Class 6 HW

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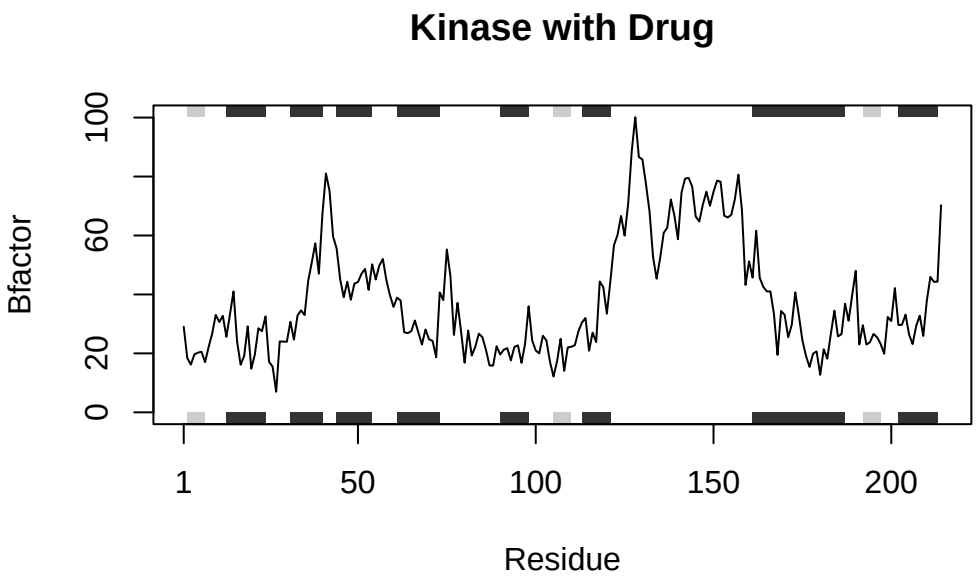
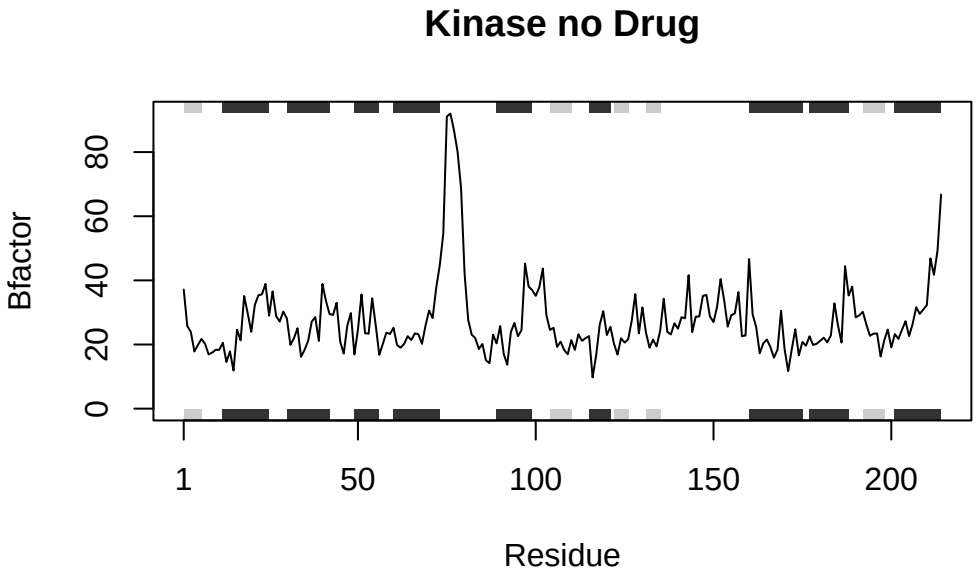
```
library(bio3d)
```

```
#Encapsulate to reduce code replication
x <- function(pdb_file, chain_id, plot_title) {
  #Read PDB file
  structure <- read.pdb(pdb_file)

  #Trim to the specified chain and extract CA atoms
  chainA <- trim.pdb(structure, chain = chain_id, elety = "CA")

  #Extract B-factors
  bfactors <- chainA$atom$b

  #Plot B-factors
  plotb3(bfactors, sse = chainA, typ = "l", ylab = "Bfactor", main = plot_title)
}

#Specify PDB files and chain IDs
pdb_files <- c("4AKE", "1AKE", "1E4Y")
chain_ids <- c("A", "A", "A")
plot_titles <- c("Kinase with Drug", "Kinase no Drug", "Kinase with Drug")

#Loop to repeat the process
for (i in 1:length(pdb_files)) {
  x(pdb_files[i], chain_ids[i], plot_titles[i])
}
```

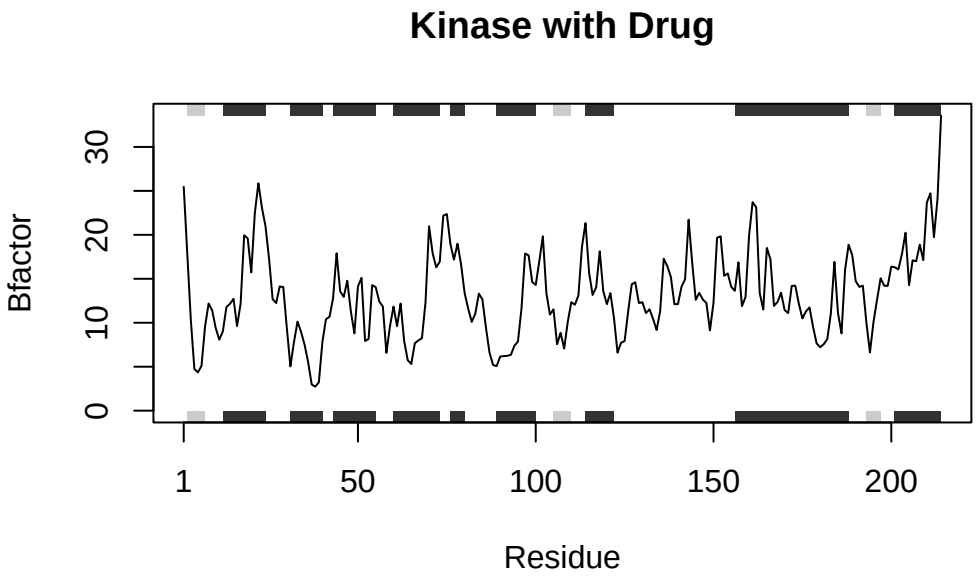
```
Note: Accessing on-line PDB file
```




```
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
```



```
Note: Accessing on-line PDB file
```



Q1. What type of object is returned from the read.pdb() function?

The object returned is a pbd, a derivation of a protein data bank file.

Q2. What does the trim.pdb() function do?

Using trim.pdb() we can select a specific from a structure multi-chain. Overall, it cleans data from any unwanted aspects of it as we are able to get specifics.

Q3. What input parameter would turn off the marginal black and grey rectangles in the plots and what do they represent in this case?

Eliminating the sse parameter would then result in turning off marginal black and grey rectangles, these are the secondary structural elements of the protein.

Q4. What would be a better plot to compare across the different proteins?

A box plot, so as to have the side by side comparisons of the factors among the different proteins we are comparing.

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this?