

**M. SC. BIOINFORMATICS SEM.-II (C.B.C.S.) (2013 COURSE)  
: WINTER - 2017**

**SUBJECT : STRUCTURAL BIOLOGY & MOLECULAR MODELLING**

Day : **Thursday**  
Date : **02/11/2017**

**W-2017-1012**

Time : **10.00 AM TO 01.00 PM**  
Max. Marks : **60**

**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
  - b) Rigid docking
  - c) De-novo drug design
  - d) Independent variable
  - e) COMPASS
- Q.2** a) Sketch the chemical structure of following amino acids: **[02]**  
i) Proline    ii) Serine    iii) Tyrosine    iv) Arginine.
- b) Explain the GOR algorithm for protein structure prediction **[04]**

**OR**

- b) Differentiate between tertiary and quaternary protein structure.
- c) How can you measure the accuracy of prediction of protein molecule **[04]**
- Q.3** a) What are the differences between similarity and identity? **[02]**
- b) Explain detailed algorithm used in PHYRE for protein structure prediction. **[04]**
- c) Explain computational approach in fold recognition of protein molecule. **[04]**

**OR**

- c) Explain importance and role of template selection in Homology modelling.
- Q.4** a) Explain the importance of protein structure comparison. **[02]**
- b) Explain algorithm FSSP. **[04]**

**OR**

- b) How DALI is used in comparison to protein structures.
- c) How the macro molecular databases are important for structure comparison? **[04]**

**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 force field. [02]

- b) Explain Newton-Raphson energy minimization algorithm. [04]

- c) Differentiate between quantum mechanics and molecular mechanics. [04]

**OR**

- c) Draw the potential energy surface graph for H<sub>2</sub>O molecule.

- Q.7** a) Write a short note on ADMET. [02]

- b) Describe Conjugate gradient algorithm in molecular optimization. [04]

**OR**

- b) Explain importance of molecular optimization.

- c) Explain energy minimization method using Simplex approach. [04]

- Q.8** a) Define long range interactions with example. [02]

- b) Describe Newtonian molecular dynamics method. [04]

- c) Write short note on radial distribution function. [04]

**OR**

- c) Write short note on Self diffusion coefficient.

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