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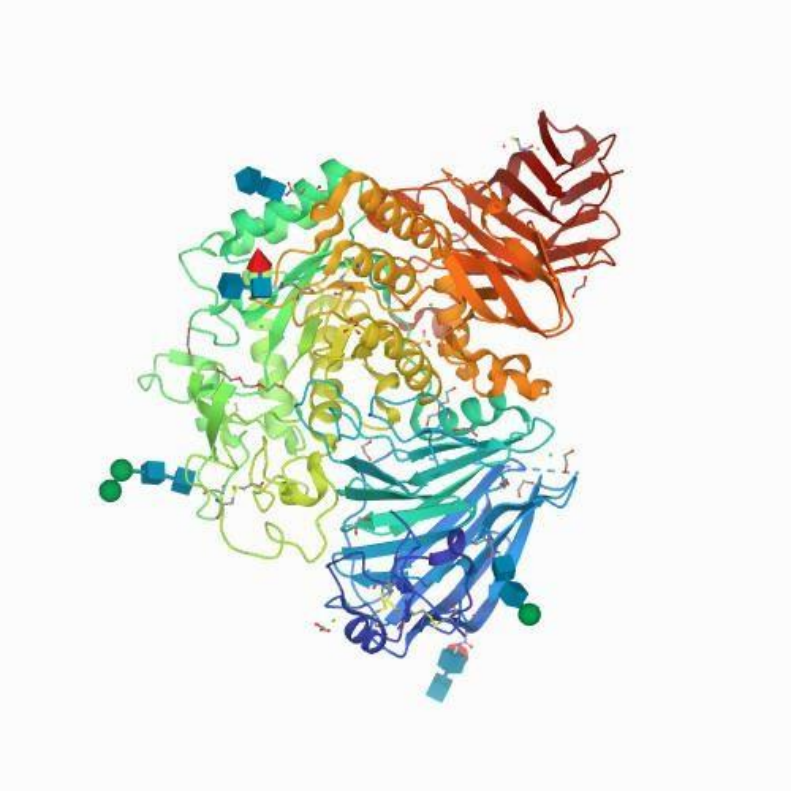
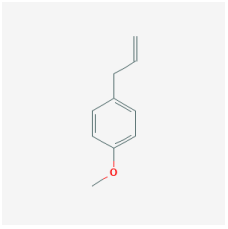
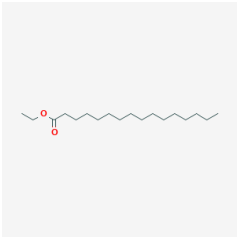
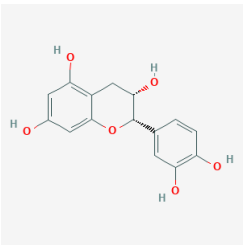
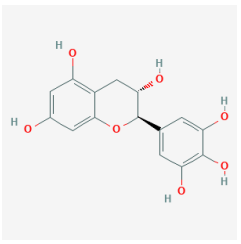
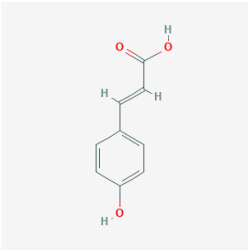
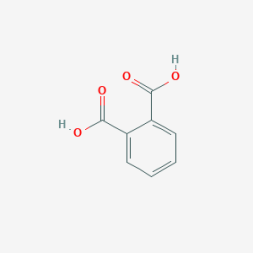
LAMPIRAN

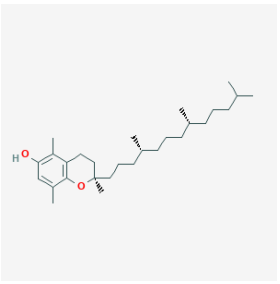
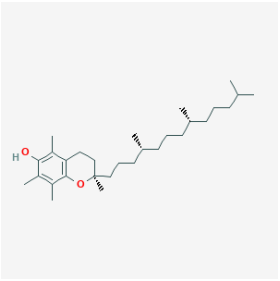
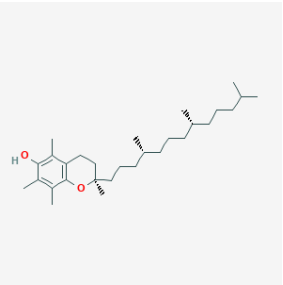
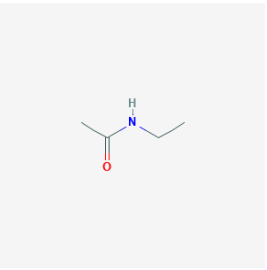
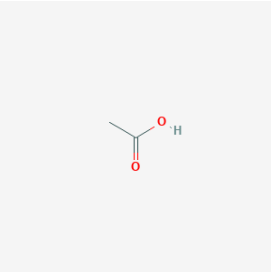
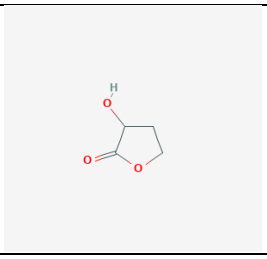
Lampiran 1. Struktur Protein (Reseptor)

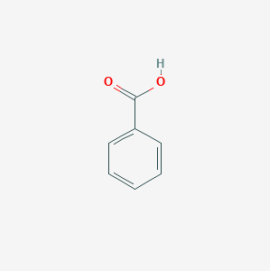
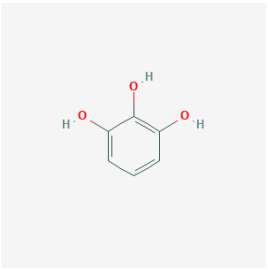
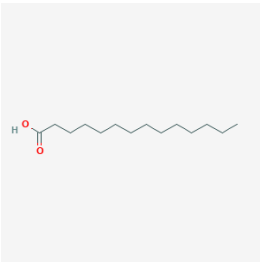
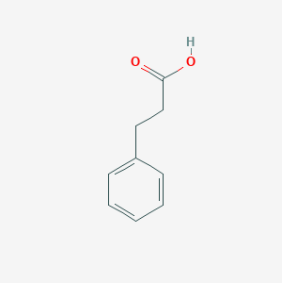
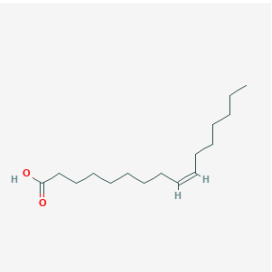


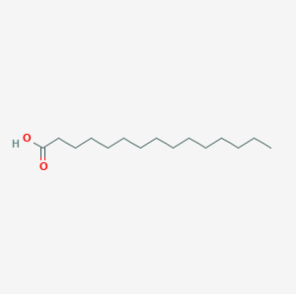
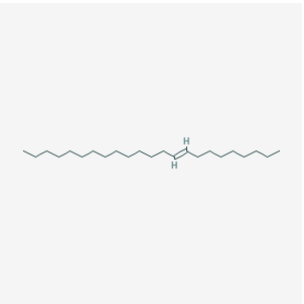
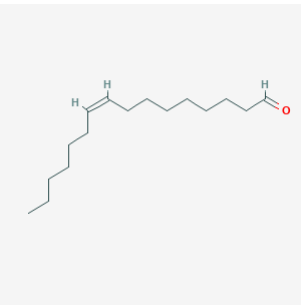
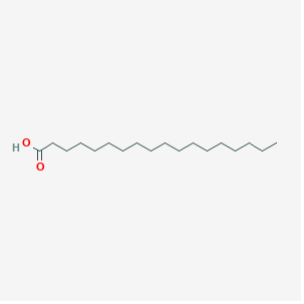
Struktur 3D dengan PDB ID 5NN3 (sumber : www.rscb.org)

Lampiran 2. Struktur Ligan Uji Ekstrak Kulit Pisang

No.	Ligan	Struktur
1	*Estragole*	
2	*Hexadecanoic acid ethyl ester*	
3	*Epicatechin*	
4	*Gallocatechin*	
5	*p-coumaric acid methyl ester*	
6	*1,2-Benzenedicarboxylic acid mono (2-ethylhexylester)*	

7	*Beta-tocopherol*	
8	*Vitamin E*	
9	*Ethanimidic acid, ethyl ester*	
10	*Acetic acid*	
11	*2-hydroxy-gammbutyrolactone*	
12	*4H-pyran-4-one, 3 hidroxy*	

13	*Benzoic acid*	
14	*Pyrogallol*	
15	*Tetradecenoic acid*	
16	*1-Nonadecene*	
17	*Benzenepropanoic acid*	
18	*Cis-9-Hexadecenoic acid*	

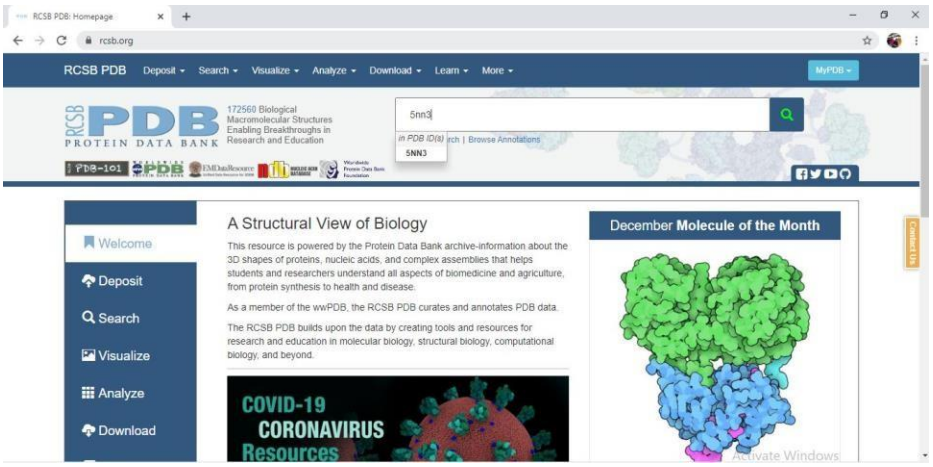
19	*Pentadecanoic acid*	
20	*9-Tricosene*	
21	*Cis-9-Hexadecenal*	
22	*Octadecanoic acid*	
23	*2,6,10,14,18,22 Tetracosahexaene*	

Lampiran 3. Hasil Pengaturan *grid box* reseptor

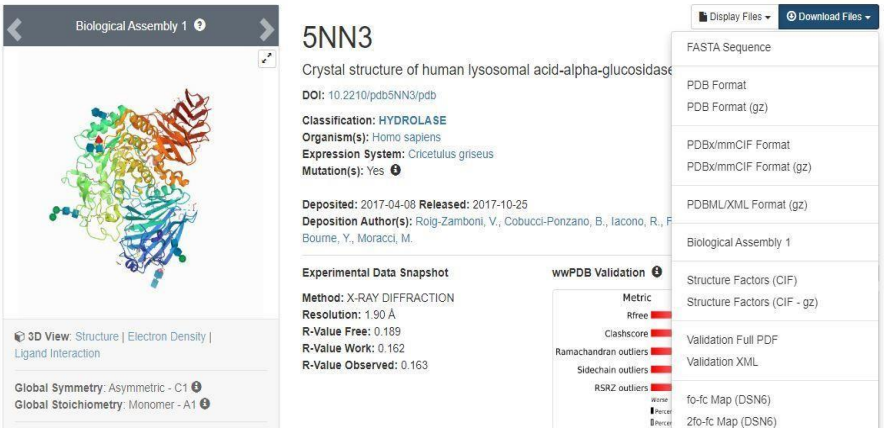
	Grid Box					
	Center			***Size***		
Makromolekul	**X**	**Y**	**Z**	**X**	**Y**	**Z**
α-glukosidase (kode 5nn3)	4,116	-13,936	75,412	14	16	14

Lampiran 4. Preparasi Struktur Reseptor

1. Struktur reseptor yang digunakan dapat diunduh dari https://www.rscb.org

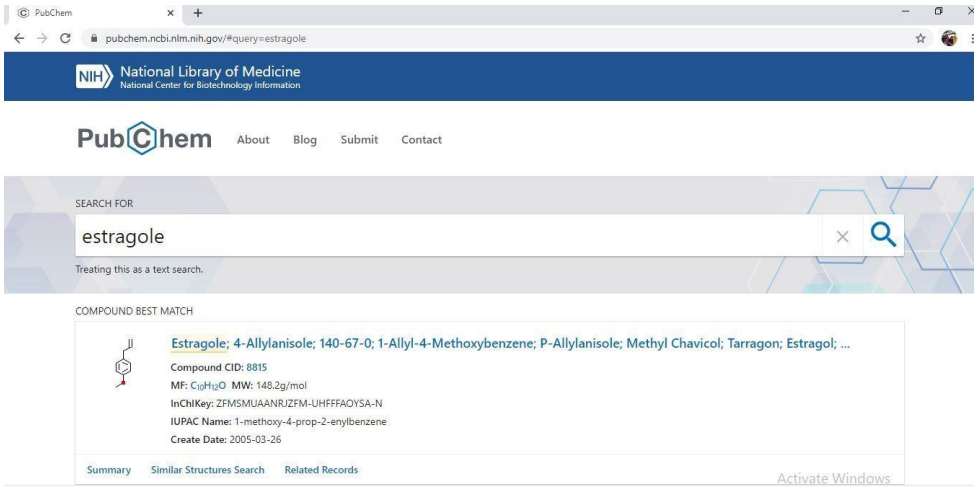


2. Reseptor *α-Glukosidase* (kode : 5NN3) dicari pada *search engine* dan diunduh dalam format PDB

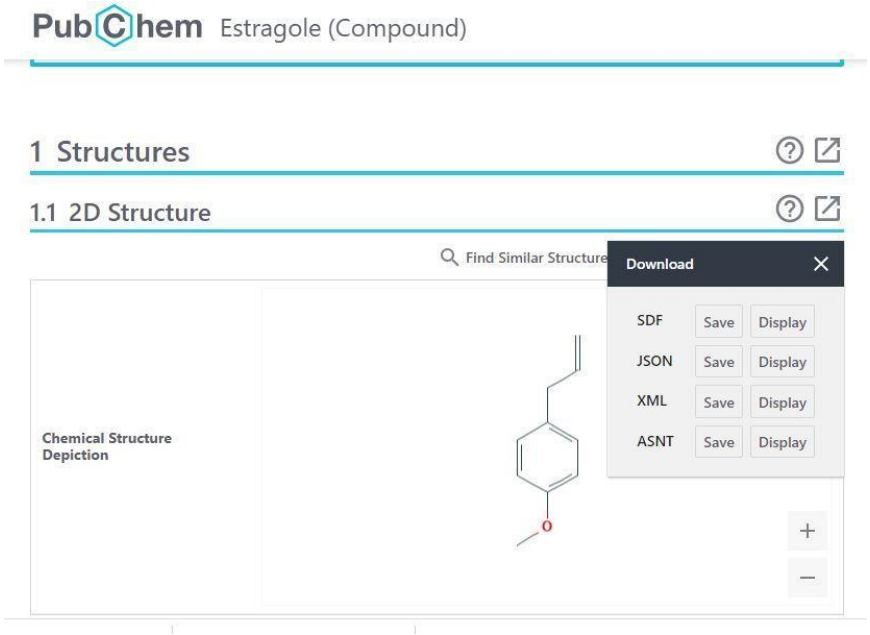


Lampiran 5. Preparasi Struktur Ligan

1. Ligan ekstrak kulit pisang yang digunakan disimpan dari situs http://pubchem.ncbi.nlm.nih.gov



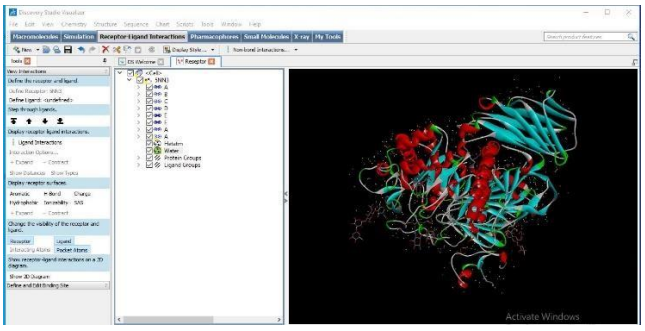
2. Struktur ligan 2D dicari dan disimpan dalam format SDF



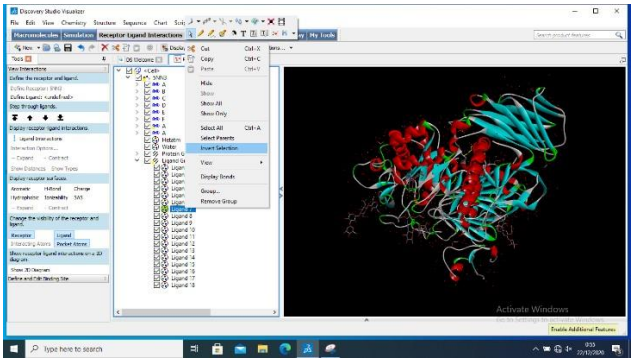
Lampiran 6. Pemisahan Ligan dan Makromolekul

1. Pemilihan Ligan

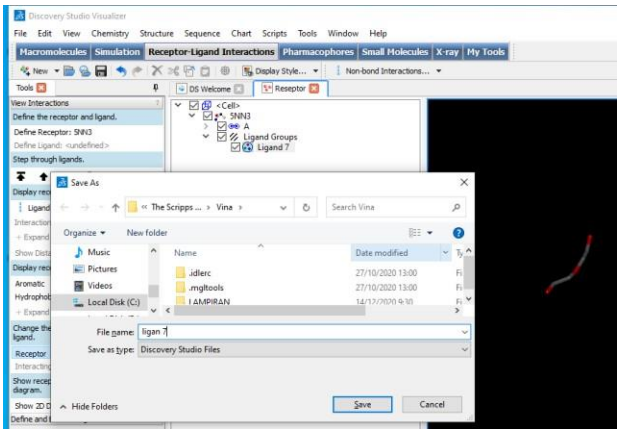
   a. Struktur 3D reseptor dalam format PDB yang diunduh dibuka dengan di*scovery studio visualizer* kemudian munculkan *view hierarcy* dengan mengetik ctrl+H pada *keyboard*.



   b. Setelah muncul struktur reseptor lakukan penghilangan molekul air dengan meng-klik kanan *mouse* lalu pilih *delete*. Kemudian, lakukan pemilihan ligan dengan meng-klik kanan *mouse*, pilih *invert selection* dan tekan *delete.*

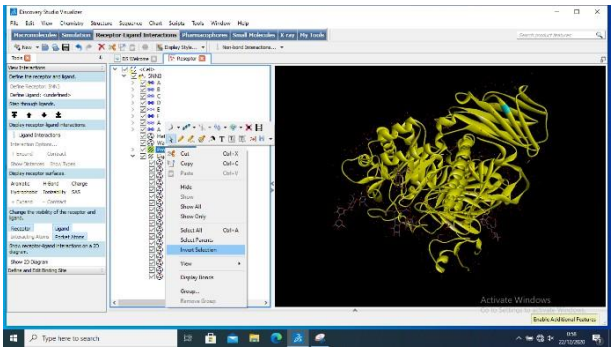


   c. Simpan file dengan format *.pdb.

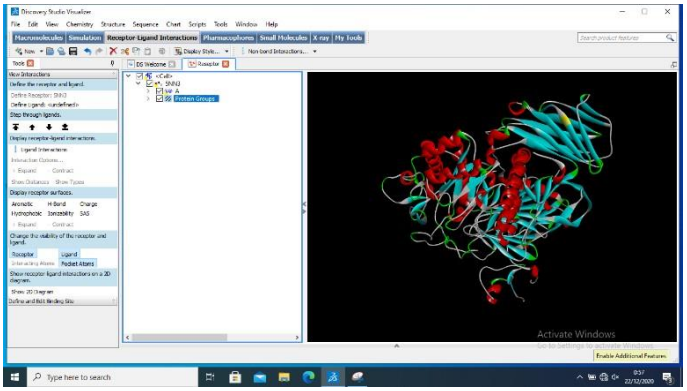


2. Pemilihan Makromolekul

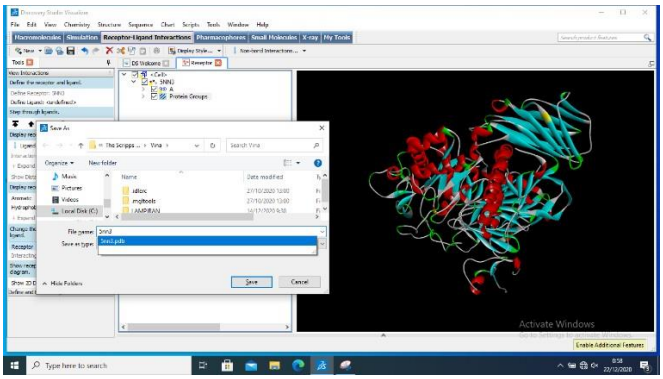
a. Hal yang sama dilakukan hingga 1b



b. Langkah selanjutnya pilih unsur protein yang ada dengan meng-klik kanan, pilih *invert selection*, dan tekan tombol *delete*.

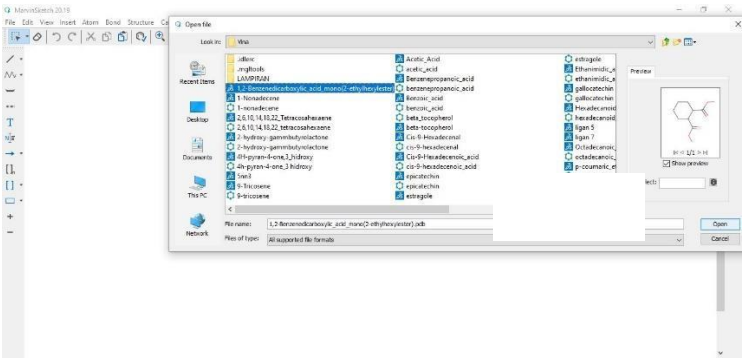


c. Kemudian, simpan *file* dengan format *.pdb.

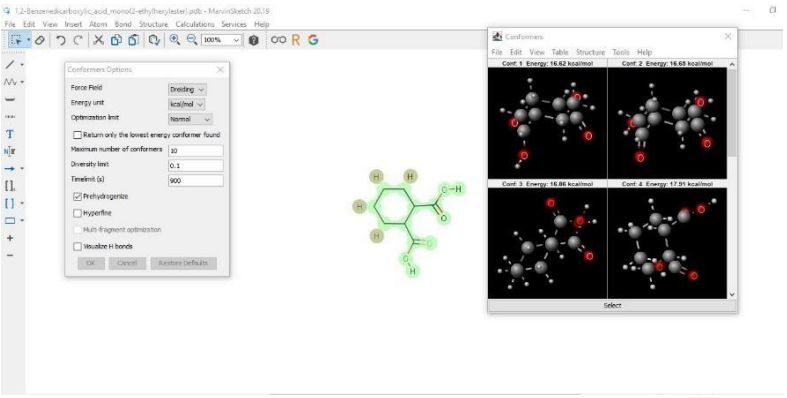


Lampiran 7. Pengubahan Struktur Ligan 2D menjadi 3D

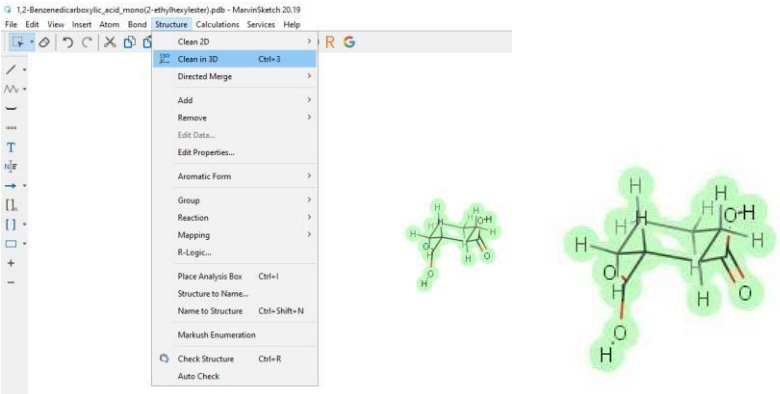
1. Pilih ligan yang telah diunduh dengan klik *open file* menggunakan *software* Marvin Sketch.



2. Blok struktur ligan, klik *calculation* > *conformation* > *conformers*, tekan ok. Setelah muncul pilih konformasi dengan enrgi yang paling rendah.

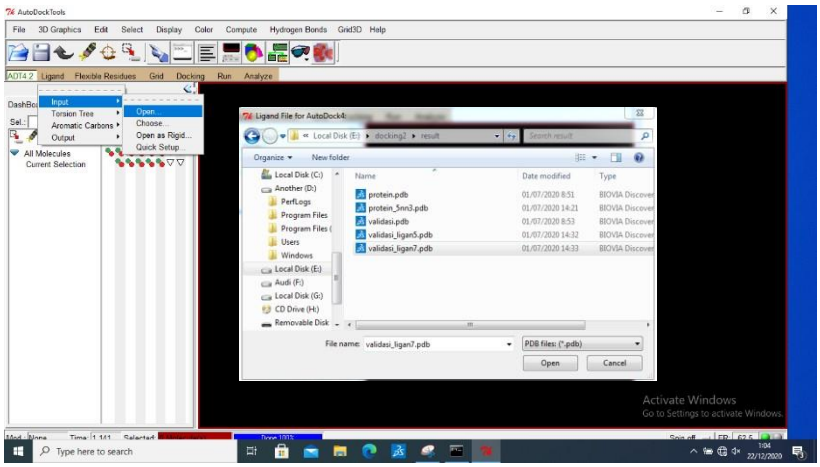


3. Setelah muncul blok kembali seluruh strukturnya, pilih *sructure* > *clean in* 3D dan file disimpan dengan format *.pdb.

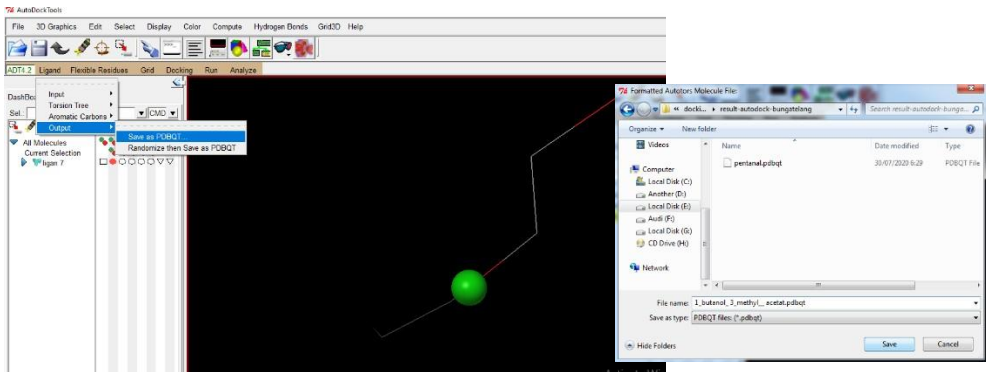


Lampiran 8. Validasi *molecular docking*

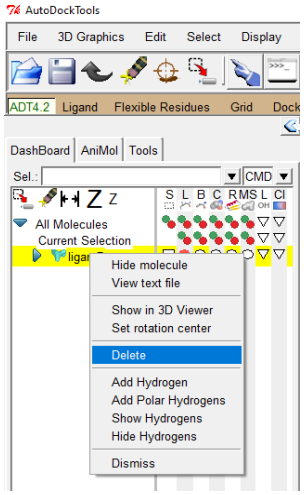
1. Buka struktur ligan dengan *software* Autodock Tools dengan klik *ligand* > *input* > open.



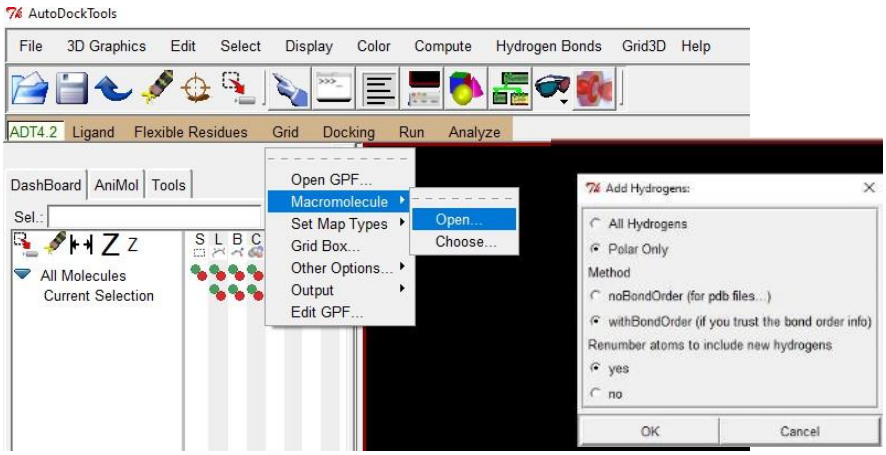
2. Dalam autodock tools struktur ligan otomatis diberi muatan *gasteiger* dan *choose torsio* sehingga dapat langsung disimpan dengan klik Ligand > Output > Save as PDBQT



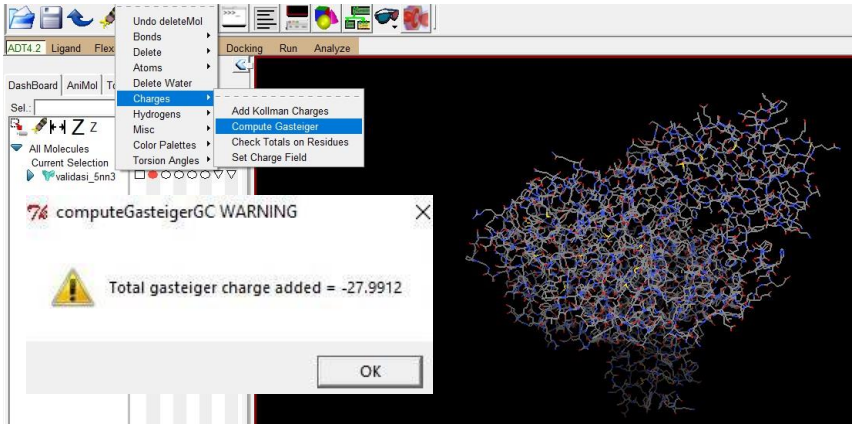
3. Setelah struktur ligan tersimpan, hapus struktur ligan pada software dengan klik kanan > *delete*.



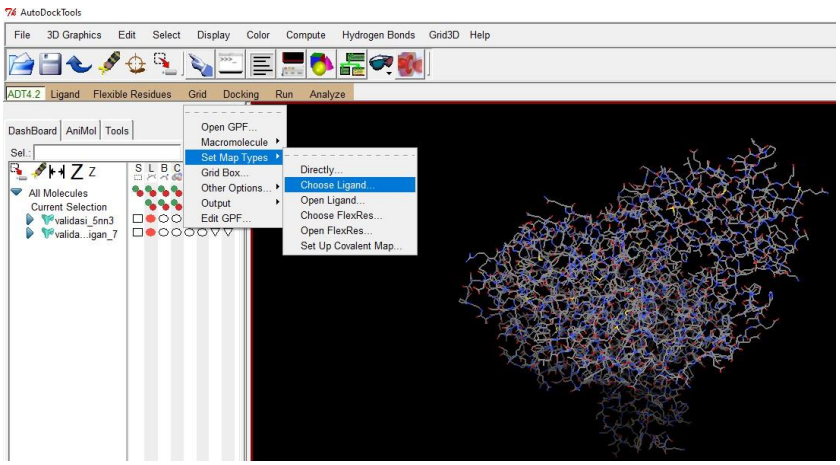
4. Buka struktur reseptor dengan meng-klik *grid* > makromolekul > open. Kemudian, tambahkan hidrogen polar dengan memilih menu *edit* > Hydrogens > Add > klik menu *Polar Only*.



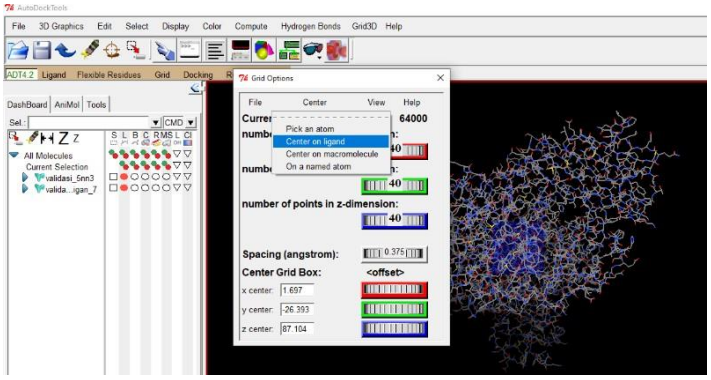
5. Hitung muatan *gasteiger* dengan klik edit > *charges* > compute *gasteiger*. Kemudian masukkan ligan yang telah disimpan dalam format PDBQT.



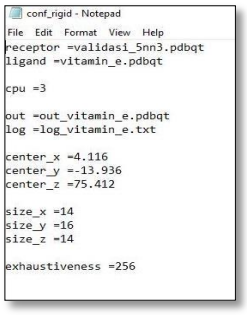
6. Pilih *grid > set map types > choose ligand > select ligand*



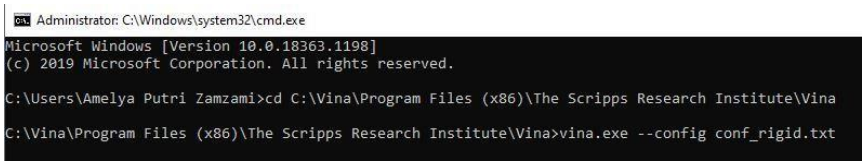
7. Tentukan *gridbox* dengan pilih *grid > grid box > center > center on ligand*



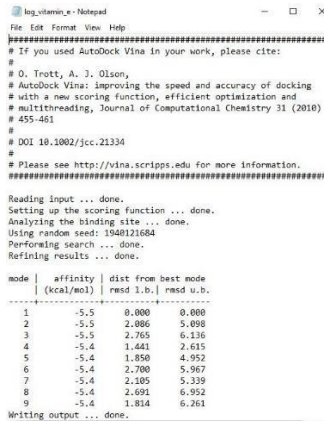
8. *Gridbox* diatur agar seluruh *box* menutupi ligan, lalu hasil validasi penambatan diketik dalam *notepad* dan disimpan dengan format *.txt serta masukkan dalam folder vina



9. Parameter penambatan dilakukan *running* dengan aplikasi *command prompt (Run as Administrator*) lalu buka file konfigurasi yang ada di folder vina.

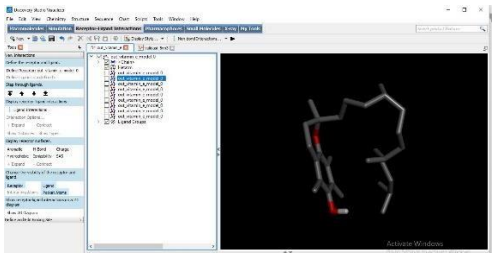


10. Tunggu proses *running* selesai. Contoh output dalam format *.txt.

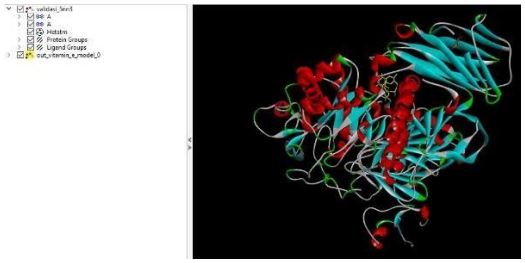


Lampiran 9. Visualisasi menggunakan *biovia* di*scovery stu*dio *visualizer*

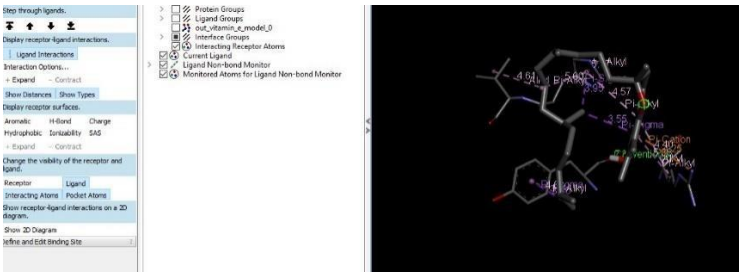
1. *File* reseptor dan hasil *out* ligan dalam format *.pdbqt dibuka.



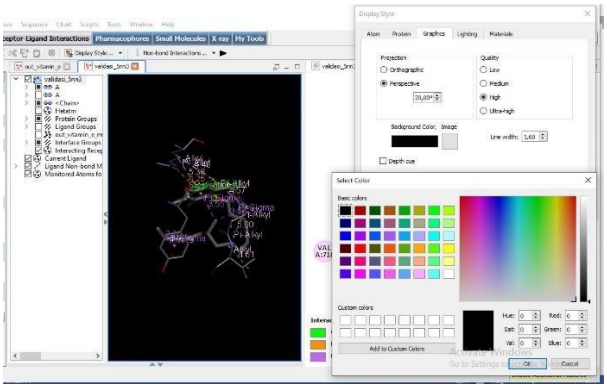
2. Hasil *out* ligan dipilih mode kedua lalu klik k*anan > Invert selection > delete*. *Out* ligan yang dipilih di *cut* dan disalin ke dalam struktur reseptor.



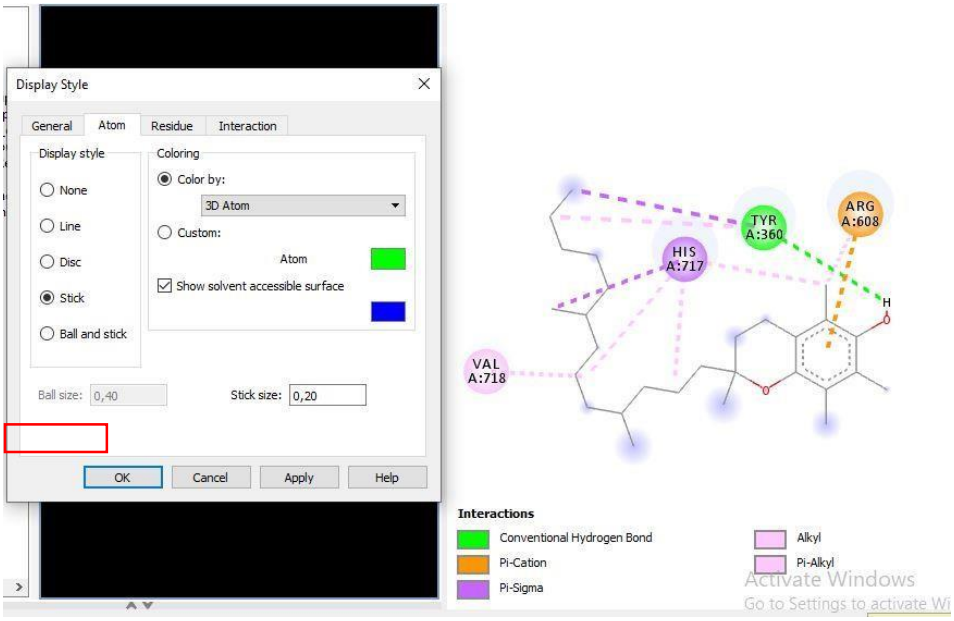
3. Untuk melihat interaksi ligan dengan reseptor pilih *Ligand Interaction > Show* D*istance > Show Types.*



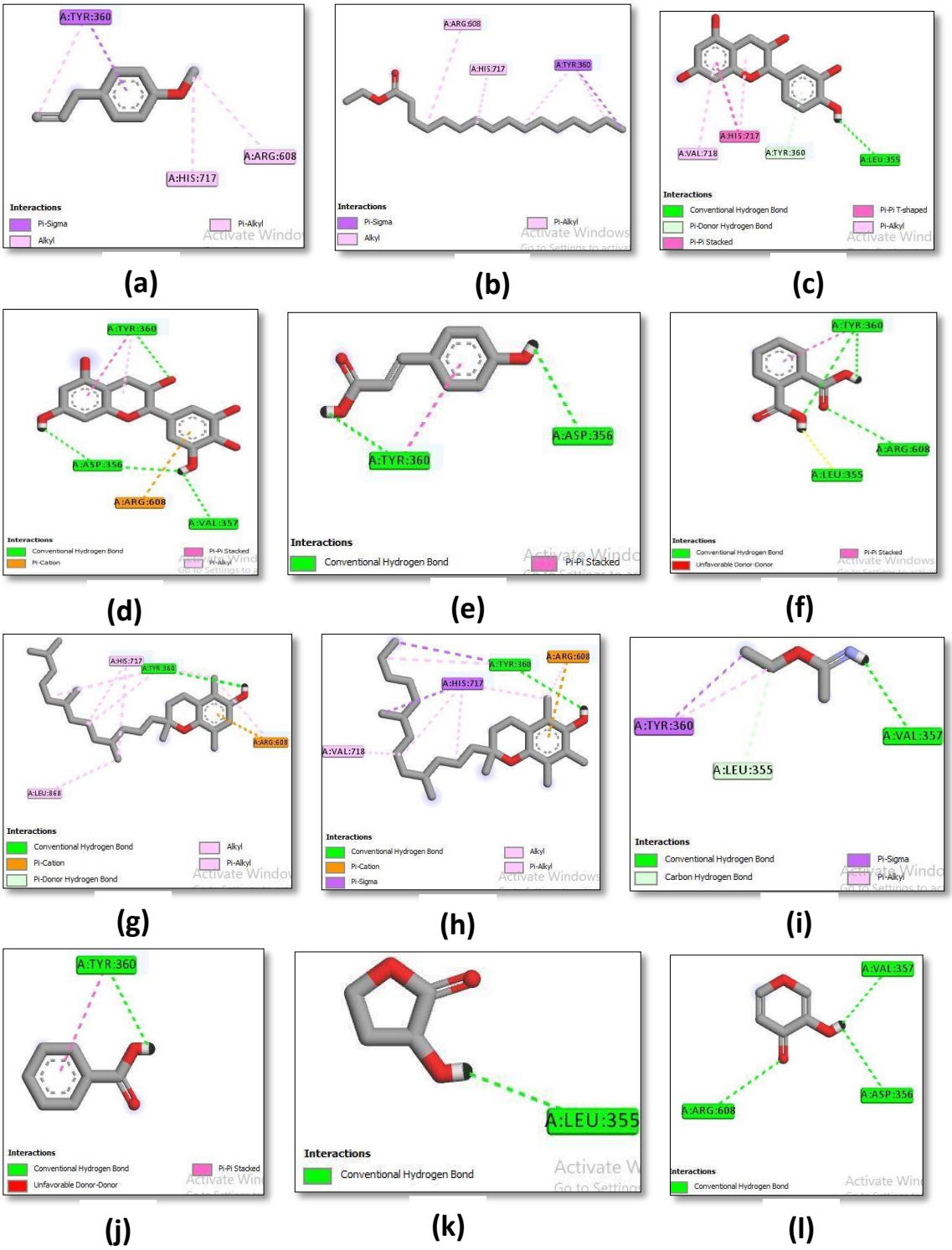
4. Agar interaksi antara ligan dengan reseptor dapat terlihat ubah *background* menjad putih dengan klik kanan > di*splay style > graphics > background*.

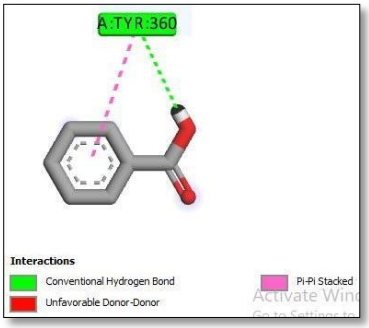


5. Agar visualisasi interaksi reseptor dan ligan lebih jelas maka ubah menjadi 2D dengan pilih *show 2D* di*agram*. Lalu agar visualisasi struktur dan ikatan dapat terlihat lebih jelas klik kanan > di*splay style* > atom > *stick* lalu tekan ok.

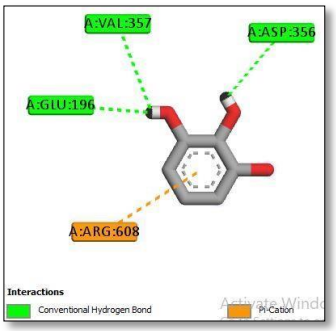


Lampiran 10. Visualisasi 2D Interaksi Ligan dengan Reseptor

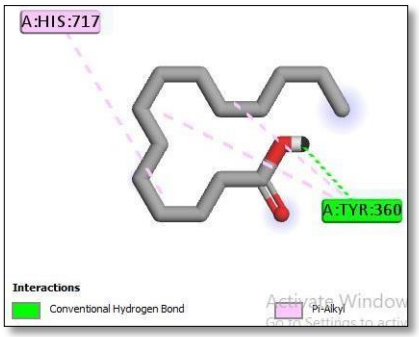




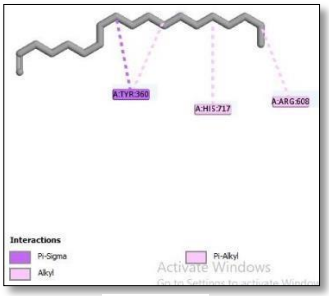
(m))



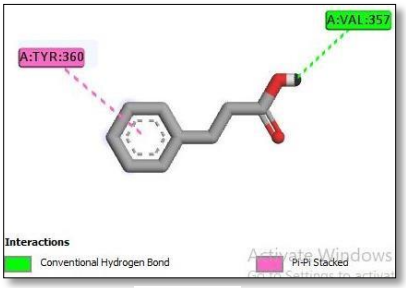
(n)



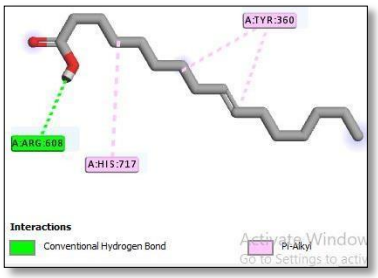
(o)



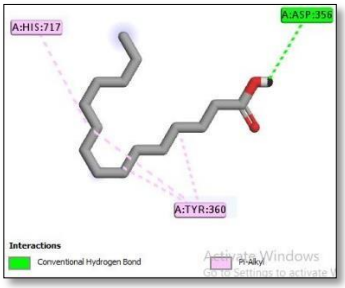
(p)



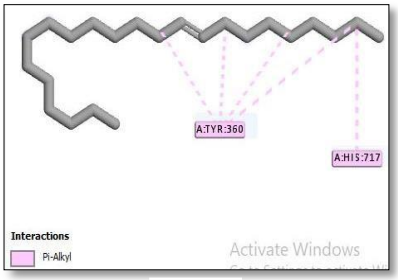
(q)



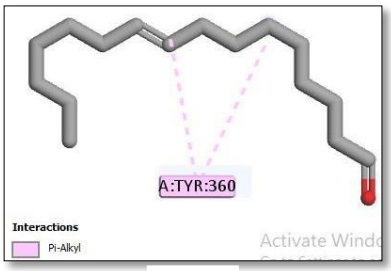
(r)



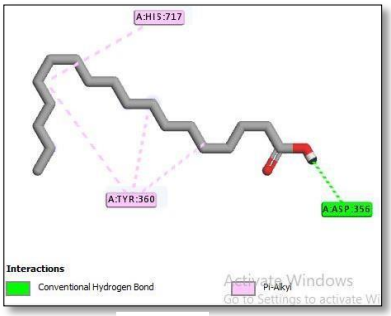
(s)



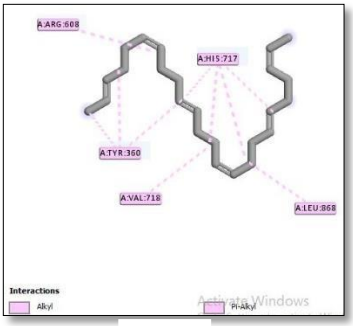
(t)



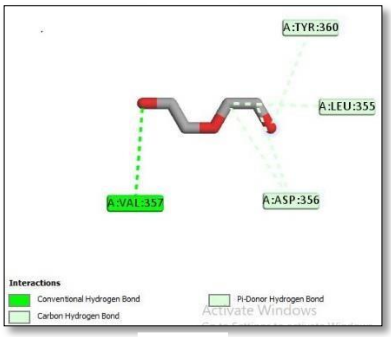
(u)



(v)



(w)



(x)

Keterangan :

Kode	Ligan uji senyawa ekstrak kulit pisang
a	*Estragole*
b	*Hexadecanoic acid ethyl ester*
c	*Epicatechin*
d	*Gallocatechin*
e	*p-coumaric acid methyl ester*
f	*1,2-Benzene*dic*arboxylic acid mono (2-ethylhexylester)*
g	*Beta-tocopherol*
h	*Vitamin E*
i	*Ethanimi*dic *acid, ethyl ester*
j	*Acetic acid*
k	*2-hydroxy-gammbutyrolactone*
l	*4H-pyran-4-one, 3 hidroxy*
m	*Benzoic acid*
n	*Pyrogallol*
o	*Tetradecenoic acid*
p	*1-Nonadecene*
q	*Benzenepropanoic acid*
r	*Cis-9-Hexadecenoic acid*
s	*Pentadecanoic acid*
t	*9-Tricosene*
u	*Cis-9-Hexadecenal*
v	*Octadecanoic acid*
w	*2,6,10,14,18,22 Tetracosahexaene*
x	Ligan 7 Validasi

Lampiran 11. Data Hasil *Docking* Vina

a. Ligan 7 Validasi

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-2,4	0,000	0,000
2	-2,4	0,108	4,086
3	-2,4	1,582	4,170
4	-2,4	1,094	4,212
5	-2,4	6,641	7,089
6	-2,4	1,937	2,260
7	-2,4	1,583	1,711
8	-2,4	6,620	8,105
9	-2,4	1,620	3,754

b. *Estragole*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,5	0,000	0,000
2	-4,5	2,899	4,049
3	-4,4	2,875	4,678
4	-4,4	2,824	5,197
5	-4,4	2,790	5,329
6	-4,4	2,892	4,122
7	-4,4	2,270	3,629
8	-4,4	2,901	4,768
9	-4,4	3,029	4,932

c. *Hexadecanoic acid ethyl ester*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,1	0,000	0,000
2	-4,1	2,198	5,437
3	-4,0	1,243	4,018
4	-4,0	2,617	5,182
5	-4,0	1,389	4,765
6	-4,0	2,611	5,932
7	-4,0	2,224	5,267
8	-4,0	1,754	4,080
9	-3,9	1,675	3,992

d. *Epicatechin*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-6,6	0,000	0,000
2	-6,4	2,628	6,420
3	-6,3	2,804	5,906
4	-6,3	1,846	2,619
5	-6,2	2,868	5,977
6	-6,2	2,803	5,926
7	-6,2	2,178	2,934
8	-6,2	3,039	4,609
9	-6,2	2,563	6,542

e. *Gallocatechin*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-6,4	0,000	0,000
2	-6,4	0,913	1,956
3	-6,3	2,482	5,356
4	-6,2	1,116	1,549
5	-6,1	2,460	5,118
6	-6,0	2,105	4,843
7	-6,0	2,074	4,559
8	-6,0	4,184	6,499
9	-6,0	1,742	5,742

f. *p-coumaric acid methyl ester*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-5,2	0,000	0,000
2	-5,2	0,316	1,436
3	-5,1	3,099	3,660
4	-5,1	3,114	3,730
5	-5,0	1,192	1,836
6	-4,9	1,270	1,485
7	-4,8	2,915	5,051
8	-4,7	2,893	4,983
9	-4,7	2,860	4,901

g. *1,2-Benzene*dic*arboxylic acid mono (2-ethylhexylester)*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-5,1	0,000	0,000
2	-5,1	0,051	2,892
3	-4,9	1,958	3,120
4	-4,9	1,970	3,391
5	-4,8	2,588	3,512
6	-4,8	2,575	4,164
7	-4,7	1,995	3,182
8	-4,7	1,993	2,903
9	-4,6	1,954	3,757

h. *Beta-tocopherol*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-5,5	0,000	0,000
2	-5,4	1,293	2,201
3	-5,3	2,897	7,442
4	-5,3	2,597	5,603
5	-5,3	1,950	4,458
6	-5,3	1,896	2,967
7	-5,3	2,081	5,165
8	-5,3	3,203	6,591
9	-5,3	2,794	5,573

i. *Vitamin E*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-5,5	0,000	0,000
2	-5,5	2,086	5,098
3	-5,5	2,765	6,136
4	-5,4	1,441	2,615
5	-5,4	1,850	4,952
6	-5,4	2,700	5,967
7	-5,4	2,105	5,339
8	-5,4	2,691	6,952
9	-5,4	1,814	6,261

j. *Ethanimid*ic *acid, ethyl ester*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,1	0,000	0,000
2	-3,1	1,742	2,010
3	-2,9	3,309	3,624
4	-2,9	1,385	2,691
5	-2,9	7,066	7,284
6	-2,9	2,527	3,431
7	-2,9	2,359	3,293
8	-2,8	6,139	6,719
9	-2,8	6,239	6,650

k. *Acetic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,6	0,000	0,000
2	-4,6	0,057	1,623
3	-4,3	2,401	2,825
4	-4,3	3,494	4,558
5	-4,3	2,397	3,030
6	-4,2	2,308	3,187
7	-4,1	2,454	3,438
8	-4,1	1,884	2,573
9	-4,1	0,858	1,835

l. *2-hydroxy-gammbutyrolactone*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,3	0,000	0,000
2	-3,2	1,558	3,150
3	-3,2	3,381	3,779
4	-3,2	1,142	2,300
5	-3,1	1,944	3,465
6	-3,1	1,865	2,342
7	-3,1	1,478	2,472
8	-3,1	2,213	2,727
9	-3,0	1,767	2,642

m. *4H-pyran-4-one, 3 hidroxy*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,5	0,000	0,000
2	-3,5	3,009	3,539
3	-3,5	1,578	1,906
4	-3,5	0,963	2,340
5	-3,4	2,342	3,359
6	-3,4	4,048	5,047
7	-3,4	2,732	3,850
8	-3,4	2,781	4,362
9	-3,4	1,882	2,685

n. *Benzoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,7	0,000	0,000
2	-4,6	0,031	1,632
3	-4,3	3,510	4,291
4	-4,3	3,497	4,566
5	-4,3	2,412	2,845
6	-4,3	2,426	3,065
7	-4,2	0,904	1,907
8	--4,2	2,468	3,471
9	-4,1	2,466	3,415

o. *Pyrogallol*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,2	0,000	0,000
2	-4,1	4,295	5,069
3	-4,1	4,293	5,198
4	-4,1	0,204	2,794
5	-4,1	4,245	5,099
6	-4,0	2,835	4,597
7	-4,0	4,080	5,556
8	-4,0	2,046	2,557
9	-4,0	1,982	2,592

p. *Tetradecenoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,1	0,000	0,000
2	-4,1	2,926	2,926
3	-4,1	1,353	1,353
4	-4,0	1,717	1,717
5	-4,0	5,406	5,406
6	-4,0	2,645	2,645
7	-3,9	5,916	5,916
8	-3,9	5,157	5,157
9	-3,9	5,396	5,396

q. *1-Nonadecene*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,8	0,000	0,000
2	-3,7	1,226	4,293
3	-3,7	1,609	5,701
4	-3,7	2,015	5,635
5	-3,7	2,231	4,076
6	-3,7	1,410	2,706
7	-3,7	2,212	5,827
8	-3,7	0,976	5,601
9	-3,6	1,596	4,891

r. *Benzenepropanoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,9	0,000	0,000
2	-4,9	0,080	1,472
3	-4,8	3,065	4,494
4	-4,8	3,067	4,441
5	-4,8	0,917	1,749
6	-4,7	3,468	4,797
7	-4,7	3,497	4,836
8	-4,6	3,962	5,506
9	-4,6	1,396	2,087

s. *Cis-9-Hexadecenoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,4	0,000	0,000
2	-4,4	1,153	1,789
3	-4,4	1,033	3,294
4	-4,3	1,094	3,713
5	-4,3	3,507	5,580
6	-4,3	3,532	5,980
7	-4,2	3,545	5,699
8	-4,2	1,545	2,809
9	-4,2	3,611	5,807

t. *Pentadecanoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,2	0,000	0,000
2	-4,2	3,561	6,060
3	-4,1	3,613	5,560
4	-4,1	1,293	2,334
5	-4,0	1,528	3,749
6	-4,0	3,514	5,870
7	-4,0	3,569	6,048
8	-4,0	3,661	5,510
9	-4,0	4,102	6,648

u. *9-Tricosene*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-3,7	0,000	0,000
2	-3,7	0,912	2,733
3	-3,7	1,710	6,150
4	-3,7	1,330	3,980
5	-3,7	1,333	3,055
6	-3,7	2,070	6,067
7	-3,6	2,564	6,533
8	-3,6	1,733	3,922
9	-3,6	1,565	6,031

v. *Cis-9-Hexadecenal*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,0	0,000	0,000
2	-4,0	1,491	2,192
3	-4,0	2,218	3,798
4	-3,9	2,511	5,615
5	-3,9	1,132	2,285
6	-3,9	2,853	5,838
7	-3,9	1,192	1,897
8	-3,9	1,306	4,192
9	-3,9	2,693	6,222

w. *Octadecanoic acid*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,0	0,000	0,000
2	-3,9	3,440	6,083
3	-3,9	3,391	5,588
4	-3,9	3,401	5,963
5	-3,9	1,019	1,999
6	-3,8	1,981	3,509
7	-3,8	3,366	5,303
8	-3,8	1,409	2,470
9	-3,8	3,305	6,525

x. *2,6,10,14,18,22 Tetracosahexaene*

Mode	Affinity (kcal/mol)	RMSD l b	RMSD u b
1	-4,4	0,000	0,000
2	-4,3	0,881	5,825
3	-4,3	2,165	5,347
4	-4,3	1,576	5,166
5	-4,2	0,825	5,636
6	-4,2	1,834	4,680
7	-4,2	2,020	6,618
8	-4,2	1,586	4,120
9	-4,2	0,424	5,590

Lampiran 12. Jarak Residu Asam Amino Reseptor dengan Ligan

a. Ikatan Hidrogen

No.	Ligan	Ikatan Hidrogen	Jarak Interaksi (Å)
1	Ligan Validasi	**VAL**^{357} **ASP**^{356} **LEU**^{355} **TYR**^{360}	3,34 3,53 ; 3,48 3,58 3,67
2	*Estragole*		
3	*Hexadecanoic acid ethyl ester*		
4	*Epicatechin*	**LEU**^{355} **TYR**^{360}	2,64 3,82
5	*Gallocatechin*	**ASP**^{356} **VAL**^{357} **TYR**^{360}	2,36 ; 2,68 2,68 3,13
6	*p-coumaric acid methyl ester*	**ASP**^{356} **TYR**^{360}	2,96 2,05
7	*1,2-Benzene*dic*arboxylic acid mono (2-ethylhexylester)*	**LEU**^{355} ARG^{608} **TYR**^{360}	2,18 3,29 3,22 ; 2,73
8	*Beta-tocopherol*	**TYR**^{360}	2,54
9	*Vitamin E*	**TYR**^{360}	2,37
10	*Ethanimi*dic *acid, ethyl ester*	**VAL**^{357} **LEU**^{355}	2,7 3,48
11	*Acetic acid*	**TYR**^{360}	2,87
12	*2-hydroxy-gammbutyrolactone*	**LEU**^{355}	2,68
13	*4H-pyran-4-one, 3 hidroxy*	ARG^{608} **ASP**^{356} **VAL**^{357}	3,39 2,92 2,41
14	*Benzoic acid*	**TYR**^{360}	2,4
15	*Pyrogallol*	GLU^{196} **VAL**^{357} **ASP**^{356}	2,35 2,45 2,1
16	*Tetradecenoic acid*	**TYR**^{360}	2
17	*1-Nonadecene*		
18	*Benzenepropanoic acid*	**VAL**^{357}	2,39
19	*Cis-9-Hexadecenoic acid*	ARG^{608}	2,28
20	*Pentadecanoic acid*	**ASP**$^{-356}$	2,93
21	*9-Tricosene*		
22	*Cis-9-Hexadecenal*		
23	*Octadecanoic acid*	**ASP**^{356}	1,97
24	*2,6,10,14,18,22 Tetracosahexaene*		

b. interaksi elektrostatik

No.	Ligan	Electrostatik	Jarak Interaksi (Å)
1	Ligan Validasi		
2	*Estragole*		
3	*Hexadecanoic acid ethyl ester*		
4	*Epicatechin*		
5	*Gallocatechin*	ARG^{608}	4,22
6	*p-coumaric acid methyl ester*		
7	*1,2-Benzene*dic*arboxylic acid mono (2-ethylhexylester)*		
8	*Beta-tocopherol*	ARG^{608}	4,33
9	*Vitamin E*	ARG^{608}	4,25
10	*Ethanimi*dic *acid, ethyl ester*		
11	*Acetic acid*		
12	*2-hydroxy-gammbutyrolactone*		
13	*4H-pyran-4-one, 3 hidroxy*		
14	*Benzoic acid*		
15	*Pyrogallol*	ARG^{608}	4,01
16	*Tetradecenoic acid*		
17	*1-Nonadecene*		
18	*Benzenepropanoic acid*		
19	*Cis-9-Hexadecenoic acid*		
20	*Pentadecanoic acid*		
21	*9-Tricosene*		
22	*Cis-9-Hexadecenal*		
23	*Octadecanoic acid*		
24	*2,6,10,14,18,22 Tetracosahexaene*		

A. Ikatan Hidrofobik

No.	Ligan	Ikatan Hidrofobik	Jarak Interaksi (Å)
1	Ligan Validasi		
2	*Estragole*	HIS^{717} ARG^{608}, **TYR^{360}**	5,19 4,29 3,98 ; 3,61
3	*Hexadecanoic acid ethyl ester*	ARG^{608} HIS^{717} **TYR^{360}**	5,17 4,05 3,82 ; 3,73 ; 4,91
4	*Epicatechin*	VAL^{718} HIS^{717}	4,78 5,04 ; 5,05
5	*Gallocatechin*	**TYR^{360}**	4,08 ; 4,7
6	*p-coumaric acid methyl ester*	**TYR^{360}**	3,82
7	*1,2-Benzene*dic*arboxylic acid mono (2-ethylhexylester)*	**TYR^{360}**	4,17
8	*Beta-tocopherol*	LEU^{868} HIS^{717} ARG^{608} **TYR^{360}**	4,59 4,42 ; 4,66 ; 5,21 4,15 5,39 ; 3,84
9	*Vitamin E*	**TYR^{360}** ARG^{608} VAL^{-718} HIS^{717}	3,8 ; 4,3 4,4 4,61 3,95 ; 5 ; 5,01
10	*Ethanimi*dic *acid, ethyl ester*	**TYR^{360}**	3,53 ; 4,1
11	*Acetic acid*	**TYR^{360}**	3,89
12	*2-hydroxy-gammbutyrolactone*		
13	*4H-pyran-4-one, 3 hidroxy*		
14	*Benzoic acid*	**TYR^{360}**	3,89
15	*Pyrogallol*		
16	*Tetradecenoic acid*	**TYR^{360}** HIS^{717}	4,86 3,92 ; 5,14
17	*1-Nonadecene*	**TYR^{360}** HIS^{717} ARG^{608}	4,8 4,71 4,23
18	*Benzenepropanoic acid*	**TYR^{360}**	3,97
19	*Cis-9-Hexadecenoic acid*	HIS^{717} **TYR^{360}**	5,04 3,71 ; 4,55
20	*Pentadecanoic acid*	HIS^{717} **TYR^{360}**	4,56 4,21 ; 4,94 ; 5,36
21	*9-Tricosene*	**TYR^{36}** HIS^{717}	3,94 ; 3,98 ; 4,86 ; 4,92 4,64

22	*Cis-9-Hexadecenal*	**TYR^{360}**	4,03 ; 4,54
23	*Octadecanoic acid*	**TYR^{360}** HIS^{717}	5,01 5,48 ; 5,35 ; 4,24
24	*2,6,10,14,18,22 Tetracosahexaene*	ARG^{608} HIS^{717} **TYR^{360}** VAL^{718} LEU^{868}	4,03 4,27 ; 4,6 ; 5,01 ; 5,08 4,14 ; 4,46 ; 5,43 5,06 4,49

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