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Daffodil International University

Department of Computer Science and Engineering

Faculty of Science & Information Technology

Final Examination, Fall-2023

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

Level:1 Term: 1 Batch: All

Time: 2 Hours **Marks: 40**

Answer ALL Questions [Optional]

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

1.	*a)*	You are a young and passionate physicist working in a world-renowned research institute, where you have access to cutting-edge equipment and collaborate with brilliant minds in your field. In your research, you are investigating a groundbreaking and elusive phenomenon in the realm of Computational Chemistry. If you could design a novel computational chemistry method that doesn't exist yet, what would it be, and how would it revolutionize our understanding of molecular interactions and chemical reactions? **Explain** its theoretical underpinnings and potential applications. **Differentiate** its significance and characteristics from other methods like DFT, Hartree-Fock or semi-empirical methods?	[7]	CO2
	b)	**Explain** Energy Minimization. **Describe** Energy Minimization with respect to Molecular mechanics.	*[3]*	
2.		You are a bioinformatics researcher working on a project that involves comparing the DNA sequences of two closely related species of butterflies to study their evolutionary relationships. The goal of your project is to identify similarities and differences in the DNA sequences, which will help you understand the genetic basis of their unique color pattern. For this purpose, **apply** the **Needleman-Wunsch** algorithm for the following sequences. **Determine** the alignment with the highest score and provide the resulting alignment. First Species: **AGCGAAT** Second Species: **AGCTAA** *Match Score: (last digit of your id)%3* *Mismatch Score: -1* *Gap Penalty: -2*	[7]	CO3
3.		The BWT is a data transformation algorithm that restructures data in such a way that the transformed message is more compressible.The idea of this method is to build an array whose rows are all cyclic shifts of the input string in dictionary order and return the last column of the array that tends to have long runs of identical characters.		CO3

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	A sequence is given below- **ATTGAA**			
	a)	**Construct** a Borrower Wheeler Matrix (BWM) for the given sequence.	**[5]**	
	b)	**Apply** LF mapping on the Borrower Wheeler Matrix (BWM) found at solution of question 3(a)	**[5]**	
	c)	**Determine** the significance of the '**$**' sign embedded in the text in BWT?	**[3]**	
4.	You are a bioinformatician working on a research project in a genomics laboratory. Your project involves the identification of specific genes responsible for a rare inherited disorder. To achieve this, you have a dataset containing a vast number of DNA sequences obtained from individuals affected by the disorder and a set of reference genomes. You decide to apply an algorithm which will compare the sequences and find similarities and dissimilarities among them. Two of the sequences are given below Query Sequence: ATCCTCGCGCCTCATCTA Target Sequence: TTCGCGCAGCGTAGAGGGT			**CO3**
	a)	**Identify** the appropriate algorithm and **apply** it on the given sequences.	**[10]**	