

(Following Paper ID and Roll No. to be filled in your Answer Book)

Paper ID : 154753

Roll No. 

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B.Tech.

(SEM. VII) THEORY EXAMINATION, 2015-16

MOLECULAR MODELING & DRUG DESIGN

[Time : 3 hours]

[Maximum Marks : 100]

Section-A

1. Attempt all sections. All sections carry equal marks.  
Write answer to each parts in short. (10×2=20)
  - (a) What is prodrug?
  - (b) In the conformational analysis of a structure, illustrate local minimum, global minimum and transition state conformations.
  - (c) What is meant by docking?
  - (d) What is the value of correlation coefficient for a perfect fit?
  - (e) What does a negative value of  $\sigma$  (Hammett Sigma constant) signify for a substituent?

- (f) What is meant by energy minimization in computational chemistry?
- (g) Expand the acronym, CoMFA and name the parameters used therein.
- (h) Explain what is 'primary structure' and 'secondary structure' of a protein.
- (i) Hansch's QSAR equation is called a linear free-energy relationship—why?
- (j) Molar refractivity (MR) is one of the originally proposed parameters of Lipinski's rule of five – True or False?

### Section-B

Attempt **any five** questions from this section. (10×5=50)

- 2. What is de novo drug design?
- 3. What is a 3D QSAR study? How it differs from a 2D QSAR study?
- 4. What is homology modeling?
- 5. Write a short note on intermolecular interactions. Identify them in the descending order of intermolecular forces.

- 6. What is the difference between quantum mechanics and molecular mechanics?
- 7. What is ADMET?
- 8. Write about Free-Wilson approach in QSAR.
- 9. What is Monte-Carlo simulation?

### Section-C

Attempt **any two** of the following : (2×15=30)

- 10. Explain the role of structure based drug design in drug discovery program.
- 11. What is molecular dynamics? Elaborate its application.
- 12. Write notes on three different conformational search algorithms.

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