Class 10: Structural Bioinformatics (pt1)

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PDB Statistics

The Protein Data Bank (PDB) is the main repository of biomolecular structures. Let's see what it contains:

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

```
           Molecular.Type   X.ray     EM    NMR Integrative Multiple.methods
1          Protein (only) 178,795 21,825 12,773         343               226
2 Protein/Oligosaccharide  10,363  3,564     34           8                11
3               Protein/NA   9,106  6,335    287          24                 7
4     Nucleic acid (only)   3,132    221  1,566           3                15
5                   Other     175     25     33           4                 0
6  Oligosaccharide (only)      11      0      6           0                 1
  Neutron Other   Total
1      84    32 214,078
2       1     0  13,981
3       0     0  15,759
4       3     1   4,941
5       0     0     237
6       0     4      22
```

```
stats$X.ray
```

```
[1] "178,795" "10,363"  "9,106"   "3,132"   "175"     "11"
```

```
sum(stats$Neutron)
```

```
[1] 88
```

The comma in these numbers leads to the numbers here being read as character.

```
c(100, 10, "barry")
```

```
[1] "100"   "10"    "barry"
```

```
library(readr)
stats <- read_csv("Data Export Summary.csv")
```

```
Rows: 6 Columns: 9
-- Column specification --------------------------------------------------------
Delimiter: ","
chr (1): Molecular Type
dbl (4): Integrative, 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.
```

```
stats
```

```
# A tibble: 6 x 9
  `Molecular Type`    `X-ray`    EM   NMR Integrative `Multiple methods` Neutron
  <chr>                 <dbl> <dbl> <dbl>       <dbl>               <dbl>   <dbl>
1 Protein (only)       178795 21825 12773         343                 226      84
2 Protein/Oligosacch~   10363  3564    34           8                  11       1
3 Protein/NA             9106  6335   287          24                   7       0
4 Nucleic acid (only)    3132   221  1566           3                  15       3
5 Other                   175    25    33           4                   0       0
6 Oligosaccharide (o~      11     0     6           0                   1       0
# i 2 more variables: Other <dbl>, Total <dbl>
```

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

```
n.xray <- sum(stats$`X-ray`)
#n.em <-
n.total <- sum(stats$Total)
n.xray/n.total
```

```
[1] 0.8095077
```

80%

```
n.em <- sum(stats$EM)
n.em/n.total
```

```
[1] 0.1283843
```

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

```
n.protein <- stats[1, "Total"]
p_protein <- n.protein/n.total
p_protein
```

```
      Total
1 0.8596889
```

85% > Q3: SKIP

Visualizing the HIV-1 protease structure

We can use the molstar viewer online: https://molstar.org/viewer/.

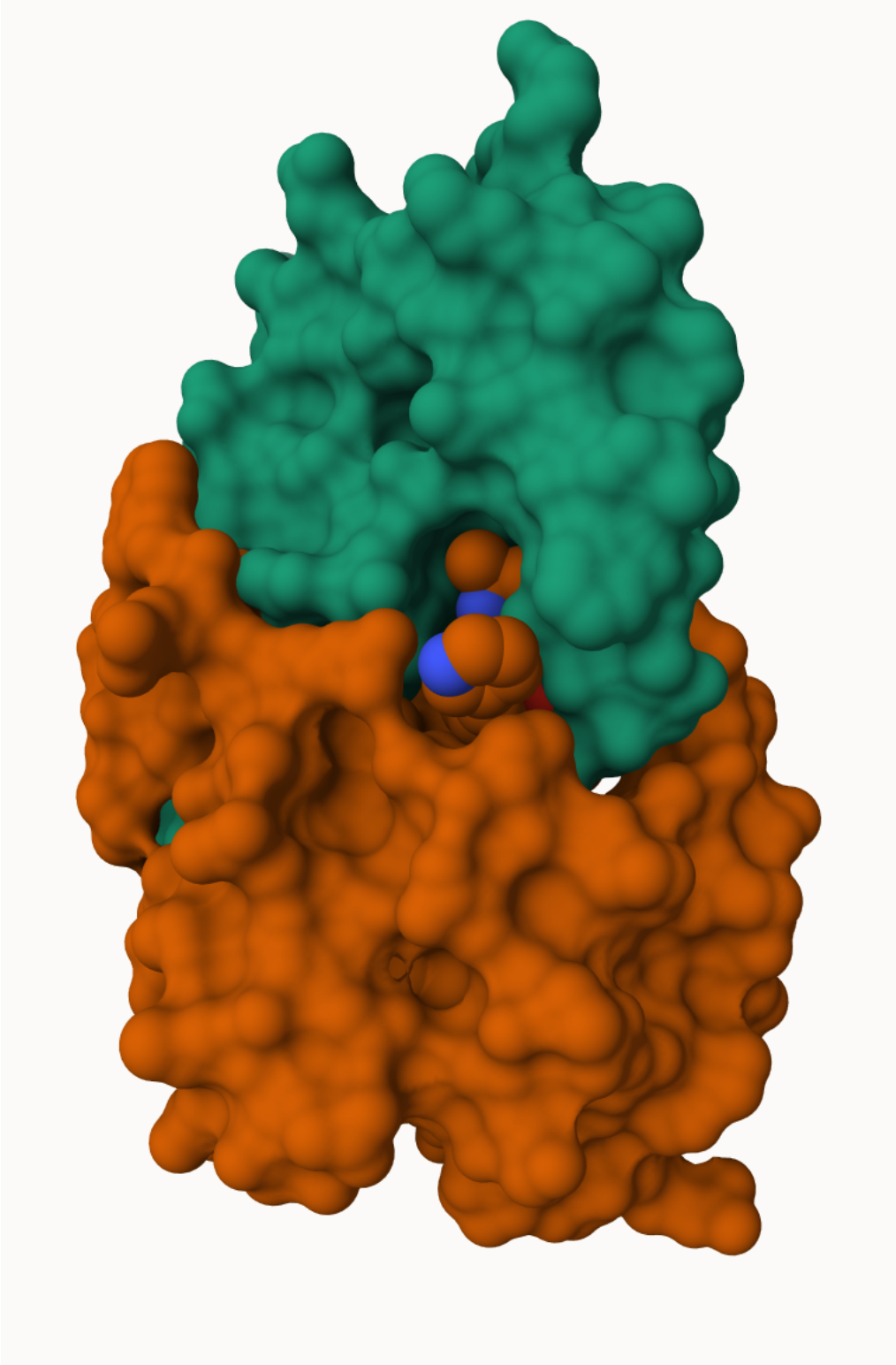


Figure 1: My first image of HIV-Pr with surface display showing ligand binding

A new clean image showing the catalytic ASP25 amino acids in both chains of the HIV-PR dimer along with the inhibitor and the all important active site water

Bio3D package foe structral bioenformatics

```
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
```

```
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>
```

```
#library(bio3dview)

#view.pdb(pdb)
```

Predicting functional motions of a single structure

Read an ADK structure from the PDB database

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

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

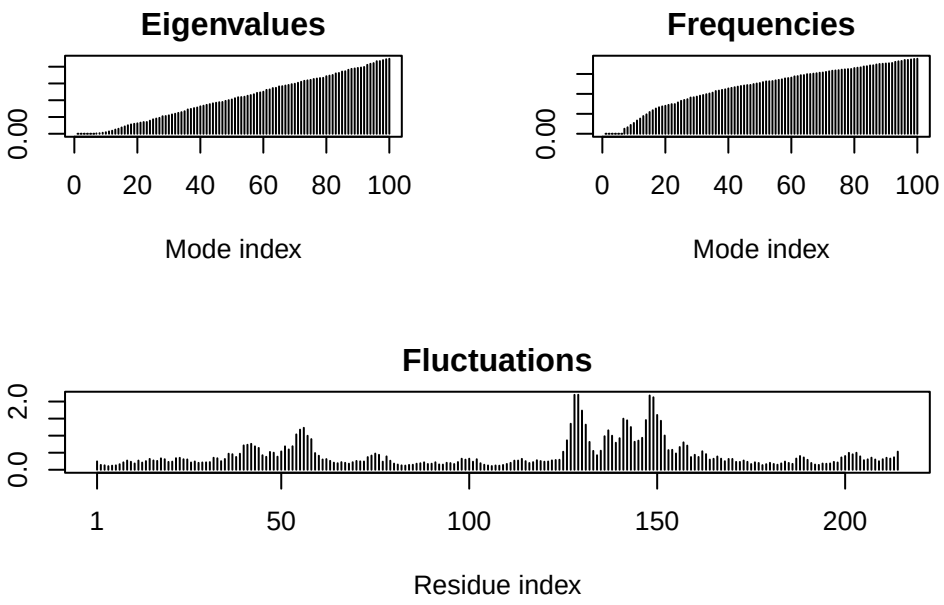
```
adk
```

```
 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 0.011 seconds.
 Diagonalizing Hessian...   Done in 0.045 seconds.
```

```
plot(m)
```



Write out results as a wee trajectory/movie of predicted motions:

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