Roll No. | | | | | | | | | | | | | **Total No. of Pages : 01**

Total No. of Questions : 06

M.Pharma. (Pharmaceutical Chemistry) (Sem.–2)

COMPUTER AIDED DRUG DESIGN

Subject Code : MPC-203

M.Code : 74957

Date of Examination : 08-07-22

Time : 3 Hrs. **Max. Marks: 75**

INSTRUCTIONS TO CANDIDATES :

1. **Attempt any FIVE questions out of SIX questions.**
2. **Each question carriesFIFTEEN marks.**

1. a. Give outline for general methodology to develop QSAR model.
   b. Write a short note on indirect methods of drug designing implemented by CADD technique.
2. a. Discuss *de novo* approach of conventional QSAR.
   b. Explain the principle of CoMFA approach of 3D-QSAR.
   c. What are the advantages of PLS analysis over other statistical methods used in building QSAR model.
3. a. Classify quantum mechanical methods used in CADD techniques. Describe their advantages and disadvantages.
   b. Describe the methods of generation of bioactive conformation of molecules inCADD techniques.
4. a. How is oral bioavailability predicted via CADD?
   b. How to predict functional components in the cavities in de novo drug designing?
   c. Discuss the template identification in homology modelling.
5. a. How doesconformational space of each ligand is determined in pharmacophore mapping?
   b. By citing at least one example of each, describe six important pharmacophorefeatures which are commonly used in pharmacophore mapping.
6. Write short note on :
   a. *De novo* designing of HIV protease inhibitor.
   b. Consensus scoring in docking analysis.

NOTE : Disclosure of Identity by writing Mobile No. or Making of passing request on any page of Answer Sheet will lead to UMC against the Student.