class06_hw

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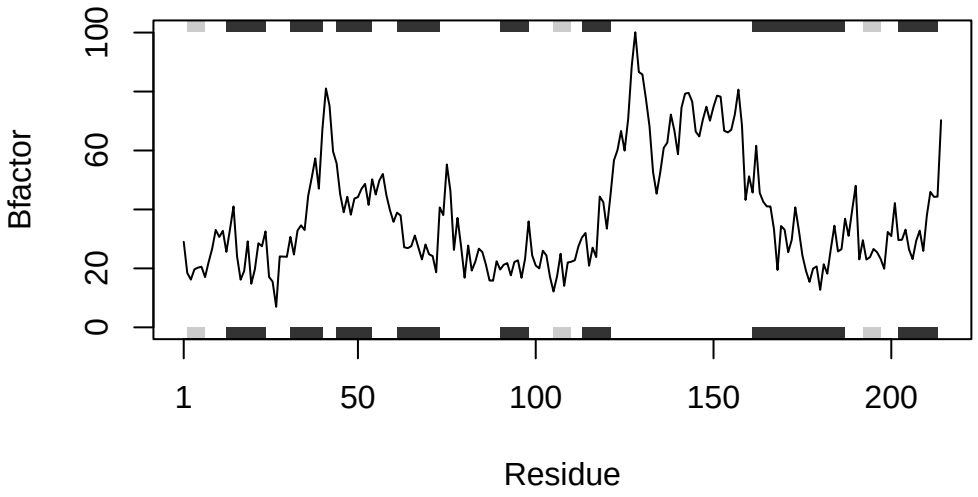
Function for the analysis of protein drug interactions

```
library(bio3d)
#Define a function named 'protein'. Inputs: ID and chain_name with a default
#chain set as "A"
protein <- function(ID, chain_name="A") {
  # Read the PDB (Protein Data Bank) file specified by the ID
  s <- read.pdb(ID)

  # Trim the PDB structure to only include the specified chain and only CA
  #(alpha carbon) atoms
  s.chain <- trim.pdb(s, chain=chain_name, elety="CA")

  # Extract the B-factor (atomic displacement parameter) values from the
  # trimmed PDB structure
  s.b <- s.chain$atom$b

  # Plot the B-factor values along the protein sequence
  # 'sse' argument stands for secondary structure elements, which are derived
  # from the trimmed chain
  # 'typ="l"' specifies the type of plot as a line plot
  # 'ylab="Bfactor"' sets the label for the y-axis as "Bfactor"
  plotb3(s.b, sse=s.chain, typ="l", ylab="Bfactor")
}
```

```
ID="4AKE"
protein(ID,"A")
```

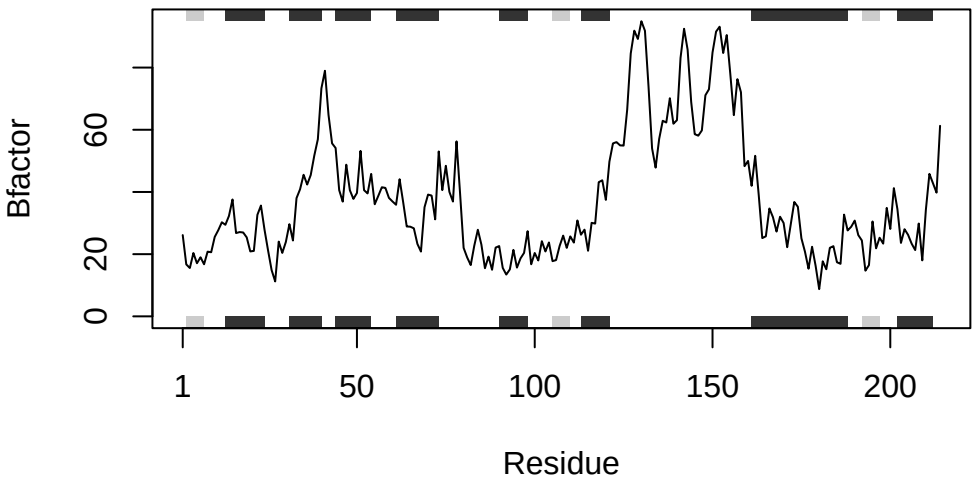
```
Note: Accessing on-line PDB file
```




```
protein(ID,"B")
```

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
C:\Users\GABYCA~1\AppData\Local\Temp\RtmpOKDAb4/4AKE.pdb exists. Skipping
download
```


Bfactor
0
20
60
1
50
100
150
200
Residue