NASKAH TUTORIAL

SIMULASI DINAMIKA MOLEKULER MENGGUNAKAN GROMACS

OLEH: APT. YENI, S.FARM., M.SI.
NIDN: 0308049102

FAKULTAS FARMASI DAN SAINS
PROGRAM STUDI FARMASI
UNIVERSITAS MUHAMMADIYAH PROF. DR. HAMKA
JAKARTA
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DOWNLOAD GROMACS

https://manual.gromacs.org/

Note:

- Gromacs merupakan aplikasi untuk ubuntu atau linux
- Pastikan pada ubuntu telah terhubung acpype, GPU, mmpbsa dan mmgbsa

FILE YANG HARUS DISIAPKAN

- Ligand.pdb
- Protein.pdb
- Hasil acepype ligand (ligand_GMX.gro dan ligand_GMX.itp dan ligand_bcc_gaff2.mol2)
- File mdp (1-5)
- File mmpbsa.in
- File mmgbsa.in

MDP1_IONS

```
; LINES STARTING WITH ';' ARE COMMENTS
title                    = Minimisasi ; Title of run

; The following lines tell the program the standard locations where to find certain files
cpp                      = /lib/cpp     ; Preprocessor
include                  = -I../top     ; Directories to include in the topology format

; Parameters describing what to do, when to stop and what to save
integrator     = steep                  ; Algorithm options
                                                ; steep = steepest descent minimization
                                                ; MD = Leap Frog algorith for integrating Newtonś equations of motion )
emtol                    = 50.0                 ; Stop minimization when the energy changes by less than emtol kJ/mol. 1000
nsteps                   = 500000       ; Maximum number of (minimization) steps to perform 1000
nstenergy      = 100                    ; Write energies to disk every nstenergy steps
nstxtcout      = 100                    ; Write coordinates to disk every nstxtcout steps
nstxout                  = 100

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions
cutoff-scheme            = Verlet
nstlist                  = 20                   ; Frequency to update the neighbor list and long range forces
ns_type                  = grid                 ; Method to determine neighbor list (simple, grid)
rlist                    = 1.4                  ; Cut-off for making neighbor list (short range forces)
coulombtype              = cut-off      ; Treatment of long range electrostatic interactions
rcoulomb       = 1.4                    ; long range electrostatic cut-off
rvdw                     = 1.4                  ; long range Van der Waals cut-off
constraints    = none                   ; Bond types to replace by constraints
pbc                      = xyz                  ; Periodic Boundary Conditions (yes/no)
```

MDP2_MINIM

```
; LINES STARTING WITH ';' ARE COMMENTS
title                    = Minimisasi ; Title of run

; The following lines tell the program the standard locations where to find certain files
cpp                      = /lib/cpp     ; Preprocessor
include                  = -I../top     ; Directories to include in the topology format

; Parameters describing what to do, when to stop and what to save
integrator     = steep                  ; Algorithm options
                                                ; steep = steepest descent minimization
                                                ; MD = Leap Frog algorith for integrating Newtonś equations of motion )
emtol                    = 100.0                ; Stop minimization when the energy changes by less than emtol kJ/mol. 1000
nsteps                   = 500000       ; Maximum number of (minimization) steps to perform 1000
nstenergy      = 100                    ; Write energies to disk every nstenergy steps
nstxtcout      = 100                    ; Write coordinates to disk every nstxtcout steps
nstxout                  = 100

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions
cutoff-scheme            = Verlet
nstlist                  = 20                   ; Frequency to update the neighbor list and long range forces
ns_type                  = grid                 ; Method to determine neighbor list (simple, grid)
rlist                    = 1.4                  ; Cut-off for making neighbor list (short range forces)
coulombtype              = cut-off      ; Treatment of long range electrostatic interactions
rcoulomb       = 1.4                    ; long range electrostatic cut-off
rvdw                     = 1.4                  ; long range Van der Waals cut-off
constraints    = none                   ; Bond types to replace by constraints
pbc                      = xyz                  ; Periodic Boundary Conditions (yes/no)
```

MDP3_NVT

```
title                    = NVT equilibration
define                   = -DPOSRES
; Run parameters
integrator       = md                    ; leap-frog integrator
nsteps                   = 250000        ; 2 * 250000 = 500 ps
dt                       = 0.002         ; 2 fs
; Output control
nstxout                  = 500           ; save coordinates every 1 ps
nstvout                  = 500           ; save velocities every 1 ps
nstfout                  = 500           ; save forces every 1 ps
nstxout-compressed = 1
compressed-x-grps  = Protein
nstenergy        = 100                   ; save energies every 0.2 ps
nstlog                   = 100           ; update log file every 0.2 ps
; Bond parameters
continuation     = no                    ; continue from short md run
constraint_algorithm = lincs             ; holonomic constraints
constraints      = all-bonds             ; all bonds (even heavy atom-H
bonds) constrained
lincs_iter       = 1                     ; accuracy of LINCS
lincs_order      = 4                     ; also related to accuracy
; Neighborsearching
ns_type                  = grid          ; search neighboring grid cells
nstlist                  = 40            ; 20/40 for GPU
rlist                    = 1.4           ; short-range neighborlist cutoff (in nm)
rcoulomb         = 1.4                   ; short-range electrostatic cutoff (in nm)
rvdw                     = 1.4           ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype      = PME                   ; Particle Mesh Ewald for long-range electrostatics
pme_order        = 4                     ; cubic interpolation
fourierspacing   = 0.16                  ; grid spacing for FFT
; Temperature coupling is on
tcoupl                   = V-rescale     ; modified Berendsen thermostat
tc-grps                  = Protein_UNL Water_and_ions                ; two coupling groups - more accurate
tau_t                    = 0.1           0.1             ; time constant, in ps
ref_t                    = 310           310             ; reference temperature, one for each group, in K
; Pressure coupling is off
pcoupl                   = no                            ; no pressure coupling in NVT
; Periodic boundary conditions
pbc                      = xyz                           ; 3-D PBC
; Dispersion correction
DispCorr         = EnerPres      ; account for cut-off vdW scheme
; Velocity generation
gen_vel                  = yes                           ; do not assign velocities
gen_seed     = -1
gen_temp     = 200
```

Suhu untuk simulasi 310 K ➔ Ssesuai suhu tubuh normal manusia

MDP4_NPT

```
title                    = minimization SIRT7m and NAM6
equilibration
define                   = -DPOSRES
; Run parameters
integrator     = md                    ; leap-frog integrator
nsteps                   = 250000      ; 2 * 250000 = 500 ps
dt                       = 0.002       ; 2 fs
; Output control
nstxout                  = 500         ; save coordinates every 1 ps
nstvout                  = 500         ; save velocities every 1 ps
nstxout-compressed = 100
;compressed-x-grps = DNA_LIG NA CL
nstenergy      = 100                   ; save energies every 0.2 ps
nstlog                   = 100         ; update log file every 0.2 ps
; Bond parameters
continuation= yes                      ; Restarting after NVT
constraint_algorithm = lincs           ; holonomic constraints
constraints    = all-bonds    ; all bonds (even heavy atom-H bonds)
constrained
lincs_iter     = 1                     ; accuracy of LINCS
lincs_order    = 4                     ; also related to accuracy
; Neighborsearching
cutoff-scheme            = Verlet      ; use Verlet to enable GPU
ns_type                  = grid        ; search neighboring grid cells
nstlist                  = 20          ; 40 fs
rlist                    = 1.4         ; short-range neighborlist cutoff (in nm)
rcoulomb       = 1.4                   ; short-range electrostatic cutoff (in nm)
rvdw                     = 1.4         ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype    = PME                   ; Particle Mesh Ewald for long-range electrostatics
pme_order      = 4                     ; cubic interpolation
fourierspacing  = 0.16                 ; grid spacing for FFT
; Temperature coupling is on
tcoupl                   = V-rescale   ; modified Berendsen thermostat
tc-grps                  = Protein_UNL Water_and_ions          ; two coupling groups - more
accurate
tau_t                    = 0.1         0.1          ; time constant, in ps
ref_t                    = 310         310          ; reference temperature, one for each group, in K
; Pressure coupling is on
pcoupl                   = Parrinello-Rahman          ; Pressure coupling on in NPT
pcoupltype     = isotropic   ; uniform scaling of box vectors
tau_p                    = 2.0                        ; time constant, in ps
ref_p                    = 1.0                        ; reference pressure, in bar
compressibility = 4.5e-5       ; isothermal compressibility of water, bar^-1
refcoord_scaling = com
; Periodic boundary conditions
pbc                      = xyz                        ; 3-D PBC
; Dispersion correction
DispCorr       = EnerPres      ; account for cut-off vdW scheme
; Velocity generation
gen_vel                  = no                         ; Velocity generation is off
```

MDP5_PRODUKSI

```
title                    =
; Run parameters
integrator       = md                    ; leap-frog integrator
nsteps                   = 100000000     ; 2 * 100000000 = 200000 ps = 200 ns
dt                       = 0.002         ; 2 fs
; Output control
nstxout                  = 5000          ; save coordinates every 10 ps
nstvout                  = 5000          ; save velocities every 10 ps
nstxout-compressed = 5000
;compressed-x-grps = Protein_UNL Water_and_ions
nstenergy        = 5000                  ; save energies every 10 ps
nstlog                   = 5000          ; update log file every 10 ps
; Bond parameters
continuation     = yes                   ; Restarting after NPT
constraint_algorithm = lincs    ; holonomic constraints
constraints      = all-bonds     ; all bonds (even heavy atom-H bonds) constrained
lincs_iter       = 1                     ; accuracy of LINCS
lincs_order      = 4                     ; also related to accuracy
; Neighborsearching
cutoff-scheme    = Verlet        ; use Verlet to enable GPU
ns_type                  = grid          ; search neighboring grid cells
nstlist                  = 20            ; 40 fs
rlist                    = 1.4           ; short-range neighborlist cutoff (in nm)
rcoulomb         = 1.4                   ; short-range electrostatic cutoff (in nm)
rvdw                     = 1.4           ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype      = PME           ; Particle Mesh Ewald for long-range electrostatics
pme_order        = 4                     ; cubic interpolation
fourierspacing   = 0.12          ; grid spacing for FFT
; Temperature coupling is on
tcoupl                   = V-rescale     ; modified Berendsen thermostat
tc-grps                  = Protein_UNL Water_and_ions            ; two coupling groups - more accurate
tau_t                    = 0.1           0.1             ; time constant, in ps
ref_t                    = 310           310             ; reference temperature, one for each group, in K
; Pressure coupling is on
pcoupl                   = Parrinello-Rahman             ; Pressure coupling on in NPT
pcoupltype       = isotropic     ; uniform scaling of box vectors
tau_p                    = 2.0                           ; time constant, in ps
ref_p                    = 1.0                           ; reference pressure, in bar
compressibility = 4.5e-5         ; isothermal compressibility of water, bar^-1
refcoord_scaling = com
; Periodic boundary conditions
pbc                      = xyz                   ; 3-D PBC
; Dispersion correction
DispCorr         = EnerPres      ; account for cut-off vdW scheme
; Velocity generation
gen_vel                  = no                    ; Velocity generation is off
```

Waktu simulasi MD 200 ns
dengan suhu 310 K

MMPBSA.IN

Sample input file for decomposition analysis
Make sure to include at least one residue from both the receptor and ligand in the print_res mask of the &decomp section. http://archive.ambermd.org/201308/0075.html. This is automally guaranteed when using "within" keyword.

```
&general
startframe=19001, endframe=20000, interval=5,
temperature=310
forcefields="oldff/leaprc.ff99SB,leaprc.gaff2"
/

&pb
istrng=0.15, inp=1, fillratio=4.0,
/
```

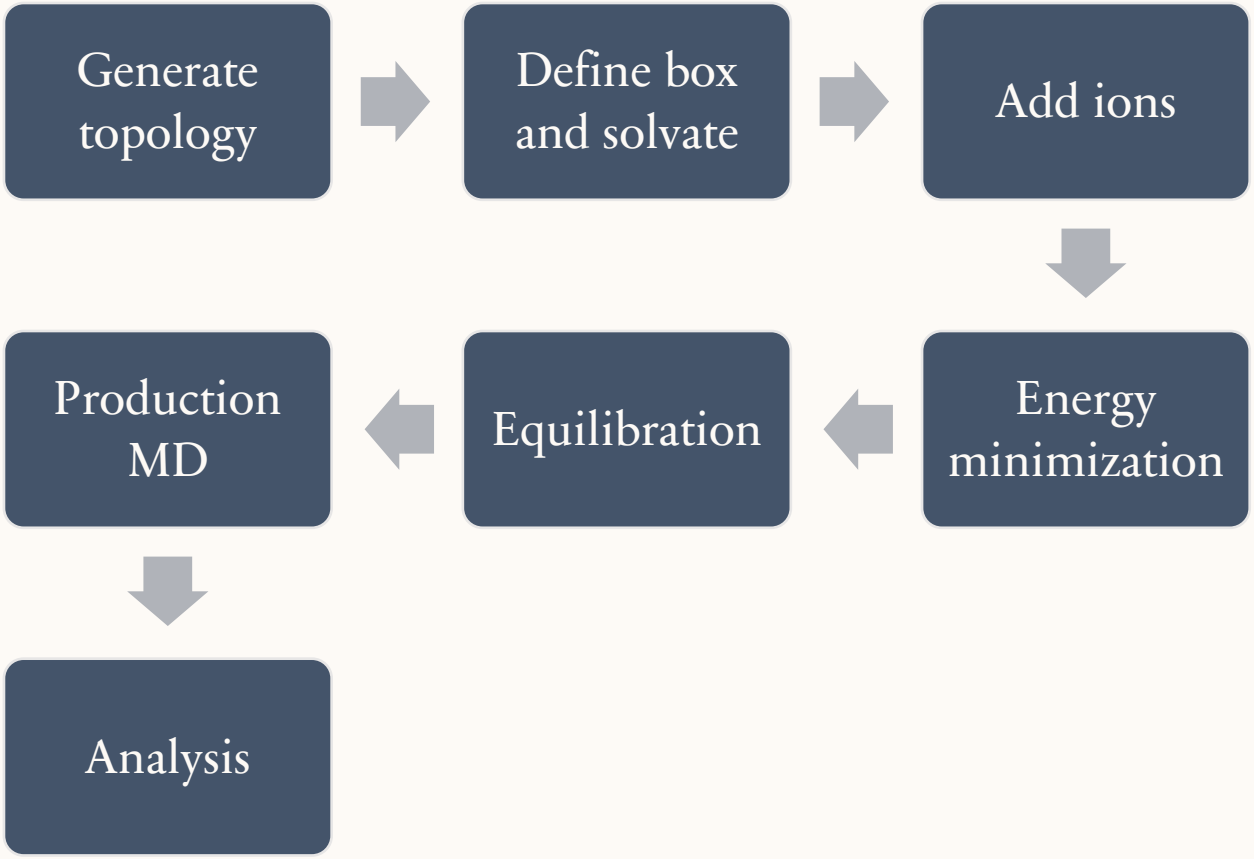
Perhitungan mmpbsa untuk 10 ns terakhir simulasi MD, suhu 310 K

MMGBSA.IN

```
#Molecular Mechanics Generalized Born Surface Area (MM-GBSA)
Sample input file for GB calculation
#This input file is meant to show only that gmx_MMPBSA works. Although,
we tried to use the input files as recommended in the
#Amber manual, some parameters have been changed to perform more
expensive calculations in a reasonable amount of time. Feel free to change
the parameters
#according to what is better for your system.
&general
sys_name="Prot-Lig-ST",
startframe=19001, endframe=20000, interval=5,
temperature=310
forcefields="oldff/leaprc.ff99SB,leaprc.gaff2"
/
&gb
igb=5, saltcon=0.150,
/
&decomp
idecomp=2, dec_verbose=3,
# This will print all residues that are less than 4 Å between
# the receptor and the ligand
print_res="within 4"
/
```

Perhitungan mmpbsa untuk 10 ns terakhir simulasi MD, suhu 310 K

TAHAP SIMULASI DINAMIKA MOLEKULER MENGGUNAKAN GROMACS



GENERATE TOPOLOGY

- Untuk membuat topologi ligan digunakan aplikasi di luar Gromacs bergantung force field yang digunakan.
- Pada tutorial ini digunakan force field amber dengan pembuatan topologi ligan menggunakan acpype
- Buka terminal folder kerja yang telah berisi file yang dibutuhkan (klik kanan pada folder kerja ➔ open terminal)
- Ketik perintah pada terminal tersebut sesuai tahap simulasi MD
- Setelah mengetik setiap perintah, tekan enter

AMBER	**Antechamber** **acpype**	Parametrizes molecules using GAFF A Python interface to Antechamber, writes GROMACS topologies
CHARMM	**CGenFF**	The official CHARMM General Force Field server
GROMOS87/GROMOS96	**PRODRG 2.5** **ATB**	An automated server for topology generation A newer server for topology generation, uses GROMOS96 54A7
OPLS-AA	**LigParGen**	A server from the Jorgensen group to produce OPLS topologies

GENERATE TOPOLOGY

conda activate
acpype -i ligand.pdb -n 1 (total charge of your molecule, for example:1 /0 /2)

conda deactivate
gmx pdb2gmx -f protein.pdb -o protein.gro atau gmx pdb2gmx -f protein.pdb -o protein.gro -ignh
pilih 6 AMBER99SB-ILDN protein, nucleic AMBER94 (Lindorff-Larsen et al., Proteins 78, 1950-58, 2010)
Select the Water Model:1: TIP3P

Buat complex.gro (copy protein.gro dahulu, ubah namanya menjadi complex.gro, gabungkan dengan ligand.gro)
Buat gabungan topologi di topol.top
; Include forcefield parameters
#include "amber99sb-ildn.ff/forcefield.itp"

; Include ligand topology
#include "ligand_GMX.itp"

[molecules]
; Compound #mols
Protein_chain_A 1
UNL 1

Ubah ligand_GMX.itp
[moleculetype]
;name nrexcl
UNL 3

protein.gro

```
5648    352SER     HB2 5646   6.963   7.955   7.467
5649    352SER      OG 5647   7.009   8.154   7.462
5650    352SER      HG 5648   6.977   8.186   7.549
5651    352SER       C 5649   7.200   7.834   7.431
5652    352SER     OC1 5650   7.226   7.816   7.526
5653    352SER     OC2 5651   7.199   7.739   7.353
5654     6.06870   4.43590   7.02300
```

complex.gro

```
Georgetown Riga Oslo Madrid Amsterdam Chisinau Stockholm
 5686
    1MET      N    1   7.034   6.309   7.093
    1MET     H1    2   6.941   6.344   7.091
    1MET     H2    3   7.058   6.284   7.187
    1MET     H3    4   7.097   6.380   7.061
    1MET     CA    5   7.044   6.196   7.011
  352SER     HG 5648   6.977   8.186   7.549
  352SER      C 5649   7.200   7.834   7.431
  352SER    OC1 5650   7.226   7.816   7.526
  352SER    OC2 5651   7.199   7.739   7.353
    1  UNL     N    1   7.745   7.251   5.844
    1  UNL    N1    2   7.759   7.305   5.964
    1  UNL     C    3   7.709   7.215   6.051
    1  UNL    N2    4   7.664   7.104   5.989
    1  UNL   C22   32   7.642   7.552   5.768
    1  UNL    N3   33   7.658   7.041   5.754
    1  UNL     H   34   7.713   7.044   5.667
    1  UNL    H1   35   7.581   6.973   5.762
  6.06870   4.43590   7.02300
```

DEFINE BOX AND SOLVATE

```
gmx editconf -f complex.gro -o box.gro -bt cubic -c -d 1.0
gmx solvate -cp box.gro -cs spc216.gro -p topol.top -o solv.gro
```

ADD IONS

gmx grompp -f mdp1_ions.mdp -c solv.gro -p topol.top -o mdp1_ions.tpr

gmx genion -s mdp1_ions.tpr -o solvions.gro -p topol.top -neutral -conc 0.15

pilih SOL (15)

ENERGY MINIMIZATION

gmx grompp -f mdp2_minim.mdp -c solvions.gro -p topol.top -o mdp2_minim.tpr
gmx mdrun -v -s mdp2_minim.tpr -deffnm minim -nb gpu
gmx energy -f minim.edr -o potential.xvg
Pilih potential (9 0)/ bisa beda untuk tiap versi Gromacs

xmgrace potential.xvg (pada terminal baru untuk melihat grafik hasil minimisasi energi)
gmx genrestr -f ligand_GMX.gro -o posre_ligand.itp
pilih UNL/LIGAND (2)

ubah topol.top
; Include forcefield parameters
#include "amber99sb-ildn.ff/forcefield.itp“

; Include ligand topology
#include "ligand_GMX.itp“

; Ligand position restraints
#ifdef POSRES
#include "posre_ligand.itp“
#endif

gmx make_ndx -f minim.gro -o index.ndx
> 1 | 13
> q

EQUILIBRATION

gmx grompp -f mdp3_nvt.mdp -c minim.gro -p topol.top -n index.ndx -o mdp3_nvt.tpr -r minim.gro
gmx mdrun -v -s mdp3_nvt.tpr -deffnm nvt -nb gpu
gmx energy -f nvt.edr -o temp.xvg
pilih temperature (15 0)
xmgrace temp.xvg (pada terminal baru untuk melihat grafik hasil ekuilibrasi suhu)

gmx grompp -f mdp4_npt.mdp -c nvt.gro -p topol.top -n index.ndx -o mdp4_npt.tpr -r nvt.gro
gmx mdrun -v -s mdp4_npt.tpr -deffnm npt -nb gpu
gmx energy -f npt.edr -o pressure.xvg
pilih pressure (17 0)
xmgrace pressure.xvg (pada terminal baru untuk melihat grafik hasil ekuilibrasi tekanan)

PRODUCTION MD

gmx grompp -f mdp5_produksi.mdp -c npt.gro -t npt.cpt -p topol.top -n index.ndx -o mdp5_produksi.tpr

gmx mdrun -v -s mdp5_produksi.tpr -deffnm produksi -nb gpu

catatan: cara ubah waktu simulasi ➔ ubah file mdp5_produksi di nstepnya

nsteps = 25000000 ; 2 * 25000000 = 50000 ps = 50 ns

dt = 0.002 ; 2 fs

Cara melanjutkan md yang awalnya 50 ns (penambahan 50 ns hingga 200 ns, yang tertera setelah extend dalam ps)

Optional

gmx convert-tpr -s mdp5_produksi.tpr -o md2.tpr -extend 50000
gmx mdrun -v -s md2.tpr -deffnm md2 -nb gpu
gmx convert-tpr -s md2.tpr -o md3.tpr -extend 50000
gmx mdrun -v -s md3.tpr -deffnm md3 -nb gpu
gmx convert-tpr -s md3.tpr -o md4.tpr -extend 50000
gmx mdrun -v -s md4.tpr -deffnm md4 -nb gpu

Gabungkan file xtc (jika dibuat potongan waktu)
gmx trjcat -f md1.xtc md2.xtc md3.xtc md4.xtc -o produksi.xtc

ANALYSIS

Buat file trajectory untuk visualisasi (we use trjconv to convert the output trajectory to remove periodic boundaries)

gmx make_ndx -f produksi.gro -o new_index.ndx
> 1| 13
> q

gmx trjconv -s mdp5_produksi.tpr -f produksi.xtc -o md_200ns_center.xtc -pbc mol -center -n new_index.ndx -ur compact (pilih 1 protein, kemudian 0 system) Choose "Protein" for centering and "System" for output.

gmx trjconv -pbc nojump -s mdp5_produksi.tpr -f md_200ns_center.xtc -o md_200ns_nojump.xtc (pilih 0 system) "System" for output (cek apakah protein dan ligan terpisah)

gmx trjconv -fit rot+trans -s mdp5_produksi.tpr -f md_200ns_nojump.xtc -o md_200ns_fit.xtc (pilih 4 Backbone, kemudian 0 system) Choose "Backbone" to perform least-squares fitting to the protein backbone, and "System" for output.

ANALYSIS

Untuk melihat perubahan tiap ns

gmx trjconv -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o 0ns.pdb -dump 0 (0 ns) pilih 0 = system

gmx trjconv -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o 25ns.pdb -dump 25000 (25 ns) 0 = system

gmx trjconv -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o 50ns.pdb -dump 50000 (50 ns) 0 = system

gmx trjconv -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o 200ns.pdb -dump 200000 (200 ns) 0 = system

PARAMETER

1. RMSD

gmx rms -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o rmsd.xvg -tu ns (pilih "backbone" 4 kemudian 4 lagi)
xmgrace rmsd.xvg

2. RMSF

gmx rmsf -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o rmsf.xvg (pilih "backbone" 4)
xmgrace rmsf.xvg

3. RADIUS GYRATION/rg

gmx gyrate -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o rg.xvg (Pilih group 1 (Protein) untuk analisis)
xmgrace rg.xvg

4. MINIMUM RESIDU DISTANCE OVERTIME

mdmat monitor the minimum distances between amino acid residues within a (protein) molecule)
gmx mdmat -s mdp5_produksi.tpr -f md_200ns_fit.xtc -mean dm.xpm -no mdmat.xvg (pilih protein 1)
xmgrace mdmat.xvg

gmx mindist computes the distance between one group and a number of other groups
gmx mindist -s mdp5_produksi.tpr -f md_200ns_fit.xtc -od mindist.xvg (pilih ligand 13 kemudian protein 1)
xmgrace mindist.xvg

5. PERUBAHAN STRUKTUR SEKUNDER SELAMA RUN

gmx do_dssp -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o dssp.xpm -sc scount.xvg

PARAMETER

6. RDF (RADIAL DISTRIBUTION FUNCTION) (calculate the rdf of protein in my system) distribusi air (sel) di sekitar protein/ligand (ref)---> protein-water/ ligand-water

gmx rdf -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o rdf_protein.xvg (pilih ref protein 116 kemudian sel water 16)----> ctrl+d
xmgrace rdf_protein.xvg

gmx rdf -s mdp5_produksi.tpr -f md_200ns_fit.xtc -o rdf_ligand.xvg (pilih ref ligand 13 kemudian sel water 16)
xmgrace rdf_ligand.xvg

7. HYDROGEN BOND

gmx hbond -s mdp5_produksi.tpr -f md_200ns_fit.xtc -ac hbond.xvg (pilih protein 1 kemudian ligand 13)
xmgrace hbond.xvg
xmgrace hbnum.xvg

8. SASA (SOLVENT ACCESSIBLE SURFACE AREA)

gmx sasa -s mdp5_produksi.tpr -f md_200ns_fit.xtc -tu ns -o sasa.xvg (pilih protein 1)
xmgrace sasa.xvg

9. Energi

gmx energy -f produksi.edr -o potential.xvg (pilih 10 0)
xmgrace potential.xvg

gmx energy -f produksi.edr -o kinetik.xvg (pilih 11 0)
xmgrace kinetik.xvg

gmx energy -f produksi.edr -o total.xvg (pilih 12 0)
xmgrace total.xvg

PARAMETER

10. MMPBSA

Perhatikan mmpbsa.in

startframe=19001, endframe=20000, interval=5 (minimal buat 1000 frame terakhir/10 ns terakhir) ➔ 100 frame untuk 1 ns, frame = nsteps:nstxout di file mdp5_produksi, jumlah frame dapat dilihat saat pembuatan trajectory

conda activate gmxMMPBSA
gmx_MMPBSA -O -i mmpbsa.in -cs mdp5_produksi.tpr -ci new_index.ndx -cg 1 13 -ct md_200ns_fit.xtc -lm ligand_bcc_gaff2.mol2
gmx_MMPBSA_ana

Lihat hasil di FINAL_RESULTS_MMPBSA.dat pada total energi

11. MMGBSA

gmx_MMPBSA -O -i mmgbsa.in -cs mdp5_produksi.tpr -ci new_index.ndx -cg 1 13 -ct md_200ns_fit.xtc -lm ligand_bcc_gaff2.mol2

PERINTAH LAINNYA

Ubah .gro ke .pdb

gmx editconf -f produksi.gro -o produksi.pdb

Ubah xpm ke xvg

gmx xpm2ps -f file.xpm -o file.xvg

Mengubah ps ke ns di sumbu x pada grafik RMSD atau lainnya (nama grafik disesuaikan)

xmgrace rmsd.xvg X=X/1000 ---> save

Mengubah nm ke angstrom

xmgrace rmsd.xvg Y=Y*10 ---> save

Kombinasi xmgrace (nama grafik yang akan digabung disesuaikan)

rmsd_lit927_1.xvg rmsd_lit927_2.xvg rmsd_54_1.xvg rmsd_54_2.xvg rmsd_57_1.xvg rmsd_57_2.xvg

xmgrace rg_lit927_1.xvg rg_lit927_2.xvg rg_54_1.xvg rg_54_2.xvg rg_57_1.xvg rg_57_2.xvg

xmgrace rmsf_lit927_1.xvg rmsf_lit927_2.xvg rmsf_54_1.xvg rmsf_54_2.xvg rmsf_57_1.xvg rmsf_57_2.xvg

xmgrace sasa_lit927_1.xvg sasa_lit927_2.xvg sasa_54_1.xvg sasa_54_2.xvg sasa_57_1.xvg sasa_57_2.xvg

xmgrace hbnum_lit927_1.xvg hbnum_lit927_2.xvg hbnum_54_1.xvg hbnum_54_2.xvg hbnum_57_1.xvg hbnum_57_2.xvg

Mengubah legenda di xmgrace

Double klik pada kurva --> grace: set appearance --> select set --> beri label/nama pada kolom string

Memindahkan legend box

ctrl + L + klik mouse kiri --> drag --> klik mouse kanan

THANK YOU