ADVANCED DIPLOMA IN BIOINFORMATICS SEM.-II
(C.B.C.S.) (2013 COURSE) : WINTER - 2017

SUBJECT: MOLECULAR MODELING & DRUG DESIGNING

Day: **Thursday** Time **02.00 PM TO 05.00 PM**

Date: **02/11/2017** **W-2017-1022** 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) Bond bending
b) Minima
c) Trajectories
d) Give the structure, one letter code and three letter code for isoleucine, tryptophan
e) What is energy minimization?

Q.2 Answer the following: (**ANY TWO**) **[10]**

a) Write the importance of energy minimization in molecular modeling.
b) Explain simplex method for energy minimization.
c) Describe the line search algorithm for energy minimization.

Q.3 Answer the following: (**ANY TWO**) **[10]**

a) Differentiate between simple water model and polarizable water model.
b) Define cross term, hydrogen bond interaction, van der Waals interaction.
c) Explain the architecture and topology of protein in any of the visualization tool.

Q.4 Answer the following: (**ANY TWO**) **[10]**

a) Write a note on Monte Carlo simulation.
b) Discuss the importance of dynamics in drug designing.
c) Describe molecular dynamics at constant temperature.

SECTION-II

Q.5 Answer in brief: **[10]**

a) Lead molecule **d)** External test set
b) CoMFA **e)** Descriptor
c) Pharmacophore

Q.6 Answer the following: (**ANY TWO**) **[10]**

a) Elaborate on ligand based drug designing. Support the answer with a flow chart.
b) Write short note on target small molecule interaction.
c) Compare between traditional and computational drug discovery process.

Q.7 Write short notes on: (**ANY TWO**) **[10]**

a) Differentiate between 2D QSAR and 3D QSAR.
b) Write a short note on topological descriptors.
c) What is the role of small molecular database in lead identification?

Q.8 Answer the following: (**ANY TWO**) **[10]**

a) What is pharmacophore modeling? Draw the flow chart.
b) Differentiate between flexible docking and rigid docking.
c) Write a note on virtual screening based on pharmacophore model.

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