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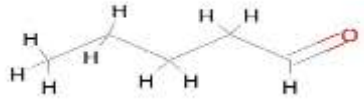
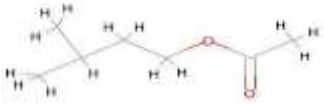
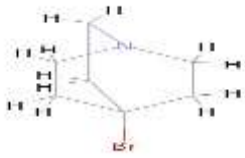
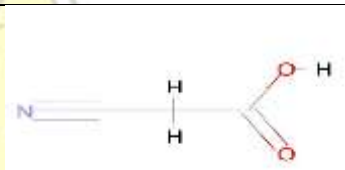
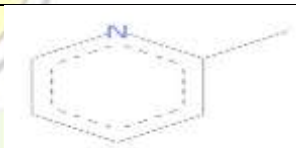
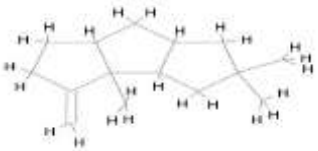
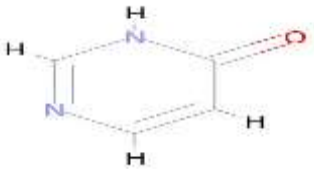
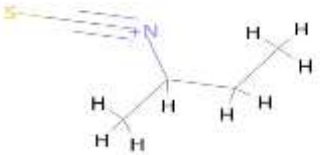
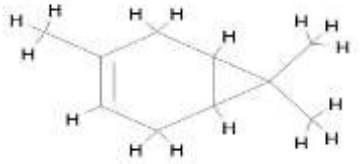
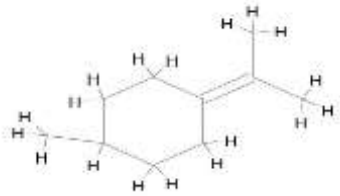
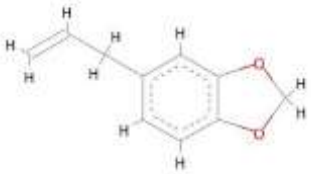
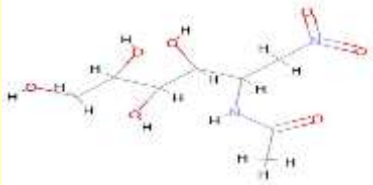
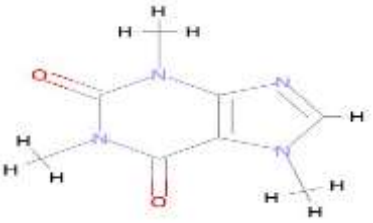
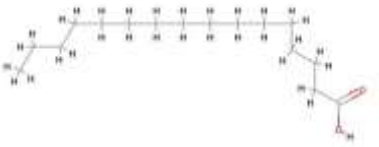
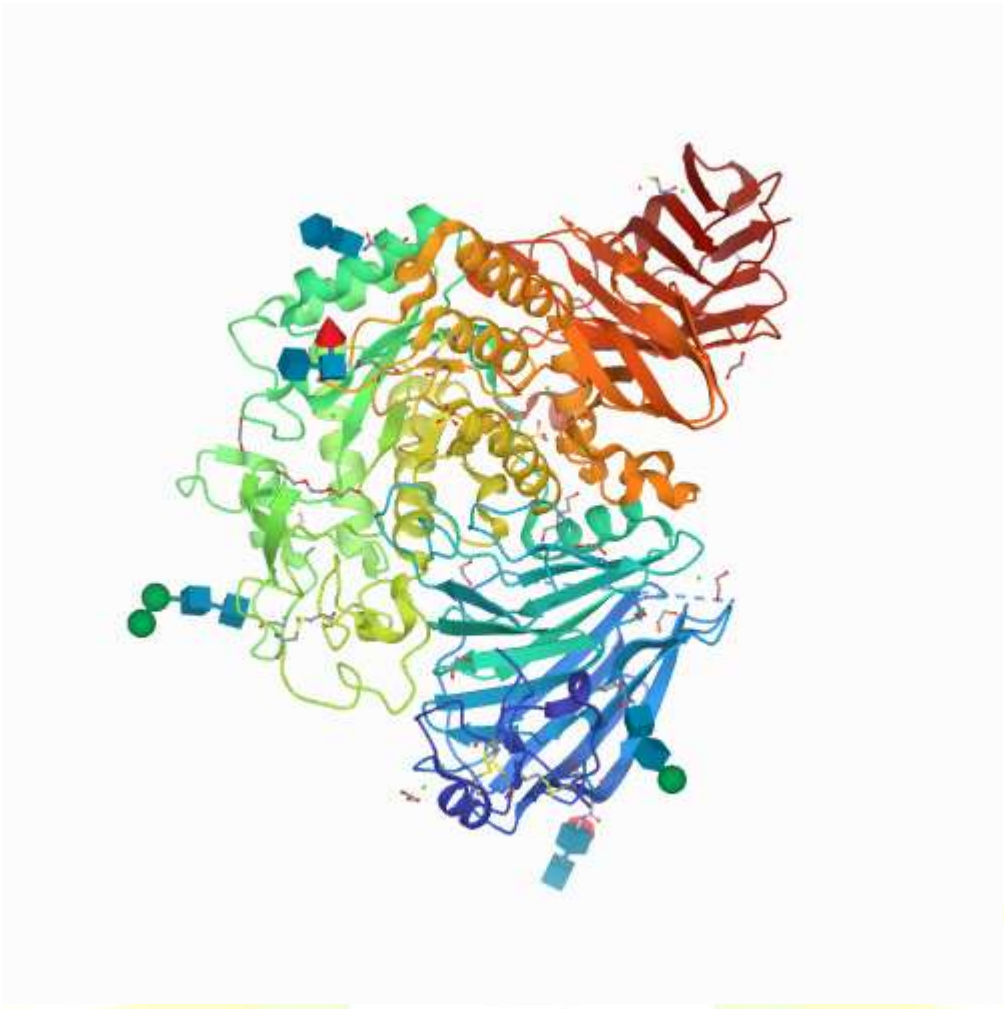
LAMPIRAN

Lampiran 1. Struktur Ligan Uji Senyawa Ekstrak Bunga Telang

No.	Ligan	Struktur
1.	*Pentanal*	
2.	*1-butanol, 3-methyl-,acetat*	
3.	*4-bromoquinuclidine*	
4.	*acetic acid, cyano-*	
5.	*pyridine-2-d, 6-methyl-*	
6.	*Hirsutene*	
7.	*pyrimidine, 4-hydroxy-*	
8.	*butane, 2-isothiocyanate*	

9.	*bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-*	
10.	*cyclohexen, 1-methyl-4-(1-methylethylideme)-*	
11.	*1,3-benzodioxole, 5-(2-propenyl)*	
12.	*1-nitro-2-acetamido-1,2-dideoxy-d-monnitol*	
13.	*Caffeine*	
14.	*hexadecanoic acid*	

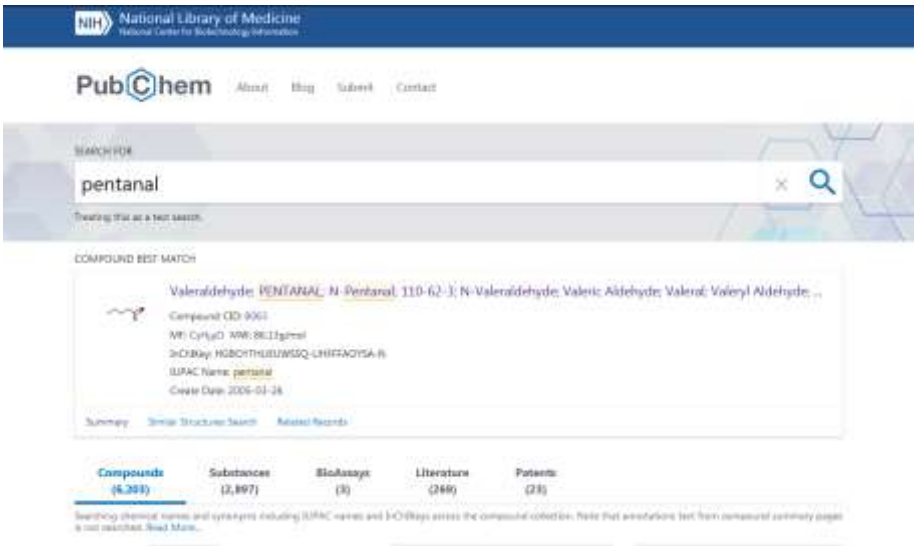
Lampiran 2. Struktur Reseptor



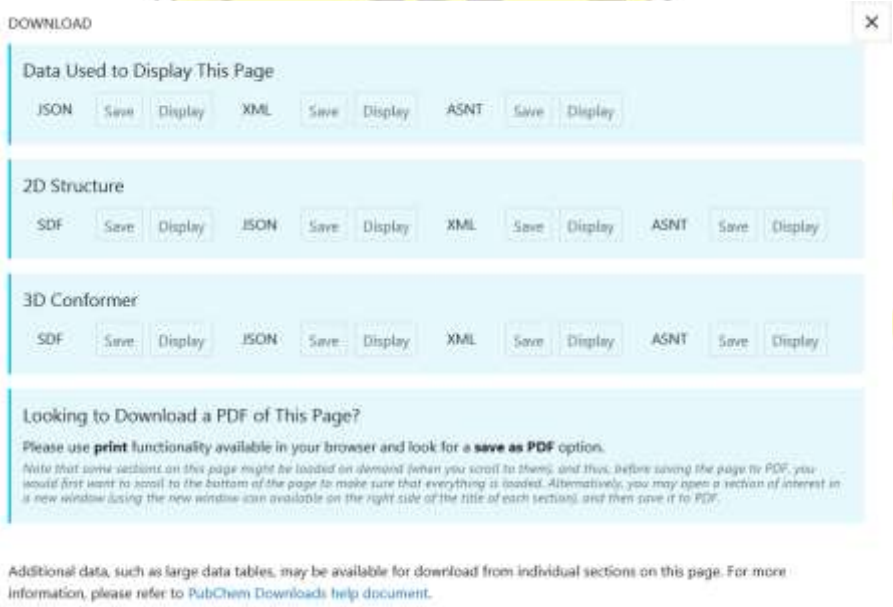
Struktur 3D dengan PDB ID 5NN3 (sumber : www.rscb.org)

Lampiran 3. Preparasi Ligan

1. Ligan yang akan digunakan diunduh dari (http://pubchem.ncbi.nlm.nih.gov).

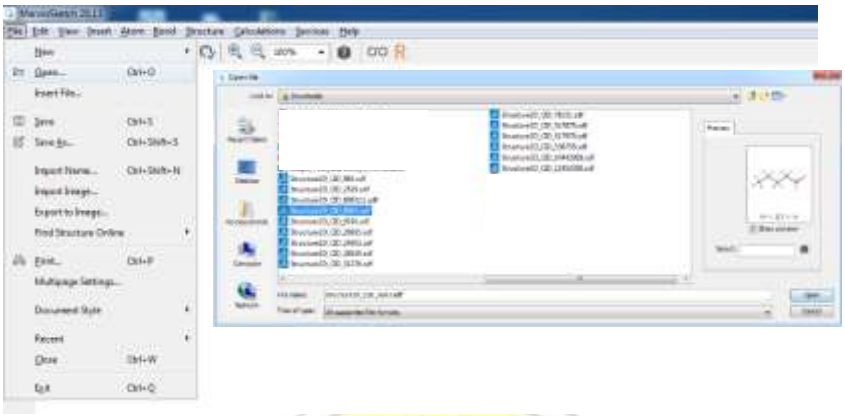


2. Ligan dalam bentuk 2D disimpan dalam format SDF

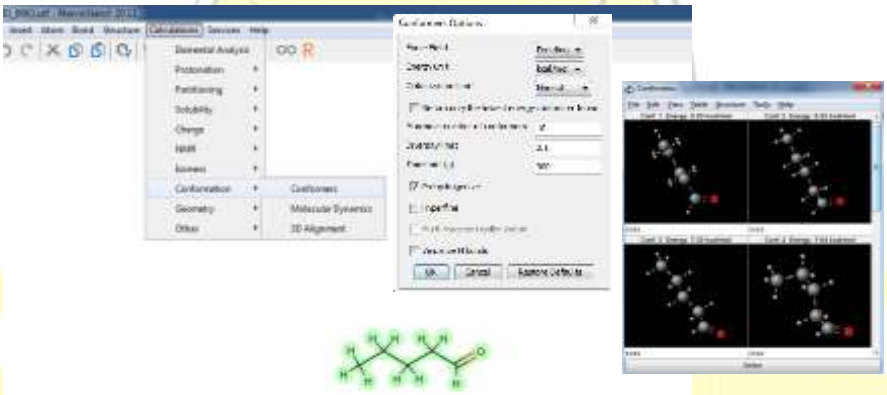


Lampiran 4. Mengubah 2D menjadi 3D

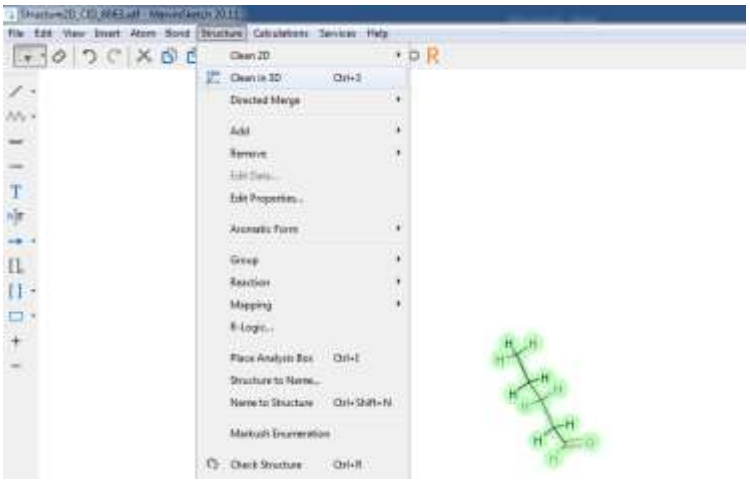
1. Buka *software* Marvin Sketch > File > Open > Pilih ligan yang telah diunduh > Klik Open.



2. Blok semua ligan, lalu pilih Calculation > Conformation > Conformers > Langsung Klik Ok > Pilih Conformers dengan nilai Energi paling rendah.

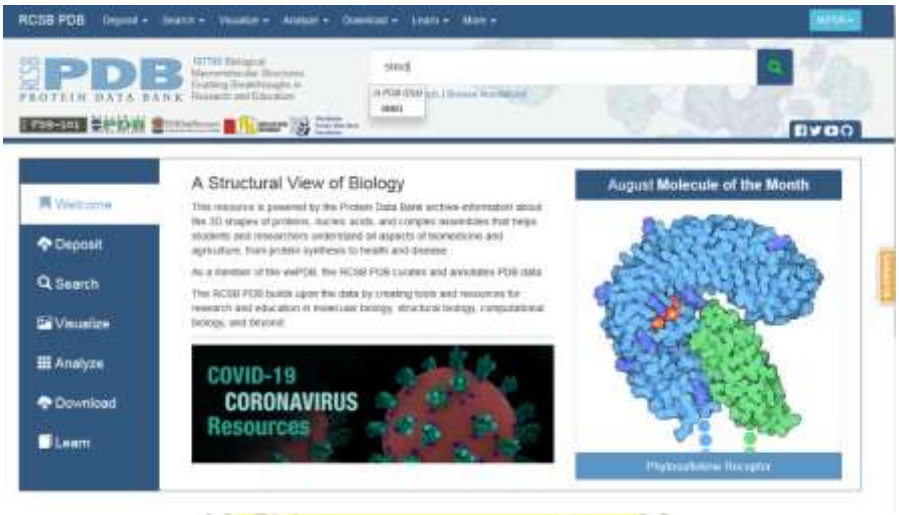


3. Blok kembali seluruhnya, lalu klik Structure > Clean in 3D > Kemudian Save dengan *.pdb

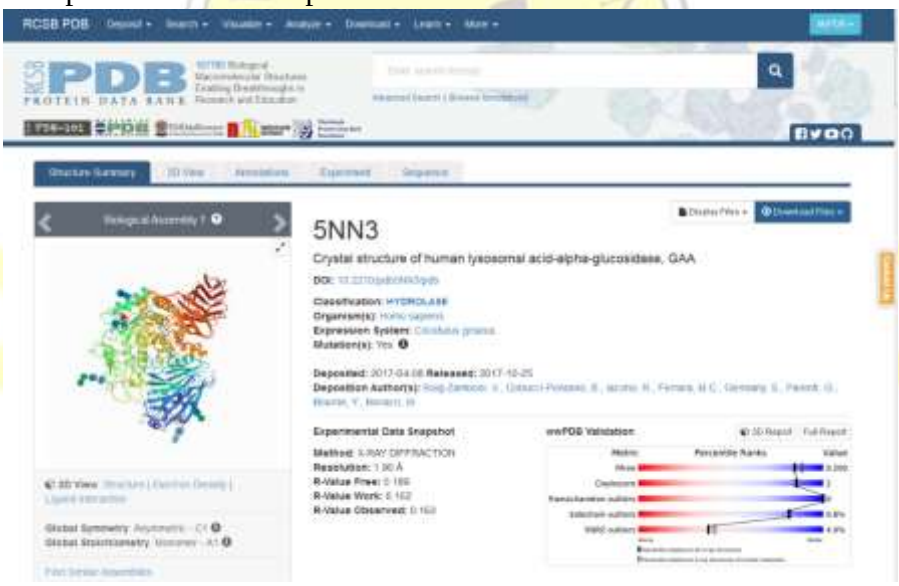


Lampiran 5. Preparasi Protein Reseptor

1. Protein (reseptor) yang akan digunakan diunduh dari (https://www.rscb.org).

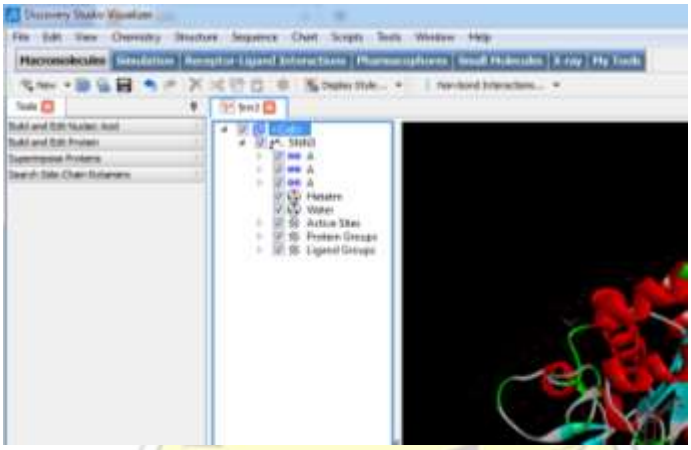


2. Reseptor tersebut disimpan dalam bentuk format PDB

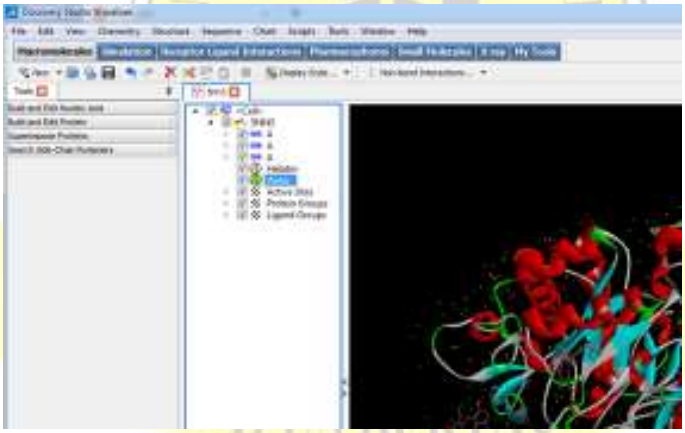


Lampiran 6. Pemisahan Makromolekul Dan Ligan

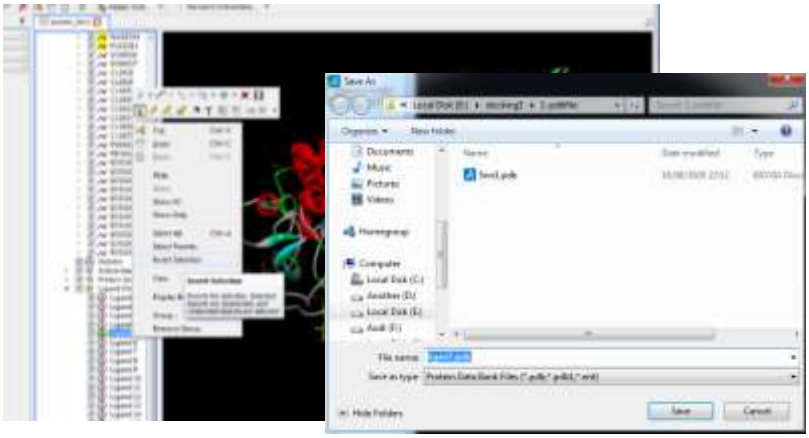
1. Pemilihan Ligan
   a. Buka file PDB yang telah diunduh dengan Discovery Studio yang akan tampak gambar 3D > Klik pada Keyboard Ctrl +H untuk memuculkan *View Hierarcy*



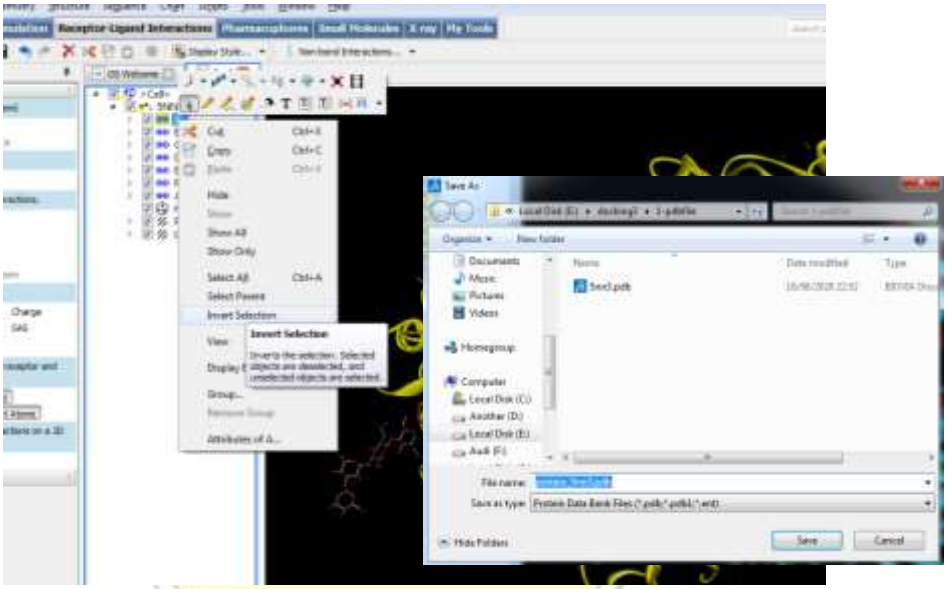
   b. Hilangkan air dengan Klik kanan pada mouse > delete



   c. Kemudian dalam view hierarcy akan dipilihnya unsur-unsur ligan yang tersedia, lalu klik kanan > *invert selection* > delete. Lalu save file dengan *.pdb.



2. Pemilihan Makromolekul
    a. Lakukan hal yang sama hingga 1b
    b. Kemudian dalam view hierarcy akan dipilihnya unsur-unsur protein yang tersedia, lalu klik kanan > *invert selection* > delete. Lalu save file dengan *.pdb.



Lampiran 7. Validasi Penambatan Molekuler (*Molecular Docking*)

1. Buka *software* Autodock Tools > Ligand > Input > Open

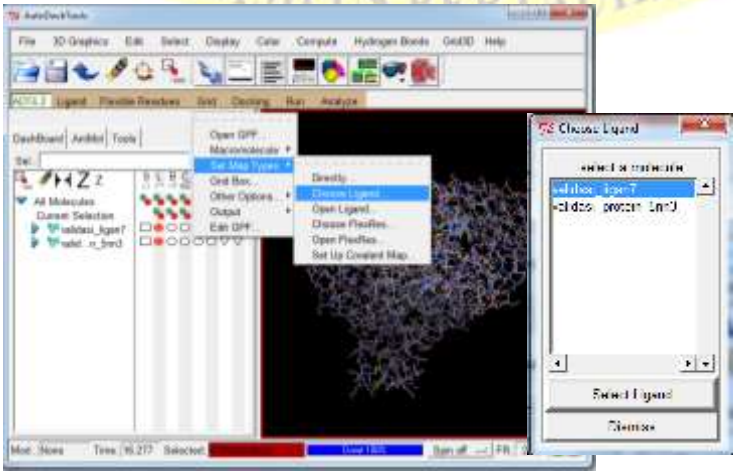
2. Otomatis sudah diberi muatan *gasteiger* dan *choose torsio.* Sehingga klik Ligand > Output > Save as PDBQT

3. Grid > Macromolekul > Open. Buka file makromolekul dan klik Open

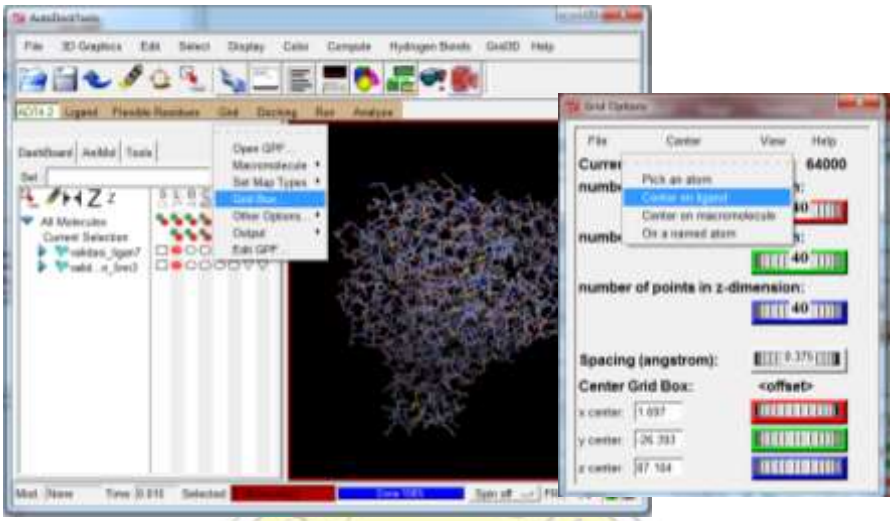
4. Edit > Hydrogens > Add > Pilih menu *Polar Only*

5. Edit > Charges > Compute Gasteiger

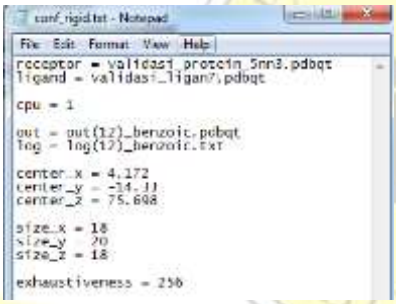
6. Untuk mengenali daerah Ligan, Klik Grid > Set Map Types > Choose Ligand > Select Ligand



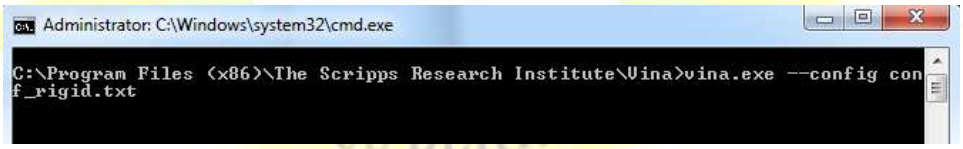
7. Atur Gridbox dengan klik Grid > Grid Box > Center > Center on Ligand (Lalu atur agar seluruh ligan tertutupi dengan Box dan catat koordinat > Save).



8. Buat parameter penambatan dalam folder vina dengan Notepad



9. Jalankan perintah untuk running Vina dengan membuka cmd.exe (*Run as Administrator*) dan masuk kedalam Command folder vina

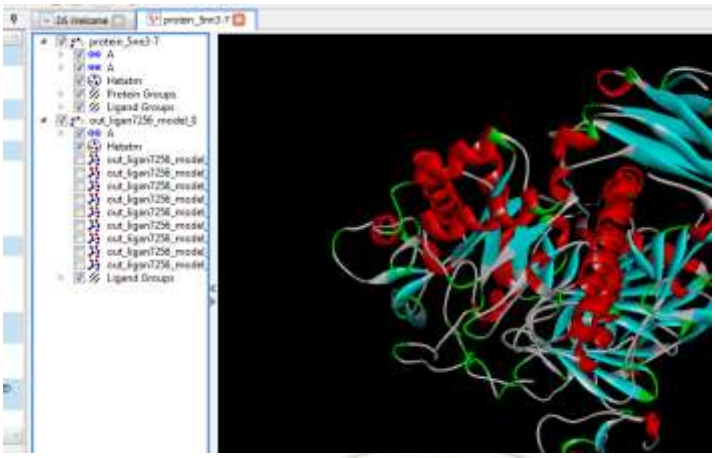


10. Contoh hasil output

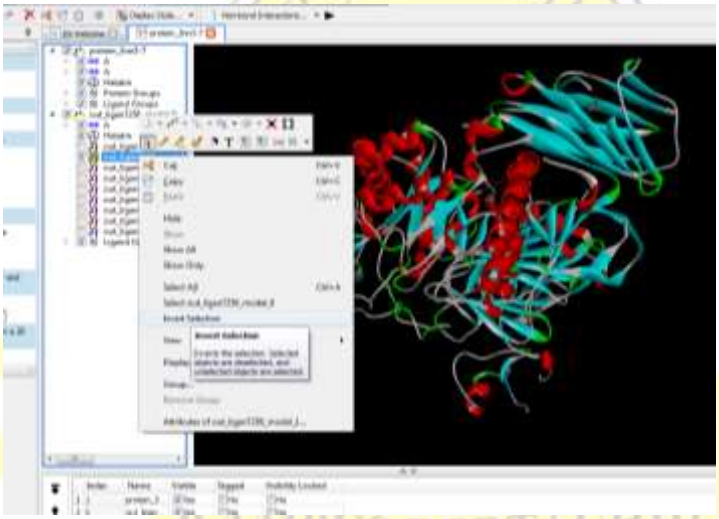
```
# AutoDock Vina: Improving the speed and accuracy of docking      #
# with a new scoring function, efficient optimization and         #
# multithreading, Journal of Computational Chemistry 31 (2010)    #
# 455-461                                                         #
#                                                                 #
# DOI 10.1002/jcc.21334                                           #
#                                                                 #
# Please see http://vina.scripps.edu for more information.        #
###################################################################

Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1052523824
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -2.9      0.000      0.000
   2        -2.8      0.434      3.936
   3        -2.5      8.959      9.614
   4        -2.5      8.076      9.799
   5        -2.5      8.565      9.791
   6        -2.5      8.871     10.183
   7        -2.5      8.480     10.250
   8        -2.4      8.116      9.415
   9        -2.4      8.902     10.003
Writing output ... done.
```

Lampiran 8. Visualisasi dengan menggunakan Discovery Studio Visualizer

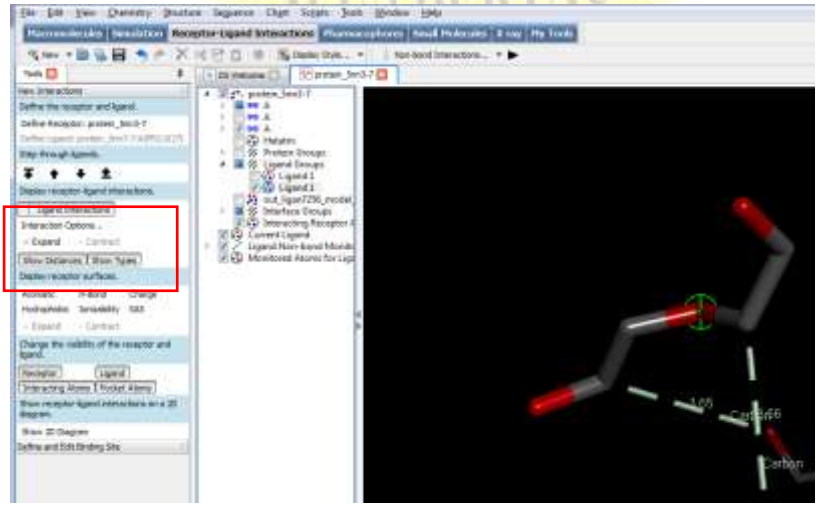
1. Buka file molekul dan hasil (out) ligan yang digunakan



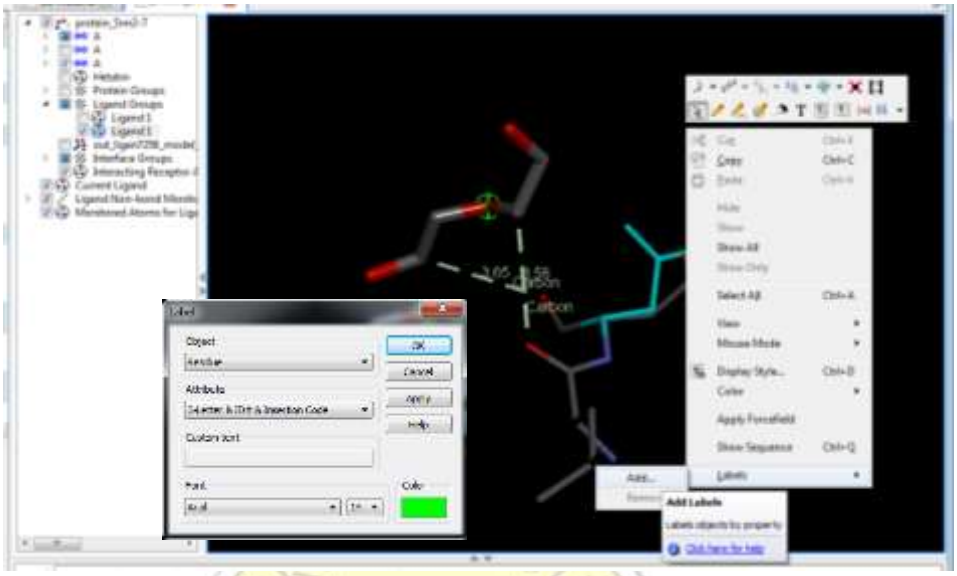
2. Pada hasil (out) ligan, pilih mode yang kedua lalu klik kanan > *Invert selection* > lalu delete. Setelah itu *drag* seluruh out ligan ke bunga telang



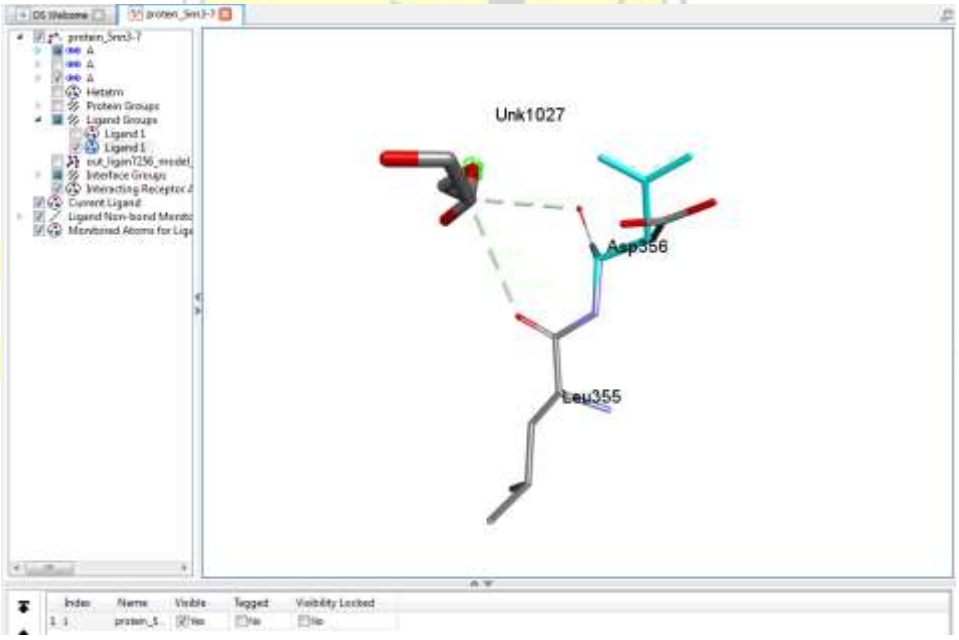
3. Klik Ligand Interaction > Show Distance > Show Types



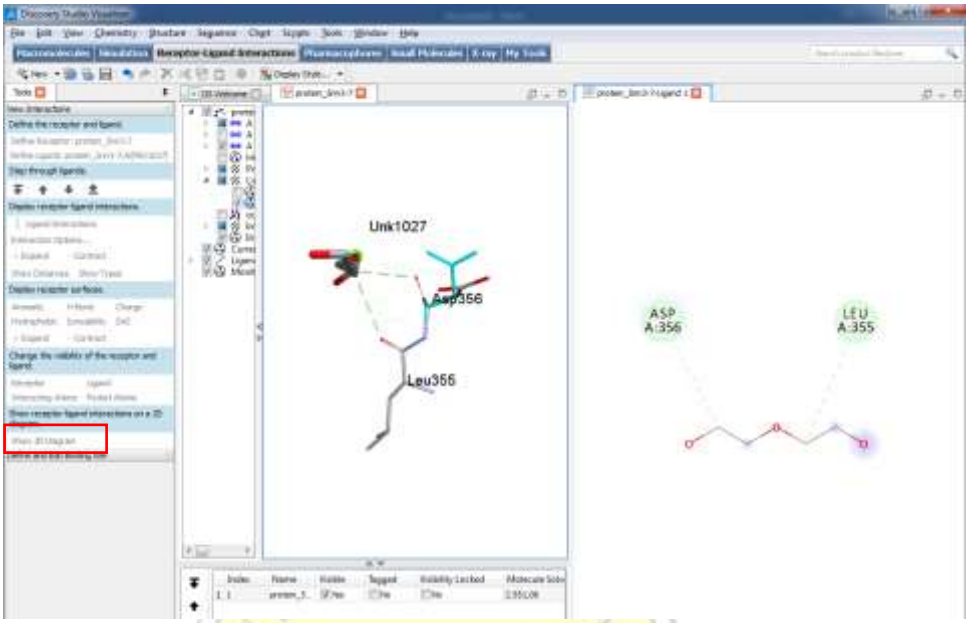
4. Klik kanan > Label > Add > Residue > 3-Letter & ID & Insertation Code > Arial > 14 > OK



5. Agar tampilan jadi lebih baik (background menjadi putih) Klik Menu Script > Visualization > Publication Quality



6. Untuk memvisualisasikan secara 2D dan mengetahui ikatan yang terjadi Klik Show 2D Diagram



Lampiran 9. Data Hasil Docking Vina

a. Ligan 7 Validasi

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-2,5	0,000	0,000
2	-2,5	1,016	4,238
3	-2,5	1,399	1,458
4	-2,4	1,580	4,353
5	-2,4	0,869	4,109
6	-2,4	1,654	1,959
7	-2,4	1,806	3,909
8	-2,4	1,474	1,744
9	-2,4	2,382	3,774

b. *pentanal*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-2,9	0,000	0,000
2	-2,9	2,345	3,283
3	-2,8	1,566	1,566
4	-2,8	9,485	10,599
5	-2,8	2,405	3,486
6	-2,8	2,525	3,339
7	-2,8	1,953	2,571
8	-2,8	1,475	1,679
9	-2,8	3,067	3,668

c. *1-butanol-3-methyl- acetate*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,5	0,000	0,000
2	-3,5	1,392	2,221
3	-3,4	1,481	2,346
4	-3,4	1,405	2,425
5	-3,4	3,233	4,312
6	-3,4	3,149	4,143
7	-3,3	1,508	2,128
8	-3,3	3,169	3,996
9	-3,2	1,815	2,583

d. *acetic acid, cyano-*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,3	0,000	0,000
2	-3,0	2,396	2,987
3	-2,9	1,250	1,257
4	-2,9	9,765	9,924
5	-2,9	12,792	13,320
6	-2,8	8,567	9,341
7	-2,8	6,947	7,492
8	-2,8	8,647	9,145
9	-2,8	8,630	9,256

e. *pyrimidine-2-d, 6-methyl-*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,4	0,000	0,000
2	-3,4	1,306	2,415
3	-3,4	0,993	1,830
4	-3,4	1,133	2,176
5	-3,3	1,445	2,493
6	-3,3	0,952	2,852
7	-3,3	0,559	2,550
8	-3,3	1,175	1,927
9	-3,3	1,625	2,379

f. *hirsutene*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-6,0	0,000	0,000
2	-5,3	2,380	4,627
3	-5,3	1,267	5,057
4	-5,2	2,116	3,997
5	-5,2	1,565	3,918
6	-5,2	1,778	4,895
7	-5,2	1,745	3,262
8	5,1	2,768	4,813
9	-5,0	1,477	3,880

g. *pyrimidine, 4-hydroxy-*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,3	0,000	0,000
2	-3,3	2,535	2,911
3	-3,2	2,119	2,724
4	-3,2	1,917	2,685
5	-3,2	1,902	2,459
6	-3,2	2,912	3,419
7	-3,2	9,528	10,214
8	-3,0	10,393	11,347
9	-3,0	8,349	9,224

h. *butane- 2-isothiocyanate*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,1	0,000	0,000
2	-3,0	2,267	2,866
3	-3,0	1,452	1,452
4	-3,0	0,956	1,006
5	-2,9	1,031	1,677
6	-2,9	2,494	2,994
7	-2,9	2,835	3,235
8	-2,9	2,874	3,438
9	-2,9	1,046	2,183

i. *bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,7	0,000	0,000
2	-4,5	0,919	1,041
3	-4,4	1,333	3,780
4	-4,2	1,602	3,419
5	-4,2	1,361	3,793
6	-4,2	0,839	3,768
7	-4,2	1,123	1,784
8	-4,1	1,409	3,455
9	-4,1	1,454	3,502

i. *cyclohexane, 1-methyl-4-(1-methylethylidene*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,6	0,000	0,000
2	-4,5	1,980	3,599
3	-4,5	2,034	4,455
4	-4,4	1,976	3,984
5	-4,3	1,559	4,205
6	-4,2	1,313	2,486
7	-4,2	2,271	3,239
8	-4,2	2,232	5,113
9	-4,1	1,759	4,379

j. *1,3-benzodioxole, 5-(2-propenyl)*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,8	0,000	0,000
2	-4,8	0,769	1,061
3	-4,6	2,962	3,990
4	-4,5	3,874	6,218
5	-4,5	2,041	2,422
6	-4,5	1,595	2,550
7	-4,5	2,510	4,839
8	-4,5	3,985	6,344
9	-4,5	2,324	4,497

k. *1-nitro-2-acetamido-1-2-dideoxy-d-mannitol*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	4,6	0,000	0,000
2	-4,5	0,937	1,043
3	-4,5	1,807	3,262
4	-4,4	6,191	8,964
5	-4,3	1,876	2,813
6	-4,3	1,958	4,952
7	-4,3	2,066	2,919
8	-4,3	3,055	5,945
9	-4,3	1,497	3,303

l. *caffeine*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,4	0,000	0,000
2	-4,4	1,412	3,061
3	-4,4	1,862	4,427
4	-4,4	1,575	3,663
5	-4,3	1,051	3,442
6	-4,3	1,339	3,750
7	-4,3	1,964	4,751
8	-4,3	2,210	3,554
9	-4,3	1,954	2,357

m. *hexadecanoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,3	0,000	0,000
2	-4,2	1,476	2,267
3	-4,2	1,110	3,517
4	-4,2	3,548	5,605
5	-4,2	1,343	1,952
6	-4,1	0,937	1,937
7	-4,1	1,532	3,382
8	-4,1	4,421	6,286
9	-4,1	3,127	6,760