bif401) (bioinformatics 1) MCQ's for final term,Organised by Muhammad Kashif

151-250

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

MS1 and MS2

theoratical 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)

$$Score = Score_{MW} + Score_{PST} + Score_{Exp <> Thr}$$

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 pH < pK for an amino acid, the amine side chains____

Gain proton and hence basic

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

1.6×10^{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 1st, overlapped and the 4th 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

$$Energy_{TOTAL} = Atoms_{VWF} \times Energy_{VWF} + Atoms_{HB} \times Energy_{HB} + Atoms_{IonicInteraction} \times Energy_{IonicInteraction}$$

To determine the structure of protein, we use_____ **X-**

Ray or NMR

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

~0.96A

Incase of hydrogen bond formation between atoms, the inter-atomic distance is : **~1.97A**

X-Ray data should have a minimum of _____ resolution

1.97A

,"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_i and N_{i+4}

_____ resides are needed to make a Beta Strand

5 to 10

The sub-structures of beta-sheets are:

- **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

Chou Fasman Algorithm helps predict

Alpha Helices, Beta Sheets and Turns

Chou Fasman can be improved to better predict secondary structures by incorporating **biochemical factors**

Structure visualization, classification and prediction are important for:

Understanding disease and designing drugs for treating them

Homology modeling is used to predict structures of proteins having _____ with other proteins with known structures **high sequence similarity** three different strategies for structure prediction are:

1. **Homology Modelling**
2. **Threading/Fold Recognition**
3. **Ab Initio Modelling**

There are_____ salient steps in any Homology Modelling pipeline **seven**

The backbone of _____ strongly prefers two rotamers and the real side-chain may fit one of them

Tyrosine

Limitations of Homology Modelling are:

Cannot study conformational changes

Cannot elicit new catalytic/binding sites

_____is a software for homology modelling **Modeller**

A _____ is defined by the way the secondary structure elements of the structure are arranged relative to each other in space **protein fold**

Common folds include _____ bundle and the TIM barrel.

4-helix

There are _____ stable folds in nature **5,000**

Fold recognition or Threading is a technique for predicting :

protein structures

Fold recognition is also called _____ **Threading** for each fold,

we must _____ of sequence matching that fold **compute the**

fitness

Threading involves _____ the amino acid sequence through each fold in the database

"passing"

Software for automated protein structure &function prediction based on the sequence-to-structure-tofunction.

Iterative threading assembly refinement (I-TASSER) server

_____ helps thread amino acid sequences on fold and secondary structure databases **iTASSER**

Fold recognition or threading is useful in cases where _____ fails to predict quality structures

homology modeling

3D-1D Bowie Algorithm was Proposed by _____

Bowie et al in 1991

3D-1D Bowie Algorithm Converts____structure into a ____ string profile for each structure in the fold library

3D, 1-D

3D-1D Bowie Algorithm Identify amino acids based on: **protein**

core, side chain positioning, solubility etc.

Inputs and outputs of 3D-1D

$P_{a:j}$= prob. of finding amino acid (a) in environment (j)

P_a=probability of finding (a) anywhere

Maximize sum of scores for the fold:

$$s_{aj} = \log\left(\frac{P_{a:j}}{P_a}\right)$$

3D-1D methods convert structure and environment information into _____

profiles

_____ attempt to identify the structure with minimum free energy

Ab initio methods

Ab Initio Modelling is Suitable for proteins with less than _____

100 residues

Energy released during the folding process is computed for _____ **predicting**

structure

_____is measured by energy released during the folding process

Stabilization

The protein structure reporting _____ is selected to be the optimal structure **lowest**

energy

_____are the very difficult to design

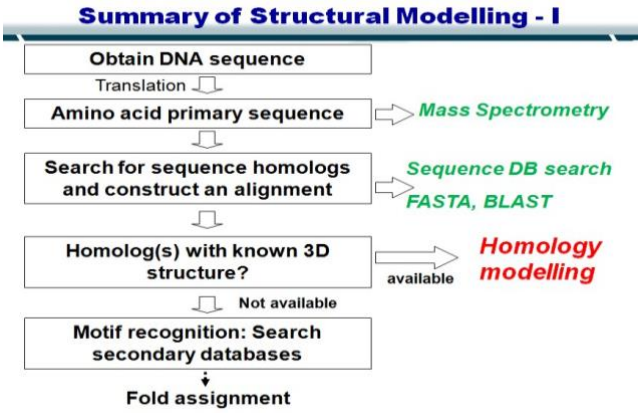
Ab initio methods

Ab initio methods are slow due to the _____ **huge**

possibilities

In Ab Initio Modelling, An order _____ steps are needed to simulate protein folding for medium sized protein structures

of 10_{12}



For low identity and alignment scores, a _____ for structure prediction exists

Twilight zone we compare

sequences by:

Pair-wise Sequence Alignment

Multiple Sequence Alignment

_____ & _____ are phylogenetic trees.

Scaled Trees/ Unscaled Trees , Rooted Trees/Unrooted Trees

Molecular evolution & mutation occur by:

Insertions, Deletions, substitution

Some of the RNA Secondary Structures are:

Hairpin Loops

Bulges

Helices

Intersection

Which is the justified statement of homology modeling?

Number of known protein sequences is much larger as compared to known proteins structures

Three Strategies for Structure Prediction are:

Homology Modelling

Fold Recognition

Ab Initio Modelling

GOOD LUCK FOR YOUR EXAMS ^_^