

COMPUTATIONAL BIOLOGY
(BTC3225)

Time Allotted : 2½ hrs

Full Marks : 60

Figures out of the right margin indicate full marks.

*Candidates are required to answer Group A and
any 4 (four) from Group B to E, taking one from each group.*

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

Group – A

1. Answer any twelve:

12 × 1 = 12

Choose the correct alternative for the following

- (i) _____ bases are not found in DNA
(a) Adenine (b) Guanine
(c) Thymine (d) Uracil
- (ii) In a protein of molecular weight 58300, the number of amino acid residues is
(a) 110 (b) 253
(c) 530 (d) 330
- (iii) _____ is a comprehensive database for the study of human genetics and molecular biology
(a) PDB (b) STAG
(c) OMIM (d) PSD.
- (iv) SCOP is
(a) primary database
(b) nucleotide sequence database
(c) based on architectural classification of protein
(d) structural database.
- (v) Molecular modelling and simulation tools are written in a variety of programming languages except
(a) C (b) fortran
(c) python (d) arabic.
- (vi) A fingerprint is a
(a) A protein family discriminator built from a set of regular expressions.
(b) A protein family discriminator built from a set of conserved motifs.
(c) A cluster of protein sequences gathered from a BLAST search.
(d) A cluster of protein sequences gathered from a FASTA search.

- (vii) Which variable can concretely define the representation of the transition model?
 (a) Single variable
 (b) Discrete state variable
 (c) Random variable
 (d) Both Single and Discrete state variable.
- (viii) Molecular dynamics approaches utilize classical mechanics based on Newton's laws of motion due to
 (a) Quantum mechanics only applies to light particles such as electrons.
 (b) Scientists have not yet developed any methods able to describe motion of atoms using quantum mechanics.
 (c) Vibrational frequencies of proteins are so incredibly small that it would be dangerous to attempt a quantum mechanical description of them.
 (d) Given the relatively high mass of atoms, it is often an acceptable approximation to neglect quantum mechanical effects when describing their motion.
- (ix) In designing OpenMM, it is essential for the API to provide support for
 (a) efficient implementations on a variety of architectures
 (b) non implementations on a variety of architectures
 (c) formation of a variety of architectures
 (d) Efficient implementations on a variety of variables.
- (x) Which of the following approaches is classified under 'Ligand-Based Drug Design'?
 (a) Molecular docking
 (b) QSAR Modeling
 (c) Pharmacophore modelling
 (d) b and c both

Fill in the blanks with the correct word

- (xi) The monosaccharides are joined by _____ bonds to synthesize the polysaccharide.
- (xii) The secondary structure of protein is stabilized by _____ bond.
- (xiii) The tool used to predict the three-dimensional structure of a Protein is _____.
- (xiv) _____ method is used for predicting protein tertiary structure in the absence of homology to a known structure.
- (xv) _____ is a template based protein modeling techniques.

Group - B

2. (a) Describe the process of DNA replication. [[CO2](Explain/IOCQ)]
 (b) How pH and pKa of an amino acids can be related? [[CO1](Derive/HOCQ)]
7 + 5 = 12
3. (a) What is the unit of protein? Classify them. [[CO1](Remember/LOCQ)]
 (b) How much ATP will be produced per mole of glucose consumption. [[CO2](Calculate/HOCQ)]
(2 + 4) + 6 = 12

Group - C

4. (a) What is a primary database and secondary database? *[[CO3) (Understand/LOCQ]]*
(b) Comment on two main functions of a biological database. *[[CO3) (Understand-knowledge/LOCQ]]*
(c) Illustrate the type of data available in biological databases? Give examples of two primary sequence databases and secondary databases. *[[CO4) (Understand-apply/HOCQ]]*
(2 + 2) + 2 + 2 + (2 + 2) = 12
5. (a) What is a domain? Give example of two databases that contain this type of data. *[[CO3)(Remember-understand/LOCQ]]*
(b) Cite the names of two secondary databases that can classify proteins according to their structure and briefly describe them. *[[CO4)(Remember-understand/LOCQ]]*
(c) State how PRINT and PROSITE is important in biological databases. *[[CO4)(Analyse/IOCQ]]*
(2 + 2) + (2 + 2) + 4 = 12

Group - D

6. (a) Define Hidden Markov Model. Discuss how it can be utilised in computational biology. *[[CO3)(Analyse/HOCQ]]*
(b) State the benefits and short comings Artificial Neural Network in computational biology? *[[CO4)(Remember/LOCQ]]*
(c) Mention one important application of ANN in computational biology. *[[CO2)(Apply/IOCQ]]*
(2 + 3) + (3 + 3) + 1 = 12
7. (a) Justify with reason for using BioLinux in biological data analysis. *[[CO5)(Analyse/HOCQ]]*
(b) Analyse the areas where BioLinux can be applied. *[[CO5)(Remember/IOCQ]]*
6 + 6 = 12

Group - E

8. (a) State how drug discovery takes place – mention the steps. *(CO6)(Describe/HOCQ)]*
(b) Justify the reasons for trials in the drug discovery process. *[[CO6)(Examine/IOCQ]]*
(c) Why drug discovery is needed? *[[CO6)(Analyse/IOCQ]]*
5 + 3 + 4 = 12
9. (a) Comment on the steepest descent method and conjugate gradient method. *[[CO6)(Describe/IOCQ]]*
(b) Discuss the steps for predicting the 3D structure of target protein by comparative modelling. *[[CO6)(Analyze/IOCQ]]*
(c) Mention a software used for predicting the 3D structure of the above protein. *[[CO6)(Remember/LOCQ]]*
(3 × 2) + 4 + 2 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	31.25	36.45	32.30