

Class 6: R functions

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BEGINNING OF MY FUNCTION

```
#a,b, and c are values stored as read.pdb("protein")
library(bio3d)
threeinone <- function(a,b,c) {
  sa.chainA <- trim.pdb(a, chain = "A", elety = "CA") #take variable "a"
  (which is a read.pdb variable for a given protein) and filter out/trim
  structures from the original PDB input and select for Chain and atom type.
  sa.b <- sa.chainA$atom$b #isolate the atoms in chain A from sa.chainA to
  get just the atom vector coordinates.
  plotb3(sa.b, sse=sa.chainA, typ = "l", ylab= "Bfactor") #plot for variable
  as a line and setting the Bfactor values on the y axis

  sb.chainA <- trim.pdb(b, chain = "A", elety = "CA")#repeat for second,b,
  variable
  sb.b <- sb.chainA$atom$b
  plotb3(sb.b, sse=sb.chainA, typ = "l", ylab= "Bfactor")#plot for second
  variable

  sc.chainA <- trim.pdb(c, chain = "A", elety = "CA") #repeat for third,c,
  variable
  sc.b <- sc.chainA$atom$b
  plotb3(sc.b, sse=sc.chainA, typ = "l", ylab= "Bfactor") #plot for third
  variable
  #now overlay all three inputs into one graph
  plotb3(sa.b, sse=s1.chainA, typ="l", ylab="Bfactor")
  points(sb.b, col="blue", typ="l")
  points(sc.b, col="red", typ="l", lwd=3)
}

#a,b, and c are values stores as read.pdb("protein")
threeinone(s1,s2,s3)
```



