STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086
(For candidates admitted from the academic year 2023 – 2024)

M. Sc. DEGREE EXAMINATION, NOVEMBER 2024
BIOINFORMATICS
THIRD SEMESTER

COURSE : CORE
PAPER : MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN
SUBJECT CODE : 23BI/PC/MC34
TIME : 3 HOURS MAX. MARKS: 100

Q. NO.	SECTION A (10 X 1=10) ALL QUESTIONS TO BE ANSWERED (OBJECTIVE TYPE)	CO	KL
1.	The chem draw files can be renamed to pdb file using _____software a) Pymol b) Discovery Studio Visualizer c) Protein Data Bank d) ChemSketch	CO1	K1
2.	The features like 'add Kollman charges' and 'compute gasteiger' are used for a) Ligand b) Protein c) Both a and b d) None	CO2	K2
3.	Which of the following is NOT used by molecular modelling software packages? a) Relative molecular mass b) Bond angles c) Bond lengths d) Torsion angles	CO1	K1
4.	Which of the following approach is considered under the 'Ligand based drug designing'? a) Molecular docking b) QSAR Modeling c) Pharmacophore modeling d) b and c both	CO2	K2
5.	Lipinski's rule of five is used for a) Docking b) Similarity search c) Drug likeness d) Dynamics simulation	CO1	K1
6.	QSAR method involves a) Target structure b) Target properties c) Ligand x-ray structure d) Ligand properties	CO2	K2
7.	Which of the following compounds has desirable properties to become a drug? a) Fit drug b) Lead c) Fit compound d) All of the above	CO1	K1
8.	AMBER is the force field used for the simulation for the following a) Proteins b) Nucleic acids and Proteins c) Carbohydrates d) All of the above	CO2	K2
9.	Lead optimization helps in a) Enhancing the most promising compound to improve the toxicity b) Obtaining lower RMSD values c) Building the target protein model d) Generating the Pharmacophore models	CO1	K1

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10.	What does the partition coefficient (P) measure? a) The solubility of a solute in a particular solvent b) The distribution of a solute between two immiscible phases c) The rate of diffusion of a solute across a membrane d) The concentration of a solute in a solution	CO2	K2
Q. No.	**SECTION B (10 X 2= 20 MARKS)** **ANSWERS IN ABOUT 50 WORDS**	**CO**	**KL**
11.	Hydrogen bond	CO3	K3
12.	Ball and stick model	CO4	K4
13.	Boundaries	CO3	K3
14.	Simplex method	CO4	K4
15.	ADMET	CO3	K3
16.	QSAR	CO4	K4
17.	Drug discovery	CO3	K3
18.	Active site prediction	CO4	K4
19.	Verlet algorithm	CO3	K3
20.	Gibbs free energy	CO4	K4
Q. No.	**SECTION C (4 X 10= 40)** **ANSWER IN ABOUT 600 WORDS - INTERNAL CHOICE**	**CO**	**KL**
21.	a) Explain the potential energy surface. **OR** b) Illustrate the Z matrix and Cartesian coordinate systems.	CO4	K4
22.	a) Discuss the significance of computer simulation. **OR** b) Brief the methods of energy minimization.	CO5	K5
23.	a) Give a detailed account molecular dynamics at constant temperature and pressure. **OR** b) Describe the De novo drug design.	CO4	K4
24.	a) Write about molecular structure representations. **OR** b) Discuss the molecular descriptors in detail.	CO5	K5
Q. No.	**SECTION D (2X 15=30)** **ANSWER ANY TWO QUESTIONS IN ABOUT 1200 WORDS**	**CO**	**KL**
25.	Elaborate the types of force fields in molecular mechanics.	CO5	K6
26.	Explain the 3D pharmacophore identification and mapping.	CO5	K6
27.	Discuss the concept of molecular docking in detail.	CO5	K6
28.	Write in brief on Monte Carlo simulation of molecules.	CO5	K6

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