Homework Class 6

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Original provided code:

```
library(bio3d)
```

```
Warning: package 'bio3d' was built under R version 4.3.3
```

```
s1 <- read.pdb("4AKE") # kinase with drug
```

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

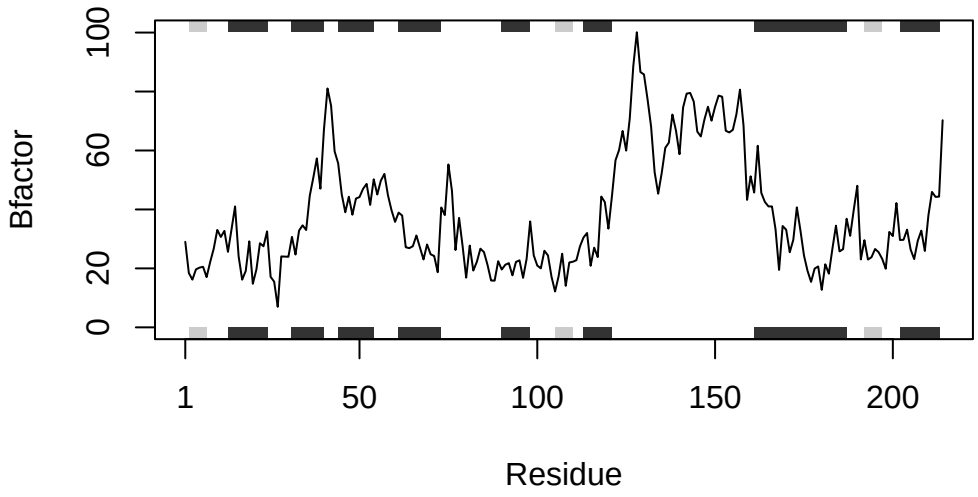
```
s2 <- read.pdb("1AKE") # kinase no drug
```

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

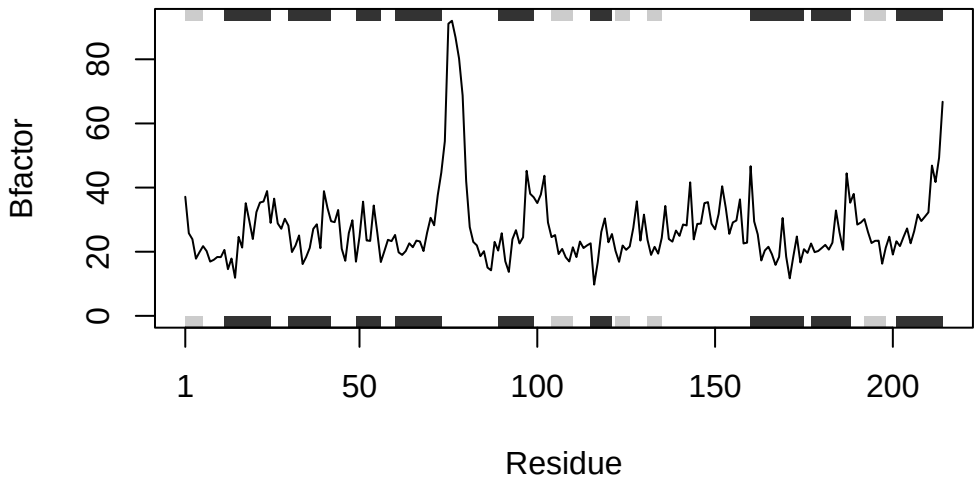
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

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

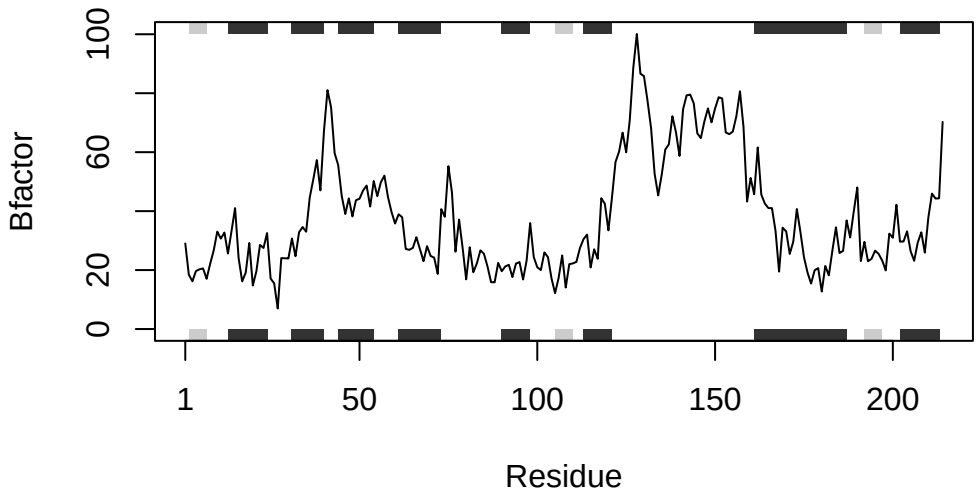
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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



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



Goal and Documentation

> I want to make a function that will condense this process. I assume that each step which is completed 3 times (downloading sequences, trimming, identifiying the b values of data, and plotting) are the targets to condense in a function
>
> Q: What are the inputs for the function? A PDB associated with a 4 letter/number code
>
> Q: What does the function do? The PDB will be trimmed, item b of the atom dataframe will be isolated, then made into a line plot of residue vs bfactor with secondary structure annotated in the margins.
>
> Q: What are the outputs for the function? A line plot of residue versus bfactor with secondary structures in the margin.

Function:

```
protein_drug <- function(input = read.pdb()) {
  s1 <- input
  s1.chainA <- trim.pdb(s1, chain= "A", elety= "CA")
  s1.b <- s1.chainA$atom$b
```

```
  plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
}
```

Testing Function:

```
protein_drug(read.pdb("1AKE"))
```

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

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

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