Roll No. | | | | | | | | | | | | |

Total No. of Pages : 01

Total No. of Questions : 06

M.Pharma(Pharmaceutical Chemistry)(2017 & Onwards) (Sem.–2)

COMPUTER AIDED DRUG DESIGN

Subject Code : MPC-203T

M.Code : 74957

Time : 3 Hrs. Max. Marks: 75

INSTRUCTIONS TO CANDIDATES :

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

1. a) Describe three substituent constants along with their mathematical expression that were used by Hansh in its QSAR model.

   b) Describe the experimental and theoretical approaches for determining lipophilicity of substituents used to correlate with biological activity in QSAR.

2. a) Compare Hansh and Free Wilson methods of traditional QSAR.

   b) What is CoMSIA? Describe its contour map analysis.

3. a) What is the principle of molecular mechanics?

   b) Give an outline for docking analysis.

   c) Discuss CADD based designing of HMG-CoA reductase.

4. a) Discuss the importance of in *silico* ADMET prediction of a NCE.

   b) How to determine active site of an enzyme in its 3D structure?

   c) What is fragment based drug designing? Give its advantages over other drug designing approaches.

5. What is virtual screening? Give detailed account on structure and ligand based protocols of virtual screening.

6. Write short notes on :

   a) Homology modeling.

   b) Statistical parameters used in QSAR 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.