BHARATHIDASAN UNIVERSITY

Tiruchirappalli- 620024,
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Programme : M.Sc., Biomedical Science

Course Title : Bioinformatics
Course Code : BM35S1BI

Unit-IV

TOPIC: FEATURES OF PROTEIN SEQUENCE AND STRUCTURES

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FEATURES OF PROTEIN SEQUENCE AND STRUCTURES

PROTEIN

DEFINITION

- Proteins are molecular devices, in nanometer scale , where biological function is exerted .They are the building blocks of cells in our bodies and in living creatures of all kingdoms.
- The information necessary for life to go on is encoded by the DNA molecule , the dynamic process of life maintenance , replication, defense and reproduction are carried out by protein.
- There are twenty natural amino acids occur in protein.
- These amino acids can be grouped together forming polypeptide chains or protein, indifferent ways determined by the genetic code and limited by stereochemical properties.

- Bioinformatics plays an important role in all aspects of protein , including sequence and structure.
- Sequence Analysis : Several bioinformatics techniques can be used to provide the sequence comparisons in which new sequence can be compared to those with known functions to study the biology of an organism.
- Structural Analysis : many available databases and bioinformatics techniques can help to find the factor govering the folding and stability of proteins and predict the secondary structures from amino acid sequence.

FEATURES OF PROTEIN SEQUENCE AND STRUCTURE

- Sequence and features are group of amino acids that confer certain characteristics upon a protein , and may be important for its overall function.
- Such features include:
- Active sites,
- Binding sites,
- PTM sites,
- Repeats.

ACTIVE SITES:

- Which contain amino acids involved in catalytic activity.

For eg: the enzyme lipase which catalyses the formation and hydrolysis of fats has two amino acids residues that are essential for its catalytic activity.

BINDING SITES:

- Containing amino acids that are directly involved in binding molecules or irons, like the iron binding site of haemoglobin.

PTM SITES:

- Which contain residues known to be chemically modified (phosphorylated, palmitoylated etc) after the process of protein translation.

REPEATS:

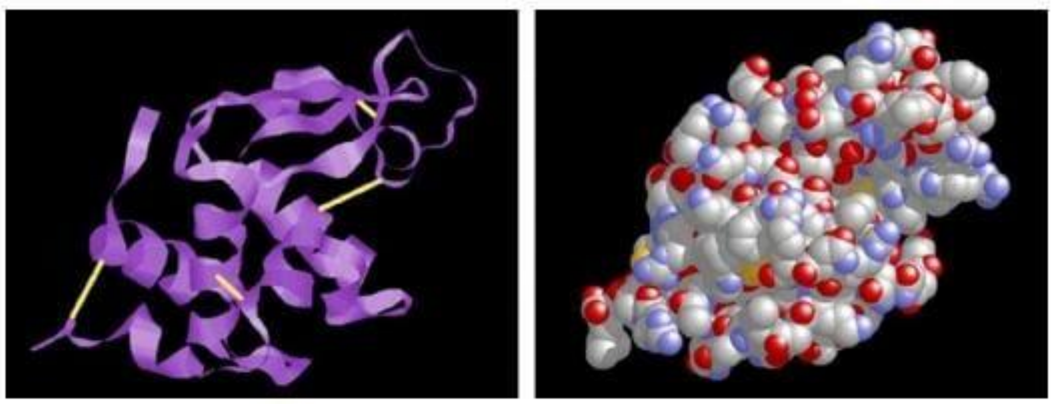
- Which are typically short amino acid sequences that are repeated within a protein and may confer binding or structural properties upon it.

PROTEIN STRUCTURE

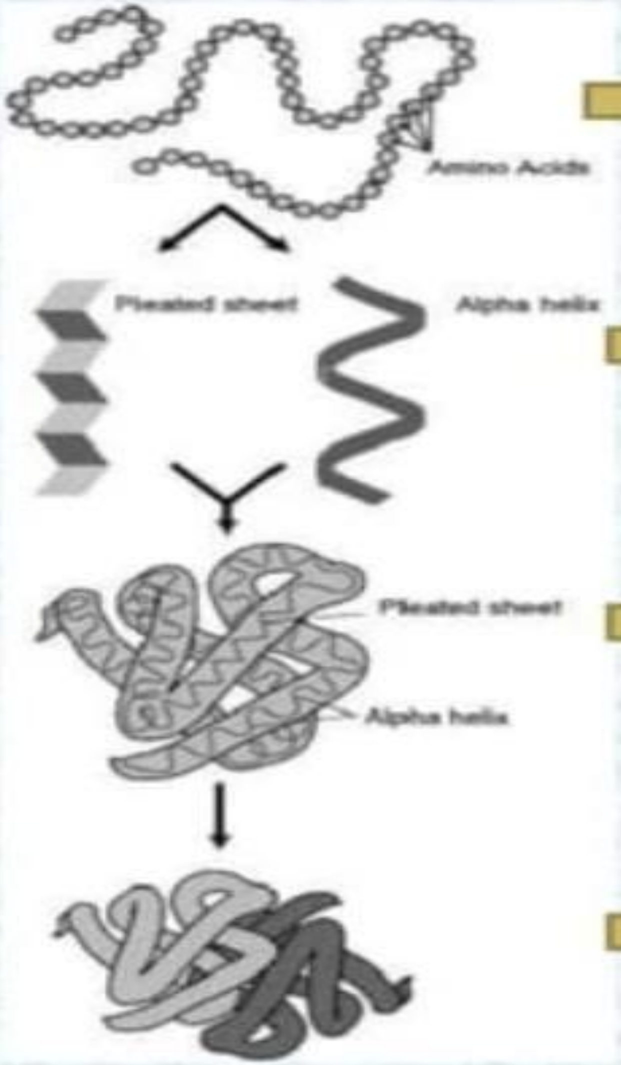
- Protein are long sequences formed out of 20 different amino acid residues that in physiological conditions adopt a unique 3-D structure.

PROTEIN HAVE DIFFERENT LEVELS OF ORGANISATION:

- Primary structure
- Secondary structure
- Tertiary structure
- Quaternary structure



PROTEIN STRUCTURE



Primary

Assembly

Secondary

Folding

Tertiary

Packing

Quaternary

Interaction

PRIMARY STRUCTURE:

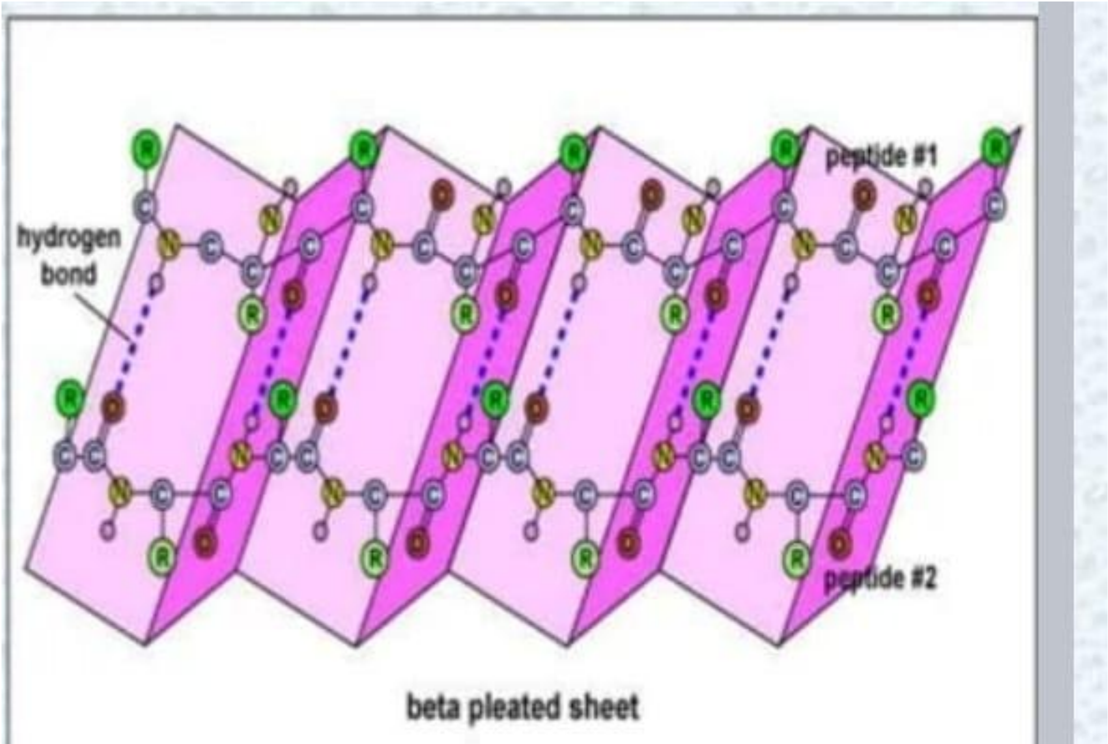
- Primary structure of protein is the linear sequence of amino acids that make up the polypeptide chain.
- The primary structure of a protein originally referred to its complete covalent structure but is more frequently interpreted as being the sequence of amino acids of each polypeptide chain of which the protein is composed.
- A perfectly linear amino acid polymer is neither functional nor energetically.

SECONDARY STRUCTURE:

- It results from hydrogen bond formation between hydrogen of –NH group of peptide bond and the carbonyl oxygen of another peptide bond.
- According to H-bonding there are two main forms of secondary structure.
- α -helix
- β -sheets

α-helix : It is a spiral structural resulting from hydrogen bonding between one peptide bond and fourth one.

β-Sheets: It is another form of secondary structure in which two or more polypeptide(or segment of the same peptide chain) are linked together by hydrogen bond between H- of NH- of one chain and carbonyl oxygen of adjacent chain.



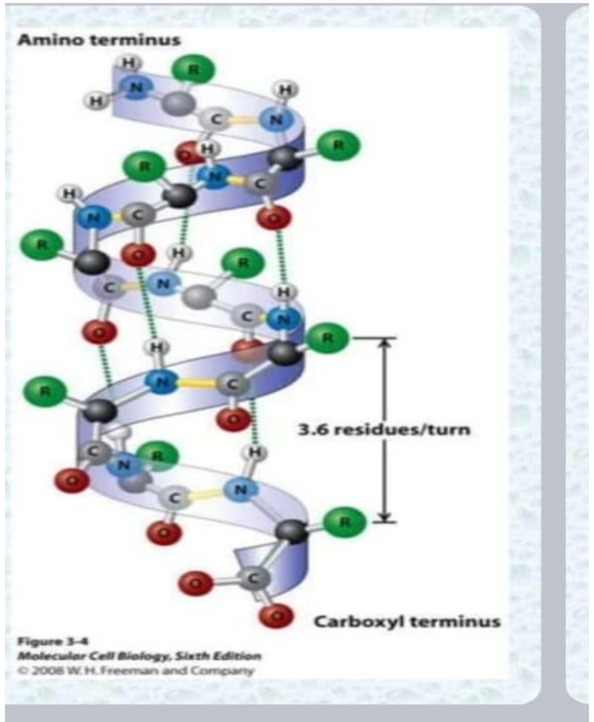


Figure 3-4
Molecular Cell Biology, Sixth Edition
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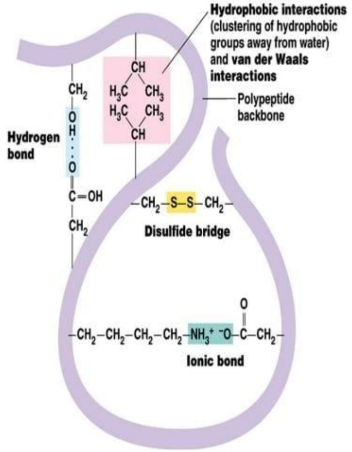
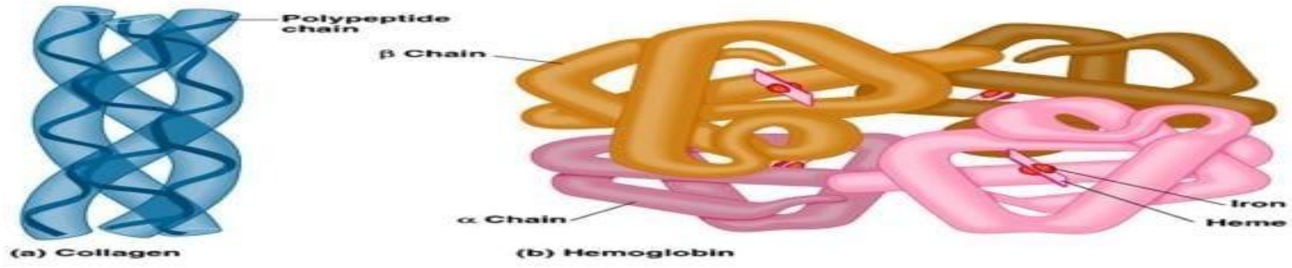
TERTIARY STRUCTURE :

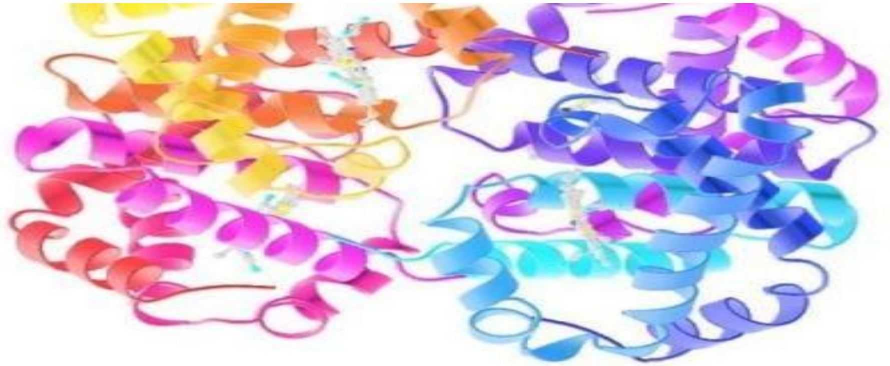
- It is non linear ,3 dimensional
- It is formed and stabilized by hydrogen bonding ,covalent bonding , hydrophobic packing toward cord and hydrophilic exposure to solvent.
- A globular amino acid polymer folded and compacted is somewhat functional(catalytic) and energetically favorable.



QUATERNARY STRUCTURE:

- Collage It results from the aggregation(combination) of two are more polypeptide subunits held together by non covalent interaction like H-bonds, ionic or hydrophobic interactions.
- n is a fibrous protein of three polypeptides (trimeric) that are supercoiled like a rope.
- This provides the structural strength for their role in connective tissue . Hemoglobin is a globular protein with four polypeptide chains insulin : two polypeptide chains (dimeric)





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THANK YOU