

3 Hours

Total Marks: 75

Q.I. Answer the following Multiple-Choice Questions. Select the most appropriate option for each statement. (20)

Sr. No.	Question	Option	
1	Computational technique used in drug discovery to search libraries of small molecules to identify those structures which are most likely to bind to a drug target is _____	a	Pharmacophore mapping
		b	Virtual screening
		c	Conformational search
		d	Homology modelling
2	Select the correct order for Pharmacophore generation	a	Input structures-evaluate hypothesis-conformational modeling-generate model
		b	Input structures-evaluate hypothesis-generate model-conformational modeling
		c	Evaluate hypothesis-input structures-generate model-conformational modeling
		d	Input structures-conformational modeling-generate model-evaluate hypothesis
3	How is π measured?	a	It is measured by calculating molecular dimensions using relevant molecular modelling software.
		b	It is measured by comparing the dissociation constants of two weak acids.
		c	It is measured by subtracting the log P value of substituted analogue from the log P value of the unsubstituted analogue.
		d	It is measured by subtracting the log P value of the unsubstituted analogue from the log P value of substituted analogue
4	Which of the following terms refers to the molecular modelling computational method that uses equations obeying the laws of classical physics?	a	Molecular mechanics
		b	Molecular calculations
		c	Quantum theory
		d	Quantum mechanics
5	The hydrophobicity of substituent is measured using	a	Hammett substituent constant
		b	Hansch substituent constant
		c	Taft substituent constant
		d	Dipole moment

6	The positive value for Taft's steric parameter represents _____	a	Substituents larger than hydrogen
		b	Substituents smaller than hydrogen
		c	Substituents smaller than methyl group
		d	Substituents larger than methyl group
7	What does E_S represent in a QSAR equation?	a	The electronic influence of a substituent as an electron withdrawing group
		b	The electronic influence of a substituent as an electron donating group
		c	The entropy associated with a substituent
		d	Taft's steric factor
8	Hansch substituent constant is represented by the symbol _____	a	σ
		b	ϕ
		c	E_S
		d	π
9	Recognize the correct sentence about the log P of Lipinski rule of 5	a	According to Lipinski's Rule of 5, an oral drug should have a Log P value <5 , ideally between 1.35-1.8 for good oral and intestinal absorption.
		b	According to Lipinski's Rule of 5, an oral drug should have a Log P value >5 , ideally between 5.35-7.8 for good oral and intestinal absorption.
		c	According to Lipinski's Rule of 5, parenteral drug should have a Log P value <5 .
		d	According to Lipinski's Rule of 5, parenteral drug should have a Log P value >5 .
10	Which of the following is a good binding energy in docking?	a	-11.7 Kcal/mol
		b	-5.6 Kcal/mol
		c	-10.5 Kcal/mol
		d	14.5 Kcal/mol
11	For compounds more soluble in water, the Log P value is _____	a	negative
		b	positive
		c	>5
		d	>10
12	Which type of interaction can be expected with receptor if the drug contains amino group	a	Ionic interaction
		b	Hydrophobic interaction
		c	Π - Π stacking interaction
		d	Coordination bond formation

13	CoMSIA is abbreviation used for	a	Comparative molecular simulation Analysis
		b	Comparative molecular similarity indices Analysis
		c	Comparative model similarity index analysis
		d	Comparative mass similarity analysis
14	What value does the regression coefficient have for a perfect fit?	a	10
		b	0.1
		c	1
		d	100
15	Lowest energy conformer found during conformational analysis is called	a	Global minima
		b	Local minimum
		c	Transition state
		d	Conformational minimum
16	Which of the following is NOT one of the steps of Homology modelling?	a	Loop modelling
		b	Alignment correction
		c	Preparation of Grid
		d	Template recognition
17	All properties given below are predicted by in-silico ADMET analysis except _____	a	P-gp substrates and inhibitors
		b	IC50
		c	Log D
		d	pKa
18	Training set in pharmacophore mapping should contain	a	actives
		b	inactives
		c	actives and inactives
		d	pseudoactives
19	Which of the following approach is used when receptor structure is known but ligand is unknown?	a	Fragment based drug design
		b	Ligand based drug design
		c	Molecular docking
		d	Homology modelling
20	Which software is NOT used in pharmacophore mapping?	a	MOE
		b	Catalyst
		c	Auto Dock Vina
		d	Phase

Q.2. Answer the following questions (Any 2)**(20)**

- Write a note on different methods of Conformational analysis in molecular docking.
- Enlist the steps involved in 3D QSAR. Explain the alignment methods in detail.
- What is QSAR? Explain the Hansch analysis and Free Wilson analysis.

Q.3. Answer the following questions (Any 7)

(35)

- A. Write a short note on Hammett equation and electronic parameters.
 - B. Explain the determination of lipophilicity in QSAR.
 - C. Write various physicochemical properties of the drug that have an influence on the ADMET of the drug. Explain any two physicochemical properties.
 - D. What is molecular docking? Distinguish between rigid docking and flexible docking.
 - E. Differentiate between Molecular mechanics and Quantum mechanics.
 - F. Define Pharmacophore. Enlist the steps involved in pharmacophore mapping.
 - G. Write a short note on model optimization and model validation steps of homology modelling.
 - H. Write a short note on conformational analysis and its significance in molecular modelling.
 - I. Explain the different approaches used in de novo drug design.
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