Daffodil International University

Department of Computer Science and Engineering (CSE)

Course Outline

Course Code:	CSE 115		
Course Title:	Introduction to Biology & Chemistry for Computation		
Program:	B.Sc. in Computer Science and Engineering		
Faculty:	Faculty of Science and Information Technology (FSIT)		
Semester:	Fall	**Year:**	2024
Credit:	3.0	**Contact Hour:**	3 Hrs/Week
Course Level:	L1-T1	**Prerequisite:**	None
Course Category:	Core Engineering		
Instructor Name:	Faria Nishat Khan		
Designation:	Lecturer		
Email:	farianishat.cse@diu.edu.bd		
Office Address:	Room#505, Knowledge Tower		

Course Content (from syllabus):

Introduction to Biology and Chemistry for Computation is a 3-credit mid-level course that introduces the basic concepts of Biology and Chemistry. As one of the important subject areas of the study of computer science and information systems, this course will focus on the theoretical aspects as gene, genome, DNA, RNA and Protein and also atom, chemical bonding, chemical reactions, acids and bases, pH, neutralization, titration, nuclear changes, radiation etc. Computational biology focuses on DNA sequence and alignment technique, database searching: read mapping, gene duplication & FASTA algorithm. Different computational chemistry methods: Molecular mechanics, quantum mechanics are core knowledge to learn in this platform. This course also explores the inner workings of a biological world from the programmer's perspective by implementing different algorithms of Computer Science.

Course Description/Rationale:

To explore a new area of expertise that emerged from a fertile field- the combination of biology, chemistry and information sciences. It also exposes the reader to the fascinating structure of biological data and explains how to treat related combinatorial and statistical problems. This describes the mathematical structure of biological data, especially from sequences and chromosomes. This course will give a prologue to field DNA sequencing and searching algorithms along with different computational chemistry methods (e.g.: molecular mechanics, quantum mechanics, etc.

Course Objective:

To provide a solid conceptual understanding of the fundamentals of Biology and Chemistry for computation. More specifically,

- To provide a solid conceptual understanding of the fundamentals of Introduction to Biology & Chemistry for Computation. More specifically,
- To learn the basic concepts of molecular and cellular biology.
- To learn the differentiation between molecular mechanics & quantum mechanics.
- To learn the importance of computational chemistry in chemical industries.
- To learn DNA sequence alignment Technique.
- To learn implementation of different searching algorithms in Computational Biology.

Course Outcome (CO): at the end of the course, students will be able to do**:**

CO1	**Illustrate** molecular & cellular biology and identify impacts/benefits of computational chemistry and Biology.
CO2	**Classify** different Computational Biology and Chemistry methods and consider the applications in real life and industry centric scenarios.
CO3	**Demonstrate** their effective knowledge of different Computational Biology Algorithms and experiment with real life scenarios

Content of the course:

Week	Course Content (as summary)	Hrs	COs
1	Introduction and Scope of Computer in Chemistry and Biology.	2.5	CO1
2	Molecular and Cellular Biology	2.5	CO1
3	DNA and RNA structural details and application	2.5	CO1
4	Role of chemistry in computer science & engineering and Computational Chemistry Methods	2.5	CO2
5	Molecular Mechanics & Molecular Dynamics basics and various methods	2.5	CO2
6	Quantum Chemistry Methods	2.5	CO2
7	Importance and real life applications of Computational Chemistry Methods.	2.5	CO2
8	Different DNA Sequence Techniques	2.5	CO3
9	Review of Week 1-8	2.5	CO1, CO2
10	DNA Sequence Alignment (Global Alignment)	2.5	CO3
11	DNA Sequence Alignment (Local Alignment)	2.5	CO3
12	Importance of Computation in Chemical Industries	2.5	CO3
13	Gene Duplication Mutation and Read Mapping	2.5	CO3
14	Genome Indexing, Confusion Matrix, Selectivity Sensitivity	2.5	CO3
15	DNA Database Searching	2.5	CO3
16	Review of Week 1-15	2.5	CO1, CO2, CO3
	Total	**48**	

Teaching Learning Activity:

TLA	Activity
TLA1	Brainstorming and peer discussion.
TLA2	Class lecture
TLA3	Video lecture and virtual practice tool
TLA4	Hands on simulative practice

Mapping of CO with PO's, TLA's, Blooms Domain, KP's, EP's and EA's

COs	POs	Teaching Learning Activity	Assessment Strategy	Blooms Taxonomy Domains and Levels	Knowledge Profile (WK)	Complex Engineering Problem (EP)	Complex Engineering Activity (EA)
CO1	PO1	TLA1, TLA2, TLA3,	Quiz, Assignment, Mid-term	C3	K1-K4	EP1	
CO2	PO4	TLA1, TLA2,	Quiz, Assignment, Mid-term, Final Exam	C4	K8	EP1 & EP2	
CO3	PO5	TLA1, TLA2, TLA3, TLA4	Quiz, Assignment, Mid-term, Final Exam	C3	K6	EP1 & EP7	

Bloom's Taxonomy Cognitive Domain	Knowledge Profile	CEP Attributes	CEA Attributes
C3: Apply *C5: Evaluate*	*K1-K4: Engineering Knowledge* *K6: Modern Tool Usage* *K8: Investigation*	*EP1: Depth of knowledge required.* *EP2: Conflicting Requirement* *EP7: Interdependence*	

Justification of CO-PO Mapping:

- The **CO1** directly aligns with the **PO1** by illustrating molecular and cellular biology, which is a fundamental aspect of engineering knowledge, especially in fields like bioengineering or biomedical engineering. It requires a deep understanding of biological principles and their applications
- The **CO2** and **PO4** demonstrate the applications in real life and industry-centric scenarios involves an investigative aspect, exploring how these methods are practically applied. This aligns with the PO related to conducting investigations of complex problems using research-based knowledge.
- The **CO3** and **PO5** consider the algorithms to be modern tools in the context of computational biology. This PO involves creating, selecting, and applying

appropriate techniques and modern tools, which aligns with the use of algorithms.

Justification of Knowledge Profile (KP) Mapping:	
CO1	Ensuring the theory-based understanding of natural sciences, mathematical and computational support for analysis and specialist knowledge of Computational Chemistry and Biology
CO2	Classifying computational methods and applying them in real-life scenarios involves engaging with and understanding the current research literature in the discipline.
CO3	Demonstrating knowledge of computational biology algorithms and experimenting in real-life scenarios involves applying engineering practices and technologies in the field

Justification of Complex Engineering Problem (CEP) Mapping (if you address PO1-PO7):	
CO1	Illustrating molecular and cellular biology and understanding computational chemistry and biology require in-depth knowledge of specific field, aligning with the need for a fundamentals based, first principles analytical approach
CO2	Classifying computational methods and applying them in real-life scenarios involves not only in-depth engineering knowledge but also navigating wide-ranging or conflicting technical and engineering issues
CO3	Demonstrating and experimenting with computational biology algorithms require deep engineering knowledge and tackling high-level problems with many component parts or sub-problems
Justification of CO and Learning Domains Mapping:	
CO1	**Applying**: Illustrating molecular and cellular biology and identifying the impacts and benefits of computational chemistry and biology involve **applying** knowledge to demonstrate understanding
CO2	**Analyzing**: Classifying computational methods and considering their applications requires **analyzing** information and breaking it down into components
CO3	**Applying:** Demonstrating knowledge of computational biology algorithms and experimenting with real-life scenarios involves **applying** theoretical concepts to practical situations

Course Delivery Plan/Lesson Delivery Plan:

Week/Lesson (hour)	**Discussion Topic and Book Reference**	**Student Activities during Online and Onsite**	**Mapping with CO and**	**Assessment Plan**

		[course teacher will decide based on the type of the contents]	**PO**	
Week-1 Lesson 1 & 2 [3 Hours]	**Lesson 1:** Overview of chemistry & biology already they have learned which will help to introduce the course. **Lesson 2:** Scope of Computer in Chemistry and Biology.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO1 PO1	Class Test, Assignment , Midterm
Week-2 Lesson 3 & 4 [3 Hours]	**Lesson 3:** Molecular and Cellular Biology (Cell Structure & Basics) **Lesson 4:** Nucleotide, DNA & RNA Structure, understanding ligand in DNA double helix structure.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO1 PO1	Class Test, Assignment , Midterm
Week-3 Lesson 5 & 6 [3 Hours]	**Lesson 5:** RNA Types & Their Applications. **Lesson 6:** DNA Replication & Visualization,	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO1 PO1	Class Test, Assignment , Midterm
Week-4 Lesson 7 & 8 [3 Hours]	**Lesson 7:** Role of chemistry in computer science & engineering (Uses and effects of chemistry Benefits of Chemistry, Applications of Chemistry Reference). **Lesson 8:** Computational Chemistry Methods (Classical & Quantum Methods)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO2 PO4	Class Test, Assignment , Midterm
Week-5 Lesson 9 &	**Lesson 9:** Molecular Mechanics & Molecular	Brainstorming sessions,	CO2 PO4	Class Test, Assignment

10 [3 Hours]	Dynamics Methods. **Lesson 10:** Schrödinger equation & Wave Function	Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		, Midterm
Week-6 Lesson 11 & 12 [3 Hours]	**Lesson 11:** Quantum Chemistry Methods (Ab Initio Methods, Density Functional Methods) **Lesson 12:** Quantum Chemistry Methods (Semiempirical Methods & Difference between them)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO2 PO4	Class Test, Assignment , Midterm
Week-7 Lesson 13 & 14 [3 Hours]	**Lesson 13:** Real life applications of Computational Chemistry Methods. **Lesson 14:** Importance of Computation in Chemical Industries (DCS, Chromatography, etc.).	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO2 PO4	Class Test, Assignment , Midterm
Week-8 Lesson 15 & 16 [3 Hours]	**Lesson 15:** DNA Sequence Technique (Sanger Method) **Lesson 16:** Difference between other DNA Sequencing Techniques	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO2 PO4	Class Test, Assignment , Midterm
Week-9 Lesson 17 & 18 [3 Hours]	**Lesson 17:** Review class on the topics discussed in Week-1 – Week-4. **Lesson 18:** Review class on the topics discussed in Week-5 – Week-8.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO1, CO2, PO1, PO4	Class Test, Assignment , Midterm
Week-10 Lesson 19 & 20 [3 Hours]	**Lesson 19:** Sequence Alignment Basics. **Lesson 20:** Global Alignment Method and	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture	CO3 PO5	Class Test, Assignment , Final Exam

	example regarding DNA sequence alignment.	video, Lecture note, Open discussion.		
Week-11 Lesson 21 & 22 [3 Hours]	**Lesson 21:** Local Alignment Basics & Method Description **Lesson 22:** How the Local and Final Exam Global Alignment methods Relate with Problem Solving in Computer Science	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO3 PO5	Class Test, Assignment , Final Exam
Week-12 Lesson 23 & 24 [3 Hours]	**Lesson 23:** Importance of Computation in Chemical Industries (Fertilizer, Water Treatment, Chemical Plant) **Lesson 24:** Presentation on Selected Topics.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO3 PO5	Class Test, Assignment , Final Exam
Week-13 Lesson 25 & 25 [3 Hours]	**Lesson 25:** Mutation, Gene Duplication (Homolog, Ortholog, Paralog and Speciation) **Lesson 26:** Read Mapping (keyword Tree, Suffix Tree, Suffix Array)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO3 PO5	Class Test, Assignment , Final Exam
Week-14 Lesson 27 & 28 [3 Hours]	**Lesson 27:** Genome Indexing (Burrows Wheeler Transform (BWT), LF Mapping) **Lesson 28:** Discussing Confusion Matrix (TP, TN, FP, FN), Selectivity & Sensitivity	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CO3 PO5	Class Test, Assignment , Final Exam
Week-15 Lesson 29 & 30 [3 Hours]	**Lesson 29:** DNA Database Searching (Hash function) and applications of it. **Lesson 30:** DNA Database Searching (FASTA Algorithms)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open	CO3 PO5	Class Test, Assignment , Final Exam

		discussion.		
Week-16 Lesson 31 & 32 [3 Hours]	**Lesson 31:** Review class on topic discussed in Week-1 – Week-8 **Lesson 32:** Review class on topic discussed in Week-10-Week-15	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	–	Class Test, Assignment, Final Exam

Assessment Pattern:

Assessment Task	CO's					Mark (Total=100)
	CO1	CO2	CO3	CO4	CO5	
Attendance	--	--	--	--	--	7
Class Test (CT1, CT2, CT3)	--	--	--	--	--	15
Assignment	--	--	--	--	--	5
Presentation	--	--	--	--	--	8
Midterm Examination	5	5	5	10	--	25
Semester Final Examination	5	10	10	15	--	40
Total Mark	10	15	15	15	--	100

CIE – Breakup (Theory) [60 marks]

Bloom's Criteria	Attendance (07)	Class Test (15)	Assignment (05)	Presentation (08)	Mid Exam (25)
Remember		02			2.5
Understand		05	02	02	7.5
Apply		05		03	12.5
Analyze		03	03	03	2.5
Evaluate					
Create					

SEE – Semester End Examination [40 marks] {Theory}

Bloom Criteria	Score for the Test
Remember	05
Understand	10

Apply	20
Analyze	05
Evaluate	-
Create	-

Learning Materials:

Textbook/Recommended Readings:

1. Introduction to Computational Chemistry by Frank Jensen.
2. An Introduction to Bioinformatics Algorithms by Neil C. Jones and Pavel A. Pevzner

Reference Books/Supplementary Readings:

1. Introduction to Bioinformatics by Arthur Lesk
2. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics by Errol G. Lewars.