Class 6 Homework: Write a Function

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In this assignment, we aim to turn the following snippet code in to a function.

```r
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
s2 <- read.pdb("1AKE")  # kinase no drug
s3 <- read.pdb("1E4Y")  # kinase with drug
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")
```

Function notes:

Input: This function will take three inputs: PDB code of enzyme with drug, PDB code of enzyme without drug, and PDB code of mutated enzyme.

Utility: This function will pull corresponding data from PDB automatically, and then clean up the data by focusing on side chain A of the protein. Finally, the function will look at the B factor of the side chain and plot it.

Output: This function will return three plots.

Function:

```r
plotBfactor <- function(noDrug = "NA", drug = "NA", mut = "NA") {
  library(bio3d)
  protein.code = c(noDrug, drug, mut)
  for (id in protein.code) {
    s <- read.pdb(id)
    s.chainA <- trim.pdb(s, chain="A", elety="CA")
    s.b <- s.chainA$atom$b
    plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")
```
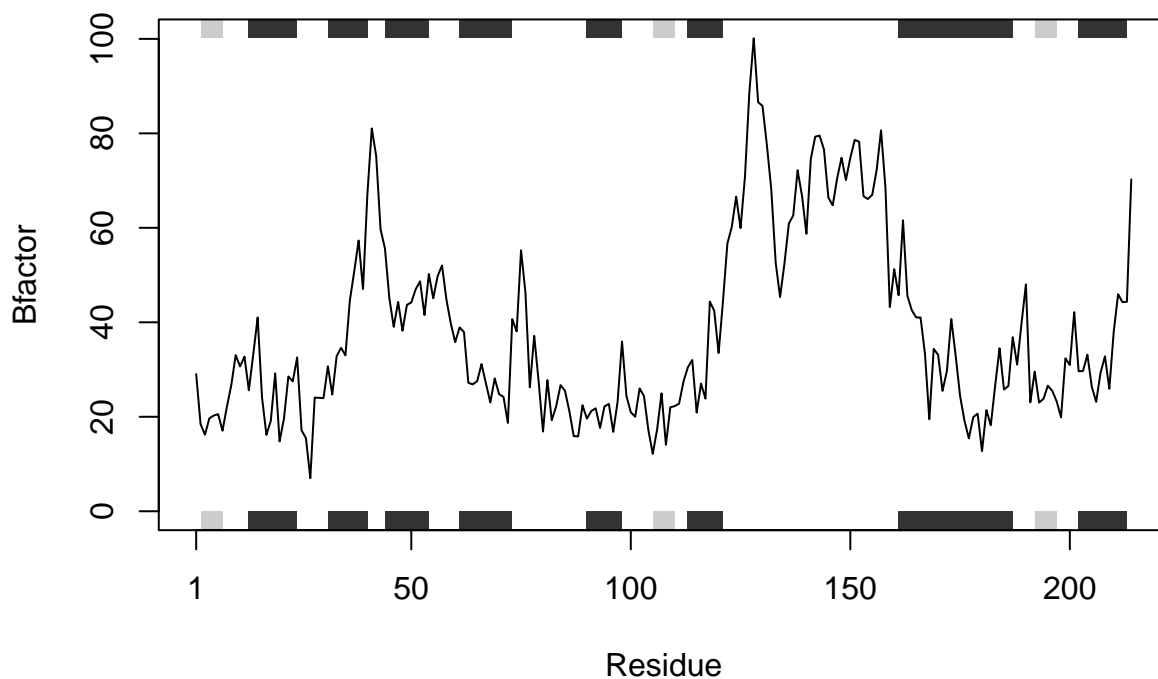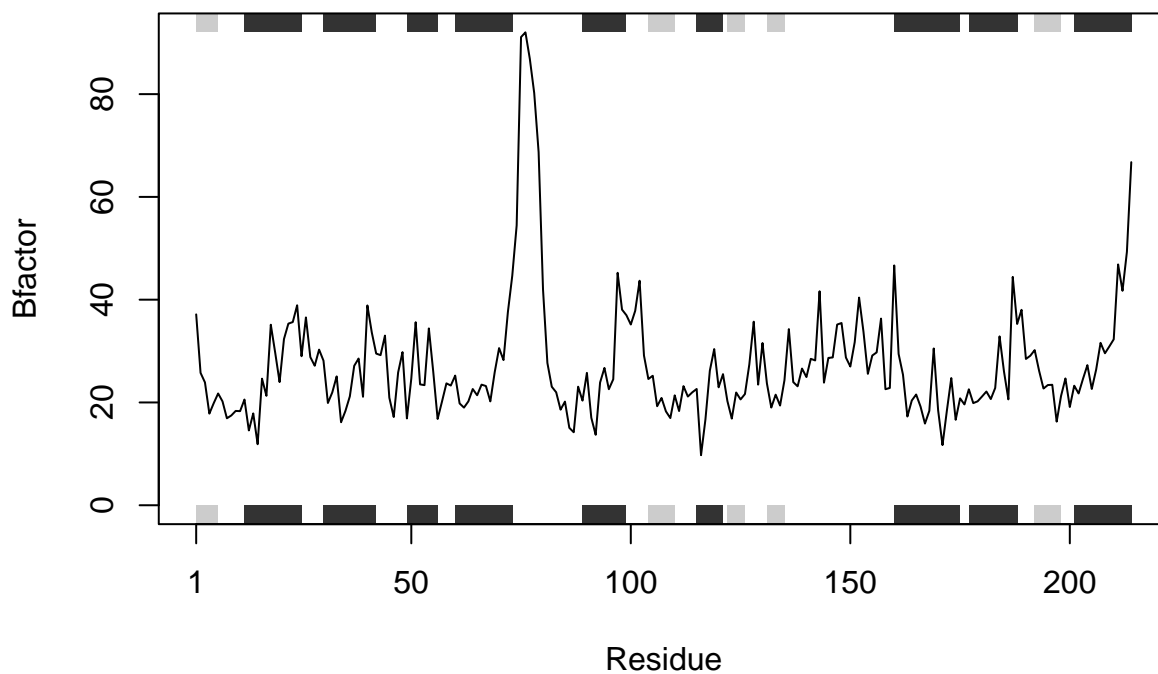
```
    }
}

plotBfactor("4AKE", "1AKE", "1E4Y")
```

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



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