Name: Enrolment No:	

UPES

End Semester Examination, May 2023

Set 2

Course: Cheminformatics & Medicinal Chemistry **Course Code: HSBT2008**

Semester: 4th **Duration: 3 Hours**

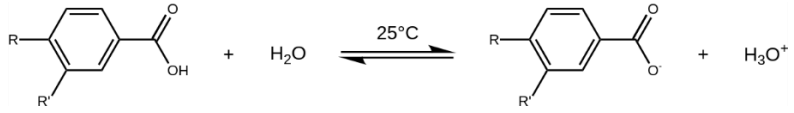
Program: B. Tech. Biotechnology **Max. Marks: 100**

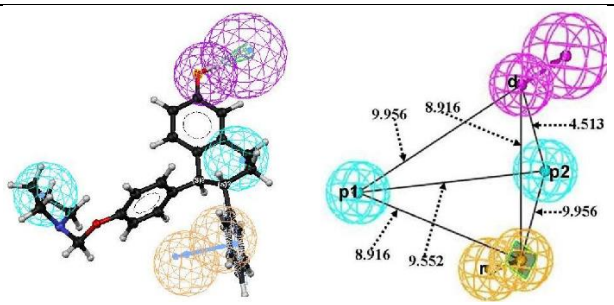
Instructions: Read all the questions carefully. All questions are compulsory.

SECTION A

(20Qx1.5M=30Marks)

S. No.		Marks	CO
Q1.	What is h-bond interaction? Give representation.	1.5	CO3
Q2.	What is Hammett's constant. Give equation.	1.5	CO2
Q3.	Sketch the chemical structure of Burimamide.	1.5	CO1
Q4.	What do you understand by the term "Pharmacodynamics"?	1.5	CO1
Q5.	Support the notion of "drug privileged scaffold", by giving the structure of drug molecule based on Coumarin?	1.5	CO5
Q6.	In computational chemistry, HTS stands for: a. High throughput system b. High throughput scintillation c. High throughput screening d. None of the above	1.5	CO1
Q7.	Interaction between a charged ion and a neutral molecule with a dipole moment is called: a. Non bonded interaction b. Charged interaction c. Dipole-dipole interaction d. Ion-dipole interaction	1.5	CO1
Q8.	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	1.5	CO1
Q9.	What are 'bioisosteres'?	1.5	CO1
Q10.	Draw the chemical structure of Paracetamol.	1.5	CO1
Q11.	Anesthetics are the compounds which: a. Induces sleep b. Treats Hypertension c. Reduces Pain d. Prevents clotting	1.5	CO1
Q12.	The process of biotransformation of foreign chemicals in the body so that they may be readily removed is referred to as _____.	1.5	CO3

Q13.	**Monoterpenes are a class of terpenes that consist of two isoprene units. (True/False)**	**1.5**	**CO3**
Q14.	**Sketch the chemical structure of Cimetidine.**	**1.5**	**CO1**
Q15.	**What is the term 'Bioinformatics'?**	**1.5**	**CO1**
Q16.	**_____ was the lead used for the development of anti-inflammatory drug Indomethacin.**	**1.5**	**CO2**
Q17.	**The molecular mechanics deals with:** **a. Number of atoms** **b. Number of orbitals** **c. Number of proton** **d. Number of molecule**	**1.5**	**CO1**
Q18.	**QSAR stands for_____.**	**1.5**	**CO2**
Q19.	**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**	**1.5**	**CO1**
Q20.	**What do you understand by the abbreviation "ADME-T", in medicinal chemistry?**	**1.5**	**CO2**
	SECTION B **(4Qx5M= 20 Marks)**		
Q21.	**Sketch the different conformations of cyclohexane?**	**5**	**CO1**
Q22.	**Critically analyze the trend followed in the discovery of Cimetidine.**	**5**	**CO5**
Q23.	**Write about the areas where molecular docking can be useful?**	**5**	**CO5**
Q24.	**Give a note on non-covalent interactions (various types, with structures and energy values).**	**5**	**CO2**
	SECTION-C **(2Qx15M=30 Marks)**		
Q25.	**In the year 1937, a researcher established a linear free-energy relationship between reaction rates and equilibrium constants for benzoic acid derivatives.**  **a) Name the substituent constant established following this research. Give brief (5 marks)** **b) Describe the physicochemical parameters used in QSAR. (10 marks)**	**15**	**CO3**
Q26.	**The following image represents one of the commonly used drug design techniques in computational medicinal chemistry.**	**15**	**CO4**

	 **a. Name the technique? Write in detail about it. (5 marks)** **b. Write in detail about h-bond acceptor, h-bond donor, hydrophobic and ring features used. (10 marks)**		
SECTION-D (2Qx10M=20 Marks)			
Q27.	**Explain the 'stepwise bond rotation' method for the determination of global energy minima.**	**10**	**CO5**
Q28.	**How phase II reactions of drug metabolism facilitate the elimination of xenobiotics (with chemical reactions)?**	**10**	**CO4**