Name: **Enrolment No:**	

UPES

End Semester Examination, May 2024

Course: Cheminformatics & Medicinal Chemistry **Semester : IV**
Program: B.Tech. Biotechnology **Duration : 3 Hours**
Course Code: HSBT2008 **Max. Marks: 100**

Instructions: The question paper comprises of FOUR sections; all sections are compulsory.
Read the instructions given before each section carefully.

S. No.	Section A Short answer questions/ MCQ/T&F (20Qx1.5M= 30 Marks)	Marks	COs
Q 1	Define partition coefficient.	**1.5**	**CO1**
Q 2	List any **THREE** examples of traditional folk medicines from whom modern drugs have been discovered.	**1.5**	**CO1**
Q 3	Define lead compound in context of drug discovery.	**1.5**	**CO1**
Q 4	List any **THREE** examples of synthetic organic chemicals first used as drugs.	**1.5**	**CO1**
Q 5	State the names of any **THREE** classes of macromolecular drug targets.	**1.5**	**CO1**
Q 6	List **THREE** alternative approaches to deliver an ionised drug.	**1.5**	**CO1**
Q 7	State any **THREE** examples of variation of alkyl or acyl substituents to alter polarity of a drug molecule.	**1.5**	**CO1**
Q 8	State the rationale of using steric shields in designing new drug candidates.	**1.5**	**CO1**
Q 9	Define bioisosteres.	**1.5**	**CO1**
Q 10	State the concept of metabolic blocker functional groups in drug design.	**1.5**	**CO1**
Q 11	Define drug biotransformation reactions.	**1.5**	**CO1**
Q 12	State the importance of drug biotransformation reactions.	**1.5**	**CO1**
Q 13	List **THREE** most important sites of drug metabolism.	**1.5**	**CO1**
Q 14	Define microsomal enzymes and list any **TWO** reactions catalysed by them.	**1.5**	**CO1**
Q 15	List any **THREE** major human forms of P450 enzymes.	**1.5**	**CO1**
Q 16	Define QSAR in context of rational drug design.	**1.5**	**CO2**
Q 17	Define Taft's steric parameter.	**1.5**	**CO2**
Q 18	List the scenarios in which ligand-based drug design will be the preferred method for drug design.	**1.5**	**CO2**
Q 19	Define a pharmacophore.	**1.5**	**CO2**

Q 20	List any **THREE** biological activities of flavones.	**1.5**	**CO3**
Section B (4Qx5M=20 Marks)			
Q 1	List **FIVE** classes of drug biotransformation reactions with **ONE** example for EACH class.	**5**	**CO1**
Q 2	List **FIVE** disadvantages of Hansch analysis.	**5**	**CO2**
Q 3	Illustrate the steps involved in pharmacophore modeling using a flow chart.	**5**	**CO2**
Q 4	Differentiate molecular mechanics and quantum mechanics based molecular modeling methods.	**5**	**CO2**
Section C (2Qx15M=30 Marks)			
Q 1	The QSAR equation relating the insecticidal activity of a series of diethyl phenylphosphonates versus σ is shown below. Interpret the QSAR equation in chemical, pharmacological and statistical terms. Log(1/C) = 2.282 σ – 0.348 (r2 = 0.952, r = 0.976, s = 0.286)	**15**	**CO2**
Q 2	Discuss in detail the medicinal chemistry of sulfonylureas.	**15**	**CO4**
Section D (2Qx10M=20 Marks)			
Q 1	Discuss any **FIVE** steps involved in 3D QSAR.	**10**	**CO2**
Q 2	Discuss any **FIVE** biological applications of alkaloids.	**10**	**CO3**