

**Advanced Diploma in Bioinformatics Sem.-II (C.B.C.S.) (2013 Course)**  
**: SUMMER - 2019**

**SUBJECT: MOLECULAR MODELING AND DRUG DESIGNING**

Day: Monday  
Date: 08/04/2019

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

**S-2019-1475**

**N.B:**

- 1) **Q. No.1 and Q. NO.5 are COMPULSORY.** Attempt **ANY TWO** from the remaining from each section.
- 2) Figures to the right indicate **FULL** marks.
- 3) Answer the both sections should be written in **SAME** answer books.

**SECTION-I**

- Q.1** a) Define Tertiary structure and secondary structure of a protein. (02)
- b) What do you mean by energy minimization? What will happen if this step is not performed in process of finding a lead identification? (04)
- c) Mention the importance of co-ordinates in drug designing. (04)
- Q.2.** a) Explain angle bending and bond stretching (02)
- b) Explain different parameters of Force Fields and connection of Hooke's Law with it. (04)
- c) Write a note on different features that are important for a visualization tool to be highly acceptable. (04)
- Q.3** a) Mention types of Geometry Optimization Methods with examples. (02)
- b) Describe simplex and Newton Raphson Methods. (04)

**OR**

Mention the First order techniques for Geometry Optimization.

- c) i) Describe Minima and Maxima on Geometry Optimization graph? (02)
- ii) Write about Quasi-newton method for energy optimization. (02)
- Q.4** a) Mention different methods used for Molecular Dynamic Simulations. (02)
- b) Discuss in detail about Monte Carlo method for performing molecular dynamics. (04)
- c) Discuss the importance Thermodynamics in M.D.S. (04)

**P.T.O.**

## SECTION-II

- Q.5** a) Give two examples each of databases and software used in Drug Discovery process. (02)
- b) Explain process of drug discovery. (04)
- c) Differentiate between ligand based and receptor based drug discovery. (04)

**OR**

Discuss the role of bioinformatics in drug discovery.

- Q.6** a) Define lead optimization. (02)
- b) Differentiate between Ligand based and structure based drug designing. (04)
- c) Given is a protein structure from PDB. Explain the different methods that can be used to predict the active site present in the protein structure. (04)
- Q.7** a) Differentiate between virtual screening and HTS. (02)
- b) Write a note on 3D QSAR. (04)

**OR**

What is ADMET? Explain its role and importance in drug designing.

- c) Write a note on different types of molecular descriptors. (04)
- Q.8** a) What is binding energy? (02)
- b) Elaborate on different types of docking. (04)

**OR**

Write a note on receptor based virtual screening.

- c) Explain receptor based as well as ligand based Pharmacophore model generation. (04)

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