

hw class06 r functions

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original 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

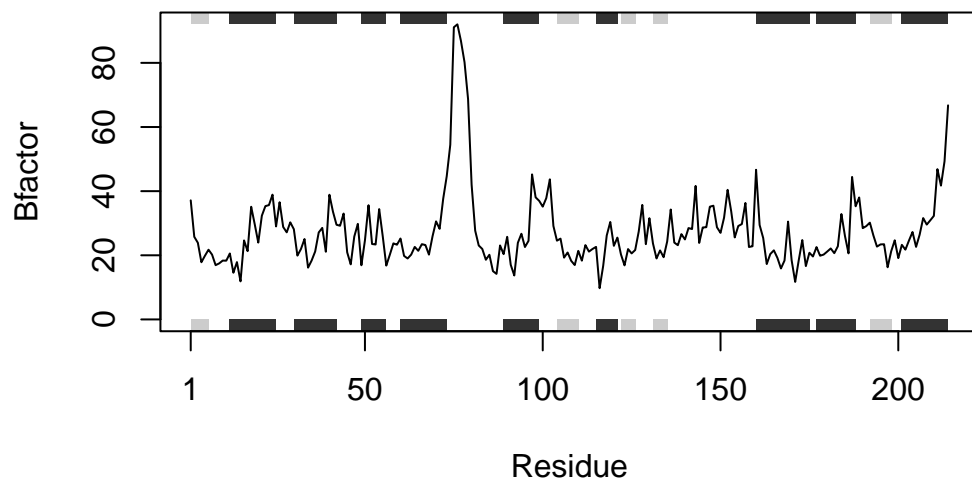
```
s3 <- read.pdb("1E4Y") # kinase with drug
```

Note: Accessing on-line PDB file

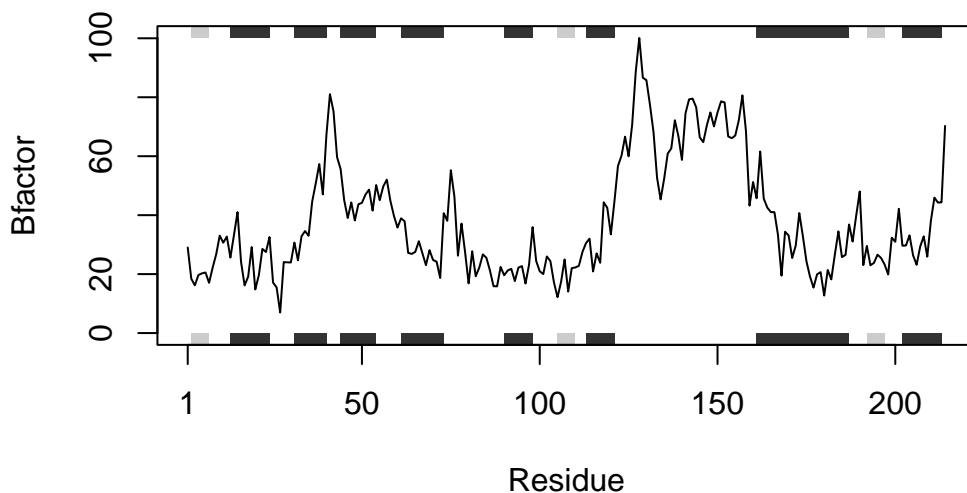
```
s1.chainA <- trim.pdb(s1, chain="A", eley="CA")
s2.chainA <- trim.pdb(s2, chain="A", eley="CA")
s3.chainA <- trim.pdb(s3, chain="A", eley="CA")
s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b
plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
```



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



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



new protein_drug_interactions_analysis function

- Input: any PDB file
- What it does and how to use it: analyzes protein-drug interactions by creating a plot of Bfactor trends and secondary structure from protein structure data. To use, call the function and enter any PDB code in ""; e.g. `protein_drug_interactions_analysis("4AKE")`
- Output: a lineplot of Bfactor trends with marginal rectangles representing secondary structure

```
protein_drug_interactions_analysis <- function(x) {
  # read protein structure file
  s <- read.pdb(x)
  # select calcium atoms in chain A
  s.chainA <- trim.pdb(s, chain="A", elety="CA")
  # save Bfactor data
  s.b <- s.chainA$atom$b
  # create a lineplot of Bfactor trends with marginal rectangles representing secondary st
```

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

example output

```
protein_drug_interactions_analysis("4AKE")
```

Note: Accessing on-line PDB file

Warning in get.pdb(file, path = tempdir(), verbose = FALSE):
/var/folders/3n/fn38j1kj1pjfx7fcf7434h1m0000gn/T//RtmpDRXign/4AKE.pdb exists.
Skipping download

