

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

**SUBJECT : CHEMINFORMATICS & DRUG DESIGN**

Day : **Saturday**  
Date : **07/04/2018**

**S-2018-1131**

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 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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