

Course Code	Course Name	Credits
26CH006	CHEMICAL BIOLOGY AND COMPUTATIONAL TOOLS	04

Course Objectives

- Apply soft computing tools and digital resources for chemical structure drawing, referencing, scientific writing, and academic integrity.
- Understand the structure, synthesis, and reactions of amino acids, peptides, and proteins, including methods of analysis.
- Analyze the chemistry and biological importance of natural products such as alkaloids, terpenoids, and steroids.
- Explain the structure and function of bioinorganic systems, including metalloproteins, ion transport, and metal-based drugs in biological processes.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Use digital and soft computing tools in chemistry.
- Understand amino acids, proteins, and their synthesis.
- Explain natural products like alkaloids, terpenoids, and steroids.
- Describe bioinorganic systems and their biological roles.

Unit 1 - Amino acids and Proteins (12 Hrs.)

List of amino acids and their structures; preparation of amino acids; reactions of amino acids; synthesis of dipeptides—protection, activation, and deprotection; Merrifield solid-phase synthesis; classification of proteins; terminal residue analysis—N-terminal (Edman degradation method) and C-terminal analysis (enzymatic and chemical methods); primary, secondary, and tertiary structures of proteins.

Unit 2 – Alkaloids, Terpenoids, and Steroids (12 Hrs.)

Introduction to alkaloids; classification, occurrence, and isolation; structural elucidation of papaverine and nicotine; structures of alkaloids—quinine, morphine, atropine, nicotine, coniine, piperine, and papaverine; classification and definition of terpenoids; isoprene rule; structure and uses of selected essential oils; structural elucidation of geraniol; structure and functions of steroids—androgens, estrogens, and cholesterol.

Unit 3 - Bioinorganic Chemistry-I (12 Hrs.)

Structure and function of chlorophyll; photosystem I and photosystem II; light reactions and dark reactions; Mn-catalyzed oxidation of H_2O to O_2 in chlorophyll; role of Mg^{2+} ion; structure and function of haemoglobin; cooperative effect in haemoglobin; role of globin; structure and function of myoglobin; structure and function of cytochrome C.

Unit 4 – Bioinorganic Chemistry-II (12 Hrs.)

Structure and function of blue copper proteins; Structure and function of vitamin B12; In vitro and in vivo nitrogen fixation; Fe-S proteins; Ionophores; Ion transport mechanism in cell membrane; Na^+/K^+ pump; Role of metal ions in DNA replication, transcription, and translation; Cis-platin and its mode of action in cancer treatment.

Unit 5 - Soft Computing in Chemistry (12 Hrs.)

Chemical Structure Drawing Tools (Origin, ChemSketch, ChemDraw); Reference Management Software (Zotero, Mendeley); Software for Paper Formatting (LaTeX, MS Office); Plagiarism Detection Software; Paraphrasing Tools; Humanizer Tools; AI Detection Tools

Reference Books:

1. R.T Morrison and R N Boyd Organic Chemistry, 7th Edition, 2011 Allyn and Bacon Ltd., New York.
2. P Y Bruice, Organic Chemistry, 8th Edition, 2011 Pearson Ltd., University of California, Santa Barbara.
3. I.L Finar , Organic Chemistry, Vol: 1 and 2, 1996 6th Edition, Addison Wesley Longman Ltd. England.
4. L. Stryer L, J.M Berg, J LTymoczko and G. Gatto Biochemistry, 2019 9th Edition, W. H. Freeman and Company, New York.
5. D. Rodwell, D Bender and K. Botham , Harper's Illustrated Biochemistry, 2018 31st Edition, McGraw Hill Professional, New York.
6. J.E Huheey , E, Keiter and R.L Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 1993 4th Edition, Harper Collins College Publishers, New York.
7. I. Bertini, H B Gray, S J Lippard and J S Valentine , Bioinorganic Chemistry, 1994 University Science Books, California.

Websites and eLearning Sources:

1. <https://archive.nptel.ac.in/content/storage2/courses/104103018/module1/lec1/3.html>
2. <https://www.youtube.com/watch?v=OSBUn5Wg0Ko&list=PL3d77NsPK1JtN30kHrxFQxG7IqmUfoROL>
3. <https://www.youtube.com/playlist?list=PL3d77NsPK1JtN30kHrxFQxG7IqmUfoROL>

COs and Bloom's Taxonomy Mapping – 26CH006		
Course Outcomes	On completing U.G. program the students will be able to	BTL
CO1	Recall and explain concepts of soft computing tools in chemistry, biomolecules (amino acids and proteins), natural products, and bioinorganic systems.	K1, K2
CO2	Apply digital tools for structure drawing, referencing, and scientific writing; use chemical knowledge to interpret biomolecular structures and reactions.	K3
CO3	Analyze structures and functions of proteins, natural products, and bioinorganic molecules, including their roles in biological systems.	K4
CO4	Evaluate the applications of computational tools, natural products, and metal ions in chemical and biological processes.	K5
CO5	Design and present scientific content using appropriate software tools and propose solutions related to biomolecules and bioinorganic chemistry.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH006													
Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)						Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	1	3	2	1	2	1	2	3	1	2	1	1	1.66
CO2	2	3	2	3	2	1	2	3	1	3	1	1	2
CO3	3	2	2	2	1	2	3	1	2	3	1	1	1.91
CO4	3	2	1	2	1	2	1	2	2	2	2	1	1.75
CO5	1	2	3	1	2	1	2	1	2	1	2	3	1.75
Total													1.81

Mean Score: 3- High, 2- Medium/Moderate, 1-Low