

Virtual University of Pakistan

**(bif401)**

**(bioinformatics 1)**

**MCQ's for final term**

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----- provide mass of intact molecules and its fragments

### **MS1 and MS2**

theoretical data is usually ----- as compared to exp. Data,

**larger**

Three scoring schemes can be applied to -----

**score the match at each stage of protein search**

Simply sum the scores up (a linear function)

$$\text{Score} = \text{Score}_{MW} + \text{Score}_{PST} + \text{Score}_{Exp} < > \text{Thr}$$

In the above scoring method, MW and PST stabs for \_\_\_\_ & \_\_\_\_ respectively

### **MS1 & MS2**

\_\_\_\_\_ are assembled by Ribosomes in cellular cytoplasm

### **Proteins**

Amino acids have characteristics like polarity, hydrophobicity, and charge states. these characteristics are governed by

### **Elemental composition of an amino acid's side chain (R group)**

Hydrophobic amino acids are non-polar due to

**very little dipole moments between H and C**

Core of amino acids is \_\_\_\_\_ and surface is \_\_\_\_\_

### **Hydrophobic & hydrophilic**

At pH \_\_\_\_ Five amino acids are charged, 2 negatively and 3 positively

7

pK values for an amino acid is the pH at which:

**Exactly half of the chargeable group is charged**

The pK of aspartic and glutamic acids are \_\_\_-& \_\_\_ respectively.

### **3.9 & 4.2**

If  $\text{pH} < \text{pK}$  for an amino acid, the amine side chains\_\_\_\_\_

### **Gain proton and hence basic**

If  $\text{pH} > \text{pK}$  for an amino acid, \_\_\_\_\_ loses a proton and hence acidic

### **The carboxyl side chain**

Lysine and arginine have pK \_\_\_ & \_\_\_ respectively.

### **10.5 & 12.5**

Glycine residues increase backbone flexibility because :

### **They have no R group (only an H)**

\_\_\_\_\_ reduce the flexibility of polypeptide chains.

### **Proline residues**

\_\_\_\_\_ Cement together by making \_\_\_\_\_ to stabilize 3-D protein structures

### **Cysteines, disulfide bonds**

Chemically \_\_\_\_\_ remain in the core of protein.

### **Inactive amino acids**

Backbone is highly polar (hydrophilic) due to polar \_\_\_ and \_\_\_ in each peptide unit

### **-NH & C=O**

A-helices & B-sheets are stabilized by\_\_\_\_\_

### **H-bonds**

The very few hydrophobic "patches" on protein surface are involved in:

### **Protein-protein interactions**

Alpha Helix is Stabilized by H-bonds between every \_\_\_\_\_ in backbone

### **~ 4th residue**

Proteins fold spontaneously to achieve:

## Thermodynamic stability

If a protein is \_\_\_\_\_, then it can lead to a lack of function in the protein

## Misfolded

Given algorithms and procedures to fold a protein, we can:

## Fold amino acid chains to form 3D proteins

Each amino acid can fold into \_\_\_\_\_, \_\_\_\_\_ & \_\_\_\_\_

## Alpha Helices, Beta Sheets and Loops

If computations of protein folding take  $1/10^{\text{th}}$  of a nano-second ( $10^{-10}$ ), then to compute all the folding possibilities will take

**$1.6 \times 10^{30}$  years**

All the information required for folding a protein into its native structure is present within the:

## Protein's amino acid sequence

(Memorize the table given below)

**Protein Structures**

---

**Energies of Various Bonds & Interactions**

Bond Type	kJ/mol
Covalent Bond	250
Electrostatic	5
van der Waals	5
Hydrogen bond	20

Primary sequence can also be referred to as \_\_\_\_\_

## 1' structure

Protein structures are organized into \_\_\_\_\_ modular conformations

**1', 2', 3' and 4'**

Edman Degradation & Tandem Mass Spectrometry are methods for obtaining \_\_\_\_\_

### **1' structures**

2' structures are also referred to as

### **Secondary structures**

C- Terminus is \_\_\_\_\_ charged

### **Negatively**

N-terminus is \_\_\_\_\_ charged

### **Positively**

2' structures or secondary protein structures are formed as a result of H-Bond formation between \_\_\_\_\_ in a protein backbone

### **N and C termini**

\_\_\_\_\_ connect helices and sheets

### **Loops**

\_\_\_\_\_ are Secondary structures that are not helices, sheets, or recognizable turns

### **Coils**

\_\_\_\_\_ are also secondary structure which form the first structures after folding of protein's amino acids

### **Loops and Coils**

Combinations of Alpha helices, Beta sheets, coils and loops help form \_\_\_\_\_

### **3' structures**

\_\_\_\_\_, \_\_\_\_\_ & \_\_\_\_\_ interactions enforce the 3' structure

### **Covalent bonds, Hydrogen bonds and hydrophobic**

The stability of all the structures of protein is as:

**4' > 3' > 2' > 1'**

The protein folding into 3D structures leads to:

### **Reduction in bond angles**

Peptide bond between two amino acids is \_\_\_\_\_

### **Planar & rigid**

The angle between the 1<sup>st</sup>, overlapped and the 4<sup>th</sup> points forms a \_\_\_\_\_

### **Dihedral angle**

\_\_\_\_\_ can be used to construct the backbone of a protein towards its visualization

### **C-Alphas**

The \_\_\_\_\_ is used to express the size of atoms, molecules and extremely small biological structures, the lengths of chemical bonds, the arrangement of atoms in crystals.

### **Angstrom**

Atoms of phosphorus, sulfur, and chlorine are \_\_\_\_\_ in covalent radius, while a hydrogen atom is \_\_\_\_\_ respectively.

**~1 Å & 0.25 Å**

Crystallography data gives \_\_\_\_\_ of atomic coordinates

### **Relative positions**

\_\_\_\_\_ Proteins are used to determine protein structures.

### **Crystallized**

(Memorize the below file format of protein data base to attempt additional mcq's in exam, for more, you can read ppt of lecture no. 179)

**HEADER** - Contains a brief description of the structure, the date and the PDB ID code.

**TITLE** - The title of the structure.

**COMPND** - Brief details of the structure.

**SOURCE** - Identifies which organism the structure came from.

**KEYWDS** - Lists a set of useful words/phrases that describe the structure.

**AUTHOR** - The scientists depositing the structure.

**REVDAT** - The date of the last revision.

\_\_\_\_\_ contains protein structure information

### **PDB**

PDB has the coordinates of C-Alphas for over \_\_\_\_\_ proteins

**50,000**

To view a protein, we need to evaluate the:

#### **physical location of its atoms**

To trace the backbone of a protein, \_\_\_\_\_ trace can be used

#### **CA atoms**

Coordinates of CA atoms can be obtained from the \_\_\_\_\_

### **PDB**

Protein structures are visualized using several online tools. These tools include:

**Rasmol, CHIME, Swiss PDB Viewer and Cn3D.**

CPK stands for:

#### **Corey-Paulin-Koltun Diagrams**

In CPK diagrams, each atom is represented by a \_\_\_\_\_

#### **Solid sphere**

Spheres are equal to atomic \_\_\_\_\_

### **Van der Waal radius**

Ribbon Diagrams represent the protein secondary structures by using:

### **Simple cartoon figures**

Balls & Stick (BS) Models have atoms as \_\_\_\_\_ and intermediate bonds as \_\_\_\_\_ respectively

### **colored balls, sticks**

“Proteins fold for a unique, stable and minimum free kinetic energy structure”. The given statement is called:

### **Anfinsen’s thermodynamic hypothesis**

There is \_\_\_\_\_ free energy accessible to each atom for further interactions.

### **Lesser**

The greater the number of bonds, the more \_\_\_\_\_ a protein becomes.

### **Stable**

The basic idea of thermodynamic stability is to \_\_\_\_\_ bonding in order to \_\_\_\_\_ the free energy

### **Maximize, minimize**

We can calculate energy of a folded protein based on the \_\_\_\_\_ of atomic interactions

### **number and types**

To determine the number of each type of interaction within a protein, we need to find its \_\_\_\_\_

### **inter-atomic distances**

Based on specific atomic distances in protein, we can guess the \_\_\_\_\_

### **type of atomic interaction**

## Energies of Interactions

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Force	Strength (kJ/mol)	Distance (nm)
Van der Waals	0.4-4.0	0.3-0.6
Hydrogen Bonds	12-30	0.3
Ionic Interactions	20	0.25
Hydrophobic Interactions	<40	varies

$$\text{Energy}_{\text{TOTAL}} = \text{Atoms}_{\text{VWF}} \times \text{Energy}_{\text{VWF}} + \text{Atoms}_{\text{HB}} \times \text{Energy}_{\text{HB}} + \text{Atoms}_{\text{IonicInteraction}} \times \text{Energy}_{\text{IonicInteraction}}$$

To determine the structure of protein, we use \_\_\_\_\_

### X-Ray or NMR

If two atoms are participating in a covalent bond, their distance is:

**~0.96Å**

In case of hydrogen bond formation between atoms, the inter-atomic distance is :

**~1.97Å**

X-Ray data should have a minimum of \_\_\_\_\_ resolution

**1.97Å**

,"Helix Formers" are generally \_\_\_\_\_ amino acids (M, A, L...)

### Hydrophobic

Alpha Helices are formed by hydrogen bonding (O-H) between \_\_\_\_\_ atoms in the protein backbone

### C<sub>i</sub> and N<sub>i+4</sub>

\_\_\_\_\_ residues are needed to make a Beta Strand

**5 to 10**

The sub-structures of beta-sheets are:

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- **Beta Strand**
- **Beta Sheet**
- **Beta Barrel**
- **Beta Sandwiches**

\_\_\_\_\_ is made of a single beta sheet that twists and coils upon itself.

### **Beta-barrel**

Beta Sandwiches are made of two beta sheets which are usually \_\_\_\_\_ so their strands are aligned

### **twisted and packed**

Loops are formed by amino acids present in the middle of \_\_\_\_\_ in a protein backbone

### **the Alpha Helices and Beta Sheets**

Variability in \_\_\_\_\_ allows loops to join Alpha Helices and Beta Sheets in a variety of ways.

### **length and conformation**

Loops are mostly comprised of \_\_\_\_\_ amino acids

### **charged and polar**

Hairpin loops are two amino acids long and join \_\_\_\_\_ Beta strands

### **anti-parallel**

Essentially, a secondary structure which is not a helix, sheet or loop, is a \_\_\_\_\_

### **coil**

Coils are apparently \_\_\_\_\_ regions

### **disordered**

\_\_\_\_\_ are semi-independent functional structures in a protein

### **Domains**

Domains have over \_\_\_\_\_ residues

~40

\_\_\_\_\_ interact (H-bonds) more internally than externally

### **Locally Compact – Domains**

Domains have a \_\_\_\_\_ core

### **hydrophobic**

various types of domains are:

- **Alpha Domains**
- **Beta Domains**
- **Alpha/Beta Domains**
- **Alpha + Beta Domains**
- **Alpha & Beta Multi-Domains**
- **Membrane & cell-surface proteins**

(must see the structures of these domains in lecture 196)

Domains can be classified into structural classes. Classes can be further classified into

### **Architecture and Topologies**

\_\_\_\_\_ classifies proteins by their structural similarity

### **CATH**

FSSP stands for \_\_\_\_\_ based on the DALI algorithm

### **Family of Structurally Similar Proteins**

SCOP stands for:–

### **Structural Classification of Proteins**

So for two different proteins, sharing the same domain, we may want to compare:

### **only a portion of the overall structure i.e. a domain**

Whole protein structures can be compared by calculating the \_\_\_\_\_ between their Alpha Carbons positions

### **root mean squared difference (RMSD)**

The \_\_\_\_\_ the RMSD, the similar are the proteins

### **Lower**

Full protein structures can be compared and ranked by the overall \_\_\_\_\_ in positions between their Alpha Carbons

### **differences**

\_\_\_\_\_ tells us about the quality of the matches

### **RMSD**

\_\_\_\_\_ mostly found in Alpha Helices

### **Alanine**

The first such algorithm to predict 2' given an amino acid sequence was the:

### **Chou-Fasman Algorithm**

we only know \_\_\_\_\_ 3D protein structures, but 10 times more sequences

### **100,000**

For a primary sequence, and a tentative 2' structure, \_\_\_\_\_ can help us compute the overall propensity

### **propensity table**

\_\_\_ amino acids are needed to start an Alpha Helix and \_\_\_ amino acids for Beta Sheet

### **4,5**

Loops are small amino acids

### **~ 3-4**

Alpha Helices are formed from 4 contiguous amino acids having an Alpha-Helix propensity over \_\_\_\_\_

### **1.0**

