class6_sec2

Xuerui HUang

4/19/2019

Section1:B

Q1: read.pdb() function return sa large pdb object

Q2: trim.pdb() function trims a PDB object to a subset of atoms, which produces a new smaller PDB object, containing a subset of atoms, from a given larger PDB object.

Q3: To turn off the marginal black and grey rectangles in the plots, we could set the top = FALSE and bot = FALSE> The rectangles represents beta strands and alpha helics

Q4: To put plots together

Q5: S1 and S3 are closer

Q6

Input: Two inputs (FileName,chain_name)

```
   FileName: a single element character vector containing the name of the PDB file
             to be read, or the four letter PDB identifier for online file access
   chain_name: a single letter string to indicate which chain you want to focus on
```

Function: Visualizing and analyzing the specific protein drug interactions by inputing the specific PBD data indicators

Ouput: A plot object for the specified protein

```
#Input: Two inputs (FileName,chain_name)
#       FileName: a single element character vector containing the name of the
#                 PDB file to be read, or the four letter PDB identifier for
#                 online file access
#       chain_name: a single letter string to indicate which chain you want
#                   to focus on
#Function: Visualizing and analyzing the specific protein drug interactions by i
#          nputing the specific PBD data indicators
#Ouput: A plot object for the specified protein
plot_drugProteinInteract <- function (fileName,chain_name){
  require(bio3d)
  #load file
  pdb_pf <- read.pdb(fileName)
  #select specific chain and info from chain
  pf_chain <- trim.pdb(pdb_pf,chain = chain_name,elety="CA")
  pf.b <- pf_chain$atom$b

  #output plot
  plotb3(pf.b, sse=pf_chain, typ="l", ylab="Bfactor")
}
```

```
#test
plot_drugProteinInteract("4AKE","A")
```

```
## Loading required package: bio3d
```

```
## Warning: package 'bio3d' was built under R version 3.4.4
```

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