M.Pharm Even Semester Examination, May, 2025

PHARMACEUTICAL SCIENCES

(2nd Semester)

Course No: MPC-203T

(Computer Aided Drug Design)

FM: 75

Time: 3 Hours

The figures in the right margin indicate full marks for the question

I. Objective type (Answer the following in brief) 2x10=20

1. Define Taft's steric factor.
2. Explain the meaning of π and σ in respect of drug design.
3. What are the polarizability parameters?
4. Identify three fundamental assumptions that form the basis of molecular mechanics methods.
5. Explain charge transfer interactions.
6. Mention the full form of AMBER and OPLS?
7. List the pros and cons of the Semi-Empirical Method.
8. Compare global energy minima and local energy minima.
9. Define virtual screening and list the different virtual screening techniques.

10. What is a similarity search? List the various similarity-based methods used in in-silico drug design.

II. Long answers (Answer two out of three questions) 10x2=20

1. What do you mean by critical reaction site and critical reaction rate? Deduce the mathematical equation of Hansch Analysis. 2+8=10

2. What is homology modeling? Explain the different stages involved in homology modeling. 1+9=10

3. Discuss(a) *Ab initio* methods(b) Density functional theory in computational chemistry. 6+4=10

III. Short answers (Answer seven out of nine questions) 5x7=35

1. Electron withdrawing group and electron donating group shows positive and negative value of substituent constant respectively. Explain it.

2. What are the basic assumptions of Free Wilson Analysis?

3. Discuss in brief about partition coefficient and lipophilic substituent constant.

4. n-octanol is the most suitable solvent for determining partition coefficient. Explain it.

5. Explain the strategies used for constructing molecules in *De Novo* Drug Design.

6. Explain the concept of molecular docking. What information can be obtained through molecular docking studies? Outline the different types of molecular docking. 1+2+2

7. Discuss the statistical methods employed in ADMET prediction. Provide examples of any three *in-silico* tools for ADMET prediction, including their developers, key features, and applications. 2+3

8. Explain the force field approach in molecular mechanics.

9. Distinguish between pharmacophore mapping and pharmacophore modeling.What are the different types of pharmacophoric features considered in pharmacophore mapping? 3+2

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