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EBT-041

(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 σ (Hammett Sigma constant) signify for a substituent?

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P.T.O.

- (f) What is meant by energy minimization in computational chemistry?
- (g) Expand the acrony, 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.

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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.

—x—

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