

CHEAT SHEET



BASIC LINUX COMMANDS

cp [filename] [path] Copies a file to the specified location

mv [filename] [path] Moves a file to the specified location

ssh Open SSh client to connect remotely

chmod Change permissions

find Search for a file

tar xvfz Create or extract .tar file

grep Print lines matching the pattern

zip Create or extract zip files

sudo Run the command in superuser mode

| Pipe or redirect the output

nohup Run command immune to hangup signal

echo Display a line of text

ctrl-c Stop current execution

vi Visual editor

nano Nano editor

DIRECTORY COMMANDS

mkdir Make a directory

rmdir Remove the directory

pwd Current path

cd [path] Change working directory

ls List all the files

ls -ltrh List all the files in human readable format

ls *.pdb List all the pub files

VI COMMANDS

Press I Insert mode

Esc+q+: Quit without saving

Esc+wq+: Quit after saving

Shift+g Navigate to the end of file

Press gg Navigate to the start of the file

Press dd Delete an entire line

Ctrl+Shift+C/V Copy/Paste content

GROMACS COMMANDS

gmx help Get information about any grimaces module

gmx pdb2gmx Convert .pdb file to a .gro format

gmx ediconf Converts .pdb to .gro along with box definition

gmx solvate Adding solvent to the prepared box

gmx grompp Producing the run input .tpr file

gmx genion Adding ions to neutralise the system

gmx mdrun Carry out mdrun using GROMACS

gmx energy Compute various thermodynamic parameters

gmx trjconv Modify the trajectory file

gmx rms Compute RMSD property for the trajectory

gmx gyrate Compute radius of gyration property

gmx rmsf Compute rms fluctutaion property

gmx sasa Compute the solvent-accessible surface area

gmx make_ndx Make an index file

gmx trjcat Concatenate trajectory files