

Indraprastha Institute of Information Technology Delhi (IIITD)

Department of Computational Biotechnology

BIO213 – Introduction to Quantitative Biology

Quiz-3 (April 23, 2024)

Name: _____

Roll no.: _____

Total time: 40 mins

Total marks: 40

Question 1. Which of the following is NOT true for GOR method of secondary structure prediction? **(2 mark)**

1. It was developed by Garnier, Osguthorpe and Robson.
 2. It is an information theory-based method.
 3. It considers a window size of 17- one central amino acid and 8 neighboring amino acids on each flanking side.
 4. It predicts four states of secondary structure- helix, strand, turn and coil.
- a) All of them
b) None of them
c) 2
d) 4
e) 2 and 3

Question 2. Which of the following is not a conformational search method? **(2 marks)**

- a) Monte Carlo
b) Genetic Algorithm
c) Simulated annealing
d) Maximum parsimony

Question 3. Which of the following is not the method that can be used for validation of the modelled protein structure? **(2 marks)**

- a) Ramachandran plot
b) ERRAT
c) Phyre
d) ANOLEA

Question 4. Which of the following is NOT a measure to reduce computational complexity of *Ab initio* modelling? **(2 marks)**

- a) Torsion angles are restricted to a finite set of values.
b) Protein sequence is searched against fold database to look for regions of structural similarity.
c) Only the polar hydrogens are given importance.
d) Bulky side chains are replaced by single pseudo-atoms.

Question 5. Homology modelling is a procedure whereby: **(2 marks)**

- a) due to low sequence similarity between proteins of unknown and known structure, the structure is predicted from first principles (i.e., ab initio).

b) due to high sequence similarity between proteins of unknown and known structure, the same function is assumed for both.

c) **due to high sequence similarity between proteins of unknown and known structure, the structure of the latter is used as a template to model the former.**

d) a protein of unknown structure is compared against a library of fold templates to find the best match.

Question 6. Secondary structure is defined by _____ . (1 mark)

a) **Hydrogen bonding**

b) Vander Waals forces

c) Covalent bonding

d) Ionic bonding

Question 7. Match the following: (5 marks)

- | | |
|---------------|---------------------------------------|
| 1. Modeller | A. Structure validation |
| 2. I-TASSER | B. Homology modelling |
| 3. ERRAT | C. Secondary structure prediction |
| 4. BHAGEERATH | D. Threading |
| 5. DSSP | E. <i>Ab Initio</i> protein modelling |

a) 1-B, 2-E, 3-A, 4-D, 5-C

b) 1-B, 2-D, 3-A, 4-E, 5-C

c) 1-B, 2-D, 3-A, 4-C, 5-E

d) 1-E, 2-E, 3-C, 4-D, 5-A

Question 8. Which of the following is untrue about Backbone Model Building Step? (2 marks)

a) Once optimal alignment is achieved, residues in the aligned regions of the target protein can assume a similar structure as the template proteins.

b) Coordinates of the corresponding residues of the template proteins can be simply copied onto the target protein.

c) If the two residues differ, everything other than the backbone atoms can be copied.

d) If the two aligned residues are identical, coordinates of the side chain atoms are copied along with the main chain atoms.

Question 9. Use the information given in the table to find out the following value: (8 marks)

	β-Sheet	Helix	Others	Total
G	200	150	30	380
V	100	400	180	680
All residues	600	2100	500	3200

a) P (SS = β-Sheet | aa = G) = **200/380 = 0.53**

b) P (SS = Helix | aa = V) = 400/680 = 0.59

c) P (SS = ~ β-Sheet | aa = G) = **(150+30)/380 = 0.47**

d) P (SS = ~ Helix | aa = V) = **(100+180)/680 = 0.41**

- e) $P(\text{SS} = \beta\text{-Sheet}) = 600/3200 = 0.19$
f) $P(\text{SS} = \sim\beta\text{-Sheet}) = (2100+500)/3200 = 0.81$
g) $P(\text{SS} = \text{Helix}) = 2100/3200 = 0.66$
h) $P(\text{SS} = \sim\text{Helix}) = (600+500)/3200 = 0.34$

Answers can be up to one decimal place or two decimal places. Slight variability is acceptable.
Deduct marks for answers left in fractions.

Question 10. How does studying the transcriptome complement our understanding of genetic instructions encoded in DNA? Give 4 reasons. **(4 marks)**

Why sequence RNA (Versus DNA)?

1. Functional studies

Genome may be constant but an experimental condition has a profound effect on the gene expression (differential expression)

Eg. Drug vs. untreated cells

Eg. Wild type vs. knock out mice cells

2. Predicting transcript sequence from genome sequence is difficult

3. Some molecular features can only be observed at the RNA level

Alternative isoforms, fusion transcripts, RNA editing

4. Understand allele specific expression

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Question 11. Differentiate between diagnostic and prognostic biomarkers with the help of an appropriate example. **(3 marks)**

- Diagnostic biomarker: To identify a disease or disease conditions. Wide range of test of disease identifications and level of severity.
- Prognostic biomarker: To predicting outcome of treatment or survival probability of patients (e.g., risk prediction). Important to understand advantage of a treatment.

Examples can be different, so check accordingly.

Question 12. List the major factors that contribute to the function for potential energy calculations. **(2 marks)**

Bond stretching, Angle bending, Dihedral torsion, H-bonding, van der Waals interactions, Electrostatic interactions.

Atleast 4 should be there.

Question 13. Which of the following are untrue about template selection step? Justify your answer. **(2 + 3 marks)**

- a) The first step in protein structural modeling is to select appropriate structural templates
- b) This forms the foundation for rest of the modeling process.

c) There is no use of heuristic alignment search programs.

Justification: BLAST, a heuristic alignment approach, is used to search for homologous protein structure to be used as a template. (Mentioning BLAST is important)

d) The template selection involves searching the non-redundant protein sequence database for homologous proteins to be used as templates.

Justification: The template selection involves searching the Protein data bank.