Week 5 Homework

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Section 1: Improving analysis code by writing functions

A. Improve this regular R code by abstracting the main activities in your own new function. Note, we will go through this example together in the formal lecture. The main steps should entail running through the code to see if it works, simplifying to a core working code snippet, reducing any calculation duplication, and finally transferring your new streamlined code into a more useful function for you.

```r
# A. Can you improve this analysis code?
df <- data.frame(a=1:10, b=seq(200,400,length=10),c=11:20,d=NA)
```

```r
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))
```

```r
# A. Improved analysis 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))
```

B. Next improve the below example code for the analysis of protein drug interactions by abstracting the main activities in your own new function. Then answer questions 1 to 6 below. It is recommended that you start a new Project in RStudio in a new directory and then install the bio3d package noted in the R code below (N.B. you can use the command install.packages("bio3d") or the RStudio interface to do this). Then run through the code to see if it works, fix any copy/paste errors before simplifying to a core working code snippet, reducing any calculation duplication, and finally transferring it into a more useful function for you.

Original

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

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

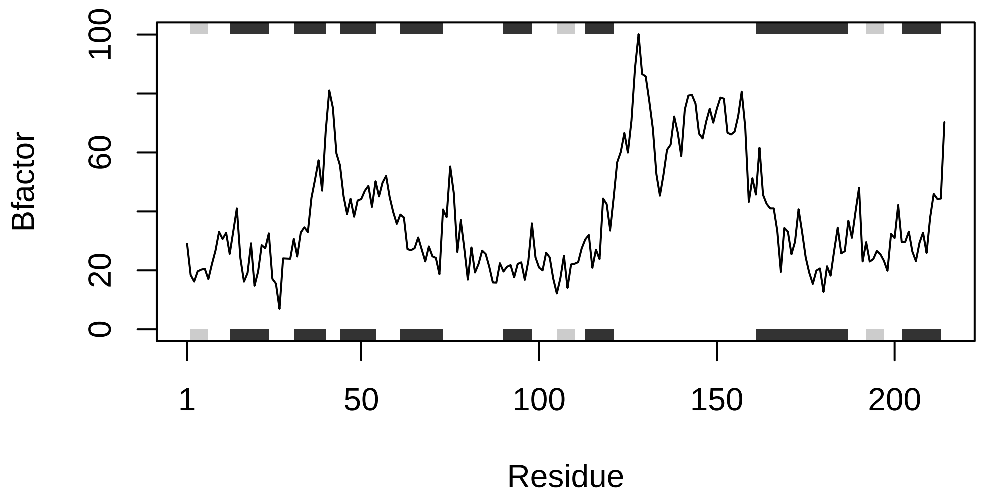
```r
s2 <- read.pdb("1AKE") # kinase no drug
```

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

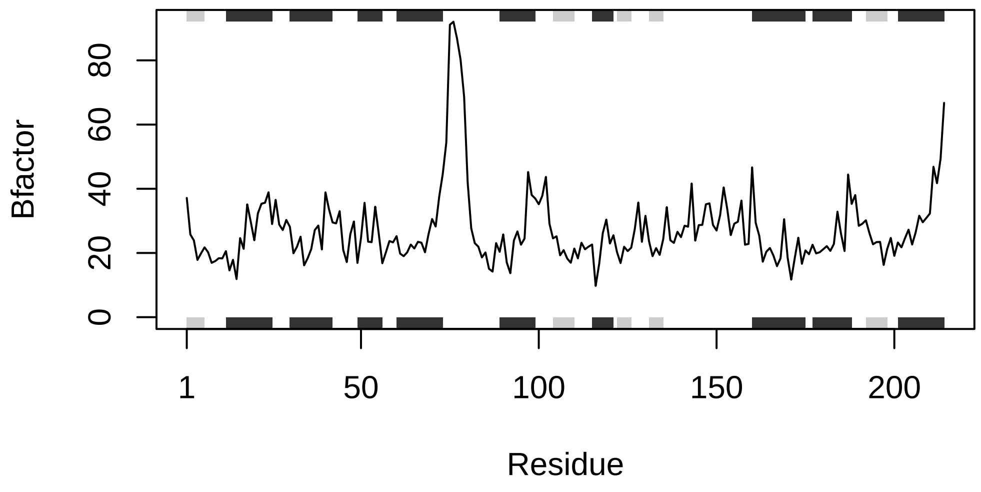
```r
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

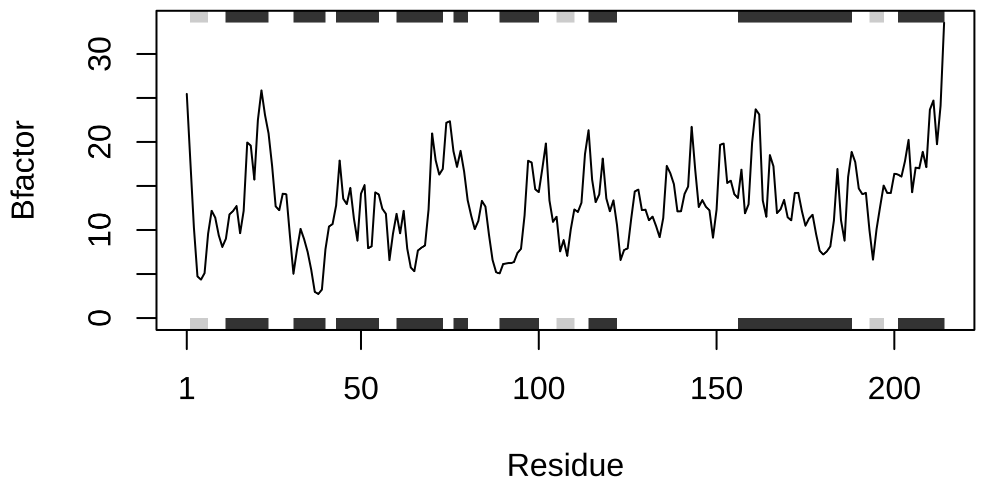
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")

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")
```

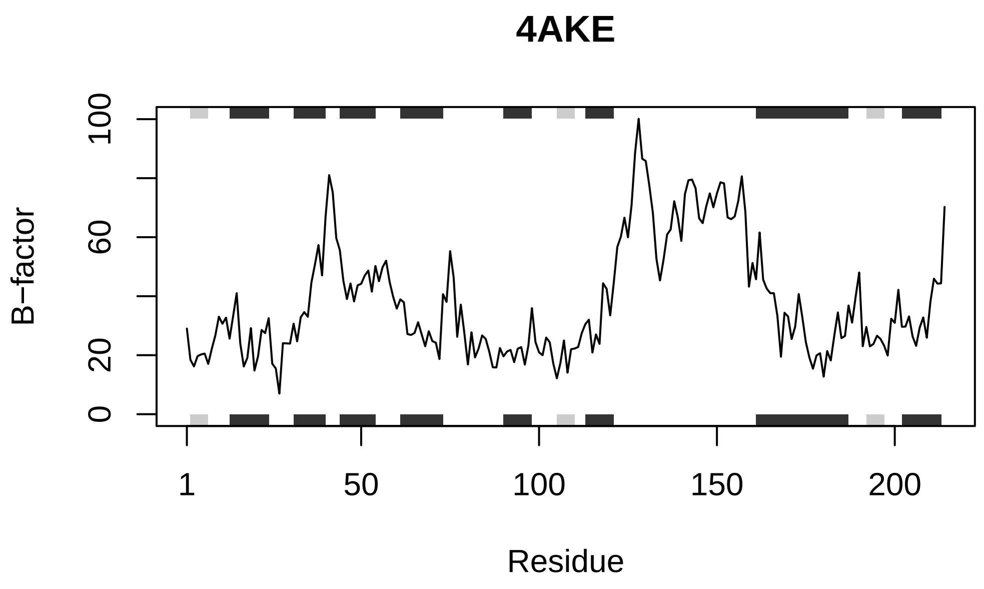


My Version

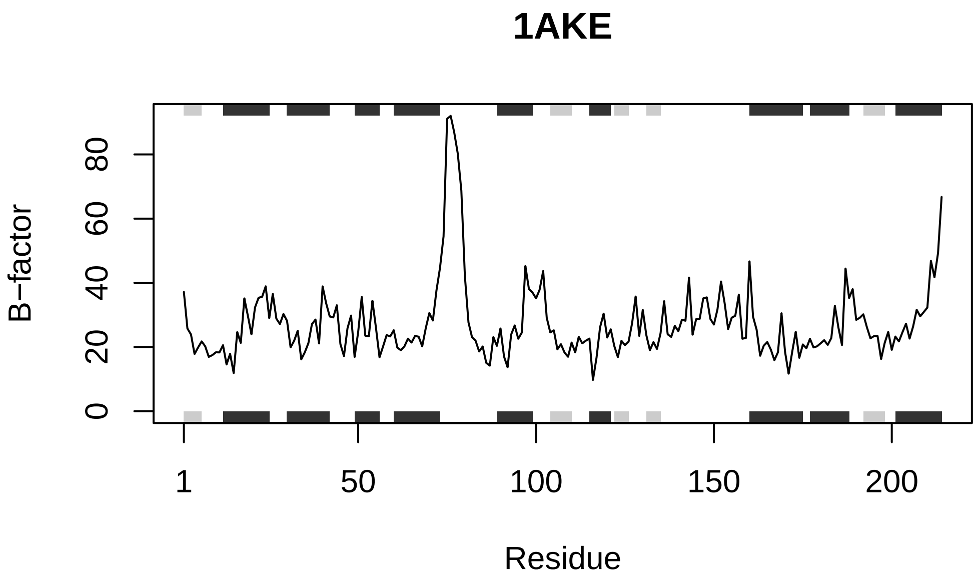
```r
generate.plot <- function(x) {
  # Applies the function to each PDB code provided in vector 'x'
  lapply(x, function(pdb_code) {

    # Reads the structure data from the Protein Data Bank using the given code
    sP <- read.pdb(pdb_code)

    # Extracts only chain A and selects alpha-carbon (CA) atoms
    # This simplifies the structure for plotting B-factors per residue
    s.chainA <- trim.pdb(sP, chain = "A", elety = "CA")

    # Retrieves the B-factor (temperature factor) values for all CA atoms
    sP.b <- s.chainA$atom$b

    # Creates a line plot of B-factor values along the sequence
    # 'sse = s.chainA' adds secondary structure information for shading
    # 'typ = "l"' makes it a line plot, and 'ylab' labels the y-axis. 'main' labels each plo
    finalplot <- plotb3(sP.b, sse = s.chainA, typ = "l", ylab = "B-factor", main = pdb_code)

    # Returns the plot for individual PDB entries
    return(finalplot)
  })
}
```

```r
# Runs the function for three PDB entries: 4AKE, 1AKE, and 1E4Y
generate.plot(c("4AKE", "1AKE", "1E4Y"))
```

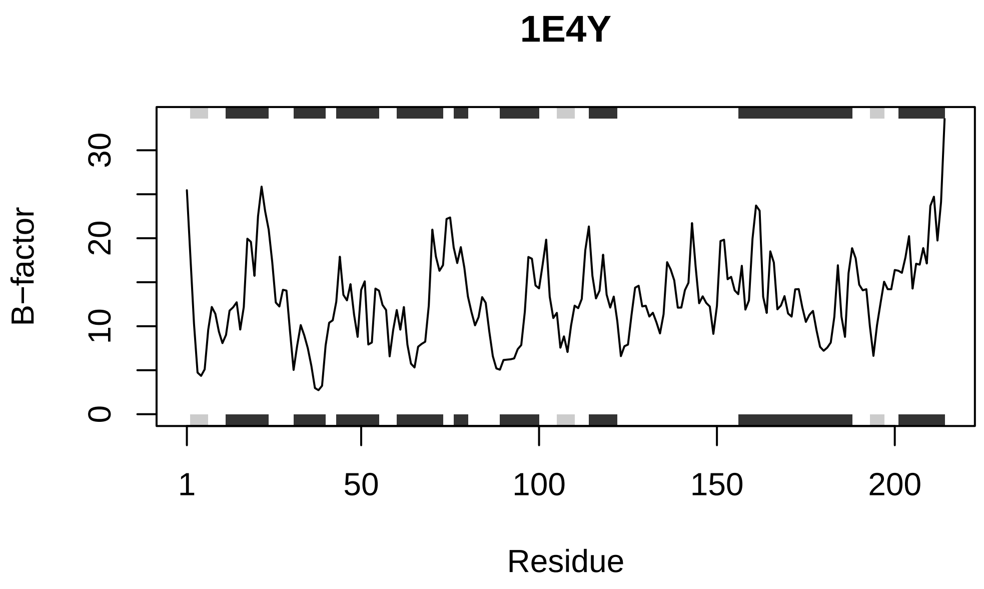
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\kavan\AppData\Local\Temp\RtmpEZQVyN/4AKE.pdb exists. Skipping download
```



```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\kavan\AppData\Local\Temp\RtmpEZQVyN/1AKE.pdb exists. Skipping download

   PDB has ALT records, taking A only, rm.alt=TRUE
```



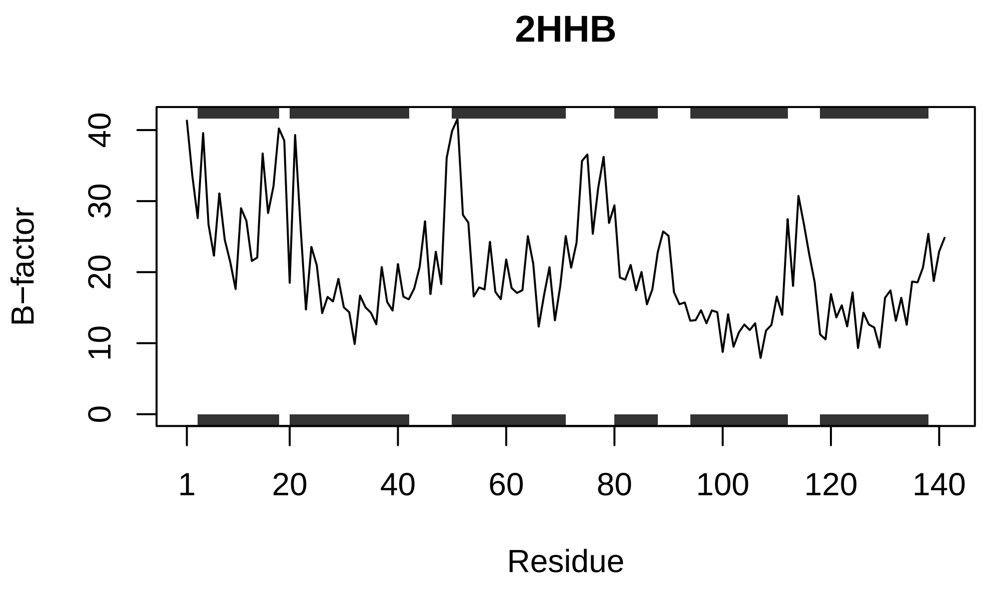
```
  Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\kavan\AppData\Local\Temp\RtmpEZQVyN/1E4Y.pdb exists. Skipping download
```



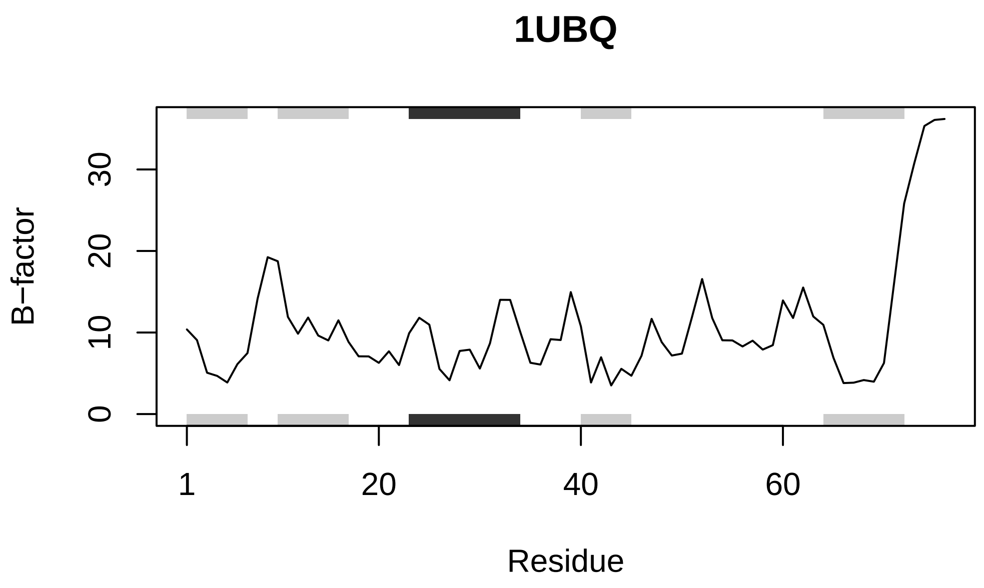
```
[[1]]
NULL

[[2]]
NULL

[[3]]
NULL
```

```
# Picked 3 random sequences, generated for those too
generate.plot(c("2HHB", "1UBQ", "4HHB"))
```

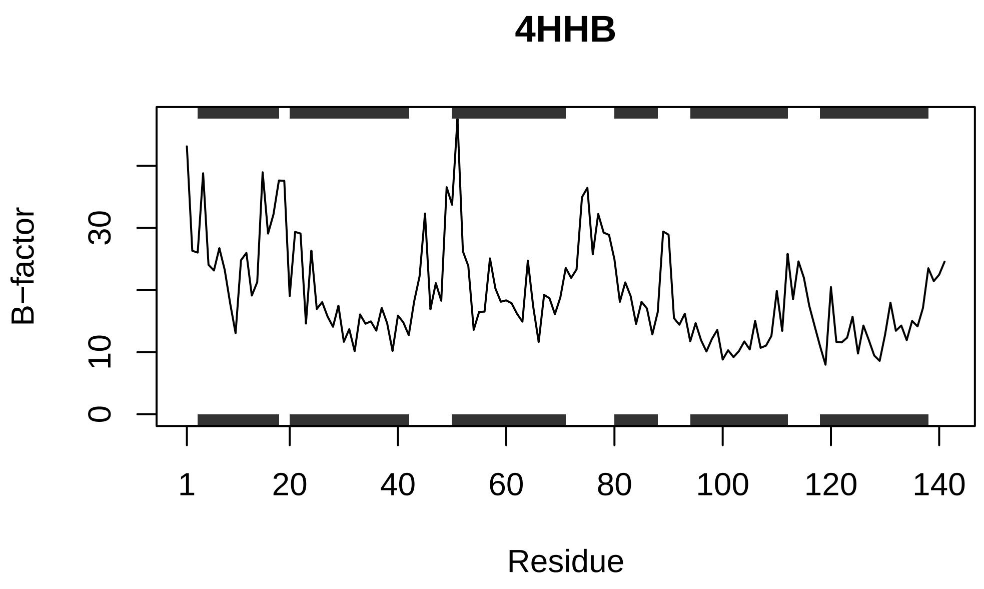
```
  Note: Accessing on-line PDB file
```



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



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



```
[[1]]
NULL

[[2]]
NULL

[[3]]
NULL
```