Class10: Structural Bioinformatics pt.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:

```
url  <- "Data Export Summary.csv"
stats <- read.csv(url, 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.

The function `as.numeric` can turn strings into numbers

```
as.numeric(c(10,"1000"))
```

```
[1]   10 1000
```

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

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

```
[1]  NA  NA  NA  NA 164  11
```

How to get rid of the commas?

```r
sum(as.numeric(sub(",", "", stats$X.ray)))
```

```
[1] 184362
```

Turning it into a fucntion:

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

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

```
[1] 219140
```

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

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

```r
apply(stats, 2, sumcomma) / n.total
```

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

X.ray: 0.8412978005 * 100 = 84.12978005 % EM: 0.0921374464 * 100 = 9.21374464 %

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

```
189750/n.total * 100
```

```
[1] 86.58848
```

> Q3: Type HIV in the PDB website search box on the home page and determine how many HIV-1 protease structures are in the current PDB?

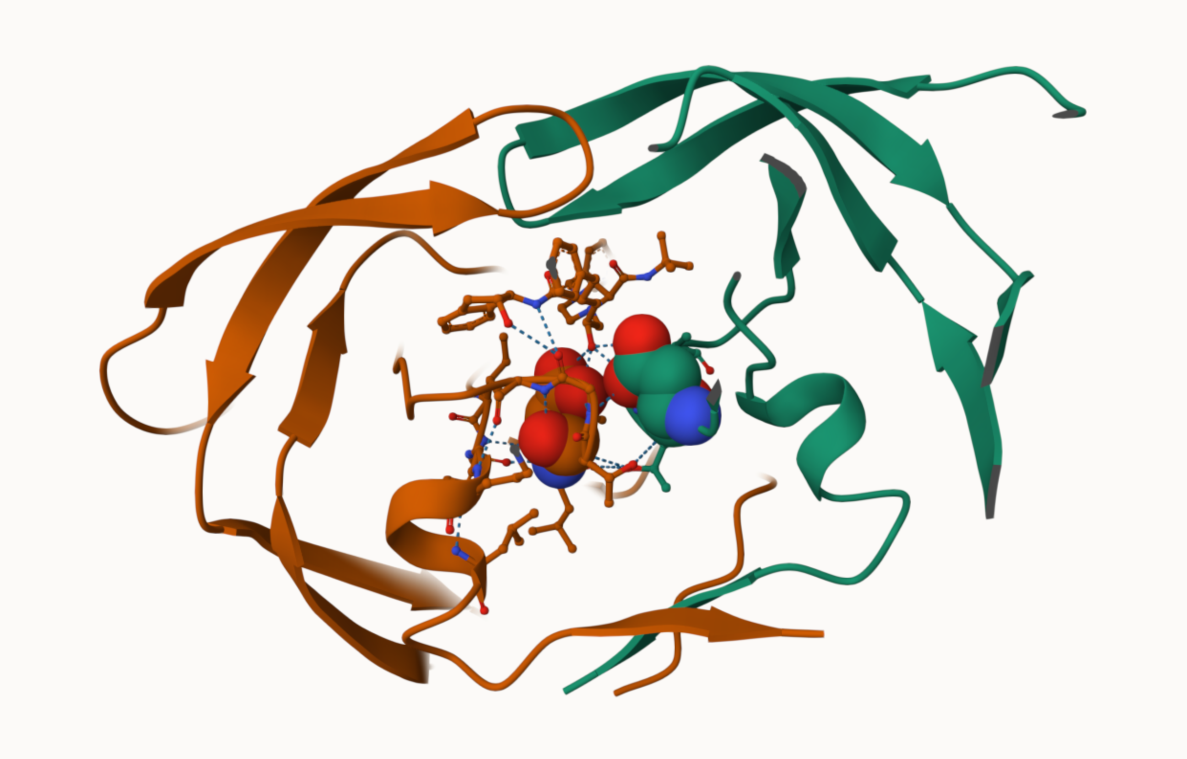
248805733 - 219140

```
219140/248805733 * 100
```

```
[1] 0.08807675
```

Visualizing the HIV-1 protease structure

Mol* ("molstar") is a web-based molecular viewer https://molstar.org/viewer/



> Q4: Water molecules normally have 3 atoms. Why do we see just one atom per water molecule in this structure?

The two H atoms are smaller than the resolution can catch, so it's not on the image.

Working with the bio3d package

```
library(bio3d)
```

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

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

```
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

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

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

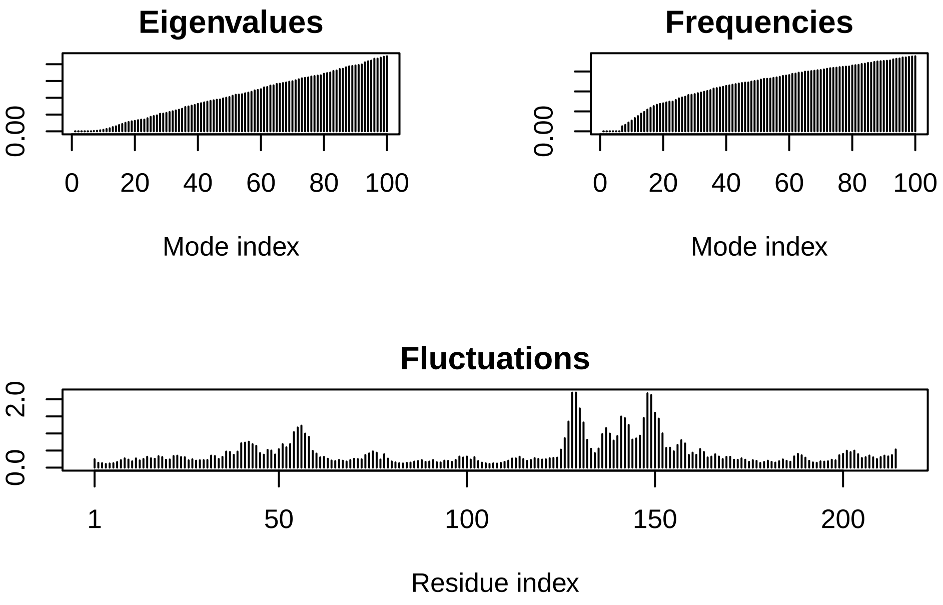
```
pdb
```

```

 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 0.013 seconds.
 Diagonalizing Hessian...   Done in 0.259 seconds.
```

```
plot(m)
```



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