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 $H_2O$ 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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