HWClass06-Q6

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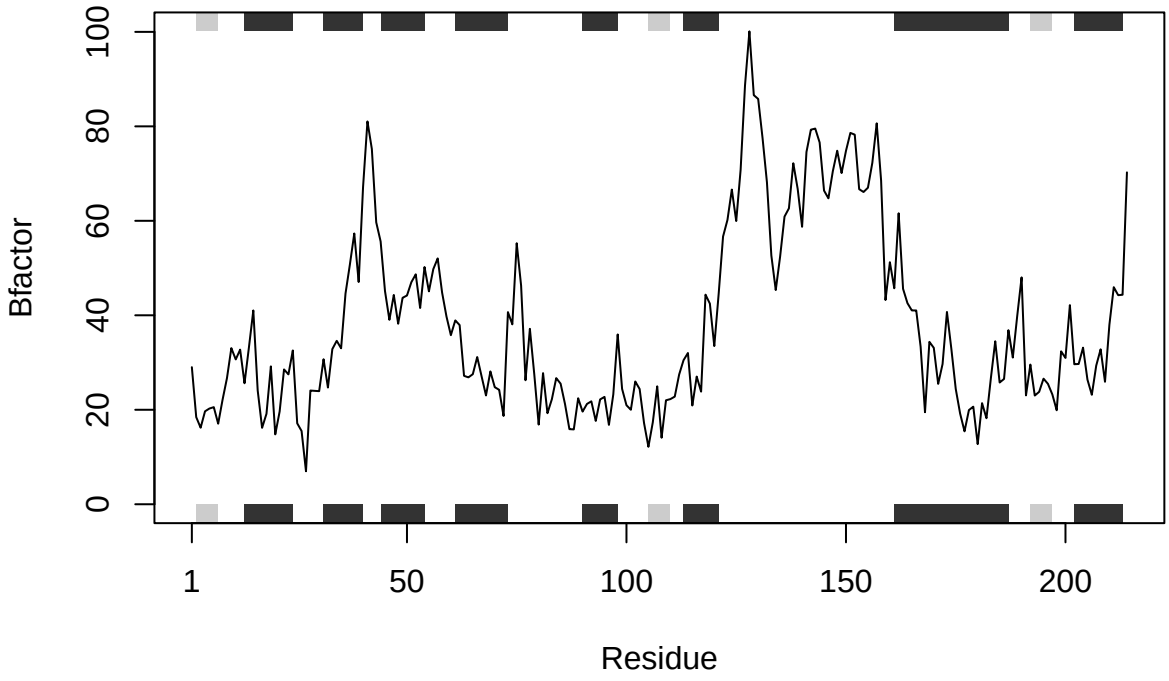
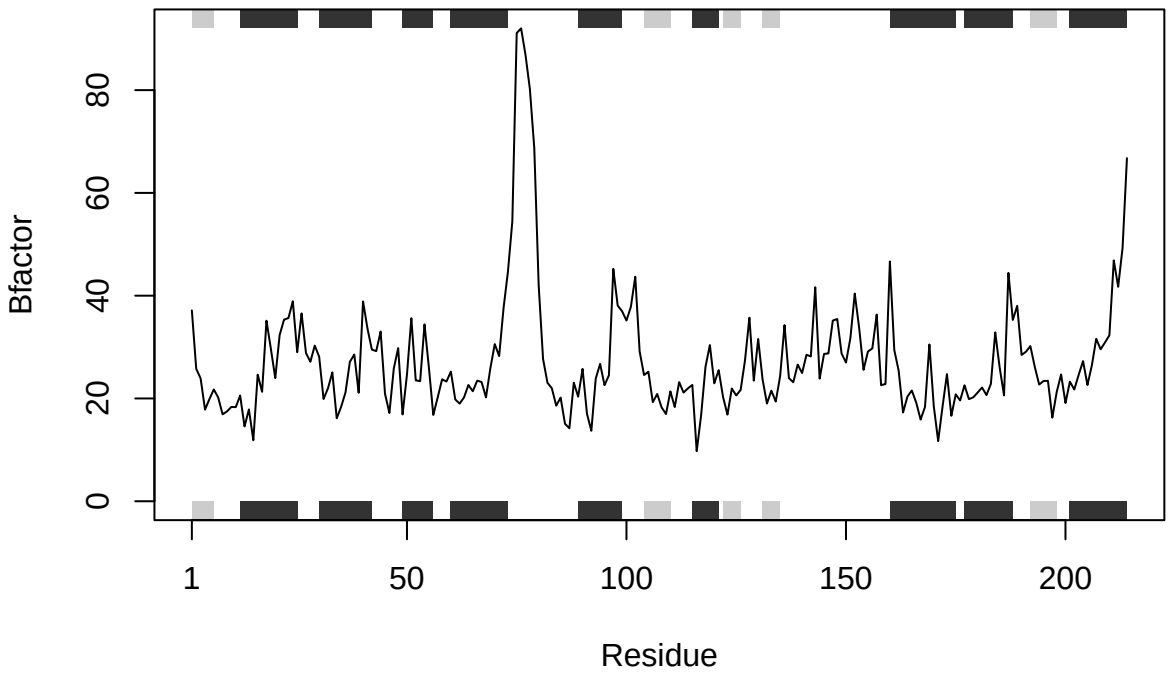
Q6. Write your own function starting from the code above that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein.

```
##install.packages("bio3d") importing bio3d

library(bio3d)
#Create any set of proteins that you want to examine
proteins2 <- list("4AKE","1AKE","1E4Y")

#Inputs are the proteins that you are examining
plottingdendrogram <- function(protein3){

  #Goes through each protein
  processing <- function(protein4){

    #Obtaining a PDB structure object
    spdb <- read.pdb(protein4)

    #Producing a new smaller PDB up to your specifications
    spdb.chainA <- trim.pdb(spdb, chain="A", elety="CA")

    #Picking your subset from smaller PDB
    spdb.b <- spdb.chainA$atom$b

    #Plotting
    plotb3(spdb.b, sse=spdb.chainA, typ="l", ylab="Bfactor")

    #Returning subset
    return(spdb.b)

  }
#Applying the processing function over the set of proteins
broteins <- sapply(protein3, processing)

#Creating a dendrogram based off the subset of the proteins you pick
hc <- hclust( dist( rbind(broteins[,1], broteins[,2], broteins[,3]) ) )

#Plotting dendrogram
plot(hc)
}
#Function plots a dendrogram based on the list of proteins you give
plottingdendrogram(proteins2)
```

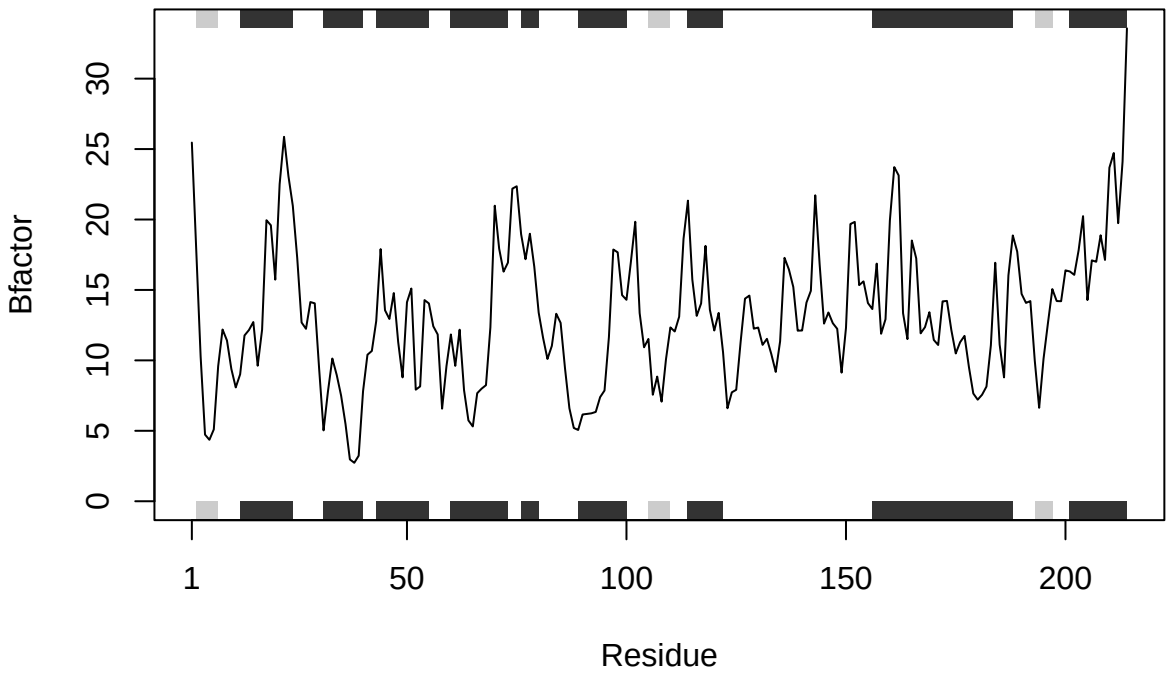
```
##   Note: Accessing on-line PDB file
```

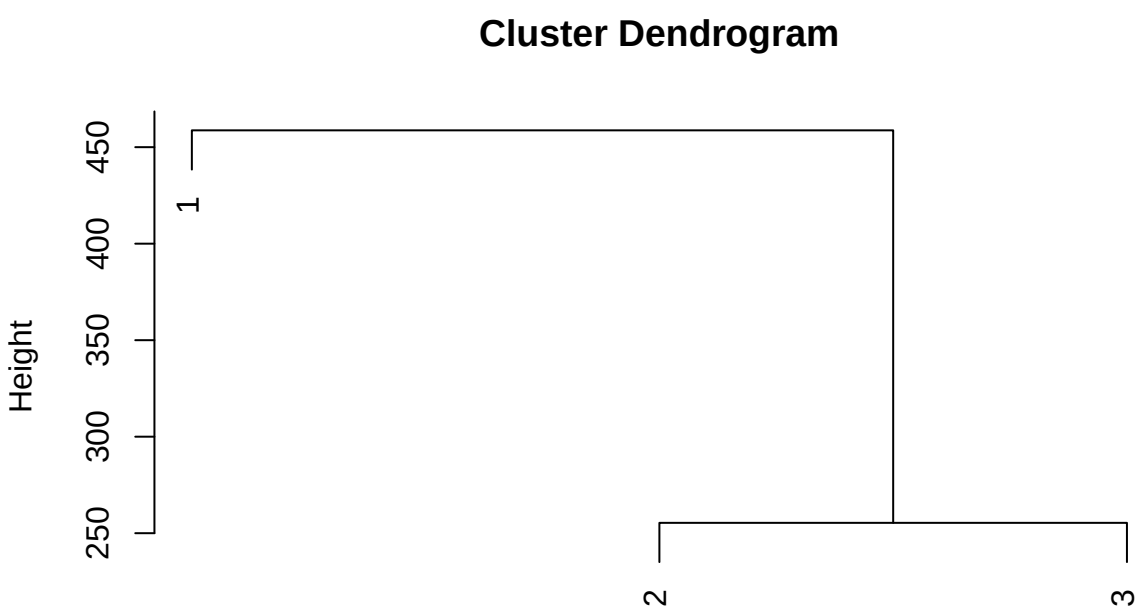



```
##   Note: Accessing on-line PDB file
##    PDB has ALT records, taking A only, rm.alt=TRUE
```




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


Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue


Cluster Dendrogram
Height
450
400
350
300
250
1
2
3
dist(rbind(broteins[, 1], broteins[, 2], broteins[, 3]))
hclust (*, "complete")