

ADVANCED BIOINFORMATICS  
(BIOT 5201)

Time Allotted : 3 hrs

Full Marks : 70

*Figures out of the right margin indicate full marks.*

*Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.*

*Candidates are required to give answer in their own words as far as practicable.*

**Group - A**  
**(Multiple Choice Type Questions)**

1. Choose the correct alternatives for the following: **10 × 1=10**

- (i) Target selection in drug discovery necessitates
- (a) linking a target molecule that affects disease by affecting its function or expression
  - (b) finding information about specific protein-protein interactions
  - (c) knowledge about differential genomics and proteomics
  - (d) all of the above.
- (ii) A Which is a data retrieving tool?
- (a) ENTREZ
  - (b) EMBL
  - (c) PHD
  - (d) all of these.
- (iii) A kissing hairpin refers to a
- (a) hydrogen bond
  - (b) hairpin-bulge contact
  - (c) hydrogen bonded interaction formed between loop residues of two hairpin structures
  - (d) all of the above

- (iv) CLUSTALW does
- |                       |                                 |
|-----------------------|---------------------------------|
| (a) Local alignment   | (b) Global alignment            |
| (c) Partial alignment | (d) Multiple sequence alignment |
- (v) A Markov model describes
- (a) a sequence of events that occur consecutively in a chain
  - (b) a sequence of events that occur in an arithmetic progression in a chain
  - (c) a sequence of events that occur in a geometric progression in a chain
  - (d) none of the above.
- (vi) An open reading frame (ORF) begins with
- |                               |                  |
|-------------------------------|------------------|
| (a) an ATG initiation codon   | (b) a stop codon |
| (c) an expressed sequence tag | (d) a TATA box.  |
- (vii) Which of the following is NOT a secondary structure prediction algorithm?
- |           |                  |
|-----------|------------------|
| (a) ZPRED | (b) PHD          |
| (c) DSSP  | (d) SWISS-MODEL. |
- (viii) Principal component analysis (PCA) is usually used to
- (a) filter redundant descriptors
  - (b) filter essential descriptors
  - (c) transfer uncorrelated variables
  - (d) all of the above
- (ix) Which of the following is true about PAM matrices?
- (a) Created by Chou-fasman.
  - (b) Created using conserved DNA families
  - (c) PAM-1 means 1 accepted point mutation per 100 residues
  - (d) Lower numbered PAM matrices are appropriate for comparing distantly related species

- (x) 10 Alignment of two sequences is performed using
- (a) dot matrix analysis
  - (b) dynamic programming algorithm
  - (c) word or K-tuple method
  - (d) all of these

**Group - B**

2. (a) In the context of similarity, mention the relationship of the following items citing definitions with suitable graphical representation: safe zone, twilight zone and midnight zone.
- (b) Briefly describe steps of BLAST algorithm. Cite the use of adjustable gap penalties in CLUSTAL.
- (c) Mention the name of the statistical indicator in BLAST result and mention how it is related to raw alignment score. Also mention the formula.

$$3 + (4+2) + (1+1+1) = 12$$

3. (a) Briefly describe the process of computational gene finding.
- (b) What are the approaches of computational gene annotations? Cite one example from each category.
- (c) Why is *ab initio* method said to be not suitable for eukaryotic gene prediction?
- (d) To evaluate the accuracy of the predicted programs mention some parameters which are important. Also state how they help in the evaluation process.

$$3 + (2+2) + 2 + 3 = 12$$

**Group - C**

4. (a) Cite one difference between phylogram and cladogram.

- (b) Find out the number of rooted trees that can be generated from six taxa.
- (c) Mention the role of biological data for constructing molecular phylogenetic tree.
- (d) Elucidate the role of synonymous and nonsynonymous substitutions in understanding the evolutionary process.
- (e) Write the objective of using Kimura substitution model over Jukes-Cantor Model
- (f) Calculate the corrected evolutionary distance by suitable substitution model of two sequence where they differ by 30%, out of which 20% of changes are a result of transitions and 10% of changes are a result of transversions.

$$2+2+2+2 +2+2 = 12$$

5. (a) Using the suitable phylogenetic tree describe the following terminologies:  
clade , lineage and paraphyletic group.
- (b) Draw an assumptive tree from the following Newick format for tree representation providing suitable reasons:  
(((X:1,Y:2),Q:2),(Z:1.5,L:3))
- (c) Describe the term 'among site rate heterogeneity' and elucidate how these artifacts can be corrected in the evolutionary models.
- (d) 'Bootstrapping is a statistical method used for evaluation of reliability of the inferred phylogeny' – justify the statement with suitable reasons.

$$4 + 3 + 3 + 2 = 12$$

**Group - D**

6. (a) How is helical membrane protein prediction undertaken?

- (b) What are the special characteristics of Phobius?
- (c) How is tertiary structure prediction undertaken in transcription regulatory proteins containing leucine zippers?

$$4 + 4 + 4 = 12$$

7. (a) Define a neural network.
- (b) Explain its method of operation with respect to protein secondary structure prediction.
  - (c) Draw a schematic diagram of a protein secondary structure prediction algorithm that uses both multiple alignments and neural networks.
  - (d) What improves the accuracy of a secondary structure prediction algorithm using a combination of factors? Explain your answer.

$$2 + 3 + 4 + 3 = 12$$

**Group - E**

8. (a) Define QSAR .
- (b) What are some typical applications of QSAR?
  - (c) What are the assumptions of QSAR techniques?
  - (d) Name two types of descriptors that are used in QSAR studies.

$$2 + 3 + 4 + 3 = 12$$

9. (a) What are the two main approaches in computer assisted drug design? Define a binding site in a protein. Specify a wet experimental method of identifying a binding site in a protein.
- (b) Define molecular docking including its essential characteristics. What is the purpose of a scoring function? Name the factors that affect the docking score explaining two of them.

$$(2+1+2) + (2+2+3) = 12$$