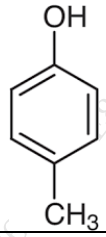
Time:3 Hours **Marks: 75**

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

Q.No.	Question		Option
1	Hansch substituent constant is represented by the symbol _____	a	σ
		b	ϕ
		c	Es
		d	π
2	The postive 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
3	Log 1/C in QSAR equation represents	a	*In vitro* biological data
		b	*In vivo* biological data
		c	*In silico* biological data
		d	Therapeutic Index of a drug
4	What two physical features (or fields) are most important in 3D QSAR studies?	a	Hydrophobic and steric fields.
		b	Electrostatic and steric fields.
		c	Hydrophobic and electrostatic fields.
		d	Steric field and dipole moment.
5	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
6	What value does the regression coefficient have for a perfect fit?	a	10
		b	0.1
		c	1
		d	100
7	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
8	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
9	_____ is an ensemble of steric and electronic features that is necessary to ensure the optimal supramolecular interactions with a specific biologic target and to trigger or block its biologic response.	a	Ligand
		b	Polar surface area
		c	Pharmacophore
		d	Agonist or antagonist
10	Which software is NOT used in pharmacophore mapping?	a	MOE
		b	Catalyst
		c	Auto Dock Vina
		d	Phase

11	Which of the following terms refers to the molecular modelling computational method that uses quantum physics?	**a**	Quantum theory
		b	molecular calculations
		c	Quantum mechanics
		d	Molecular mechanics
12	Pharmacophore is_____	**a**	group on a molecule that interact with a receptor and responsible for biological activity
		b	a collection of structural features of the molecules.
		c	group on a receptor that is responsible for biological activity.
		d	an aromatic ring of molecule that interact with a receptor and responsible for activity
13	Training set: test set molecules in pharmacophore mapping is	**a**	1:1
		b	10:1
		c	3:1
		d	100:1
14	_____ is one of the computational structure prediction methods that is used to determine protein 3D structure from its amino acid sequence.	**a**	Homology modeling
		b	De Novo drug design
		c	Molecular docking
		d	Pharmacophore mapping
15	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
16	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
17	_____ is a method which analyses the conformation and orientation of molecules into the binding site of a macromolecular target.	**a**	Molecular modeling
		b	Homology modeling
		c	Pharmacophore mapping
		d	Molecular docking
18	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	Inputstructures-conformational modeling-generate model-evaluate

			hypothesis
19	Calculate the log *P* value for the structure shown; log *P* for benzene = 2.13; π(OH) -0.67; π(CH3) 0.52. 	**a**	1.98
		b	3.32
		c	0.94
		d	2.13
20	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

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

A) What is QSAR? Explain the Hansch analysis and Free Wilson analysis.

B) Write a short note on 3D QSAR approaches.

C) Write a note on different methods of Conformational analysis in molecular docking.

Q.3. Answer the following questions (Any 7) **(35 Marks)**

A) Which computational technique is used to find out 3D structure of unknown protein or target? Explain it with the limitations.

B) Explain in detail the different types of Pharmacophore elements.

C) What is *in-silico* ADMET prediction? Write its importance in drug design.

D) Write a short note on Hammett equation and electronic parameters.

E) Explain contour map analysis in QSAR.

F) What is molecular docking? Distinguish between rigid docking and flexible docking.

G) Write a short note on model optimization and model validation steps of homology modelling.

H) Define the term pharmacophore. Explain about the pharmacophore mapping with suitable example

I) Write a short note on different components of forcefield.

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