M. SC. BIOINFORMATICS SEM.-III (2013 COURSE)
(CHOICE BASED CREDIT SYSTEMS) : WINTER - 2017

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : Saturday
Date : 28/10/2017

W-2017-1016

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

N.B :

1) **Q. 1** and **Q. 5** are **Compulsory.** Out of the remaining questions, attempt **any 2** from each sections.
2) Figures to the right indicate **Full** marks.
3) Answers to both the sections should be written in **Separate** answer books.

Section - I

Q. 1 Define : **(10)**

a) Hosoya index **b)** Adjacency Matrix
c) E-state **d)** Pharmacophore
e) Molecular Shape

Q. 2
a) Explain SMARTS. **(02)**
b) Describe electro-topological and refracto-topological descriptors. **(04)**
c) Write short note on cheminformatics. **(04)**

OR

c) Define descriptors. Explain shape indices descriptors.

Q. 3
a) What is Vertex partition algorithm? **(02)**
b) Explain followings: **(04)**
1) Tanimoto coefficient **2)** Euclidean distance
c) Explain Multiple Linear Regression (MLR). **(04)**

OR

c) How molecular databases are important in drug discovery research?

Q. 4
a) Define principal moment of inertia. **(02)**
b) Write short note on ADMET. **(04)**
c) How combinatorial library play important role in drug discovery research? **(04)**

OR

c) Discuss Lipinski's rule of five and define lead molecule.

Section - II

Q. 5 Answer in brief: **(10)**

a) Name any four 3D descriptors.
b) Define SMIRKS
c) Write full form of SMILES.
d) What is Tversky Index?
e) Write a brief account on Autodock.

Q. 6
a) What is lead optimization? **(02)**
b) Differentiate between ligand-based and structure-based drug design approaches with examples. **(04)**

OR

b) How can you identify and validate target site?
c) Discuss ab-initio drug design approach. **(04)**

Q. 7
a) Define structure-activity relationship (SAR). **(02)**
b) Differentiate between 2D and 3D QSAR techniques with examples. **(04)**
c) Explain stepwise derivation of 2D QSAR model. **(04)**

OR

c) Why validation of in-silico models are important?

Q. 8
a) Define virtual screening. **(02)**
b) Differentiate between flexible and rigid docking. **(04)**

OR

b) Write short note on Scoring function.
c) Define pharmacophore. Explain steps of derivation of pharmacophore models. **(04)**

* * * * *