M. SC. BIOINFORMATICS SEM.-III (2013 COURSE)
(CHOICE BASED CREDIT SYSTEMS) : SUMMER - 2018

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : **Saturday** Time : **02.00 PM TO 05.00 PM**
Date : **07/04/2018** **S-2018-1131** 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 matrices
c) E-state **d)** Tanimoto coefficient
e) Lipinski's rule

Q. 2
a) What is the full form of SMILES and SDF in molecular file format? **(02)**
b) How can you search molecular patterns using SMARTS? **(04)**
c) Explain the role of cheminformatics in pharmaceutical research. **(04)**

OR

c) Explain descriptors with example of 1D, 2D and 3D descriptors.

Q. 3
a) Explain molecular graph in brief. **(02)**
b) What is the lead molecule? How molecular databases are crucial to find lead molecules? **(04)**

OR

b) Explain Partial Least Square method.
c) Explain – "Role of similarity matrix in molecular similarity search". **(04)**

Q. 4
a) Define molecular refractivity. **(02)**
b) Write short note on electronic descriptors. **(04)**
c) Discuss importance of ADMET profile being a drug molecule. **(04)**

OR

c) Explain – "Role of small molecular databases to identify potential lead molecules".

Section - II

Q. 5 Define : **(10)**

a) Pharmacophore keys **b)** Lead optimization
c) Scoring function **d)** Test set
e) SMIRKS

Q. 6
a) Define receptor. **(02)**
b) Write short note on ligand-based drug design. **(04)**

OR

b) Discuss the role of drug design in pharmaceutical industry.
c) How bioinformatics merged to cheminformatics to develop lead molecules? **(04)**

Q.7
a) Define QSPR. **(02)**
b) Write short note on 3D QSAR. **(04)**

OR

b) Write short note on applicability domain of QSAR.
c) Write short note on quantum chemical descriptors. **(04)**

Q.8
a) Define scoring function in molecular docking. **(02)**
b) Define virtual screening. Explain role of virtual screening for identification of lead molecules. **(04)**
c) Explain receptor-based pharmacophore model. **(04)**

OR

c) Differentiate between ligand-based and receptor-based drug designing.

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