

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATIONS- 2026

B.Tech-VI Semester (BI)

COURSE CODE(CREDITS): 18B11BI612 (3)

MAX. MARKS: 25

COURSE NAME: Computer Aided Drug Design

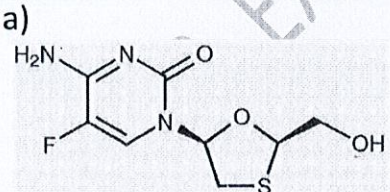
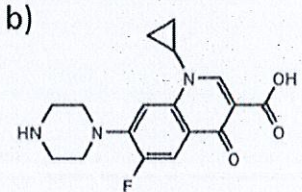
COURSE INSTRUCTOR: Dr. Raj Kumar

MAX. TIME: 1 Hour 30 Min

Note: (a) All questions are compulsory.

(b) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems

(c) Use of calculator is not allowed

Q.No	Question	CO	Marks
Q1	Discuss the properties of a good drug target. How do researchers prioritize potential drug targets for further investigation and validation?	1	3
Q2	Describe how biological pathway such as Glycolysis can be targeted for cancer therapeutics?	2	3
Q3	Analyze how CASTp distinguishes between surface pockets and internal cavities?	3	5
Q4	Describe the working of genetic algorithm used by Autodock program.	3	4
Q5	Create SMILES string for the given molecules: a)  b) 	4	4
Q6	Create 2D structures for the given SMILES strings: a) <chem>NC(O)C(=O)O</chem> b) <chem>CC(=O)Oc1ccccc1C(=O)O</chem> c) <chem>CNC[C@H](O)c1ccc(O)c(O)c1</chem>	4	1 × 3 =3
Q7	Short notes: a) RNA interference b) CAS Registry Number c) Blind docking	3	1 × 3 =3