

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -2 EXAMINATION- 2024

B.Tech-V Semester (BI)

COURSE CODE (CREDITS): 18B1WBI531 (3)

MAX. MARKS: 25

COURSE NAME: Structural Bioinformatics

COURSE INSTRUCTORS: Dr. Raj Kumar

MAX. TIME: 1 Hour 30 Minutes

**Note:** (a) All questions are compulsory.

(b) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems

| Q.No | Question   | CO  | Marks |
|------|--|-----|-------|
| Q1   | Formulate an energy function which can be utilized to calculate an optimal sequence-structure alignment in fold recognition method?  | 3   | 2     |
| Q2   | Cite some fundamental differences between the Chou-Fasman and GOR methods.   | 3   | 2     |
| Q3   | Discuss the three core factors on which successful <i>ab initio</i> modeling depends?  | 3,4 | 2     |
| Q4   | The level of sequence identity between the target protein and the template affect the accuracy of the homology model. Provide examples of what may happen at different thresholds of identity?   | 3,4 | 3     |
| Q5   | Evaluate the effect of different factors, such as sequence alignment accuracy and template resolution affect the quality of the generated backbone structure. What are the potential consequences of these factors?  | 4   | 3     |
| Q6   | A researcher has predicted the secondary structure of a protein containing 100 amino acids. The actual secondary structure is as follows: Helix (H): 40 residues, Sheet (E): 30 residues, and Coil (C): 30 residues. The predicted secondary structure contains: Helix (H): 35 residues, Sheet (E): 25 residues, and Coil (C): 40 residues. Calculate the Q3 score for the above protein structure prediction. | 4   | 3     |
| Q7   | Calculate the statistical propensities of Alanine and Arginine residues in helix conformation of the given sequence.<br><br>SS- HHHHHCCCCCCCCCHHHHHCCCCCCC<br>Seq- AVLLTSAPLPTPLESRYRARIYRGNAITV   | 4,5 | 6     |

Q8

Evaluate the first seed window for the given sequence using the given Chou-Fasman parameters.

| Residue | $P_{\alpha}$      |
|---------|-------------------|
| Glu     | $H_{\alpha}$ 1.53 |
| Ala     | 1.45              |
| Leu     | 1.34              |
| His     | $h_{\alpha}$ 1.24 |
| Met     | 1.20              |
| Gln     | 1.17              |
| Trp     | 1.14              |
| Val     | 1.14              |
| Phe     | 1.12              |
| Lys     | $I_{\alpha}$ 1.07 |
| Ile     | 1.00              |
| Asp     | $i_{\alpha}$ 0.98 |
| Thr     | 0.82              |
| Ser     | 0.79              |
| Arg     | 0.79              |
| Cys     | 0.77              |
| Asn     | $b_{\alpha}$ 0.73 |
| Tyr     | 0.61              |
| Pro     | $B_{\alpha}$ 0.59 |
| Gly     | 0.53              |

4,5

4

JUIT TEST-2 EXAMINATION-OCT-2024