ourdiu.com | Shared by Md. Oliul Islam Bappy

Daffodil International University

Faculty of Science & Information Technology

Department of Computer Science & Engineering

Final Examination, Summer 2025

Course Code: CSE115 Course Title: Introduction to Biology and Chemistry for Computation

Level: 1 Term: 1 Batch: 69

Time: 02:00 Hrs **Marks: 40**

Answer ALL Questions

[The figures in the right margin indicate the full marks and corresponding course outcomes. All portions of each question must be answered sequentially.]

1.	Mr. Max is analyzing the Pentane (C_5H_{12}) molecule using molecular mechanics to determine its total potential energy. He has gathered data for various energy components involved in the system, which include bond stretching energy of 2.5 kcal/mol, angle bending energy of 1.8 kcal/mol, torsional energy of 3.0 kcal/mol, and non-bonded interaction energy of 0.7 kcal/mol. As part of his analysis, he rotates one of the methyl groups around the central carbon–carbon bond and records how the torsional energy varies with the dihedral angle. He observes that the torsional energy is 3.0 kcal/mol at 0°, 120°, 240°, and 360°, while it drops to 0.0 kcal/mol at 60°, 180°, and 300°.			
	a)	**Define** Energy Minimization. Compute the total potential energy of the Pentane molecule using the given data.	**[4]**	**CO2**
	b)	**Plot** the torsional energy versus dihedral angle graph and **explain** which conformations are most and least stable based on the trends shown in the plot and the given data.	**[6]**	
2.	You are working in a bioinformatics lab tasked with storing genome data efficiently while monitoring cancer-related mutations in patients. The patient's DNA sequence has already been transformed using the Burrows-Wheeler Transform (BWT) for storage efficiency. You are given the original reference sequence before mutation: AGCTGA and the BWT of the patient's mutated sequence: AATTGG$GA AG$GTAATG			**CO3**
	a)	**Apply** LF mapping to retrieve the mutated genome from the BWT. Then **Generate** the Burrows-Wheeler Matrix from the calculated mutated sequence.	**[7]**	
	b)	**Compare** the recovered genome with the original and **classify** the types of mutations observed.	**[3]**	

ourdiu.com | Shared by Md. Oliul Islam Bappy

3.	Dr. Khalid, a bioinformatician, and Dr. Rehnuma, a computational physicist, are decoding a noisy signal intercepted from a distant star system. The transmission appears to contain both DNA-like sequences and symbolic message fragments. Khalid is responsible for extracting all occurrences of the nucleotide T from the DNA-like portion of the signal: T C A G C A T G A G C A G T T T C T G C T A G G He should have extracted TTTTTTT, but his system returned TATTTGT. On the other hand Dr. Rehnuma studies a symbolic part of the signal. She compares the query QWERTYU with the known alien fragment XDTWERTYUQ using k = 1 to find matching symbols.			CO3
	a)	Analyze the model's performance by calculating and interpreting the Selectivity and Sensitivity based on Khalid's extraction results.	[4]	
	b)	Choose a suitable algorithm that Dr. Rehnuma used to show the match between the query sequence and the target sequence, and find out at what positions the sequences match.	[6]	
4.	Dr. Nadia Malik, a molecular geneticist, is investigating two short DNA sequences retrieved from different ancient bacterial genomes. She suspects these sequences may contain conserved short segments of DNA that could be functionally important due to evolutionary conservation. She applies an alignment strategy usihg the Smith-Waterman algorithm. She uses the following scoring scheme: **Match:** +2 **Mismatch:** –1 **Gap penalty:** –2 **Sequence 1 (S1):** G G G A T T G **Sequence 2 (S2):** A A T T C G G			
	a)	Apply the sequence alignment algorithm to find the best possible alignments. Then find the alignment score matrix and calculate the optimal similarity score based on the given scoring scheme.	[10]	CO3