Ref. No. : Ex/MPC2031/2025

M. PHARMACY FIRST YEAR SECOND SEMESTER - 2025

COMPUTER AIDED DRUG DESIGN

Time : 3 h **Full Marks : 75**

Answer any five questions taking at least ONE from each group

Group A

1. Write all steps for deriving a multiple linear regression equation starting from a standard QSAR table. [15

2. Discuss on different validation metrics (both regression-based and classification-based). [15

3. Write notes on: [3 x 5
   (i) Solvent accessible surface area
   (ii) Topological descriptors
   (iii) Partial least squares regression
   (iv) Symmetry equations
   (v) LFER model

Group-B

4. Write notes on different qualitative validation parameters used to assess the quality of a Pharmacophore model? [15

5. Define Pharmacophore and virtual screening? What are the different steps/layers used to screen a molecule from a large database? Discuss elaborately. [5+10

6. Write short notes on (***any three***)
   i) Ionic bonding interactions used to define docking score [5
   ii) Hydrogen bonding interactions used to define docking score [5
   iii) Reverse docking [5
   iv) Rigid docking and flexible docking [5

Group-C

7. Discuss the different steps of homology modeling. What are the opportunities and limitations of homology modelling? [9+6

8. Write the advantages of computational fragment-based drug design. Discuss common strategies of the fragment-based approach. Write the steps of the computational fragment-based drug design approach. [3+7+5

9. Write short notes on [3x5
   (a) Rule of three
   (b) Importance of protein structure in drug discovery
   (c) Significance of ADME prediction
   (d) Prediction of Cytochrome P450 activity
   (e) Ramachandran plot