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Daffodil International University

Department of Computer Science and Engineering

Faculty of Science & Information Technology

Midterm Examination, Fall 2023

Course Code: CSE 115, Course Title: Introduction to Biology and Chemistry for Computation

Level: 1 Term: 1 Batch: All

Time: 01:30 Hrs **Marks: 25**

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.	**Explain** the benefits of computational chemistry in the field of scientific research and drug discovery. Provide at least three key advantages, each briefly described.	[5]	CO1
2.	You are a lead scientist at a cutting-edge biotechnology research lab. Your team is currently working on a groundbreaking project that involves sequencing the DNA of a rare and elusive species of deep-sea microorganisms. These microorganisms have unique genetic adaptations that allow them to thrive in extreme underwater conditions, making them of great interest to scientists studying extremophiles. Being an extraordinary researcher, you decided to apply a classic sequencing technique that was developed in 1977 for identifying the gene sequence. ***Identify*** the process and **describe** it step by step with appropriate figure	[7]	CO1
3.	You are a research scientist at a leading pharmaceutical company tasked with designing a new drug molecule to combat a rapidly spreading infectious disease. The success of your project relies on understanding the molecular interactions between the drug candidate and the target protein responsible for the disease. Primarily you will have to find out the molecular orbital energy where bond-breaking and bond forming energies play a crucial part. However, you must choose between two different computational approaches: molecular mechanics and quantum mechanics.		CO2
	a) **Explain** the equation for finding out the total potential energy of the molecule.	[3]	
	b) **Distinguish** between molecular mechanics and quantum mechanics and choose one of these for your research.	[5]	
4.	You are a production manager at a large chemical manufacturing facility. The plant produces various chemical products through a complex and interconnected series of reactors, distillation columns, and storage tanks. Considering you have optimum facilities you have established a top-down system where the system will react to sudden changes in the process of the plant and regardless of that change the system will be running smoothly. **Implement** DCS for the above mentioned situation using supporting diagrams.	[5]	CO4