Registration no: | | | | | | | | | | |

Total Number of Pages: 02 **B.Tech**
PEBT 5302

6th Semester Regular Examination – 2016-17
MOLECULAR MODELING AND DRUG DESIGNING
BRANCH: BIOTECHNOLOGY
Time: 3 Hours
Max Marks: 70
Q.CODE: Z695

Answer Question No.1 which is compulsory and any FIVE from the rest.
The figures in the right hand margin indicate marks.

Q1 **Answer the following question**s: **(2 x 10)**

a) What is global minimum in protein conformation?

b) Define van der waals force of interaction.

c) Define the electrostatic potential

d) What is "implicit" versus "explicit" solvation?

e) What is a lead module?

f) Why do you always energy minimize before running MD?

g) Why does a protein's structure depend on the pH of the solution?

h) What is the role of bond stretch and angle bending in molecular modeling?

i) What is template-based modeling (TBM)

j) What are the differences between local and global alignment?

Q2 **a)** How *ab-initio* modeling used for prediction of protein domains? **(5)**

b) Write a note on tertiary structure of protein and its importance **(5)**

Q3 What is structure based drug designing? Explain the *De-novo* Ligand design in details. **(10)**

Q4 **a)** Describe the amphipathic (hydrophobic/hydrophilic) patterns found in alpha helices and beta strands. Explain why they exist. **(5)**

b) What is Lipinski's rule of 5? **(5)**

Q5 **a)** Explain molecular docking. In molecular docking, what is the difference between ligand and cofactor? **(5)**

b) Explain molecular descriptors and their types? Describe physicochemical parameter and molecular descriptors. **(5)**

Q6 **a)** Explain conformation Searching of Polypeptides. **(5)**

b) Explain QSAR and differentiate between 2D and 3D QSAR. **(5)**

Q7 Explain molecular modeling and its applications biomolecular modeling problems. **(10)**

Q8 Write Short Notes *(Any two)* **(5 x 2)**

a) Pharmacophores

b) Weak interactions

c) Combinatorial libraries

d) Protein threading