

2056

B.Sc. (Hons.) Bio-Informatics (FYUP)

Fourth Semester

BINF-404: Introduction to Molecular Modeling

Time allowed: 3 Hours

Max. Marks: 60

**NOTE:** Attempt five questions in all, including Question No. 1 which is compulsory and selecting two questions from each Unit.

x-x-x

I. Answer briefly:-

- a) Simplex method for energy minimization
- b) Basic concept of Periodic box
- c) PubChem
- d) Conjugate gradient method of energy minimization
- e) Two applications of Molecular dynamics
- f) Protein-ligand interactions (6x2)

### UNIT - I

- II. a) Discuss the interactions stabilizing the protein tertiary structure.  
b) Differentiate between a helix and  $\beta$  pleated sheet. (2x6)
- III. a) Define cheminformatics and explain its scope. Discuss different chemical structure representations such as SMILES, SDF, and MOL formats.  
b) Define 1D, 2D, and 3D molecular descriptors. Explain simple counts and pharmacophore descriptors. (2x6)
- IV. a) Define molecular graphics and explain its importance in molecular modeling.  
b) Discuss different types of molecular surfaces and their significance in studying biomolecular interactions. (2x6)

### UNIT - II

- V. a) Explain torsional terms and their role in molecular mechanics.  
b) Discuss non-bonded interactions in molecular mechanics force field. (2x6)

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- VI. a) Define molecular docking. Differentiate between rigid body docking and flexible ligand docking.
- b) Explain scoring functions in docking: force field-based and empirical scoring functions. (2x6)
- VII. a) Explain the Born–Oppenheimer approximation and its importance in molecular mechanics.
- b) Describe bond stretching and angle bending interactions in a molecular mechanics force field. (2x6)

x-x-x