lab6_hw

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2022-10-15

```
library(bio3d)
```

```
## Warning: package 'bio3d' was built under R version 4.0.5
```

Q6

This function evaluates the b-factor similarity of different proteins. Enter the wanted chain and elety to be compared and the proteins being compared as a vector. The function would output a hierarchical cluster dendrogram based on protein b-factor similarity.

Inputs: chain: the chain identifier that user wants to compare within proteins elety: atom type to be compared within proteins proteins: the list of proteins to be compared as a vector

Output: a hierarchical cluster dendrogram showing b-factor correlation among proteins.

```r
protein_comp <- function(chain,elety,proteins){
  labs <- c()
  for (i in 1:length(proteins)){
    protein <- read.pdb(proteins[i])
    protein.subset <- trim.pdb(protein, chain=chain,elety=elety)
    protein.b <- (protein.subset$atom$b)
    labs <- c(labs,proteins[i])
    if (i==1){
      protein.list <- protein.b
    }
    else{
      protein.list <- rbind(protein.list,protein.b)
    }
  }
  hc <- hclust(dist(protein.list))
  return(plot(hc,labels=labs))
}
```

```r
protein_comp("A","CA",c("4AKE","1AKE","1E4Y"))
```

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

Cluster Dendrogram
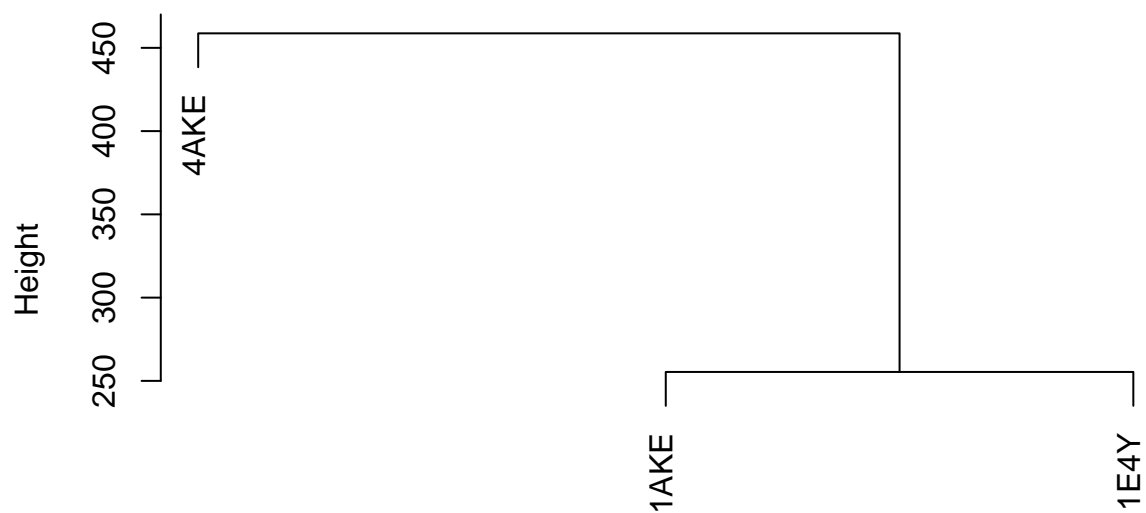
dist(protein.list)
hclust (*, "complete")