

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.
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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 is 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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