High-throughput MD tutorial

Login to cluster

from Linux OS

cp ./dd-23-13-01 ~/.ssh/

chmod 600 ~/.ssh/dd-23-13-01

ssh -i ~/.ssh/dd-23-13-01 dd-23-13-XX@login1.karolina.it4i.cz

from Windows OS:

Use PuTTY.

PuTTY Configuration:

Host name: *dd-23-13-XX@login1.karolina.it4i.cz*

SSH - Auth - add Private key file for authentication

XX - your user ID

Automated Molecular Docking

https://github.com/ci-lab-cz/docking-scripts

1) Prepare working directory and files

mkdir docking_tutorial
cd docking_tutorial
cp /mnt/proj2/dd-23-13/docking_tutorial/{ligands_pH74.smi,protein_prepared.pdbqt,config.txt} .

2) Run calculations on the Karolina cluster

qsub -A DD-23-13 -v input=$(pwd)/ligands_pH74.smi,protein=$(pwd)/protein_prepared.pdbqt,config=$(pwd)/config.txt /mnt/proj2/dd-23-13/script_vina.pbs

3) Convert sdf of docked poses to mol files for further molecular dynamics simulation with added by RDKit hydrogens

module load Anaconda3
source activate vina

python /mnt/proj2/dd-23-13/md-scripts/scripts/sdf2mols.py -i ligands_pH74_protein_prepared_docking_vina_output.sdf -o mols

Automated Molecular Dynamics

https://github.com/ci-lab-cz/md-scripts/tree/master/Protein-Ligand_MD_PBGBSA

1) Prepare working directory and files

cd
mkdir md_tutorial
cd md_tutorial
cp /mnt/proj2/dd-23-13/md_tutorial/{protein_prepared.pdb,ligand.mol} .

2) Run molecular dynamics simulation for 0.1 ns on the Karolina cluster

qsub -A DD-23-13 -v
lfile=$(pwd)/ligand.mol,pfile=$(pwd)/protein_prepared.pdb,script_path=/mnt/proj2/dd-23-13/md-scripts/scripts/,wdir=ligand_01ns,mdtime=0.1,gromacs_version='GROMACS/2021.4-foss-2020b-PLUMED-2.7.3'
/mnt/proj2/dd-23-13/md-scripts/Protein-Ligand_MD_PBGBSA/01_complex_preparation_md.pbs

3) Run GBSA energy calculation

qsub -A DD-22-13 -v
tpr=md_out.tpr,xtc=md_fit.xtc,script_path=/mnt/proj2/dd-23-13/md-scripts/scripts/,wdir=ligand_01ns/,NP=11
/mnt/proj2/dd-23-13/md-scripts/Protein-Ligand_MD_PBGBSA/02_pbsa.pbs

4) Collect GBSA energies

wdir=$(pwd) bash
/mnt/proj2/dd-23-13/md-scripts/Protein-Ligand_MD_PBGBSA/03_sum_result_pbsa.pbs

5) Analysis of molecular dynamics simulation

module load grace
cd ligand_01ns/
for i in *.xvg; do gracebat -hdevice PNG $i;done

6) To copy files from cluster to computer

from Linux OS

scp -I ~/.ssh/dd-23-13-XX dd-23-13-XX@login1.karolina.it4i.cz:md_tutorial/ligand_01ns/{frame.pdb,md_fit.xtc,*.png} .

from Windows OS

use PowerShell.

pscp -i path_to_your_ppk\dd-23-13-XX.ppk dd-23-13-XX@login1.karolina.it4i.cz:md_tutorial/ligand_01ns/frame.pdb .

pscp -i path_to_your_ppk\dd-23-13-XX.ppk dd-23-13-XX@login1.karolina.it4i.cz:md_tutorial/ligand_01ns/md_fit.xtc .

pscp -i path_to_your_ppk\dd-23-13-XX.ppk dd-23-13-XX@login1.karolina.it4i.cz:md_tutorial/ligand_01ns/*.png .

XX - user ID