Class 9: Structural Bioinformatics (pt1)

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2/15/2022

The PDB database

The PDB is the main repository for 3D structure data of biomolecules.

Here we explore it's composition. We obtained the most recent stats from https://www.rcsb.org/stats/summary

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

```
##                           X.ray   NMR   EM Multiple.methods Neutron Other  Total
## Protein (only)          144301 11877 6676              182      70    32 163138
## Protein/Oligosaccharide   8528    31 1116                5       0     0   9680
## Protein/NA                7617   274 2153                3       0     0  10047
## Nucleic acid (only)       2393  1398   61                8       2     1   3863
## Other                      150    31    3                0       0     0    184
## Oligosaccharide (only)      11     6    0                1       0     4     22
```

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

```
tot.method <- colSums(tbl)
round(tot.method/tot.method["Total"] * 100, 3)
```

```
##            X.ray              NMR               EM Multiple.methods
##           87.197            7.284            5.354            0.106
##          Neutron            Other            Total
##            0.039            0.020          100.000
```

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

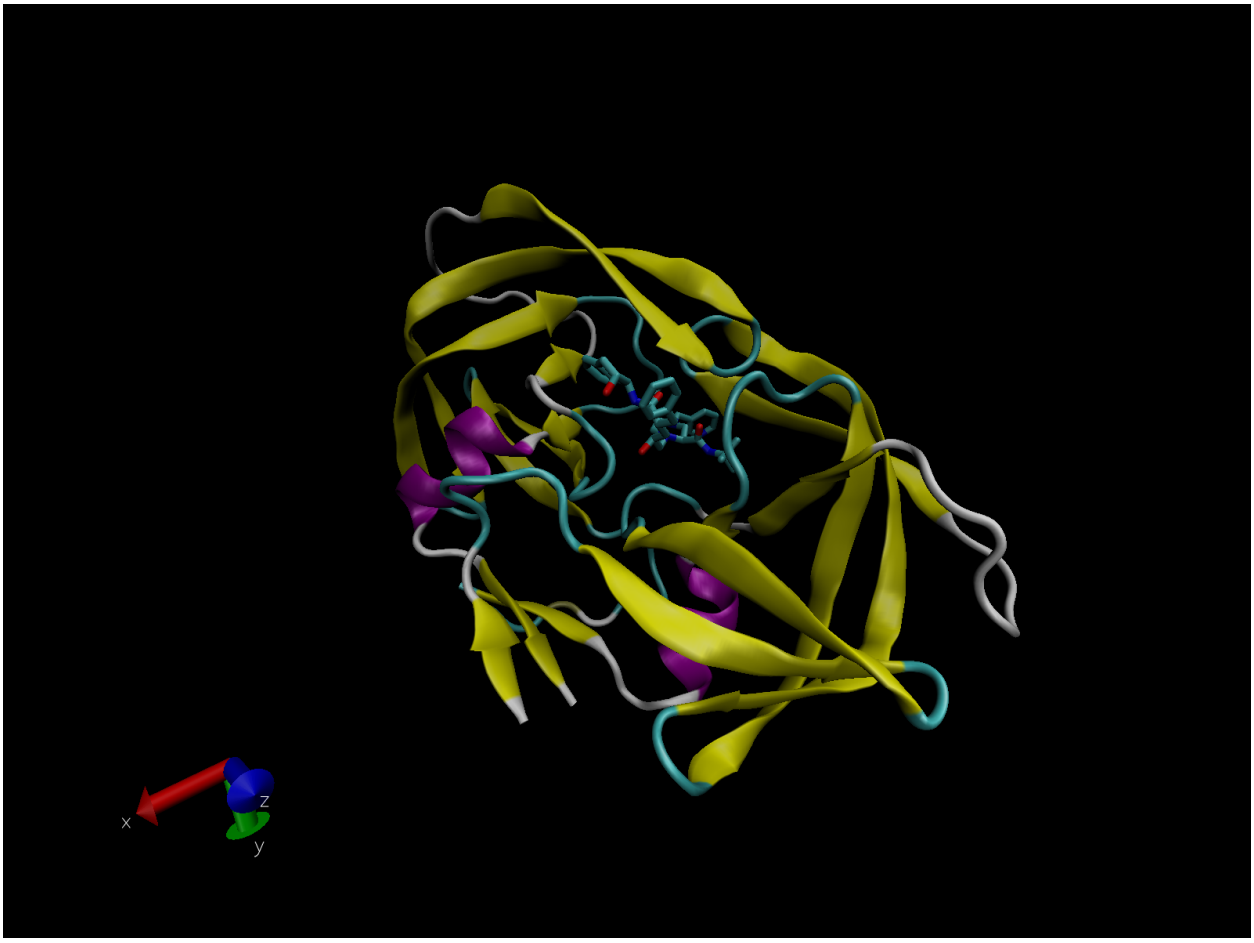
```
ans <- tbl$Total[1]/sum(tbl$Total) * 100
round(ans, 3)
```

```
## [1] 87.27
```

The answer to this question is 87.27 % of total structures.

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?

Here is a VMD generated image of HIV-protease, PDB code: 1hsg



Bio3D package for structural bioinformatics

We will load the bio3d package.

```
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>
```

Extract the sequence for ADK:

```
aa <- get.seq("1ake_A")
```

```
## Warning in get.seq("1ake_A"): Removing existing file: seqs.fasta
```

```
## Fetching... Please wait. Done.
```

```
aa
```

```
##              1        .         .         .         .         .         60
## pdb|1AKE|A   MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##              1        .         .         .         .         .         60
##
##             61        .         .         .         .         .         120
## pdb|1AKE|A   DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##             61        .         .         .         .         .         120
##
##            121        .         .         .         .         .         180
## pdb|1AKE|A   VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##            121        .         .         .         .         .         180
##
```

```
##            181        .         .         .   214
## pdb|1AKE|A   YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##            181        .         .         .   214
##
## Call:
##   read.fasta(file = outfile)
##
## Class:
##   fasta
##
## Alignment dimensions:
##   1 sequence rows; 214 position columns (214 non-gap, 0 gap)
##
## + attr: id, ali, call
```

```
#blast <- blast.pdb(aa)
```

```
#hits <- plot(blast)
```

```
#hits$pdb.id
```

Normal mode analysis (NMA)

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

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

```
pdb
```

```
##
##  Call:  read.pdb(file = "1ake")
##
##    Total Models#: 1
##      Total Atoms#: 3804,  XYZs#: 11412  Chains#: 2  (values: A B)
##
##      Protein Atoms#: 3312  (residues/Calpha atoms#: 428)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 492  (residues: 380)
##      Non-protein/nucleic resid values: [ AP5 (2), HOH (378) ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILGMRIILLGAPGA...<cut>...KILG
##
## + attr: atom, xyz, seqres, helix, sheet,
##         calpha, remark, call
```

Trim to chain A only.

```
chain <- trim.pdb(pdb, chain="A")
chain
```

```
##
##  Call:  trim.pdb(pdb = pdb, chain = "A")
##
##    Total Models#: 1
##      Total Atoms#: 1954,  XYZs#: 5862  Chains#: 1  (values: A)
##
##      Protein Atoms#: 1656  (residues/Calpha atoms#: 214)
##      Nucleic acid Atoms#: 0  (residues/phosphate atoms#: 0)
##
##      Non-protein/nucleic Atoms#: 298  (residues: 242)
##      Non-protein/nucleic resid values: [ AP5 (1), HOH (241) ]
##
##    Protein sequence:
##       MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVT
##       DELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRI
##       VGRRVHAPSGRVYHVKFNPPKVEGKDDVTGEELTTRKDDQEETVRKRLVEYHQMTAPLIG
##       YYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG
##
## + attr: atom, helix, sheet, seqres, xyz,
##         calpha, call
```

Run a bioinformatics method to predict the flexibility and "functional motions" of this protein chain.

```
modes <- nma(chain)
```

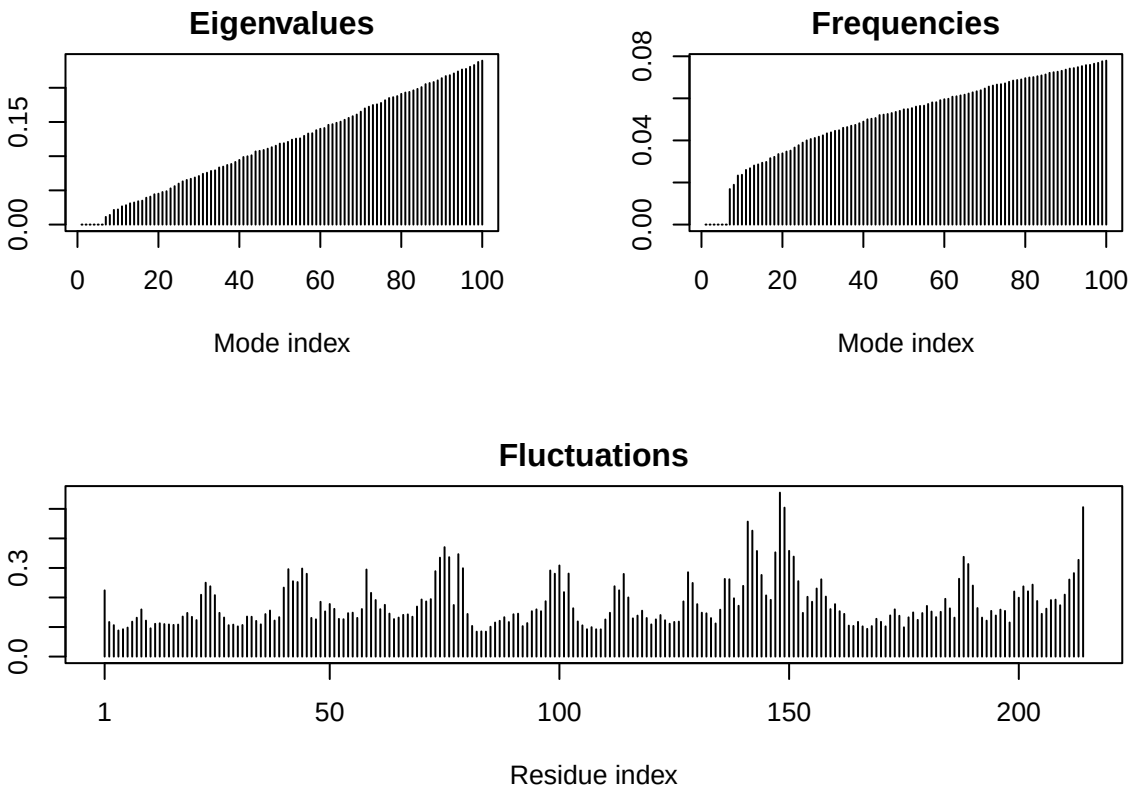
```
##  Building Hessian...     Done in 0.07 seconds.
##  Diagonalizing Hessian...    Done in 0.445 seconds.
```

```
modes
```

```
##
## Call:
##   nma.pdb(pdb = chain)
##
## Class:
##   VibrationalModes (nma)
##
## Number of modes:
##   642 (6 trivial)
##
## Frequencies:
##   Mode 7:    0.017
##   Mode 8:    0.019
##   Mode 9:    0.023
##   Mode 10:   0.024
##   Mode 11:   0.026
##   Mode 12:   0.027
```

```
##
## + attr: modes, frequencies, force.constants, fluctuations,
##         U, L, xyz, mass, temp, triv.modes, natoms, call
```

```
plot(modes)
```




```
m7 <- mktrj.nma(modes, mode=7, file= "mode_7.pdb")
```

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

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

## Warning in get.pdb(file, path = tempdir(), verbose = FALSE): /var/folders/gt/
## jh52x5y13_q65qj_w8clp6dc0000gn/T//RtmpVDDn4V/1ake.pdb exists. Skipping download

##    PDB has ALT records, taking A only, rm.alt=TRUE
```

```
chain <- trim.pdb(pdb, chain="A")
modes <- nma(chain)
```

```
##  Building Hessian...     Done in 0.054 seconds.
##  Diagonalizing Hessian...    Done in 0.505 seconds.
```

```
mktrj.nma(modes, mode=7, file="mode_7.pdb")
```