



**HDS-003-006509**

Seat No. \_\_\_\_\_

**B. Sc. (Bioinformatics) (Sem. V) (CBCS) Examination**

November / December – 2017

**BI - 505 A : Molecular Modelling & Drug Designing**

**Faculty Code : 003**

**Subject Code : 006509**

Time :  $2\frac{1}{2}$  Hours]

[Total Marks : 70

- Instructions :** (1) All questions are compulsory.  
(2) The right-side figure indicates total marks of the question.

**PART – A**

- 1 The average angle between the orbitals of the central atom containing the bonding electron pairs in the molecule is known as \_\_\_\_\_ between the atoms.
- 2 Non-covalent interactions can be classified into different categories, such as involve the attraction of ions or molecules with full permanent charges of opposite signs.
- 3  $\pi$ -effects can be broken down into numerous categories, including u \_\_\_\_\_
- 4 Full form of SMD?
- 5 What is the abbreviation of SUMO protein?
- 6 The function performed by SUMO proteins is known as \_\_\_\_\_?
- 7 Why the product is formed unstable in the active site?
- 8 What is the aim of virtual screening?
- 9 ADMET
- 10 Covalent Bonds are \_\_\_\_\_ and \_\_\_\_\_ with respect to drug binding receptor.
- 11 What type of interactions in hydrogen bonding provides extension of attraction of opposite charges?

- 12 \_\_\_\_\_ is a group of diseases involving abnormal cell growth with the Potential to invade or spread to other parts of the body.
- 13 What are oncogenes?
- 14 Define malignancy.
- 15 Define infectious disease.
- 16 \_\_\_\_\_ and \_\_\_\_\_ have been used to generate a model of the FDA-approved inhibitor Sustiva bound to HIVRT.
- 17 How we get semisynthetic drugs?
- 18 Which theory of the activated complex by enzymes was first proposed by Pauling?
- 19 Define suicide inhibition.
- 20 Data mining approaches used for target identification

### PART – B

- 1 (A) Explain Any **Three** : **6**
  - (1) Bond length
  - (2) Define Valence. bond method.
  - (3) Application of pharmacophore
  - (4) What is cancer? Mention types of cancer.
  - (5) What are proto onco genes?
  - (6) Which are the steps to increase accuracy in modeling the solvent effect during scoring?
  
- (B) Explain Any **Three** : **9**
  - (1) Use of molecular mechanism
  - (2) What are the Empirical potentials?
  - (3) Virtual Screening
  - (4) Describe mechanisms of anti-cancer drugs.
  - (5) What are the steps involved in post screening analysis focusing on protein-ligand interaction in Structure based drug design?
  - (6) Steps involved in the concept of Enzyme inhibition.

- (C) Attempt Any **Two** : **10**
- (1) Non-covalent interactions
  - (2) Explain molecular dynamics example of applications?
  - (3) Explain in detail about ab initio method.
  - (4) Ligand based drug design
  - (5) Describe mechanisms of antibiotics and antibiotic resistance.
- 2** (A) Explain Any **Three** : **6**
- (1) Bond Angle
  - (2) Define Canonical ensemble (NVT).
  - (3) Features of pharmacophore
  - (4) What is p53 and what does it do?
  - (5) How drug design is useful in drug discovery?
  - (6) Features of enzyme structures and reaction pathways
- (B) Explain Any **Three** : **9**
- (1) Explain molecular dynamics algorithms.
  - (2) MMFF
  - (3) Explain drug-induced autophagy
  - (4) Challenges of Structure based drug design.
  - (5) Steps involved in evaluating a structure for Structure based drug design.
  - (6) Active site identification
- (C) Attempt Any **Two** : **10**
- (1) Write a note on Monte Carlo Simulation for conformational analysis
  - (2) Drug-receptor interactions
  - (3) Explain diseases related to cancer
  - (4) How proto oncogene converts to an oncogene?
  - (5) Describe infectious disease and its mechanisms in detail.