class06HW_function

Siyu Xie (PID:A16438448)

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Analysis code snippet

```
#install.packages("bio3d")
```

Can you improve this analysis code?

```
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
```

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

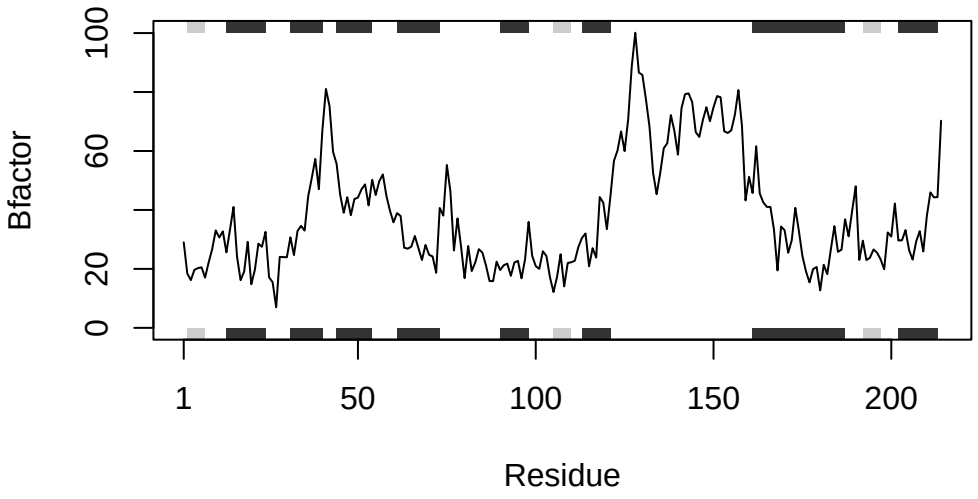
```
s2 <- read.pdb("1AKE")  # kinase no drug
```

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

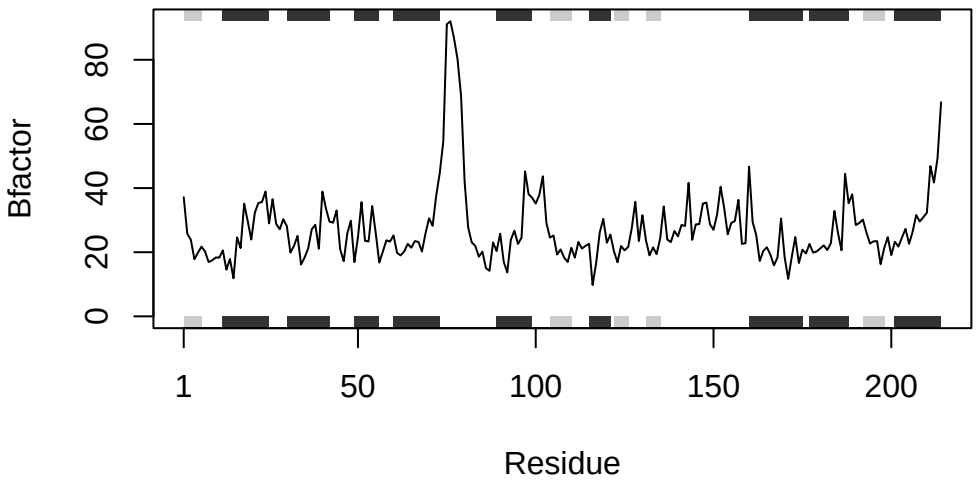
```
s3 <- read.pdb("1E4Y")  # kinase with drug
```

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

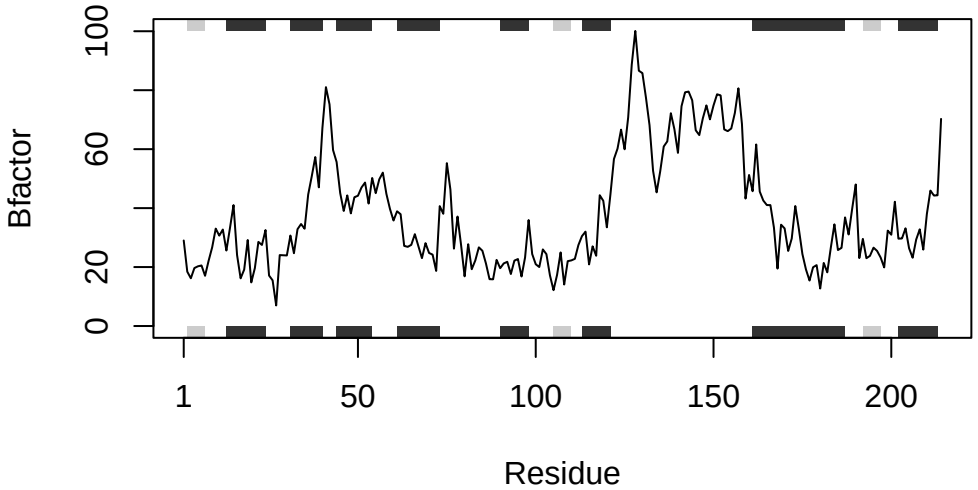
```
s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```




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




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



Improved R function

Documentation:

1. comments on the inputs to the function

PDB_data: the PDB file name extracted from the PDB data for analysis chain_name: chain interested in analysis

2. what the function does and how to use it

The function analyzes protein drug interactions by reading any protein's PDB data. To use the function, input the protein's PDB data name and the corresponding chain ID.

3. what's the output of the function

The function outputs a plot displaying the B-factor trends of the specified protein upon drug interactions.

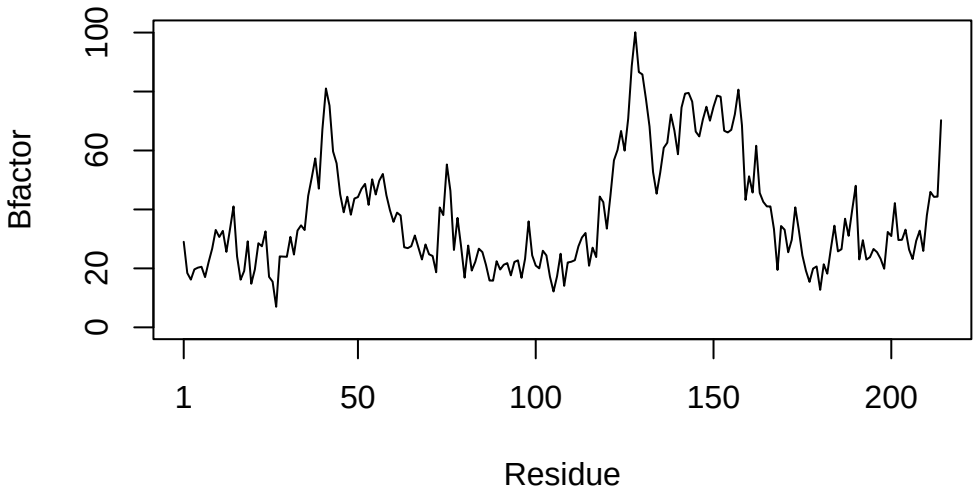
```
protein <- function(PDB_data, chain_name){
  library(bio3d)
# reading PDB file and trim the data
    protein_chain <- trim.pdb(read.pdb(PDB_data), chain = chain_name, elety ="CA")
# getting b factors from data
    b_factor <- protein_chain$atom$b
# plotting b factor trend for the specified protein
    plotb3(b_factor, sse=chain_name, typ="l", ylab="Bfactor")
}

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

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

```
Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/jp/lp84gwy56qb6ndccpw543lww0000gn/T//RtmpKh32QC/4AKE.pdb exists.
Skipping download
```

```
Warning in plotb3(b_factor, sse = chain_name, typ = "l", ylab = "Bfactor"):
Length of input 'sse' does not equal the length of input 'x'; Ignoring 'sse'
```


Bfactor
0
20
60
100
1
50
100
150
200
Residue