

MASTER 2 BIOINFORMATICS

ASSIGNMENT OF SECONDARY STRUCTURES OF PROTEINS

Jeyani George Clement

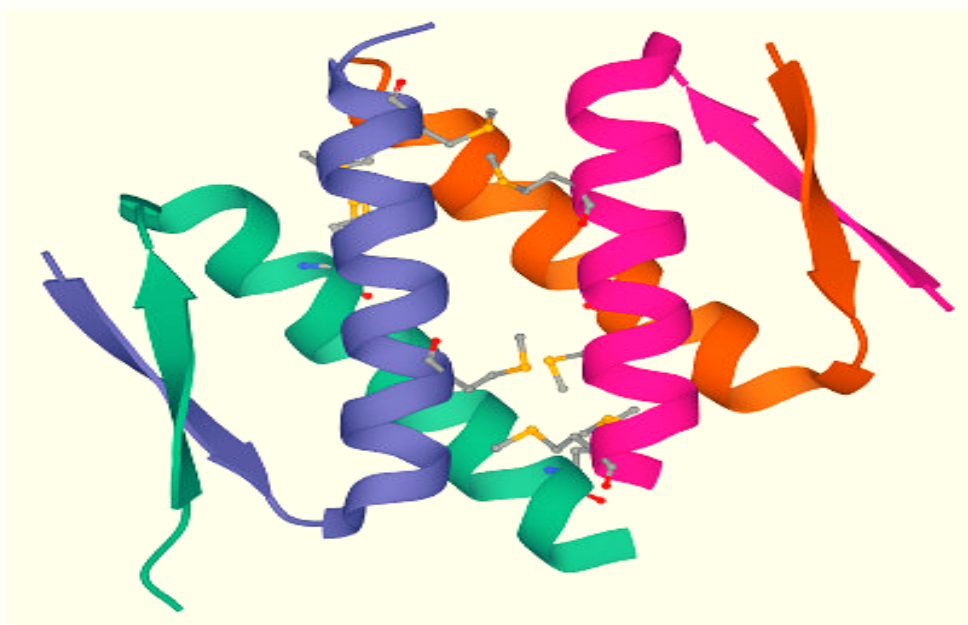
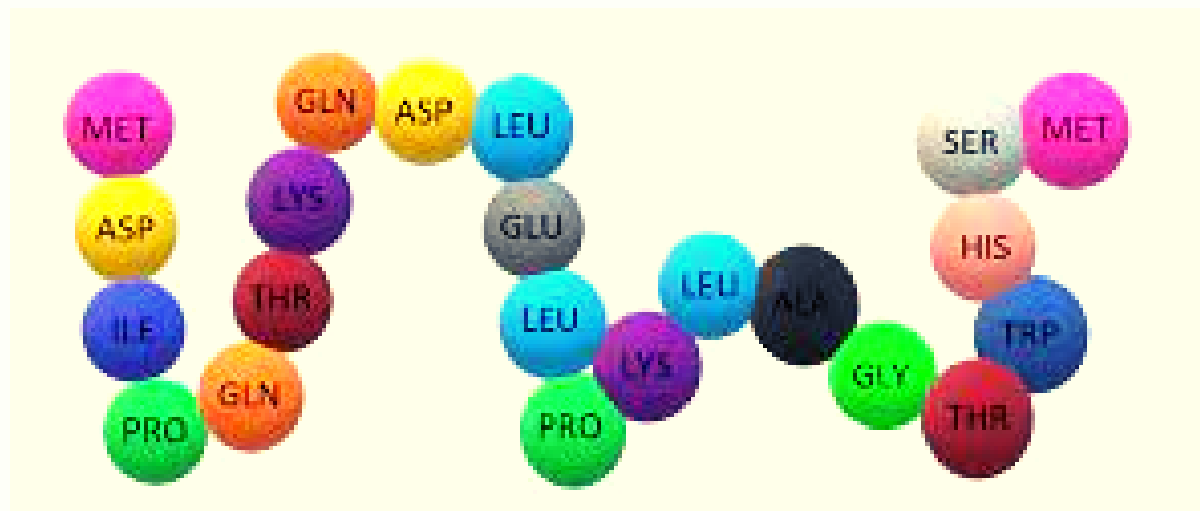
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BACKGROUND

**

Can simple rules be defined to
assign the secondary structure of
proteins ?

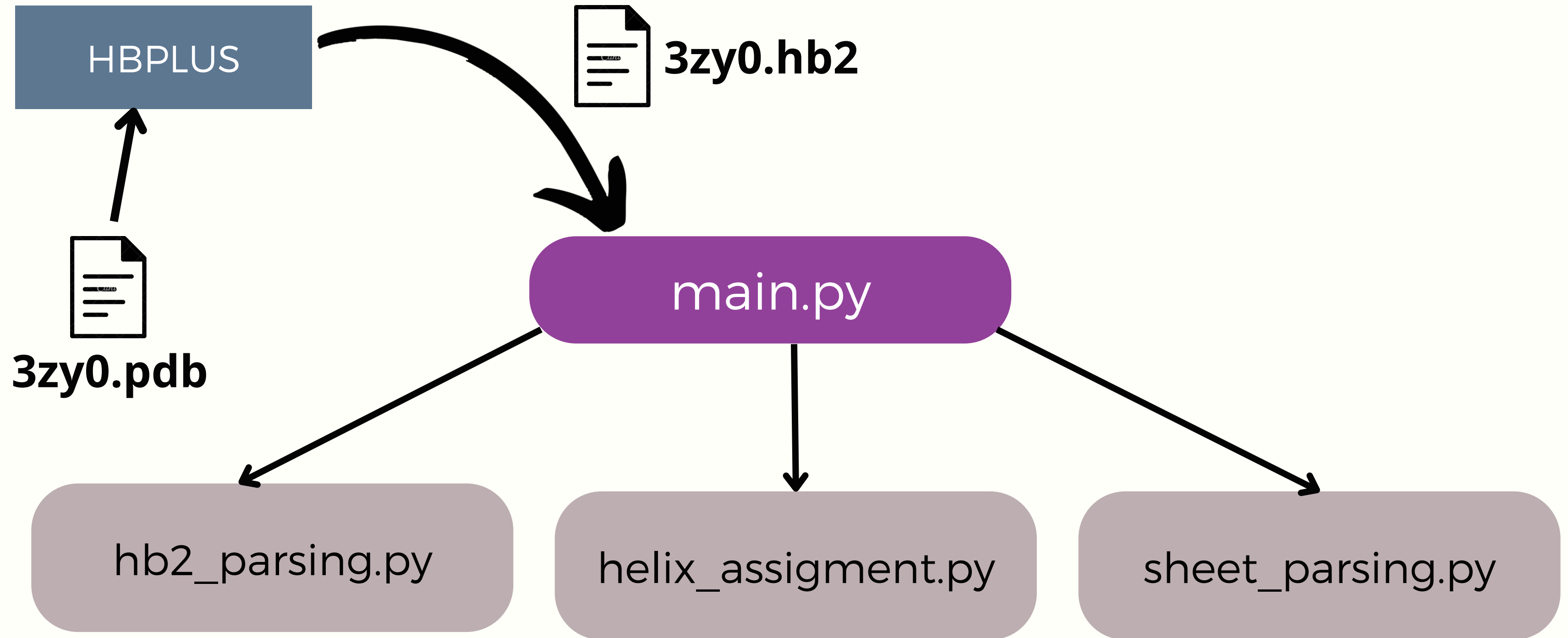
Lignes directrices de la marque Tobago



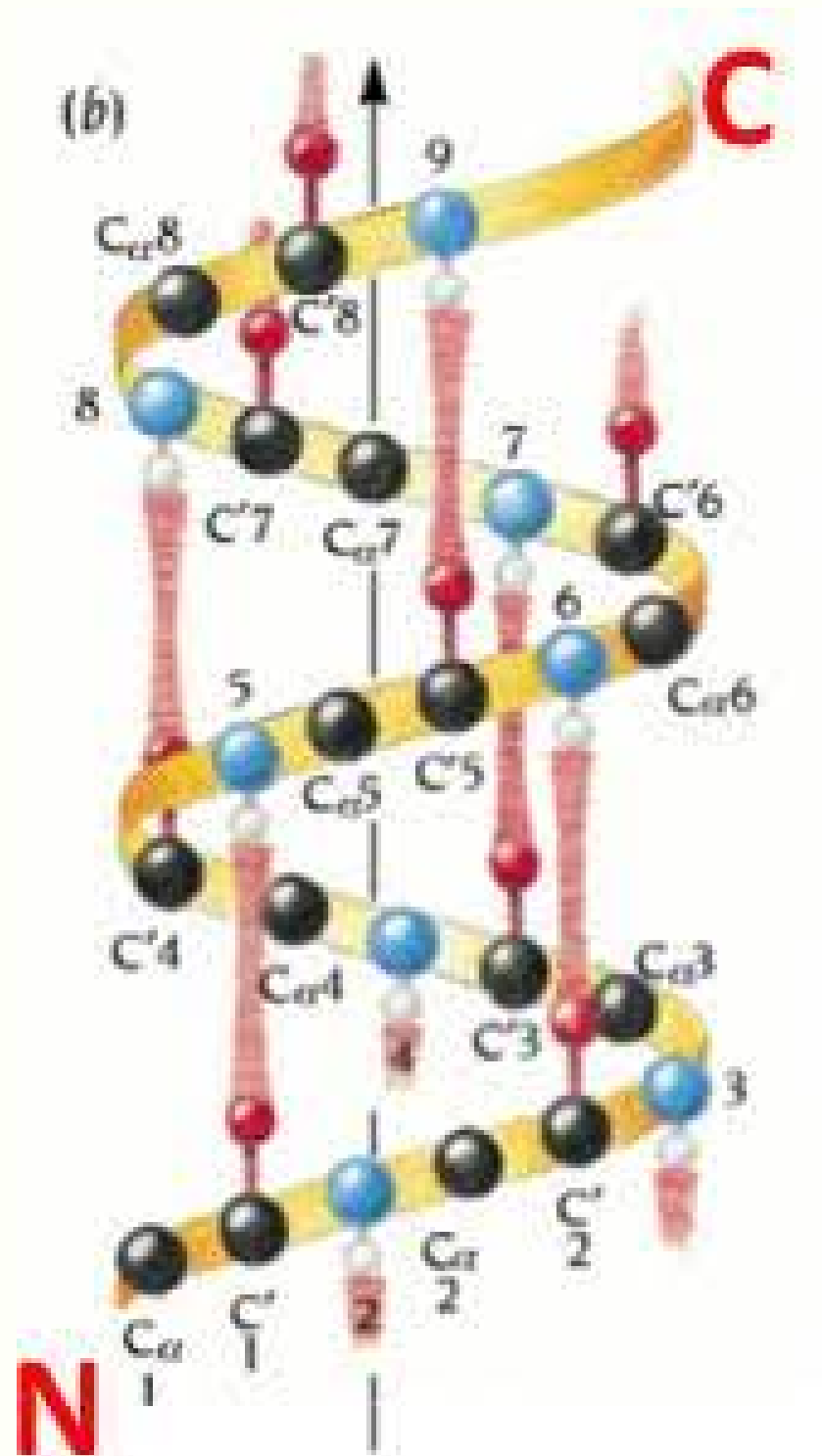
MAIN OBJECTIVE

**Implement a tool for the
assignment of secondary structures**

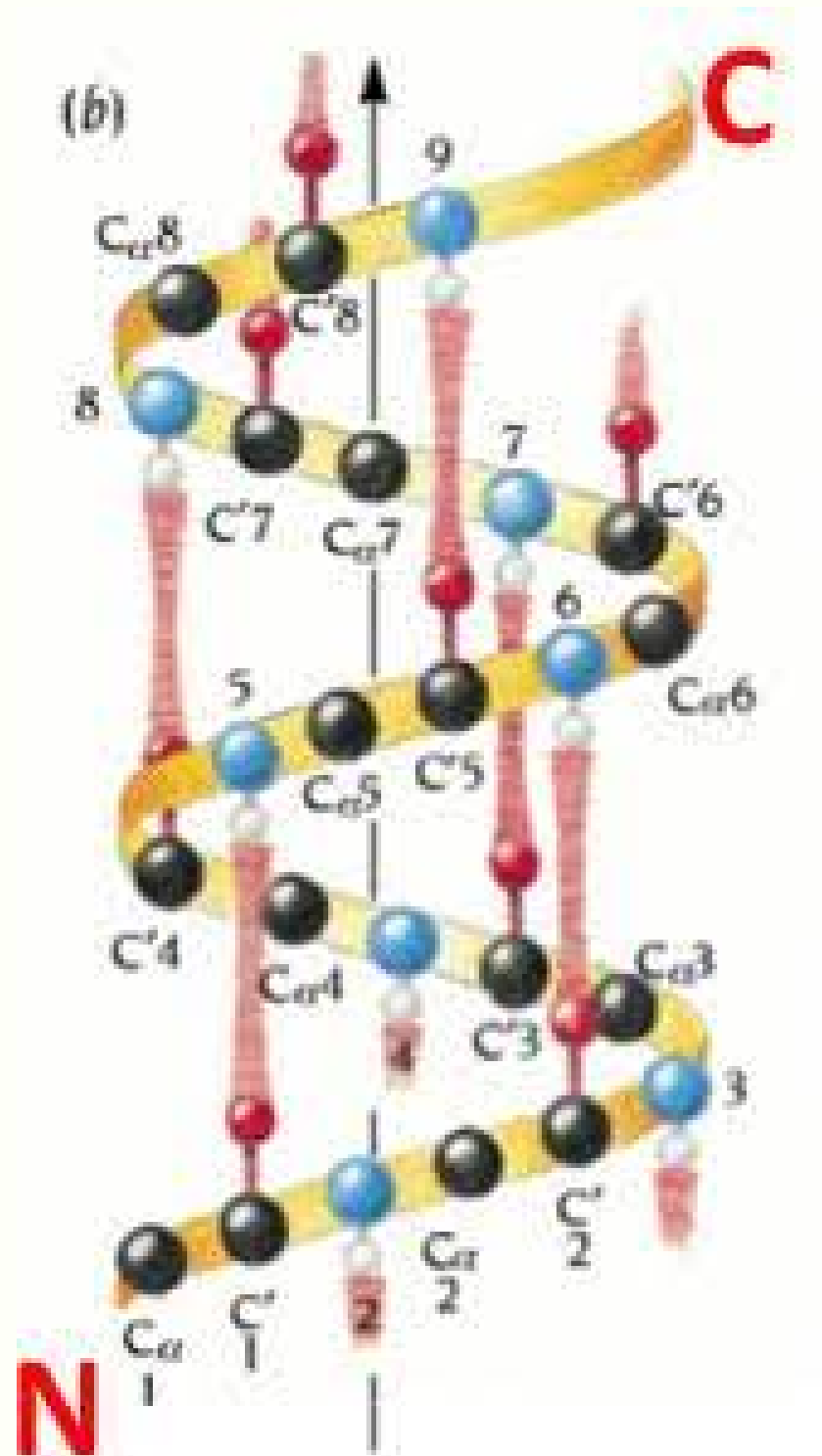
The steps of the algorithm



Helix assignment



Helix assignment



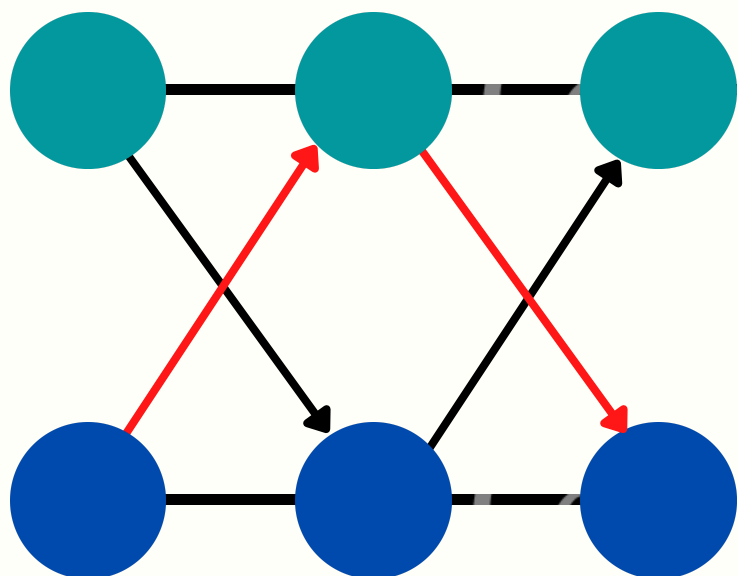
TURN



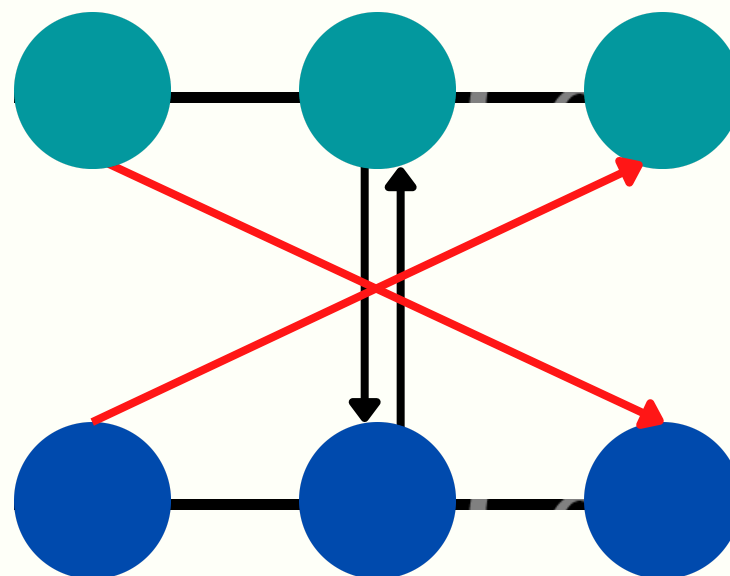
HELIX

Sheet assignment

Parallel bridge

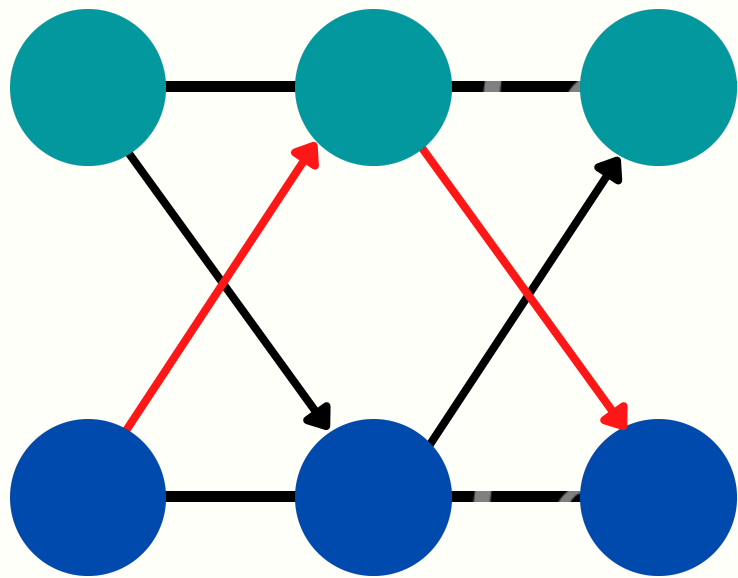


Antiparallel bridge

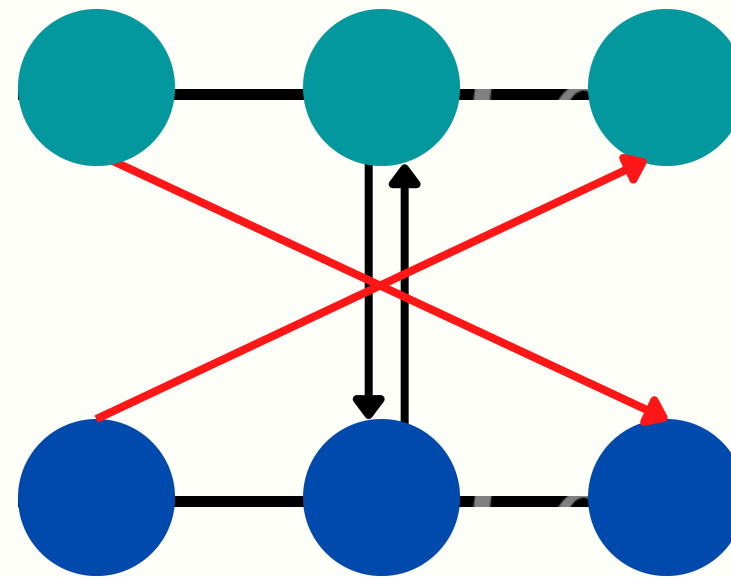


Sheet assignment

Parallel bridge



Antiparallel bridge



BRIDGE



LADDER

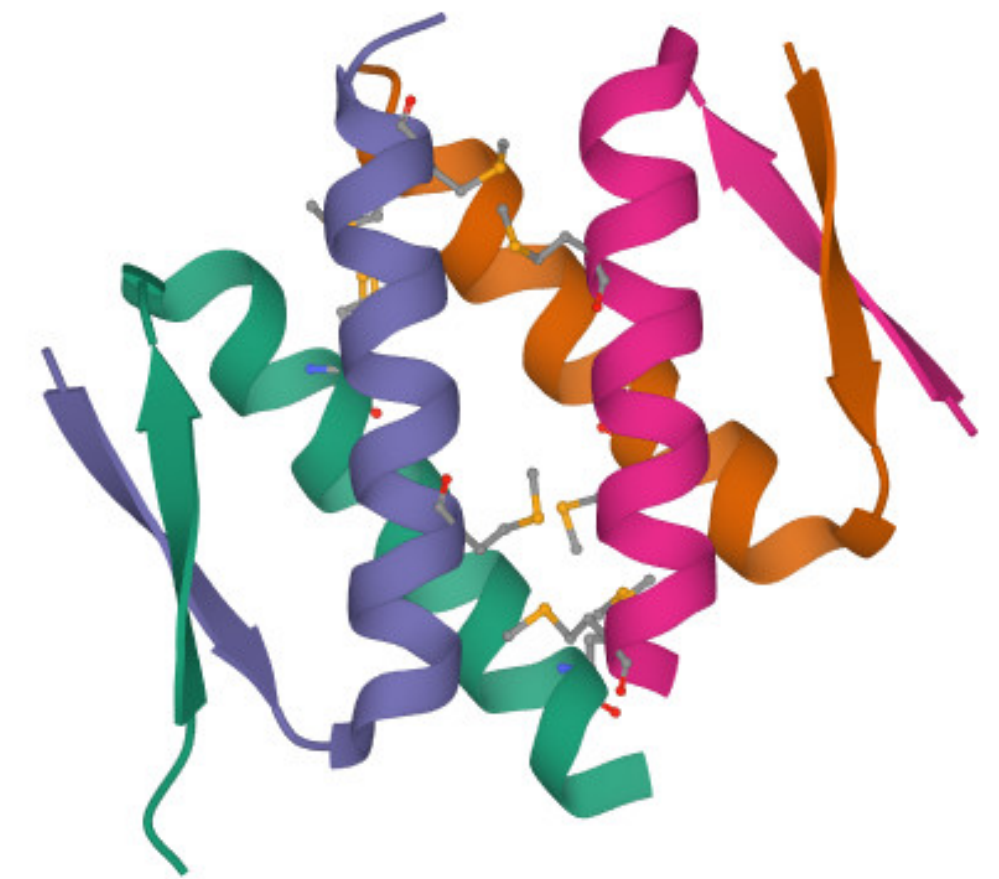


SHEET

RESULT

```
Chaine A : T---T--HHTHHHT--HH
Chaine B : T---T--T--HHT---
Chaine C : T---T--HHTHHHT---
Chaine D : T---T--HHHHH
```

My output



3ZY0

```
- , - , E , E , E , E , E , S , S , H , H , H , H , H , H , H , H , H , H , H , H ,
| H , H , H , H , H ,
- , - , E , E , E , E , E ,
- , S , H , H , H , H , H , H , H , H , H , H , H , H , H , H , T , T ,
| - , - , E , E , E , E , E , S , - , H , H , H , H , H , H , H , H , H , H , H , H , H , H , H ,
```

DSSP output

CONCLUSION & PROSPECT

- **Improving the code to obtain the assignation of sheet**
- **Distinction between the different types of helixes**
- **Improved display of results**

Thank you for listening

Any questions ?

APPENDICES

.HB2 FILE

- CHARLES EAMES

```
HBPLUS Hydrogen Bond Calculator v 3.2          Sep 10 03:23:53 CEST 2022
(c) I McDonald, D Naylor, D Jones and J Thornton 1993 All Rights Reserved.
Citing HBPLUS in publications that use these results is condition of use.
|      <- Brookhaven Code "data/3zy0_new.pdb" <- PDB file
<---DONOR---> <-ACCEPTOR-->      atom      ^
c      i      cat <-CA-CA->      ^      H-A-AA      ^      H-
h      n      atom resd res      DA || num      DHA      H-A      angle D-A-AA      Bond
n      s      type num  typ      dist DA aas      dist angle      dist      angle      num
A0362-LEU N      C0366-VAL 0      2.81 MM -1 5.10 156.4 1.86 170.9 162.9      1
C0366-VAL N      A0362-LEU 0      2.75 MM -1 5.10 156.1 1.80 158.9 161.6      2
A0364-LEU N      C0364-LEU 0      2.85 MM -1 4.90 161.5 1.89 145.7 139.8      3
C0364-LEU N      A0364-LEU 0      2.91 MM -1 4.90 155.2 1.97 148.1 141.1      4
C0379-LYS NZ     A0365-PRO 0      3.25 SM -1 9.54 139.1 2.42 129.0 140.5      5
A0366-VAL N      C0362-LEU 0      2.78 MM -1 5.20 159.2 1.82 156.9 157.0      6
C0362-LEU N      A0366-VAL 0      2.76 MM -1 5.20 173.2 1.76 169.4 167.7      7
A0372-TYR N      A0368-GLY 0      3.00 MM 4 6.08 164.7 2.02 149.2 154.2      8
A0373-GLU N      A0369-ARG 0      2.93 MM 4 5.92 162.6 1.96 149.3 152.4      9
A0376-LEU N      A0372-TYR 0      2.89 MM -1 6.08 148.0 1.99 144.9 154.6     10
A0377-LYS N      A0373-GLU 0      3.12 MM -1 6.32 154.6 2.19 143.6 148.7     11
A0379-LYS N      A0375-LEU 0      2.80 MM 4 5.83 162.3 1.83 144.5 150.0     12
A0380-GLU N      A0376-LEU 0      3.20 MM 4 6.40 157.5 2.26 146.2 151.2     13
A0381-SER N      A0377-LYS 0      3.25 MM 4 6.56 163.0 2.28 146.0 149.1     14
A0381-SER OG     A0377-LYS 0      3.46 SM 4 6.56 166.7 2.48 145.3 145.6     15
A0382-LEU N      A0378-ILE 0      2.83 MM 4 6.08 161.0 1.86 158.4 164.1     16
```