

Homework 6 - (R Functions)

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Drug_analysis function takes a set of proteins from a database and runs analysis on drug interactions and displays results graphically.

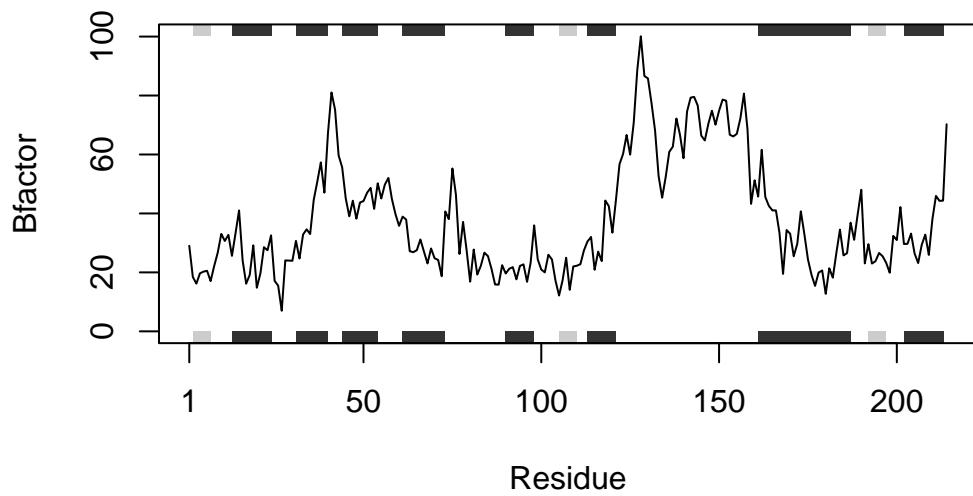
To use this function, call the `drug_analysis()` function with a single or multiple 4 character protein tag from the protein database to run analysis.

```
drug_analysis <- function(pdb_id){  
  # pdb_id input is a set of ID inputs from the pdb database  
  library(bio3d)  
  
  for(i in 1:length(pdb_id)){  
    s <- read.pdb(pdb_id[i])  
    s.chainA <- trim.pdb(s, chain="A", elety = "CA")  
    s.b <- s.chainA$atom$b  
    plotb3(s.b, sse=s.chainA, typ="l", ylab="Bfactor")  
  }  
}
```

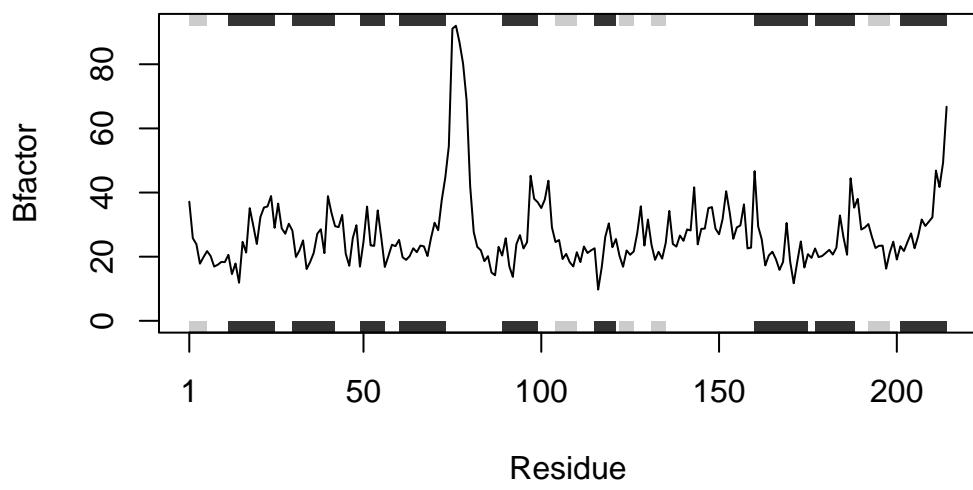
Test code that displays the results of the function, `drug_analysis()` of 3 different proteins.

```
drug_analysis(c("4AKE", "1AKE", "1E4Y"))
```

Note: Accessing on-line PDB file



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



Note: Accessing on-line PDB file

