Bio3D

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17/12/2019

Matériel et Méthodes

Outils

Bio3D offre différent outils pour manipuler les objets pdb contenant les structures des protéines.

```
aa <- get.seq("P21554")

blast <- blast.pdb(aa)

hits <- plot.blast(blast, cutoff = 45)

files <- get.pdb(hits$pdb.id, path = "pdbs", split = TRUE, gzip = TRUE)
```

Voici maintenant le graphique d'alignement obtenu à l'ai de MUSCLE

```
pdbs <- pdbaln(files, fit=TRUE, web.args=list(email="mon.email@gmail.com"))

ids <- basename.pdb(pdbs$id)

anno <- pdb.annotate(ids)

ID <- gsub("crystal structure of the ", "", tolower(anno$structureTitle))
ID <- gsub(".* crystal structure of the ", "", ID)
ID <- gsub("crystal structure of ", "", ID)
ID <- gsub("r 1 ", "r 1\n", ID)
ID <- gsub("1 c", "1\n c", ID)

annoID <- paste0(ids, "\n", ID)

plot(pdbs, labels = annoID, mar4 = 14)
```

Nous voulons maintenant concentrer nos analyses sur la chaine R de la prot puisque c'est celle-ci qui est homologue aux structures trouvées par le blast

```
pdb <- read.pdb("6N4B")

sele <- atom.select(pdb, chain = "R")

ca.pdb <- trim.pdb(pdb, sele)
```

Nous pouvons ensuite obtenir le coeur protéique

```
# find invariant core

core <- core.find(pdbs, outpath = "core", write.pdbs = T)

core.inds <- print(core, vol = 1.0)

#write.pdb(xyz = pdbs$xyz[1, core.inds$xyz], file = "6nb_core.pdb")
```

```
#write.pdb(pdbs$xyz, file = "64nb_pdbs.pdb")

# superimpose all structures to core

pdbs$xyz = pdbfit(pdbs, core)
```

PCA

```
pc <- pca.xyz(pdbs$xyz[,gaps.pos$f.inds], rm.gaps = T)

plot(pc)

##Clustering
# Calculate RMSD

rd <- rmsd(pdbs)

# Structure-based clustering

hc.rd <- hclust(dist(pc$z[,1:2]))

grps.rd <- cutree(hc.rd, h=90)

cols <- c("red", "green", "blue")[grps]

plot(pc, col=cols)
```

```
plot.bio3d(pc$au[,1], resno=ref.pdb, sse=ref.pdb, ylab="PC1")

plot.bio3d(pc$au[,2], resno=ref.pdb, sse=ref.pdb, ylab="PC2")

plot.bio3d(pc$au[,3], resno=ref.pdb, sse=ref.pdb, ylab="PC3")
```

```
mktrj(pc, pc=1, file="pc_1.pdb")

mktrj(pc, pc=2, file="pc_2.pdb")
```

NMA

voici maintenant les commandes pour faire la NMA sur la structure de la chaine R

```
modes.pdb <- nma(ca.pdb, ff="calpha")

print(modes.pdb)

plot(modes.pdb)

mktrj(modes.pdb, mode=7, file = "6N4B_R_nma7_mktrj.pdb")

mktrj(modes.pdb, mode=8, file = "6N4B_R_nma8_mktrj.pdb")

mktrj(modes.pdb, mode=10, file = "6N4B_R_nma10_mktrj.pdb")
```

La NMA sur l'ensemble des structures alignées

```
modes <- nma(pdbs)

plot(modes, pdbs, col=grps)
```

Analyses postérieures

```
r <- rmsip(modes.pdb, pc)

mypalette<-brewer.pal(11,"GnBu")

plot(r, xlab="NMA", ylab="PCA", col = mypalette, zlim = c(0, 0.2))
```