

**ADVANCED DIPLOMA IN BIOINFORMATICS SEM.-II  
(C.B.C.S.) (2013 COURSE) : SUMMER - 2018**

**SUBJECT: MOLECULAR MODELING & DRUG DESIGNING**

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

**S-2018-1137**

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

**N.B:**

- 1) **Q.No1 and Q.No 5 are COMPULSORY.** Out of the remaining questions, attempt Any **TWO** from each sections.
- 2) Answer to both the sections should be written in **SEPARATE** answer book.
- 3) Figures to the right indicate **FULL** marks.
- 4) Draw neat labeled diagram **WHEREVER** necessary.

**SECTION-I**

- Q.1** Answer in brief: [10]
- a) Torsional angle
  - b) Saddle point
  - c) Metropolis algorithm
  - d) Give the structure, one letter code and three letter code for tyrosine, cysteine.
  - e) Give names of any two non – derivative energy minimization method.
- Q.2** Answer the following: ( **ANY TWO**) [10]
- a) Are all the energy minimization method valid for each system? Explain.
  - b) Differentiate between first order derivative & second order derivative methods for energy minimization.
  - c) Explain the role of minima, maxima, and saddle point in energy minimization.
- Q.3** Answer the following: ( **ANY TWO**) [10]
- a) Explain the architecture and topology of DNA in any visualization tool.
  - b) Write a short note on- **i) All atom force field ii) United atom force field**
  - c) What is the importance of force field in molecular modeling studies?
- Q.4** Answer the following: ( **ANY TWO**) [10]
- a) Explain Newtonian dynamics.
  - b) Write about simulated annealing technique.
  - c) Describe molecular dynamics at constant pressure.

**SECTION-II**

- Q.5** Answer in brief: [10]
- a) LBDD
  - b) QSPR
  - c) Rigid docking
  - d) Test set
  - e) Receptor
- Q.6** Answer the following: ( **ANY TWO**) [10]
- a) Differentiate between SBDD and LBDD.
  - b) Discuss the importance of drug designing in pharmaceutical industry.
  - c) Explain the method to identify and validate the target site.
- Q.7** Write short notes on: ( **ANY TWO**) [10]
- a) Write a short note on CoMSIA.
  - b) Write in detail about the various types of descriptors used in QSAR studies.
  - c) What is multiple linear regression? How is it related to QSAR?
- Q.8** Answer the following: ( **ANY TWO**) [10]
- a) What is docking? Give the importance of scoring function in docking.
  - b) Write a note on receptor based pharmacophore model.
  - c) What is virtual screening? Explain the role of virtual screening for lead identification?