Class10 - Structural Bioinformatics Part 1

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What is in the PDB databse

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

Let's see what this 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

We have to get rid of the commas in the data so it can be read as numeric instead of characters.
- we can use the `sub()` function which is a type of "find and replace" function

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

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

```
[1] 184362
```

Now we need to turn this into a function so it can be used for the other columns of data using `apply()`

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

sumcomma(stats$X.ray)
```

```
[1] 184362
```

Applying the function to each column for the whole table (the two indicates column)

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

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

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

```
[1] 219140
```

These are the percentages of structures solved by each method.

```
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
```

```
#applying the sumcomma function to each column in the table, and then dividing by the tota
```

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

```
n.protein <- sumcomma(stats[1,"Total"])
n.protein
```

```
[1] 189750
```

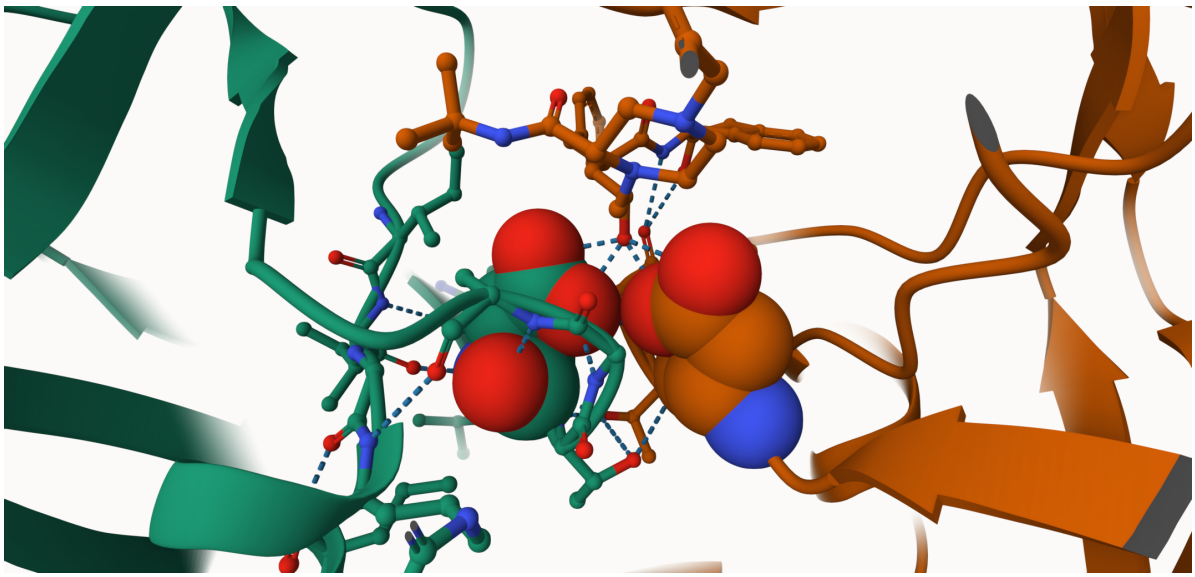
```
n.protein/n.total
```

```
[1] 0.8658848
```

Visualizing the HIV-1 protease structure

Mol* viewer is now everywhere. The homepage is https://molstar.org/viewer/ .

I want to insert my image from Mol* here.



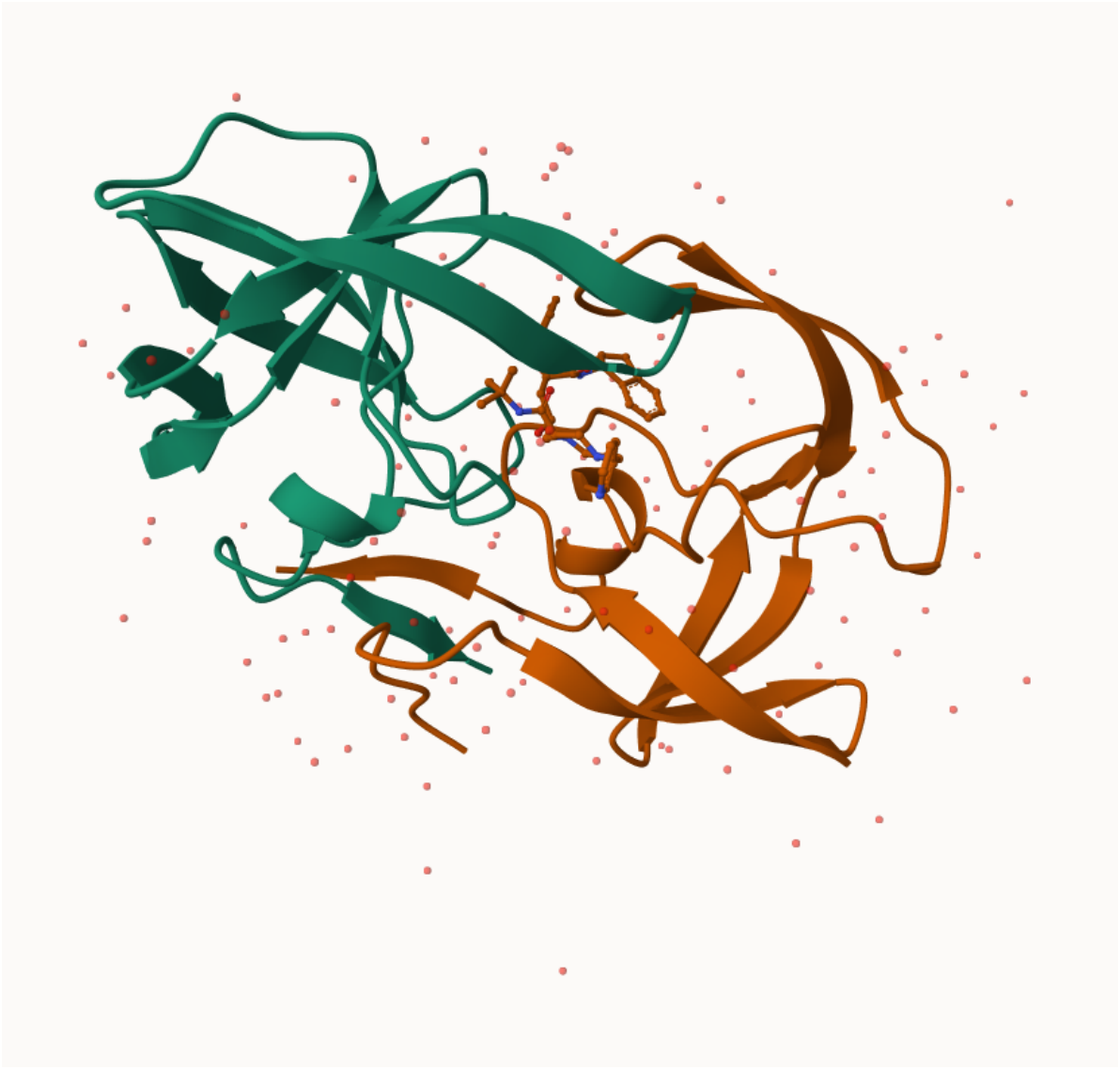


Figure 1: The first molecular image

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 strcture

We can do bioinformatics prediction of functional motions (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:
```

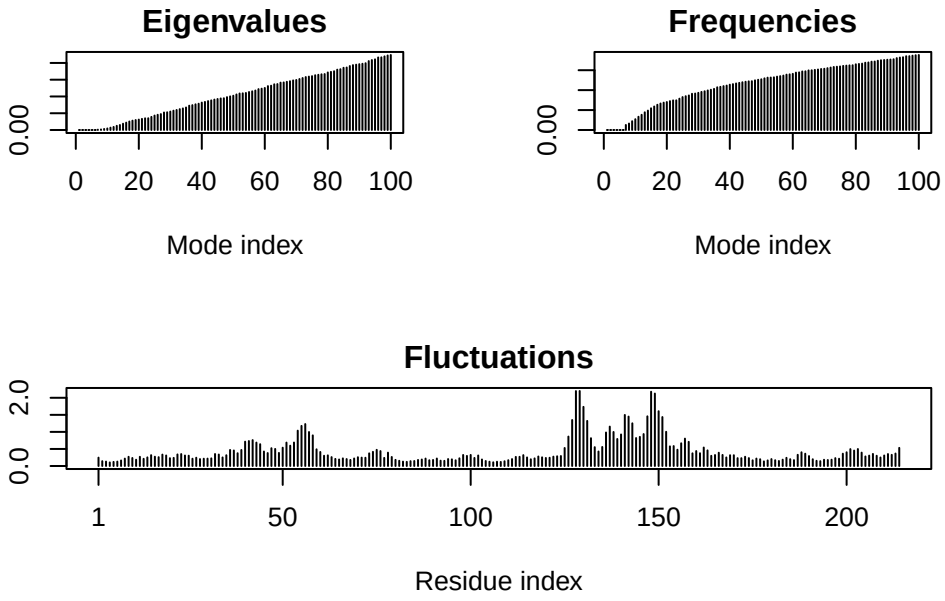
```
      MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

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

nma is normal mode analysis

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

```
 Building Hessian...        Done in 0.047 seconds.
 Diagonalizing Hessian...   Done in 0.359 seconds.
```

```
plot(m)
```



Saving a pdb file to the directory - we can open this in Mol*

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