# class6 supplement

Hetian Su

## Generalize code into function

```r
# load the bio3d package
#install.packages('bio3d')

library(bio3d)

#function name - protDrugInt
#description - read in any given protein sequence from PDB, extract the data of chain A fr
#Input - prot: the protein code as in PDB
#Output - the plot of the selected chain of the given protein

protDrugInt <- function(prot){

  S <- c()

  for (p in 1:length(prot)){
    # retrieve sturctural data from pdb
    s <- read.pdb(prot[p])

    # extract chain A and atom data
    s.A <- trim.pdb(s, chain='A', elety='CA')
    s.b <- s.A$atom$b

    # store the individual protein data
    S <- rbind(S, s.b)

    # plot the chain
    # plotb3(s.b, sse=s.A, typ='l', ylab='Bfactor')
  }
```

```
    #name the rows to the names of the proteins
    row.names(S) <- prot

    hc <- hclust( dist( S ) )
    plot(hc)
}

# test output
Prot = c('4AKE','1AKE','1E4Y')

protDrugInt(Prot)
```
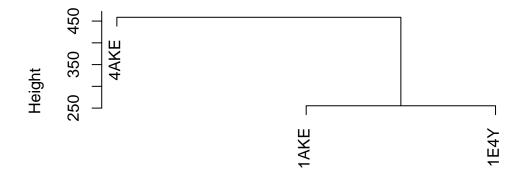
```
Note: Accessing on-line PDB file
Note: Accessing on-line PDB file
 PDB has ALT records, taking A only, rm.alt=TRUE
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```

## Cluster Dendrogram



dist(S)
hclust (*, "complete")