Name: Enrolment No:	

UPES

End Semester Examination, May 2023

Set 1

Course: Computer Aided Drug Design | **Course Code: BP807ET**

Semester: 8th | **Duration: 3 Hours**

Program: B. Pharmacy | **Max. Marks: 75**

Instructions: Read all the questions carefully. Follow the instructions mentioned against each section.

SECTION A

(2Qx10M=20 Marks)

(Answer all the questions)

S. No.		Marks	COs
Q1.	Sketch the chemical structure of Cimetidine.	2	CO1
Q2.	In computational chemistry, HTS stands for: a. High throughput system b. High throughput scintillation c. High throughput screening d. None of the above	2	CO1
Q3.	Which bioisosteres have been successfully employed in the development of H2 receptor antagonists. a. Halogen bioisosteres b. Thiourea bioisosteres c. Amide bioisosteres d. Classical bioisosteres	2	CO1
Q4.	_____ was the lead used for the development of anti-inflammatory drug Indomethacin.	2	CO1
Q5.	ADME stands for_____.	2	CO1
Q6.	Sketch the structure of Serotonin.	2	CO1
Q7.	The measure value of the electron withdrawing or donating ability of a substituent is known as: a. logP b. Taft's constant c. Free Wilson analysis d. Hammett's substitution constant	2	CO1
Q8.	Draw the chemical structure of Aspirin.	2	CO1
Q9.	The molecular mechanics deals with: a. Number of atoms b. Number of orbitals c. Number of proton d. Number of molecule	2	CO1

Q10.	**Multiple protein structures are utilized as an ensemble for docking with ligand in one of the following techniques:** **a. Induced fit docking** **b. Lock and key docking** **c. Ensemble docking** **d. Rigid docking**	**2**	**CO1**
SECTION B **(2Qx10M=20 Marks)** **Long Answers (Answer 2 out of 3)**			
Q11.	**Using Newman's projection of n-butane, determine the global conformation minima.**	**10**	**CO4**
Q12.	**Describe the various stages of drug discovery. Critically analyze the trend followed in the discovery of Cimetidine.**	**10**	**CO5**
Q13.	**Explain the concept of 3D-QSAR (CoMFA) in detail.**	**10**	**CO2**
SECTION C **(7Qx5M=35 Marks)** **Short Answers (Answer 7 out of 9)**			
Q14.	**Write a note on applications of molecular docking.**	**5**	**CO3**
Q15.	**Give brief on Lead compound. Give example.**	**5**	**CO3**
Q16.	**Describe a case study for analog based drug design.**	**5**	**CO3**
Q17.	**Describe the physicochemical parameters based on "Steric effects", used in QSAR.**	**5**	**CO3**
Q18.	**What is bioisosterism? Classify bioisosteres.**	**5**	**CO3**
Q19.	**What is h-bond interaction? Give its importance in drug design.**	**5**	**CO3**
Q20.	**Write a note on quantum mechanics.**	**5**	**CO3**
Q21.	**Discuss about drug-likeliness screening.**	**5**	**CO3**
Q22.	**What is the main focus of medicinal chemistry?**	**5**	**CO3**