HW 06

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Section 1

Problem A

```
#Original code
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
df$a <- (df$a - min(df$a)) / (max(df$a) - min(df$a))
df$b <- (df$b - min(df$a)) / (max(df$b) - min(df$b))
df$c <- (df$c - min(df$c)) / (max(df$c) - min(df$c))
df$d <- (df$d - min(df$d)) / (max(df$a) - min(df$d))
```

```
#Improved code
x<-function(column){
  (column - min(column)) / (max(column) - min(column))
}
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
apply(df, 2, x)
```

```
             a         b         c  d
 [1,] 0.0000000 0.0000000 0.0000000 NA
 [2,] 0.1111111 0.1111111 0.1111111 NA
 [3,] 0.2222222 0.2222222 0.2222222 NA
 [4,] 0.3333333 0.3333333 0.3333333 NA
 [5,] 0.4444444 0.4444444 0.4444444 NA
 [6,] 0.5555556 0.5555556 0.5555556 NA
 [7,] 0.6666667 0.6666667 0.6666667 NA
 [8,] 0.7777778 0.7777778 0.7777778 NA
 [9,] 0.8888889 0.8888889 0.8888889 NA
[10,] 1.0000000 1.0000000 1.0000000 NA
```

Problem B (Intended HW) Installation of Bio3d in the terminal.

```
# Can you improve this analysis code?
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

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

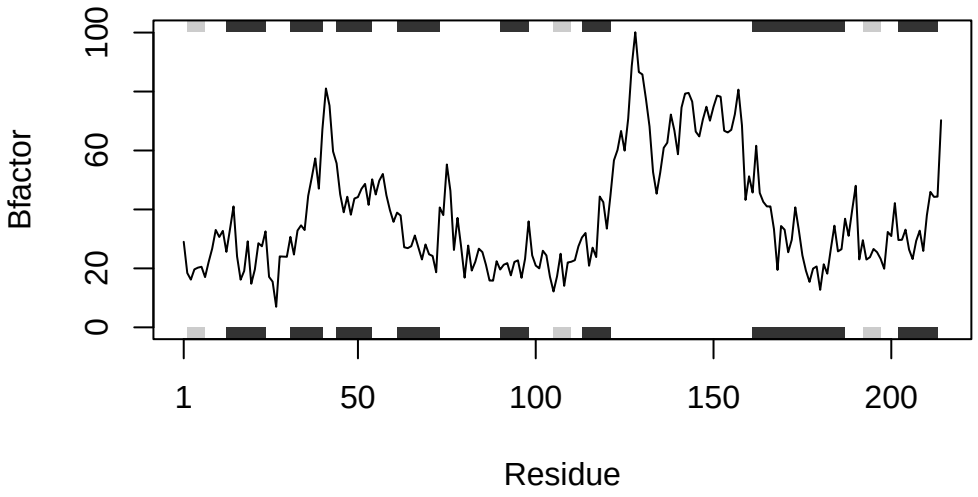
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

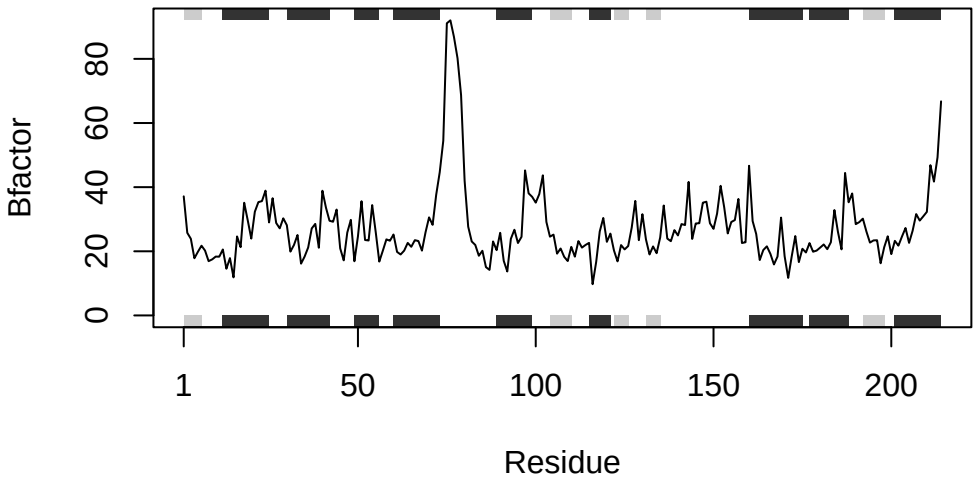
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

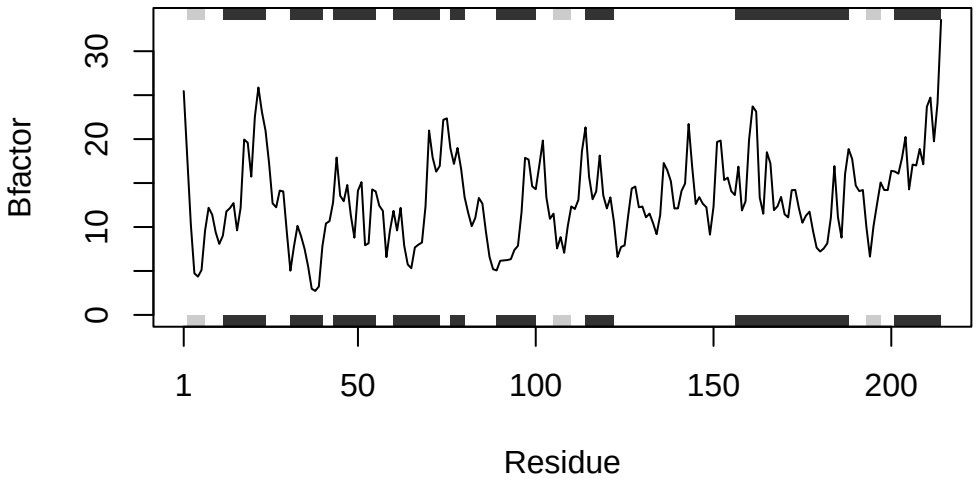
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```



```
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```



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

It is accessing the on-line PDB files. It is now a list contains a lot information including lists and characters.

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

It allows to produce a smaller dataset with the elements indicated in the arguments.

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

Delet the sse argument. They represent the secondary structure object.

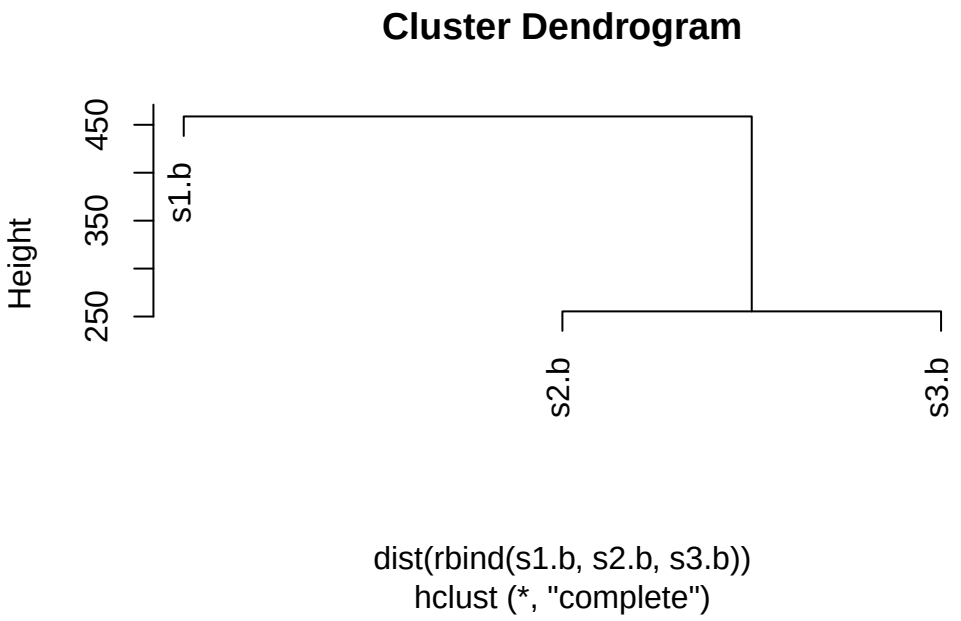
Q4. What would be a better plot to compare across the different proteins?

Using ggplot, just add mutiple y geom layers from different proteins.

Q5. Which proteins are more similar to each other in their B-factor trends. How could you quantify this? HINT: try the rbind(), dist() and hclust() functions together with a resulting dendrogram plot. Look up the documentation to see what each of these functions does.

```
?rbind()
?dist()
?hclust()

hc <- hclust( dist( rbind(s1.b, s2.b, s3.b) ) )
plot(hc)
```



Q6. How would you generalize the original code above to work with any set of input protein structures?

```
#Function y: It will produce produce a vector and
#a graph summarizing binding factor index "Bfactors" based on residues.

#The input of the function is PDB_code like "4AKE",
#the chain info such as "A",
#and the atom name info (elety) such as "CA".
y<-function(PDB_code, chain, elety){
  # Just in case
  library(bio3d)
  # All information of the protein
  all_info <- read.pdb(PDB_code)
```

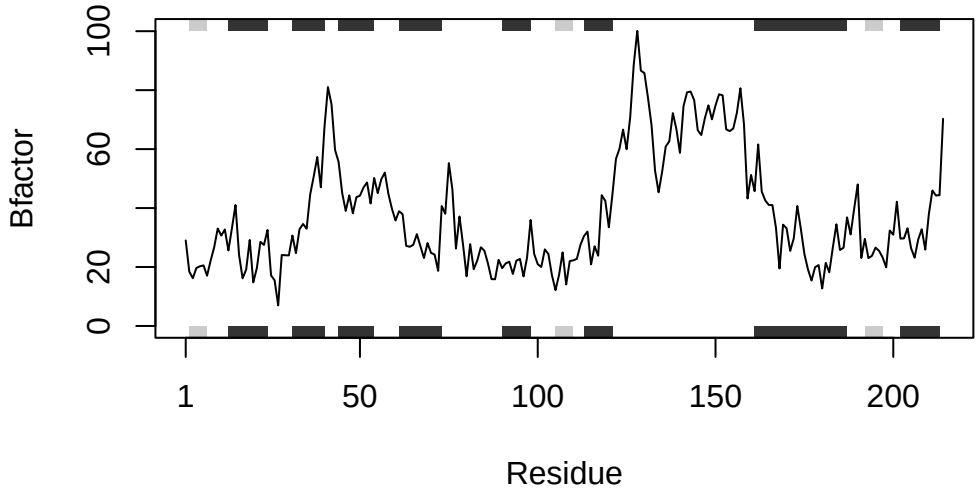
```
  # specific information of the protein.
  specific_info<- trim.pdb(all_info, chain=chain, elety=elety)
  #This will access the b vector in the specific information.
  specific_info.b<-specific_info$atom$b
  #This will return the a vector and a graph
  #summarizing the b factor variable across residues.
  plotb3(specific_info.b, sse=specific_info, typ="l", ylab="Bfactor")
  print (specific_info.b)
}
```

Test run

```
y("4AKE", "A", "CA")#How to use this function
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/wl/tlb448512xb2441v7vw4jms40000gn/T//RtmppkaLHI/4AKE.pdb exists.
Skipping download
```




```
 [1]  29.02  18.44  16.20  19.67  20.26  20.55  17.05  22.13  26.71  33.05
```

```
 [11]  30.66  32.73  25.61  33.19  41.03  24.09  16.18  19.14  29.19  14.79
 [21]  19.63  28.54  27.49  32.56  17.13  15.50   6.98  24.07  24.00  23.94
 [31]  30.70  24.70  32.84  34.60  33.01  44.60  50.74  57.32  47.04  67.13
 [41]  81.04  75.20  59.68  55.63  45.12  39.04  44.31  38.21  43.70  44.19
 [51]  47.00  48.67  41.54  50.22  45.07  49.77  52.04  44.82  39.75  35.79
 [61]  38.92  37.93  27.18  26.86  27.53  31.16  27.08  23.03  28.12  24.78
 [71]  24.22  18.69  40.67  38.08  55.26  46.29  26.25  37.14  27.50  16.86
 [81]  27.76  19.27  22.22  26.70  25.52  21.22  15.90  15.84  22.44  19.61
 [91]  21.23  21.79  17.64  22.19  22.73  16.80  23.25  35.95  24.42  20.96
[101]  20.00  25.99  24.39  17.19  12.16  17.35  24.97  14.08  22.01  22.26
[111]  22.78  27.47  30.49  32.02  20.90  27.03  23.84  44.37  42.47  33.48
[121]  44.56  56.67  60.18  66.62  59.95  70.81  88.63 100.11  86.60  85.80
[131]  77.48  68.13  52.66  45.34  52.43  60.90  62.64  72.19  66.75  58.73
[141]  74.57  79.29  79.53  76.58  66.40  64.76  70.48  74.84  70.11  74.82
[151]  78.61  78.24  66.70  66.10  67.01  72.28  80.64  68.54  43.23  51.24
[161]  45.72  61.60  45.61  42.57  41.03  41.02  33.34  19.48  34.38  33.11
[171]  25.48  29.68  40.71  32.91  24.41  19.20  15.43  19.93  20.66  12.72
[181]  21.40  18.21  26.68  34.50  25.77  26.52  36.85  31.05  39.84  48.03
[191]  23.04  29.57  23.00  23.80  26.59  25.49  23.25  19.89  32.37  30.97
[201]  42.16  29.64  29.69  33.15  26.38  23.17  29.35  32.80  25.92  38.01
[211]  45.95  44.26  44.35  70.26
```