Time: 3 Hours **Marks: 75**

Q. 1 Attempt all multiple-choice questions (MCQ) **20M**

Sr No	Questions		Options
1	The first step after a target has been identified is to _____ it	a	Optimize
		b	Validate
		c	Process
		d	Rectify
2	What is a significant factor contributing to the high cost of drug discovery?	a	Rapid approval process
		b	Low research and development costs
		c	High failure rates in clinical trials
		d	Short duration of drug development
3	Antisense-oligonucleotides usually consist of 15–20 nucleotides, which are complementary to their target _____	a	Receptor
		b	mRNA
		c	Enzyme
		d	Protein
4	Which technique allows the simultaneous study of the expression levels of thousands of genes?	a	Zinc finger proteins
		b	Antisense technologies
		c	Protein microarrays
		d	Nucleic acid microarrays
5	Which phase of drug discovery is often the most costly and time-consuming?	a	Target Identification
		b	Clinical Trials
		c	Lead Identification
		d	Target Validation
6	Which of the following statements best describes a lead compound?	a	A compound that contains the element lead.
		b	A compound from the research laboratory that is chosen to go forward for preclinical and clinical trials.
		c	A molecule that shows some activity for the property of interest and serves as the starting point for the development of a drug.
		d	The first compound of a structural class of compounds to reach the market.

7	Lipinski's rule of five is used for	a	Docking
		b	Similarity search
		c	Drug likeness
		d	Dynamics simulation
8	Identify the kind of interactions that are not typically involved in binding a drug to the binding site of a protein	a	Predominantly van der Waals interaction
		b	Predominantly ionic bonds
		c	Predominantly hydrogen bonds
		d	Predominantly covalent bonds
9	What is meant by docking?	a	The process by which two different structures are compared by molecular modeling
		b	The process by which a lead compound is simplified by removing excess functional groups
		c	The process by which drugs are fitted into their target binding sites using molecular modeling.
		d	The process by which a pharmacophore is identified.
10	Which of the following approaches is considered under the 'Ligand based drug designing' ?	a	Molecular docking
		b	Pharmacophore modeling and QSAR modeling
		c	Rigid docking
		d	Rigid modeling
11	What does the symbol P represent in a QSAR equation?	a	pH
		b	Plasma Concentration
		c	Partition coefficient
		d	Prodrug
12	Which of the following statements is true in de novo drug design?	a	The design of rigid molecules is superior to flexible ones.
		b	Molecules should be designed to fit as snugly as possible into the target binding site.
		c	Molecules that have to adopt an unstable conformation in order to bind should be rejected.
		d	Desolation energies can be ignored since they are likely to be the same for different molecules having the same pharmacophore.

13	Which of the following statements is untrue when comparing 3D QSAR with conventional QSAR?	a	Only drugs of the same structural class should be studied by 3D QSAR or QSAR.
		b	3D QSAR has a predictive quality unlike QSAR.
		c	Experimental parameters are not required by 3D QSAR, but are for QSAR.
		d	Results can be shown graphically in 3D QSAR, but not with QSAR.
14	What is meant by de novo drug design?	a	The synthesis of a compound from simple starting materials.
		b	The design of the synthesis required to generate a novel range of structures.
		c	The design of a novel drug based on molecular modeling studies of a binding site.
		d	The modification of a drug based on molecular modeling studies into how it binds to its target binding site.
15	In case of Protein-ligand docking, _____ ligands are often _____ in adapting their shape to fit the receptor binding pocket.	a	small molecule, highly flexible
		b	large molecule, highly flexible
		c	large molecule, more flexible
		d	small molecule, less flexible
16	What is advantage of Levodopa over Dopamine	a	Improved Membrane permeability
		b	Reduction in production cost
		c	Improved taste
		d	No odour
17	Which of the following is a prodrug	a	Neostigmine
		b	Enalapril
		c	Esmolol
		d	Captopril
18	Methenamine is a prodrug of —--	a	Mechlorethamine
		b	Metoprolol
		c	Formaldehyde
		d	Mannitol
19	Which of the following will be the pharmacokinetic application of prodrugs?	a	Improvement of taste
		b	Improvement of odour
		c	Site-specific drug delivery
		d	Reduction in GI irritation

20	Which of the following is an example of a mutual prodrug?	a	Prontosil is the prodrug for sulfanamide
		b	Aspirin is the prodrug of salicylic acid
		c	Benorylate prodrug for NSAIDs and paracetamol
		d	Diesters pro-prodrug for pilocarpic acid

Q 2. Attempt any two of the following questions **10M**

1. Explain the significance of High Throughput Screening (HTS) in Lead Identification.
2. Discuss and elaborate 'Pharmacophore Modeling' and how it serves as a tool for novel drug discovery.
3. Discuss in detail about De Novo drug design. Elaborate flexible docking methods with suitable examples.

Q 3. Attempt any Seven of the following questions **35M**

1. Discuss process of target identification in new drug discovery
2. Explain hierarchy of protein. Discuss domains, motifs, and folds in Protein Structure?
3. Define combinatorial Chemistry. Discuss solid phase synthesis.
4. What are the different approaches for traditional drug design?
5. Explain in detail ligand based drug design.
6. Define and explain the parameters used to define 2D QSAR model by Hansch analysis.
7. Trace the history and development of Quantitative Structure-Activity Relationship (QSAR) in the field of medicinal chemistry.
8. What is QSAR? Give advantages and disadvantages of QSAR? Write a note on 3D QSAR.
9. Write a note on carrier linked prodrug.

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