Class6 HW - Script

Aries Chavira

1/27/2020

# Generate standard scatter plots of specific selection of atoms from a Protein Data Bank object

## Installing Bio3D

Here we will utilize specific functions from the Bio3D v2.3 package. To being we need to install the Bio3D package so that it can be used for subsequent analyses. To do this run the following code in the R Console:

**install.packages(‘bio3d’)**

Next we will load the Bio3D library. To be able to access the Bio3D functions, run the following code into the R studio interface.

library(bio3d)

## Code to generate a scatter plot for a specific selection of atoms from a PDB object

Below is the code behind the easypdb.plot function, and how it works.

It was generated to be able to take any four letter PDB identifier, and generate a subsequent scatter plot.

**See next section for an example**

easypdb.plot <- function(x) { # x = the four letter PDB identifier  
   
 y <- read.pdb(x)   
   
  
 A.chainA <- trim.pdb(y, chain="A", elety="CA")  
  
 Z <- A.chainA$atom$b  
   
 plotb3(Z, sse=A.chainA, typ="l", ylab="B Factor", col = "coral", lwd=2, main = x)  
   
}

* read.pdb reads a PDB coordiate file using the four letter PDB identifier
* Trim.pdb(y, chain="A", elety="CA") taked the protein identified, and produces a smaller new object that only conatins the Alpha chain, and the CA nucleic atoms.
* Finally, plotb3 generates a per-residue line plot of your trimmed PDB object.
* The color, y label (ylab), Color(col), and line width(lwd) can all be adjusted.
* The plot is automatically labeled with the four letter PDB identifier. \*\*To remove this feature, simply delete the main = x argument in the last line.

Run the code to generate the easypdb.plot function.

Next, insert your four letter PDB identifier into the function to generate your plot ## Example

easypdb.plot("4AKE")

## Note: Accessing on-line PDB file

