Class10: Structural Bioinformatics pt.1

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##What is in the PDB database

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

Let's see what the database contains:

```
stats=read.csv("Data Export Summary.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)
```

```
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] 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
```

84% of the structures were X-ray and 9.2% were EM

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

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?

```
186898/248805733 * 100
```

```
[1] 0.07511804
```

##Visualizing the HIV-1 protease structure

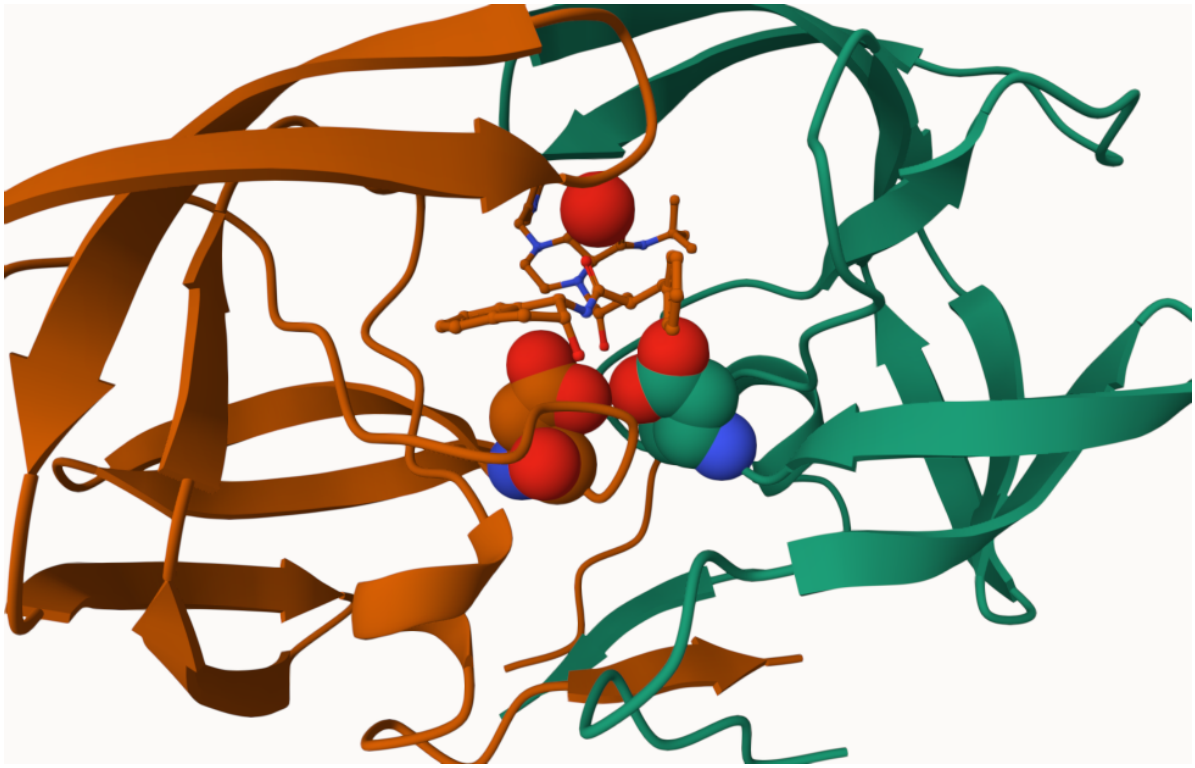
Mol*("mol-star") viewer is now everywhere.

I want to insert my image from Mol* here.

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

Q5: There is a critical "conserved" water molecule in the binding site. Can you identify this water molecule? What residue number does this water molecule have

Figure 1: My first molecular image



##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)
```

```
    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 predictions 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
```

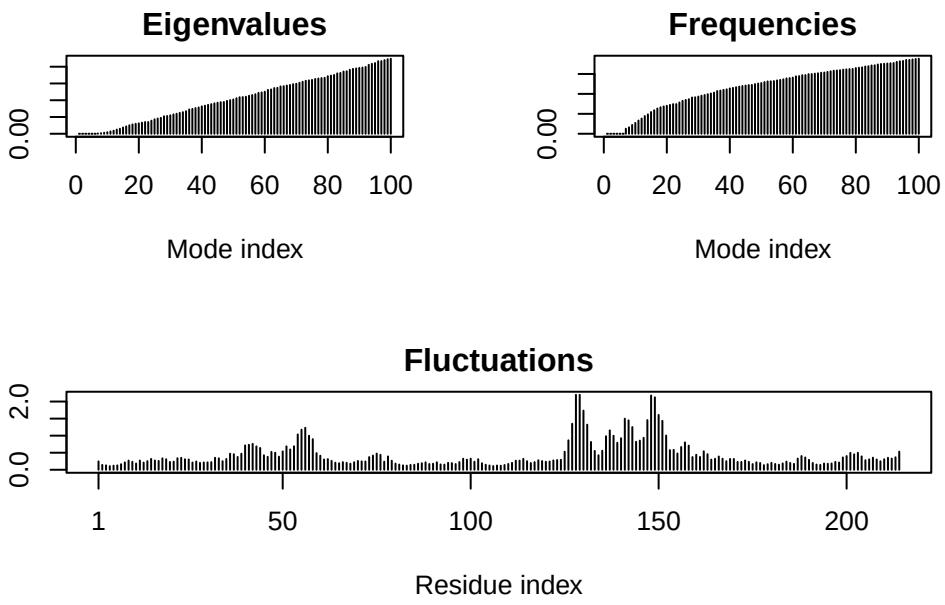
```
pdb
```

```

 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 0.05 seconds.
 Diagonalizing Hessian...   Done in 0.31 seconds.
```

```
plot(m)
```




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