STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI 600 086 (For candidates admitted from the academic year 2023 – 2024) M.A / M.Com / M. Sc. DEGREE EXAMINATION, APRIL 2024 BIOINFORMATICS SECOND SEMESTER

COURSE : ELECTIVE

PAPER : COMPUTER AIDED DRUG DESIGN

SUBJECT CODE : 23BI/PE/CD23

TIME : 3 HOURS MAX. MARKS: 100

Q. No.	SECTION A (10 x 1=10)	CO	KL
	All questions to be answered (Objective type)		
1	What is the primary goal of drug development?	CO1	K1
2	What is the purpose of preclinical phase studies in drug development?	CO2	K2
3	Name one ethical consideration in drug discovery.	CO1	K1
4	What are small molecules in drug design?	CO2	K2
5	Give an example of a database used for retrieving protein structures.	CO1	K1
6	What is the role of ligand-based drug design in drug discovery?	CO2	K2
7	Expand FDA.	CO1	K1
8	Name a commonly used chemical database for drug discovery.	CO2	K2
9	What does ADME stand for in pharmacokinetics?	CO1	K1
10	Define pharmacodynamics.	CO2	K2
Q. No.	$\begin{array}{ccc} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$	CO	KL
	Answers in about 50 words		
11	List the main phases of drug discovery?	CO3	K3
12	Explain the role of regulations in drug discovery.	CO4	K4
13	State the role of IND.	CO3	K3
14	How do computational inferences contribute to target discovery and validation?	CO4	K4
15	Define active site.	CO3	К3
16	Explain the drug targets.	CO4	K4
17	Discuss the significance of natural products and their analogues in screening lead molecules.	CO3	К3
18	Comment on Lipinski' rule.	CO4	K4
19	What is scoring in molecular docking?	CO3	K3
20	Explain how molecules are scored and evaluated in molecular docking studies.	CO4	K4
Q. No.	SECTION C (4 x 10= 40)	CO	KL
2.110	Answer in about 600 words - Internal choice		
21	a) Discuss the significance of each phase in the drug discovery	CO4	K4
	process.		
	OR		
	b) Analyze the impact of FDA regulations on drug development.		

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22	a) Evaluate the effectiveness of Indian regulatory systems in	CO5	K5
	ensuring drug safety and efficacy.		
	OR		
	b) Justify the need for ethics in drug discovery studies		
23	a) Explain how computational methods aid in target discovery	CO4	K4
	and validation in drug discovery.		
	OR		
	b) Compare different databases used for drug target		
	identification and retrieval of protein structures.		
24	a) Comment on different file formats.	CO5	K5
	OR		
	b) Evaluate the utility of PubChem and Drug Bank databases		
	for drug discovery research.		
Q. No.	SECTION D (2x 15=30)	CO	KL
C			
	Answer any TWO questions in about 1200 words		
25	Answer any TWO questions in about 1200 words Explore the challenges and opportunities associated with the		
25	Explore the challenges and opportunities associated with the	CO5	K6
25	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief		
	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development.	CO5	K6
25	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development. Critically analyze the ethical implications of drug discovery in		
26	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development. Critically analyze the ethical implications of drug discovery in relation to vulnerable populations.	CO5	K6
	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development. Critically analyze the ethical implications of drug discovery in relation to vulnerable populations. Evaluate the potential impact of molecular docking studies in	CO5	K6
26 27	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development. Critically analyze the ethical implications of drug discovery in relation to vulnerable populations. Evaluate the potential impact of molecular docking studies in rational drug design and lead optimization.	CO5 CO5	K6 K6
26	Explore the challenges and opportunities associated with the changing landscape of drug development with a brief description on the timeline and phases in drug development. Critically analyze the ethical implications of drug discovery in relation to vulnerable populations. Evaluate the potential impact of molecular docking studies in	CO5	K6
