Homework6

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Load the library for bio3d:

```
#load the packages
library("bio3d")
```

First, let's look at what the given code does:

```
# this is the demo code provided in the pdf
#first of all, specify the protein file to be read
s1 <- read.pdb("4AKE") # kinase with drug
```

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

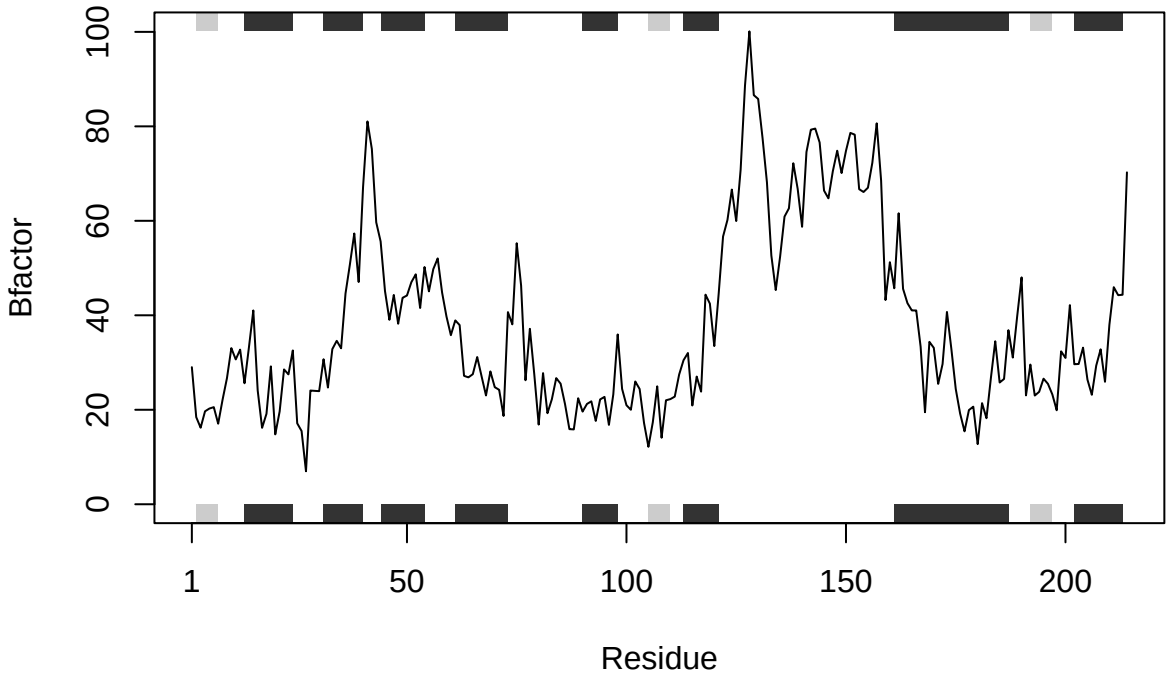
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

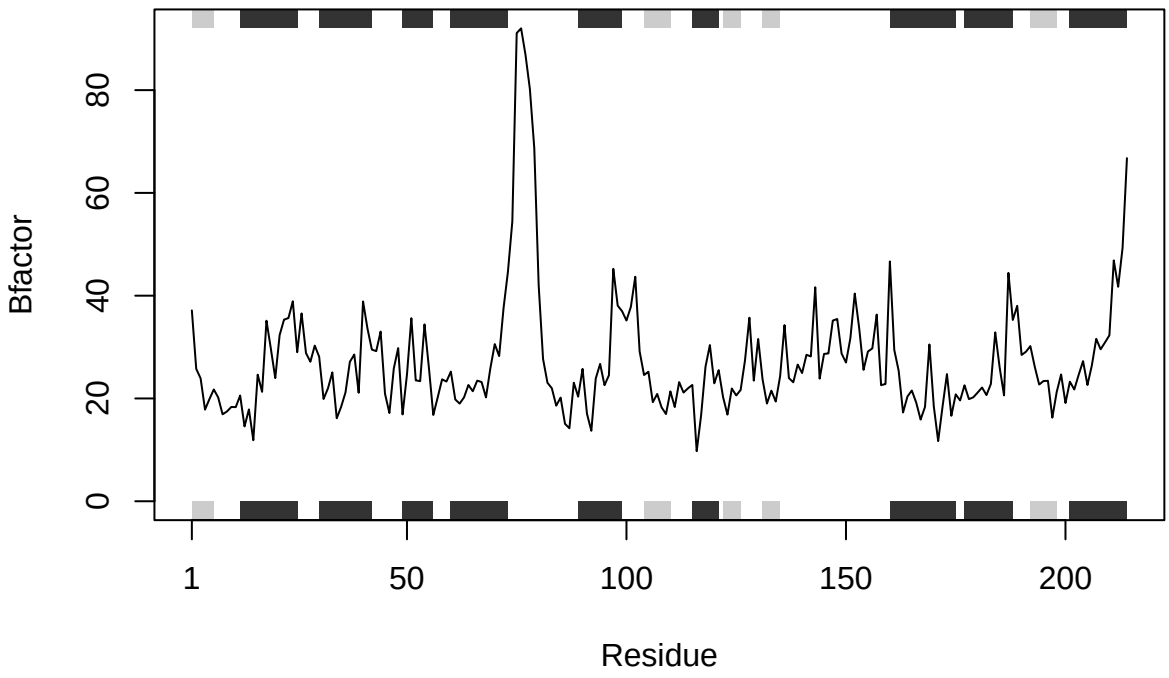
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

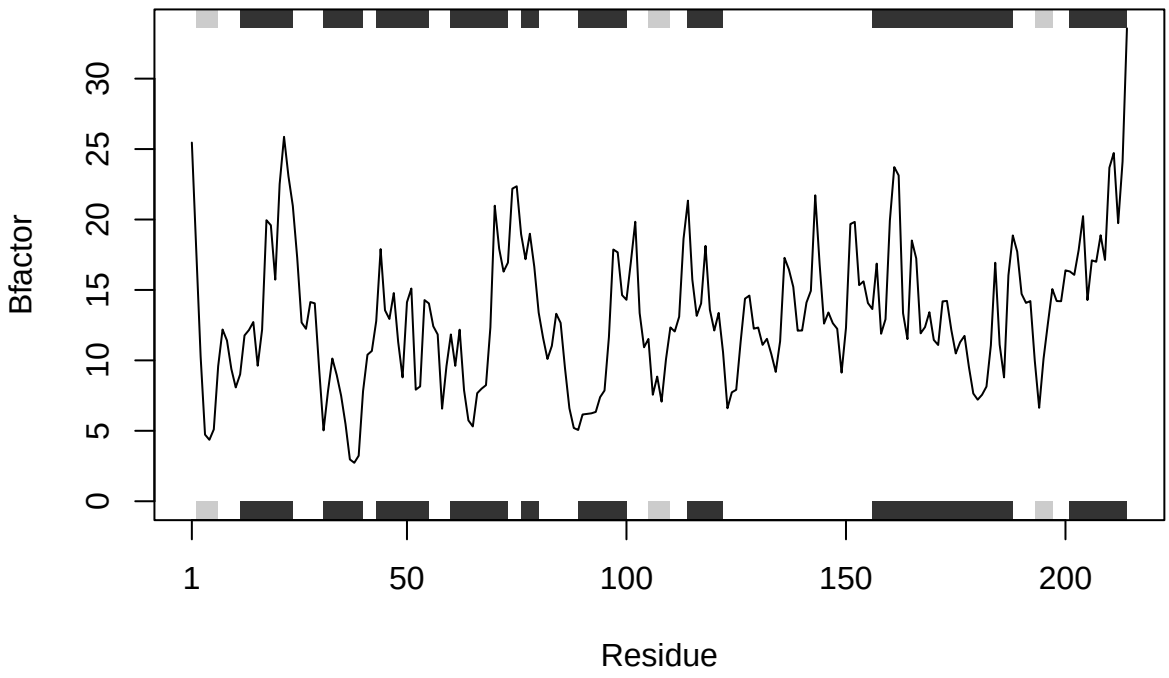
```
#get the chain information by trimming the protein sequence
#set the chain identifier as A, and the element type as CA
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s3, chain="A", elety="CA")
#I modified the line above because there's a paste mistake s1>>s3

#access the atom data for each amino acid residue on A chain of the proteins
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
 #generate the plot information on the protein sequence
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")
```



The code above takes in protein names, and generate graphs indicate the mobility of different amino acid residues on a protein chain

Based on the given information, my function's inputs are the protein names with quotes, so that specifies it to **read in the *files **on that specific kind of protein, and trims the sequence by looking at the atom data of its A chain, then uses the data to generate graphs as outputs on residue mobility. This is the function that** takes in a random protein name in quotes **and do the same analysis as above, and** outputs a graph** that indicates the interaction between different residues with the binding factor and the mobility of different residues.

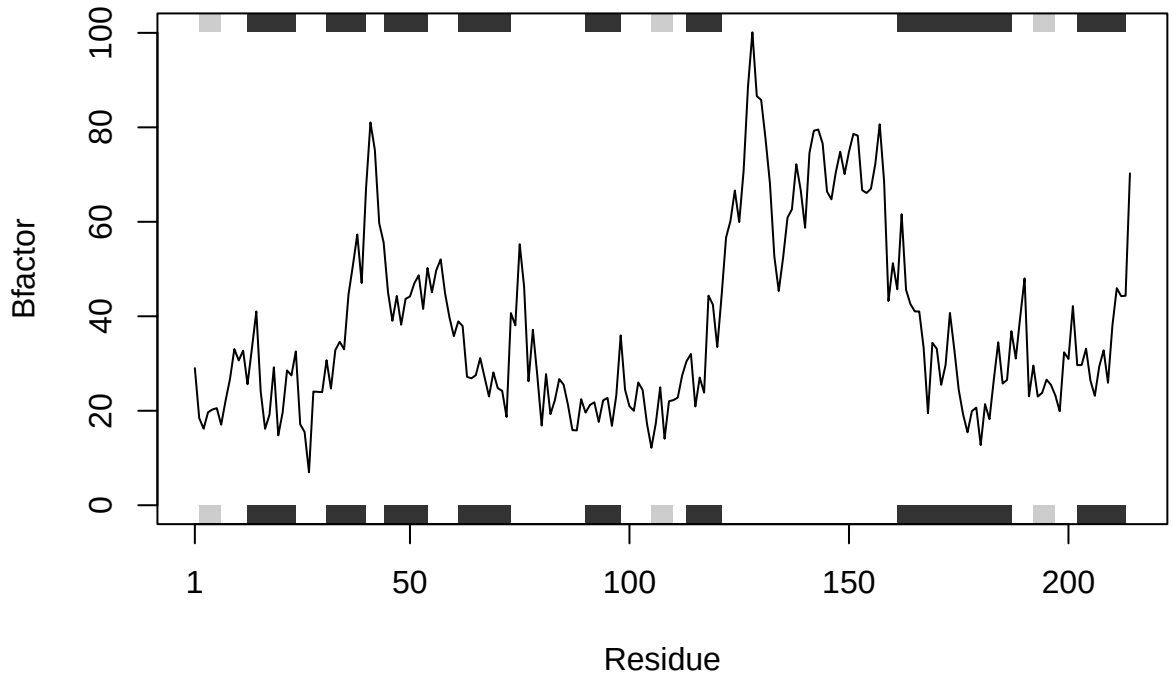
```
#input x is the protein name
proteinP<-function(x){
  #first of all, specify the protein file to be read
  s<-read.pdb(x)
  #get the chain information by trimming the protein sequence
  #set the chain identifier as A, and the element type as CA
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  #access the atom data for each amino acid residue on A chain of the proteins
  s.b <- s.chainA$atom$b
  #generate the plot information on the protein sequence
  plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")


}
```

Now test the function on the three proteins:

```
#this is generating the graph for the first protein kinase with drug
proteinP("4AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\zhang\AppData\Local\Temp\Rtmpu4avcK/4AKE.pdb exists. Skipping download
```

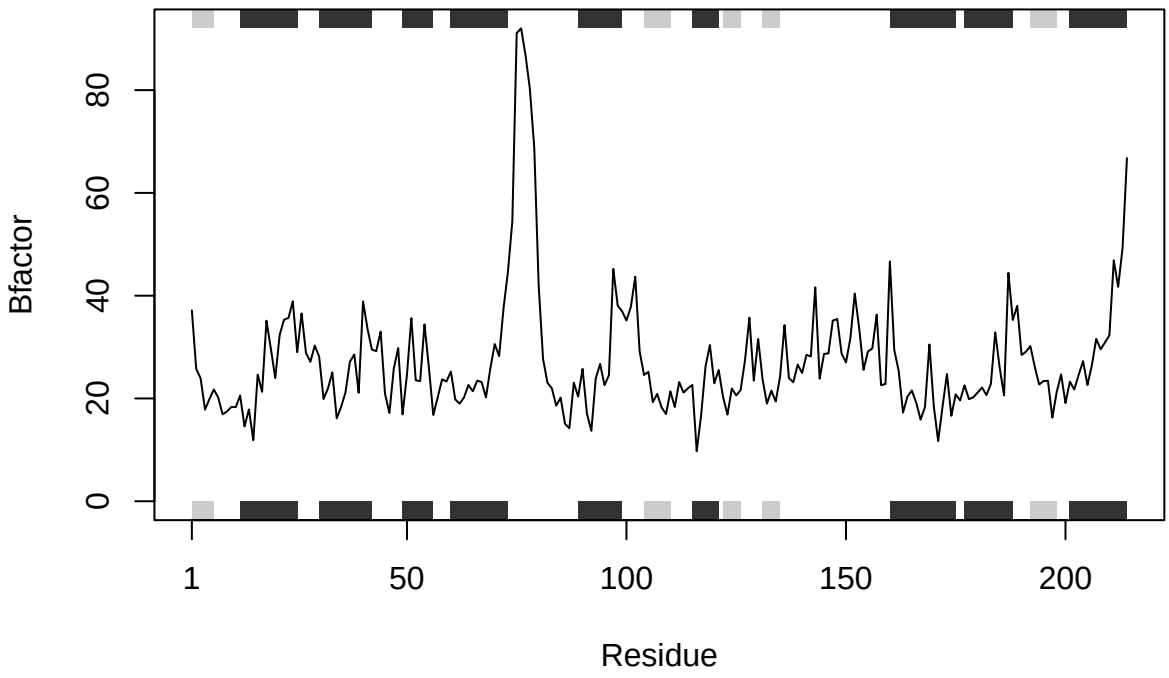



```
#this generates the graph for the second protein with no drug
proteinP("1AKE")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\zhang\AppData\Local\Temp\Rtmpu4avcK/1AKE.pdb exists. Skipping download
```

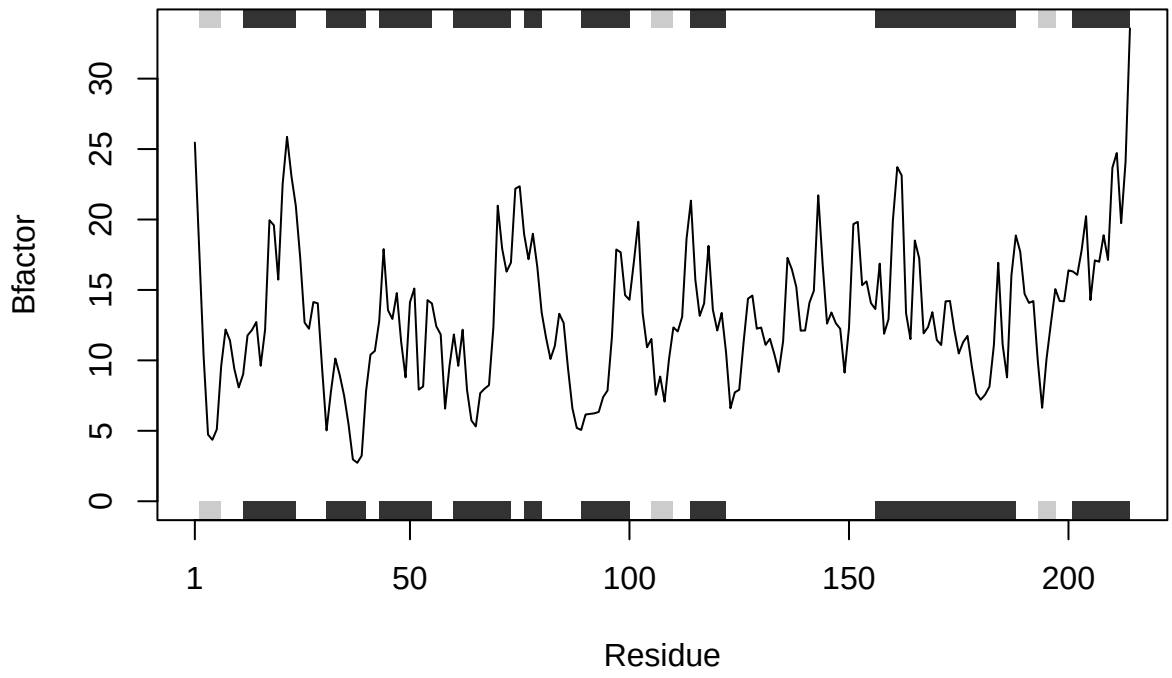
```
##    PDB has ALT records, taking A only, rm.alt=TRUE
```




```
#this generates the graph for the third protein with drug
proteinP("1E4Y")
```

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

```
## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): C:
## \Users\zhang\AppData\Local\Temp\Rtmpu4avcK/1E4Y.pdb exists. Skipping download
```




```
#the graphs indicate the mobility of different residues on the protein chain
```

Hooray! The graphs are generated as shown above. :) They are the same as the graphs generated by the separate analysis.