Homework6 (R Functions)

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Function that can analyze protein drug interactions by reading in any protein PDB data and will output a plot.

```r
library(bio3d)
```

```r
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))
```

```r
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

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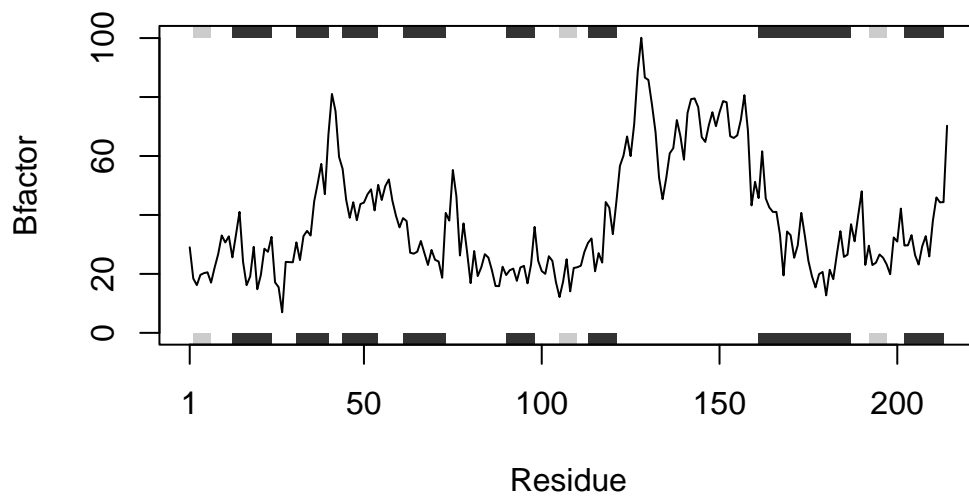
```
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

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")
```
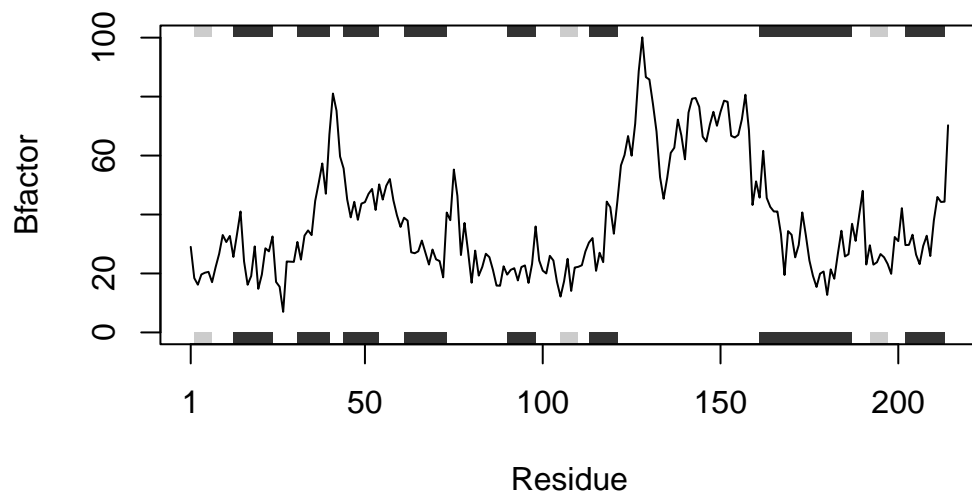


```
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
```

2

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


3

```r
protein_plot <- function(file, chain, elmnt, fctr) {

  #Loop over vector elements
  s1 <- lapply(file, read.pdb)
  s1.chain <- lapply(s1, trim.pdb, chain = chain, elety = elmnt)

  #Accessing columns
  s1.fctr <- lapply(s1.chain, function(x) x$atom[, fctr])

  #Set a color scheme
  color_set <- c("green", "red", "blue")

  #Creating the plot
  plotb3(s1.fctr[[1]], sse = s1.chain[[1]], typ = "l",
       ylab = paste(toupper(fctr), "factor", sep = ""),
       col = color_set[1])

  for(i in 2:length(file)) {
    lines(s1.fctr[[i]], col = color_set[i])
  }
}
```

```r
files <- c("4AKE", "1AKE", "1E4Y")
chains <- "A"
elements <- "CA"
factors <- "b"

protein_plot(files, chains, elements, factors)
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/xl/2bn6mry96sg0xqp5m20jl1lw0000gn/T//RtmpPorfMZ/4AKE.pdb exists.
Skipping download
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/xl/2bn6mry96sg0xqp5m20jl1lw0000gn/T//RtmpPorfMZ/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):
/var/folders/xl/2bn6mry96sg0xqp5m20jl1lw0000gn/T//RtmpPorfMZ/1E4Y.pdb exists.
Skipping download
```