Class 10: Structural Bioinformatics (pt.1)

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1. The BDP Database

The main repository of biomolecular structure data is called the Protein Data Bank (PDB for short). It is the second oldest database (after GenBank)

What is currently in the PDB? We can access current composition stats here

```
stats <- read.csv("Data Export Summary.csv", row.names=1)
head(stats)
```

	X.ray	EM	NMR	Multiple.methods	Neutron	Other
Protein (only)	171,959	18,083	12,622	210	84	32
Protein/Oligosaccharide	10,018	2,968	34	10	2	0
Protein/NA	8,847	5,376	286	7	0	0
Nucleic acid (only)	2,947	185	1,535	14	3	1
Other	170	10	33	0	0	0
Oligosaccharide (only)	11	0	6	1	0	4

	Total
Protein (only)	202,990
Protein/Oligosaccharide	13,032
Protein/NA	14,516
Nucleic acid (only)	4,685
Other	213
Oligosaccharide (only)	22

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

```
x <- stats$X.ray

#Substitute comma for nothing
y <- gsub(",","",x)

#Convert to numeric
sum(as.numeric(y))
```

```
[1] 193952
```

Turn this snippet into a function so I can use it any time I have this comma problem (i.e. the other columns of this `stats` table)

```
comma.sum <- function(x) {
  #Substitute comma for nothing
  y <- gsub(",","",x)
  #Convert to numeric
```

```
  return(sum(as.numeric(y)))
}
```

```
xray.sum <- comma.sum(stats$X.ray)
em.sum <- comma.sum(stats$EM)
total.sum <- comma.sum(stats$Total)
```

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

```
protein <- comma.sum(stats[1,"Total"])
protein_percent <- protein / total.sum * 100
protein_percent
```

```
[1] 86.2107
```

> 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

2. Visualizing with Mol-star

Explore the HIV-1 protease structure with PDB code: `1HSG` Mol-star homepage at https://molstar.org/viewer/.

![Figure2.] (1HSG.2.png) ![Figure3.] (1HSG.3.png)

3. Using the bio3d package in R

The Bio3D package is focued on 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
```

We can see atom data with `pdb$atom`:

```
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>
```

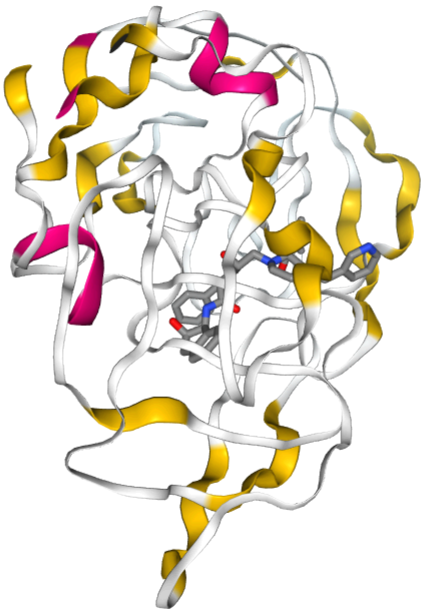
```
head(pdbseq(pdb))
```

```
  1   2   3   4   5   6
"P" "Q" "I" "T" "L" "W"
```

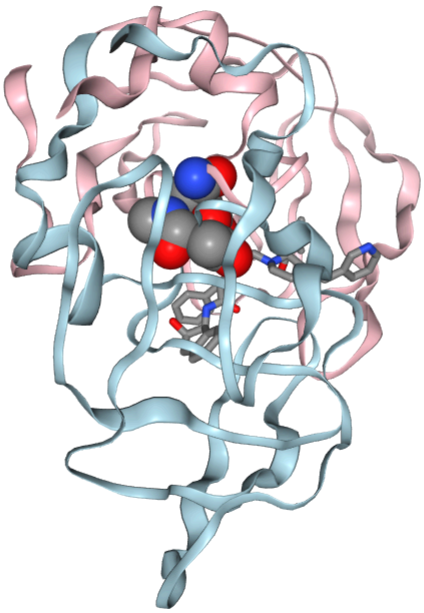
3. Visualization in R

We can make quick 3D viz with the

```
library(bio3dview)
view.pdb(pdb, backgroundColor = "lightblue", colorScheme = "sse")
```



```
sel <- atom.select(pdb, resno=25)
view.pdb(pdb, cols=c("pink","lightblue"),
         highlight = sel,
         highlight.style = "spacefill")
```



Predicting functional motions of a single structure

We can finish off today with a bioinformatics prediction of the functional motions of a protein

We will run a Normal Mode Analysis (NMA)

```
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
```

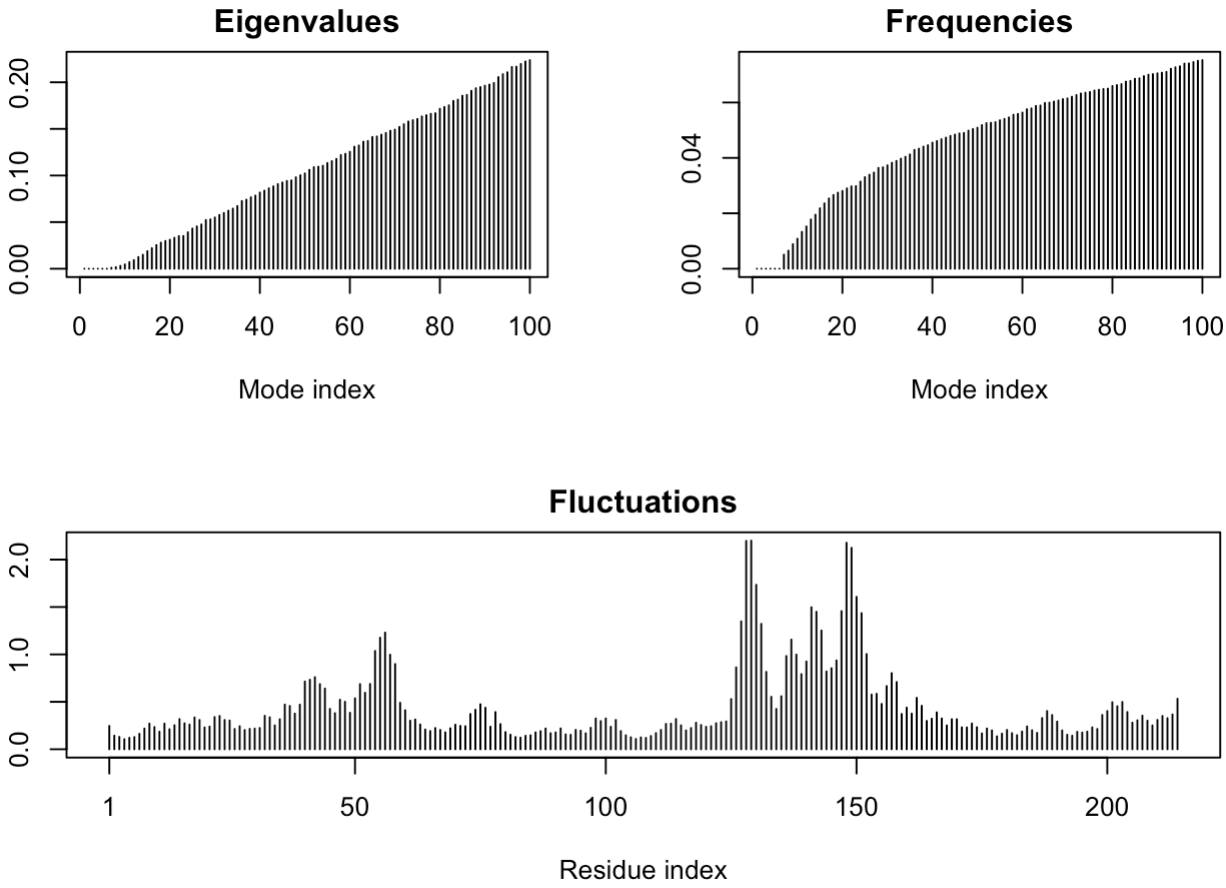
```
      DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDKI
      VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
      YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG

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

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

```
 Building Hessian...        Done in 0.021 seconds.
 Diagonalizing Hessian...   Done in 0.458 seconds.
```

```
plot(m)
```




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

```
view.nma(m, pdb=adk)
```