Class09

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PDB Statistics

The PDB is the main database for structural information on biomolecules let's see what it contains:

```
db <- read.csv("Data Export Summary.csv")
db
```

```
           Molecular.Type   X.ray     EM    NMR Multiple.methods Neutron Other
1          Protein (only) 154,766 10,155 12,187              191      72    32
2 Protein/Oligosaccharide   9,083  1,802     32                7       1     0
3              Protein/NA   8,110  3,176    283                6       0     0
4     Nucleic acid (only)   2,664     94  1,450               12       2     1
5                   Other     163      9     32                0       0     0
6  Oligosaccharide (only)      11      0      6                1       0     4
    Total
1 177,403
2  10,925
3  11,575
4   4,223
5     204
6      22
```

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

```
db$X.ray
```

```
[1] "154,766" "9,083"   "8,110"   "2,664"   "163"     "11"
```

Remove the commas!

```r
db$X.ray <- gsub(",", "", db$X.ray)
```

```r
write.csv(db)
```

```
"","Molecular.Type","X.ray","EM","NMR","Multiple.methods","Neutron","Other","Total"
"1","Protein (only)","154766","10,155","12,187",191,72,32,"177,403"
"2","Protein/Oligosaccharide","9083","1,802","32",7,1,0,"10,925"
"3","Protein/NA","8110","3,176","283",6,0,0,"11,575"
"4","Nucleic acid (only)","2664","94","1,450",12,2,1,"4,223"
"5","Other","163","9","32",0,0,0,"204"
"6","Oligosaccharide (only)","11","0","6",1,0,4,"22"
```

```r
xray.total<- sum(as.numeric(gsub(",","", db$X.ray)))
```

```r
db$EM <- gsub(",", "", db$EM)
```

```r
em.total <-sum(as.numeric(gsub(",","", db$EM)))
```

Now we have to write a function:

```r
# I will work with `x` as input

sum_comma <- function(x) {
  # Substitute the comma and convert to numeric
  sum(as.numeric(gsub(",","",x)))
}
```

```r
sum_comma(db$X.ray)
```

```
[1] 174797
```

```r
sum_comma(db$Total)
```

```
[1] 204352
```

For X.ray

```r
sum_comma(db$X.ray) / sum_comma(db$Total)
```

```
[1] 0.8553721
```

For EM:

```r
sum_comma(db$EM)
```

```
[1] 15236
```

```r
sum_comma(db$EM) / sum_comma(db$Total)
```

```
[1] 0.07455763
```

> Q2. What proportion of structures in the PDB are protein?

```r
round (sum_comma(db$Total[1]) / sum_comma(db$Total),2)
```

```
[1] 0.87
```

> 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?

skipped!

Visualizing the HIV-1 protease structure

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

We are not able to see the hydrogen atoms because it is too small for it to be visualized in the technology that we have today, since it is smaller than 2 angstroms

> 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

HOH308

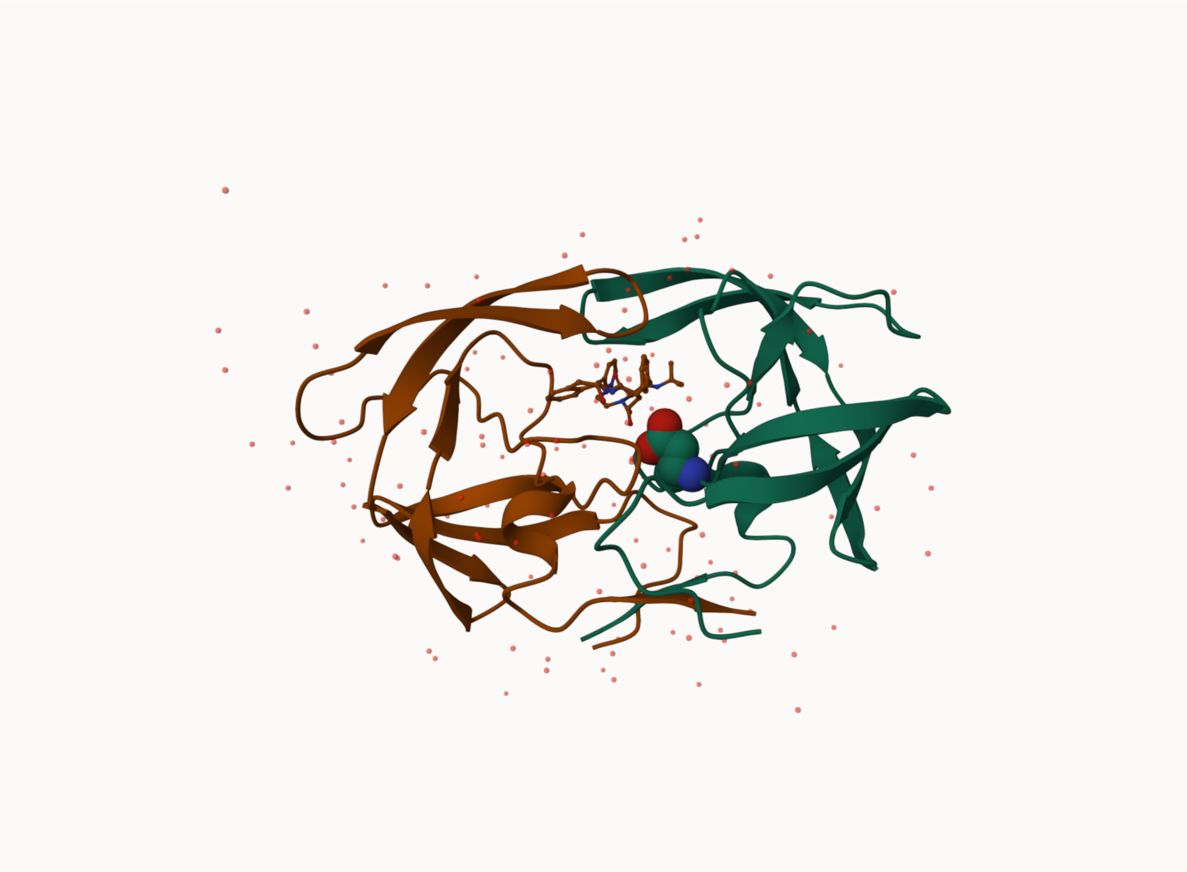


Figure 1: HIV-PR structure from MERK with a bound drug

Working with Structure in R

We can use the bio3d package to read and perform bioinformatics calculations on PDB structures.

```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
attributes(pdb)
```

```
$names
[1] "atom"   "xyz"    "seqres" "helix"  "sheet"  "calpha" "remark" "call"
```

```
$class
[1] "pdb" "sse"
```

```
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>
```

Read an ADK structure

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

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

```
adk
```

```

 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
```

Perform a prediction of flexibility with a technique called NMA (Normal Mode Analysis)

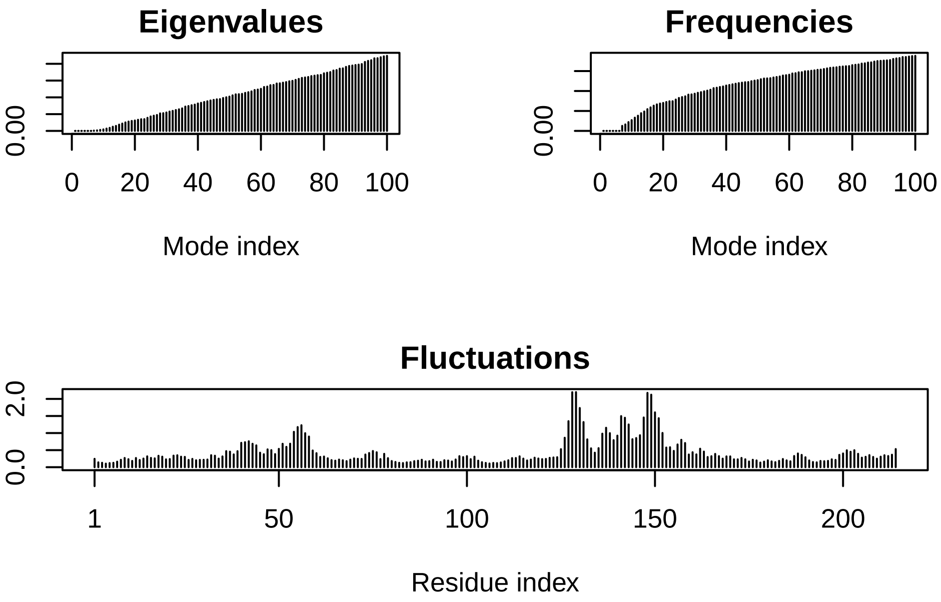
```r
# perform flexibility prediction
m<- nma(adk)
```

```
 Building Hessian...        Done in 0.039 seconds.
 Diagonalizing Hessian...   Done in 0.412 seconds.
```

```r
m
```

```

Call:
  nma.pdb(pdb = adk)

Class:
  VibrationalModes (nma)

Number of modes:
  642 (6 trivial)

Frequencies:
  Mode 7:   0.005
  Mode 8:   0.007
  Mode 9:   0.009
  Mode 10:  0.011
  Mode 11:  0.013
  Mode 12:  0.015

+ attr: modes, frequencies, force.constants, fluctuations,
        U, L, xyz, mass, temp, triv.modes, natoms, call
```

```
plot(m)
```



Write out a “movie” (aka trajectory) of the motion for viewing in MOLstar

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

The created file can be read in MOLstar

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

198

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

HOH

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

2