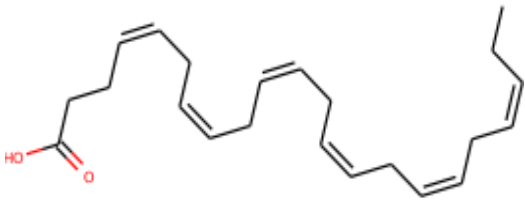
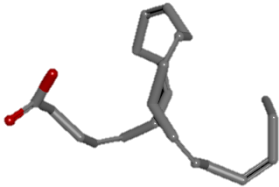
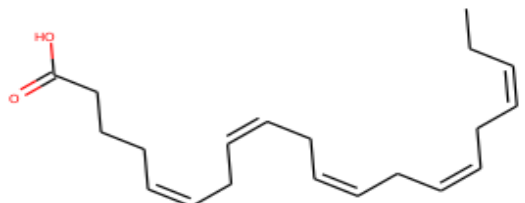
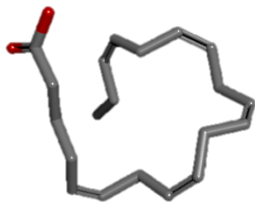
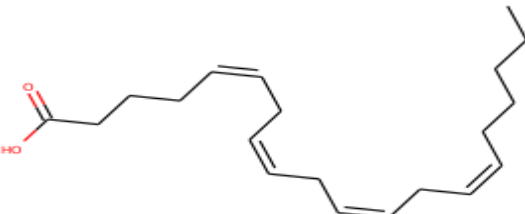
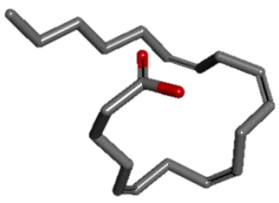
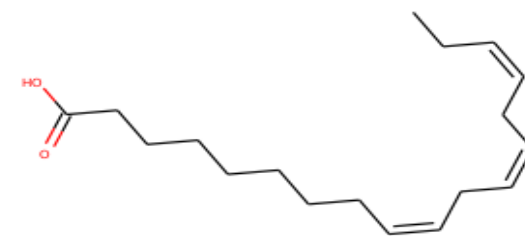
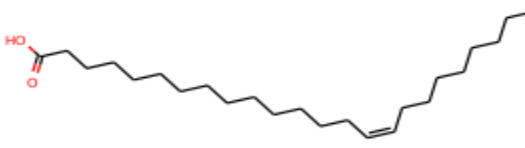
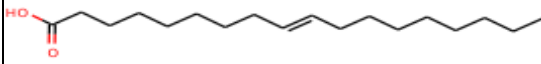
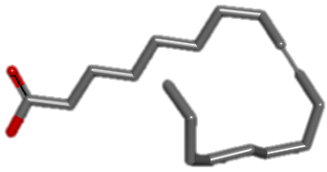
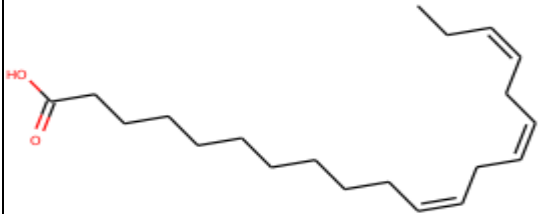
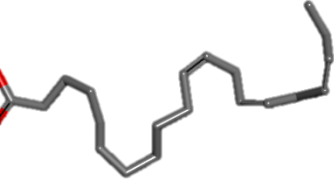
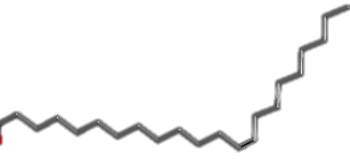
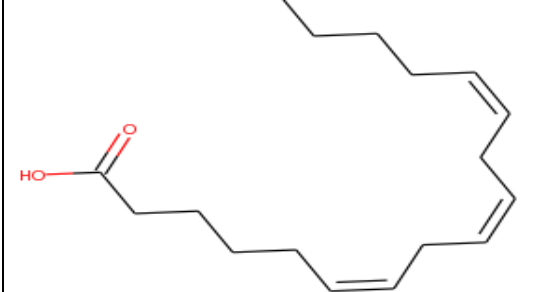
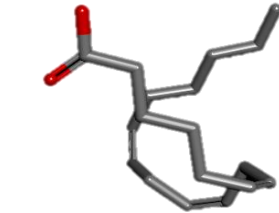
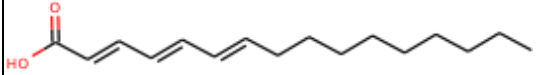
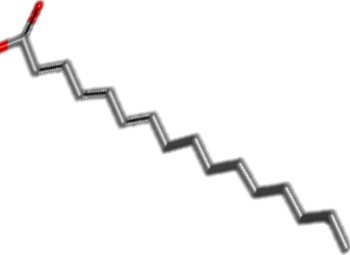
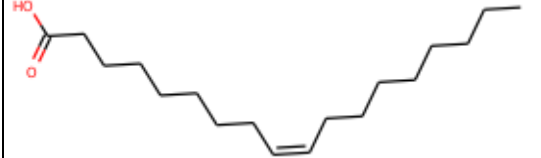
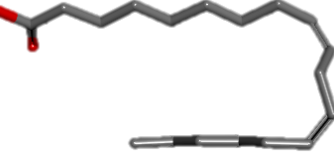
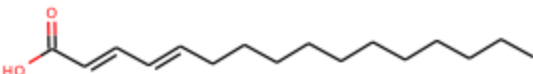
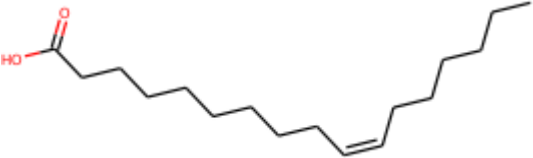
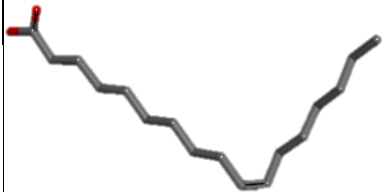
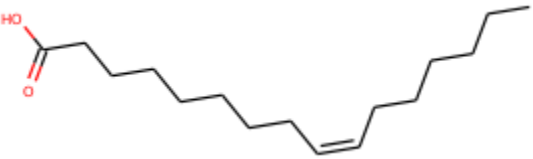
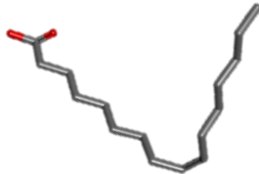
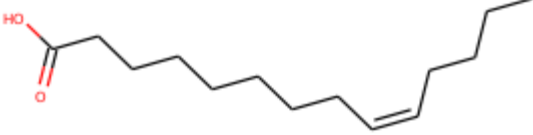
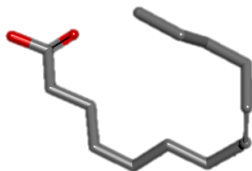


LAMPIRAN

Lampiran 1 15 senyawa uji asam lemak tak jenuh

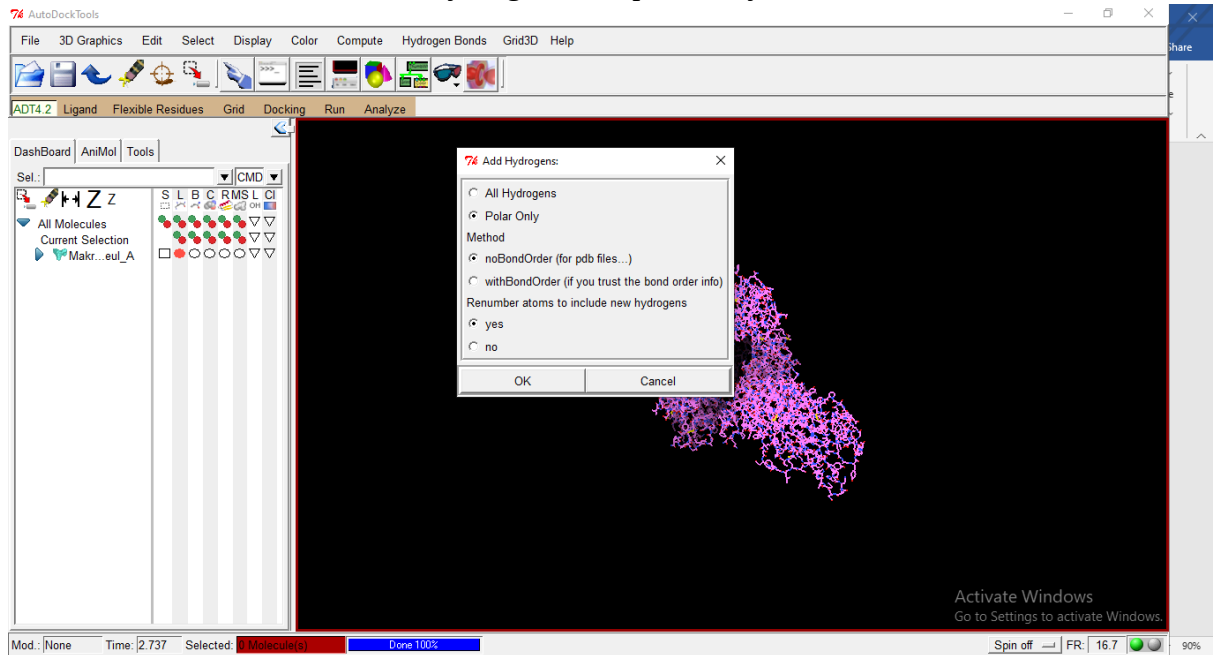
Struktur senyawa uji 2D dan 3D		
Nama Ligan	Struktur 2D	Struktur 3D
LU1 Docosahexaenoic acid		
LU2 Eicosapentaenoic acid		
LU3 Arachidonic acid		
LU4 alpha-linolenic acid		
LU5 Nervonic acid		

LU6 Elaidic Acid		
LU7 Eicosatrienoic acid		
LU8 Erucic acid		
LU9 Gamma linoleic acid		
LU10 Hexadecatrienoic acid		
LU11 Oleic acid		

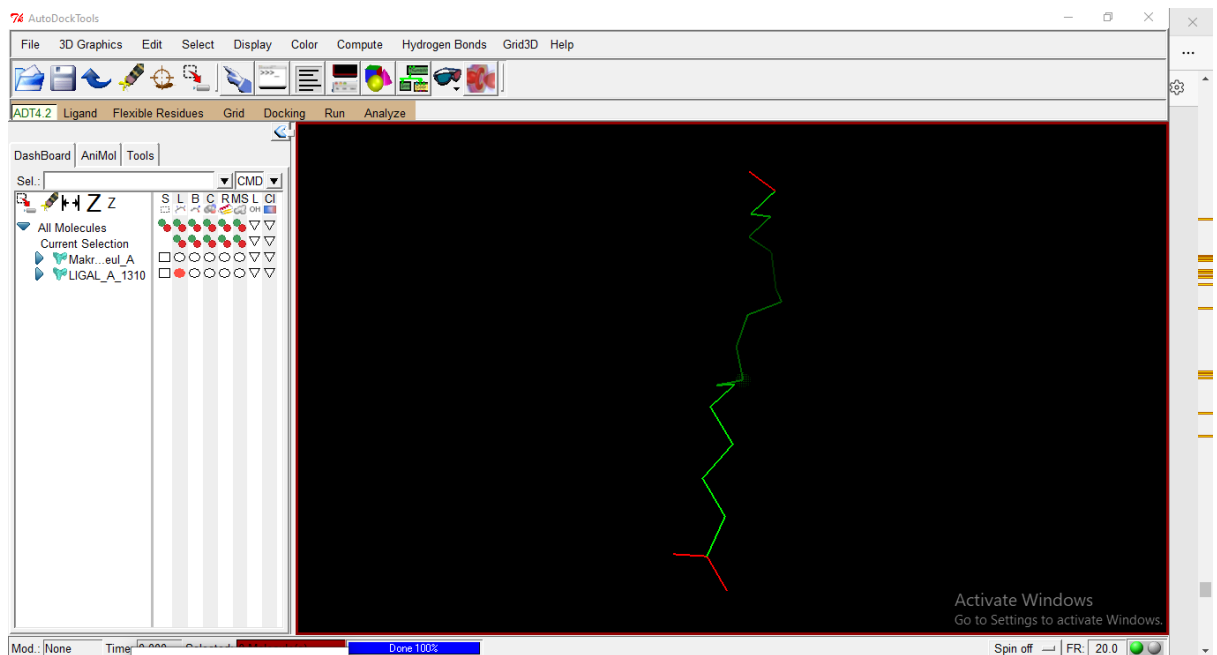
LU12 Hexadecadienoic acid		
LU13 Cis10 Heptadecenoic acid		
LU14 Palmitoleic Acid		
LU15 Myristoleic acid		

Lampiran 2 Prosedur penambatan molekul

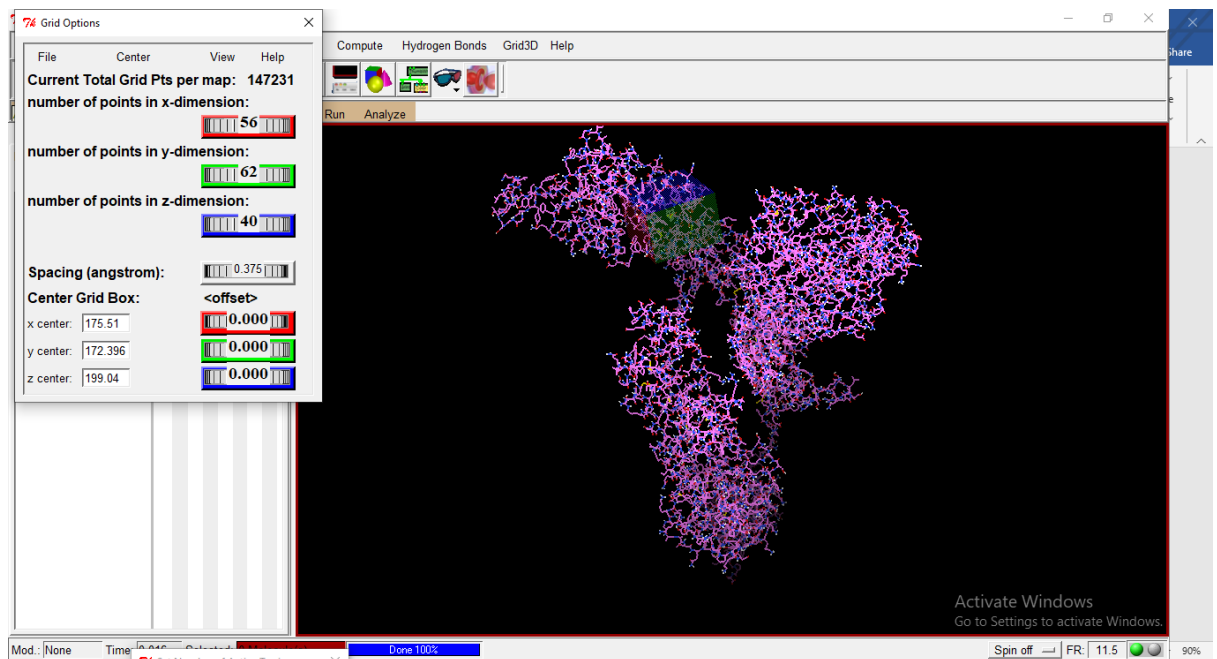
1. Add hydrogen bond polar only



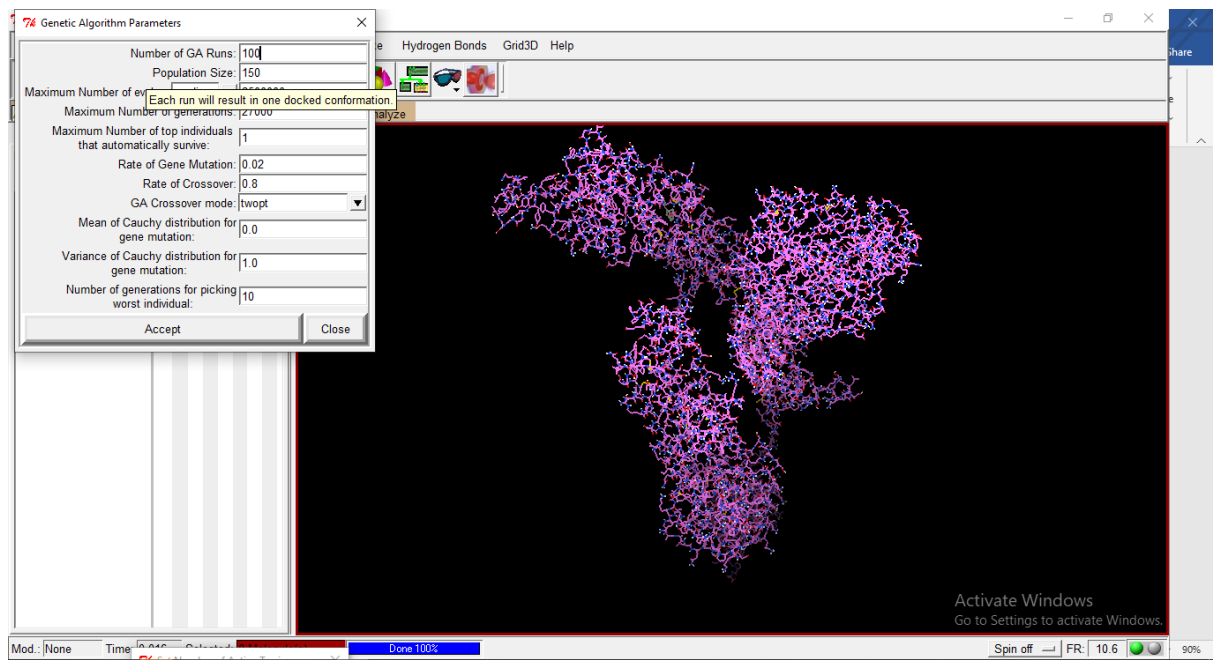
2. Set torsion root default



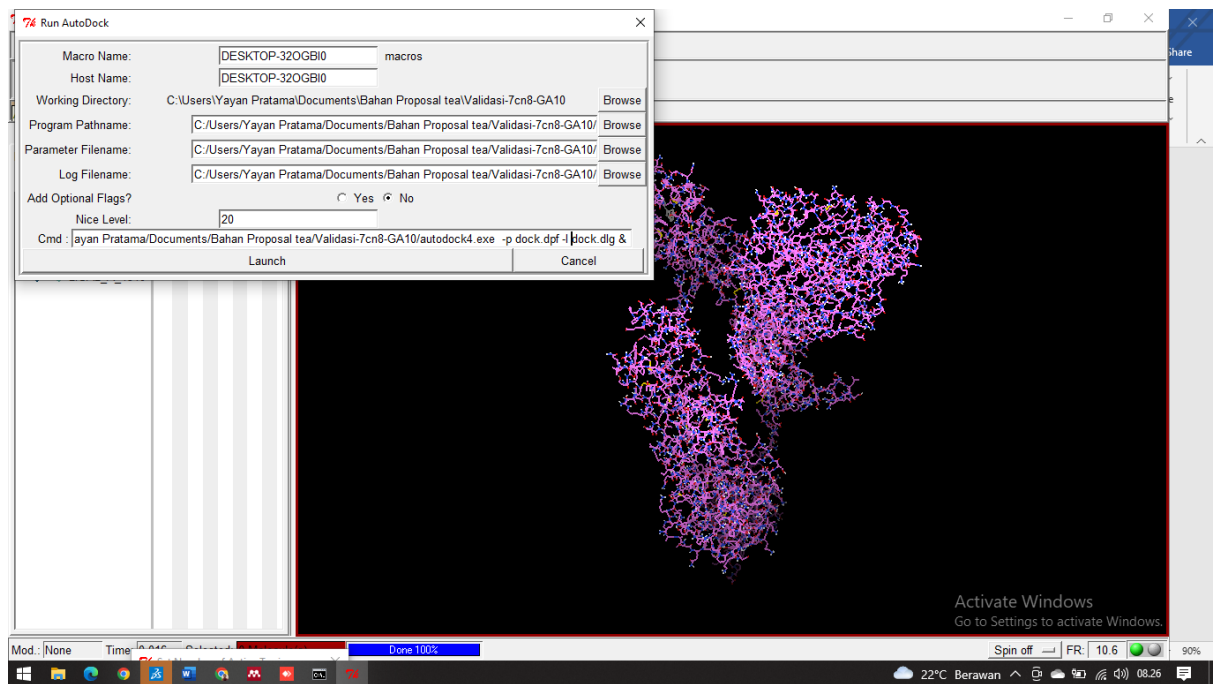
3. Set point & coordinate gridbox



4. Set parameter docking



5. Run autogrid & autodock



Lampiran 3 Prosedur dan script MD

1. Memperbaiki struktur protein

```
$ grep ATOM protein.pdb* > protein_rec.pdb*  
  
$ pdb4amber -i protein_rec.pdb --reduce -o protein_amber.pdb  
  
$ tleap  
  
$ source leaprc.protein.ff14SB  
  
$ x = loadpdb protein_amber.pdb  
  
$ savepdb x protein_fix.pdb  
  
$ quit  
  
*nama file protein
```

2. Ligand Parameterization

```
$ antechamber -i ligan.pdb* -fi pdb -o lig.mol2** -fo mol2 -c bcc -s 2  
  
$ parmchk2 -i lig.mol2** -f mol2 -o lig.frcmod  
  
$ tleap  
  
$ source leaprc.protein.ff14SB  
  
$ source leaprc.gaff2  
  
$ LIG = loadmol2 lig.mol2**  
  
$ loadamberparams lig.frcmod  
  
$ check LIG  
  
$ saveoff LIG LIG.lib  
  
$ saveamberparm LIG LIG.prmtop LIG.inpcrd  
  
$ quit  
  
*nama file ligan  
  
**tiga huruf ligan
```

3. Upload protein & ligan

```
$ tleap
```

```
$ source leaprc.protein.ff14SB
```

```
$ source leaprc.gaff2
```

```
$ loadoff LIG.lib
```

```
$ loadamberparams lig.frcmod
```

```
$ LIG = loadmol2 lig.mol2
```

```
$ PRO = loadpdb protein_fix.pdb
```

```
$ complex = combine {PRO LIG}
```

```
$ check complex
```

```
$ saveamberparm complex complex.prmtop complex.inpcrd
```

```
$ savepdb complex complex.pdb
```

4. Menyiapkan simulasi dinamika molekul

```
$ charge complex
```

```
$ source leaprc.water.tip3p
```

```
$ addions complex Na+ 0 (atau addions complex Cl- 0)
```

```
$ charge complex
```

```
$ solvatebox complex TIP3PBOX 10.0
```

```
$ check complex
```

```
$ saveamberparm complex solvated.prmtop solvated.inpcrd
```

```
$ savepdb complex solvated.pdb
```

```
$ quit
```

4. Minimization

```
$ sander -O -i min1.in -o min1.out -p solvated.prmtop -c solvated.inpcrd -x min1.crd -r  
min1.rst -ref solvated.inpcrd
```



```
$ sander -O -i min2.in -o min2.out -p solvated.prmtop -c min1.rst -x min2.crd -r min2.rst -ref min1.rst
```

```
$ sander -O -i min3.in -o min3.out -p solvated.prmtop -c min2.rst -x min3.crd -r min3.rst
```

5. Heating

```
$ pmemd.cuda -O -i heat1.in -o heat1.out -p solvated.prmtop -c min3.rst -x heat1.crd -r heat1.rst -ref min3.rst
```

```
$ pmemd.cuda -O -i heat2.in -o heat2.out -p solvated.prmtop -c heat1.rst -x heat2.crd -r heat2.rst -ref heat1.rst
```

```
$ pmemd.cuda -O -i heat3.in -o heat3.out -p solvated.prmtop -c heat2.rst -x heat3.crd -r heat3.rst -ref heat2.rst
```

6. Equilibration

```
$ mpiexec -n 4 pmemd.MPI -O -i eq1.in -o eq1.out -p solvated.prmtop -c heat3.rst -x eq1.crd -r eq1.rst -ref heat3.rst
```

```
$ pmemd.cuda -O -i eq2.in -o eq2.out -p solvated.prmtop -c eq1.rst -x eq2.crd -r eq2.rst -ref eq1.rst
```

```
$ pmemd.cuda -O -i eq3.in -o eq3.out -p solvated.prmtop -c eq2.rst -x eq3.crd -r eq3.rst
```

```
$ mkdir analysis
```

```
$ cd analysis
```

```
$ process_mdout.perl ../heat1.out ../heat2.out ../heat3.out ../eq1.out ../eq2.out ../eq3.out
```

```
$ xmgrace summary.ETOT summary.EPTOT summary.EKTOT
```

7. PRODUCTION

```
$ pmemd.cuda -O -i prod1.in -o prod1.out -p solvated.prmtop -c eq3.rst -x prod1.crd -r prod1.rst
```

8. TRAJECTORY ANALYSIS

```
$ cpptraj solvated.prmtop strip.in
```

```
$ cpptraj complex.prmtop rmsd.in
```

```
$ cpptraj complex.prmtop rmsf.in
```

```
$ xmgrace rms_pro.txt rms_lig.txt
```

```
$ xmgrace rmsf.out
```

9. MMGBSA

```
$ ante-MMPBSA.py -p solvated.prmtop -c complex2.prmtop -s '!:1-1125' -r PRO.prmtop -m
```

```
:1-1125 -l LIG.prmtop*
```

```
$ MMPBSA.py -O -i MM/GBSA.in -sp solvated.prmtop -cp complex.prmtop -rp PRO.prmtop  
-lp
```

```
LIG.prmtop* -y prod1.crd
```

Lampiran 4 hasil turnitin

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MOLEKULAR SENYAWA ASAM LEMAK TAK JENUH DARI
NAVICULA SALINICOLA TERHADAP TARGET PROTEIN SPIKE
DARI SARS-COV-2**

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Yayan Pratama
11181146

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NPM 11181146

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