M. Sc. Bioinformatics Sem.-II (C.B.C.S.) (2013 Course) : WINTER - 2018

SUBJECT: STRUCTURAL BIOLOGY AND MOLECULAR MODELING

Day : Monday
Date : 22/10/2018

W-2018-1256

Time : 02.00 PM TO 05.00 PM
Max. Marks : 60

N. B. :

1) **Q. No. 1** and **Q. No. 5** are **COMPULSORY**. Out of remaining attempt **ANY TWO** questions from each section.
2) Figures to the right indicate **FULL** marks.
3) Answers to both the sections should be written in **SEPARATE** answer books.
4) Draw neat and labeled diagram **WHEREVER** necessary.

SECTION - I

Q. 1 Explain the following: **(10)**

a) Mathew's correlation coefficient.

b) Draw structure of the following amino acid

i) Alanine **ii)** Leucine

c) Ramchandran Plot.

d) Secondary structure of protein.

e) CASP.

Q. 2 Answer **ANY TWO** of the following: **(10)**

a) Briefly explain GOR for secondary structure prediction.

b) Write short note on protein secondary structure.

c) Write short note on Segment Overlap.

d) Explain 3 D structure visualization tools.

Q. 3 Answer **ANY TWO** of the following: **(10)**

a) Define sequence similarity and sequence identity.

b) Briefly explain the fundamental principles of protein folding.

c) What is Homology modeling? What are steps involved in the Homology modeling.

d) Differentiate between PHYRE and PSI-PRED method.

Q. 4 Answer **ANY TWO** of the following: **(10)**

a) Explain VAST and DALI.

b) Write short note on SCOP.

c) Discuss the application of 3D protein structure comparison.

d) Differentiate between CATH and SCOP.

P. T. O.

SECTION - II

Q. 5 Define the following: **(10)**

a) Define molecular mechanics

b) Simplex

c) Bond length

d) Maxima and Minima

e) Non-bonded interactions

Q. 6 Answer **ANY TWO** of the following: **(10)**

a) Write a note on Bond stretching.

b) Discuss the role of bond length, bond angle and torsional term in field approach.

c) What is simple water model?

d) Write short note on Mulliken method.

Q. 7 Answer **ANY TWO** of the following: **(10)**

a) Explain simplex minimization method.

b) Briefly explain the Newton-Raphson energy minimization method.

c) Differentiate between derivative and non-derivative energy minimization methods.

d) Describe first order minimization method.

Q. 8 Answer **ANY TWO** of the following: **(10)**

a) How in Newton's law applied in molecular dynamics simulation?

b) Explain molecular dynamics using simple models.

c) Write note on Random number generator

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