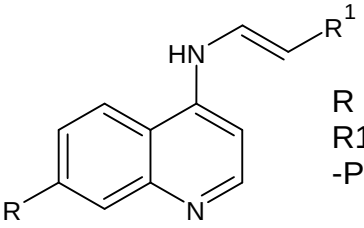
Name: **Enrolment No:**			
	UPES **End Semester Examination** **May 2025** **Course: Rational Drug Discovery** **Semester: VIII** **Program: B. Tech Biotechnology** **Time: 03 hrs.** **Course Code: HSCR4001** **Max. Marks: 100**		
	SECTION A **1. Each Question will carry 1.5 Marks.** **2. Instruction: Complete the statement / Select the correct answer(s)**		
S. No.	**Give answers of all following MCQs**	**(20 X 1.5) = 30**	**CO**
Q 1	**Select the correct method from following approaches which is considered under the 'Ligand based drug design'?** a) Molecular docking b) Pharmacophore modeling c) QSAR Modeling d) b and c both	**1.5**	**CO1**
Q2	**Find the following sets contains all aromatic residues?** a) G, D, N, E b) I, V, L, M c) R, K, H d) F, Y, W	**1.5**	**CO1**
Q3	**Find the type of database EBI is?** a) Protein db b) Pathway db c) Nucleotide db d) Specialized db	**1.5**	**CO2**
Q4	**'Procheck' tool is used for** a) Alignment b) Protein Validation c) Simulation d) None of these	**1.5**	**CO1**
Q5	**Two sequences are said to be homologous if:** a) they have diverged from a common ancestor. b) their alignments share 30% identity or more. c) they belong to the same family. d) they have converged to share similar functional properties.	1.5	CO3
Q6	**Find the correct process from the following methods which is commonly used for virtual screening?** a) ADMET analyses b) QSAR modeling c) Pharmacophore modeling d) All of the above	**1.5**	**CO1**
Q7	**CoMFA method is used for** a) 4D-QSAR b) 3D-QSAR c) 5D-QSAR d) 6D-QSAR	**1.5**	**CO4**
Q8	**With homology modelling, if there are major errors in the template, the model will:** a) be very good b) be just as good as the template c) be unable to be built using current modelling programs d) be completely wrong	**1.5**	**CO2**

Q9	**Lipinski's rule of five is used for _____.** a) Docking b) Similarity search c) Drug likeness d) Dynamics simulation	**1.5**	**CO3**
Q10	**Select the correct model used for gene prediction algorithm?** a) UPGMA b) Hidden Markov Model c) Maximum parsimony d) None of these	**1.5**	**CO2**
Q11	**Find the kind of interactions that are typically involved in binding a drug to the binding site of a protein.** a) van der Waals interactions b) ionic bonds c) hydrogen bonds d) a combination of all the above	**1.5**	**CO2**
Q12	**Identify the correct descriptions that most accurately describe binding sites and binding regions?** a) A binding site is part of a binding region b) A binding region is part of a binding site c) A binding region is the same as a binding site d) a binding region is on a drug whereas a binding site is on a macromolecular target	**1.5**	**CO2**
Q13	**Define the meaning of ADME in pharmacokinetics?** a) Affinity, dosage, marketing, efficacy b) Absorption, distribution, metabolism, excretion c) Agonism, dependence, mobility, efficiency d) Antagonism, deficiency, mean, efflux	**1.5**	**CO4**
Q14	**Select one of the following statements best describes an induced fit?** a) the process by which a binding site alters shape such that it is ready to accept a drug b) the process by which a drug adopts the correct binding conformation before entering a binding site c) the process by which binding of a drug to a binding site alters the shape of the binding site d) The process by which a binding site alters the shape of the drug into the binding conformation before binding	**1.5**	**CO1**
Q15	**Identify the correct process to be established before the search for a lead compound takes place?** a) the pharmacophore b) Structure-activity relationships c) a bioassay d) patents	**1.5**	**CO2**
Q16	**Select the term used for the automated in vitro testing of large numbers of compounds using genetically modified cells?** a) robotic testing b) high throughput screening c) multi-screening d) nanotechnology	**1.5**	**CO4**
Q17	**There are several sources and methods of discovering new compounds. Which of the following is most likely to lead to the discovery of a complex structure quite unlike any other previously discovered?** a) combinatorial chemistry b) database mining c) screening plant extracts d) me too drugs	**1.5**	**CO2**

Q18	**Select the term used for drugs that are similar in structure to a known drug, and which are used for the same purpose?** a) 'copycat' drugs b) 'me-too' drugs c) 'derivative' drugs d) 'analogue' drugs	**1.5**	**CO3**
Q19	**Find out the term used for small molecules that bind to different regions of a binding site?** a) epimers b) isomers c) isotopes d) epitopes	**1.5**	**CO2**
Q20	**The software which is not used for molecular docking?** a) Auto Dock b) Gold c) Glide d) Chem-draw	**1.5**	**CO3**
	SECTION B **Each question will carry 5 marks.** **Write short / brief notes (any four)**		
Q1	a) Define fragment-based drug design. b) Describe the advantages and disadvantages of fragment-based drug design.	**2+3**	**CO2**
Q2	Briefly discuss the antisense technology for target validation.	**5**	**CO4**
Q3	a) Illustrate the differences between 2D and 3D QSAR for lead optimization. b) Write down the process of 3D QSAR study.	**1+4**	**CO2**
Q4	a) Define pharmacophore mapping. b) Discuss the significance and its limitations for drug design.	**1+4**	**CO4**
Q5	a) Clarify the importance of molecular docking for drug discovery. b) Draw a flow chart to explain the method of docking study.	**1+4**	**CO1**
	SECTION C **Each question contains 15 marks.** **Write short / brief notes**		
Q1	a) Explain homology modeling. b) Draw a flow-chart to explain the process of homology modeling. c) Discuss the need of loop refinement in homology modeling? d) Illustrate the advantages and disadvantages of homology modeling.	**1+6+3+5**	**CO1**
Q2	a) What do you mean by rational drug design? b) Ranitidine (Zantac) is a medicine that reduces indigestion, heartburn, and acid reflux. Describe the steps which were utilized to discover this drug via rational drug design approach? c) Briefly discuss the types of rational drug design methods used for developing new drug like molecules.	**3+7+5**	**CO4**
	SECTION D		

	Each question contains 10 marks **Write short / brief notes**		
Q1	a) Explain the Hansch rule? b) Discuss the difference between Hansch analysis and Free Wilson analysis. c) Discuss the Hansch analysis which can be utilized to optimize the quinoline derivative which is mentioned below. Find out the best lead compound based on craig plot. (K1 = 0.152, K2 = 1.681, K3 = 4.053 and K4 = 7.212)  R = Cl, Br R1 = -CH3, -C2H5, -Phenyl, -COOH, -NO2	**1+2+7**	**CO2**
Q2	a) Define DNA microarray. b) Explain the function of zinc finger proteins (ZFPs). c) Explain the reason for using shotgun sequencing method than sanger sequencing process during target identification. d) Illustrate 2D electrophoresis.	**2+2.5+3.5+2**	**CO3**