

Centre for Computational Biology and Bioinformatics CENTRAL UNIVERSITY OF HIMACHAL PRADESH (Established under Central Universities Act 2009, Accredited with NAAC A') Shahpur, District: Kangra, Himachal Pradesh-176206 MID-TERM EXAMINATIONS, APRIL-2024 (SPRING SESSION) M.SC. BIOINFORMATICS

ological

same of the Course: Computer Aided Drug Discovery

Time Duration: 1 Hour Date of Exam: 15-4-2024 Course Code: BIN465 Semester: II Maximum Marks: 20 Roll No:

SECTION-A

Q1). ANSWER ALL THE FOLLOWING QUESTIONS

5 X 1 = 5 M

i). Factors affecting Van der Waals forces are?

- ii). In electronic substituent X represents_
 - a) 70
- b) 75
- c) 76
- d) 72

iii). The biological activity is normally expressed as 1/C, where C is

- iv). What is the logP value of Benzene?
 - a) 2.13
- b) 2.31
- c) 1.23
- d) 3.21

v). P= Concentration of drug in octanol /Concentration of drug in aqueous solution is

True (or) False?

SECTION-B

2 X 2.5= 5 M

ANSWER ANY $\underline{\text{TWO}}$ OF THE FOLLOWING QUESTIONS

- Q2). Write a short note on applications of Computer Aided Drug Discovery.
- Q3). Write a short note on the History of Computer Aided Drug Discovery.
- Q4). Write a short note on Hydrophobicity and partition co-efficient.
- Q5). Write a short note on electronic effects.

ANSWER ANY TWO OF THE FOLLOWING QUESTIONS

2 X 5= 10 M

- Q6). Discuss the ADMET properties.
- Q7). Discuss Steric and Taft's steric factors.
- Q8). Explain the Hansch Analysis
- Q9). Explain non-bonded interactions in detail.