## **BioPhysics - BIO361** Quiz1 19.09.24

Total marks:20

Time: 1hr

## MCQ(1 mark each)

- A. Which among the following is the primary protein structure database?
  - a. PDB
  - b. UniProt
  - c. Chembl
  - d. Both a & b
- B. Channels are classified as
  - a. Fibrous protein
  - b. Membrane Protein
  - C. Globular protein
  - d. Both b&c
- C. Transfer of information from RNA -> DNA is described as
  - a. Reverse transcription
  - b. Translation
  - C. Reverse translation
  - d. Transcription
- D. Which scoring method do we use to evaluate the quality of our modeled structure?
  - a. RMSD
  - b. RMSF
  - c. e-value
  - d. **DOPE score**
- E. Which of the following is/are aromatic amino acids?
  - a. Proline
  - b. Tryptophan
  - c. Tyrosine
  - d. Both b&c

## **Very Short answer type questions (1 Mark each)**

A. Differentiate between nucleotide and nucleoside.

Presence of phosphate group in nucleotide

B. Why is RNA molecule more reactive than a DNA molecule?

Presence of 2'OH

C. State Levinthal's paradox.

Levinthal's paradox is that finding the native folded state of a protein by a random search among all possible configurations can take an enormously long time.

D. Name any 2 fully automatic servers available for homology modeling.

3D-jigsaw, EsyPred3D,Swissmodel,Pcons,itasser

E. Template 1 has %identity of 95% and resolution 4A°. Template 2 has %identity of 90% and resolution 1.5A°. Which one will you choose and why?
One with lower resolution

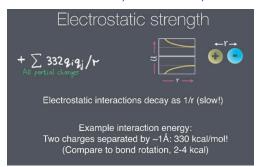
## Short answer type questions (2 Marks each)

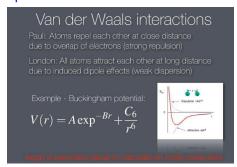
A. What are the classical and quantum mechanical differences that are considered in MD simulation and why?

**Classical MD** is computationally efficient and sufficient for large systems (e.g., proteins, lipids) because it simplifies the motion of atoms as continuous and deterministic. Classical MD doesn't account for quantum effects, such as electronic excitations, bond breaking/forming, or tunneling.

**QM** methods are necessary for systems where electronic effects, chemical reactions, or bond formation/breaking are critical. It provides an accurate description of atomic interactions at short distances and is useful in areas like catalysis, charge transfer, or enzymatic reactions. QM calculations are computationally expensive, making them impractical for large systems or long timescales.

- B. What is the major difference in formation of helices and sheets? Explain with reference to H-bonding.
   In Helices, h-bonding is observed within the protein chain(i—>i+n), whereas in sheets H-bonding
  - In Helices, h-bonding is observed within the protein chain(i—>i+n), whereas in sheets H-bonding is observed between different strands (parallel/antiparallel).
- C. Briefly explain the role of BLAST in homology modeling? How do you interpret its result? BLAST is performed to obtain the template for homology modeling. Best template is selected on the basis of %identiti, query coverage and e-value.
- D. Describe any 2 types of non-bonded interactions observed in the protein-water system. Electrostatic interaction, vanderwaal, Hbonding, hydrophobic





E. Which type of interaction does the following graph show? Label the forces accordingly and the logic. Vander waal/ lennard jones

