Class06 Homework

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Load library bio3d.

```
library(bio3d)
```

Write a function plot_pdb() that will read a PDB file and trim it to contain just chain A and alpha carbons.

```
plot_pdb <- function(x) {
  trim.pdb(read.pdb(x), chain="A", elety="CA")
}
```

Execute new function plot_pdb() for each PDB file and assign a new variable name for each.

```
s1 <- plot_pdb("1AKE") #without drug
```

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

```
s2 <- plot_pdb("4AKE") #with drug A
```

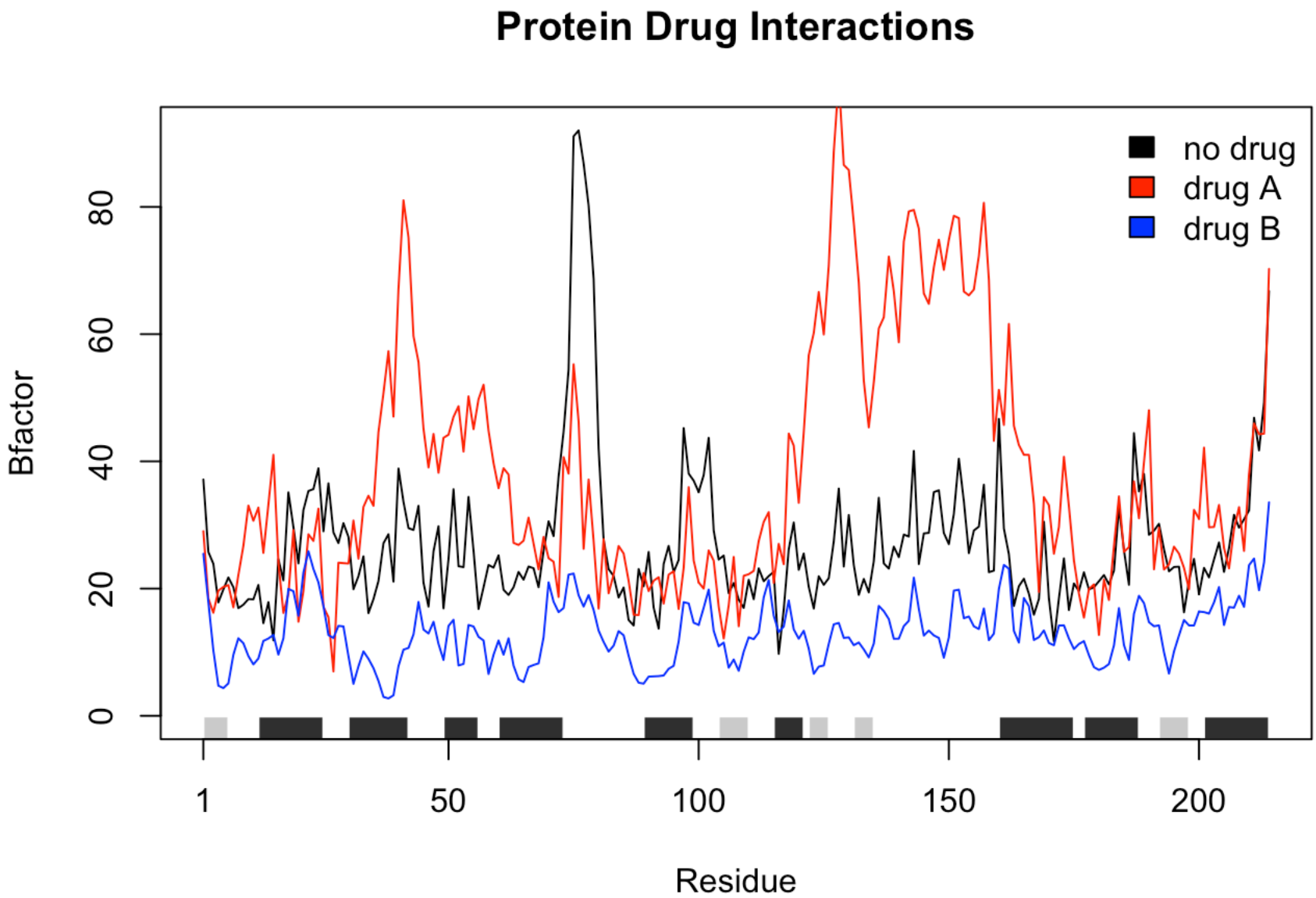
```
##   Note: Accessing on-line PDB file
```

```
s3 <- plot_pdb("1E4Y") #with drug B
```

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

Make a line plot of the “atom” and “b” columns from the first variable (s1), along with SSE along the x axis (Residue). The y axis is Bfactor. Now add the other 2 variable sets (s2 and s3) in different colors to the line plot. Generate a color-coded legend in the top right corner and a title at the top.

```
plotb3(s1$atom$b, sse=s1, top = FALSE, typ="l", ylab="Bfactor") #plot the first varia
ble
points(s2$atom$b, typ="l", ylab="Bfactor", col="red") #add a second variable
points(s3$atom$b, typ="l", ylab="Bfactor", col="blue") #add third variable
leg = c("no drug", "drug A", "drug B") #define legend text
legend("topright", legend = leg, fill = c("black", "red", "blue"), bty = "n", inset =
0) #generate a legend
title(main = "Protein Drug Interactions") #generate a title
```


Protein Drug Interactions
no drug
drug A
drug B
Bfactor
0
20
40
60
80
1
50
100
150
200
Residue