Ex/MPC2031/2024

M. PHARMACY FIRST YEAR SECOND SEMESTER - 2024

COMPUTER AIDED DRUG DESIGN

Time: 3 hrs **Full Marks: 75**

Answer any five questions taking at least one from each group

Group A

1. Staring from a hypothetical QSAR Table, show the construction of an MLR model. How do you compute standard error of an individual regression coefficient? [12 + 3

2. Write notes on:
   a. Determination coefficient and regression coefficient
   b. Mathews correlation coefficient and Pearson's correlation coefficient
   c. Regression through origin and regression with intercept
   d. Explained and unexplained variances [4+4+4+3

3. Discuss the parabolic dependence of the biological activity on lipophilicity. What is bilinear dependence of the biological activity on lipophilicity? Are lipophilicity and molar volume correlated? Is molar refractivity a purely steric parameter? [4+3+4+4

Group B

1. What are the different validation parameters used to assess the quality of a pharmacophore model? [15]
2. Define Pharmacophore, docking, and virtual screening. What are the different types of binding interactions used to define docking score? [6+9]
3. Write a note on reverse docking. What are the different layers used to screen a molecule from a large database? Discuss elaborately. [5+10]

Group C

4. Why is computational modeling of protein structure important? Write the procedures and advantages of homology modeling. [3+12]
5. Discuss the limitations of experimental fragment-based drug design. Write the strategies and overall procedure of computational fragment-based drug design. [3+12]