Name:

Enrolment No:

UPES

End Semester Examination, May 2024

Course: Computer Aided Drug Design **Semester: 8th**

Program: B. Pharm. **Duration: 3 Hours**

Course Code: BP807ET **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.	**1**	**CO1**
Q2.	Ab initio program is? a. MNDO b. GAUSSIAN c. AMI d. PRDDO	**1**	**CO5**
Q3.	In computational chemistry, HTS stands for: a. High throughput system b. High throughput scintillation c. High throughput screening d. None of the above	**1**	**CO3**
Q4.	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	**1**	**CO1**
Q5.	What is partition coefficient?	**1**	**CO2**
Q6.	_____ was the lead used for the development of anti-inflammatory drug Indomethacin.	**1**	**CO1**
Q7.	ADME stands for_____.	**1**	**CO4**
Q8.	Semi-empirical method computes for: a. Electron b. Orbitals c. Valence electrons d. Proton	**1**	**CO5**
Q9.	Sketch the structure of Serotonin.	**1**	**CO2**
Q10.	Write the formula used to calculate number of conformations.	**1**	**CO5**
Q11.	The measure value of the electron withdrawing or donating ability of a substituent is known as:	**1**	**CO2**

	a. logP b. Taft's constant c. Free Wilson analysis d. Hammett's substitution constant		
Q12.	Partial least square is used in: a. SAR b. 2D-QSAR c. 3D-QSAR d. None	**1**	**CO2**
Q13.	Draw the chemical structure of Aspirin.	**1**	**CO5**
Q14.	Sildenafil is used for the treatment of: a. Colon cancer b. Dengue c. Malaria d. Erectile Dysfunction	**1**	**CO1**
Q15.	The molecular mechanics deals with: a. Number of atoms b. Number of orbitals c. Number of proton d. Number of molecule	**1**	**CO5**
Q16.	Name of the program in which fragments from bioactive conformation are joint with spacer to generate a new structure to fit the model. a. SCROUT b. UNITY c. NEWLEAD d. QSAR	**1**	**CO2**
Q17.	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	**1**	**CO3**
Q18.	From computational point of view which system is used for drug safety development: a. DEREK b. Topkat c. MultiCASE d. All of the above	**1**	**CO3**
Q19.	NIH's molecular libraries and imaging initiatives are the experimental projects of: a. Cheminformatics b. Bioinformatics c. Chemical database d. Biochemical database	**1**	**CO4**

Q20.	What do you understand by Single Nucleotide Polymorphisms (SNPs)?	**1**	**CO4**
SECTION B **(2Qx10M=20 Marks)** **Long Answers (Answer 2 out of 3)**			
Q1.	Using Newman's projection of n-butane, determine the global conformation minima.	**10**	**CO5**
Q2.	Describe the various stages of drug discovery. Critically analyze the trend followed in the discovery of Cimetidine.	**7** **3**	**CO1**
Q3.	Explain the concept of 3D-QSAR (CoMFA) in detail.	**10**	**CO2**
SECTION C **(7Qx5M=35 Marks)** **Short Answers (Answer 7 out of 9)**			
Q1.	Write a note on applications of molecular docking.	**5**	**CO3**
Q2.	Give brief on Lead compound. Give example.	**3** **2**	**CO1**
Q3.	Describe a case study for analog based drug design.	**5**	**CO1**
Q4.	Describe the physicochemical parameters based on “Steric effects”, used in QSAR.	**5**	**CO2**
Q5.	Explain bioisosterism. Classify bioisosteres.	**2** **3**	**CO1**
Q6.	Explain h-bond interaction. Give its importance in drug design.	**2** **3**	**CO5**
Q7.	Write a note on quantum mechanics.	**5**	**CO5**
Q8.	Discuss about drug-likeliness screening.	**5**	**CO4**
Q9.	Discuss the objectives of medicinal chemistry.	**5**	**CO4**