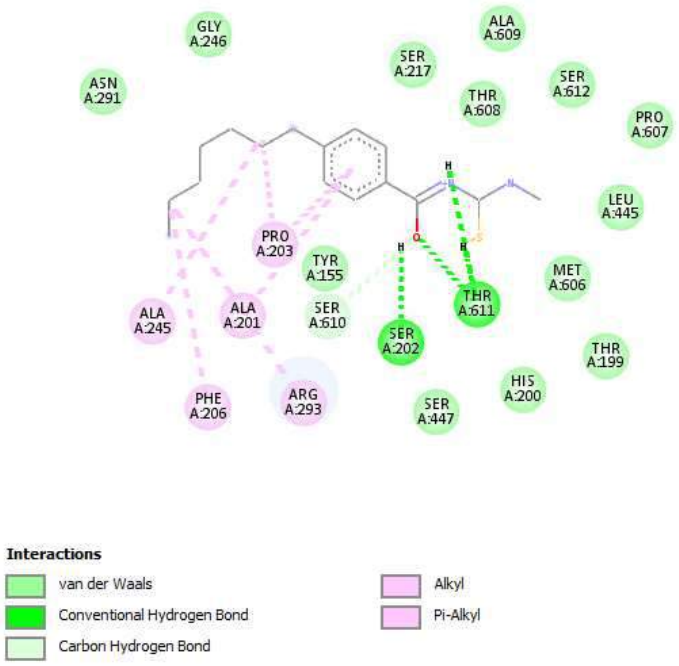
Visualisasi 2D dan 3D hasil *docking* senyawa kompleks menggunakan *discovery studio visualizer*



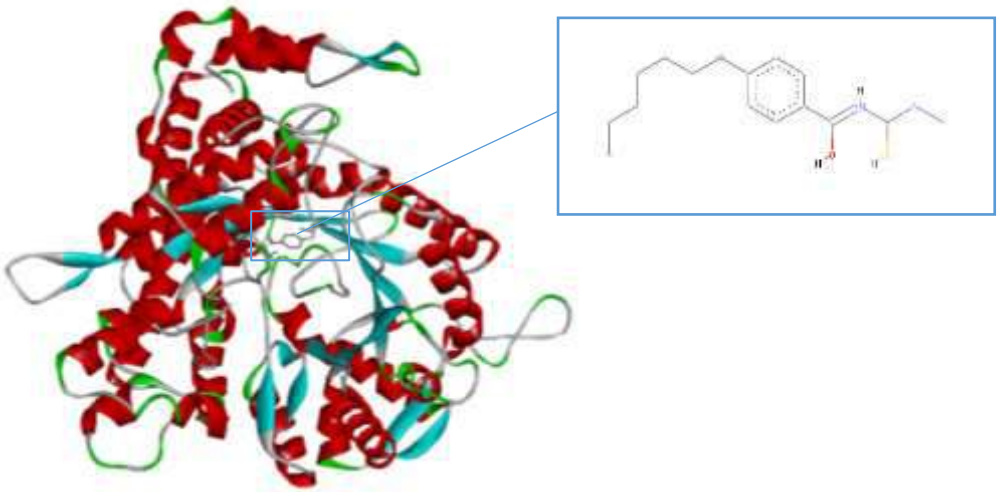
Hasil visualisasi 2D ligan alami atau reseptor target 2EUD



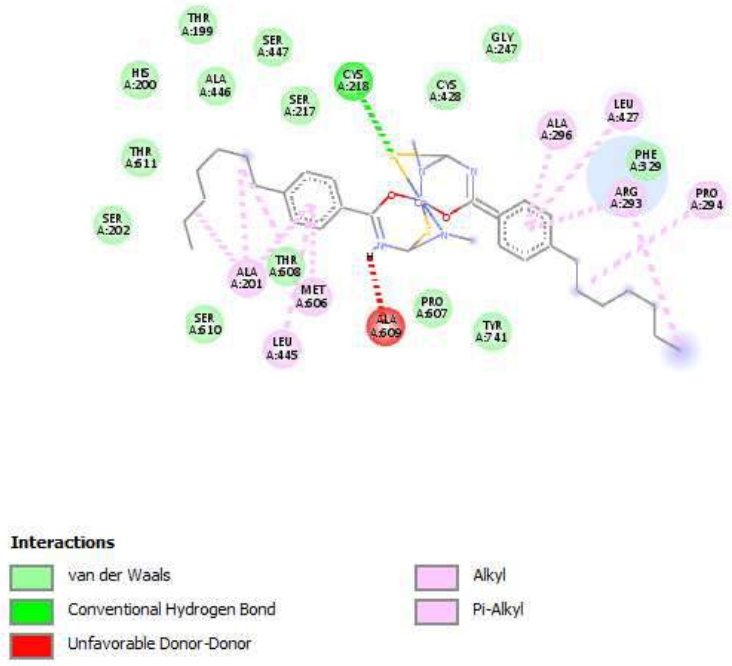
Hasil visualisasi 3D ligan alami atau reseptor target 2EUD



Hasil visualisasi 2D senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*

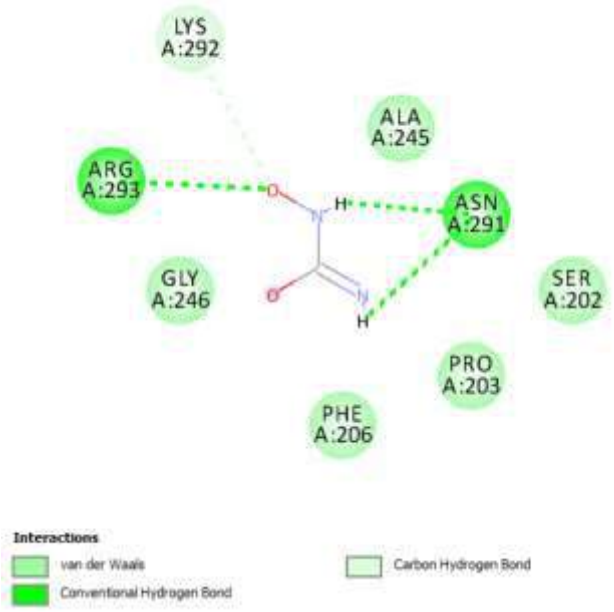


Hasil visualisasi 3D senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*

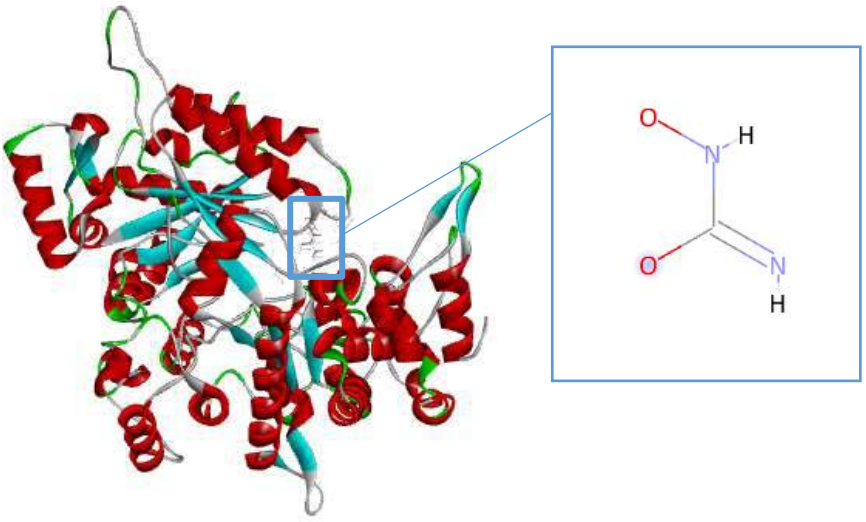


Hasil visualisasi 2D senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

Hasil visualisasi 3D senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*



Hasil visualisasi 2D senyawa *Hydroxyurea*

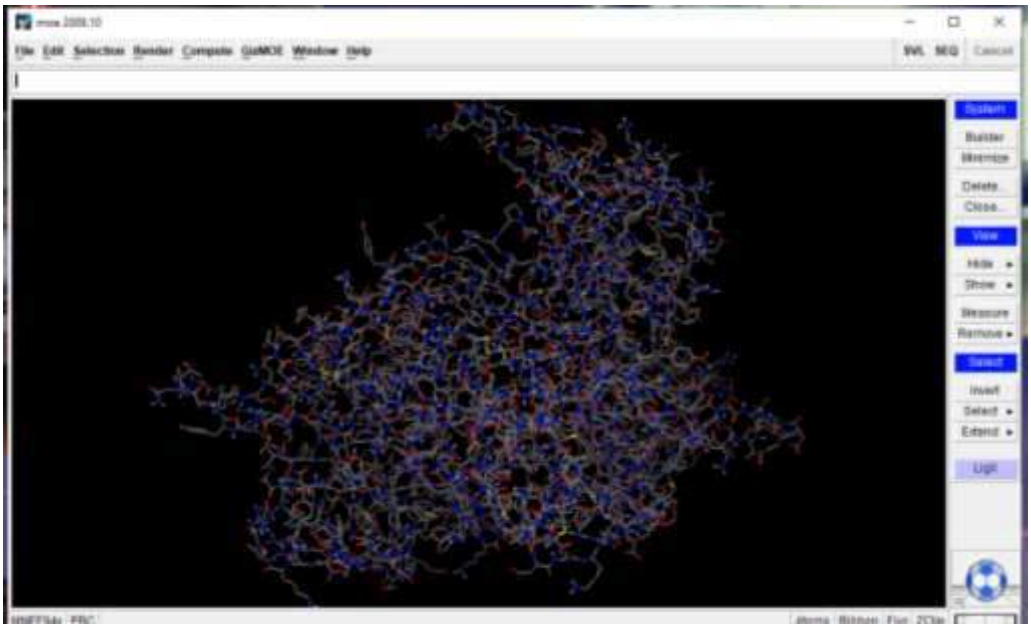


Hasil visualisasi 3D senyawa *Hydroxyurea*

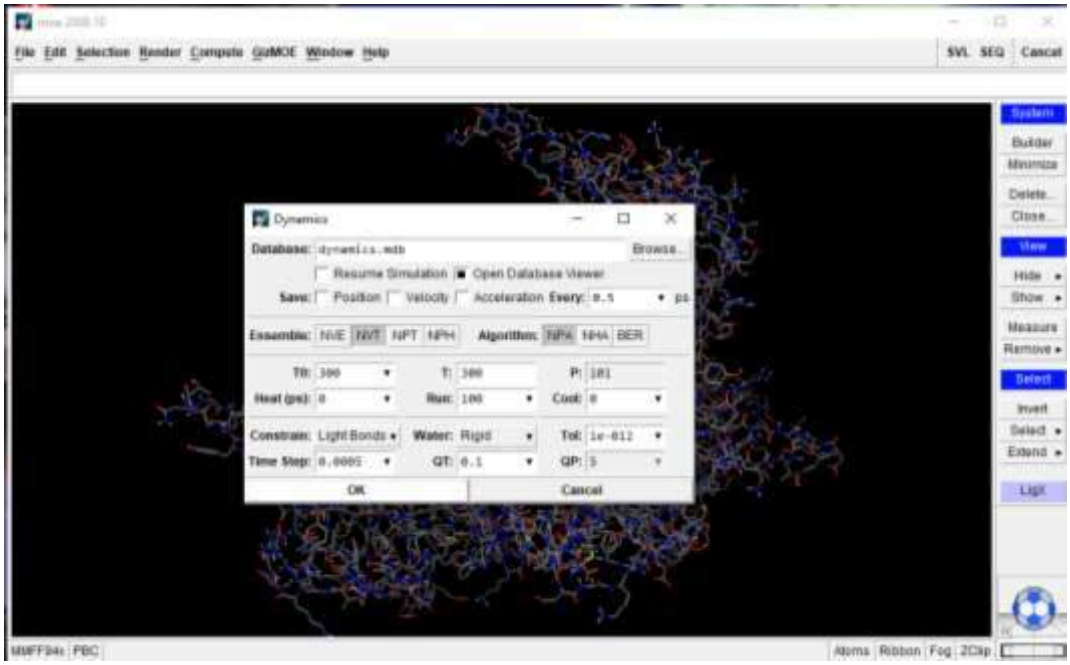
LAMPIRAN XI

MOLECULAR DYNAMIC

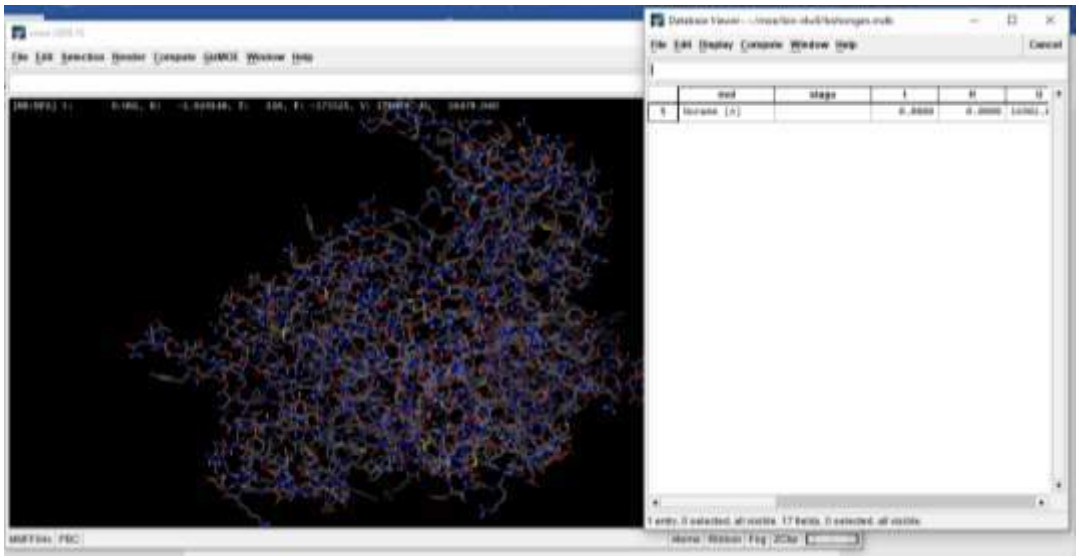
Tahapan dalam melakukan *molecular docking* saat meng-*input* data



Ligand uji yang sudah di *input*



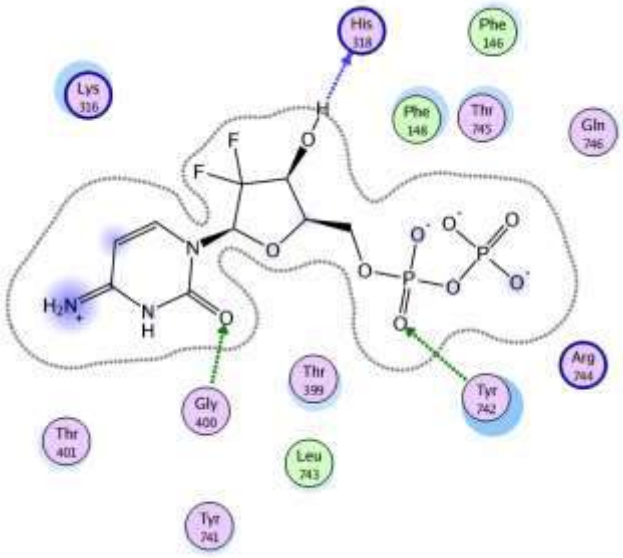
Tahapan pengaturan dalam proses *molecular docking*



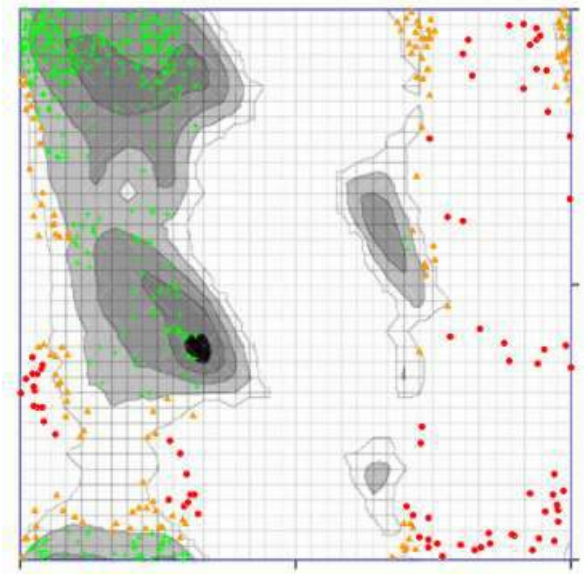
Proses *molecular docking* pada senyawa uji

Berikut merupakan hasil dari *molecular docking* menggunakan aplikasi *software MOE* :

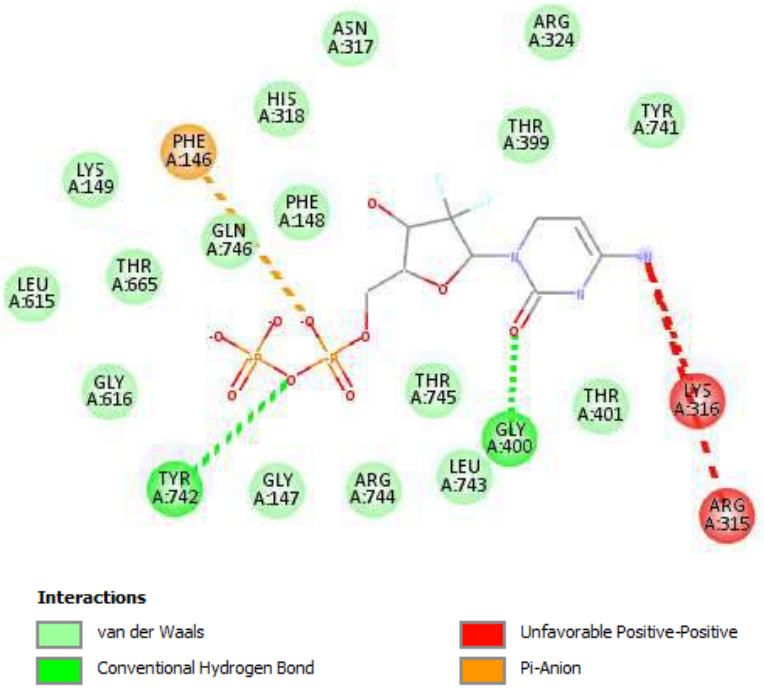
1. *Ligand* alami atau reseptor protein 2EUD



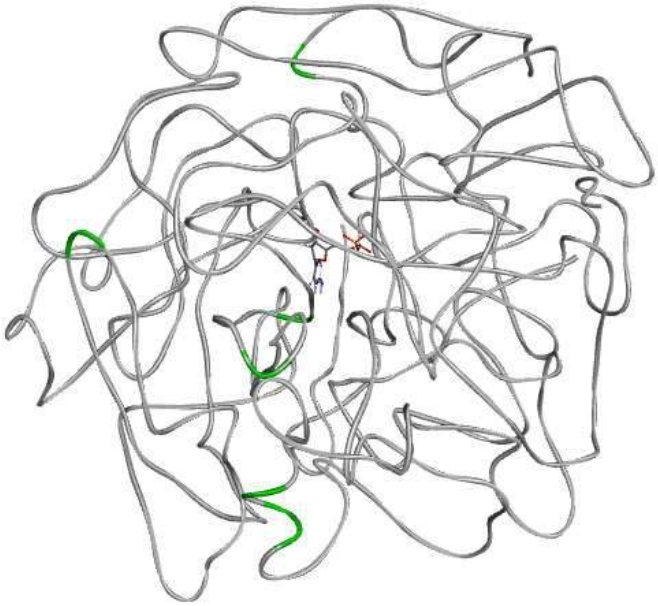
Hasil interaksi *ligand* dengan antar molekul dari protein reseptor 2EUD



Hasil plot *Ramachandran* dari *ligand* alami 2EUD

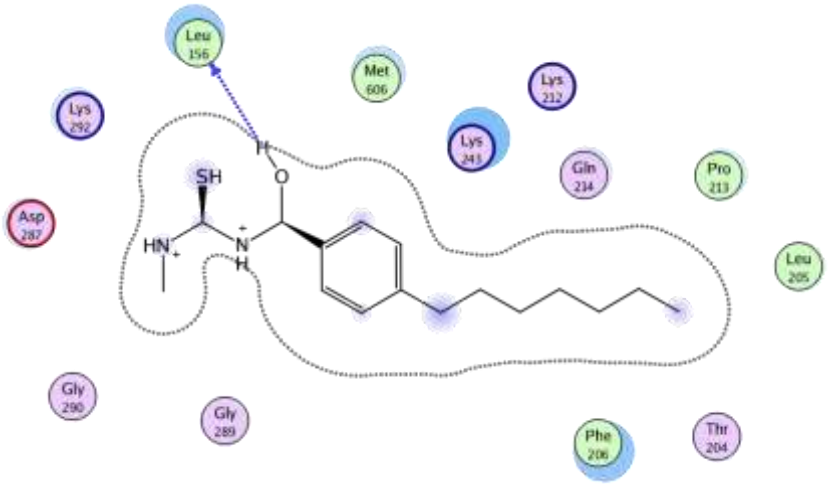


Hasil visualisasi MD *ligand* alami secara 2D

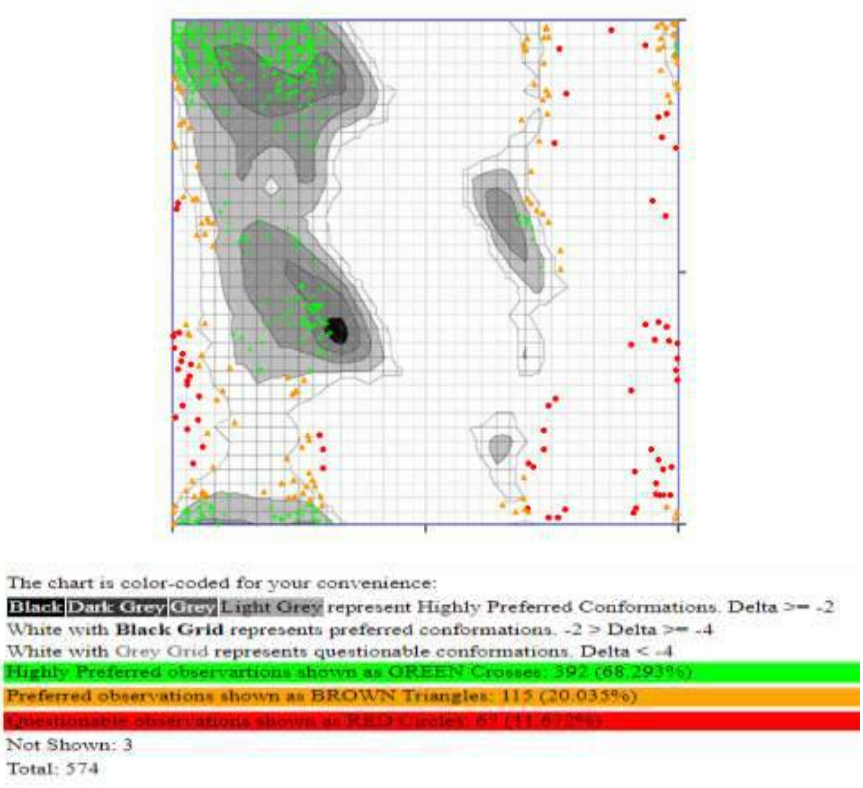


Hasil visualisasi MD senyawa *ligand* alami secara 3D

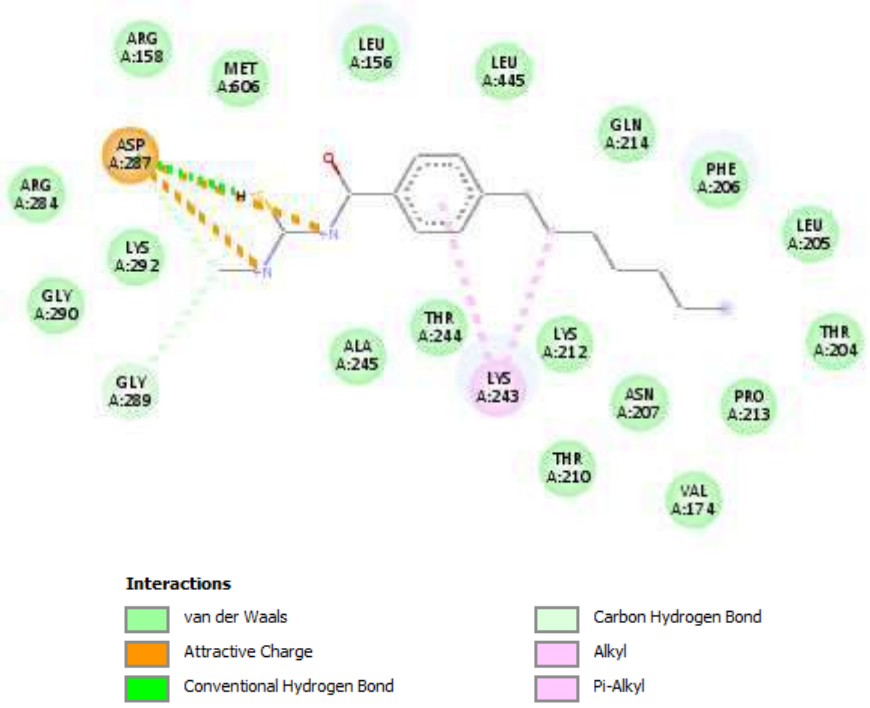
2. Senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*



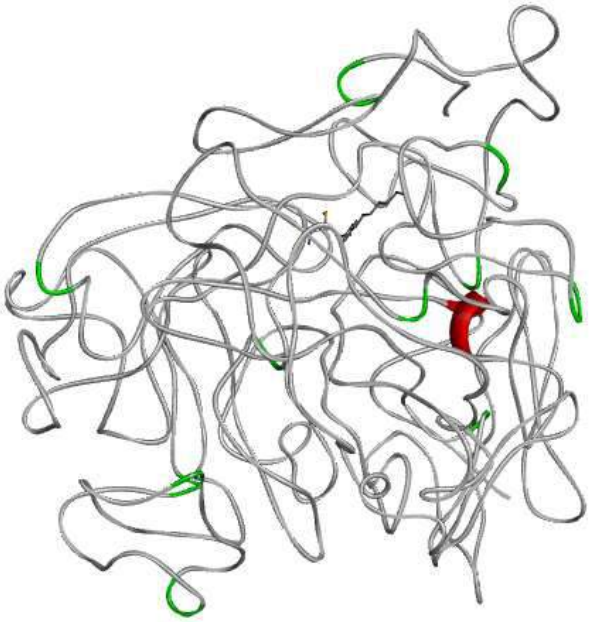
Hasil interaksi *ligand* dengan antar molekul dari senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*



Hasil plot *Ramachandran* dari senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea*

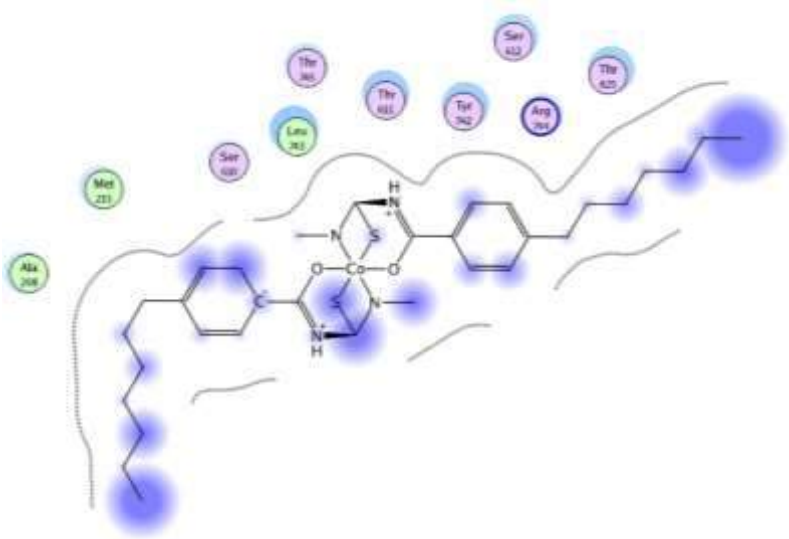


Hasil visualisasi MD senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea* secara 2D

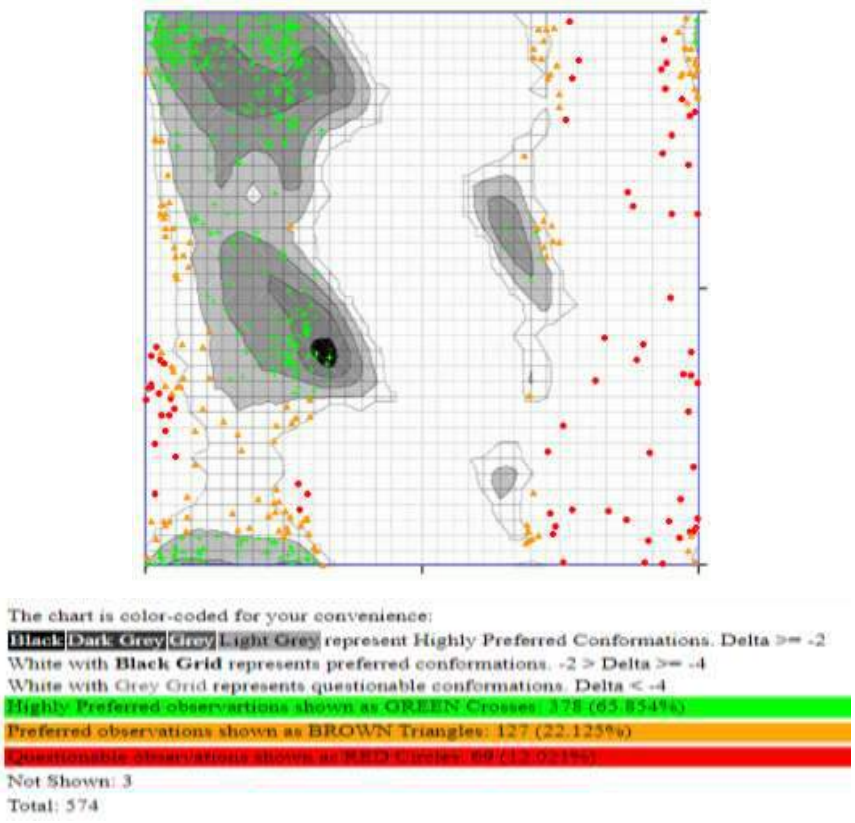


Hasil visualisasi MD senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea* secara 3D

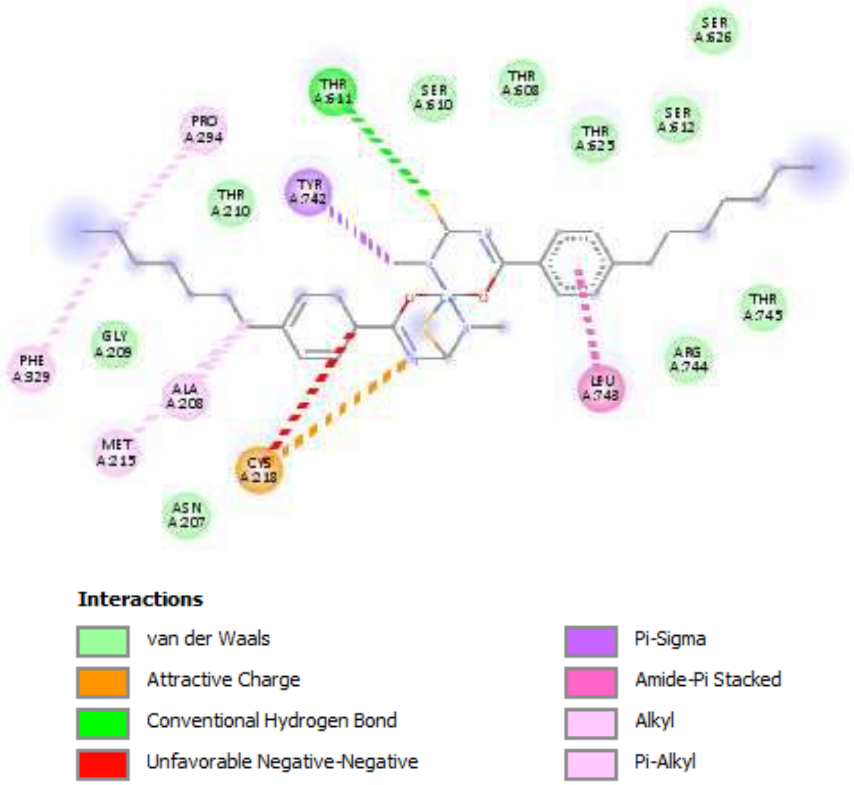
3. Senyawa Kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*



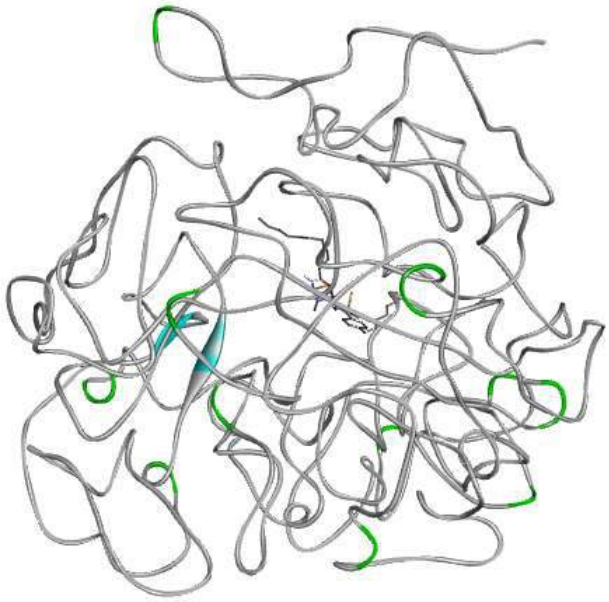
Hasil interaksi *ligand* dengan antar molekul dari senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*



Hasil plot *Ramachandran* dari senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

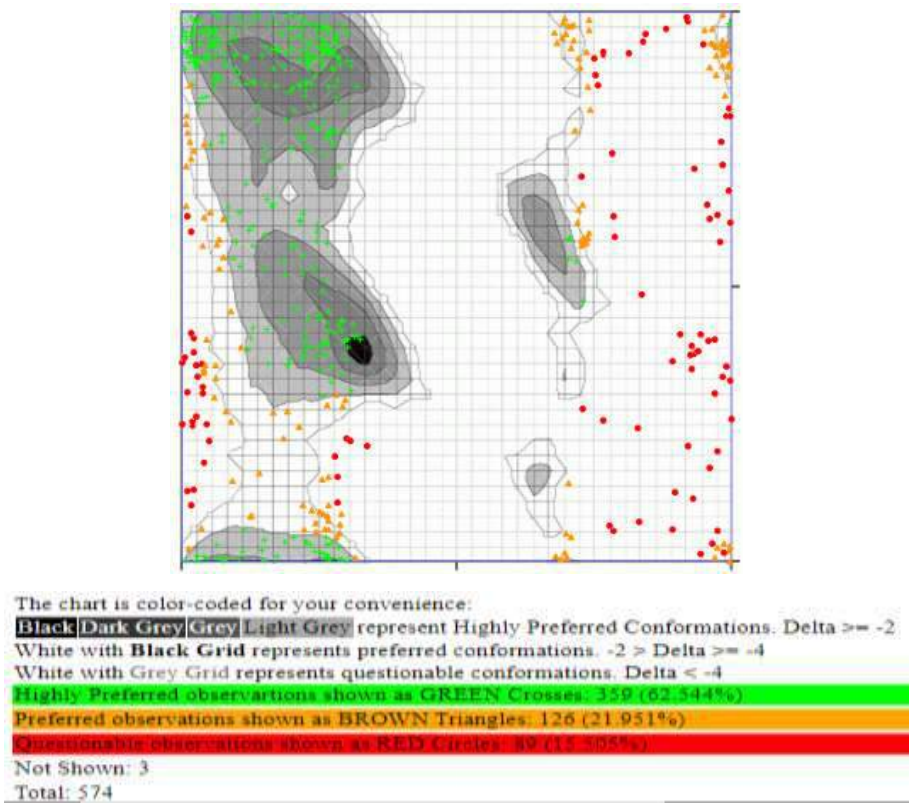


Hasil visualisasi MD senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

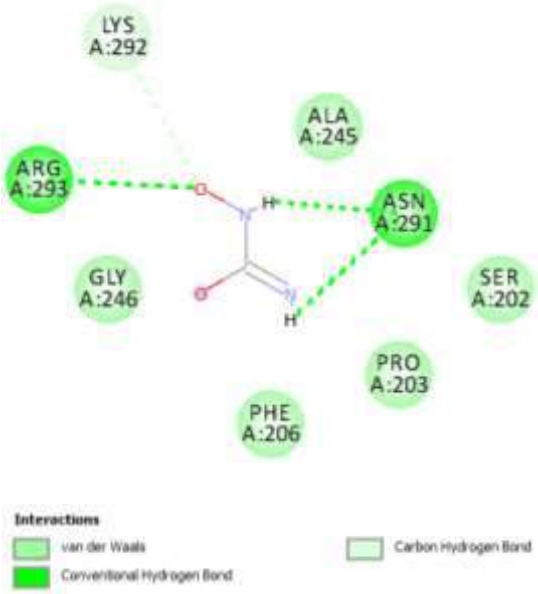


Hasil visualisasi MD senyawa kompleks *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

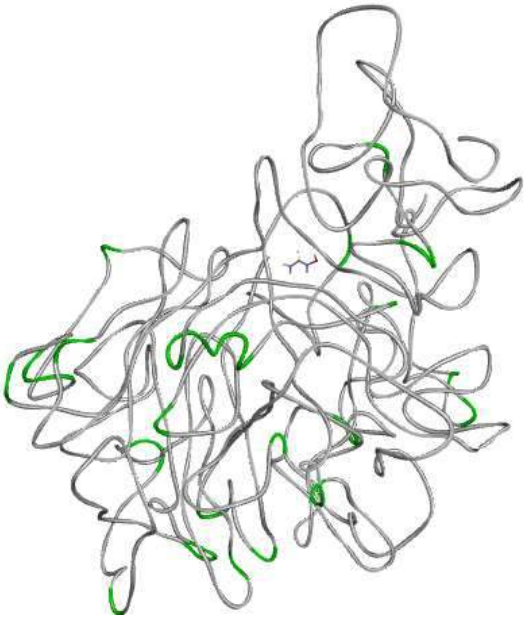
4. Senyawa *Hydroxyurea*



Hasil plot *Ramachandran* dari senyawa *Hydroxyurea*



Hasil visualisasi MD senyawa *Hydroxyurea* secara 2D



Hasil visualisasi MD senyawa *Hydroxyurea* secara 3D

LAMPIRAN XII

PREDIKSI ADME DAN TOKSISITAS

1. *1-(4-hepthylbenzoyl)-3-methylthiourea*

ADME

ID	Value
BBB	4.3011
Buffer_solubility_mg_L	19.3217
Caco2	37.5731
CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non
CYP_3A4_inhibition	Non
CYP_3A4_substrate	Non
HIA	94.381510
MDCK	1.98576
Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	100.000000
Pure_water_solubility_mg_L	2.57504
Skin_Permeability	-1.32909
SKlogD_value	4.613370
SKlogP_value	4.613370
SKlogS_buffer	-4.179990
SKlogS_pure	-5.055250

Toksisitas

ID	Value
algae_at	0.0060754
Ames_test	mutagen
Carcino_Mouse	negative
Carcino_Rat	negative
daphnia_at	0.0102775
hERG_inhibition	medium_risk
medaka_at	0.000223827
minnow_at	0.000183596
TA100_10RLI	negative
TA100_NA	positive
TA1535_10RLI	negative
TA1535_NA	negative

Perolehan data hasil ADMET senyawa *1-(4-hepthylbenzoyl)-3-methylthiourea* menggunakan *software PreADMET* yang berbasis *online*

2. *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)*

ADME

ID	Value
BBB	3.68989**
Buffer_solubility_mg_L	8.13122e-008**
Caco2	20.2862**
CYP_2C19_inhibition	Non
CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Non
CYP_2D6_substrate	Weakly
CYP_3A4_inhibition	Inhibitor
CYP_3A4_substrate	Substrate
HIA	98.222658**
MDCK	0.0436534**
Pgp_inhibition	Inhibitor
Plasma_Protein_Binding	88.393140**
Pure_water_solubility_mg_L	4.05318e+006**
Skin_Permeability	-4.15248**
SKlogD_value	2.714800**
SKlogP_value	2.714800**
SKlogS_buffer	-12.897240**
SKlogS_pure	0.800400**

Toksisitas

ID	Value
algae_at	0.000294023**
Ames_test	mutagen
Carcino_Mouse	out of range
Carcino_Rat	out of range
daphnia_at	0.000123406**
hERG_inhibition	medium_risk
medaka_at	7.395e-008**
minnow_at	5.08294e-007**
TA100_10RLI	negative
TA100_NA	negative
TA1535_10RLI	positive
TA1535_NA	positive

Perolehan data hasil ADMET senyawa *Bis-(1-(4-heptylbenzoyl)-3-methylthiourea*) *Cobalt (III)* menggunakan *software* PreADMET yang berbasis *online*

3. Senyawa *Hydroxyurea*

ADME

ID	Value
BBB	0.156784
Buffer_solubility_mg_L	1645.27
Caco2	2.3587
CYP_2C19_inhibition	Inhibitor
CYP_2C9_inhibition	Non
CYP_2D6_inhibition	Inhibitor
CYP_2D6_substrate	Weakly
CYP_3A4_inhibition	Non
CYP_3A4_substrate	Non
HIA	61.074276
MDCK	293.367
Pgp_inhibition	Non
Plasma_Protein_Binding	4.835029
Pure_water_solubility_mg_L	151115
Skin_Permeability	-3.88489
SKlogD_value	-1.570750
SKlogP_value	-1.570750
SKlogS_buffer	-1.664890
SKlogS_pure	0.298180

Toksisitas

ID	Value
algae_at	0.446487
Ames_test	mutagen
Carcino_Mouse	negative
Carcino_Rat	positive
daphnia_at	5.40892
hERG_inhibition	low_risk
medaka_at	28.0847
minnow_at	11.0734
TA100_10RLI	negative
TA100_NA	negative
TA1535_10RLI	positive
TA1535_NA	negative

Perolehan data hasil ADMET senyawa *Hydroxyurea* menggunakan *software* PreADMET yang berbasis *online*