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## SARDAR PATEL UNIVERSITY

M.Sc. (BIOINFORMATICS)

SEMESTER - III External Examination PS03CMBI02: Computational Structural Biology Wednesday, 5th December 2012

Time: 2:30p.m. to 05:30 p.m.

Max Marks: 70

[8]

| Q1. | Choose the most appropriate option for each   | question.  |  |
|-----|---|--|--|
| a.  | is induced electrical interacti<br>conformational stability in the interior of the<br>A) Hydrophilic interactions | ons which contribute significantly to protein.  B) Covalent interactions |  |
|     | C) Van der Waals interactions   | D) Hydrophobic interactions  |  |
|     | E) None of above.   |  |  |
| b.  | DALI and the results are organized into the database.   |  |  |
|     | A) SCOP   | B) SARF  |  |
|     | C) FSSP   | D) MMDB  |  |
|     | E) None of Above  |  |  |
| c.  | phi (φ) bond corresponds to the bond between A) Alpha carbon & amide nitrogen                                     | i.<br>B) Alpha carbon & alpha carbon                                     |  |
|     | C) Carbonyl carbon & amide nitrogen   | D) Alpha carbon & carbonyl carbon  |  |
|     | E) None of above.   |  |  |
| d.  | may or may not be an indicator of an evolutionary relationship.   |  |  |
|     | A) Sequence similarity  | B) Genome similarity   |  |
|     | C) Structural similarity  | D) All of Above  |  |
|     | E) None of Above  |  |  |
| e.  | are structural analogs that bind to a receptor and mimic the effects of its                                       |  |  |
|     | natural ligand.   |  |  |
|     | A) Agonists   | B) Antagonists   |  |
|     | C) Pharmacophore  | D) Hit molecule  |  |
|     | F) None of Above  |  |  |

| f.       | The leucine zipper motif is typically made to<br>by interactions between hydrophobic leuci  | ap of two antiparallel α helices held toget<br>ne residues located at every pos | her<br>on |
|----------|---|---|-----------|
|          | in each helix:  A) 8 <sup>th</sup>  | B) 5th  |           |
|          | C) 6th  | D) 7 <sup>th</sup>  |           |
|          | E) None of Above  |   | •         |
| g.       | Gaussian nodal function used in NN is:<br>A) Bell-shaped  | B) SShaped  |           |
|          | C) V shaped   | D) N Shaped   |           |
|          | E) None of Above  |   | 235       |
| h.       | In a sequence alignment, the presence of may be an indication of a  A) Loop   | more substitutions, insertions, and deleti<br>B) helix                          | ions      |
|          | C) Sheet  | D) All of Above   |           |
|          | E) None of Above  | D) I III of 1100 to   | 000       |
|          | 744.V   |   | eff.      |
| Q2.      |   |   |           |
| a.<br>b. | List and discuss any three classes of protein based on the types and arrangements of secondary elements.  Explain various types of single and double stranded regions in RNA secondary                |   |           |
|          | structures.   |   |           |
| c.       | Explain file structure of Brookhaven Protein Data Bank with example.  |   |           |
| d.<br>e. | Which are the major secondary structures in protein? List types of possible helix in protein and discuss structure of $\pi$ -helix in detail. Explain Lipinski Rule of Five to evaluate druglikeness. |   |           |
| f.       | Write short note on CASP.   |   |           |
| g.       | Describe structural 3-D profile table method for detecting matches of a sequence to a structural profile.   |   |           |
| h.       | Describe chameleon sequence in protein structure analysis.  |   |           |
| i.       | Explain Ramp Node function and its uses.  |   |           |
| Q3.      | Answer the following questions:   |   |           |
| a.       | Explain method of construction of environmental vectors, vector matrices and  |   | and [6]   |
|          | summary matrix of double dynamic programming method for aligning structures using $C_{\beta}$ vectors of amino acids by giving example.   |   |           |
|          |   |   |           |

Give structural detail of most abundant type of secondary structures in proteins and [6] b. discuss about Helical structure in detail. Discuss structural role of Prolin and Glycine amino acids in polypeptide. OR Discuss structural details of possible secondary structures in proteins other than helix. [6] b. Answer the following questions: Q4. What is HMM? How it is useful in preparing discrete state-space model of protein [6] three-dimensional structure. Discuss Chou-Fasman method for secondary structure prediction of protein and [6] b. describe how it differs from GOR method. Explain Garnier, Osguthorpe, and Robson method for secondary structure prediction of [6] protein. Answer the following questions: Q5. Discuss neural network architecture for protein sequence processing through five [6] a. modules, A, C, D, H and M, to quantify the five types of compositional attributes. Describe structural 3-D profile method for detecting matches of a sequence to a [6] b. structural profile. OR List two main approaches of RNA secondary structure prediction and describe method [6] used in dynamic programming analysis for identifying the most energetically favorable configuration of linear RNA molecule in detail. Answer the following questions: Q6. List descriptors used in QSAR studies and discuss about ligand-receptor interaction [6] a. complementarities. Describe Sanjeevini a complete drug designing software suite of IIT Dolhi with [6] b. necessary details. OR Explain the base covariation method used to make RNA secondary structure predictions also discuss major difficulties of this method.

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