Lecture 6 HW

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1/31/2020

Protein Drug Interactions Homework Using Bio3d

Q6. Write a function that analyzes protein drug interactions by reading in any protein PDB data and outputs a plot for the specified protein.

Submit as R markdown file and either an HTML or PDF with the code and output saved.

What are the inputs of the function?

4 main sets of inputs: 1. read.pdb (read the protein pdb file) 2. trim.pdb (reduce the data to a smaller pdb file) 3. chain.pdb (find possible chain breaks based on the Calpha or peptide bond atom separation) 4. plot3b (make a graph of the protein drug interactions from PDB)

Since these are the lines of code that get repeated, it's best to divvy them up into a function.

What does the function do? How do you use it?

The function **pdi_plot** should generate a plot for the given parameters to analyze a PDB file (a chain, an element, and a specified atom).

To use the function, you can fill in the parameters for the vectors PDB file, chain, and element.

What is the output of the function?

The output is a graph labeled with the file name.

HOMEWORK CODE

```
library(bio3d)

#change variables to desired
files <- "4AKE"
chains <- "A"
elem <- "CA"

pdi_plot <- function(files) {

#input 1: read
    s <- read.pdb(files)

#input 2: trim
    s.chain <- trim.pdb(s, chain = chains, elety = elem)

#input 3: chain.pdb on atom "b"
```

```
    s.x <- s.chain$atom$b

#input 4: generate the plot
      plotb3(s.x, sse = s.chain, typ = "l", ylab = "Bfactor", main = (files))

}
```

Final Output

```
pdi_plot(files)
```

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