Total number of printed pages – 4 **B. Tech**

PEBT 8303

Sixth Semester Examination – 2008

MOLECULAR MODELLING AND DRUG DESIGNING

Full Marks – 70

Time : 3 Hours

*Answer Question No. **1** which is compulsory and any **five** from the rest.*

The figures in the right-hand margin indicate marks.

1. Answer the following questions : 2×10

   (a) Write an algorithm for Ewald summation method for the long range forces.

   (b) What is boundary conditions and what are the different boundary conditions to simulate methane molecule ?

   (c) Define time average. If 'p^N' and 'r^N' represent the 'N' momenta and position respectively and 'M' is the number of time steps. Then define thermodynamic average '<A>' as time average using above parameter ?

   (d) Define Morse potential to explain the bond stretching and deduce an mathematical expression for it.

   (e) Define conformational flexibility with respect to Monte Carlo simulation method and molecular dynamics.

   (f) Initial probability vector is (1, 0) with Boltzmann factor 2 : 1, calculate the distribution probability of two different state of a molecule.

   (g) Differentiate between Lattice model and Continuous model of the polymer simulation.

   (h) What are the potential applications of Hooke's law on bond stretching of biomolecules ?

(i) Write down the differences between equilibrium phase and production phase in molecular dynamic simulation.

(j) What are the attributes we can use for the simulation of simple water molecule ?

2. (a) A methane molecule is subjected to the external mechanical force and found that it has got 15^{o} angular bending. Calculate the potential energy being stored in the molecule. 3

(b) If the molecule is being subjected to torsional bending of 15^{o}, what will be the effect on that molecule- illustrate it in brief ? 7

3. Write the prototype program for the simulation of the simple water molecule keeping the temperature and pressure as constant and interaction of non bonded force as variable parameter. 10

4. What is van der Waal interaction ? Discuss in brief about the repulsive contribution. Simulate an ethane molecule by using van der Waals interaction with respect to Leannard Jones potential. 2+3+5

5. (a) Describe the various force field models for the simulation of lipid bilayer in biological membrane. 5

(b) Write a mathematical note on energy conservation in molecular dynamics. 5

6. What are the advantages of molecular dynamics over Monte Carlo simulation method ? Briefly discuss about the constant temperature and pressure dynamics. 5+5

7. (a) Write down the salient feature of Metropolis Method for simulation and compare it with Monte Carlo method of simulation for the water molecule. 6

(b) Briefly explain the steps involved during the process of molecular dynamic simulation. 4

8. What do you mean by protein folding simulation constraints ? What are the strategies used to overcome it and write the program to solve the problem ? 2+3+5

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