class10

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First let's see what is in the PDN database-the mainrepository of protein structures.

Downloaded composition stats from: https://www.rcsb.org/stats/summary

For context: Release 2023_04 of 13-Sep-2023 of UniProtKB/TrEMBL contains 251600768 sequence entries.

http://tinyurl.com/statspdb

```
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
```

There is a problem here due to the commas in the numbers. this cause R to treat them as characters.

```
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$X.ray)
```

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

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
```

```
totals <-apply(pdbstats, 2, sum)
totals
```

```
           X.ray               EM              NMR Multiple.methods 
          179316            17602            14119              226 
         Neutron            Other            Total 
              77               37           211377 
```

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

```r
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 
```

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

```r
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: What proportion of structures in the PDB are protein?

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

```
[1] 86.67
```

> 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?

SKIPED for time

Protein structures in PDB as a fraction of Uniprot sequences. See:https://www.uniprot.org/help/release-statistics

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

```
[1] 0.07
```

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

This is a 2 Angstrom structure and hydrogen is not visible at this resolution. In X-ray crystal structure, hydrogen atoms are generally not detected because they have only one electron. This means they contribute very little to the electron density maps that are used to determine atom positions.But the oxygen atom have 8 electrons so it is more visible, hence for the water molecules we can just see one atom which is the oxygen in the molecule in this sturcture.

> 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

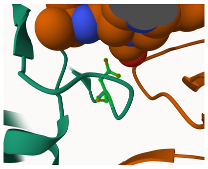
Water HDH 308

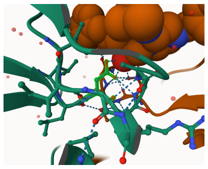
> Q6: Generate and save a figure clearly showing the two distinct chains of HIV-protease along with the ligand. You might also consider showing the catalytic residues ASP 25 in each chain and the critical water (we recommend "Ball & Stick" for these side-chains). Add this figure to your Quarto document.

```
getwd()
```

```
[1] "/Users/zhaokai/Desktop/Rbimm/class10"
```

Here are 2 lovely figures of HIP-Pr with the catalytic ASP residues,the MK1 compound and the all important water 308(1 is the simple one, one is with surroundings).





```r
library(bio3d)

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

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

```r
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
```

```r
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>
```

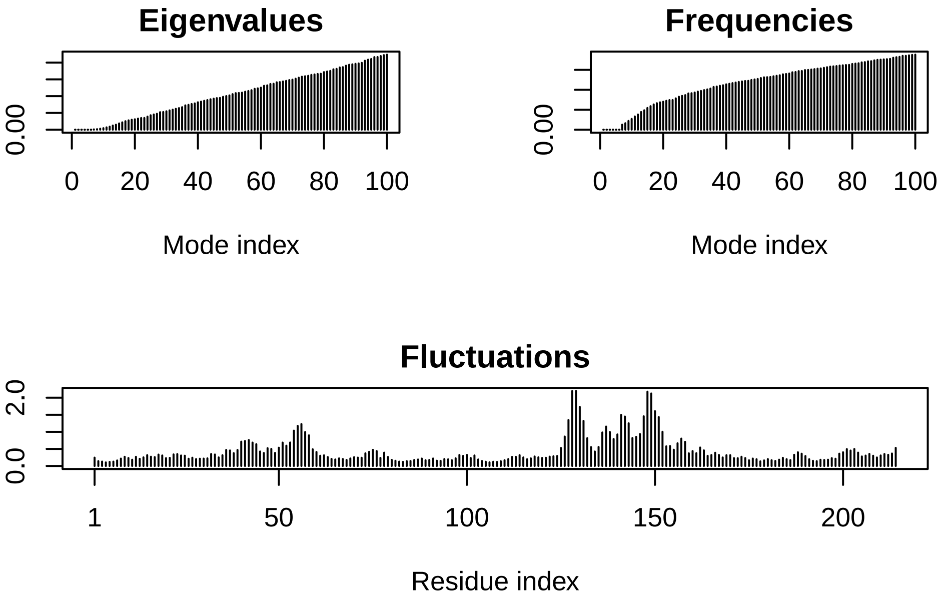
```r
adk <- read.pdb("6s36")
```

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

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

```
Building Hessian...        Done in 0.033 seconds.
Diagonalizing Hessian...   Done in 0.387 seconds.
```

```r
plot(m)
```



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

> Q7: How many amino acid residues are there in this pdb object?

198

> Q8: Name one of the two non-protein residues?

MK1

> Q9: How many protein chains are in this structure?

2

> Q10. Which of the packages above is found only on BioConductor and not CRAN?

msa

> Q11. Which of the above packages is not found on BioConductor or CRAN?:

bio3d-view

> Q12. True or False? Functions from the devtools package can be used to install packages from GitHub and BitBucket?

TRUE

> Q13. How many amino acids are in this sequence, i.e. how long is this sequence?

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