Class 10: Structural Bioinformatics

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PDB Database

The Protein Data Bank (or PDB) is the second oldest database and is the main one for biomolecular structure data.

```r
stats <- read.csv("Data Export Summary.csv", row.names=1)
stats[] <- lapply(stats, function(x) as.numeric(gsub(",", "", x)))
head(stats)
```

```
                         X.ray    EM   NMR Multiple.methods Neutron Other
Protein (only)          171959 18083 12622              210      84    32
Protein/Oligosaccharide  10018  2968    34               10       2     0
Protein/NA                8847  5376   286                7       0     0
Nucleic acid (only)       2947   185  1535               14       3     1
Other                      170    10    33                0       0     0
Oligosaccharide (only)      11     0     6                1       0     4
                         Total
Protein (only)          202990
Protein/Oligosaccharide  13032
Protein/NA               14516
Nucleic acid (only)       4685
Other                      213
Oligosaccharide (only)      22
```

Here is how you write it as a function:

```r
comma.sum <- function(x){
  y <- gsub(",","",x)
  ##G sub makes it , to no ,
  return (sum(as.numeric(y)))
}
```

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

```r
xray.sum <- comma.sum(stats$Neutron)
em.sum <- comma.sum(stats$EM)
total.sum <- comma.sum (stats$Total)
```

```r
xray.sum/total.sum*100
```

```
[1] 0.03779867
```

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

```r
protein.sum <- stats["Protein (only)","Total"]
protein.sum/total.sum*100
```

```
[1] 86.2107
```

86% of the structures are proteins.

Visualizing with Mol-star

We will be analyzing the HIV-1 protease structure with PDB code: `1HSG` Mol-star homepage at: https://molstar.org/viewer/.

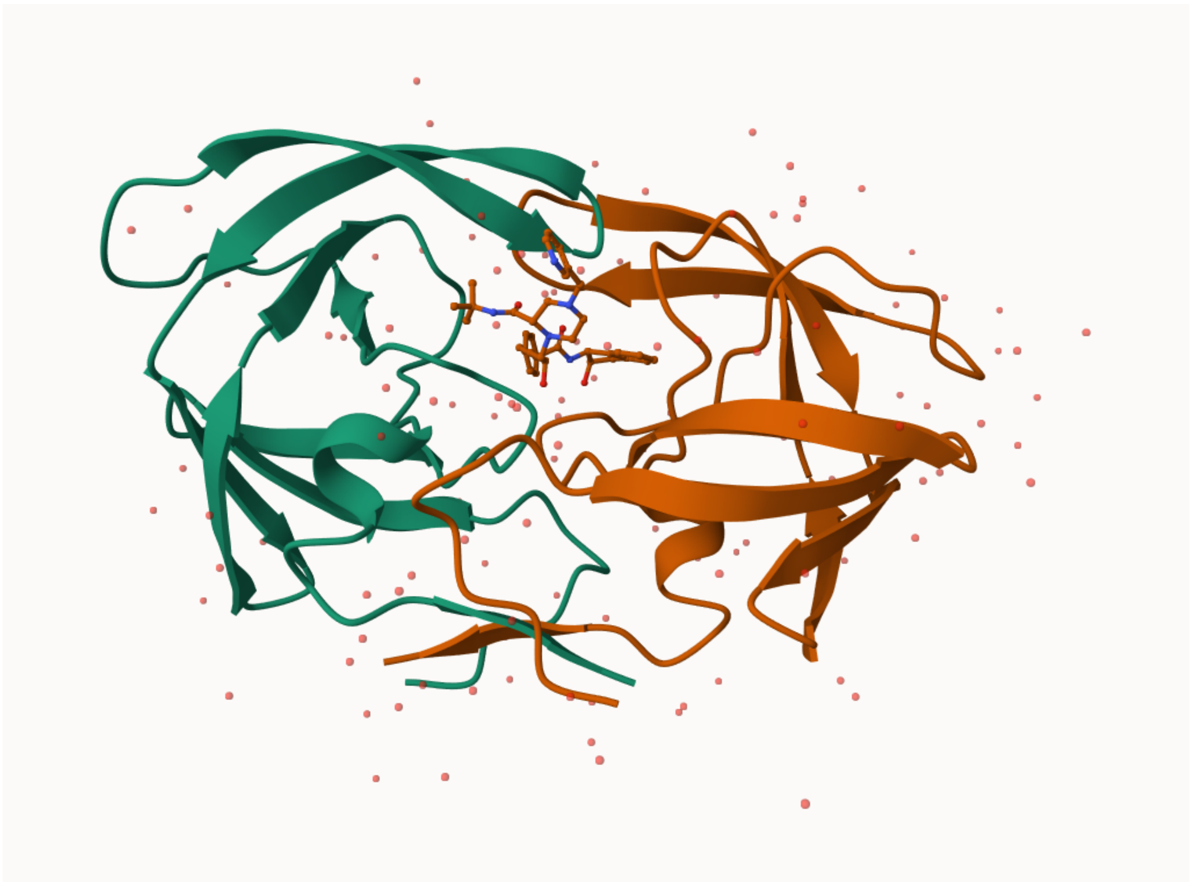


Figure 1: Figure 1. A first view of HIV-Pr

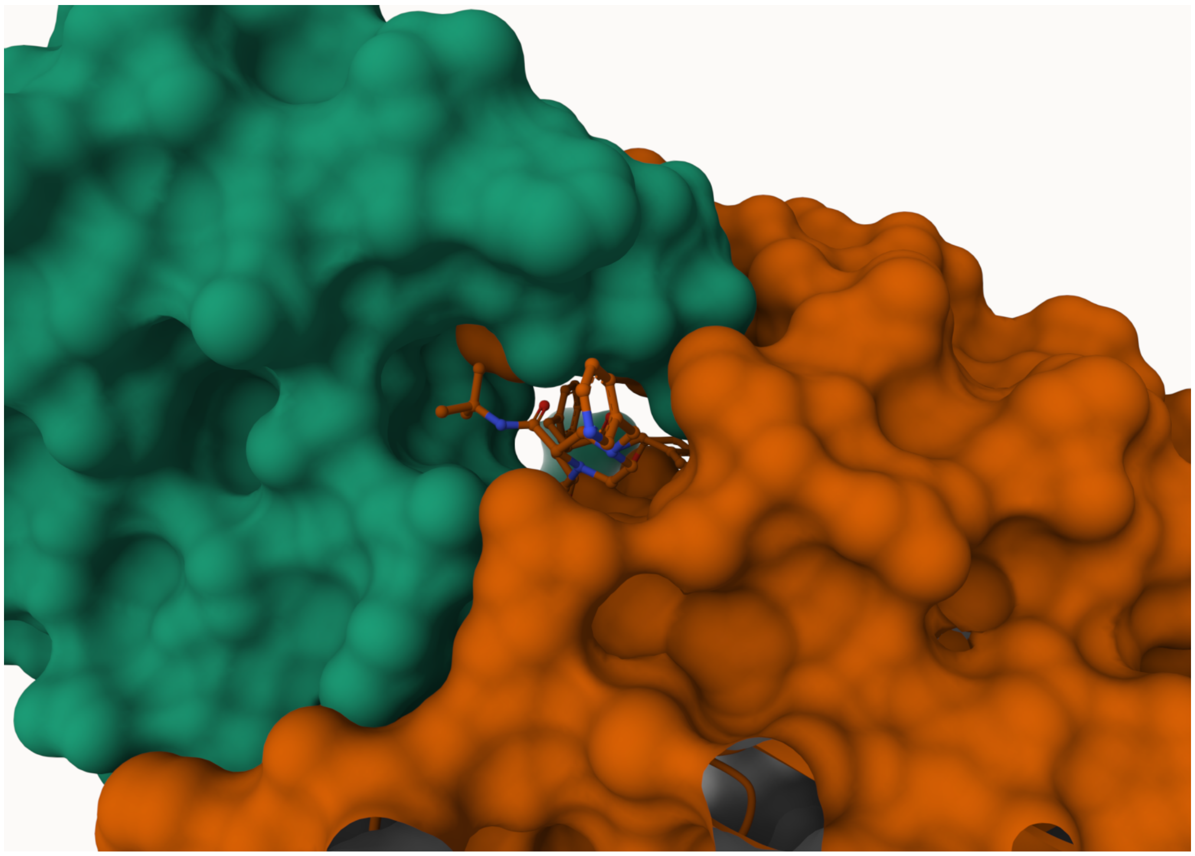


Figure 2: Figure 2. A view of where the ligand attaches in HIV-Pr

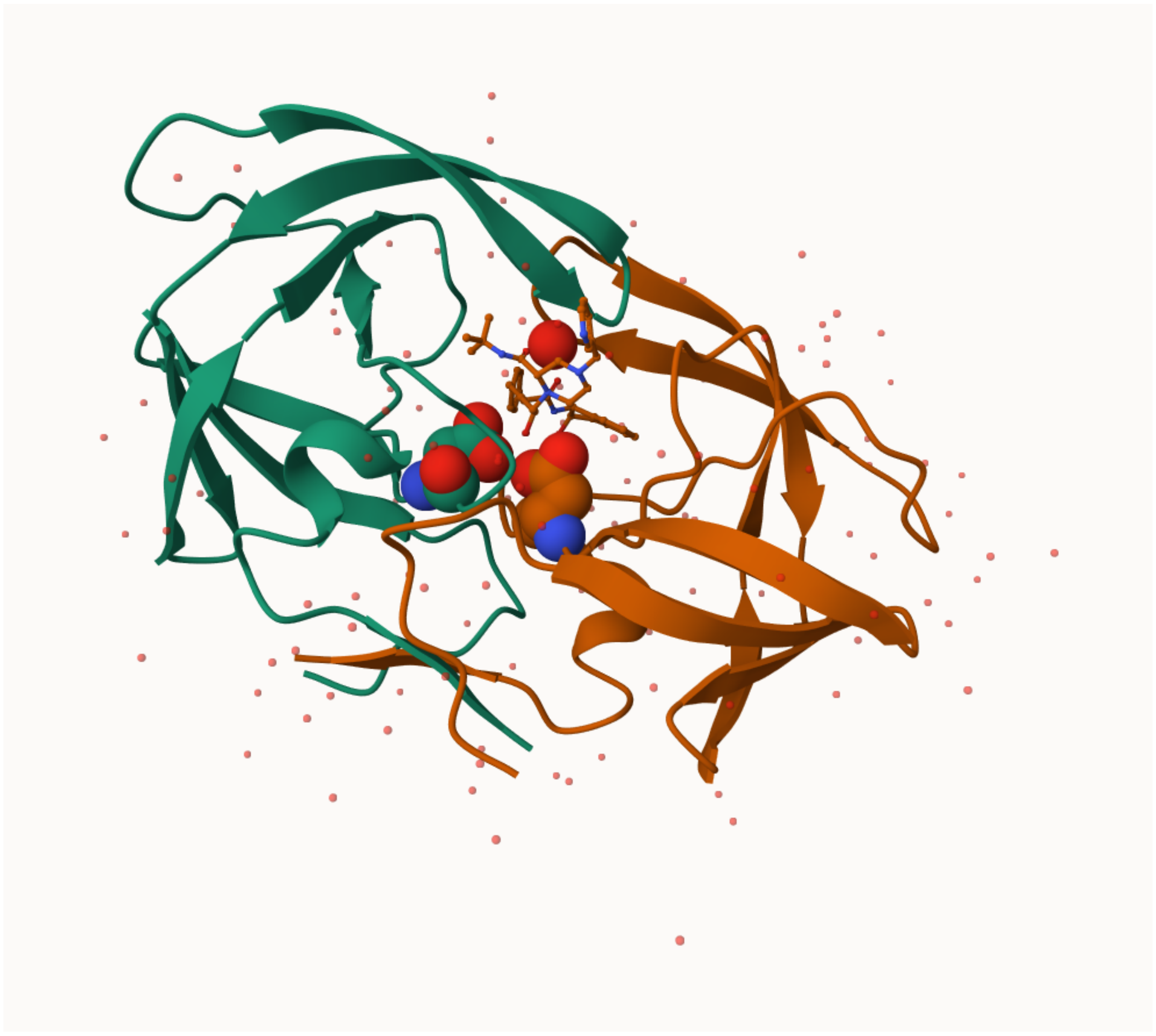


Figure 3: Figure 3. A view of Aspartic Acid residue with Water

Using bio3d package in R

Bio3D package can help focus on structural bioinformatics analysis. It allows us to read and analyze PDB data.

```
library (bio3d)
```

```
pdb <- read.pdb("1hsg")
```

```
  Note: Accessing on-line PDB file
```

```r
pdb
```

```
 Call:  read.pdb(file = "1hsg")

   Total Models#: 1
     Total Atoms#: 1686,  XYZs#: 5058  Chains#: 2  (values: A B)

     Protein Atoms#: 1514  (residues/Calpha atoms#: 198)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 172  (residues: 128)
     Non-protein/nucleic resid values: [ HOH (127), MK1 (1) ]

   Protein sequence:
      PQITLWQRPLVTIKIGGQLKEALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYD
      QILIEICGHKAIGTVLVGPTPVNIIGRNLLTQIGCTLNFPQITLWQRPLVTIKIGGQLKE
      ALLDTGADDTVLEEMSLPGRWKPKMIGGIGGFIKVRQYDQILIEICGHKAIGTVLVGPTP
      VNIIGRNLLTQIGCTLNF

+ attr: atom, xyz, seqres, helix, sheet,
        calpha, remark, call
```

```r
attributes(pdb)
```

```
$names
[1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"

$class
[1] "pdb" "sse"
```

We will see atom data with `pdb$atom`

```r
head(pdb$atom)
```

```
  type eleno elety  alt resid chain resno insert      x      y     z o     b
1 ATOM     1     N <NA>   PRO     A     1   <NA> 29.361 39.686 5.862 1 38.10
2 ATOM     2    CA <NA>   PRO     A     1   <NA> 30.307 38.663 5.319 1 40.62
```

```
3 ATOM     3      C <NA>   PRO     A     1   <NA> 29.760 38.071 4.022 1 42.64
4 ATOM     4      O <NA>   PRO     A     1   <NA> 28.600 38.302 3.676 1 43.40
5 ATOM     5     CB <NA>   PRO     A     1   <NA> 30.508 37.541 6.342 1 37.87
6 ATOM     6     CG <NA>   PRO     A     1   <NA> 29.296 37.591 7.162 1 38.40
  segid elesy charge
1  <NA>     N   <NA>
2  <NA>     C   <NA>
3  <NA>     C   <NA>
4  <NA>     O   <NA>
5  <NA>     C   <NA>
6  <NA>     C   <NA>
```

```
head(pdbseq(pdb))
```

```
  1   2   3   4   5   6 
"P" "Q" "I" "T" "L" "W" 
```

We can make 3D visualizations we can use

```
#library(bio3dview)
#library(NGLVieweR)

#view.pdb(pdb, colorScheme = "sse", backgroundColor = "skyblue") |>
#  setSpin()
```

```
#library (bio3d)
#sel <- atom.select(pdb, resno=25)
#view.pdb(pdb, highlight = sel,
#         highlight.style = "spacefill")
```

Predicting Functional Motions of a Single Structure

Normal Mode Analysis (NMA)

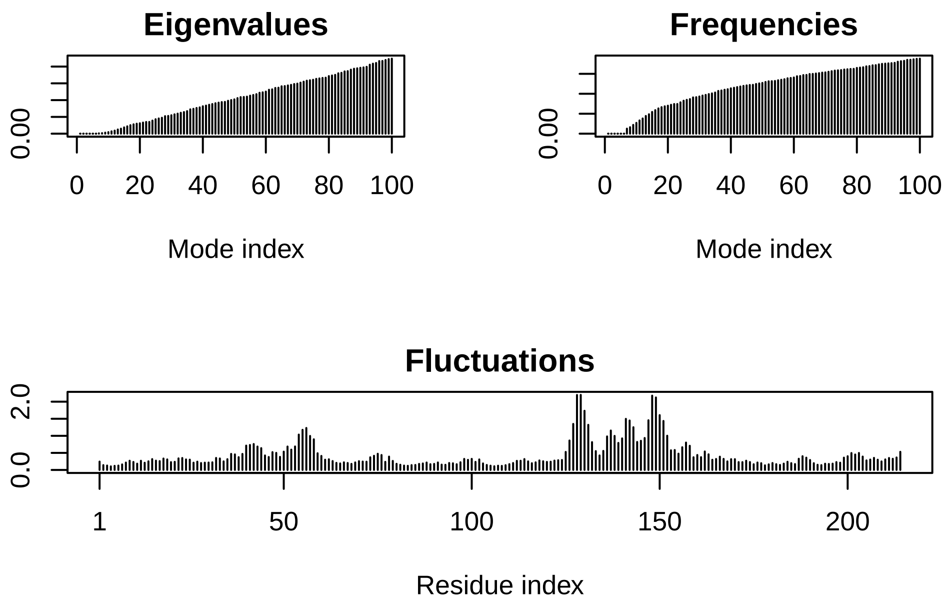
```
adk <- read.pdb("6s36")
```

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

```r
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.015 seconds.
 Diagonalizing Hessian...   Done in 0.282 seconds.
```

```r
plot (m)
```



```r
#view.nma(m)
```

We can write out a trajectory of predicted dynamics and view it in Mol-star

```r
#mktrj(m, file="nma.pdb")
```