Class10: Structural Bioinformatics Part 1

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What is in the PDB database?

The main repository of biomolecular structure info is the PDB < www.rcsb.org >.

Let's see what this database contains:

```
stats <- read.csv("pdb_stats.csv", row.names = 1)
stats
```

```
                         X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)         163,468 13,582 12,390              204      74    32
Protein/Oligosaccharide  9,437  2,287     34                8       2     0
Protein/NA               8,482  4,181    286                7       0     0
Nucleic acid (only)      2,800    132  1,488               14       3     1
Other                      164      9     33                0       0     0
Oligosaccharide (only)      11      0      6                1       0     4
                          Total
Protein (only)         189,750
Protein/Oligosaccharide  11,768
Protein/NA               12,956
Nucleic acid (only)       4,438
Other                       206
Oligosaccharide (only)       22
```

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

```
#as.numeric(stats$X.ray)
```

We got to get rid of the commas. Can you find a function to get rid of the commas?

```
x<-stats$X.ray
sum(as.numeric(gsub(",","",x)))
```

```
[1] 184362
```

I am going to turn this into a function and then use `apply()` to work on the entire table of data.

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

sumcomma(stats$X.ray)
```

```
[1] 184362
```

```
n.total <- sumcomma(stats$Total)
n.total
```

```
[1] 219140
```

```
sumcomma(stats$EM)
```

```
[1] 20191
```

```
apply(stats, 2, sumcomma)
```

```
        X.ray            EM           NMR Multiple.methods
       184362         20191         14237              234
      Neutron         Other         Total
           79            37        219140
```

```
apply(stats, 2, sumcomma) / sumcomma(stats$Total)
```

```
        X.ray            EM           NMR Multiple.methods
 0.8412978005  0.0921374464  0.0649676006  0.0010678105
      Neutron         Other         Total
 0.0003605001  0.0001688418  1.0000000000
```

```
as.numeric(c(10, "10,000"))
```

```
Warning: NAs introduced by coercion
```

```
[1] 10 NA
```

```
(184362/219140)*100
```

```
[1] 84.12978
```

About 84% solved by X-ray.

```
(20191/219140)*100
```

```
[1] 9.213745
```

About 9% solved by EM.

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

248,805,733 - 186,898

```
186898/248805733 * 100
```

```
[1] 0.07511804
```

Visualizing the HIV-1 protease structure

Mol* ("mol-star") viewer is now everywhere. The homepage is here: https://molstar.org/viewer/

I want to insert my image from Mol* here.

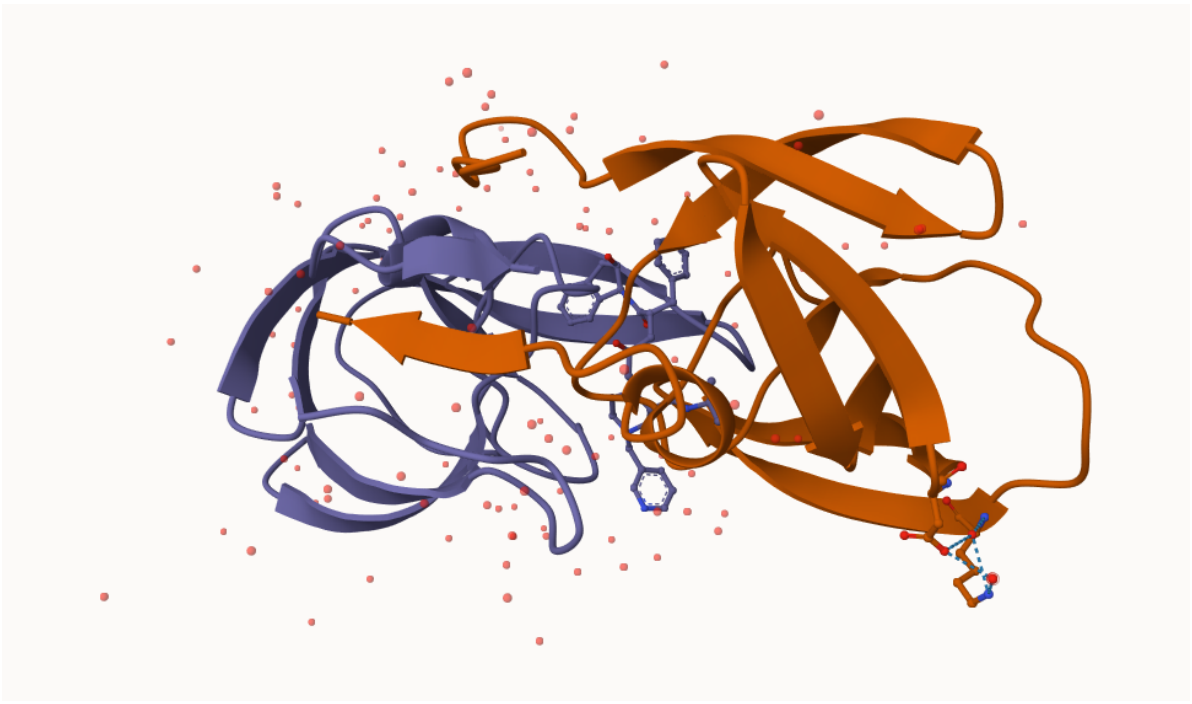
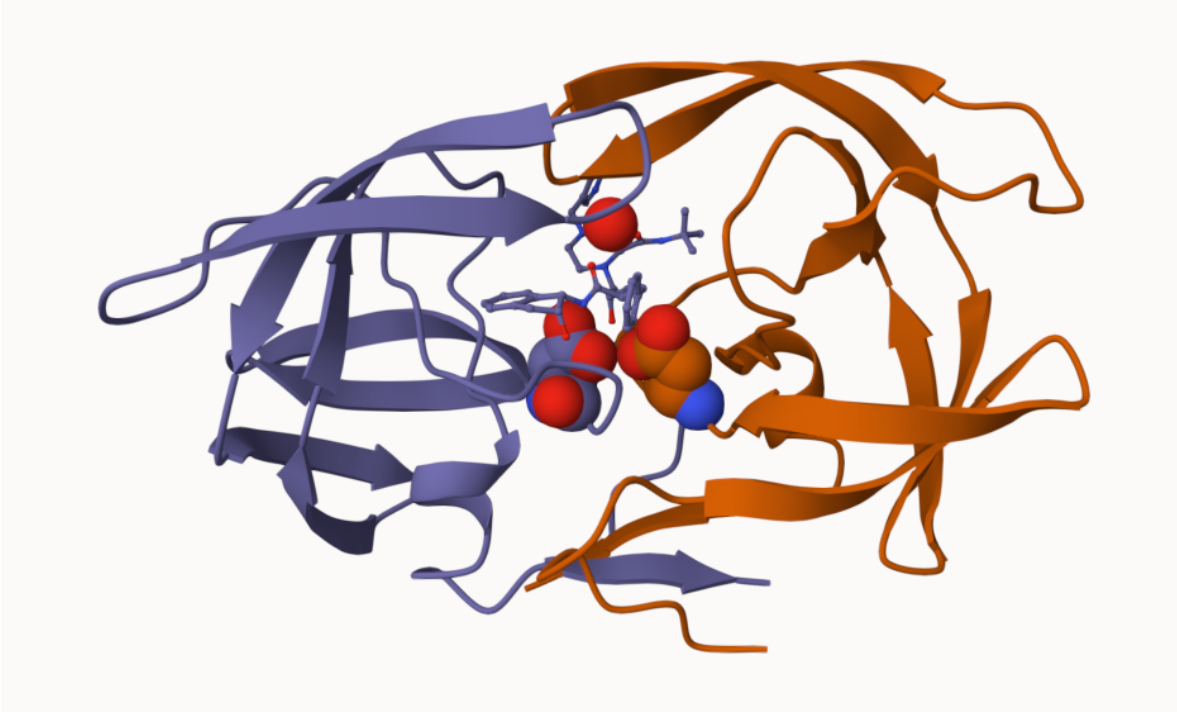


Figure 1: My first molecular image

This image highlights an important water molecule and ASP25 on both chains by changing



them into spacefill

Working with bio3d package

```
library(bio3d)
```

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

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

```
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
```

```
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>
```

```
pdbseq(pdb)[25]
```

```
 25
"D"
```

Predicting functional motions of a single structure

We can do a bioinformatics prediction of functional motions (i.e. flexibility/dynamics):

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

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

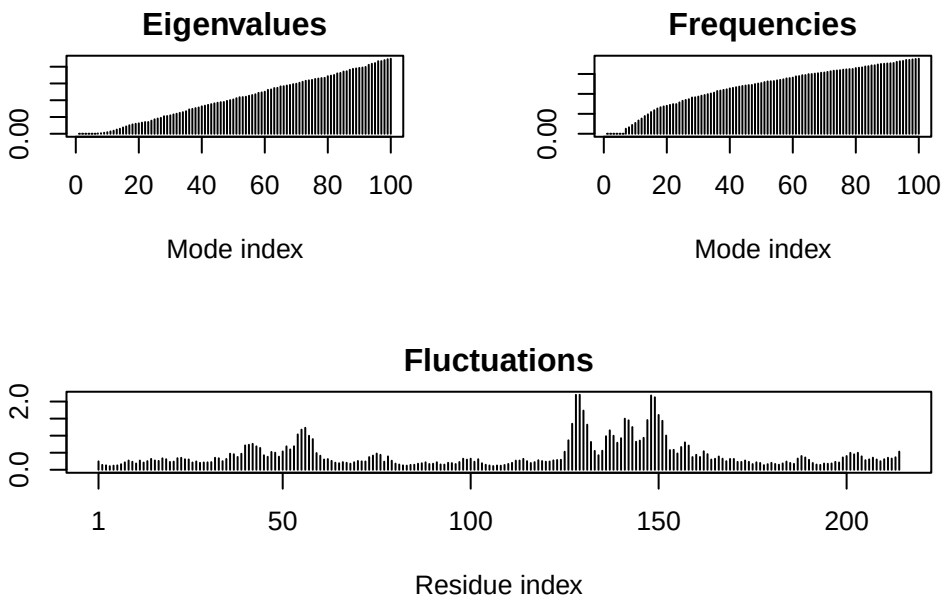
```
pdb
```

```
 Call:  read.pdb(file = "6s36")

   Total Models#: 1
     Total Atoms#: 1898,  XYZs#: 5694  Chains#: 1  (values: A)

     Protein Atoms#: 1654  (residues/Calpha atoms#: 214)
     Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)

     Non-protein/nucleic Atoms#: 244  (residues: 244)
     Non-protein/nucleic resid values: [ CL (3), HOH (238), MG (2), NA (1) ]

   Protein sequence:
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

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

```
m <- nma(pdb)
```

```
 Building Hessian...        Done in 0.014 seconds.
 Diagonalizing Hessian...   Done in 0.276 seconds.
```

```
plot(m)
```




```
mktrj(m, file="adk_m7.pdb")
```