PG (CBCS) EVEN SEMESTER EXAMINATION, 2024

PHARMACEUTICAL SCIENCES
(M.Pharm. 2nd Semester)

Course No: MPC 203T
(Computer Aided Drug Design)

Full Marks : 75

Time : 3 hours

The figures in the margin indicate full marks for the questions

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

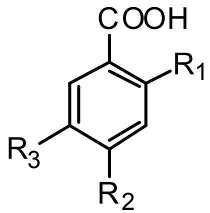
1. What do you mean by critical reaction site and critical reaction rate?
2. What are the chromatographic factors considered as physicochemical parameters?
3. What is pharmacophore mapping and De novo drug design?
4. Mention two conformational search strategies.
5. Differentiate between global energy minima and local energy minima.
6. List three assumptions underlying molecular mechanics methods.
7. Define Potential Energy Surface and Force Field.
8. Mention the full form of COMPASS and MNDS?
9. Mention the benefits and limitations of Semi-Empirical Method.

(Turn Over)

10. What is the basic principle behind Quantum Mechanics?

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

1. Write the basic assumptions of Free Wilson Analysis. Calculate the number of possible equations necessary to find out the contribution of substituents as well as parent moiety of substituted benzoic acid derivatives having anti cholinergic activity. The details are as follows:



Comp Number	R_1	R_2	R_3	IC_{50} (M)
1	Me	Et	H	402.5
2	Et	H	Et	308.5
3	Pr	Me	Et	290.0
4	Bu	H	Me	250.5
5	Amyl	Et	Et	200.0
6	Amyl	H	Me	180.5
7	Amyl	H	Et	165.5
8	Hexyl	Me	Me	151.0
9	Hexyl	Me	Et	135.5
10	Desyl	H	H	125.5
11	Desyl	H	Et	110.5

2. Discuss the various steps of homology modeling.

3. Write a note on Born-Oppenheimer approximation and Density function theory. 3+7

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

1. Why is n-octanol used for estimation of partition coefficient?

2. Write the utility of sigma and rho in Hammett equation.

3. Write notes on partition coefficient and lipophilic substituent constant.

4. Discuss in brief about polarizability parameter.

5. Explain the role of H-bond donor and H-bond acceptor in the analysis of ADMET properties.

6. What is molecular docking. Describe its types.

7. Mention the limitations of conformational analysis.

8. Describe Hartree-Fock approximation along with its advantages and disadvantages. 2+2+1

9. Mention a typical docking workflow and explain the key stages in molecular docking. 1+4

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