Class 10: Structural Bioinformatics

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```
pdbstats <- read.csv("Data_Export_Summary.csv")
x <- pdbstats$Total
as.numeric(x)
```

```
Warning: NAs introduced by coercion
```

```
[1]  NA  NA  NA  NA 213  22
```

```
# Read the CSV file
data <- read.csv("Data_Export_Summary.csv", stringsAsFactors = FALSE)

# Remove commas within each value
data <- as.data.frame(lapply(data, function(x) gsub(",", "", x)))

# Convert only specific columns to numeric (replace with your column names or indices)
# For example, if columns 2 and 3 are numeric
data[, c(2:8)] <- lapply(data[,c(2:8)], as.numeric)

# Check the cleaned data
print(data)
```

```
           Molecular.Type  X.ray    EM   NMR Multiple.methods Neutron Other
1          Protein (only) 167317 15698 12534               208      77    32
2 Protein/Oligosaccharide   9645  2639    34                 8       2     0
3              Protein/NA   8735  4718   286                 7       0     0
4     Nucleic acid (only)   2869   138  1507                14       3     1
5                   Other    170    10    33                 0       0     0
6  Oligosaccharide (only)     11     0     6                 1       0     4
   Total
1 195866
```

```
2  12328
3  13746
4   4532
5    213
6     22
```

```
library(readr)
pdbstats <- 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.
```

```
pdbstats
```

```
# A tibble: 6 x 8
  `Molecular Type`   `X-ray`    EM   NMR `Multiple methods` Neutron Other  Total
  <chr>                <dbl> <dbl> <dbl>              <dbl>   <dbl> <dbl>  <dbl>
1 Protein (only)      167317 15698 12534                208      77    32 195866
2 Protein/Oligosacc~    9645  2639    34                  8       2     0  12328
3 Protein/NA            8735  4718   286                  7       0     0  13746
4 Nucleic acid (onl~    2869   138  1507                 14       3     1   4532
5 Other                  170    10    33                  0       0     0    213
6 Oligosaccharide (~      11     0     6                  1       0     4     22
```

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

```
xray <-  sum(data$X.ray) / sum(data$Total) * 100
xray
```

```
[1] 83.25592
```

```
EM <-  sum(data$EM) / sum(data$Total) * 100
EM
```

```
[1] 10.2348
```

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

```
sum(pdbstats[1:3,8]) / sum(data$Total) * 100
```

```
[1] 97.89729
```

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?

4,563

#Using Mol*

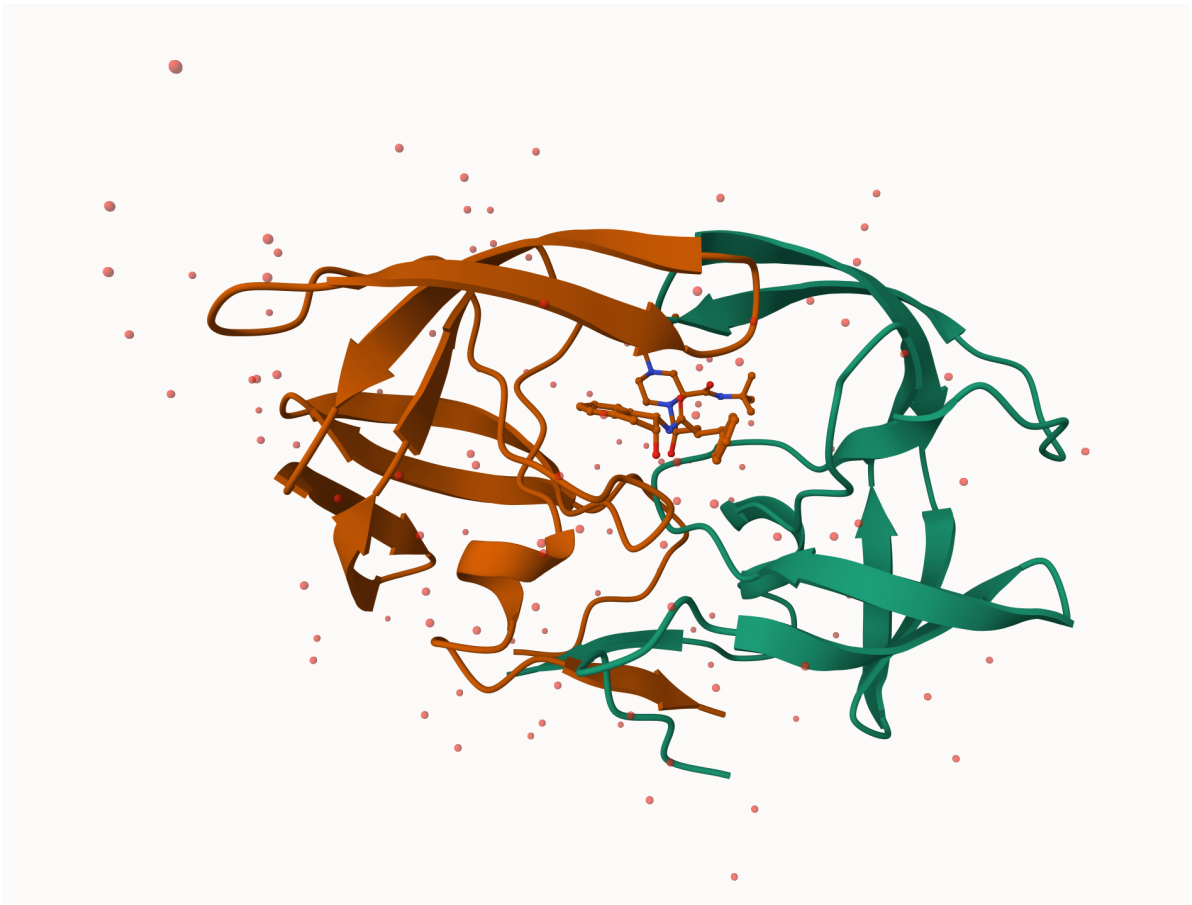
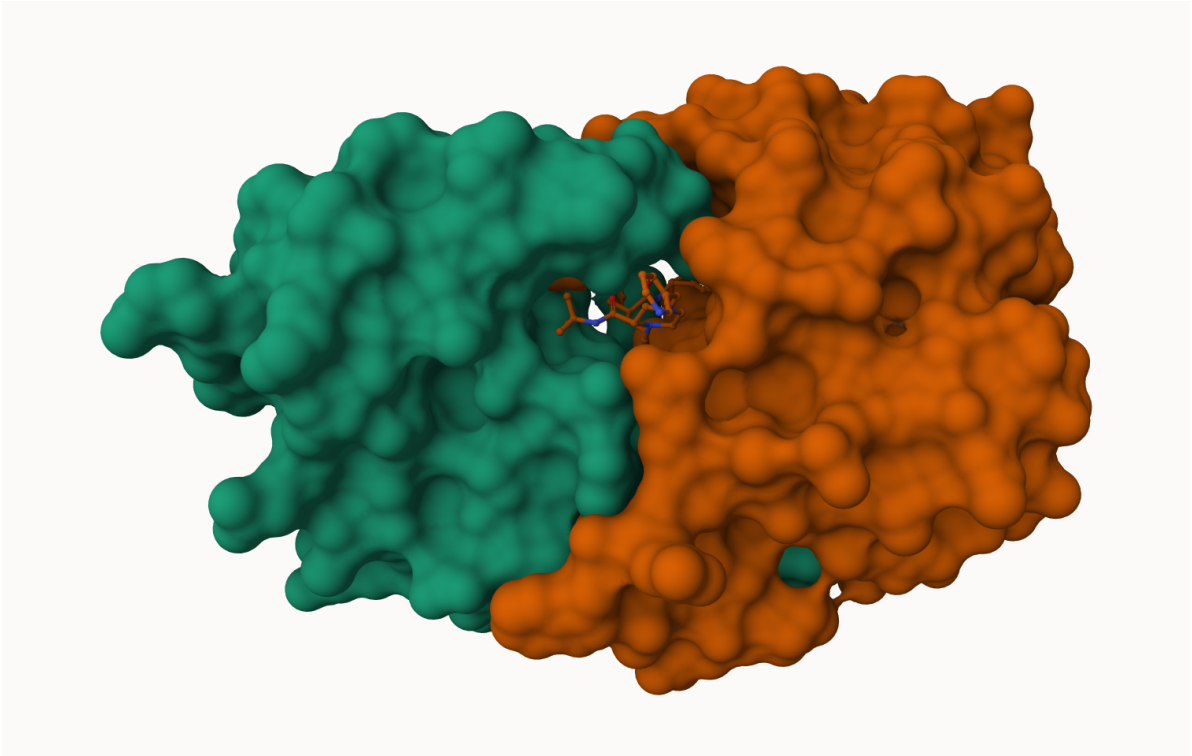


Figure 1: My first image from Mol-star



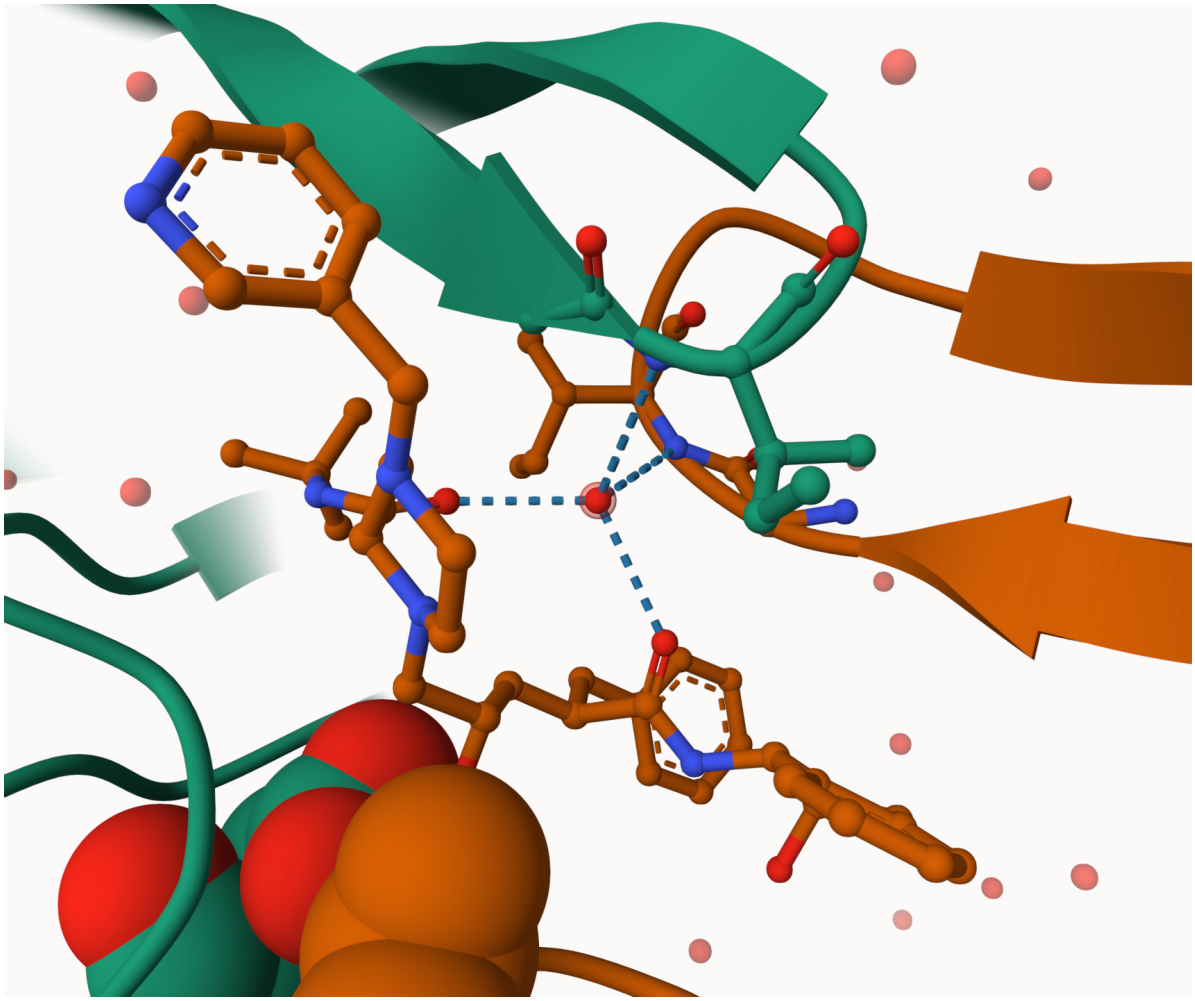


Figure 2: Water

pdb <- read.pdb(“1hsg”)

```
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
```

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

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

Q9: How many protein chains are in this structure?

```
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>
```

**Predicting functional motions of a single 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
```

Performing flexibility prediction

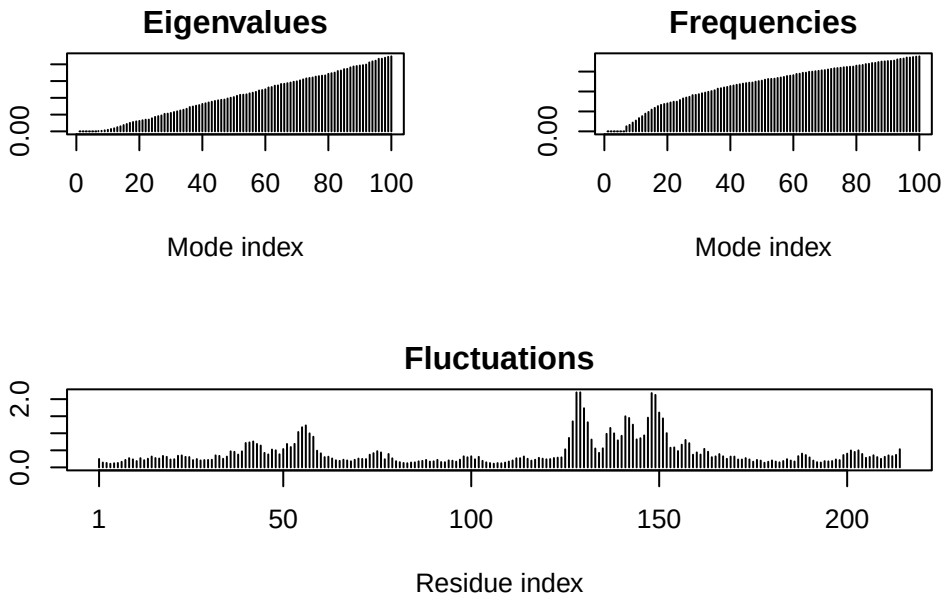
```
#source("https://tinyurl.com/viewpdb")
#install.packages("r3dmol")
#library(r3dmol)

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

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

```
modes <- nma(adk)
```

```
 Building Hessian...        Done in 0.015 seconds.
 Diagonalizing Hessian...   Done in 0.29 seconds.
```

```
plot(modes)
```




```
mktrj(modes, pdb = adk, file="adk_m7.pdb")
```