Class06 Hands-on Supplement Q6

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Q6. How would you generalize the original code above to work with any set of input protein structures?

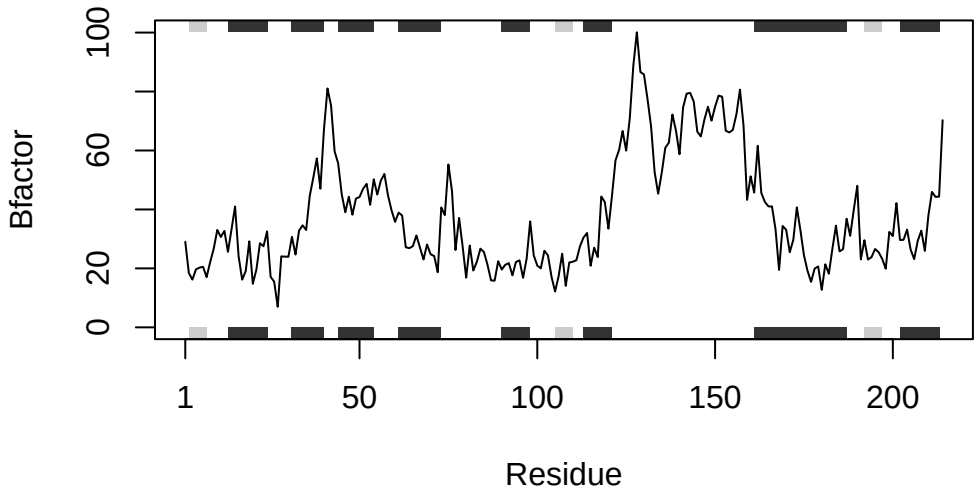
The main input for the function is the name of the PDB file. This is a generalized function that analyzes protein drug interactions. The output of this function is a plot for the specific protein.

```
library(bio3d)   #to be able to obtain file from bio3d
PDIxn <- function(file) {   #creating a new function
  s1 <- read.pdb(file)
  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")
}
```

Example of the function

```
PDIxn("4AKE")
```

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


Bfactor
0
20
60
100
1
50
100
150
200
Residue