	UNIVERSITY OF PETROLEUM AND ENERGY STUDIES **End Semester Examination, December 2021** **Course: Drug Discovery and Development** **Semester: I** **Program: MSc (N&D)** **Duration: 03 hr** **Course Code: HSCR7008** **Max. Marks: 100**		
	SECTION A **(Type the answers in test box)**	**(20Q x1.5M= 30 Marks)**	**CO**
Q1	**Which of the following approach is considered under the 'Ligand based drug designing'?** a) Molecular docking b) Pharmacophore modeling c) QSAR Modeling d) b and c both	**1.5**	CO1
Q2	**Which of 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	**Which type of data base EBI is?** a) Protein db b) Pathway db c) Nucleotide db d) Specialized db	1.5	CO2
Q4	**'Procheck' tool is use 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 fold family. d) they have converged to share similar functional properties.	1.5	CO3
Q6	**Which of the following method 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	**Which of these is gene prediction algorithm?** a) UPGMA b) Hidden Markov Model c) Maximum parsimony d) None of these	1.5	CO2
Q11	**Identify the kind of interactions that are typically involved in binding a drug to the binding site of a protein.**	1.5	CO2

	a) van der Waals interactions b) ionic bonds c) hydrogen bonds d) a combination of all of the above		
Q12	**Which of the following descriptions most accurately describes 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	**What is meant by 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	**Which 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	**Which of the following needs 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	**What is 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	**What is 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	**What is 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) Chemdraw	1.5	CO3

	SECTION B **(Scan and upload)**	**(4Qx5M =20 Marks)**	**CO**
	Short Answer Type Question (5 marks each)		
Q1	a) What is QSAR? b) Explain the importance of QSAR for lead optimization.	1+4	CO1
Q2	a) What are the needs of drug discovery? b) Illustrate the process used for drug discovery?	2+3	CO3
Q3	a) What is molecular docking? b) How this technique can be utilized to predict binding affinity of new biologically active molecules?	2+3	CO2
Q4	Write a short note on target based virtual high throughput screening.	5	CO4
	SECTION C **(Scan and upload)**	**(2Qx15 M=30 Marks)**	**CO**
	Two case studies 15 marks each subsection		
Q1	a) What is role of fragment-based drug discovery? b) Describe the method of fragment-based drug discovery by giving an example. c)Illustrate the advantage and disadvantages of pharmacophore mapping.	3+6+6	CO1
Q2	a) What do you mean by rational drug design? b) Ranitidine (Zantac) is a medicine that reduce 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 **(Scan and upload)**	**(2Qx10 M=20 Marks)**	**CO**
	Long Answer type Question		
Q1	a) Discuss the importance of homology modelling? b) Briefly describe the method ofhomology modelling of a targeted protein.	4+6	CO2
Q2	a) Write down the different characteristics of drug target. b) What is the role of proteomics intarget identification.	4+6	CO3