

SUBJECT: STRUCTURAL BIOLOGY AND MOLECULAR MODELING

Day : Monday
Date : 08/04/2019

S-2019-1465

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 **SAME** answer books.
- 4) Draw neat and labeled diagram **WHEREVER** necessary.

SECTION - I

Q. 1 Discuss the following: (10)

- a) Q_3 coefficient.
- b) Propensity value.
- c) Molecular Chaperons.
- d) Draw structure of the following amino acid:
 - i) Histidine
 - ii) Serine
- e) SCOP.

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

- a) Explain the various protein visualization tools.
- b) Write a note on Chou-Fasman method.
- c) Explain Mathew's correlation coefficient.

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

- a) Differentiate between Homology modeling and fold recognition methods.
- b) Write short note on CASP.
- c) Explain comparative modeling techniques using flow diagram.
- d) Write a note on Ramchandran Plot.

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

- a) Write short note on Structural databases.
- b) Explain the 3D structure comparison and alignment.
- c) Differentiate between CE and DALI.

P. T. O.

SECTION - II

Q. 5 Define the following: (10)

- a) Force field
- b) Conformation
- c) Saddle point
- d) Angle bending
- e) Hydrophobic interaction

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

- a) What is potential truncation?
- b) What is Van der Waals interactions?
- c) What is Cross term? Explain in brief.

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

- a) Differentiate between Maxima and Minima.
- b) Describe line-search energy minimization algorithm.
- c) Write short note on application of energy minimization of molecular system.
- d) Describe Derivative Energy minimization method.

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

- a) Write a note on Metropolis algorithm.
- b) Explain Monte Carlo simulation method.
- c) Write short note on non-periodic boundary method.
- d) Write note on Leap frog algorithm.

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