LAMPIRAN

Lampiran 1. Hasil Data Reseptor Target pada Obat

Nama obat	Common name	Probability
Atorvastatin	FUCA1	0,048952898
	GBA	0,048952898
	PNP	0,048952898
	MTAP	0,048952898
	PYGL	0,048952898
	MAN1B1	0,048952898
	DPP4	0,048952898
	MAN2B1	0,048952898
	UGCG	0,048952898
	GAA	0,048952898
	GBA2	0,048952898
	PIM1	0,048952898
	GLB1	0,048952898
	CDC7	0,048952898
	MGAM	0,048952898
	SI	0,048952898
	CDC25C	0,048952898
	ADRB2	0,048952898
	HTR2A	0,048952898
	MAN2A1	0,048952898
	ANPEP	0,048952898
	AMD1	0,048952898
	GSR	0,048952898
	PRKCI	0,048952898
	YARS	0,048952898
	NOS1	0,048952898
	NOS3	0,048952898
	EGFR	0,048952898
Rosuvastatin	PDE6D	0,998137005
	HMGCR	0,998137005
	HDAC6	0,150917042
	HDAC2	0,150917042

HDAC1	0,150917042
CASP3	0,100634432
CASP7	0,100634432
CASP1	0,100634432
TBXAS1	0,100634432
GSK3B	0,100634432
GSK3A	0,100634432
CASP8	0,100634432
CTSA	0,100634432
PTGER1	0,100634432
PTGER4	0,100634432
SLC5A2	0,100634432
TBXA2R	0,100634432
PTGER2	0,100634432
P2RY12	0,100634432
PDE5A	0,100634432
MME	0,100634432
ECE1	0,100634432
PPARG	0,100634432
NR3C1	0,100634432
MAPK14	0,100634432
MAPK10	0,100634432
EGLN1	0,100634432
IMPDH1	0,100634432
IMPDH2	0,100634432
LTB4R	0,100634432
ITGB7 ITGA4	0,100634432
PTGIR	0,100634432
CYP2C9	0,100634432
PTGDR	0,100634432
AURKA	0,100634432
PTGIS	0,100634432
GALK1	0,100634432
PGR	0,100634432
ITGB1 ITGA4	0,100634432
PTGER3	0,100634432
FNTA FNTB	0,100634432

THRA	0,100634432
THRB	0,100634432
CCKBR	0,100634432
EDNRB	0,100634432
ACE	0,100634432
EDNRA	0,100634432
SYK	0,100634432
HSD17B2	0,100634432
SIRT1	0,100634432
MMP1	0,100634432
AMPD3	0,100634432
MMEL1	0,100634432
FOLH1	0,100634432
EGFR	0,100634432
PARP1	0,100634432
HSP90AB1	0,100634432
IKBKB	0,100634432
CPA1	0,100634432
SRC	0,100634432
MMP8	0,100634432
TYMS	0,100634432
PTGFR	0,100634432
REN	0,100634432
SLC10A2	0,100634432
INSR	0,100634432
CCNE2 CDK2 CCNE1	0,100634432
CCNB3 CDK1 CCNB1	0,100634432
CCNB2	0,100634432
CDK2 CCNA1 CCNA2	0,100634432
NTRK1	0,100634432
CDK2	0,100634432
CDK1	0,100634432
MAPK3	0,100634432
CDK5	0,100634432
NTRK2	0,100634432
TOP1	0,100634432
OPRD1	0,100634432

	MMP9	0,100634432
	MMP2	0,100634432
	AKR1B1	0,100634432
	ITGAV ITGB3	0,100634432
	ITGA2B ITGB3	0,100634432
	OPRM1	0,100634432
	PPARD	0,100634432
	CMA1	0,100634432
	CASP2	0,100634432
	ITGB5 ITGAV	0,100634432
	ITGAV ITGB6	0,100634432
	SOAT1	0,100634432
	MMP13	0,100634432
	DPP4	0,100634432
	ITK	0,100634432
	CASP6	0,100634432
	CSNK2A1	0,100634432
	ADAM17	0,100634432
	CYP26A1	0,100634432
	BTK	0,100634432
	DGAT1	0,100634432
	TNF	0,100634432
	MMP16	0,100634432
Niasin	HCAR2	0,999487275
	DDO	0,054487947
	SIRT3	0,03397069
	SIRT2	0,03397069
	SLC22A6	0,023832743
	FYN	0,023832743
Gemfibrozil	TTR	0,935895337
	FABP1	0,935895337
	SLC22A12	0,053556076
	FABP4	0,053556076
	FABP5	0,053556076
	PPARA	0,053556076
	TBXA2R	0,053556076
	BMP1	0,053556076

PTGER4	0,053556076
PTGIR	0,053556076
AKR1C1	0,053556076
TBXAS1	0,053556076
CMA1	0,053556076
CXCL8	0,053556076
NOS2	0,053556076
AKR1C2	0,053556076
AKR1B10	0,053556076
ABAT	0,053556076
MAPK14	0,053556076
MAPK1	0,053556076
MMP12	0,053556076
TOP1	0,053556076
ACE	0,053556076
MDM2	0,053556076
CSNK2A1	0,053556076
AKR1A1	0,053556076
MIF	0,053556076
CA1	0,053556076
CA12	0,053556076
CA9	0,053556076
PTGER1	0,053556076
PTGER3	0,053556076
PTGDR	0,053556076
FFAR4	0,053556076
FABP3	0,053556076
GSR	0,053556076
CTSG	0,053556076
SRD5A1	0,053556076
SRD5A2	0,053556076
PTGES2	0,053556076
MME	0,053556076
CSNK2A2	0,053556076
BCL2	0,053556076
SLC22A6	0,053556076
BCL2L1	0,053556076

	ECE1	0,053556076
	SLC16A1	0,053556076
	PDPK1	0,053556076
	ALOX5AP	0,053556076
	KDM2B	0,053556076
	KDM4C	0,053556076
	PIN1	0,053556076
	BAD	0,053556076
	DHODH	0,053556076
	RXRA	0,053556076
	AGTR1	0,053556076
	GLO1	0,053556076
	CCR2	0,053556076
	HNF4A	0,053556076
	KMO	0,053556076
	MARS	0,053556076
	ADAMTS5	0,053556076
	CCKAR	0,053556076
	PSEN2 PSENEN NCSTN APH1A	0,053556076
	PSEN1 APH1B	0,053556076
	PDE10A	0,053556076
	AGTR2	0,053556076
	DUSP3	0,053556076
	DAGLA	0,053556076
	PPARG	0,053556076
	PFKFB3	0,053556076
	BCAT2	0,053556076
	PIK3CA	0,053556076
	MAP3K8	0,053556076
	BRD4	0,053556076
	CTSA	0,053556076
	VCP	0,053556076
	PTPN22	0,053556076
	PLA2G2A	0,053556076
	RPA1	0,053556076
	AKR1C4	0,053556076
	KDM6B	0,053556076

	NR3C2	0,053556076
	PGR	0,053556076
	CPA1	0,053556076
	FNTA FNTB	0,053556076
	ITGB1 ITGA2	0,053556076
	ACE2	0,053556076
	CHRM1	0,053556076
	EPRS	0,053556076
	PTGFR	0,053556076
	KDM5C	0,053556076
	CPB1	0,053556076
	CPB2	0,053556076
	NTSR1	0,053556076
	CD38	0,053556076
	RHOA	0,053556076
	DYRK2	0,053556076
	PIM2	0,053556076
	MKNK1	0,053556076
	CAMKK1	0,053556076
Bezafibrate	PPARA	1
	PTGIR	0,10560828
	PTGDR2	0,097239989
	CSNK2A1	0,097239989
	PTPRF	0,097239989
	CTSA	0,097239989
	MTNR1A	0,097239989
	DHODH	0,097239989
	MMP2	0,097239989
	LDHA	0,097239989
	ITGA2B ITGB3	0,097239989
	FLT1	0,097239989
	PDGFRB	0,097239989
	NR1H4	0,097239989
	FGFR1	0,097239989
	AURKC	0,097239989
	NQO2	0,097239989
	DUSP26	0,097239989

	LDHB	0,097239989
	PIM1	0,097239989
	PIM2	0,097239989
	SERPINE1	0,097239989
	MMP14	0,097239989
	VCP	0,097239989
	FNTA FNTB	0,097239989
	CPB1	0,097239989
	NTRK1	0,097239989
	PPARG	0,097239989
	PLA2G1B	0,097239989
	PDE10A	0,097239989
	TNNC1 TNNT2 TNNI3	0,097239989
	PTPN22	0,097239989
	HCAR2	0,097239989
	CHEK1	0,097239989
	KDM6B	0,097239989
	NEK2	0,097239989
	ALOX5AP	0,097239989
	SCN10A	0,097239989
	GPR35	0,097239989
	RPA1	0,097239989
	CCKAR	0,097239989
	MPO	0,097239989
	TGFBR1	0,097239989
	ITGB1 ITGA4	0,097239989
	IKBKB	0,097239989
	PIK3CB	0,097239989
	PIK3CA	0,097239989
	LIPG	0,097239989
	CSF1R	0,097239989
	FABP4	0,097239989
	PFKFB3	0,097239989
	FABP3	0,097239989
	FFAR1	0,097239989
	WEE1	0,097239989
	PDE3A	0,097239989

MTOR	0,097239989
PDE7A	0,097239989
MAP3K8	0,097239989
CCNE2 CDK2 CCNE1	0,097239989
CCNB3 CDK1 CCNB1	0,097239989
CCNB2	0,097239989
CHUK	0,097239989
PPARD	0,097239989
ITGB7 ITGA4	0,097239989
PRKAG1 PRKAB1 PRKAA2	0,097239989
MMEL1	0,097239989
AGPAT2	0,097239989
SGK1	0,097239989
CPB2	0,097239989
ENPP2	0,097239989
PPIA	0,097239989
MAPK10	0,097239989
MAP2K1	0,097239989
MAPK11	0,097239989
PLEC	0,097239989
ADORA1	0,097239989
CA4	0,097239989
RHOA	0,097239989
HPSE	0,097239989
NR4A1	0,097239989
ITGAL	0,097239989
ZAP70	0,097239989
PGK1	0,097239989
TERT	0,097239989
MKNK2	0,097239989
BDKRB1	0,097239989
CD38	0,097239989
NGFR	0,097239989
PLA2G5	0,097239989
PLA2G10	0,097239989
OXER1	0,097239989
FLT4	0,097239989

	FLT3	0,097239989
	PDGFRA	0,097239989
	EPHA2	0,097239989
	YES1	0,097239989
	KMO	0,097239989
	BLK	0,097239989
	KDM5A	0,097239989
	RPS6KA1	0,097239989
	CSK	0,097239989

Lampiran 2. Perintah Docking pada YASARA #

```
YASARA MACRO
    # TOPIC: 5. Structure prediction
    # TITLE: Docking a ligand to a receptor
    # REQUIRES: Structure
    # AUTHOR: Elmar Krieger
    # LICENSE: GPL
    # DESCRIPTION: This macro runs VINA or AutoDock to predict the structure of
    a ligand-receptor complex. It can also continue a docking run that got interrupted.
    An analysis log file is written at the end.

    # Parameter section - adjust as needed, but NOTE that some changes only take
    effect
    # if you start an entirely new docking job, not if you continue an existing one.
    #
    ============================================================
    Processors 10
    Processors GPU=1
    Antialias 0
    Console Off

    # You can either set the target structure by clicking on Options > Macro > Set
    target,
    # by providing it as command line argument (see docs at Essentials > The
    command line),
    # or by uncommenting the line below and specifying it directly.
    #MacroTarget '/home/myname/projects/docking/1sdf'

    # Docking method, either VINA (CPU only) or AutoDockLGA (runs on the GPU
    if enabled at Options > Processors > Set compute GPU)
    method='AutoDockLGA'

    # Number of docking runs (maximally 999, each run can take up to an hour)
    runs=100

    # Docking results usually cluster around certain hot spot conformations,
    # and the lowest energy complex in each cluster is saved. Two complexes belong
    to
    # different clusters if the ligand RMSD is larger than this minimum [A]:
    rmsdmin=5.0

    # Set to 1 to keep the ligand completely rigid (alternatively you can provide
    # the ligand as a *.yob file and fix certain dihedral angles only).
    rigid=0
```

Lampiran 3. Perintah md_runmembrane

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Running a molecular dynamics simulation of a membrane protein with normal or fast
speed
# REQUIRES: Dynamics
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro sets up and runs a simulation of a membrane protein. It scans the
protein for secondary structure elements with hydrophobic surface residues, orients it accordingly
and embeds it in a membrane of adjustable lipid composition. Finally a 250 ps restrained
equilibration simulation is run, which ensures that the membrane can adapt to the newly embedded
protein. Then the real simulation starts.

# Include library functions
include md_library

# Parameter section - adjust as needed, but NOTE that some changes only take
# effect if you start an entirely new simulation, not if you continue an existing one.
#
=========================================================================
==============

#nice -n 20 /home/al/yasara/yasara -txt
"/home/al/yasara/2021/desti/03_md/md_runmembrane.mcr"

Processors CPUThreads=50,GPU=1
Antialias 0
Console Off

# The structure to simulate must be present with a .pdb or .sce extension.
# If a .sce (=YASARA scene) file is present, the membrane and cell must have been added.
# You can either set the target structure by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below and specifying it directly.
#MacroTarget 'c:\MyProject\1crn'
MacroTarget /home/al/yasara/2021/desti/03_md/1hwl.yob,Remove=Extension
# Extension of the cell on each side of the protein in the membrane plane (=XZ plane)
# '15' means that the membrane will be 30 A larger than the protein
memextension=15

# Extension of the cell on each side of the protein along the third (water) axis (=Y-axis)
# '10' means that the cell will be 20 A higher than the protein
waterextension=10

# Flag to use a square membrane. This makes sure that also elongated proteins
# embedded in the membrane can rotate freely during very long simulations. If
# only a short simulation is planned, it can be speeded up by setting the flag
# to 0, creating a rectangular membrane that fits the solute more tightly.
square=1

# Membrane composition: The three letter names of phosphatidyl-ethanolamine (PEA),
# phosphatidyl-choline (PCH, also known as POPC), phosphatidyl-serine (PSE), phosphatidyl-
glycerol (PGL),
```

```
# cholesterol (CLR) and cardiolipin (CDL) are each followed by the mass percentage for
# each membrane side, and must sum up to 100. CDL conntent cannot exceed 30%.
# All lipids are 1-palmitoyl, 2-oleoyl by default, except CDL with four 18:2 tails.
# The first percentage is for the bottom side of the membrane, the second is for the top side.
# When YASARA shows you the suggested membrane embedding, you need to check that the
protein
# orientation matches the membrane composition. If not, flip first and second percentages below
and
# rerun the macro. Note that PCH has a large headgroup which cannot form hydrogen bonds, and
# thus reduces membrane stability. PEA is the most stable membrane lipid.
memcomplist()='PEA',100,100,'PCH',0,0,'PSE',0,0,'PGL',0,0,'CLR',0,0,'CDL',0,0
# Or uncomment below to use your own membrane template with 10x10 lipids on each side,
# see membrane simulation recipes for details. In this case, 'memcomplist' will be ignored.
# The 'usermemlist' contains the name of your membrane template followed by its X and Z size.
# If your membrane template name is 'YourChoice', it must be saved as
yasara/yob/membrane_YourChoice.yob
usermemlist()='' # Default
#usermemlist()='YourChoice',77.21,73.24 # Example: Use own membrane 'YourChoice' of 77.21
x 73.24 A size
# pH at which the simulation should be run, by default physiological pH 7.4.
ph=7.4
# The ion concentration as a mass fraction, here we use 0.9% NaCl (physiological solution)
ions='Na,Cl,0.9'
# Forcefield to use (this is a YASARA command, so no '=' used)
ForceField AMBER14
# Simulation temperature, which also serves as the random number seed (see Temp command).
# If you increase the temperature significantly by X%, you also need to reduce the timestep by X%
# by changing the 'tslist' that matches your speed below.
temperature='310'
# Pressure at which the simulation should be run [bar].
pressure=1
# Cutoff
cutoff=8
# Equilibration period in picoseconds:
# During this initial equilibration phase, the membrane is artificially stabilized
# so that it can repack and cover the solute, while solvent molecules are kept outside.
equiperiod=250
# Delay for animations, 1=maximum speed
delay=100
# The format used to save the trajectories: YASARA 'sim', GROMACS 'xtc' or AMBER 'mdcrd'.
# If you don't pick 'sim', a single *.sim restart file will be saved too, since the other
# two formats don't contain velocities, only positions.
format='sim'
# Duration of the complete simulation, must be longer than equiperiod above.
# Alternatively use e.g. duration=5000 to simulate for 5000 picoseconds
# 'if !count duration' simply checks if variable 'duration' as been defined previously (e.g. by an
including macro)
if !count duration
 duration=20000
```

Lampiran 4. Perintah md_convert-sim2pdb.mcr

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Convert between Sim, XTC, MDCrd and PDB simulation trajectories
# REQUIRES: Dynamics 9.5.10
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro converts an existing MD trajectory between various formats.
Supported are conversions between YASARA Sim, GROMACS XTC and AMBER MDCrd
trajectories, as well as conversion to PDB files
# Parameter section - adjust as needed
# ==================================
Antialias 0
Console Off
Processors cputhreads=1, gpu=0
#nice -n 20 /home/gerry/yasara/yasara -txt "/home/gerry/pafr/2_md/md_convert-sim2pdb.mcr"
# The trajectory to convert must be present with a .sim, .xtc or .mdcrd extension.
# The starting scene *_water.sce is also required.
# You can either set the target by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below and specifying it directly.
#MacroTarget = 'c:\MyProject\1crn'
#MacroTarget /home/gerry/pafr/2_md/5zkp.sce,Remove=Extension
# Source format (srcformat) can be 'sim' (see SaveSim/LoadSim), 'xtc' (see SaveXTC/LoadXTC)
# or 'mdcrd' (see SaveMDCrd/LoadMDCrd).
# Destination format (dstformat) can be 'sim', 'xtc', 'mdcrd', 'pdb' (a series of PDB files)
# or 'pdbw' (a series of wrapped PDB files, where all atoms are inside the cell
# and potentially wrapped around periodic boundaries (i.e. broken molecules)).
# If one is left empty, YASARA will ask for the formats interactively.
srcformat='sim'
dstformat='pdb'
# Flag if water object should be included (1) or not (0)
waterincluded=0
# Forcefield to use
ForceField AMBER14
```

Lampiran 5. Perintah md_analyze.mcr

```
# YASARA MACRO
# TOPIC: 3. Molecular Dynamics
# TITLE: Analyzing a molecular dynamics trajectory
# REQUIRES: Dynamics
# AUTHOR: Elmar Krieger and Kornel Ozvoldik
# LICENSE: GPL
# DESCRIPTION: This macro analyzes a simulation and creates a detailed report with a large
number of plots, e.g. energies, RMSDs, hydrogen bonds. It also tries to identify the main ligand
and provides ligand-specific data. All results are additionally written to a simple text table, which
can be imported into your favorite spreadsheet program. Your own analysis can often be added
with just one line of code, search for 'Example:'.
RequireVersion 20.1.1
# MD report initialization parameters and flags
# ============================================
# The structure to analyze must be present with a .sce extension.
# You can either set the target structure by clicking on Options > Macro > Set target,
# by providing it as command line argument (see docs at Essentials > The command line),
# or by uncommenting the line below (=remove the '#') and specifying it directly.
#MacroTarget 'c:\MyProject\1crn'
# Set common beginning for all result filenames. By default,
# this is the same as the macro target, but you can change
# it to run multiple analyses at the same time.
resultbase=MacroTarget # Default
#resultbase='(MacroTarget)_run1' # Example
# Forcefield to use for analysis, should be the same as the one used to run the simulation
ForceField AMBER14,SetPar=Yes # Default
#ForceField YASARA2,SetPar=Yes # Example: Add a quality Z-score in YASARA Structure
# Number of the solute object whose RMSDs from the starting conformation will be calculated
# If the protein is an oligomer, check the documentation of the 'Sup' command at 'analyzing a
simulation' to avoid pitfalls.
soluteobj=1
# Flag to convert the entire trajectory to PDB format (solute object only)
pdbsaved=0
# The B-factors calculated from the root-mean-square fluctuations can be too large to fit them
# into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale them down to 10%
bfactorscale=1.0
# Trajectory block to be analyzed. The 'if not count block' skips this part if this macro is included
# by the md_analyzeblock macro, that analyzes the trajectory in blocks (see 'Analyzing a
trajectory' in the docs).
if not count block
 # First snapshot to be analyzed, increase number to ignore an equilibration period.
 firstsnapshot=0
 # Number of snapshots to be analyzed
 snapshots='all'
```

Lampiran 6. Nilai RMSD bb

0.577	4.709	4.729	4.333	4.507	4.305	4.625
5.189	5.239	5.363	5.510	4.969	5.297	5.211
5.421	5.279	5.782	5.170	4.925	5.324	5.155
5.331	5.134	5.387	5.741	5.402	5.704	6.067
6.124	5.594	5.885	5.560	5.366	5.497	5.838
5.724	5.875	5.834	5.724	5.677	6.159	5.853
5.644	6.150	6.167	6.065	5.648	5.578	5.300
5.345	5.097	5.111	5.308	5.254	5.026	5.470
5.785	5.577	5.370	5.527	5.819	5.766	6.097
5.521	5.726	5.885	6.341	5.784	5.550	5.670
5.708	5.880	6.179	6.216	6.033	5.968	6.101
5.716	5.823	6.027	6.497	6.158	6.635	6.046
6.438	6.289	6.510	6.814	6.672	6.513	6.523
6.356	6.627	6.277	6.617	6.517	6.392	6.612
6.179	6.070	6.612	6.255	6.574	6.884	6.708
6.613	6.913	6.938	6.863	6.641	6.929	6.479
6.587	6.269	6.224	6.216	6.328	6.593	5.923
5.880	5.834	6.196	6.195	6.140	6.356	6.193
6.562	6.257	5.924	6.117	5.975	5.769	5.688
6.445	6.255	6.470	6.703	6.361	6.179	6.477
7.025	6.269	6.587	6.532	6.327	5.914	5.607
5.807	5.914	5.729	5.872	6.240	6.765	6.861
6.901	6.621	6.636	6.791	6.541	6.749	6.339
6.851	6.497	6.762	6.459	6.380	6.633	6.153
6.765	6.533	6.333	6.450	6.007	6.183	6.214
6.113	6.231	5.923	5.732	5.932	6.044	6.045
6.175	6.015	5.638	5.815	5.628	5.999	6.152
6.497	6.127	6.270	6.463	6.310	6.217	6.617
6.502	6.613	6.848	6.823	6.511	6.005	0.577
7.025						

Lampiran 7. Perintah BEcalculation.mcr

```
Antialias 0
Console Off
Processors cputhreads=1, gpu=0
#nice -n 20 /home/gerry/yasara/yasara -txt "/home/gerry/2_H2R/7_sce/BEcalculation.mcr"
#konversi pdb ke sce
for k=00001 to 00200
 LoadPDB (MacroDir)\1hwl(k).pdb,Center=No,Correct=No
 SplitObj 1
 DelObj 3
 NiceOriAll
 Cell Auto,Extension=5,Shape=Cuboid,Obj 2
 FixAll
 ForceField NOVA,SetPar=Yes
 Boundary Wall
 SaveSce (MacroDir)\1hwl(k)_complex.sce
 Clear
#Calculation
method = 'VINALS'
runs = 1
rmsdmin = 5.0
rigid = 1
for j=00001 to 00200
 LoadSce (MacroDir)\1hwl(j)_complex.sce
 NameObj 1,receptor
 NameObj 2,ligand
 ForceField AMBER03
 Boundary Wall
 Longrange None
```

Lampiran 8. Mengambil Nilai Terendah Dengan Ubuntu

Open terminal
Grep 001 *.log > grep_log
Ambil kolom ketiga awk ‘{print $3}’ grep_log > awk_log
Mengurutkan nilai sort awk_log > spasi sort_awk
Mencari data yang terdapat nilai terendah grep 13.5130 *.log

Lampiran 9. Nilai RMSD Kompleks Ligan-Reseptor 1hwl Selama Simulasi *Molecular Dynamics*

Time(ns)	RMSD	Time(ns)	RMSD	Time(ns)	RMSD
0.1		5.9	0.2456	13	0.2394
0.2		6	0.2418	13.1	0.2066
0.3		6.1	0.3458	13.2	0.3108
0.4	0.2116	6.2	0.225	13.3	0.3384
0.5	0.1948	6.3	0.2648	13.4	0.4374
0.6	0.2868	6.4	0.278	13.5	0.6242
0.7	0.468	6.5	0.393	13.6	0.1918
0.8	0.6392	6.6	0.3304	13.7	0.2146
0.9	0.5602	6.7	0.3072	13.8	0.259
1	0.285	6.8	0.296	13.9	0.37
1.1	0.3066	6.9	0.2606	14	0.2832
1.2	0.301	7	0.1684	14.1	0.3284
1.3	0.3126	7.1	0.2474	14.2	0.309
1.4	0.2664	7.2	0.2606	14.3	0.279
1.5	0.187	7.3	0.2952	14.4	0.4118
1.6	0.2026	7.4	0.1752	14.5	0.5864
1.7	0.3904	7.5	0.1314	14.6	0.4304
1.8	0.371	7.6	0.2908	14.7	0.3068
1.9	0.3462	7.7	0.2122	14.8	0.1872
2	0.256	7.8	0.211	14.9	0.1788
2.1	0.2488	7.9	0.3168	15	0.1834
2.2	0.1322	8	0.3282	15.1	0.375
2.3	0.2156	8.1	0.405	15.2	0.5644
2.4	0.265	8.2	0.2456	15.3	0.6558
2.5	0.3396	8.3	0.3088	15.4	0.4376
2.6	0.2732	8.4	0.2672	15.5	0.1358
2.7	0.4056	8.5	0.3376	15.6	0.141
2.8	0.3762	8.6	0.3734	15.7	0.157
2.9	0.2808	8.7	0.2556	15.8	0.1266
3	0.286	8.8	0.2706	15.9	0.2722
3.1	0.3398	8.9	0.0964	16	0.3152
3.2	0.2144	9	0.2196	16.1	0.2564
3.3	0.2632	9.1	0.1822	16.2	0.3006
3.4	0.231	9.2	0.1822	16.3	0.2426
3.5	0.294	9.3	0.203	16.4	0.2098
3.6	0.2566	9.4	0.2018	16.5	0.1662
3.7	0.075	9.5	0.209	16.6	0.3244
3.8	0.0898	9.6	0.206	16.7	0.325
3.9	0.1768	9.7	0.2844	16.8	0.3398

4	0.1724	9.8	0.284	16.9	0.3304
4.1	0.1674	9.9	0.303	17	0.2938
4.2	0.2526	10	0.2756	17.1	0.4106
4.3	0.3506	10.1	0.268	17.2	0.2942
4.4	0.3318	10.2	0.409	17.3	0.2304
4.5	0.2908	10.3	0.3516	17.4	0.1864
4.6	0.3436	10.4	0.3518	17.5	0.1426
4.7	0.4516	10.5	0.1644	17.6	0.2098
4.8	0.2872	10.6	0.1982	17.7	0.3106
4.9	0.2966	10.7	0.194	17.8	0.2542
5	0.1892	10.8	0.1806	17.9	0.2404
5.1	0.1352	10.9	0.2158	18	0.2032
5.2	0.126	11	0.291	18.1	0.2536
5.3	0.1332	11.1	0.2208	18.2	0.1102
5.4	0.2078	11.2	0.312	18.3	0.3454
5.5	0.3426	11.3	0.2736	18.4	0.2996
5.6	0.3964	11.4	0.139	18.5	0.2262
5.7	0.4196	11.5	0.1088	18.6	0.191
5.8	0.1758	11.6	0.11	18.7	0.2184
5.9	0.2456	11.7	0.3338	18.8	0.3902
6	0.2418	11.8	0.308	18.9	0.4526
6.1	0.3458	11.9	0.2776	19	0.21
6.2	0.225	12	0.2512	19.1	0.1748
6.3	0.2648	12.1	0.1716	19.2	0.2064
6.4	0.278	12.2	0.215	19.3	0.1504
6.5	0.393	12.3	0.3102	19.4	0.1584
6.6	0.3304	12.4	0.076	19.5	0.2048
6.7	0.3072	12.5	0.1492	19.6	0.2348
6.8	0.296	12.6	0.1616	19.7	0.3424
6.9	0.2606	12.7	0.3344	19.8	0.1786
7	0.1684	12.8	0.2866	19.9	0.1574
7.1	0.2474	12.9	0.243	20	0.1574

	SURAT	No Dokumen	Form-A1
		Berlaku Sejak	
	PERMOHONAN IZIN PENELITIAN PROGRAM STUDI S-1 FARMASI UNIVERSITAS AISYIYAH PALEMBANG	Revisi	000

Hal : Permohonan Izin Penelitian

1	Skripsi
2	PKM/I.KTI
3	Penelitian Dosen
4	Luar

Kepada Yth
Kabag Laboratorium Terpadu
Universitas 'Aisyiyah Palembang

Assalamualaikum Wr. Wb.
Sehubungan dengan penelitian kami dalam bidang Kimia komputasi, dengan:
Judul Penelitian : Membangun Protokol Structure-Based Virtual Screening (SBVS) untuk Identifikasi Kandidat Ligan Anti-Hiperlipidemia
Nama Pembimbing : 1. Gerry Nugraha, M.Sc., M.Farm
2. Suprayetno, S.Si., M.T.

No	Nama	NIM/NIP/NIK	No. HP
1	Desti kurnia sari	21482010 3006	089684333063
2			
3			
4			
5			

Bermaksud mengajukan izin penelitian di Laboratorium*): **Farmasetika Dasar / Teknologi Farmasi / Kimia Farmasi / Biologi Farmasi / Farmakologi / Mikrobiologi / Komputasi** Prodi S1 Farmasi Universitas 'Aisyiyah Palembang.
Penelitian tersebut akan kami laksanakan selama: 6 bulan,
yang terhitung dari : 19 | 03 | 2025 s.d 19 | 08 | 2025

Sebagai bahan pertimbangan, bersama ini dilampirkan lembar pengesahan proposal penelitian.
Demikian permohonan kami, atas perhatiannya diucapkan terima kasih.

Palembang, 19 Maret 2025

Mengetahui,
Dosen Pembimbing

Gerry Nugraha, M.Sc., M.Farm

Pemohon

Desti kurnia sari

Menyetujui,
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Heni Riyanti, Akm., M.Kes

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apt. Ady Indriadi, M.Farm

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بِسْمِ اللَّهِ الرَّحْمَٰنِ الرَّحِيمِ

FORMULIR
PERNYATAAN SELESAI REVISI PROPOSAL/ NASKAH SKRIPSI*)
(S-06)

Yang bertandatangan dibawah ini, tim penguji Skripsi 1/ Skripsi 2*):

Nama Mahasiswa : Desti kurnia sari

NIM : 2148201032006

Judul Penelitian : Membangun Protokol Structure - Based Virtual Screening (SBVS) untuk Identifikasi Kandidat Ligan Anti - Hiperlipidemia

Pembimbing 1 : Gerry Nugraha,M.Sc., M.Farm

Pembimbing 2 : Suprayetno, S.Si., MT

Tanggal Ujian : 11 Januari 2025

Menerangkan bahwa naskah Proposal/ ~~Skripsi~~*) telah **selesai** direvisi oleh tim penguji.

Nama	Tanda Tangan	Tanggal
1. Gerry Nugraha,M.Sc., M.Farm		15/04-2025
2. Suprayetno, S.Si., MT		15/04-2025
3. Ade Oktasari, M.Sc		15/04-2025
4. Apt. Onny Indriani, M.Farm		24/04-2025

*) : Coret yang tidak perlu.

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FORMULIR BIMBINGAN SKRIPSI

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Nama Pembimbing :1. Dr. Gerry Nugraha,.Sc., M.Farm
2.Suprayetno, S.Si., MT
Judul Skripsi :MEMBANGUN PROTOKOL *STRUCTURE-BASED VIRTUAL SCREENING* (SBVS) UNTUK IDENTIFIKASI KANDIDAT LIGAN ANTI-HIPERLIPIDEMIA

No.	Tanggal Konsultasi	Keterangan	Paraf Pembimbing
1.	14 mei 2025	Revisi Tujuan	
2.	27 Mei 2025	Revisi Rumusan Masalah	
3.	2 Juni 2025	Revisi Bab 1	
4.	3 Juni 2025	Revisi Bab 1	
5.	4 Juni 2025	Revisi Bab 2	
6.	3 Juli 2025	Revisi Bab 2	
7.	4 Juli 2025	Revisi Bab 2	
8.	5 Juli 2025	Revisi Metode penelitian	
9.	9 Juli 2025	Revisi Pembahasan	
10.	17 Juli 2025	Revisi Pembahasan	
11.	20 Juli 2025	Revisi Pembahasan	
12.	22 Juli 2025	Revisi Pembahasan	
13.	24 Juli 2025	Revisi Kesimpulan	
14.	26 Juli 2025	Revisi Kesimpulan	
15.	2 Agustus 2025	Revisi Lampiran	