Class 10: Structural Bioinformatics

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First let's see what is in the PDB database - the main repository of protein structures.

Download composition stats from: https://tinyurl.com/statspdb

For context: a variable

```
stats=read.csv("PDBstats.csv",row.names=1)
stats
```

```
                         X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)         158,844 11,759 12,296              197      73    32
Protein/Oligosaccharide  9,260  2,054     34                8       1     0
Protein/NA               8,307  3,667    284                7       0     0
Nucleic acid (only)      2,730    113  1,467               13       3     1
Other                      164      9     32                0       0     0
Oligosaccharide (only)      11      0      6                1       0     4
                         Total
Protein (only)         183,201
Protein/Oligosaccharide 11,357
Protein/NA              12,265
Nucleic acid (only)      4,327
Other                      205
Oligosaccharide (only)      22
```

```
x=stats$X.ray
x
```

```
[1] "158,844" "9,260"   "8,307"   "2,730"   "164"     "11"
```

```
as.numeric(gsub(",","", x))
```

```
[1] 158844   9260   8307   2730    164     11
```

```
rm.comma=function(x){
  as.numeric(gsub(",","", x))
}
```

```
rm.comma(stats$EM)
```

```
[1] 11759  2054  3667   113     9     0
```

I can use `apply()` to fix the whole table.

```
pdbstats=apply(stats,2,rm.comma)
rownames(pdbstats)=rownames(stats)
head(pdbstats)
```

```
                         X.ray    EM   NMR Multiple.methods Neutron Other
Protein (only)          158844 11759 12296               197      73    32
Protein/Oligosaccharide   9260  2054    34                 8       1     0
Protein/NA                8307  3667   284                 7       0     0
Nucleic acid (only)       2730   113  1467                13       3     1
Other                      164     9    32                 0       0     0
Oligosaccharide (only)      11     0     6                 1       0     4
                         Total
Protein (only)          183201
Protein/Oligosaccharide  11357
Protein/NA               12265
Nucleic acid (only)       4327
Other                      205
Oligosaccharide (only)      22
```

Q1.84.83%, 8.33%

```
totals=apply(pdbstats,2,sum)
round(totals/totals["Total"]*100,2)
```

```
      X.ray               EM              NMR Multiple.methods
      84.83             8.33             6.68             0.11
    Neutron            Other            Total
       0.04             0.02           100.00
```

Q2. 86.67%

```
round(pdbstats[,"Total"]/sum(pdbstats[,"Total"])*100,2)
```

```
      Protein (only) Protein/Oligosaccharide              Protein/NA
               86.67                    5.37                    5.80
 Nucleic acid (only)                   Other  Oligosaccharide (only)
                2.05                    0.10                    0.01
```

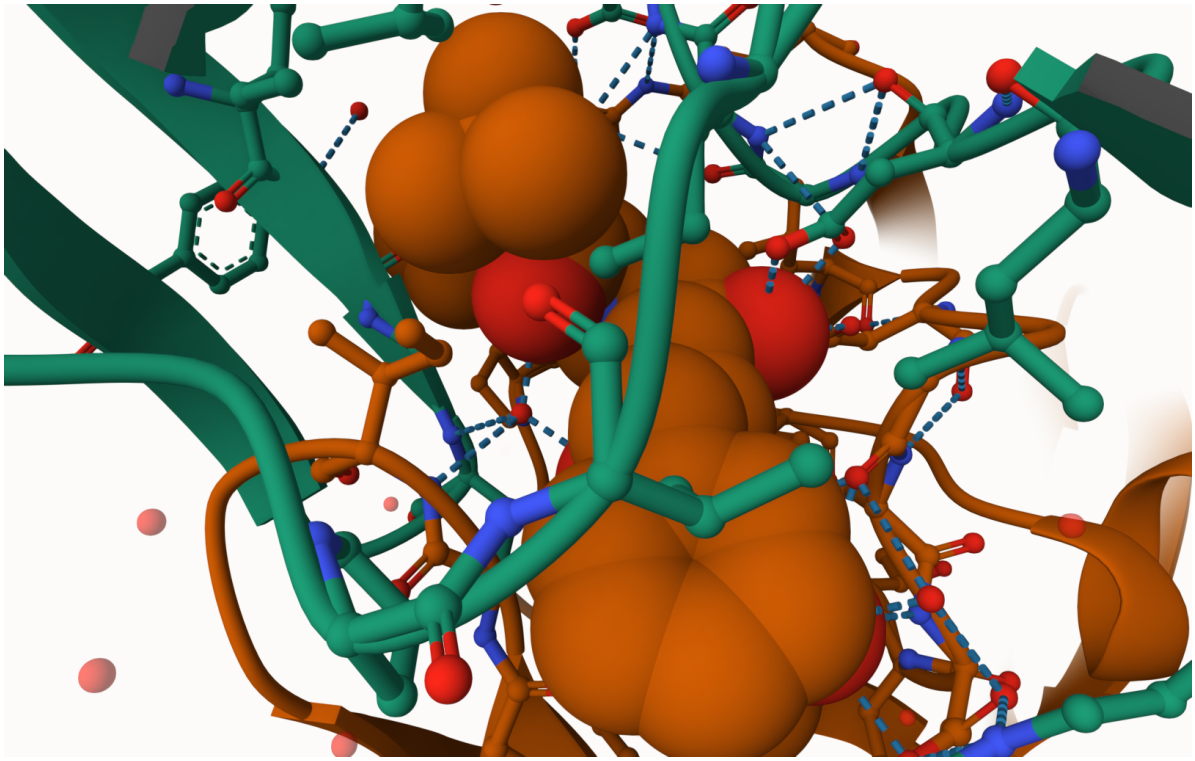
```
round((pdbstats[1,"Total"]/251600768)*100,2)
```

```
[1] 0.07
```

Q4. We see just one atom per water molecule in this structure due to the limited resolution. The hydrogens are too small to be displayed.

Q5. Yes, 308

Q6. Here is a lovely figure of the HIP-Pr with the catalytic ASP residues, the MK1 compound and the important water 308



##The bio3d package for structural bioinformatics

```
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>
```

##Predicting functional motions of a single structure

Let's finish today with a bioinformatics calculation to predict the functions motions of a PDB structure.

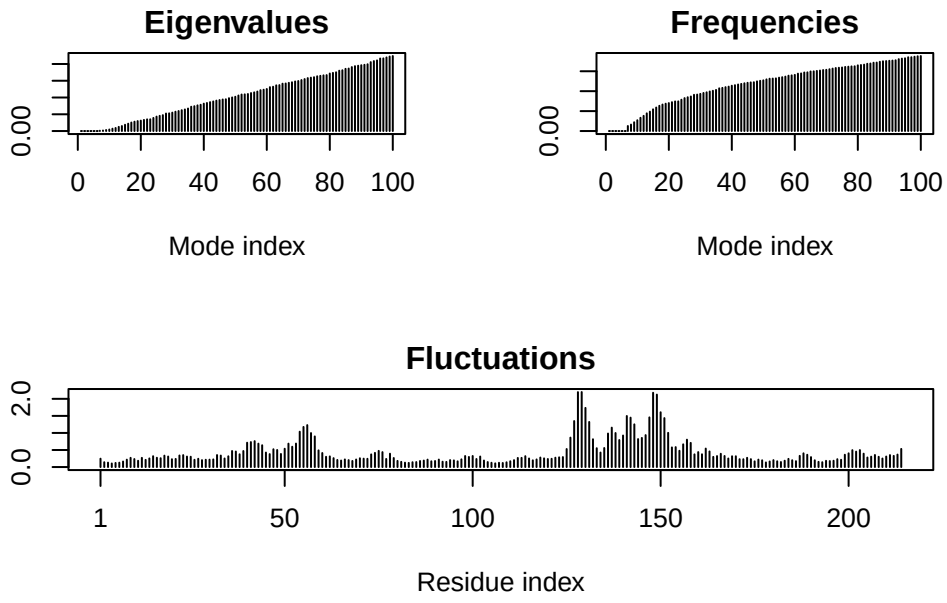
```
adk <- read.pdb("6s36")
```

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

```
m <- nma(adk)
```

```
Building Hessian...         Done in 0.016 seconds.
Diagonalizing Hessian...    Done in 0.287 seconds.
```

```
plot(m)
```




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