

Roll No. _____

B.Sc-M. Sc-INTEGRATED PROGRAMME
SCHOOL OF CHEMICAL AND LIFE SCIENCES
SEMESTER V EXAMINATION 2019
PAPER TITLE: MOLECULAR MODELLING AND DRUG DESIGN
PAPER CODE: BCH-DSE02TH

(Write your roll no. at the top immediately after receipt of this question paper.)

Time: 3h

Max Marks: 75

Attempt all the questions. All parts of a question must be attempted in continuation.

Start answer of a fresh question on a new page.

Q1a. Define ANY FIVE of following terms.

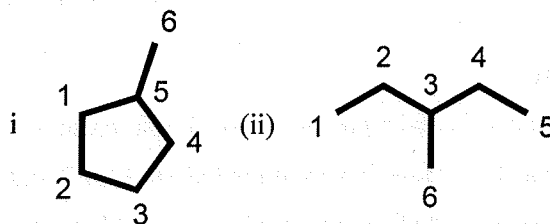
5 x 1 = 5

- A. Lipinski's rule of five
- B. Pharmacophore
- C. Descriptor
- D. Indicators
- E. IC_{50}
- F. Active Site
- G. Catalytic Triad
- H. AM1 stands for _____; PM3 stands for _____; the noble prize for computation chemistry was awarded to _____ in _____.

Q1b: Answer briefly ANY FIVE the following questions

5 x 2 = 10

- A. Justify that Occupancy model is also known as multiple docking theory.
- B. Differentiate between Restricted, Restricted Open and Open system with an appropriate example of H^+ , H and H^- .
- C. The mechanism of ATP synthase could be best explained by which docking model. Justify briefly your answer.
- D. Write Smile notation for (i) C_2H_5OH ; (ii) $CH_3CH_2CH_2OH$; (iii) $CH_2=CHCH_2OH$; (iv) $CHCl_3$
- E. Write Z-matrices for the following compounds
(i) methane; (ii) H_2O
- F. Write the matrix notation for the following:



Q2. Attempt ANY THREE of the following:

3 x 5 = 15

- A. Explain Ramachandran Plot in protein, mention the psi, phi and theta clearly in the representative diagram.
- B. What do you stand from (i) open system; Unrestricted Systems (ii) Closed System; Restricted System. Explain with proper representations and examples (if possible).
- C. Draw and mention the Z-matrix for
 - (i) CH_4 (ii) ClCH_2CH_3 (iii) ClCH_2CF_3
- D. What is the difference between the following terms (any two)
 - (i) Bond angle and Dihedral angle (ii) Atomic Radii and Van der waal Radii
 - (iii) Maxwell Distribution and Brownian motion (iv) Coordinate system and Z-matrices
- E. Explain Born Oppenhiemer Approximation Theory (BOAT) on the Basis of SHM.

Q3. Attempt ANY THREE of the following:

3 x 5 = 15

- A. Define transition state and intermediate. Explain the difference between both the terms with a suitable example.
- B. Explain the forcefields for Ligands, Protein and Protein-Ligand Complex.
- C. Define Hydrogen-bond. What are the different types of hydrogen bonds? Arrange them in increasing order of interaction energy.
- D. Briefly explain and mathematical proves for correlating the Damping mechanics and SHM.
- E. Differentiate between the following:
 - (i) Molecular mechanics and molecular modelling

OR

- (ii) Molecular dynamics and molecular mechanics

Q4. Attempt ANY THREE of the following:

3 x 5 = 15

- A. Classify the following (any two)
 - (i) protein (ii) Ligand (iii) Docking
- B. Explain the steps used for docking and briefly explain each step.
- C. Explain docking in terms of mechanics and thermodynamics.
- D. Define grid. How grid of protein differs from DNA?
- E. Explain mathematically that induced fit model is complementary to Induced fit model.

Q5. Attempt ANY THREE of the following:

3 x 5 = 15

- A. Explain the preparation of correlation matrix and regression through test, training and external set.
- B. Explain Hammett plot and Hansch equation. How they useful in QSAR, QSPR and QSTR.
- C. *In silico* understanding of racemic mixtures and Chiral resolution is possible through matrix notation. Justify.
- D. Explain Cheminformatics and how designing drug molecule could be achieved using intrinsic and extrinsic properties.
- E. Explain a Protein-ligand complex using ONIOM theory.