Class 10: PDB and Structural Bioinformatics

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```
pdb_data <- read.csv("data_export_summary.csv", row.names = 1)
head(pdb_data)
```

```
                          X.ray     EM    NMR Multiple.methods Neutron Other
Protein (only)          167,317 15,698 12,534               208      77    32
Protein/Oligosaccharide   9,645  2,639     34                 8       2     0
Protein/NA                8,735  4,718    286                 7       0     0
Nucleic acid (only)       2,869    138  1,507                14       3     1
Other                       170     10     33                 0       0     0
Oligosaccharide (only)       11      0      6                 1       0     4
                          Total
Protein (only)          195,866
Protein/Oligosaccharide  12,328
Protein/NA               13,746
Nucleic acid (only)       4,532
Other                       213
Oligosaccharide (only)       22
```

```
#create a function
comma_number <- function(x){
  x <- gsub(",", "", x)
  x <- as.numeric(x)

  return(x)
}
```

```
x.ray_num <- comma_number(pdb_data$X.ray)
x.ray_tot <- sum(x.ray_num)

total_sum <- sum(comma_number(pdb_data$Total))
```

The `apply()` function can take any function and apply it over rows or cols.

```
colSums(apply(pdb_data, 2, comma_number)) / total_sum
```

```
          X.ray              EM             NMR Multiple.methods
   0.8325592064    0.1023479646    0.0635181093    0.0010498132
        Neutron           Other           Total
   0.0003617003    0.0001632063    1.0000000000
```

```
#can also use this package that will read it in as a numeric and take out commas for you

library(readr)
pdb_csv <- read_csv("data_export_summary.csv")
```

```
Rows: 6 Columns: 8
-- Column specification --------------------------------------------------------
Delimiter: ","
chr (1): Molecular Type
dbl (3): Multiple methods, Neutron, Other
num (4): X-ray, EM, NMR, Total

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

Q1: X ray solves 83.25% and EM solves 10.23% for a total of 93.48%.

```
sum(comma_number(pdb_data[1:3,7])) / total_sum
```

```
[1] 0.9789729
```

Q2: 97.9% are protein.

##Using Mol*

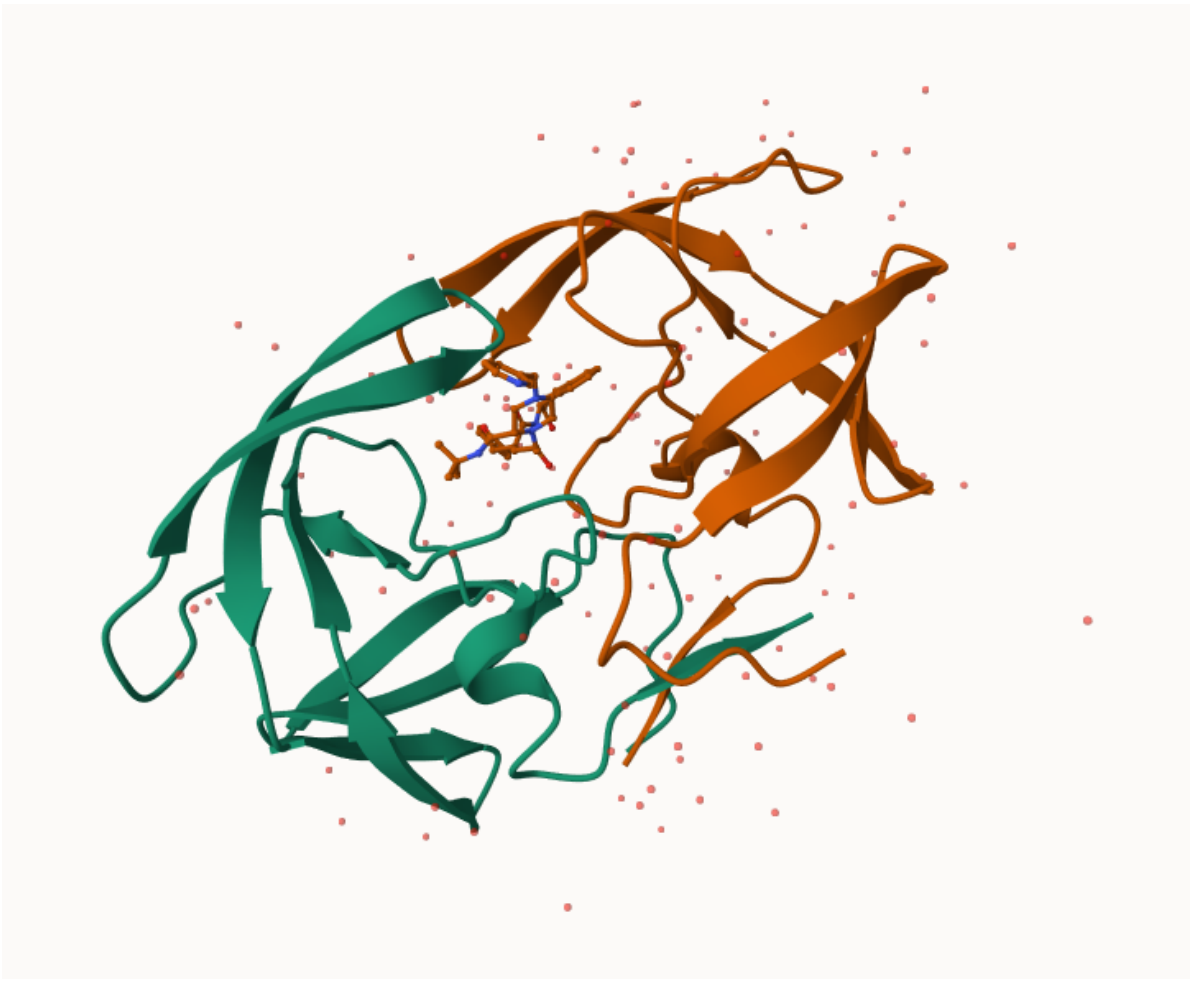


Figure 1: My first image from Mol-star

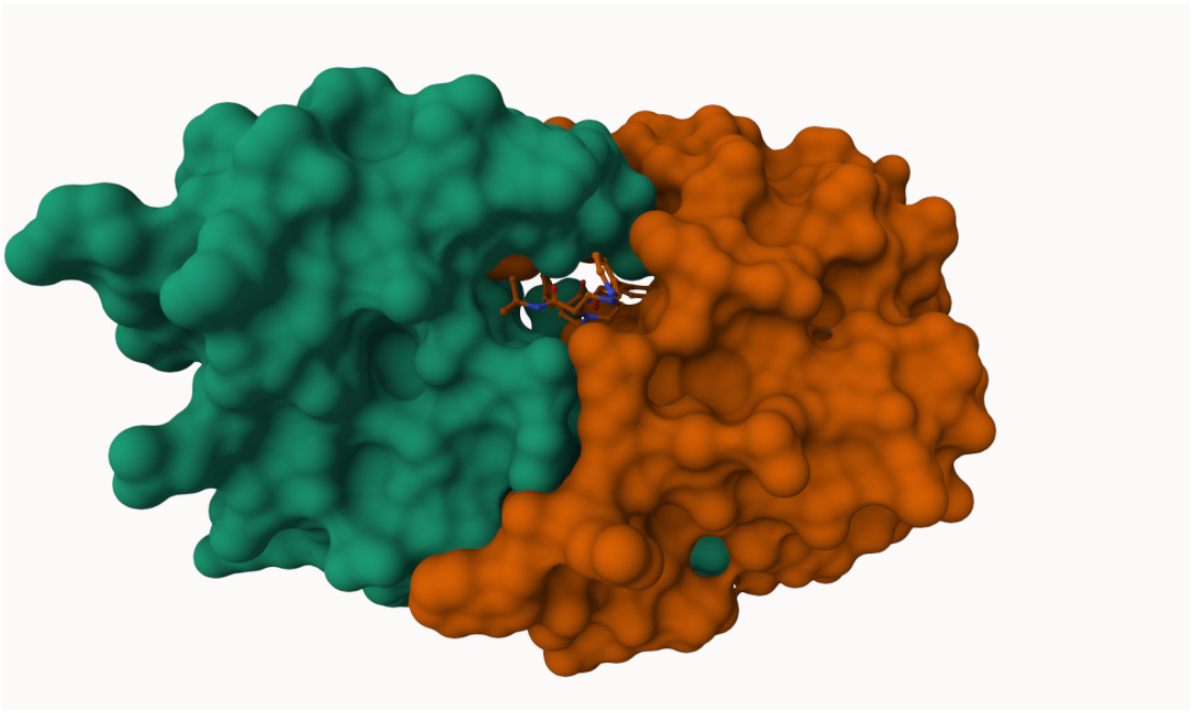


Figure 2: Protein with molecular surface overlay

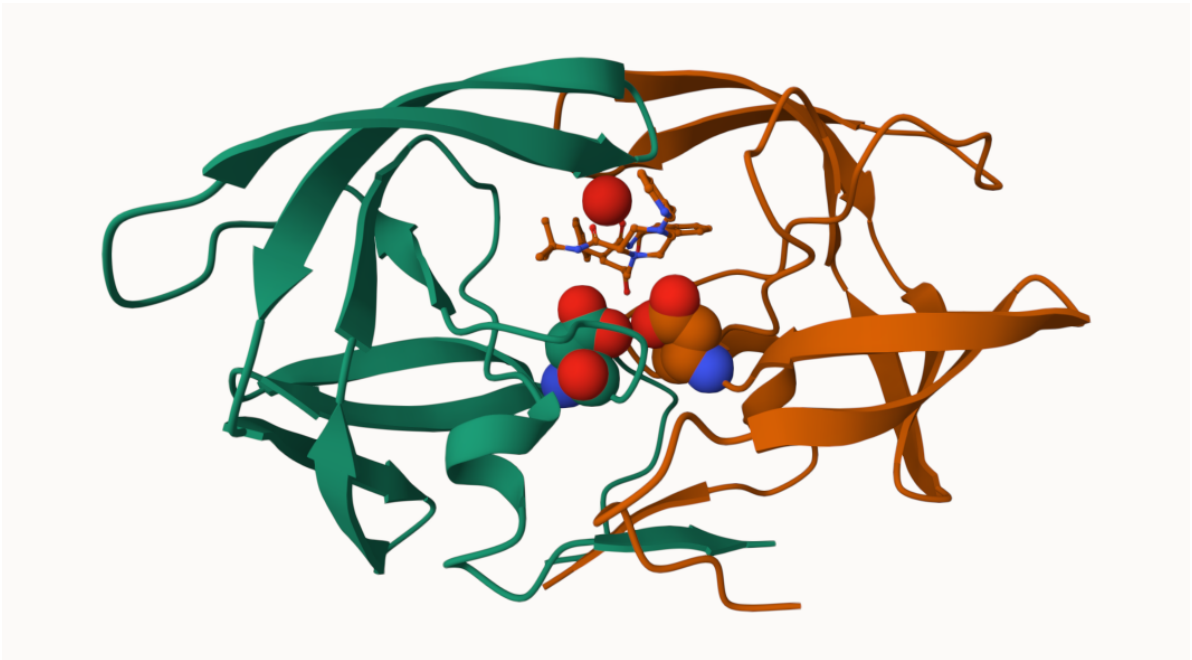


Figure 3: Protein with important water and aspartic acid residues

Q4: The hydrogens do not show up because they are too small.

Q5: Water molecule (HOH) 308

Bio3D package for Structural Bioinformatics

```
library(bio3d)
```

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

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

```
summary(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) ]

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

```
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>
```

```
pdbseq(pdb)[25]
```

```
 25
"D"
```

Q7: There are 198 amino acid residues

Q8: The non-protein residues are the waters and the MK1 (drug)

Q9: 2 protein chains

Functional dynamics prediction

```
#library(r3dmol)
#source("https://tinyurl.com/viewpdb")
```

```
#view.pdb(pdb, backgroundColor = "lightpink")
```

```
#view.pdb(adk, backgroundColor = "lightgrey")
```

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

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

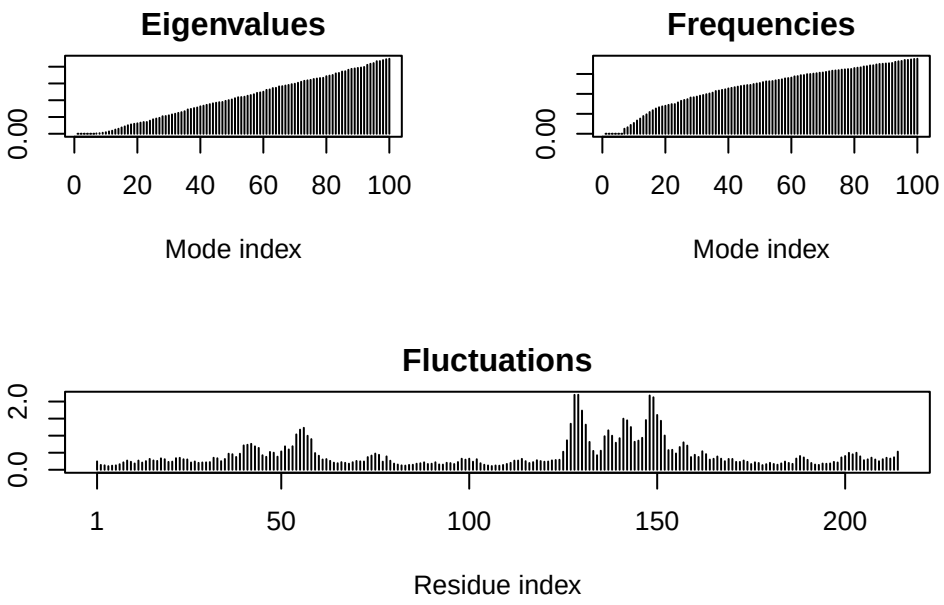
```
adk
```

```
 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
```

```
#flexibility prediction
flex_pred <- nma(adk)
```

```
 Building Hessian...        Done in 0.03 seconds.
 Diagonalizing Hessian...   Done in 0.25 seconds.
```

```
plot(flex_pred)
```




```
mktrj(flex_pred, pdb=adk, file= "adk-m7.pdb")

#view the file this outputs in Mol-star by opening the file created by `mktrj()`
#if you don't add the "pdb" argument, the sequence will not show up in Mol-star correctly
```