HOMEWORK 6

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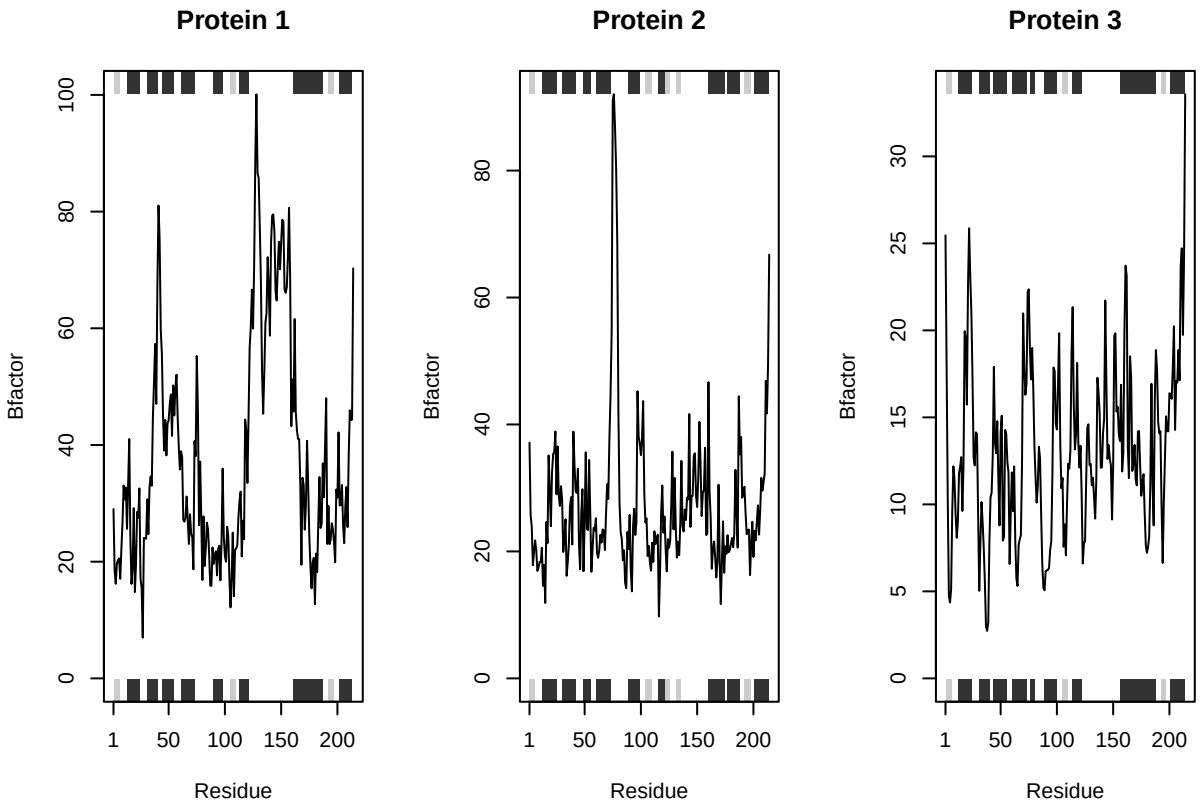
```
analyze_protein_drug_interactions <- function(pdb_files, chain = "A", elety = "CA") {
  # Load required package
  library(bio3d)

  # Read and trim PDB files
  pdb_data <- lapply(pdb_files, function(file) {
    pdb <- read.pdb(file)
    trim.pdb(pdb, chain = chain, elety = elety)
  })

  # Calculate B-factors
  b_factors <- lapply(pdb_data, function(data) data$atom$b)

  # Define plotting function
  plot_b_factors <- function(b_factors, sse, main = "", ylab = "Bfactor") {
    plotb3(b_factors, sse = sse, typ = "l", ylab = ylab, main = main)
  }

  # Generate plots
  par(mfrow = c(1, length(b_factors)))
  for (i in 1:length(b_factors)) {
    plot_b_factors(b_factors[[i]], sse = pdb_data[[i]], main = paste0("Protein ", i))
  }

  return(pdb_data)
}
```

```
# Define PDB files
pdb_files <- c("4AKE", "1AKE", "1E4Y")

# Call the function with the specified PDB files
pdb_data <- analyze_protein_drug_interactions(pdb_files)
```

```
##   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
```


Protein 1
Bfactor
0
20
40
60
80
100
1
50
100
150
200
Residue
Protein 2
Bfactor
0
20
40
60
80
1
50
100
150
200
Residue
Protein 3
Bfactor
0
5
10
15
20
25
30
1
50
100
150
200
Residue