Name: Enrolment No:	

UPES

End Semester Examination, May 2025

Course: Computer Aided Drug Design **Semester: VIII**

Program: B. Pharm **Duration: 03 Hours**

Course Code: BP807ET **Max. Marks: 75**

Instructions: Read the question paper carefully. Attempt the questions as mentioned.

SECTION A

(20Qx1M=20 Marks)

S. No.	Multiple Choice Questions/objective/one line	Marks	COs
Q 1	Define the term log D.	**1**	**CO1**
Q 2	Differentiate between SP and XP method of docking in schrodinger.	**1**	**CO1**
Q 3	Write the full form for SAR.	**1**	**CO1**
Q 4	A lead is a _____compound.	**1**	**CO1**
Q 5	Ligand efficiency is defined as_____.	**1**	**CO1**
Q 6	Define the RO5.	**1**	**CO1**
Q 7	Give four examples of software used for pharmacophore mapping.	**1**	**CO1**
Q 8	The bark of _____tree was used to treat malaria.	**1**	**CO1**
Q 9	Give examples of hydrogen bond acceptors.	**1**	**CO1**
Q 10	Write the full form for HTVS.	**1**	**CO1**
Q 11	_____database consists of publically available DNA sequence.	**1**	**CO2**
Q 12	SIDER contains information on _____and their_____.	**1**	**CO2**
Q 13	PACT-F stands for_____.	**1**	**CO2**
Q 14	Write the full form for HBD.	**1**	**CO2**
Q 15	DDBJ stands for_____.	**1**	**CO2**
Q 16	The orange book provides_____.	**1**	**CO2**
Q 17	Write the full form for HBA.	**1**	**CO2**
Q 18	Define Free wilson approach.	**1**	**CO2**
Q 19	Verloop stearic parameter can be calculated using____software.	**1**	**CO2**
Q 20	Write the full form of CoMFA.	**1**	**CO2**

SECTION B (20 Marks)

(2Qx10M=20 Marks)

Attempt 2 Question out of 3

Q 1	Explain drug discovery without a lead. Write the case study of two drugs discovered through this approach.	**10**	**CO5**
Q 2	Discuss different types of docking. Write applications of molecular docking.	**10**	**CO5**

Q 3	Define cheminformatics. Explain with suitable examples the use of cheminformatics in drug discovery.	**2+8**	**CO4**
SECTION-C (35 Marks) **(7Qx5M=35 Marks)** **Attempt 7 Question out of 9**			
Q 1	Differentiate between random and non-random screening approach in drug discovery.	**5**	**CO4**
Q 2	Classify different types of databases in Bioinformatics. Give a minimum of two examples of each category.	**2.5+2.5**	**CO4**
Q 3	Discuss the concept of pharmacophore. Elaborate pharmacophore-based screening approach.	**2.5+2.5**	**CO4**
Q 4	Differentiate between SAR and QSAR.	**5**	**CO4**
Q 5	Write a case study involving the use of bioisosterism.	**5**	**CO3**
Q 6	Differentaite between COMFA and COMSIA.	**5**	**CO3**
Q 7	Write in detail about induced fit docking.	**5**	**CO3**
Q 8	Discuss the use of HTVS in drug discovery.	**5**	**CO3**
Q 9	Draw a flowchart showing steps used in lead identification using pharmacophore-based 3D database searching.	**5**	**CO3**