BT305

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Lab 2

① install vi editor → sudo apt install vim

:qa ↵ (to exit)

② vim <filename>

③ to delete text : highlight text, press dd to be deleted

OR

(no. of lines to be deleted) dd (Ex: 240dd)

* place cursor at the start, from where you want to start deleting.

④ to save

:w <filename>

⑤ grep "CA" file1.pdb > file2.pdb (Q3)

(to save)

⑥ :%s/ATOM/Yourname/g (Q4)

:w <filename> # to save

⑦ to concatenate

cat file1.pdb file2.pdb > file3.pdb

(saved as file3.pdb)

cat <filename>

↓

to open the file on the terminal.

⑧ to count no. of lines

wc -l <filename>

⑨ awk '{print $7, $8, $9}' <filename>

↓

(column number, starting from 1)

cat file11.txt | awk '{sum += $1} END {print sum}'

prints 1st column's sum.

Lab5 → to do (not ribosome)

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Lab 3

for both main & side table.

Use VADAR, save the main & side table
Use grep to extract helix values " H "
Use awk to get phi, psi values ka column. → direct edit

* Remove the 'I' → gives an error → considered as a separate column.

column-wise concatenation

paste file1.txt file2.txt -d " " > file_result.txt
(delimiter)

↓

has phi psi chi values.

Install Ribosome (fortran as well)
shift .zmat to labse pehla directory
edit the file_result.txt on excel

↓

res ala phi -69.2 psi -32.2 chi1 360
(amino acid)

↓

save as text file.

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Lab 6

download models from 'swiss model'

align model-03, model_04
you get the rmsd value automatically
(about the PyMOL>

VAST Score is the sequence identity.

Lab 8 (doesn't exist)

Lab 9

./agfrgui

Lab 10

download from drugbank.