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

SUBJECT: MOLEULAR 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)**

Q2. **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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