

M.Sc. Semester—IV (CBCS Pattern) Examination

BIO—INFORMATICS

(Chemo Informatics)

Paper—XIV

Time : Three Hours]

[Maximum Marks : 80

Note :—(1) **ALL** questions are compulsory and carry equal marks.

(2) Draw suitable diagram wherever necessary.

1. (a) What do you understand by Chemical indexing ? 5
- (b) Describe scope and applications of Chemoinformatics. 5
- (c) Give an account of primary, secondary and tertiary sources of Chemical Information. 6

OR

- (p) Describe database search method for substructure searching. 5
- (q) Which type of chemoinformatics resources are used for synthetic polymers ? Elaborate with suitable examples. 6
- (r) Describe basics of Chemo-informatics. 5
2. (a) What is SMILES coding ? How these codings are used in Chemoinformatics ? 6
- (b) Explain Combinatorial Chemistry of Chemoinformatics. 5
- (c) Discuss Salient features of Zinc database. 5

OR

- (p) How to represent molecules and their chemical reactions ? 6
- (q) What are the advantages of Combinatorial synthesis ? 5
- (r) Discuss the advantages and limitations of Combinatorial Library design. 5
3. (a) Explain structure-activity relationships with suitable example. 8
- (b) Describe Chemical Safety information. 8

OR

- (p) How are spectroscopic and analytical information used for structure determination of compound ? 8
- (q) Give an account of QSAR-data analysis. 8

4. Write in brief :

- (a) Prediction of Pharmacological Properties. 6
- (b) Visualization and validation of the molecule. 5
- (c) Target identification. 5

OR

- (p) Homology modelling. 5
 - (q) Chemical Libraries. 5
 - (r) Advantages and limitations of Virtual Screening. 6
5. (a) What do you understand by Pharmacophore ? Describe the process of Pharmacophore based drug design. 8
- (b) The knowledge of ADME property of a Chemical is important to develop it as a drug. Justify the statement with suitable examples. 8

OR

- (p) Describe the Software MOLINSPIRATION in brief. Enlist the properties of compounds which can be predicted by this Software. 8
- (q) Discuss the salient features of lead compound. Elaborate the steps involved in structure based designed of lead compound. 8