Class 10: Structural Bioinformatics Pt1

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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)         161,663 12,592 12,337              200      74    32
Protein/Oligosaccharide  9,348  2,167     34                8       2     0
Protein/NA               8,404  3,924    286                7       0     0
Nucleic acid (only)      2,758    125  1,477               14       3     1
Other                      164      9     33                0       0     0
Oligosaccharide (only)      11      0      6                1       0     4
                         Total
Protein (only)         186,898
Protein/Oligosaccharide 11,559
Protein/NA              12,621
Nucleic acid (only)      4,378
Other                      206
Oligosaccharide (only)      22
```

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

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

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

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] 182348
```

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] 182348
```

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

```
[1] 215684
```

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

```
        X.ray                EM               NMR Multiple.methods
0.8454405519     0.0872433746     0.0657118748     0.0010663749
     Neutron            Other            Total
0.0003662766     0.0001715473     1.0000000000
```

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

```
sum(sumcomma(stats$X.ray), sumcomma(stats$EM)) / sumcomma(stats$Total)
```

```
[1] 0.9326839
```

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

```
sumcomma(stats$Total[1]) / sumcomma(stats$Total)
```

```
[1] 0.8665362
```

In Uniprot there are 258,805,733 entries which compare to PDB protein entries (186,898) means there are only ~7% of known sequences with a known structure.

```
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 to insert my image from Mol* here

Working with the 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)
```

Figure 1: My first molecular image

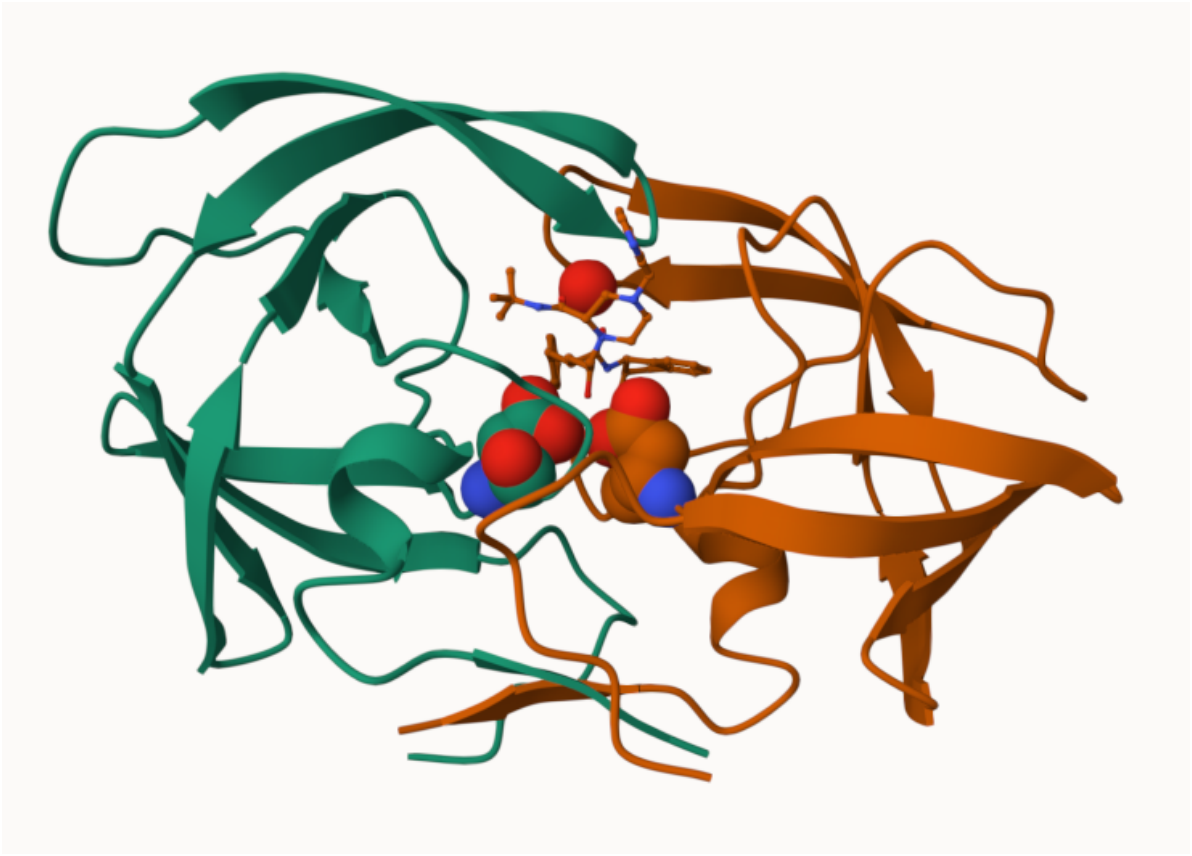


Figure 2: 1HSG with D25 and water as spacefill

```
     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 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
```

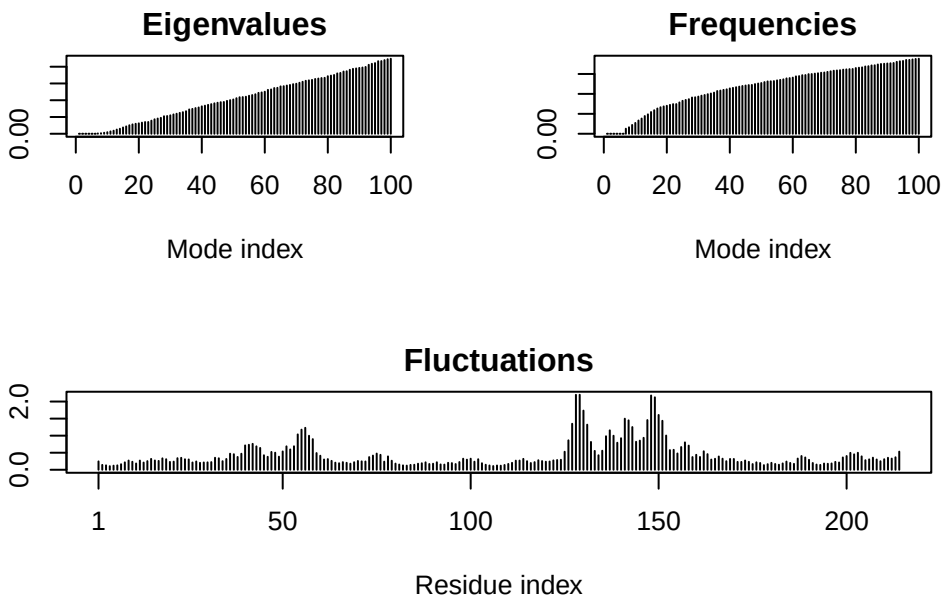
```
pdb
```

```
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 0.03 seconds.
Diagonalizing Hessian...   Done in 0.17 seconds.
```

```
plot(m)
```




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