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

Total No. of Pages : 01

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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) Briefly explain Lipinsky's Rule of five. 7

   b) What do you mean by term preADME. Discuss the significance of preADME prediction in drug discovery process. 8

2. a) Write short note on Fragment based Denovo drug designing. 5

   b) Write a short note on global energy minimization. 5

   c) Briefly explain Craig plot. 5

3. a) Explain in detail Homology modelling and the method adopted for the generation of the 3D structure of a protein. 7

   b) Give a detailed account of Pharmacophore mapping. 8

4. a) Explain Topliss Decision Tree for aromatic substituents in deciding on newer analogues with improved biological activity. 5

   b) Discuss Structure based in silico virtual careening. 5

   c) Discuss different Statistical approached used in QSAR. 5

5. Enumerate the different physicochemical properties of a drug molecule that influence the biological activity and describe in detail about hydrogen bonding and ionization influences on biological activity. 15

6. Define and classify QSAR with their advantages. Elaborate on the multi-parametric approach to QSAR as enunciated by Hansch. 15

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.