

M. Sc. Bioinformatics Sem.-III (2013 Course) (Choice Based Credit Systems) : SUMMER - 2019

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : Wednesday
Date : 03/04/2019

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

S-2019-1469

N.B.:

- 1) Q.No.1 and Q.No.5 are **COMPULSORY**. Out of the remaining attempt **ANY TWO** questions from each section.
- 2) Answers to both the sections should be written in **SAME** answer books.
- 3) Figures to the right indicate **FULL** marks.

SECTION – I

- Q.1** Define: [10]
- | | | |
|--------------------|------------------|-------------------|
| a) Cheminformatics | c) MLR | e) Hydrophobicity |
| b) SMILES | d) Linker groups | |
- Q.2** Answer the following: [10]
- a) Explain the chemical structure representation file format with suitable examples.
 - b) Describe different molecular descriptors.
- Q.3** Write short notes on: [10]
- a) Lipinski's Rule
 - b) Virtual Screening
- Q.4** Answer the following: [10]
- a) Discuss about different electronic charges.
 - b) Give applications of ADMET in drug discovery process.

SECTION – II

- Q.5** Explain in brief: [10]
- | | |
|---------------------------|--------------------------|
| a) Kappa shape index | d) Target identification |
| b) E-State | e) Molecular Scaffolds |
| c) Molecular refractivity | |
- Q.6** Answer the following: [10]
- a) What do you mean by lead optimization and validation?
 - b) Explain structure based drug design.
- Q.7** Write short notes on: [10]
- a) QSARs and QSPRs
 - b) CoMPA and CoMSIA
- Q.8** Explain in detail receptor based and ligand based pharmacophore modeling. [10]

OR

What is docking? How flexible and rigid docking works? Explain with example.

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