

2020

## CHEMISTRY — HONOURS

Paper : DSE-A-1

(Molecular Modelling and Drug Design)

Full Marks : 50

*The figures in the margin indicate full marks.**Candidates are required to give their answers in their own words as far as practicable.*Answer **question no. 1** and **any eight** questions from the rest (**Q. 2 to Q. 13**)

1. Answer **any ten** questions : 1×10
- (a) What approximation leads to the concept of potential energy surface?
  - (b) What types of points on a potential energy surface are particularly relevant in understanding a molecular structure?
  - (c) What are the internal coordinates of a molecular system?
  - (d) For a linear molecule with 4 atoms (ABCD), comment on the dimensionality of the potential energy surface.
  - (e) Write an expression for the diatomic bond stretching energy and draw the graphical representation of the energy.
  - (f) Name one first-order energy minimization method. Identify the key step.
  - (g) What is the significance of Temperature in the context of a Molecular Dynamics simulation?
  - (h) What is Metropolis algorithm?
  - (i) Name one three-site water model and mention the features of the model.
  - (j) What is the active conformation of a drug molecule?
  - (k) What is meant by a binding site?
  - (l) Mention the significance of integration time-step in a classical Molecular Dynamics simulation.
2. What is meant by 'docking'? How is it used in drug design? 2+3
3. For n-Butane molecule draw a rough potential energy diagram keeping the bond lengths and bond angles fixed. Explain your diagram. 2+3
4. What is a molecular mechanics force field? Write down the term that represents torsion angle energy explaining all the variables in the expression. 2+3

Please Turn Over

5. What are non-covalent interactions? Suggest how they are important in stabilizing a glucose molecule in aqueous medium. 2+3
  6. What do you mean by optimization of molecular geometry? Explain a method by which this can be achieved. 2+3
  7. Mention the steps involved in a classical molecular dynamics simulation. Explain briefly how initial velocity is assigned to individual atoms. 3+2
  8. From a molecular dynamics simulation of liquid water done at a particular temperature, identify two structural and / or dynamic properties of water molecules that can be estimated. Explain the process. 2+3
  9. Briefly outline the steps of a Monte Carlo simulation. Which one, in your opinion, is the most critical step? 3+2
  10. What are numerical errors? Suggest a possible source of such errors in a classical molecular dynamics simulation. 2+3
  11. What is Lennard–Jones potential? Give an expression clearly explaining the variables used. Draw its graphical representation. 2+3
  12. Name one first-order energy minimization method. Briefly outline the steps involved. 5
  13. What do you mean by ‘Sequence Alignment’ in connection with the structure prediction of a protein? Name these general types of ‘Sequence Alignment’ methods. 5
-