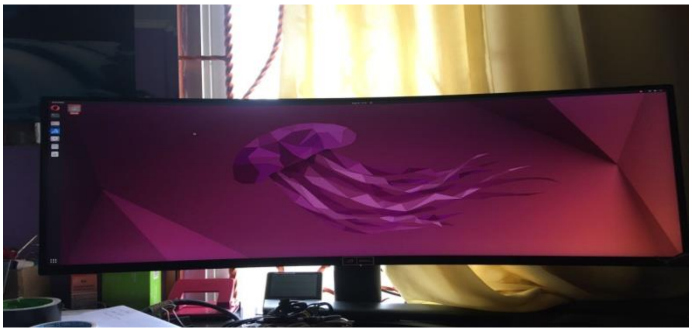
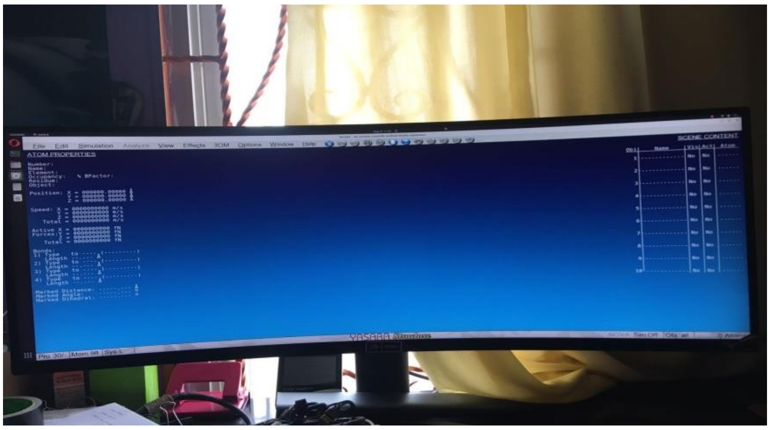
LAMPIRAN

Lampiran 1. Perangkat keras CPU Komputer

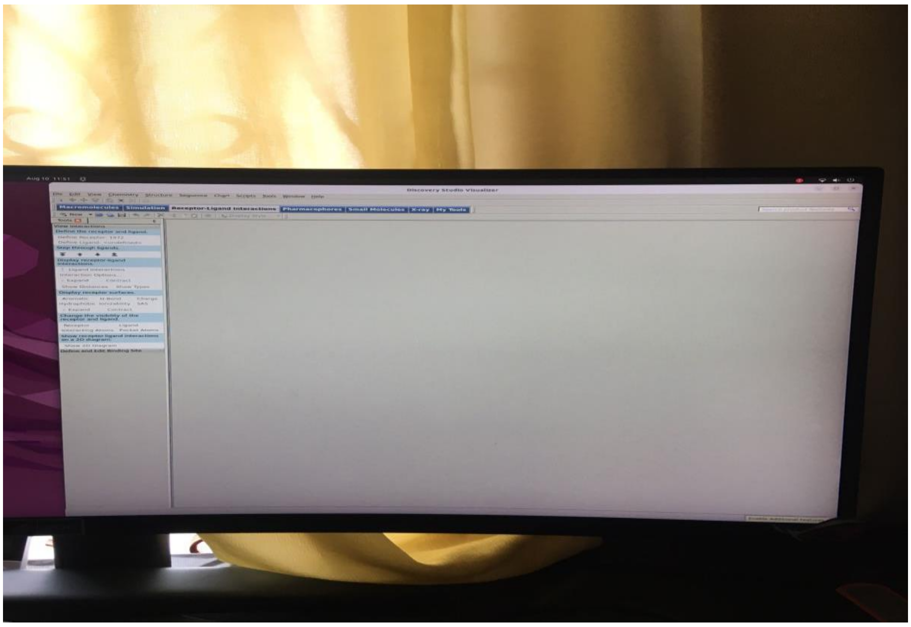
Lampiran 2. Perangkat keras Monitor Ubuntu



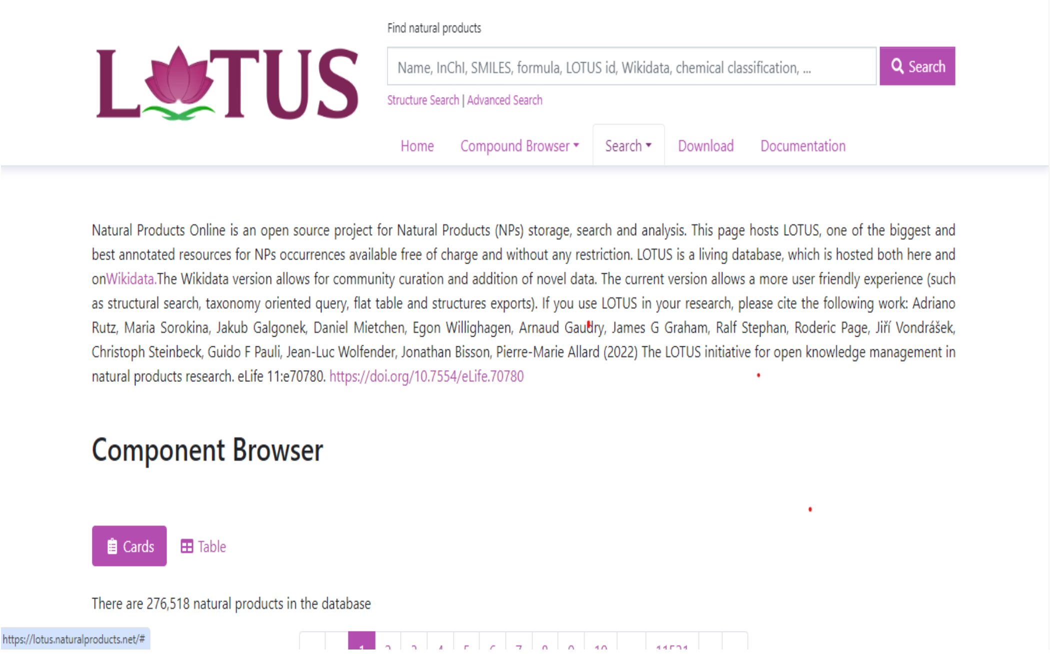
Lampiran 3. Perangkat lunak YASARA-*structure*



Lampiran 4. Perangkat lunak *Discovery Studio*



Lampiran 5. *Lotus Natural Product*

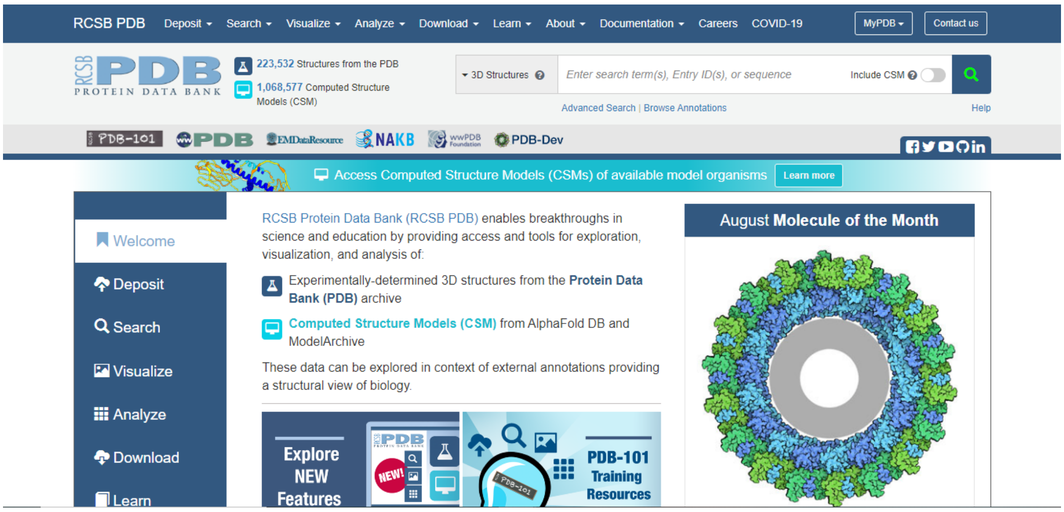


Natural Products Online is an open source project for Natural Products (NPs) storage, search and analysis. This page hosts LOTUS, one of the biggest and best annotated resources for NPs occurrences available free of charge and without any restriction. LOTUS is a living database, which is hosted both here and onWikidata.The Wikidata version allows for community curation and addition of novel data. The current version allows a more user friendly experience (such as structural search, taxonomy oriented query, flat table and structures exports). If you use LOTUS in your research, please cite the following work: Adriano Rutz, Maria Sorokina, Jakub Galgonek, Daniel Mietchen, Egon Willighagen, Arnaud Gaudry, James G Graham, Ralf Stephan, Roderic Page, Jiří Vondrášek, Christoph Steinbeck, Guido F Pauli, Jean-Luc Wolfender, Jonathan Bisson, Pierre-Marie Allard (2022) The LOTUS initiative for open knowledge management in natural products research. eLife 11:e70780. https://doi.org/10.7554/eLife.70780

Component Browser

There are 276,518 natural products in the database

Lampiran 6. laman RCSB PDB



RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive

Computed Structure Models (CSM) from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

Lampiran 7. Perintah smi2pdb.mcr

```
Processors 6
Processors GPU=0
Antialias 0
Console Off

CD (MacroDir)
libname='(MacroTarget)'
OnError Continue
Clear
for line in file (libname).smi
  # Extract SMILES and name
  smiles,name=split line
  # Build SMILES
  obj = BuildSMILES '(smiles)'
  # Minimize with NOVA to close any long bonds that BuildSMILES left
  # (QM optimization doesn't know where bonds should be)
  pH value=7.4,update=Yes
  Cell Auto,Extension=10
  ForceField NOVA,SetPar=yes
  Experiment Minimization
  Experiment On
  Wait ExpEnd
  # Set compound name
  CompoundMol Obj (obj),'(name)'
  SaveSDF !SimCell,(name).sdf
  SavePDB !SimCell,(name).pdb
  DelObj (obj)
Clear
```

Lampiran 8. Perintah dock_runscreening.mcr

```
# YASARA MACRO
# TOPIC:      5. STRUCTURE PREDICTION
# TITLE:      DOCKING MANY LIGANDS TO A RECEPTOR TO PERFORM VIRTUAL SCREENING
# REQUIRES:   STRUCTURE
# AUTHOR:     ELMAR KRIEGER
# LICENSE:    GPL
# DESCRIPTION: THIS MACRO RUNS VINA OR AUTODOCK TO DOCK MULTIPLE LIGANDS
AGAINST A RECEPTOR AND SAVES A SORTED TABLE of their binding energies, as well as the
corresponding complexes

# 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 20
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 AutoDockLGA or VINA
method='AutoDockLGA'

# Number of docking runs per ligand (maximally 999, 0 lets YASARA choose based on the number of CPUs)
runs=25

# Number of best poses per ligand saved and reported
bestposes=1

# 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

# A selection of receptor residues whose side-chains should be kept flexible, e.g.
# flexres='Lys 91 Leu 100', or (if the receptor is not a monomer)
# flexres='Res Lys 91 Mol A or Res Leu 100 Mol B'.
# Alternatively you can provide the receptor as a *.sce or *.yob file with fixed
# atoms, which gives better control (e.g. you can keep only part of a side-chain
# or even a terminal backbone flexible).
flexres=''

# Sort results either by ligand number ('ligandnum'), binding energy ('bindnrg') or by
# efficiency ('effi'), i.e. binding energy per heavy atom, which addresses the bias towards
# larger ligands in screening.
sortby='bindnrg'

# Force field used for charge assignment (AutoDock only, not VINA) and to determine which ligand bonds can
rotate.
# Do not change to an in vacuo force field (NOVA), all other force fields should work too (not tested).
ForceField AMBER03
```

```
# Uncomment below to set a certain random seed (a YASARA command, no '=')
# RandomSeed 1000

# Normally no change required below this point
# ==
============================================

if !runs
  # For an optimum speed/accuracy tradeoff, we select at least 8 runs, but more if CPUs are available
  cpus=Processors
  runs=cpus
  while runs<8
    runs=runs+cpus

# Sanity checks
if MacroTarget==''
  RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to
choose a target structure"
if runs>999
  RaiseError 'Too many docking runs selected, (runs) would take forever'
if runs<bestposes
  RaiseError 'You need to choose at least (bestposes) docking runs to keep the best (bestposes) poses per ligand'

structlist='receptor','ligand'

# Load receptor and ligand
Clear
# Do we already have a receptor scene?
scefilename='(MacroTarget)_receptor.sce'
scene=FileSize (scefilename)
if !scene
  # No, load PDB or YOB files of receptor
  receptor=0
  for type in 'yob','pdb'
    filename='(MacroTarget)_receptor.(type)'
    exists=FileSize (filename)
    if exists
      receptor=Load(type) (filename)
      break
  if !receptor
    RaiseError 'The receptor was not found at (MacroTarget)_receptor.* Please follow the instructions in the
"Recipes" section exactly, especially when setting the macro target'
  # Orient receptor along the major axes
  NiceOriObj (receptor)
else
  # Yes, a scene is present
  LoadSce (scefilename)
  # Verify that the cell is present
  simcell=CountObj SimCell
  if !simcell
    RaiseError 'If you provide a scene, it must contain a simulation cell, but none was found in (scefilename)'
  # The receptor is the object containing the first atom
  receptor=ListObj Atom 1
  if Objects>2
```

```
    ShowMessage 'Your scene contains (Objects) objects, while only the receptor and the docking cell are expected.'
    Wait ContinueButton
    HideMessage
# Load the ligands and determine the maximum radius
for type in 'yob','pdb','sdf'
  filename='(MacroTarget)_ligands.(type)'
  exists=FileSize (filename)
  if exists
    ligandlist()=Load(type) (filename)
    break
ligands=count ligandlist
if not ligands
  RaiseError 'No ligands were found at (MacroTarget)_ligands.* Please follow the instructions in the "Recipes" section exactly, especially when setting the macro target'
if ligands==1
  # Maybe ligands are separate molecules, not objects
  ligandlist()=SplitObj (ligandlist1)
  ligands=count ligandlist
if ligands==1
  # If there is really just one ligand, raise an error (otherwise dock_play won't work)
  RaiseError 'Only a single ligand was found at (filename), you need at least two for screening'
# Determine maximum ligand radius
radiuslist()=RadiusObj (join ligandlist)
radiusmax=max radiuslist
# Rename objects to make sure they can be identified later, ligands are 'Waiting' to be docked.
NameObj (receptor),Receptor
NameObj (join ligandlist),Waiting
RemoveObj (join ligandlist)
# Keep selected side-chains flexible
if flexres!="
  FixObj Receptor
  FreeAtom Res (flexres) Sidechain and Obj Receptor
  FixRes Cys Atom SG with bond to Atom SG or Ala Pro and Obj Receptor
# Add a cell if not already present
cellfound=CountObj SimCell
if !cellfound
  if scene
    RaiseError 'The receptor scene (scefilename) does not contain a cell'
  Cell Auto,Extension=(radiusmax*2)
# Warn if the cell is too large
x,y,z=Cell
if method!='VINA' and (x>384 or y>384 or z>384)
  # AutoDock now uses dynamic memory allocation for grids up to 1024x1024x1024 (int MAX_GRID_PTS=1025 in autocomm.h)
  # Given the standard grid spacing of 0.375 A, these are 384 A. VINA doesn't have a compile-time limit
  ShowMessage "A cell axis is longer than 384 A, which may reduce docking accuracy. Consider focusing on the active site, or remove unusually long ligands from the library"
  Wait ContinueButton
HideMessage
# The segment name C*** is used to tag ligand Conformations, and cannot be used for the receptor
hit=ListAtom Segment C??? Obj Receptor
if hit
  MarkAtom (hit)
  segname=SegAtom (hit)
```

```
  RaiseError 'Segment names starting with "C" are unfortunately reserved to identify ligand conformations, please
click "Edit > Name > Segment", double-click object (receptor) on the right, and click OK to set an empty segment
name'
# The molecule name 'l' is reserved for the ligand
hit=ListAtom Mol l
if hit
  RaiseError 'The receptor must not contain a molecule named "l", please click Edit > Name > Molecule and try
again'
# Docking is done without periodic boundaries
Boundary Wall
Longrange None

# Do we have a checkpoint file from a previous run?
checkpointfilename='(MacroTarget)_checkpoint.sce'
restarted=FileSize (checkpointfilename)
if restarted
  LoadSce (checkpointfilename)
# Loop over the ligands
for i=1 to ligands
  # Has this ligand been docked in a previous run?
  ligand=ligandlist(i)
  ligname=NameObj (ligand)
  if ligname=='Done' or ligname=='Broken'
    ShowMessage 'Ligand (i) has been docked before...'
    continue
  # Place only the ligand in the soup
  AddObj (ligand)
  RemoveObj (receptor)
  # Check that ligand is not internally disconnected
  conatoms=CountAtom Obj (ligand) with connection to 1
  if conatoms!=Atoms
    # Ligand has bonds missing, cannot be docked
    failure=1
  else
    # See if the ligand can be simulated or is broken. Try three times.
    # This must be done without receptor, which may not have been cleaned yet.
    OnError Continue
    for j=1 to 3
      # Initialize force field parameters, but do not stop if it fails
      failure=Sim Init
      if !failure
        # All OK
        break
      if failure==434
        # User pressed escape
        OnError Stop
        RaiseError "Screening was interrupted. All progress has been saved, so you can simply run this macro again
to continue"
      if j==1
        # Try to retype the bonds
        TypeBond all,all
      if j==2
        # Try to re-add the hydrogens
        DelHydObj (ligand)
        failure=CleanObj (ligand)
```

```
        if failure==768
          # Molecule disappeared during cleaning, don't leave an empty object slot
          obj=BuildAtom C
          SwapObj (obj),(ligand)
          break
    OnError Stop
  AddObj (receptor)
  if failure
    # This compound is hopeless, skip it
    NameObj (ligand),Broken
    BFactorObj (ligand),-9999
    SegObj (ligand),C001
  else
    # This compound is OK
    NameObj (ligand),Docking
    # Get the ligand compound name and display it at the top
    ligandname=CompoundMol Obj (ligand)
    LabelAll 'Screening ligand (i)/(ligands), (ligandname)',Height=0.5,Color=Yellow,Y=4,Z=2
    # Move the ligand out of the cell, so that it does not block the view
    cellpos()=PosObj SimCell
    PosObj (ligand),(cellpos1),(cellpos2+y*0.5+radiusmax),(cellpos3)
    # Perform rigid docking if requested
    if rigid
      FixObj (ligand)
    # Align ligand with the cell (to end up with the same local atom coordinates independent
    # of cell orientation, which are used to calculate the checksum for the *.adr file)
    TransferObj (ligand),SimCell,Local=Keep
    # Perform the docking
    Experiment Docking
      Method (method)
      ReceptorObj (receptor)
      LigandObj (ligand)
      Runs (runs)
      # We only want a single result, the best complex
      ClusterRMSD 1000
      # In case of docking failures (e.g. cell too small) don't stop, but assign this binding energy to the ligand
[kcal/mol]
      FailureEnergy -9998
      # Result file number must be separated with '_', in case MacroTarget also ends with number
      # If we exceed 999, an additional digit will be inserted.
      # If PDB files are needed too, replace .yob with .pdb to get both
      ResultFile (MacroTarget)_(000+i).yob
      # Uncomment below to set the number of energy evaluations (AutoDock ga_num_evals):
      # DockPar ga_num_evals 25000000
      # Uncomment the two lines below to provide your own atom parameters (VdW radii etc.)
      # GridPar parameter_file /Path/To/Custom/AD4_parameters.dat
      # DockPar parameter_file /Path/To/Custom/AD4_parameters.dat
    Experiment On
    Wait ExpEnd
    UnlabelAll
    NameObj (ligand),Done
  RemoveObj (ligand) RecepFlex
  NameObj RecepFlex,RecFlex(ligand)
  # Save checkpoint
  SaveSce (checkpointfilename)
```

```
# Add the objects back to the soup, except the broken ligands (Sim On would fail) and flexible side-chains
AddObj not Receptor and not Broken and not RecFlex?????
# Clear surface environment to calculate contact surface
RemoveEnvAll
# Must be done during simulation so that the contact surface between different objects can be calculated
Sim Pause
Sim On
# Save a log file with an analysis
Console Off
RecordLog (MacroTarget)
print 'Ligand screening result'
print '======================='
print
print '(ligands) different ligands were docked with (runs) runs each to the receptor object (receptor) yielding the
following results,'
print 'sorted by binding energy [more positive energies indicate stronger binding, and negative energies mean no
binding].'
print '"Effi" is the binding efficiency [binding energy per heavy atom], "Con.Surf" is the molecular contact
surface.'
print 'The best (bestposes) poses of each ligand are reported.'
print
print "Lig.|Effi[kcal/(mol*Atom)]|Bind.energy[kcal/mol]|Dissoc. constant [pM]| Con.Surf[A^2] | Name |
Contacting receptor residues"
print '----+---------------------+---------------------+---------------------+---------------+------+-----------------------------'
idx=1
for i=1 to ligands
  for j=001 to bestposes
    resultlist(idx),bindnrglist(idx),effilist(idx)=DockingResult i,'Obj (receptor)','Segment C(j) Obj (ligandlist(i))'
    idx=idx+1
  if !(i%5)
    ShowMessage 'Analyzing docking results, (100*i/ligands)% completed...'
    Wait 1
Sim Off
# Load original scene without hydrogens on flexible side-chains
LoadSce (checkpointfilename)
AddObj all

if sortby!='ligandnum'
  # Sort results by binding energy or binding efficiency
  SortResults 'resultlist','(sortby)list'
for i=1 to ligands
  NameObj (ligandlist(i)) and not Broken,Ligand(i)
for i=1 to count resultlist
  print (resultlist(i))
print
rndseed=RandomSeed
print 'The random seed used during docking was (rndseed).'
fof=ForceField
print 'Point charges and dihedral barriers were obtained from the (fof) force field.'
StopLog
HideMessage
SaveSce (MacroTarget)
# Temporarily delete all except the bestposes
selection='Segment C??? and not Segment'
```

```
for i=001 to bestposes
  selection=selection+' C(i)'
DelRes (selection)
DelObj SimCell Broken
RenumberObj all
# Rename ligand molecules so that the compound info can be kept, but don't use receptor molecule names
objlist()=ListObj Ligand??????
recmolnamelist()=NameMol Obj Receptor
for range in '"A" to "Z"','"a" to "z"','"0" to "9"'
  for molname=(range)
    if molname not in recmolnamelist
      ligmolnamelist(count ligmolnamelist+1)=molname
for i=1 to count objlist
  NameMol Obj (objlist(i)),(ligmolnamelist(1+(i-1)%count ligmolnamelist))
# Make each ligand a separate object, keep atom numbers and shift objects ahead
SplitObj (join objlist),Center=No,Keep=AtomNum
# Save SDF file with the best ligand poses, coordinate system matches receptor if both are loaded without centering
SaveSDF Ligand??????,(MacroTarget)_bestposes,Transform=No
# Save PDB file with the receptor and best ligand poses
SavePDB all,(MacroTarget)_bestposes,Transform=No
# Bring back the complete scene
LoadSce (MacroTarget)
Console On

# Exit YASARA if this macro was provided as command line argument in console mode and not included from another macro
if runWithMacro and ConsoleMode and !IndentationLevel
  Exit

# EXTRACT DOCKING RESULT
# =====================
# Returns a result string and binding energy, extracted from atomic BFactor and Property.
# 'num' is a sequential number, 'recsel' selects the receptor, 'ligsel' the ligand.
def DockingResult num,recsel,ligsel
  # Is ligand broken and not in the soup?
  heavyatoms=CountAtom Element !H (ligsel)
  if !heavyatoms
    bindnrg=-9999
    consurf=0,0
    obj = ListObj (ligsel)
    compound='Ligand (num)'
    effi=0
  else
    # Get the binding energy from the B-factor...
    bindnrg=BFactorAtom (ligsel)
    # ...and the dissociation constant from the atomic property.
    dissconst=PropAtom (ligsel)
    # Calculate contact surface in both directions to average result
    consurf1=ConSurfAtom (recsel),(ligsel)
    consurf2=ConSurfAtom (ligsel),(recsel)
    # Get compound name
    compound=CompoundMol (ligsel)
    if compound==''
      compound=NameRes (ligsel)
```

```
      compound=compound+' '
    # Get receptor residues that contact the ligand
    reslist()=ListRes (recsel) with distance<4.0 from (ligsel),Format='MOLNAME RESNAME RESNUM'
    # Calculate ligand efficiency, i.e. binding energy divided by heavy atoms
    effi=bindnrg/heavyatoms
  if bindnrg<=0
    dissconst='              None'
  else
    dissconst=00000000000000.0000+dissconst
  if bindnrg<=-9999
    reslist='Broken molecule, no docking possible'
  elif bindnrg<=-9998
reslist='Docking failed. Check if cell is too small for ligand'
  elif !count reslist
    reslist='No residues in contact'
  else
    reslist=join reslist
  result='(0000+num)|        (000000.0000+effi) |        (000000.0000+bindnrg) | (dissconst) |     (000000.00+mean consurf) | (compound) | (reslist)'
  return result,bindnrg,effi

# SORT KEYLIST BY VALUES, HIGHEST FIRST
# ====================================
# Lists are passed by reference, see Yanaconda doc section 'Calls to user-defined functions..'
def SortResults keylist,vallist
  caller (keylist),(vallist)

  elements=count (keylist)
  do
    sorted=1
    for i=1 to elements-1
      if (vallist)(i)<(vallist)(i+1)
        swap=(vallist)(i)
        (vallist)(i)=(vallist)(i+1)
        (vallist)(i+1)=swap
        swap=(keylist)(i)
        (keylist)(i)=(keylist)(i+1)
        (keylist)(i+1)=swap
        sorted=0
  while not sorted
```

Lampiran 9. Hasil screening ligands

```
Ligand screening result
======================

2228 different ligands were docked with 25 runs each to the receptor object 1 yielding the following results,
sorted by binding energy [more positive energies indicate stronger binding, and negative energies mean no
binding].
"Effi" is the binding efficiency [binding energy per heavy atom], "Con.Surf" is the molecular contact surface.
The best 1 poses of each ligand are reported.

Lig.|Effi[kcal/(mol*Atom)]|Bind.energy[kcal/mol]|Dissoc. constant [pM]| Con.Surf[A^2] | Name | Contacting
receptor residues
----+---------------------+---------------------+---------------------+---------------+------+-----------------------------
```

```
0089|     000000.2233 |     000007.5920 | 00000002722640.0000 |    000266.54 | LTS0087137 | A PHE 103
A LEU 111 A GLN 112 A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A
ASP 122 A LEU 123
1637|     000000.2409 |     000007.4680 | 00000003356475.0000 |    000297.72 | LTS0029382 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
1635|     000000.2225 |     000007.3420 | 00000004151859.5000 |    000203.33 | LTS0023016 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
1172|     000000.2334 |     000007.2350 | 00000004973644.0000 |    000301.09 | LTS0045802 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG
121 A ASP 122 A LEU 123 A SER 124
1491|     000000.2371 |     000007.1130 | 00000006110853.5000 |    000296.38 | LTS0210884 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG
121 A ASP 122 A LEU 123 A SER 124
1680|     000000.2371 |     000007.1130 | 00000006110853.5000 |    000296.38 | LTS0210884 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG
121 A ASP 122 A LEU 123 A SER 124
1881|     000000.2371 |     000007.1130 | 00000006110853.5000 |    000296.38 | LTS0210884 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG
121 A ASP 122 A LEU 123 A SER 124
2202|     000000.2371 |     000007.1130 | 00000006110853.5000 |    000296.38 | LTS0210884 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG
121 A ASP 122 A LEU 123 A SER 124
0070|     000000.2075 |     000007.0550 | 00000006739325.5000 |    000232.47 | LTS0071002 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122 A LEU 123
0182|     000000.2038 |     000006.9280 | 00000008350426.5000 |    000265.16 | LTS0221614 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP 120 A
ARG 121
1433|     000000.2388 |     000006.9250 | 00000008392816.0000 |    000263.03 | LTS0184081 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU
123 A SER 124
1972|     000000.2095 |     000006.9120 | 00000008579003.0000 |    000277.39 | LTS0097986 | A ASP 67 A
TYR 69 A VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A
ARG 121 A ASP 122 A LEU 123 A SER 124
1681|     000000.2081 |     000006.8670 | 00000009255977.0000 |    000201.14 | LTS0213060 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
0203|     000000.2079 |     000006.8600 | 00000009365982.0000 |    000212.59 | LTS0256404 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1664|     000000.2079 |     000006.8600 | 00000009365982.0000 |    000232.67 | LTS0150063 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1226|     000000.2207 |     000006.8410 | 00000009671203.0000 |    000274.86 | LTS0068076 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU
123 A SER 124
1678|     000000.2010 |     000006.8350 | 00000009769640.0000 |    000204.50 | LTS0207894 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
0781|     000000.2274 |     000006.8220 | 00000009986371.0000 |    000310.25 | LTS0197417 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
1462|     000000.2274 |     000006.8220 | 00000009986371.0000 |    000310.25 | LTS0197417 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
0168|     000000.2003 |     000006.8110 | 00000010173510.0000 |    000237.99 | LTS0201400 | A LEU 111
A GLN 112 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0019|     000000.1886 |     000006.7890 | 00000010558373.0000 |    000231.58 | LTS0154111 | A LEU 111
A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
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0067|     000000.1995 |     000006.7830 | 00000010665840.0000 |    000214.47 | LTS0066533 | A LEU 111
A GLN 112 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A
LEU 123
0154|     000000.2055 |     000006.7830 | 00000010665840.0000 |    000212.64 | LTS0183189 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1167|     000000.2042 |     000006.7400 | 00000011468708.0000 |    000229.21 | LTS0043372 | A PHE 80 A
TYR 101 A LYS 113 A SER 116 A TRP 120 A ARG 121 A ASP 122
1710|     000000.2042 |     000006.7400 | 00000011468708.0000 |    000229.21 | LTS0043372 | A PHE 80 A
TYR 101 A LYS 113 A SER 116 A TRP 120 A ARG 121 A ASP 122
1119|     000000.2167 |     000006.7190 | 00000011882497.0000 |    000167.87 | LTS0019099 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1440|     000000.2094 |     000006.7000 | 00000012269726.0000 |    000234.32 | LTS0187108 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
1693|     000000.2161 |     000006.6990 | 00000012290453.0000 |    000210.27 | LTS0121682 | A LEU 111
A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0051|     000000.2085 |     000006.6710 | 00000012885230.0000 |    000191.21 | LTS0035167 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ARG 121 A ASP 122
0470|     000000.2085 |     000006.6710 | 00000012885230.0000 |    000191.21 | LTS0035167 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ARG 121 A ASP 122
0983|     000000.2085 |     000006.6710 | 00000012885230.0000 |    000191.21 | LTS0035167 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ARG 121 A ASP 122
0684|     000000.2218 |     000006.6540 | 00000013260299.0000 |    000253.42 | LTS0121467 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0729|     000000.2218 |     000006.6540 | 00000013260299.0000 |    000253.42 | LTS0248998 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0076|     000000.2135 |     000006.6170 | 00000014114799.0000 |    000167.63 | LTS0075888 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
2133|     000000.2135 |     000006.6170 | 00000014114799.0000 |    000167.63 | LTS0075888 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
0018|     000000.1834 |     000006.6040 | 00000014427923.0000 |    000173.90 | LTS0134711 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0108|     000000.1931 |     000006.5650 | 00000015409594.0000 |    000218.87 | LTS0103861 | A LEU 111
A GLN 112 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
2170|     000000.2113 |     000006.5510 | 00000015778050.0000 |    000289.79 | LTS0145614 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LEU 111 A GLN 112 A LYS 113 A SER 116 A LEU 118 A PRO
119 A TRP 120 A ARG 121 A ASP 122 A SER 124
0503|     000000.2338 |     000006.5470 | 00000015884932.0000 |    000205.31 | LTS0234779 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LEU 118 A PRO 119 A ARG 121 A ASP 122 A SER 124
1016|     000000.2338 |     000006.5470 | 00000015884932.0000 |    000205.31 | LTS0234779 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LEU 118 A PRO 119 A ARG 121 A ASP 122 A SER 124
0507|     000000.2045 |     000006.5440 | 00000015965569.0000 |    000212.09 | LTS0272446 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1020|     000000.2045 |     000006.5440 | 00000015965569.0000 |    000212.09 | LTS0272446 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1506|     000000.2110 |     000006.5410 | 00000016046615.0000 |    000193.27 | LTS0221024 | A PHE 80 A
VAL 81 A ASN 82 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1031|     000000.1979 |     000006.5310 | 00000016319751.0000 |    000214.65 | LTS0080592 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
1694|     000000.2105 |     000006.5270 | 00000016430303.0000 |    000197.55 | LTS0168383 | A LEU 111
A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
1523|     000000.2167 |     000006.5020 | 00000017138420.0000 |    000183.73 | LTS0233379 | A GLY 78 A
PHE 80 A VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
1289|     000000.1968 |     000006.4960 | 00000017312862.0000 |    000240.68 | LTS0103100 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0778|     000000.2092 |     000006.4840 | 00000017667088.0000 |    000181.89 | LTS0191529 | A PHE 80 A
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TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0825|      000000.2092 |      000006.4840 | 00000017667088.0000 |     000181.89 | LTS0191529 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0930|      000000.2092 |      000006.4840 | 00000017667088.0000 |     000181.89 | LTS0191529 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1448|      000000.2092 |      000006.4840 | 00000017667088.0000 |     000181.89 | LTS0191529 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
2192|      000000.2092 |      000006.4840 | 00000017667088.0000 |     000181.89 | LTS0191529 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1023|      000000.2818 |      000006.4820 | 00000017726826.0000 |     000221.34 | LTS0005376 | A ASP 67 A
GLU 68 A TYR 69 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
1395|      000000.2024 |      000006.4770 | 00000017877058.0000 |     000202.87 | LTS0162125 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
0415|      000000.2085 |      000006.4650 | 00000018242828.0000 |     000242.59 | LTS0210386 | A PHE 80 A
LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0622|      000000.2085 |      000006.4650 | 00000018242828.0000 |     000242.59 | LTS0210386 | A PHE 80 A
LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
1155|      000000.2229 |      000006.4650 | 00000018242828.0000 |     000279.37 | LTS0037765 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LEU 111 A GLN 112 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
1645|      000000.2081 |      000006.4500 | 00000018710582.0000 |     000296.04 | LTS0059737 | A ASP 67 A
TYR 69 A HIS 99 A VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
2038|      000000.2016 |      000006.4500 | 00000018710582.0000 |     000161.48 | LTS0015363 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1165|      000000.2015 |      000006.4480 | 00000018773850.0000 |     000194.24 | LTS0041775 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
1127|      000000.2149 |      000006.4470 | 00000018805564.0000 |     000201.18 | LTS0021583 | A PHE 80 A
VAL 81 A ASN 82 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0034|      000000.1895 |      000006.4430 | 00000018932954.0000 |     000234.65 | LTS0001309 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0217|      000000.1895 |      000006.4430 | 00000018932954.0000 |     000234.65 | LTS0275722 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0410|      000000.2078 |      000006.4410 | 00000018996972.0000 |     000241.49 | LTS0194153 | A PHE 80 A
LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0726|      000000.2074 |      000006.4280 | 00000019418404.0000 |     000184.86 | LTS0221009 | A PHE 80 A
HIS 99 A TYR 101 A TRP 120 A ASP 122 A LEU 123
0102|      000000.1889 |      000006.4240 | 00000019549946.0000 |     000202.16 | LTS0101613 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ARG 121 A ASP 122
1690|      000000.2065 |      000006.4000 | 00000020358126.0000 |     000305.86 | LTS0275815 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP
120 A ARG 121 A ASP 122 A LEU 123 A SER 124
2096|      000000.1999 |      000006.3960 | 00000020496034.0000 |     000202.60 | LTS0008603 | A LYS 113
A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0206|      000000.1878 |      000006.3840 | 00000020915390.0000 |     000219.92 | LTS0261397 | A LYS 113
A SER 116 A SER 117 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1152|      000000.2126 |      000006.3770 | 00000021163964.0000 |     000268.89 | LTS0034537 | A TYR 69 A
VAL 100 A LEU 111 A GLN 112 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP 120 A
ARG 121 A ASP 122 A LEU 123 A SER 124
1432|      000000.2124 |      000006.3720 | 00000021343324.0000 |     000258.14 | LTS0183297 | A ASP 67 A
TYR 69 A ALA 70 A VAL 100 A TYR 101 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP
122 A LEU 123
1190|      000000.1806 |      000006.3200 | 00000023301216.0000 |     000225.89 | LTS0053359 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0211|      000000.1856 |      000006.3120 | 00000023617974.0000 |     000231.63 | LTS0269282 | A LEU 111
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A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0749|      000000.2036 |      000006.3120 | 00000023617974.0000 |     000188.57 | LTS0041890 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0805|      000000.2036 |      000006.3120 | 00000023617974.0000 |     000188.57 | LTS0041890 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0860|      000000.2036 |      000006.3120 | 00000023617974.0000 |     000188.57 | LTS0041890 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1166|      000000.2036 |      000006.3120 | 00000023617974.0000 |     000188.57 | LTS0041890 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
2110|      000000.2036 |      000006.3120 | 00000023617974.0000 |     000188.57 | LTS0041890 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1529|      000000.2102 |      000006.3050 | 00000023898670.0000 |     000249.44 | LTS0237196 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0746|      000000.2099 |      000006.2980 | 00000024182700.0000 |     000184.79 | LTS0024392 | A SER 79 A
PHE 80 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1134|      000000.2099 |      000006.2980 | 00000024182700.0000 |     000184.79 | LTS0024392 | A SER 79 A
PHE 80 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0504|      000000.1850 |      000006.2910 | 00000024470106.0000 |     000279.30 | LTS0246099 | A PHE 80 A
TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1017|      000000.1850 |      000006.2910 | 00000024470106.0000 |     000279.30 | LTS0246099 | A PHE 80 A
TYR 101 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1028|      000000.2731 |      000006.2810 | 00000024886622.0000 |     000216.92 | LTS0043560 | A ASP 67 A
GLU 68 A TYR 69 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
0191|      000000.1846 |      000006.2760 | 00000025097532.0000 |     000216.27 | LTS0239149 | A LEU 111
A LYS 113 A SER 116 A SER 117 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0494|      000000.1961 |      000006.2750 | 00000025139928.0000 |     000180.67 | LTS0191991 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
1007|      000000.1961 |      000006.2750 | 00000025139928.0000 |     000180.67 | LTS0191991 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
1419|      000000.2506 |      000006.2660 | 00000025524726.0000 |     000197.30 | LTS0176089 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1559|      000000.2089 |      000006.2660 | 00000025524726.0000 |     000218.13 | LTS0250010 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
1090|      000000.2087 |      000006.2610 | 00000025741044.0000 |     000281.28 | LTS0002885 | A TYR 69 A
VAL 100 A TYR 101 A LEU 111 A GLN 112 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A
ARG 121 A ASP 122 A LEU 123
0475|      000000.2086 |      000006.2580 | 00000025871712.0000 |     000202.46 | LTS0064000 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A LYS 113 A TRP 120 A ASP 122
0988|      000000.2086 |      000006.2580 | 00000025871712.0000 |     000202.46 | LTS0064000 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A LYS 113 A TRP 120 A ASP 122
0922|      000000.2018 |      000006.2570 | 00000025915416.0000 |     000179.88 | LTS0175295 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1662|      000000.1955 |      000006.2550 | 00000026003044.0000 |     000219.19 | LTS0143436 | A PHE 80 A
HIS 99 A TYR 101 A TRP 120 A ASP 122 A LEU 123 A SER 124 A GLU 125
1273|      000000.1952 |      000006.2470 | 00000026356534.0000 |     000198.62 | LTS0091769 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
1219|      000000.2013 |      000006.2410 | 00000026624800.0000 |     000198.06 | LTS0065765 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1722|      000000.2013 |      000006.2410 | 00000026624800.0000 |     000198.06 | LTS0065765 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0373|      000000.1891 |      000006.2400 | 00000026669776.0000 |     000205.81 | LTS0250838 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
1058|      000000.1891 |      000006.2400 | 00000026669776.0000 |     000205.81 | LTS0250838 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
1902|      000000.1891 |      000006.2400 | 00000026669776.0000 |     000205.81 | LTS0250838 | A PHE 80 A
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PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
2219|      000000.1891 |      000006.2400 | 00000026669776.0000 |    000205.81 | LTS0250838 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
0188|      000000.1834 |      000006.2350 | 00000026895796.0000 |    000191.63 | LTS0228816 | A LEU 111
A LYS 113 A SER 116 A SER 117 A LEU 118 A TRP 120 A ARG 121 A ASP 122
1430|      000000.1886 |      000006.2250 | 00000027353600.0000 |    000247.57 | LTS0182529 | A TYR 69 A
VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A
LEU 123
1156|      000000.1944 |      000006.2220 | 00000027492456.0000 |    000211.63 | LTS0038802 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
0014|      000000.1728 |      000006.2200 | 00000027585416.0000 |    000233.00 | LTS0093930 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0673|      000000.2221 |      000006.2190 | 00000027632016.0000 |    000223.27 | LTS0073114 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1229|      000000.2071 |      000006.2130 | 00000027913264.0000 |    000230.12 | LTS0069946 | A LYS 113
A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1607|      000000.1827 |      000006.2110 | 00000028007648.0000 |    000204.41 | LTS0271661 | A GLY 78 A
PHE 80 A HIS 99 A TYR 101 A TRP 120 A ASP 122 A LEU 123 A SER 124 A GLU 125
0820|      000000.2070 |      000006.2100 | 00000028054960.0000 |    000189.27 | LTS0176364 | A PHE 80 A
VAL 81 A ASN 82 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0923|      000000.2070 |      000006.2100 | 00000028054960.0000 |    000189.27 | LTS0176364 | A PHE 80 A
VAL 81 A ASN 82 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
0099|      000000.1773 |      000006.2060 | 00000028245006.0000 |    000214.66 | LTS0098924 | A LEU 111
A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0130|      000000.1821 |      000006.1900 | 00000029018158.0000 |    000241.31 | LTS0145330 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
1668|      000000.1821 |      000006.1900 | 00000029018158.0000 |    000183.14 | LTS0167194 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
0038|      000000.1815 |      000006.1720 | 00000029913278.0000 |    000215.17 | LTS0003728 | A LYS 113
A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0751|      000000.2057 |      000006.1710 | 00000029963810.0000 |    000191.89 | LTS0048893 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
2114|      000000.2057 |      000006.1710 | 00000029963810.0000 |    000191.89 | LTS0048893 | A PHE 80 A
VAL 81 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1253|      000000.1928 |      000006.1690 | 00000030065128.0000 |    000186.95 | LTS0079372 | A PHE 80 A
TYR 101 A TRP 120 A ARG 121 A ASP 122
1585|      000000.1990 |      000006.1690 | 00000030065128.0000 |    000160.22 | LTS0263482 | A PHE 80 A
VAL 81 A TYR 101 A TRP 120 A ASP 122
1761|      000000.1990 |      000006.1690 | 00000030065128.0000 |    000160.22 | LTS0263482 | A PHE 80 A
VAL 81 A TYR 101 A TRP 120 A ASP 122
1841|      000000.1814 |      000006.1680 | 00000030115914.0000 |    000145.25 | LTS0122037 | A PHE 80 A
TYR 101 A TRP 120 A ARG 121 A ASP 122
2160|      000000.1814 |      000006.1680 | 00000030115914.0000 |    000145.25 | LTS0122037 | A PHE 80 A
TYR 101 A TRP 120 A ARG 121 A ASP 122
1577|      000000.1986 |      000006.1570 | 00000030680268.0000 |    000176.33 | LTS0257989 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
1325|      000000.1809 |      000006.1510 | 00000030992544.0000 |    000233.81 | LTS0124339 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122
1469|      000000.1862 |      000006.1430 | 00000031413860.0000 |    000198.52 | LTS0200073 | A PHE 80 A
HIS 99 A TYR 101 A PHE 103 A THR 105 A LEU 111 A TRP 120 A ASP 122
2166|      000000.1919 |      000006.1400 | 00000031573326.0000 |    000168.22 | LTS0136738 | A PHE 80 A
TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1650|      000000.1855 |      000006.1230 | 00000032492378.0000 |    000198.86 | LTS0086923 | A PHE 80 A
HIS 99 A TYR 101 A TRP 120 A ASP 122 A LEU 123 A SER 124
1316|      000000.2352 |      000006.1150 | 00000032934082.0000 |    000190.32 | LTS0120161 | A PHE 80 A
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LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122
0585|      000000.2444 |      000006.1110 | 00000033157182.0000 |     000258.80 | LTS0130084 | A ASP 67 A
TYR 69 A VAL 100 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP
122
0619|      000000.2444 |      000006.1110 | 00000033157182.0000 |     000258.80 | LTS0206837 | A ASP 67 A
TYR 69 A VAL 100 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP
122
2157|      000000.2263 |      000006.1110 | 00000033157182.0000 |     000234.00 | LTS0119092 | A TYR 69 A
VAL 100 A LEU 111 A LYS 113 A SER 116 A SER 117 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A
ASP 122 A LEU 123
1488|      000000.2036 |      000006.1090 | 00000033269298.0000 |     000199.11 | LTS0209719 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1320|      000000.1851 |      000006.1080 | 00000033325498.0000 |     000278.05 | LTS0122404 | A ASP 67 A
TYR 69 A ALA 70 A VAL 100 A TYR 101 A LYS 113 A ASP 114 A SER 116 A LEU 118 A ARG 121 A ASP
122 A LEU 123 A SER 124
0065|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0212|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0754|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0796|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0808|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0834|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0871|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0969|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1214|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1601|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1780|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1807|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
2126|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0062833 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
2225|      000000.1969 |      000006.1050 | 00000033494668.0000 |     000231.67 | LTS0269561 | A PHE 80 A
LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A LEU 123
1113|      000000.2105 |      000006.1040 | 00000033551248.0000 |     000174.34 | LTS0016921 | A PHE 80 A
HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1634|      000000.2105 |      000006.1040 | 00000033551248.0000 |     000174.34 | LTS0016921 | A PHE 80 A
HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1911|      000000.2105 |      000006.1040 | 00000033551248.0000 |     000174.34 | LTS0016921 | A PHE 80 A
HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
2100|      000000.2105 |      000006.1040 | 00000033551248.0000 |     000174.34 | LTS0016921 | A PHE 80 A
HIS 99 A TYR 101 A PHE 103 A LEU 111 A TRP 120 A ASP 122
1211|      000000.1743 |      000006.1010 | 00000033721564.0000 |     000251.26 | LTS0061079 | A PHE 80 A
TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A
```

```
LEU 123
2206|      000000.2033 |      000006.1000 | 00000033778528.0000 |    000235.36 | LTS0221217 | A TYR 69 A
VAL 100 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A ASP 122 A
LEU 123
0485|      000000.1905 |      000006.0950 | 00000034064792.0000 |    000245.52 | LTS0120993 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
0998|      000000.1905 |      000006.0950 | 00000034064792.0000 |    000245.52 | LTS0120993 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
1530|      000000.2030 |      000006.0900 | 00000034353484.0000 |    000255.91 | LTS0237547 | A TYR 69 A
HIS 99 A VAL 100 A TYR 101 A LYS 113 A SER 116 A ARG 121 A ASP 122 A LEU 123 A SER 124
0575|      000000.2254 |      000006.0870 | 00000034527876.0000 |    000249.69 | LTS0117764 | A TYR 69 A
VAL 100 A TYR 101 A LEU 111 A LYS 113 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121 A
ASP 122 A LEU 123
1125|      000000.2099 |      000006.0860 | 00000034586200.0000 |    000194.29 | LTS0020786 | A PHE 80 A
VAL 81 A ASN 82 A HIS 99 A TYR 101 A TRP 120 A ASP 122
0383|      000000.2433 |      000006.0820 | 00000034820492.0000 |    000202.79 | LTS0024698 | A LEU 111
A LYS 113 A ASP 114 A SER 116 A LEU 118 A PRO 119 A TRP 120 A ARG 121
0711|      000000.1901 |      000006.0820 | 00000034820492.0000 |    000186.50 | LTS0192817 | A LYS 113
A SER 116 A LEU 118 A TRP 120 A ARG 121 A ASP 122 A LEU 123
0676|      000000.1962 |      000006.0810 | 00000034879312.0000 |    000179.81 | LTS0088634 | A PHE 80 A
PHE 103 A LEU 111 A LYS 113 A ASP 114 A TRP 120 A ASP 122
The random seed used during docking was 0.
Point charges and dihedral barriers were obtained from the AMBER03 force field.
```

Lampiran 10. Perintah BEcalculation.mcr

```
Antialias 0
Console Off
Processors cputhreads=30, 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 00100
  LoadPDB (MacroDir)\ok3iol_006(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)\ok3iol_006(k)_complex.sce
  Clear

#Calculation
method = 'VINALS'
runs = 1
rmsdmin = 5.0
rigid = 1
for j=00001 to 00100
  LoadSce (MacroDir)\ok3iol_006(j)_complex.sce
  NameObj 1,receptor
  NameObj 2,ligand
  ForceField AMBER03
```

```
  Boundary Wall
  Longrange None
#FixAll

  Experiment Docking
    Method (method)
    ReceptorObj (1)
    LigandObj 2
    Runs (runs)
    ClusterRMSD (rmsdmin)
  # Result file number must be separated with '_', in case MacroTarget also ends with number
    ResultFile temp_001
  # Uncomment below to set the number of energy evaluations (AutoDock ga_num_evals):
  # DockPar ga_num_evals 25000000
  # Uncomment the two lines below to provide your own atom parameters (VdW radii etc.)
  # GridPar parameter_file /Path/To/Custom/AD4_parameters.dat
  # DockPar parameter_file /Path/To/Custom/AD4_parameters.dat
  # If you want to keep all temporary files, uncomment below
  # TmpFileID YourChoice
  Experiment On
  Wait ExpEnds
  # Save a scene with receptor and all ligand conformations
  SaveSce (MacroDir)\ok3iol_006(j)_result.sce
  # Save a log file with an analysis

  Console Off
  RecordLog (MacroDir)\ok3iol_006(j)_result.log
  print 'Local docking result analysis'
  print '============================'
  print
  print '(runs) (method) docking runs of the ligand object 2 to the receptor object 1 yielded the following results,'
  print 'sorted by binding energy: [More positive values indicates stronger binding, and negative values mean no
binding]'
  print
  print 'Run |Bind.energy[kcal/mol]|Dissoc.constant[pM]| Contacting receptor residues'
  print '----+-------------------+----------------+--------------------------'
  clusters=0
  for i=001 to runs
    # Ligands have SegmentID C001, C002 etc.
    result = DockingResult i,'Obj 1','Segment C(i)'
    print (result)
    StopLog
  HideMessage
  Console On
  LoadSce (MacroDir)\ok3iol_006(j)_result.sce
  # Exit YASARA if this macro was provided as command line argument in console mode
  if runWithMacro and ConsoleMode
    Exit

# EXTRACT DOCKING RESULT
# =====================
# Returns a result string. 'num' is a sequential number, 'recsel' selects the receptor, 'ligsel' the ligand.
  def DockingResult num,recsel,ligsel
  # Get the binding energy from the B-factor...
    bindnrg = BFactorAtom (ligsel)
```

```
# ...and the dissociation constant from the atomic property.
 dissconst = PropAtom (ligsel)
 if bindnrg<=0
  dissconst='              None'
 else
  dissconst= 00000000000000.0000+dissconst
# Get receptor residues that contact the ligand
 reslist() = ListRes (recsel) with distance<4.0 from (ligsel),Format='MOLNAME RESNAME RESNUM'
 if !count reslist
  reslist='No residues in contact'
 else
  reslist=join reslist
 result='(000+num) |        (000000.0000+bindnrg) | (dissconst) | (reslist)'
 return result
Clear
```

Lampiran 11. 1972_hasil rmsd

```
214.746
0.48496
0.48782
0.4888
0.49594
0.50362
0.51246
0.39396
0.40674
0.3955
0.4009
0.41142
0.41992
0.4273
0.43886
0.32736
0.289
0.29838
0.30852
0.31452
0.3124
0.31196
0.311
0.31194
0.31496
0.29376
0.28314
0.31398
0.30988
0.31192
0.31356
```

0.3118
0.3129
0.31318
0.31274
0.31816
0.3275
0.33718
0.34814
0.35216
0.35458
0.35404
0.36226
0.36186
0.36278
0.36104
0.367
0.3708
0.37234
0.3828
0.38874
0.3827