

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- April-2023

MSc (Biotechnology)-4<sup>th</sup> Sem (BT)

COURSE CODE(CREDITS): 20MSWBT432 (2)

MAX. MARKS: 25

COURSE NAME: Drug Discovery and Development

COURSE INSTRUCTORS: Dr Udayabanu

MAX. TIME: 1hour 30 minutes

*Note: All questions are compulsory. Marks are indicated against each question in square brackets.*

1. Identification of relevant groups on a molecule that interact with a receptor are responsible for biological activity. How would you optimize the relevant groups and activity with the help of QSAR? [5 Marks]
2. Is Clavulanic acid a suicide substrate? What is the use of clavulanic acid and what is the combination drug that is most commonly used? Explain the mechanism involved in it. [5 Marks]
3. The substituent hydrophobicity constant ( $\pi$ ) can be used to optimize the lead molecule. Log P value of benzene is 2.13.  $\pi$  value of different groups are given below. Calculate the Log P value of Chlorobenzene, Dichlorobenzene, Bromobenzene, Phenol, 2-Chlorophenol. [5 Marks]

Group	CH <sub>3</sub>	t-Bu	OH	OCH <sub>3</sub>	CF <sub>3</sub>	Cl	Br	F
$\pi$ (aliphatic substituents)	0.50	1.68	-1.16	0.47	1.07	0.39	0.60	-0.17
$\pi$ (aromatic substituents)	0.52	1.68	-0.67	-0.02	1.16	0.71	0.86	0.14

4. Most DNA Intercalating drugs are compounds that contain planar or heteroaromatic features which slip between the base-pair layers of the DNA double helix. Discuss some planar/heteroaromatic drugs that act as DNA intercalating drugs. [5 Marks]
5. Write a note on the following
  - a. Homology modeling [2.5 Marks]
  - b. Selection of animal model could affect preclinical studies [2.5 Marks]