Class 10 - Structural Bioinformatics

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1. Introduction to PDB

The main repository of bio-molecular structure data is called the Protein Data Bank (PDB). It is the second oldest database ever (after GenBank)

What is currently in the PDB? We can access current composition stats here

```
pdb.stats <- read.csv("Data Export Summary.csv", row.names=1)
head(pdb.stats)
```

```
                        X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)        171,959 18,083 12,622              210      84    32
Protein/Oligosaccharide  10,018  2,968     34               10       2     0
Protein/NA                8,847  5,376    286                7       0     0
Nucleic acid (only)       2,947    185  1,535               14       3     1
Other                       170     10     33                0       0     0
Oligosaccharide (only)       11      0      6                1       0     4
                        Total
Protein (only)        202,990
Protein/Oligosaccharide  13,032
Protein/NA               14,516
Nucleic acid (only)       4,685
Other                       213
Oligosaccharide (only)       22
```

> Q1: What percentage of structures in the PDB are solved by X-Ray and Electron Microscopy.

```
comma.sum <- function(x){
  y <- gsub(",","",x)
  return(sum(as.numeric(y)))}

(comma.sum(pdb.stats$X.ray) + comma.sum(pdb.stats$EM)) / (comma.sum(pdb.stats$Total)) * 100
```

```
[1] 93.6787
```

> Q2: What proportion of structures in the PDB are protein?

```
comma.sum(pdb.stats["Protein (only)","Total"]) / comma.sum(pdb.stats[,"Total"])
```

```
[1] 0.862107
```

2. Visualizing with Mol-star

Mol (pronounced "molstar") is a new web-based molecular viewer that is rapidly gaining in popularity and utility. At the time of writing it is still a long way from having the full feature set of stand-alone molecular viewer programs like VMD, PyMol or Chimera. However, it is gaining new features all the time and does not require any download or complicated installation.

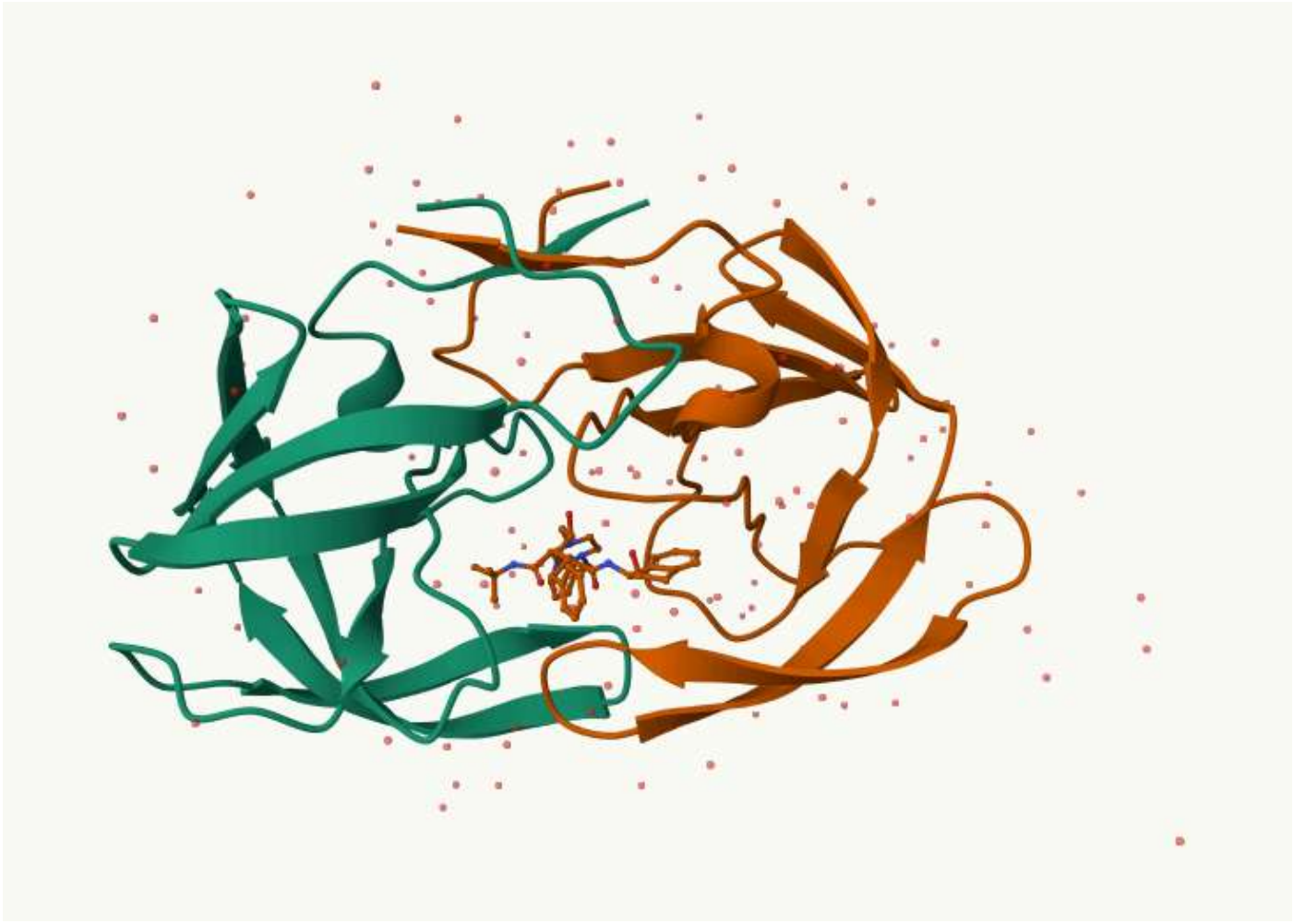


Figure 1. A first look at HIV-pr

4. Comparative Structure Analysis

```
library(bio3d)
aa <- get.seq("1ake_A")
```

```
Warning in get.seq("1ake_A"): Removing existing file: seqs.fasta

Fetching... Please wait. Done.
```

```
blast <- blast.pdb(aa)
```

```
Searching ... please wait (updates every 5 seconds) RID = 1MHHXJNF016
.................
Reporting 90 hits
```

```
attributes(blast)
```

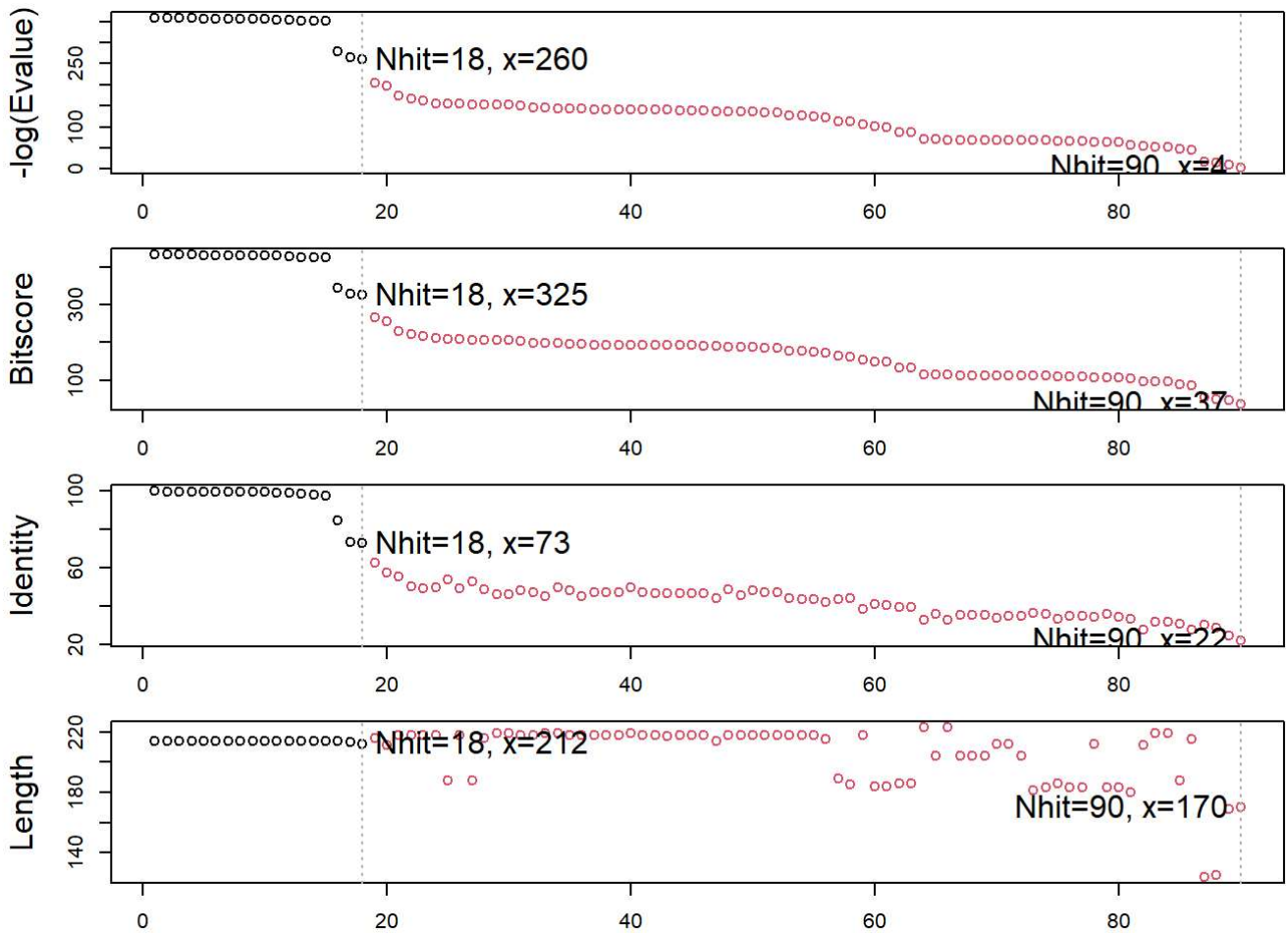
```
$names
[1] "hit.tbl" "raw"     "url"

$class
[1] "blast"
```

```
hits <- plot(blast)
```

```
 * Possible cutoff values:    260 3
          Yielding Nhits:    18 90

 * Chosen cutoff value of:    260
          Yielding Nhits:    18
```




```
head(hits$pdb.id)
```

```
[1] "1AKE_A" "8BQF_A" "4X8M_A" "6S36_A" "8Q2B_A" "8RJ9_A"
```

```
# Download releated PDB files
#files <- get.pdb(hits$pdb.id, path="pdbs", split=TRUE, gzip=TRUE)
#pdbs <- pdbaln(files, fit = TRUE)
```

```
#pc <- pca(pdbs)
#plot(pc)
```

Write a PDB “trajectory” for mol-star

```
#mktrj(pc, file="pca_results.pdb")
```