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

Paper ID : 154753 Roll No. | | | | | | | | | | |

B.Tech.

(SEM. VII) THEORY EXAMINATION, 2015-16

MOLECULAR MODELING & DRUG DESIGN

[Time : 3 hours] [MaximumMarks : 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?

(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.

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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