Roll No. | | | | | | | | | | | | | Total No. of Pages : 1

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

COMPUTER AIDED DRUG DESIGN

Subject Code : MPC-203T

Paper ID : [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.

Q1 a. Explain fundamental principle of QSAR. (7.5)

b. Give outline for drug designing approaches which can be employed using CADD technique. (7.5)

Q2 a. Discuss the extra thermodynamic approach of conventional QSAR. (5)

b. Describe generation of 3D field in CoMFA analysis. (5)

c. Describe five thumb rules for deriving of Hansch QSAR equations. (5)

Q3 a. How will you parameterize potential energy in CADD techniques? (5)

b. Bioactive conformation is not always global energy minima; sometime it is local energy minima. Explain. (5)

c. Flexible docking is superior to rigid docking. Justify with example. (5)

Q4 a. What is Lipinski rule of five? Describe its importance in CADD. (5)

b. Describe the validation of 3D structure of protein generated by homology modelling. (5)

c. Discuss cavity size prediction in *de novo* designing. (5)

Q5 a. What is pharmacophore mapping? (5)

b. Comment on conformation search in pharmacophore mapping. (5)

c. Name standard pharmacophoric techniques alongwith one structural example used in pharmacophore modelling. (5)

Q6 Write short note on :

a. Electronic parameters used in QSAR. (7.5)

b. Structure based designing of DHFR inhibitors. (7.5)