

**M. SC. BIOINFORMATICS SEM.-II (C.B.C.S.) (2013
COURSE) : SUMMER - 2018**
SUBJECT : STRUCTURAL BIOLOGY & MOLECULAR MODELLING

Day : **Friday**
Date : **06/04/2018**

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

S-2018-1127

N.B.:

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

SECTION – I

- Q.1** Explain the following terms: [10]
- a) Molecular database c) De-novo drug design e) Independent variable
b) Rigid docking d) COMPASS
- Q.2** a) Sketch the chemical structure of following amino acids: [02]
i) Isoleucine ii) Threonine iii) Tyrosine iv) Glutamic acid
- b) Describe role of visualization tools in molecular modelling approach. [04]
- c) Differentiate between Chau-Fasman and GOR methods of secondary structure prediction. [04]

OR

- c) Explain in details analysis procedure of predicted secondary structure of protein.
- Q.3** a) Define protein domain. [02]
- b) Explain comparative protein modelling technique with flow diagram. [04]

OR

- b) Describe ab-initio protein prediction algorithm.
- c) Write short note on PSI – PRED. [04]
- Q.4** a) Write short note on protein structure comparison. [02]
- b) How significant is protein structure prediction using computational methods. [04]
- c) Write short note on protein structure databases. [04]

OR

- c) Write short note on VAST and DALI.

P.T.O.

SECTION – II

- Q.5** a) Show with the diagrams: [05]
i) Hydrogen bonds
ii) Ionic bonds
iii) Van der Waal's interactions
iv) Overlapping bond
v) Hydrophobic interactions

- b) Explain the following terms with example (databases and tools): [05]
i) Chemical substance databases ii) SAR

- Q.6** a) Define torsions and improper torsions. [02]

- b) Explain all atoms and united atoms force field. [04]

OR

- b) Describe bond stretching and angle bending parameters in force field.

- c) Define non-bonded interactions with examples. [04]

- Q.7** a) Define minima, global minima, maxima and global maxima. [02]

- b) Explain non-derivative energy minimization method. [04]

- c) Discuss second order derivative energy minimization method. [04]

OR

- c) Describe potential energy surface.

- Q.8** a) What is potential? [02]

- b) Explain importance of solvation of the systems in molecular dynamics by the water molecules. [04]

- c) Explain metropolis algorithm. [04]

OR

- c) Define boundary condition of the system and minimum image conversion.

* * * *