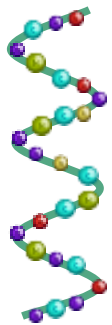
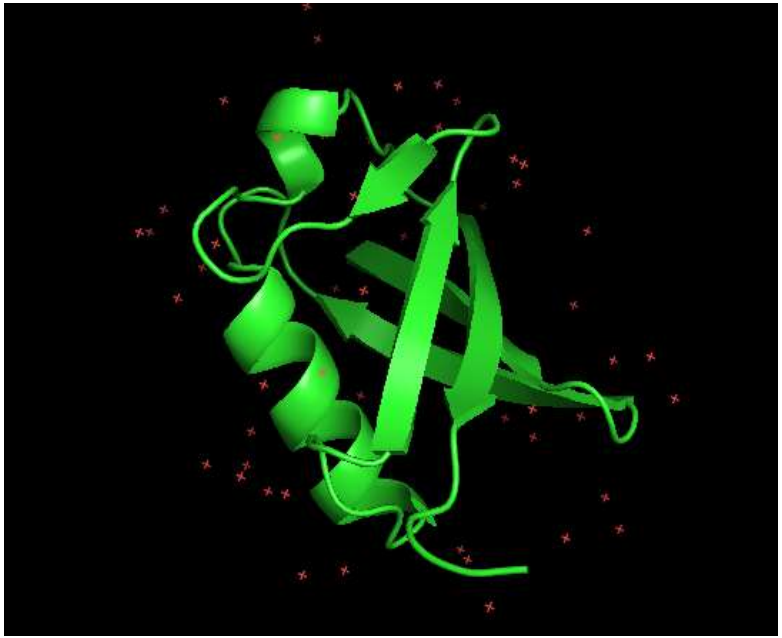
Protein secondary structure assignment



Presented by : Insaf ElEbri


01
02
03
04
Secondary Structure
DSSP Program
Implemented Program
Results

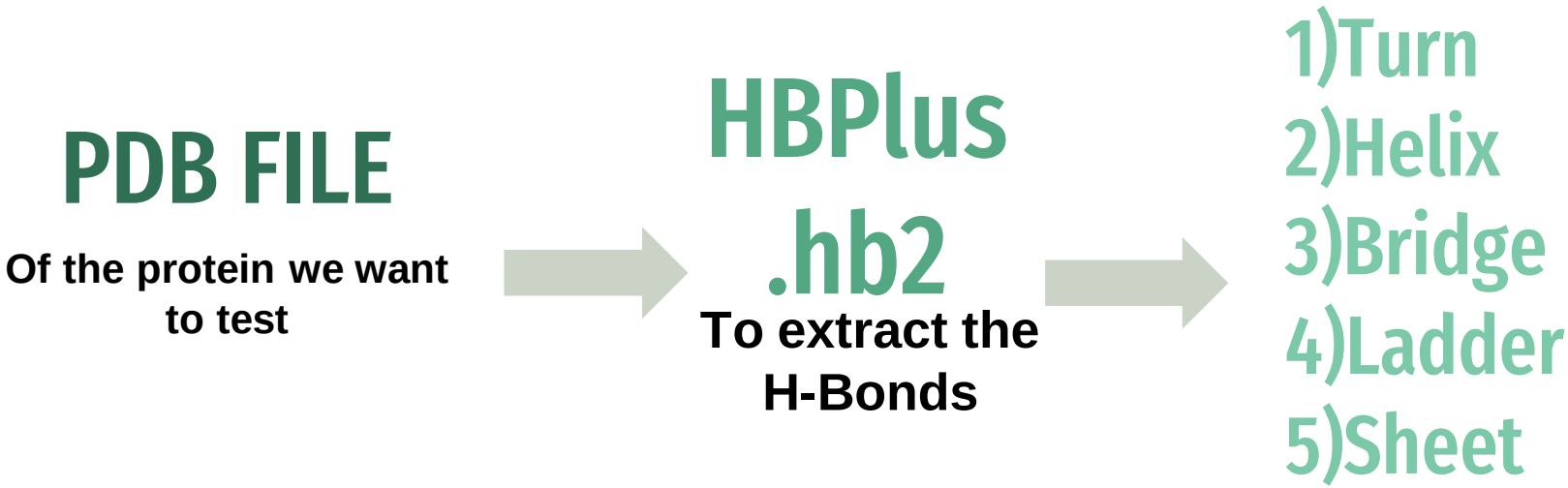


Definition

Secondary structure refers to regular, recurring arrangements in space of adjacent amino acid residues in a polypeptide chain. It is maintained by hydrogen bonds between amide hydrogens and carbonyl oxygens of the peptide backbone. The major secondary structures are α-helices and β-structures.

DSSP Program

- Is a program designed by Wolfgang Kabsch and Chris Sander to standardize secondary structure assignment.
- Is not designed to predict secondary structure.


PDB FILE
Of the protein we want to test
HBPlus
.hb2
To extract the H-Bonds
1)Turn
2)Helix
3)Bridge
4)Ladder
5)Sheet

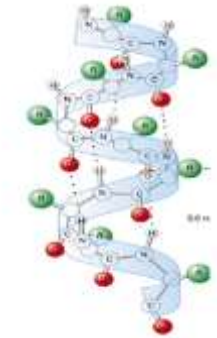
The 5 main sections of the program

Turn

A loop for will browse these to lists to calculate the distance between both involved residues. If it is equal to FOUR then a list called TURN will append the two of them.

01

Helix



02

Bridge

1) Parallel
2) Antiparalle

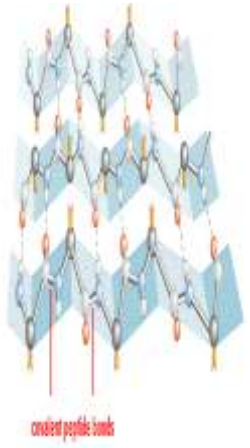
03

Ladder

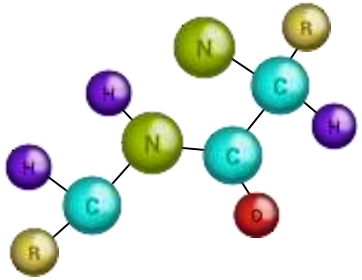
If there's a set of one or more consecutive bridges of identical type, the program will identify it as a Ladder.

04

Sheet



05



Results

Liaison d'une Hélice alpha : [[26, 22], [27, 23], [28, 24], [29, 25], [30, 26], [31, 27], [32, 28], [33, 29], [34, 30]]

23	23	A	I	H
24	24	A	E	H
25	25	A	N	H
26	26	A	V	H
27	27	A	K	H
28	28	A	A	H
29	29	A	K	H
30	30	A	I	H
31	31	A	Q	H
32	32	A	D	H
33	33	A	K	H
34	34	A	E	H