Class 11.1: AlphaFold

Emily Chen (PID:A16925878)

Here we read the results from AlphaFold and try to interpret all the models and quality scores metrics:

```
library(bio3d)
pth <- "dimer_23119"
pdb.files<-list.files( path=pth, full.names=TRUE, pattern= ".pdb")
```

Align and supperpose all these models

```
file.exists(pdb.files)
```

```
[1] TRUE TRUE TRUE TRUE TRUE
```

```
pdbs<- pdbaln(pdb.files, fit=TRUE, exefile="msa")
```

```
Reading PDB files:
dimer_23119/dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1_seed_000.pdb
dimer_23119/dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3_seed_000.pdb
.....

Extracting sequences

pdb/seq: 1   name: dimer_23119/dimer_23119_unrelaxed_rank_001_alphafold2_multimer_v3_model_2
pdb/seq: 2   name: dimer_23119/dimer_23119_unrelaxed_rank_002_alphafold2_multimer_v3_model_5
pdb/seq: 3   name: dimer_23119/dimer_23119_unrelaxed_rank_003_alphafold2_multimer_v3_model_4
pdb/seq: 4   name: dimer_23119/dimer_23119_unrelaxed_rank_004_alphafold2_multimer_v3_model_1
pdb/seq: 5   name: dimer_23119/dimer_23119_unrelaxed_rank_005_alphafold2_multimer_v3_model_3
```

```
library(bio3d)
#view.pdbs(pdbs)
```

```
plot(pdbs$b[1,], typ= "l", ylim=c(0,100), ylab= "pLDDR Score")
lines(pdbs$b[2,], typ= "l", col=("blue"))
lines(pdbs$b[3,], typ= "l", col=("hotpink"))
lines(pdbs$b[4,], typ= "l", col=("purple"))
lines(pdbs$b[5,], typ= "l", col=("lightgreen"))
```