Class 09: Structural Bioinformatics

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Section 1 - Intro to RCSB Protein Data Bank (PDB)

```
pdb <- read.csv('Data_Export_Summary.csv')
```

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

92.99% of structures in the PDB are solved by X-Ray and Electron Microscopy with each making up approximate 86 and 7% respectively.

```
#xray <- sum(154766, 9083, 8110, 2664, 163, 11)
#em <- sum(10155, 1802, 3176, 94, 9 ,0 )
#total <- sum(177403, 10925, 11575, 4223, 204, 22)

#(xray + em )/ total


xtot <- sum(as.numeric(gsub(',', '' , pdb$X.ray)))

etot <- sum(as.numeric(gsub(',','',pdb$EM)))

ttot <- sum(as.numeric(gsub(',','', pdb$Total)))

(xtot + etot)/ttot
```

```
[1] 0.9299297
```

Make this a function

```
tot <- function(z) {
  #Take inuput z and remove commas
    #then make it numeric and then take the sum
  #Save the sum as y
  y <- sum(as.numeric(gsub(',', '', z)))
  #return output
  return(y)
}

Q1 <- 100* (tot(pdb$X.ray) + tot(pdb$EM)) / tot(pdb$Total)


xprop <- round(tot(pdb$X.ray) / tot(pdb$Total), 2)
```

```
eprop <- round(tot(pdb$EM) / tot(pdb$Total), 2)
```

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

86.81% of structures in the PDB are protein (only).

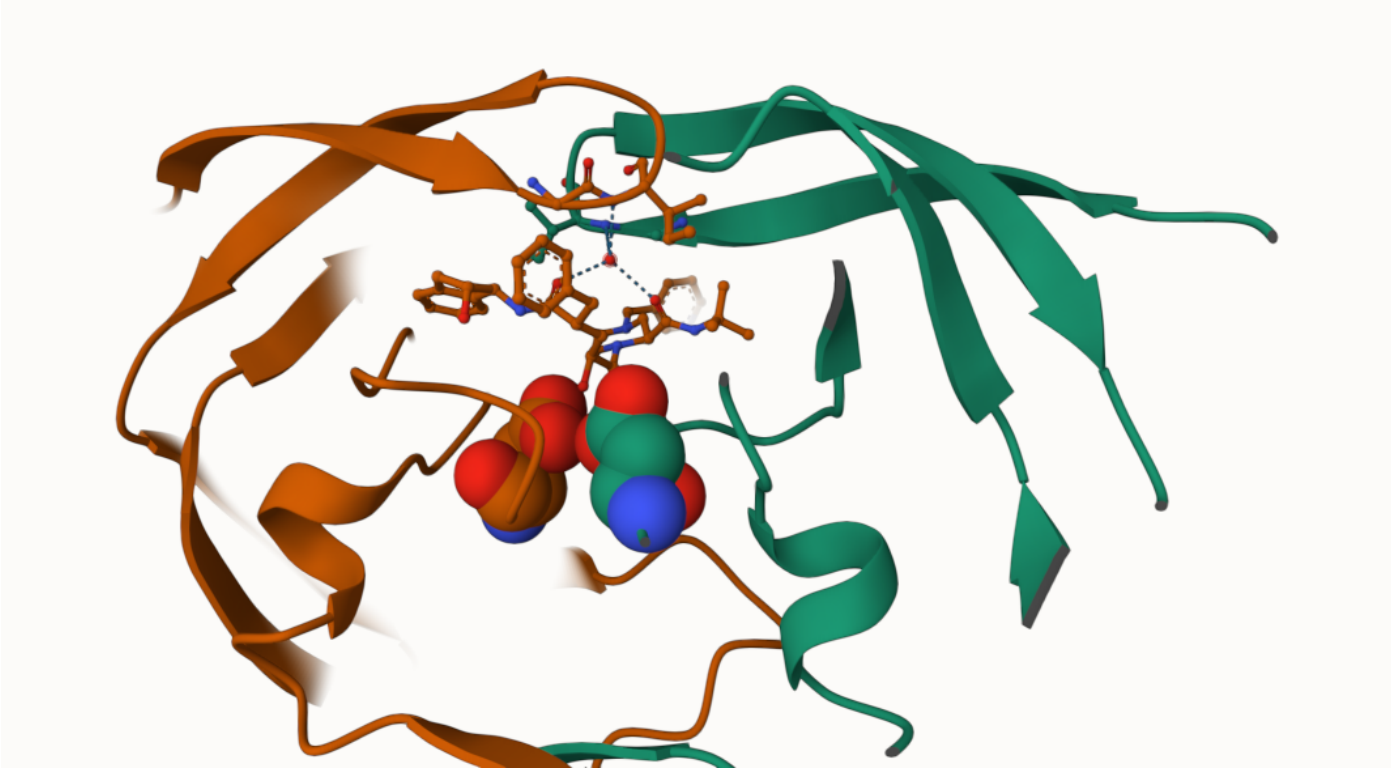
```
rmcomma <- function(input){
 input <- as.numeric(gsub(',','', input))
}

pdb$Total <- as.numeric(gsub(',', '',pdb$Total))

prot <- sum(pdb$Total[1])

prot/sum(pdb$Total)
```

```
[1] 0.8681246
```

> 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?

There are 239 HIV-1 protease structures in the current PDB.

Part 2 - Visualizing the HIV-1 protease structure



HIV-PR Structure from MERK with a bound drug

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

The hydrogen molecules are extremely small and are not rendered due to the low resolution representation,

> 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

The molecule is HOH 308.

Part 3 - Introduction to Bio3D in R

Working with Structures in R

We can use the `bio3d` package to read and perform bioinformativcs calculations on PDB structures

```
library(bio3d)

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

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

```
hsg
```

```
 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
```

```
attributes(hsg)
```

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

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

```
head(hsg$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>
```

Part 4 - Comparative structure analysis of Adenylate Kinase

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

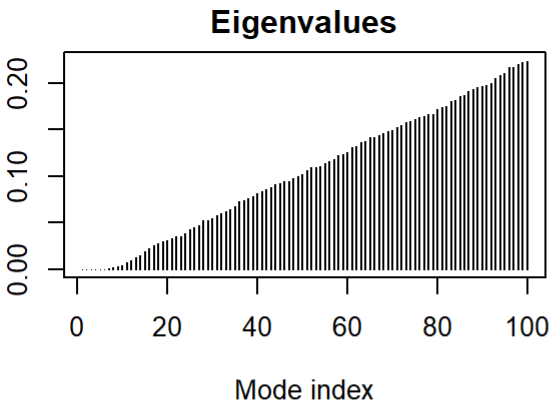
```
  Note: Accessing on-line PDB file
   PDB has ALT records, taking A only, rm.alt=TRUE
```

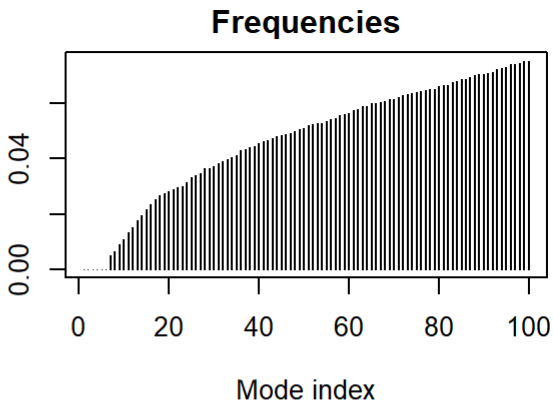
Perform a prediction of flexibility with a technique called NMA (normal mode analysis)

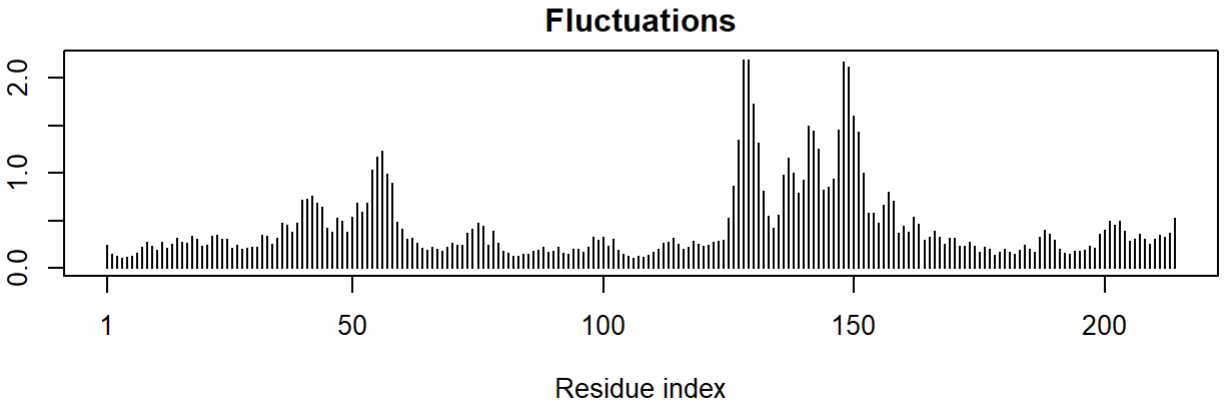
```
#perform a flexibility prediction
m <- nma(adk)
```

```
 Building Hessian...        Done in 0.03 seconds.
 Diagonalizing Hessian...   Done in 0.34 seconds.
```

```
plot(m)
```







Write out a 'movie' (a.k.a trajectory) of the motion for viewing in MOlstar

```
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?

HOH

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

2 protein chains