

<b>Course Code: CSE 115</b>	<b>CIE Marks: 60</b>
<b>Course Title: Introduction to Biology &amp; Chemistry for Computation</b>	<b>SEE Marks: 40</b>
<b>Credits: 3</b>	

### **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 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 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 importance of computational chemistry in chemical industries.
- To learn DNA sequence alignment Technique.
- To learn implementation of different searching algorithms in Computational Biology.

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

CLO1	Illustrate molecular & cellular biology and identify impacts/benefits of computational chemistry and Biology.
CLO2	Classify different Computational Chemistry methods and consider the applications in real life.
CLO3	Demonstrate different Algorithms related to Computational Biology and experiment with real life scenario.
CLO4	Identify importance of computation in Chemical Industries.

**Content of the course:**

SL	Course Content (as summary)	Hrs	CLO's
1	Overview and real-life applications of computational biology & chemistry	6	CLO-1
2	Molecular and Cellular Biology, Nucleotide, DNA & RNA Structure, DNA replicational and sequence technique	9	CLO-2
3	Schrödinger equation, different computational chemistry methods & applications in chemical industries	6	CLO-3
4	DNA sequence alignment techniques & their differences, DNA Database Searching algorithms, Read mapping & genome indexing,	24	CLO-3, CLO-4

**Mapping of Course Learning Outcomes to Program Learning Outcomes [attainment level used for CLO's from 1(weak)-3(strong) correlation]**

	PLO-1	PLO-2	PLO-3	PLO-4	PLO-5	PLO-6	PLO-7	PLO-8	PLO-9	PLO-10	PLO-11	PLO-12
CLO-1		✓										
CLO-2				✓								
CLO-3	✓											
CLO-4			✓									

**Mapping Course Learning Outcome (CLOs) with the Teaching-Learning and Assessment Strategy:**

CLO's	Teaching Learning Strategy	Assessment Strategy	Corresponding PLO number	Domain Level/ Learning Taxonomy
	[course teacher will decide based on the type of the contents]			
CLO-1	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video,	Class Test/Assignment/ Midterm examination	PLO-2	L2

	Lecture note, Open discussion			
<b>CLO-2</b>	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion	Class Test/Assignment/ Midterm examination	PLO-4	L2, L3
<b>CLO-3</b>	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion	Class Test/Assignment/ Final examination	PLO-1	L2
<b>CLO-4</b>	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion	Class Test/Assignment/ Final examination	PLO-3	L5

**Course Delivery Plan/Lesson Delivery Plan:**

<b>Week/Lesson (hour)</b>	<b>Discussion Topic and Book Reference</b>	<b>Student Activities during Online and Onsite</b> [course teacher will decide based on the type of the contents]	<b>Mapping with CLO and PLO</b>	<b>Assessment Plan</b>
<b>Week-1</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Overview of chemistry & biology already they have learned which will help to introduce the course.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-1, PLO-2	Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Scope of Computer in Chemistry and Biology.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-2</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Molecular and Cellular Biology (Cell Structure & Basics)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Nucleotide, DNA & RNA Structure, understanding ligand in DNA double helix structure.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture		

		video, Lecture note, Open discussion.		
<b>Week-3</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> RNA Types & Their Applications.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Midterm
	<b>Lesson 2:</b> DNA Replication & Visualization,	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-4</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Role of chemistry in computer science & engineering (Uses and effects of chemistry Benefits of Chemistry, Applications of Chemistry Reference).	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Computational Chemistry Methods (Classical & Quantum Methods)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-5</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Molecular Mechanics & Molecular dynamics Methods.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-2 PLO-4	Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Schrödinger equation & Wave Function	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-6</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Quantum Chemistry Methods (Ab Initio Methods, Density Functional Methods)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Quantum Chemistry Methods (Semi-empirical Methods & Difference between them)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture		

		video, Lecture note, Open discussion.		
<b>Week-7</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Real life applications of Computational Chemistry Methods.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-4 PLO-3	Class Test, Assignment, Midterm
	<b>Lesson 2:</b> Importance of Computation in Chemical Industries (DCS, Chromatography, etc.).	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-8</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> DNA Sequence Technique (Sanger Method)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-3 PLO-1	Class Test, Assignment, Midterm Exam
	<b>Lesson 2:</b> Difference between other DNA Sequencing Techniques	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-9</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Review class on topic discussed in Week-1 - Week-4.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	--	None
	<b>Lesson 2:</b> Review class on topic discussed in Week-5 - Week-8.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-10</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Sequence Alignment Basics.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-3 PLO-1	Class Test, Assignment, Final Exam
	<b>Lesson 2:</b> Global Alignment Method and example regarding DNA sequence alignment.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		

<b>Week-11</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Local Alignment Basics & Method Description	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Final Exam
	<b>Lesson 2:</b> How the Local and Global Alignment methods Relate with Problem Solving in Computer Science	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-12</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Importance of Computation in Chemical Industries (Fertilizer, Water Treatment, Chemical Plant)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-4 PLO-1	Class Test, Assignment, Final Exam
	<b>Lesson 2:</b> Presentation on Selected Topics.	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-13</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Mutation, Gene Duplication (Homolog, Ortholog, Paralog and Speciation)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		Class Test, Assignment, Final Exam
	<b>Lesson 2:</b> Read Mapping (keyword Tree, Suffix Tree, Suffix Array)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-14</b> Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Genome Indexing (Burrows Wheeler Transform (BWT), LF Mapping)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	CLO-3 PLO-1	Class Test, Assignment, Final Exam
	<b>Lesson 2:</b> Discussing Confusion Matrix (TP, TN, FP, FN), Selectivity & Sensitivity	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-15</b>	<b>Lesson 1:</b> DNA Database Searching (Hash function) and applications of it	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture		

Lesson 1 & 2 [3 Hours]		video, Lecture note, Open discussion.		
	<b>Lesson 2:</b> & DNA Database Searching (FASTA Algorithms)	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		
<b>Week-16</b>  Lesson 1 & 2 [3 Hours]	<b>Lesson 1:</b> Review class on topic discussed in Week-1 - Week-8	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.	--	None
	<b>Lesson 2:</b> Review class on topic discussed in Week-10-Week-15	Brainstorming sessions, Classroom discussion, Voice over PPT, Lecture video, Lecture note, Open discussion.		

#### 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	10	5	5	5	--	25
Semester Final Examination	0	10	20	10	--	40
Total Mark	10	15	25	15	--	100

**CIE – Breakup (Theory) [60 marks]**

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

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

Bloom Criteria	Score for the Test
Remember	05
Understand	05
Apply	10
Analyze	10
Evaluate	05
Create	05

**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.