HWclass6: R function

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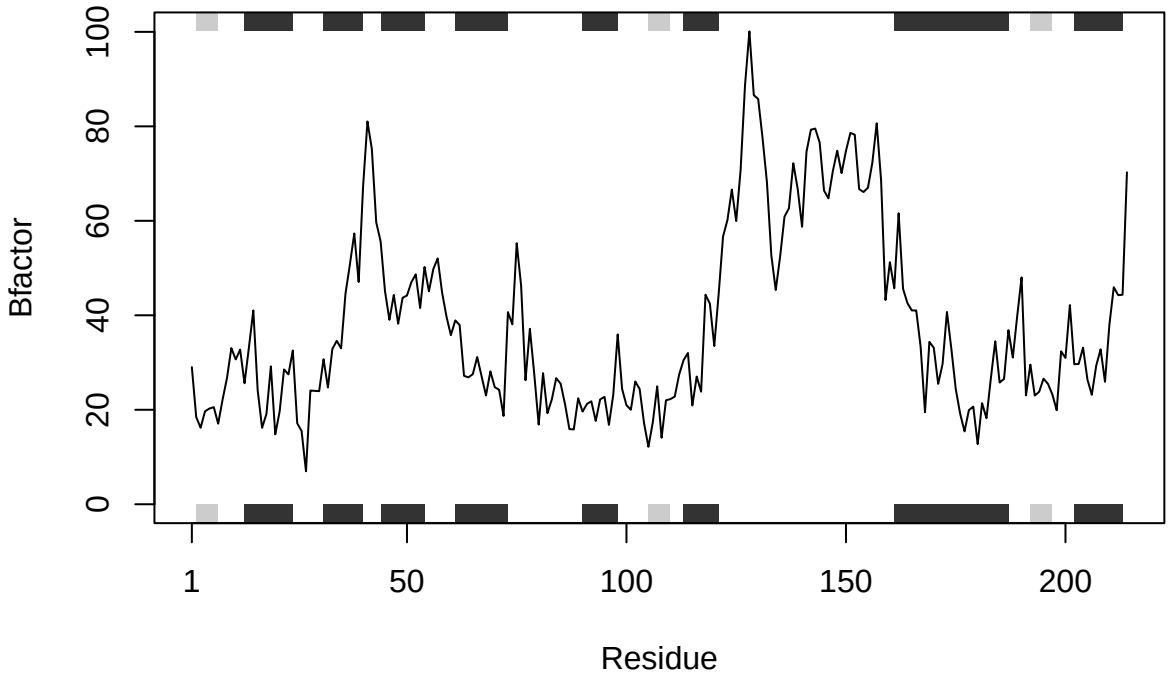
```
#1.The input of the function "PDB" is the protein structure file
#from protein data bank of the protein we are interested.
#2.This function reads a protein structure file and plots the b factors
#for only the alpha carbons in chain A of the protein.
#This allows us to visualize and get insights of flexibility of the protein structure in the specific p
#The output the function is a graph that plots the b factor against the residues.
protein.drug.interactions <- function(PDB) {
  library(bio3d)
  s <- read.pdb(PDB) #
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  s.b <- s.chainA$atom$b
 return(plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor"))
}
```

```
protein.drug.interactions("4AKE")
```

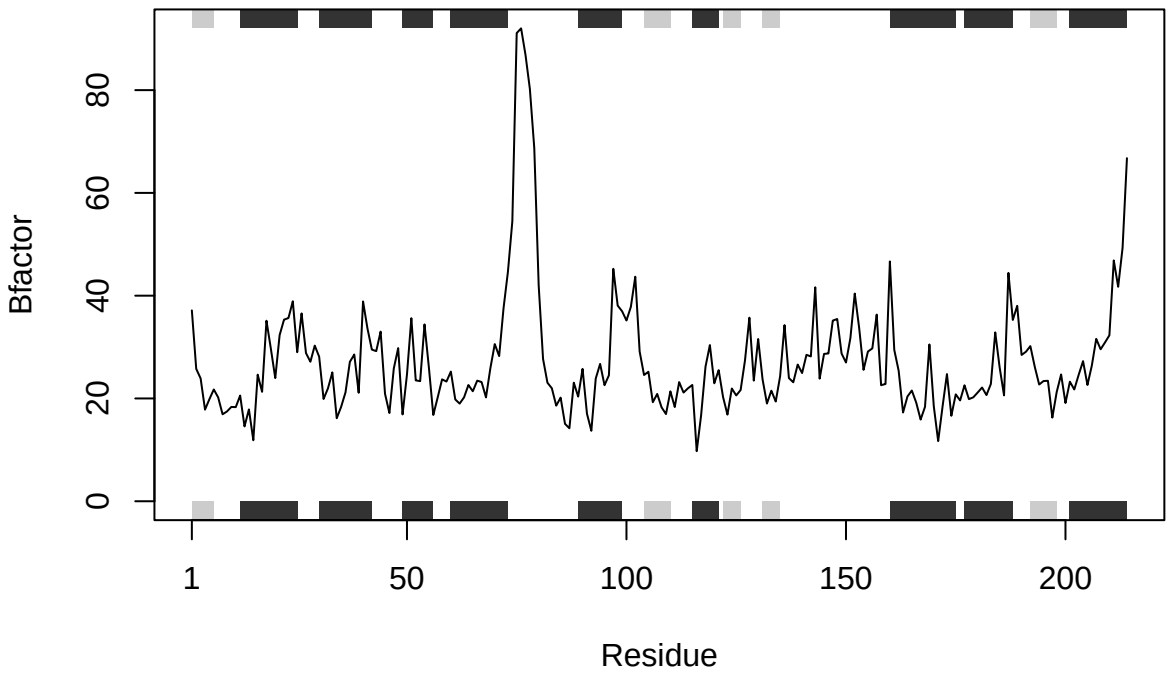
```
## Warning: package 'bio3d' was built under R version 4.3.3
```

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



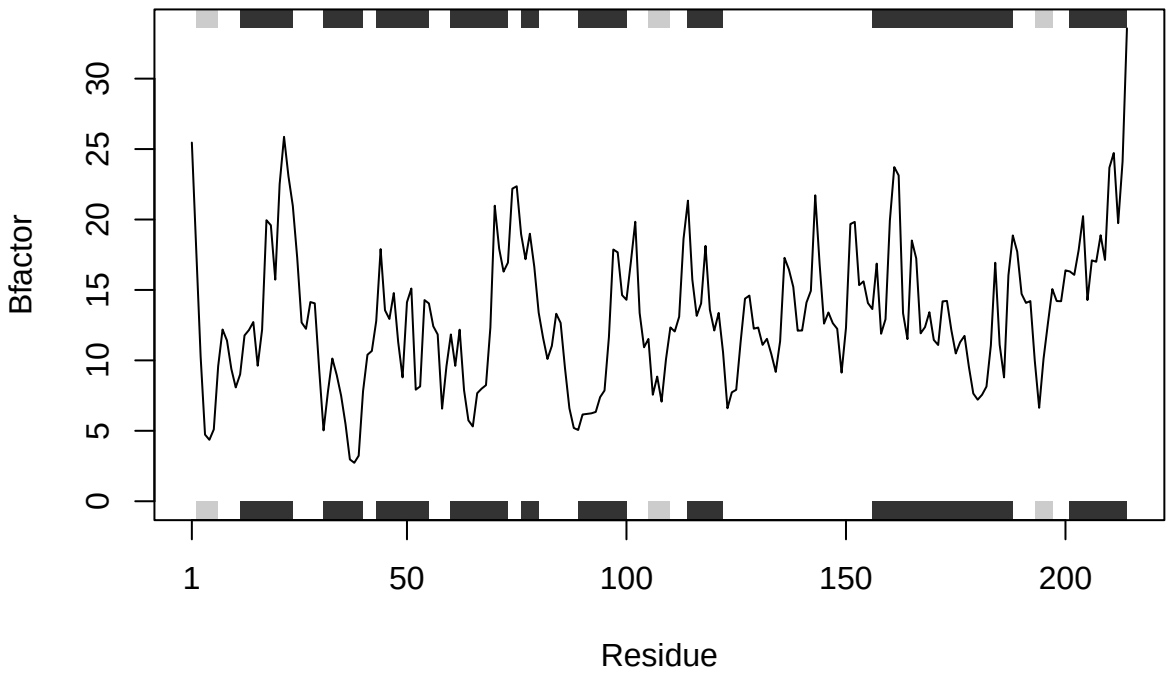

```
protein.drug.interactions("1AKE")
```

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




```
protein.drug.interactions("1E4Y")
```

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


Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue