2017

BIOTECHNOLOGY

Paper : 402

COMPUTATIONAL BIOLOGY

Full Marks: 80
Time: 3 hrs

The figures in the margin indicate full marks for the questions

1. Find out the correct answer of the following questions (any five) 1×5=5

A) The Protein Data Bank (PDB):
   a) Functions primarily as the major worldwide repository of macromolecular secondary structures.
   b) Contains approximately as many structures as there are protein sequences in SwissProt / TrEMBL.
   c) Includes data on proteins, DNA-protein complexes as well as carbohydrates.
   d) Is operated jointly by the NCBI and EBI.

B) A CATH database offers a hierarchical classification of protein structures. The first three levels, Class, architecture and Topology, all describe:
   a) Protein tertiary structure
   b) Protein secondary structure
   c) Protein domain structure
   d) Protein superfamilies grouped according to homologous domains.

C) The substitution of one amino acid for another
   a) will change the primary structure of the polypeptide.
   b) can change the secondary structure of the polypeptide.

P.T.O.

c) can change the tertiary structure of the polypeptide.

d) All of these are correct.

D) Protein motifs are considered a type of Loop region

a) Primary structure

b) Secondary structure

c) No specific secondary structure

d) Tertiary structure

E) Proteins, nucleic acids, lipids and carbohydrates all have certain characteristics in common. Which of the following is not a common characteristic?

a) They are organic, which means they are all living substances.

b) They all contain the element carbon.

c) They contain simpler units that are linked together making larger molecules.

d) They contain functional groups.

F) In the practical application of molecular dynamics simulations the fundamental equation is that of

a. Lagrangian equation

b. Schroedinger's equation

c. Langevin's equation

d. Newton's equation of motion

G) Proteins have regions that show specific patterns of folding or function and are called

a) Domains

b) Sites

c) Subunits

d) Motifs

2. Match the following items in column X with appropriate items in column Y: (any five) 1×5=5

Column X	Column Y	
2.1 Microarray	A	Protein family
2.2 Pubmed	B	Software for phylogenetic analysis
2.3 X-ray crystallography	C	Gene expression
2.4 Pharmacogenomics	D	database for abstracts related to medicine
2.5 GenBank	E	Single nucleotide polymorphisms in drug metabolizing genes
2.6 Pfam	F	Protein structure
2.7 Phylip	G	Accession number

3. Define any five from the following. 2×5=10

a) Ramachandran plot b) Docking

c) Threading d) TrEMBL

e) Chou-Fasman Algorithm f) Edman Degradation

g) ADMET property prediction

4. Distinguish Between (any four) 4×5=20

a) Local and Global Energy Minimization method

b) Molecular Mechanics and ab initio method for molecular modelling

c) Ligand based and Structure based Drug Designing

d) Tertiary and Quaternary structure of protein

e) Protein Sequence database and Protein Structure database

f) Database and Databank.

5. Describe any two from the following. 8×2=16

a) Why is the lower right quadrant called a "forbidden" region in the Ramachandran plot? What makes Gly special when it comes to Ramachandran plots? 4+4=8

b) The amino acids of a polypeptide chain affect the shape of the protein. Predict where each of the following amino acid pairs would be found in the protein-facing toward the outside or folded in toward the interior-and explain your answer. 2+2+2+2=8

i) Both amino acids are valine.

ii) One amino acid is aspartic acid, and the other is serine.

iii) Both amino acids are glycine.

iv) One amino acid is alanine, and the other is isoleucine

c) What is loop modelling? How would you validate/assess a protein structure predicted by homology modelling? Name two other methods of protein structure prediction. 2+4+2=8

d) State the structural features of alpha helix and beta sheet. Compare parallel and anti parallel strand. 4+4=8

6. Answer any two from the following. 12×2=24

a) Describe the secondary structure prediction method for globular proteins. What are the applications of protein secondary structure prediction? 8+4=12

b) What are the two prediction methods used for Secondary Structure of RNA. Discuss any one of them. 2+10=12

c) Describe the methods of Computer Aided Drug Designing. 12

d) What are the techniques used to investigate Protein- Protein Interactions? Describe briefly. 12

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