Department of Bioinformatics

[VALUE ADDED COURSE (VAC)]

Regulations, Description and Syllabus

[For candidates admitted form the Academic year 2021onwards]

DEPARTMENTOFBIOINFORMATICS

(DST-FIST, DBT-BIC and PURSE Sponsored Department)

ALAGAPPAUNIVERSITY

(A State University Accredited with "A+" grade by NAAC (CGPA: 3.64) in the Third Cycle and Graded as Category-I University by MHRD-UGC)

KARAIKUDI-630003, TAMIL NADU, INDIA

DEPARTMENT: BIOINFORMATICS

ALAGAPPA UNIVERSITY, KARAIKUDI

(A State University Accredited with "A+" grade by NAAC (CGPA: 3.64) in the Third Cycle and Graded as Category-I University by MHRD-UGC)

M.Sc BIOINFORMATICS

(For those who join the Course in July 2021 onwards)

VALUE ADDED COURSE SYLLABUS

[For candidates admitted form the Academic year 2021 onwards]

Name of the Department	:	Bioinformatics
Name of the Subject Discipline	:	Bioinformatics
Program of Level	:	M.Sc
Course name	:	Value Added Course

Introduction: Value-added courses are part of the curriculum designed to impart the necessary skills to increase employability and equip students with the essential skills to succeed in life. The Department of Bioinformatics offers a variety of value added courses which are conducted after class hours (5.30-6.30 pm). These courses are conducted by in-house staff and help students stand out from the rest in the job market by adding value to their resume. These value-added courses are often independent of each type of department.

General Objectives of the Program: The general objective of the M.Sc program in Bioinformatics is to develop strong-minded graduates with high-quality skills in the field of Structural Bioinformatics and Computer Aided Drug Design. The curriculum designed is to assist the students in understanding the vital concept of fundamentals involved in the structure determination through various Molecular Biology, Biochemical and Cell Biology experimental methods with practical hands-on training in the usage of Bioinformatics tools for Drug Discovery. At the end of the program, the student will gain in-depth knowledge in Bioinformatics and play an active role in biological research, government or non-government organization, and private sectors.

Courses: 'Course' is a component (Department paper) of a programme. Each course offered by the Department is identified by a unique course code. A course contains lectures to meet effectively the teaching and learning needs.

The students have to undergo any one value added course in each semester ofered by Department of bioinformatics and the exam should be announced before the end of university exam.

General Objectives of the Course:

- To improve employability skills of students.
- To provide an opportunity to students develop their inter-disciplinary skills.
- To bridge the skill gaps and make students industry ready.

- To provide the novel information about form the course to the students.

Guidelines for conducting value added courses

- Value Added Course is not mandatory to qualify for any program.
- It is a teacher assisted learning course open to all students without any additional fee.
- The value added courses may be also conducted class hours (evening 5.30-6.30 pm) .
- A student will be permitted to register only one Value Added Course in each Semester.
- The students may be allowed to take value added courses offered by parent department offering the course.

Duration and Venue

The duration of value added course should not be less than 30 hours.

Value added course shall be conducted in the respective faculty itself.

Attendance

- Each faculty members shall be maintenance of for all courses Attendance and Assessment Record for candidates who have registered for the course.
- The record shall contain details of the students' attendance and marks obtained in the Internal Assessment Tests.
- The record shall be submitted to the Head of the Department once a month for monitoring the attendance and syllabus coverage.
- At the end of the semester, the record shall be duly signed by the Course Instructor and the Head of the Department and placed in safe custody for any future verification.
- Each student shall have a minimum of 75% attendance in all the courses of the particular semesterfailing which he or she will not be permitted to write the End-Semester Examination.

Medium of Instruction

The medium of instruction is English only.

Passing Requirement and Grading

- The passing requirement for value added courses shall be 40% of the marks prescribed for thecourse.
- A candidate who has not secured a minimum of 40% of marks in a course (internal and end-term) shall reappear for the course in the next semester/year.
- The grades obtained in course will not be included for calculating the CGPA.

Course Completion

- Learners will get a certificate after they have registered for, written the exam and successfully passed.

- The students who have successfully completed the Value Added Course shall be issued with a Certificate duly signed by the Authorized signatories.

S.No	Paper Code	Title of the Paper	Th/Pr	Hrs	Marks
FIRST YEAR (SEMESTER Ist & IInd)					
1	502VAC01	Plant Bioinformatics	Th/Pr	6	50
2	502VAC02	Pharmacoinformatics	Th/Pr	6	50
3	502VAC03	Cyber Security	Th/Pr	6	50
4	502VAC04	Computational Diagnosis of Human Diseases	Th/Pr	6	50
5	502VAC05	Recent Techniques in Biophysics	Th/Pr	6	50
SECOND YEAR (SEMESTER IIIrd & IVth)					
6	502VAC06	Cheminformatics	Th/Pr	6	50
7	502VAC07	Artificial Intelligence	Th/Pr	6	50
8	502VAC08	Immunoinformatics	Th/Pr	6	50
9	502VAC09	Microbial Genetics	Th/Pr	6	50
10	502VAC010	Medical Coding	Th/Pr	6	50
11	502VAC011	Synthetic Organic Chemistry	Th/Pr	6	50
12	502VAC012	Next Generation Sequencing Data Analytics	Th/Pr	6	50

Th-Theory, Pr-Practical

FIRST YEAR (SEMESTER Ist & IInd)

PLANT BIOINFORMATICS


Course Timeline: 30 Hrs

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Course Code	502VAC01	**Plant Bioinformatics**	**L**	**T**	**P**	**C**
Core/Elective/Supportive		**Value Added Course**				
Pre-requisite		**Basic Knowledge in Plant Bioinformatics**	**Syllabus Version**		**2021-2022**	

Course Objectives:

1. To provide an understanding of the importance of plant bioinformatics in the context of modern plant research.
2. To provide an understanding of the importance of phytochemicals and biophysical techniques in the context of modern plant research.
3. To provide an understanding of the importance of bioinformatics tools and software in the context of modern plant-based drug designing.
4. To provide an understanding of the importance of network pharmacology in the context of modern plant research.
5. To provide an understanding of the importance of network pharmacology in the context of modern plant research.

Expected Course Outcomes:

1.	Lead a way to understand the basics of plant bioinformatics and itsapplications in plant research.
2	Students will be able to appreciate the importance of phytochemicals andbiophysical techniques in the context of modern plant research.
3	Students will be able to use different databases and resources available forplant-based drug designing.

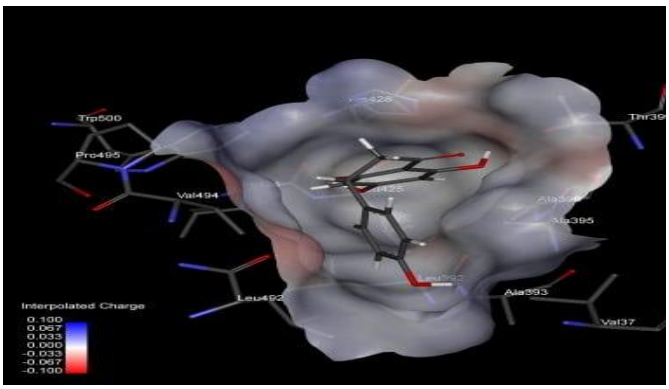
4	To be able to appreciate the importance of network pharmacology in thecontext of modern plant research.
5.	Students will be able to appreciate the importance of next-generationsequencing in the context of modern plant research.

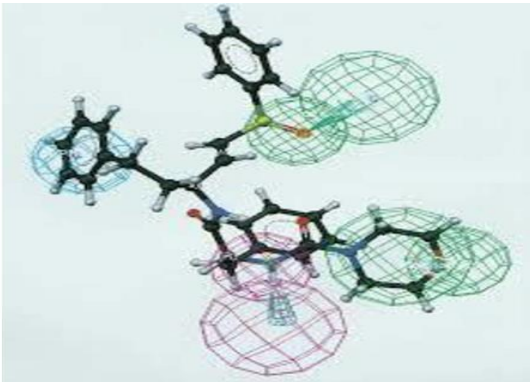
UNIT-I	**Introduction to Plant Bioinformatics**	**6 hours**
Overview, scope and applications of plant bioinformatics in understanding plant biology and drug discovery. Integration of computational tools and biological data, role of plant bioinformatics in analyzing and interpreting genomic information, and its advances of plant-based research.		
UNIT-II	**Phytochemicals and Biophysical Techniques**	**6 hours**
Types of phytochemicals and its significance, Phytochemistry, Role of phytochemicals in drug discovery, synthesis, extraction methods and potential health benefits. Techniques used for identification and quantification of compounds such as HPLC, GC-MS and FTIR, NMR, XRD, MS, LC-MS.		
UNIT-III	**Bioinformatics Tools and Software for Plant-Based Drug Designing**	**6 hours**
Tools and software used in plant-based drug designing. PubChem, ChEMBL, and Phyto Chem DB for data mining and compound selection. Application of molecular docking and virtual screening tools like AutoDock and Vina. Molecular dynamics simulation and modeling software such as GROMACS and AMBER.		
Unit-IV	**Network Pharmacology**	**6 hours**
Network pharmacology, complex interactions in biological networks. Construction and analysis of protein-protein interaction networks, metabolic pathways and their relevance in plant-based drug discovery.		
Unit-V	**Next Generation Sequencing in Plants**	**6 hours**
Introduction - Illumina sequencing, PacBio and Oxford Nanopore long-read sequencing. Principles and applications of next-generation sequencing (NGS) technologies in plant genomics - De novo genome assembly and annotation, Comparative genomics, Transcriptomics (RNA-seq), Epigenomics (ChIP-seq, bisulfite sequencing), Metagenomics. Data analysis tools and pipelines for NGS data.		
Total Lecture		**30 hours**

References:

1	Cagney, G., & Emili, A. (2011). Network biology: methods and applications. New York, NY: Humana Press.
2	Rao, V. (2012). Phytochemicals: a global perspective of their role in nutrition and health.
3	Choudhuri, S. (2014). Bioinformatics for beginners: genes, genomes, molecular evolution, databases and analytical tools.
4	Edwards, D. (2016). Plant Bioinformatics. Methods in Molecular Biology. Doi: 10.1007/978-1-4939-3167-5.
5	Müllertz, A., Perrie, Y., & Rades, T. (2016). Analytical techniques in the pharmaceutical sciences, (pp. 171-222). New York, NY, USA

PHARMACOINFORMATICS





Course Timeline: 30 Hrs

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Course Code	**502VAC02**	**Pharmacoinformatics**	**L**	**T**	**P**	**C**
Core/Elective/Supportive		**Value-Added Course**		**-**		
Pre-requisite		**Basic Knowledge of drug discovery**	**Syllabus Version**		**2020-23**	

Course Objectives:

The students will be able to understand the basics aspects of drug metabolism and delve into their kinetics and dynamics that are crucial in the functioning of the drugs.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Explain the basics of pharmacoinformatics and its application in medicine
2	Summarize the various biomolecules as drug targets
3	Retrieve data from the drug databases
4	Select the right approach to design molecules for a particular disease
5	Study the properties of drug metabolism in silico
6	Understand the mechanism of action of drugs

Unit-I	**Introduction**	**5 hours**

Basics of pharmacoinformatics: Definition, branches, scope and applications. Concepts of drugs: Classification, Major sources, Common filters for drugs design.

Unit-II	**Drug targets**	**6 hours**

Classification of drug targets: intrinsically disordered proteins, ions channels, chromatin-associated proteins, noncoding RNAs, membranes; Drug-target interactions, Drug-target network.		
Unit-III	**Drug Design**	**6 hours**
Concepts of drug design, Fragment based drug design, Artificial intelligence and Deep learning in drug design, Biomarkers in drug design.		
Unit-IV	**Pharmacokinetics**	**6 hours**
Overview, One-compartment model, Two-compartment model, Multi-compartment models, Pharmacokinetic parameters, Bioavailability.		
Unit-V	**Pharmacodynamics**	**6 hours**
Drug receptor action, direct physiological action, Drug-drug interactions, drug metabolism, Drug potency and efficacy, Therapeutic index.		
Total Lecture		**30 hours**

References

1.	Durai Ananda Elementary Pharmacoinformatics BSP 2014
2.	Tagelsir Mohamed Gasmelseid Pharmacoinformatics and Drug Discovery Technologies: Theories and Applications: Idea Group,U.S.; 1 edition 2012
3.	Sara E. Rosenbaum Basic Pharmacokinetics and Pharmacodynamics: An Integrated Textbook and Computer SimulationsWiley; 1 edition 2011
4.	Thomas N. TozerPharmD, Malcolm Rowland Introduction to Pharmacokinetics and Pharmacodynamics: The Quantitative Basis of Drug Therapy 1st Edition LWW; 1 edition

CYBER SECURITY

Course Timeline: 30 Hrs

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Course Code	502VAC03	Cyber Security	L	T	P	C
Core/Elective/Supportive		Value-Added Course		-	-	
Pre-requisite		Basic Knowledge in Cyber Security	Syllabus Version		2020-23	

Course Objectives:

- To offer an understanding of principle concepts, central topics and basic approaches in information and cyber security.
- To know the basics of cryptography.
- To acquire knowledge of standard algorithms and protocols employed to provide confidentiality, integrity and authenticity.
- To enhance awareness about Personally Identifiable Information (PII), Information Management, cyber forensics.

Expected Course Outcomes:

1	Gauge the security protections and limitations provided by today's technology.
2	Identify cyber security threats.
3	Analyze threats in order to protect or defend it in cyberspace from cyber-attacks.
4	Build appropriate security solutions against cyber-attacks

Unit-I	Introduction	6 hours

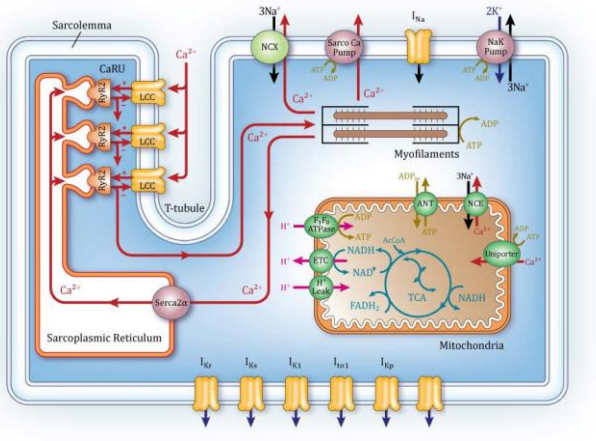
Introduction, Elements of Information Security, Security Policy, Techniques, Steps, Categories, Operational Model of Network Security, Basic Terminologies in Network Security. Threats and Vulnerability, Difference between Security and Privacy.

Unit-II	Data Encryption Techniques And Standards	6 hours
Introduction, Encryption Methods: Symmetric, Asymmetric, Cryptography, Substitution Ciphers. Transposition Ciphers, Stenography applications and limitations, Block Ciphers and methods of operations, Feistal Cipher, Data Encryption Standard (DES), Triple DES, Weak Keys in DES Algorithms, Advance Encryption Standard (AES).		
Unit-III	**Public Key And Management**	**6 hours**
Public Key Cryptography, RSA Algorithm: Working, Key length, Security, Key Distribution, Deffie-Hellman Key Exchange, Elliptic Curve: Arithmetic, Cryptography, Security, Authentication methods, Message Digest, Kerberos, X.509 Authentication service. Digital Signatures: Implementation, Algorithms, Standards (DSS), Authentication Protocol.		
Unit-IV	**Security Requirements**	**6 hours**
IP Security: Introduction, Architecture, IPV6, IPv4, IPSec protocols, and Operations, AH Protocol, ESP Protocol, ISAKMP Protocol, VPN. WEB Security: Introduction, Secure Socket Layer (SSL), SSL Session and Connection, SSL Record Protocol, Change Cipher Spec Protocol, Alert Protocol, Handshake Protocol. Electronic Mail Security: Introduction, Pretty Good Privacy, MIME, S/MIME, Comparison. Secure Electronic Transaction (SET).		
Unit-V	**Cyber Forensic, Hacking& its countermeasures**	**6 hours**
Personally Identifiable Information (PII), Cyber Stalking, Cybercrime, PII Confidentiality Safeguards, Information Protection Law: Indian Perspective. Hacking: Remote connectivity and VoIP hacking, Wireless Hacking, Mobile Hacking, countermeasures		
Total Lecture		**30 hours**

References

1.	William Stallings, “Cryptography and Network Security: Principles and Practice”, 7/e, Pearson, ISBN:9789332585225.
2.	https://pearsoned.co.in/web/books/9789332585225_Cryptography-and-Network-Security_William-Stallings.aspx
3.	Atul Kahate, “Cryptography and Network Security”, Mc Graw Hill Publication, 2nd Edition, 2008, ISBN : 978-0-07-064823-4
4.	Dr. V.K. Pachghare, Cryptography and Information Security, PHI, ISBN 978-81-303- 5082-3
5.	Nina Godbole,SunitBelapure, Cyber Security,Wiley India, ISBN:978-81-345-2179-1
6	PDF Digital Content : Stuart McCLURE, Joel Scambray, George Kurtz, Hacking Exposed Network Security Secrets and Solutions, McGrowHill, 2012 ISBN: 978-0-07-178028-5 Digital Ref: http://84.209.254.175/linux-pdf/Hacking-Exposed-7-Network-Security-Secrets.pdfCollege libraries are requested to purchase the copy

COMPUTATIONAL DIAGNOSIS OF HUMAN DISEASES



Course Timeline: 30 Hrs

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Course Code	**502VAC04**	**Computational Diagnosis of Human Diseases**	**L**	**T**	**P**	**C**
Core/Elective/Supportive		**Value-Added Course**		**-**	**-**	
Pre-requisite		**Basic Knowledge in Genetics and Artificial Intelligence**	**Syllabus Version**		**2020-23**	

Course Objectives:

The main objectives of this course are to:

1. To obtain knowledge about AI and ML.
2. To understand the need and application of computational approaches in disease diagnosis.
3. Analyze the future perspective of AI in Human Disease Diagnosis.

Expected Course Outcomes:

On the successful completion of the course, students will be able to:

1	Understand the computational perspective of Disease Diagnosis.
2	Apply the concept of deep learning to improve the genome editing technique
3	Analyzing the different kinds of tools available to predict genes and genetic variants responsible for human diseases.
4	Evaluate the application of computational techniques in the diagnosis of human diseases.
5	Create and Evaluate the Neural Network Model

Unit-I	**Computational Diagnosis of Common Diseases**	**6 hours**

Cancer, Diabetes, CVD, CKD - Identification of marker genes-similarity based searches- Ab-initio prediction- pathway analysis- Geneset Enrichment analysis- Molecular Network analysis.

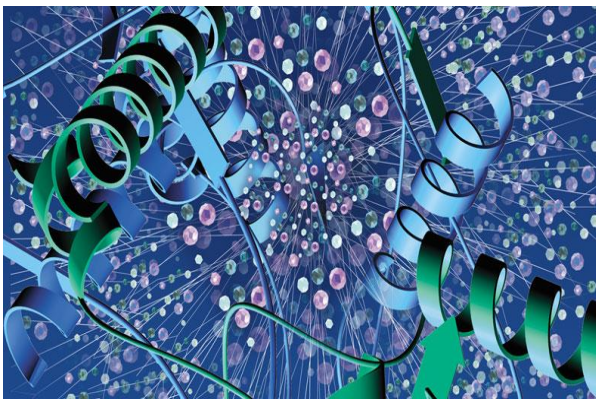
Unit-II	**Computational Diagnosis of Rare Diseases**	**6 hours**

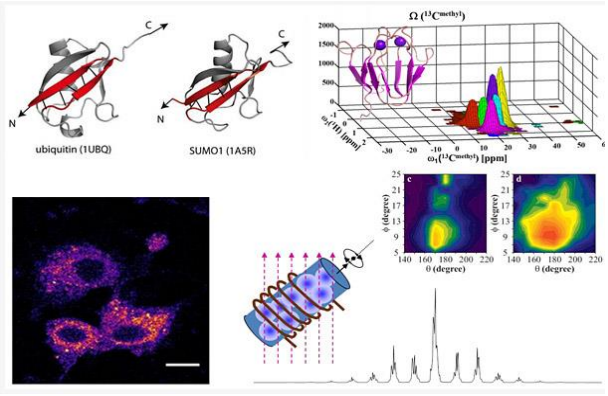
Parkinson's disease, Alzheimer's disease, and Muscular Dystrophy- gene enrichment analysis, Supervised/ Unsupervised based Gene selection, Interpreting genetic variants, and Analyzing DNA expression arrays, Clustering or Network Construction, Network Integration.		
Unit-III	**Computational Diagnosis of Mitochondrial Diseases**	**6 hours**
Mitochondrial encephalopathy, Maternally Inherited Diabetes and Deafness (MIDD) - Multi-Omics Data analysis, Gene Co-Expression network, Genome-scale metabolic modeling, Genome engineering (CRISPR-CAS)		
Unit-IV	**Computational Diagnosis of Severity/Vulnerability of Viral Diseases**	**6 hours**
H1N1, SARS COVID-Dataset Description, Feature selection, Convolutional Neural Network based model prediction-Model training, Model evaluation-Statistical analysis		
Unit-V	**Case study**	**6 hours**
Chronic Kidney Disease-Gene selection-Computational Identification of genetic variants- Deep Learning based Genome editing-Next Generation Sequencing Analysis		
Total Lecture & Practical hours		**30 hours**

References

1	Cannataro, M., Pietro Hiram Guzzi, Agapito, G., Zucco, C., & Milano, M. (2022). *Artificial Intelligence in Bioinformatics*. Elsevier.
2	Setubal, J. C., & Waldeyr Mendes Silva. (2020). *Advances in Bioinformatics and Computational Biology*. Springer Nature.
3	Mei, J., Desrosiers, C., & Frasnelli, J. (2021). Machine learning for the diagnosis of Parkinson's disease: a review of literature. *Frontiers in aging neuroscience*, *13*, 633752.
4	Glaab, E. (2018). Computational systems biology approaches for Parkinson's disease. *Cell and tissue research*, *373*, 91-109.
5	Jayaraj, J. M., Kuriakose, B. B., Alhazmi, A. H., & Muthusamy, K. (2021). Structural and functional insights on vitamin D receptor and CYP24A1 deleterious single nucleotide polymorphisms: A computational and pharmacogenomics perpetual approach. *Cell Biochemistry and Function*, 39(7), 874-885.
6	https://nptel.ac.in/courses/102106065

RECENT TECHNIQUES IN BIOPHYSICS





Course Timeline: 30 Hrs

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Course Code	502VAC05	Recent Techniques in Biophysics	L	T	P	C
Core/Elective/Supportive		Value-Added Course		-	-	
Pre-requisite		Basic Knowledge in Biophysics	Syllabus Version		2022-23	

Course Objectives:

The main objectives of this course are to:

1. Enlighten the students to have a glimpse of recent advances in biophysical techniques.
2. Understand the important role of Biophysics for better visualization in scientific Research.
3. Further, the interdisciplinary area of biophysics explains the interactions of biomolecules with electromagnetic radiations and biological phenomena in terms of physical and chemical properties of a molecule.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

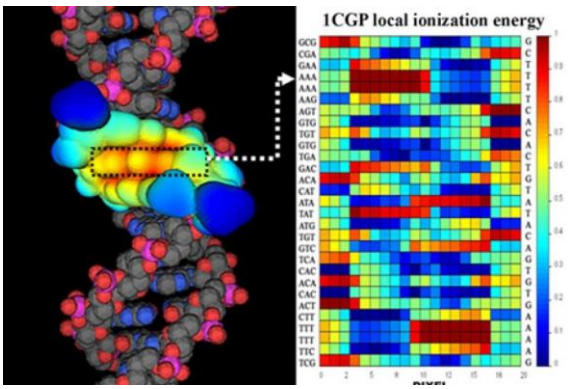
1	Understand the intricacies of future in depth knowledge about the functioning and applications on various biophysical techniques.
2	Identify the specializations they would like to opt for future and would also enhance their capabilities to understand various cutting-edge technologies.
3	Students will be exposed to the techniques and methods to elucidate the structure, function, dynamics, interaction and complexities of biomolecular system.
4	Critically analyze and improve existing technologies and develop the next generation of devices.

5	Have implications in enhancement of the scientific data and interpretations in research.	
Unit-I	**Electron Paramagnetic Resonance**	**6 hours**
External Magnetic Field, Microwave Frequencies, Detection, Hyperfine Coupling, Advantages and Disadvantages, Applications in Biology.		
Unit:II	**X-ray Protein Crystallography**	**6 hours**
Technique of Obtaining crystals, Protein production and purification, Crystallization, obtaining x-ray diffraction data, X-ray sources, Sample preparation, X-ray scattering, obtaining an electron density map and Obtaining a three-dimensional model of protein.		
Unit:III	**Dynamic Force Spectroscopy**	**6 hours**
Experimental Methods and Applications of Atomic Force Microscope (AFM), Biomembrane Force Probe (BFP).		
Unit:IV	**Raman Spectroscopy and Surface Enhanced Raman Spectroscopy**	**6 hours**
Advantages and Disadvantages, Applications of Raman Spectroscopy and surface enhanced Raman Spectroscopy in Biology.		
Unit:V	**Transient Photobiology**	**6 hours**
Lasers, Setting up Ultrashort Pulses, Pump-Probe Technique, Applications.		
Total Lecture hours		**30 hours**

References

1	Glusker JP and Trueblood KN, 1972. Crystal structure analysis: a primer. Oxford University Press. [Reprint: OUP Oxford, May 27, 2010].
2	S Eaton, G. Eaton, 'Electron Paramagnetic Resonance', Ewing's Analytical Instrumentation Handbook. CRC Press.
3.	Evstigneev, M., et al. Dynamic Force Spectroscopy on Single Molecules. Arizona State University, 2012.
4.	Eric C. Le Ru, and Pablo G. Etchegoin, *Principles of Surface-Enhancemed Raman Spectroscopy and relatied plasmonic effects*, First Edition, Elsevier
5.	Lozovoy, Vadim V., Yair Andegeko, Xin Zhu, and Marcos Dantus. "Applications of Ultrashort Shaped Pulses in Microscopy and for Controlling Chemical Reactions." *Chemical Physics*: 118-24. Web. 3 Mar. 2015.
6.	https://phys.libretexts.org/Courses/University_of_California_Davis/UCD%3A_Biophysics_200A_-_Current_Techniques_in_Biophysics

CHEMINFORMATICS



Course Timeline: 30 Hrs

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Course Code	502VAC06	Cheminformatics	L	T	P	C
Core/Elective/Supportive		Value-Added Course		-	-	
Pre-requisite		Basic Knowledge in Biology or Chemistry	Syllabus Version		2020-23	

Course Objectives:

The main objectives of this course are to:

1. Predict oral availability of chemical compounds by understanding its physicochemical features.
2. Analyze the structure and functional properties of chemical compounds using chemical databases and softwares.
3. Predict the biological activity of chemical compounds relevant to process of drug discovery.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

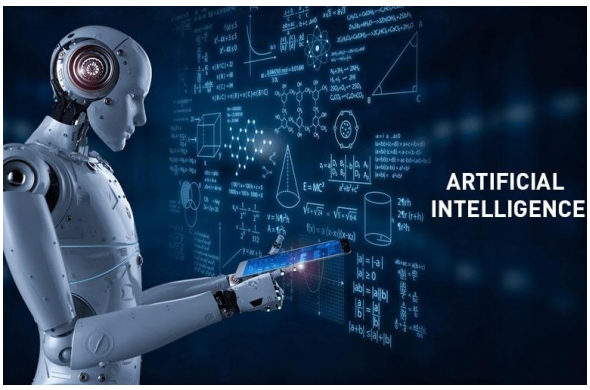
1	Understand the representation of chemical compounds in a linear format file.
2	Apply knowledge of chemical databases, drawing of molecular structures and softwares in drug design.
3	Analyze physicochemical and structural features of chemical compounds.
4	Predict pharmacokinetic properties, bioactivity, or safety profile of chemical compounds.
5	Have hands-on experience on salvaging chemical properties and structure of the chemical compounds to predict its biological activity.

Unit-I	Concept of Cheminformatics	6 hours
Units to describe biological activity. Concept of SMILES in chemistry and cheminformatics.		
Unit-II	**Chemical Databases**	**6 hours**
Small molecule databases: PUBCHEM, PUBCHEM sketcher, ZINC database and ChemSpider database		
Unit-III	**ADME Concepts**	**6 hours**
Softwares to analyze physical chemical features of compounds: Physical-chemical descriptors of bioavailability, cheminformatics software: Molinspiration, Swiss ADME, PRO-Tox-II.		
Unit-IV	**Structure and Biological Activity**	**6 hours**
Strategies to change the structure of bioactive compounds: Strategy of combinatorial library, fragment-based approach, peptideomimetics and bio isosterism in medicinal chemistry. Introduction to the software Swiss Bioisostere.		
Unit-V	**Artificial Intelligence in Drug Discovery**	**6 hours**
Role of artificial intelligence in the process of drug discovery. Rationale for choosing drug molecules and deducing their possible pharmacokinetic properties such as plasma concentration, or biological activity, based on their functional groups, molecular weight, cLogP, etc.		
Total Lecture & Practical Hours		**30 hours**

References

1.	Gary Wiggins, "Chemical Information Sources", Mcgraw-Hill Series in Advanced Chemistry.
2.	Hans-Dieter Holtje, Wolfgang Sippl, Didier Rognan, Gerd Folkers,"Molecular Modeling: Basic Principles and Applications",Wiley publications.
3.	Thomas Engel and Johann Gasteiger,"Applied Chemoinformatics - Achievements and Future Opportunities", Wiley-VCH publication.
4.	Andrew R. Leach and Valerie J. Gillet,"An Introduction to Chemoinformatics", Springer Publication.
5.	https://chem.libretexts.org/Courses/Intercollegiate_Courses/Cheminformatics_OLCC_(2019)

ARTIFICIAL INTELLIGENCE



Course Timeline: 30 Hrs

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Course Code	502VAC07	Artificial Intelligence	L	T	P	C
Core/Elective/Supportive		Value Added Course				
Pre-requisite		Programming and Problem solving	Syllabus Version		2021-2022	

Course Objectives:

- To understand the concept of Artificial Intelligence (AI) in the form of various Intellectual tasks
- To understand Problem Solving using various peculiar search strategies for AI
- To understand multi-agent environment in competitive environment
- To acquaint with the fundamentals of knowledge and reasoning
- To devise plan of action to achieve goals as a critical part of AI
- To develop a mind to solve real world problems unconventionally with optimality

Expected Course Outcomes:

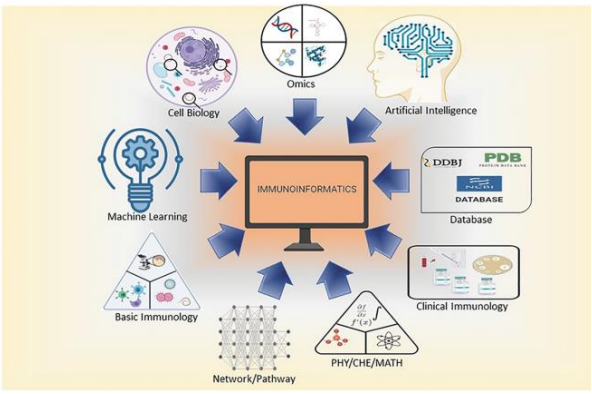
1.	Identify and apply suitable Intelligent agents for various AI applications
2	Build smart system using different informed search / uninformed search or heuristic approaches
3	Identify knowledge associated and represent it by ontological engineering to plan astrategy to solve given problem
4	Apply the suitable algorithms to solve AI problems
5.	Implement ideas underlying modern logical inference systems
6	Represent complex problems with expressive yet carefully constrained language of representation

UNIT-I	Introduction	6 hours
Introduction to Artificial Intelligence, Foundations of Artificial Intelligence, History of Artificial Intelligence, State of the Art, Risks and Benefits of AI, Intelligent Agents, Agents and Environments, Good Behavior: Concept of Rationality, Nature of Environments, Structure of Agents.		
UNIT-II	**Problem-solving**	**6 hours**
Solving Problems by Searching, Problem-Solving Agents, Example Problems, Search Algorithms, Uninformed Search Strategies, Informed (Heuristic) Search Strategies, Heuristic Functions, Searchin Complex Environments, Local Search and Optimization Problems.		
UNIT-III	**Adversarial Search and Games**	**6 hours**
Game Theory, Optimal Decisions in Games, Heuristic Alpha–Beta Tree Search, Monte Carlo Tree Search, Stochastic Games, Partially Observable Games, Limitations of Game Search Algorithms, Constraint Satisfaction Problems (CSP), Constraint Propagation: Inference in CSPs, Backtracking Search for CSPs.		
Unit-IV	**Knowledge**	**6 hours**
Logical Agents, Knowledge-Based Agents, The Wumpus World, Logic, Propositional Logic: A Very Simple Logic, Propositional Theorem Proving, Effective Propositional Model Checking, Agents Based on Propositional Logic, First-Order Logic, Representation Revisited, Syntax and Semantics of First-Order Logic, Using First-Order Logic, Knowledge Engineering in First-Order Logic.		
Unit-V	**Planning**	**6 hours**
Automated Planning, Classical Planning, Algorithms for Classical Planning, Heuristics for Planning, Hierarchical Planning, Planning and Acting in Nondeterministic Domains, Time, Schedules, and Resources, Analysis of Planning Approaches, Limits of AI, Ethics of AI, Future of AI, AI Components, AI Architectures.		
Total Lecture		**30 hours**

References:

1	Stuart Russell and Peter Norvig, “Artificial Intelligence: A Modern Approach”, Third edition,Pearson, 2003, ISBN :10: 0136042597
2	Elaine Rich, Kevin Deepak Khemani, “A First Course in Artificial Intelligence”, McGraw Hill Education(India),2013, ISBN : 978-1-25-902998-1
3	Knight and Nair, “Artificial Intelligence”, TMH, ISBN-978-0-07-008770-5
4	Nilsson Nils J , “Artificial Intelligence: A new Synthesis”, Morgan Kaufmann Publishers Inc. San Francisco, CA, ISBN: 978-1-55-860467-4
5	Patrick Henry Winston, “Artificial Intelligence”, Addison-Wesley Publishing Company, ISBN: 0-201-53377-4
6	Andries P. Engelbrecht-Computational Intelligence: An Introduction, 2nd Edition-Wiley India-ISBN: 978-0-470-51250-0

IMMUNOINFORMATICS



Course Timeline: 30 Hrs

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Course Code	502VAC08	Immunoinformatics	L	T	P	C
Core/Elective/Supportive		Value-Added Course		-	-	
Pre-requisite		Basic Knowledge Immunoinformatics	Syllabus Version		2020-23	

Course Objectives:

The main objectives of this course are to:

1. Introduce about reverse vaccinology and computational vaccine design.
2. Make understand the various immunoinformatics tools used in vaccine design pipeline.
3. Analyze the structure of antigens and antibodies and their interaction.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Retrieve sequence of the antigenic protein.
2	Apply structural features of the antigenic proteins like secondary structures, domains, and motifs in vaccine design.
3	Analyze various types of epitopes in antigenic proteins.
4	Model the structure of antigen and antibodies to analyze their interaction.
5	Have hands-on experience on functional analysis of antigenic protein including antigenicity, allergic nature and physicochemical properties of antigenic proteins.

Unit-I	Functional Analysis of Antigenic Proteins	6 hours

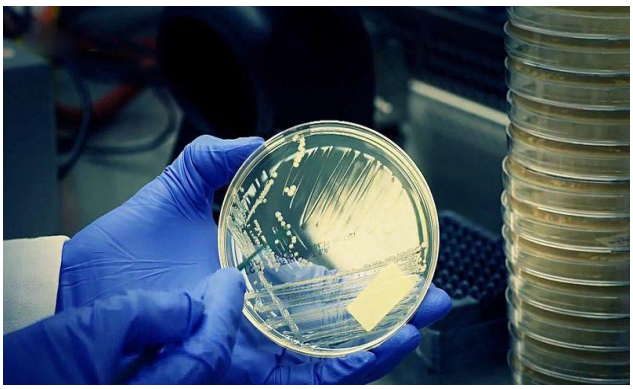
Prediction of Primary structure, antigenicity, allergic nature of antigenic protein and physiochemical properties of antigenic proteins.

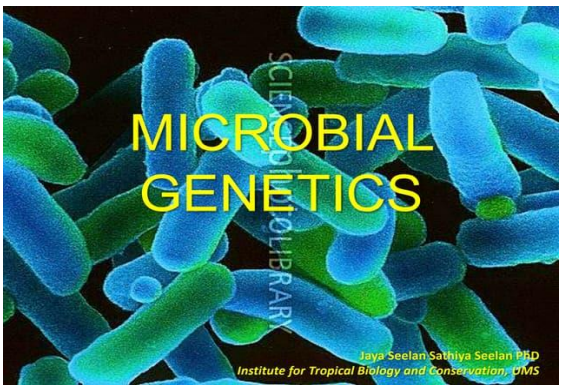
Unit-II	**Structural Analysis of Antigenic Proteins**	**6 hours**
Prediction of the secondary structure, domains and important sites in antigenic protein.		
Unit-III	**Epitope Prediction (B-cell)**	**6 hours**
Prediction of continuous B-cell epitope, Discontinuous B-cell epitope, glycoprotein antigen epitopes and immunogenic regions in antigenic proteins.		
Unit-IV	**Epitope Prediction (T-cell and MHC)**	**6 hours**
Prediction of epitopes for T cell, cytotoxic T cells, MHC (class I & II) and T cell epitopes processing. Prediction of Immunogenicity.		
Unit-V	**Antigen and Antibody Modelling**	**6 hours**
Automated antigen modelling, Alignment based antigen modelling, Antibody modelling, and Antigen-Antibody Docking.		
Total Lecture		**30 hours**

References

1.	Darren R Flower, "Immunoinformatics: Predicting Immunogenicity in Silico", Humana Press, 2007.
2.	Shoba Ranganathan, Vladimir Brusic, Christian Schonbach, "Immunoinformatics (Immunomics Reviews)" Springer publication.
3.	Rammensee, "Immunoinformatics - Bioinformatics Strategies for better understanding of Immune Function", Wiley, 2003.
4.	Thomas J. Kindt , Barbara A. Osborne, Richard A. Goldsby , " Kuby Immunology", WH Freeman, Sixth Edition, 2006.
5.	https://nptel.ac.in/courses/102/103/102103038/ https://nptel.ac.in/courses/102/105/102105083/

MICROBIAL GENETICS





Course Timeline: 30 Hrs

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Course code	502VAC09	MICROBIAL GENOMICS	L	T	P	C
Core/Elective/Supportive		Certificate course	4	-	-	4
Pre-requisite		Basic knowledge in Biology	Syllabus Version		2022-23	

Course Objectives:

The main objectives of this course are to:

1. Provide knowledge about the normal microbial flora and interactions.
2. Understand the methods to clone, propogate and maintain metagenomic libraries
3. Study the functioning of microbial communities using metagenomic approaches.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Explain genomic technologies and the ways in which genomic data are stored.
2	Have hands-on experience on various bioinformatics tools available for analyzing genes and genomes.
3	To handle biological big data generated by the sequencing projects and its analysis.
4	Adequate awareness on plant and clinical trancriptomics and epigenomics evaluation.
5	Get the clear idea in theories of various NGS technologies.

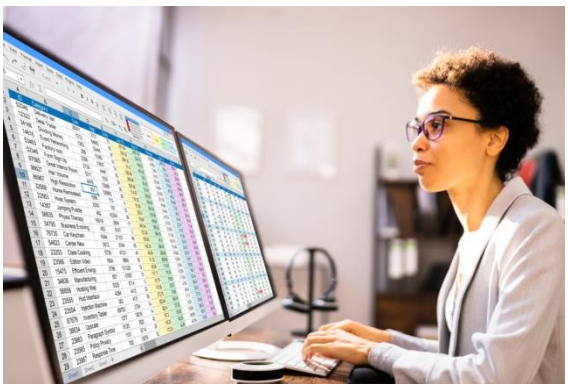
Unit-I	Microbes and Environment	5 hours

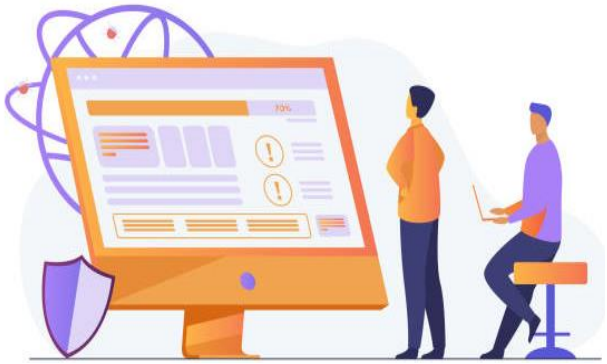
Diversity of Microorganisms, Comparison of three domains – Bacteria, Protista, Fungi, Viral and Algae diversity, Microbial habitats, Metagenomics, Microbe-microbe interactions, Microbe-host interactions, Microbial communities- Biofilms, Quorum sensing, Bioremediation.

Unit-II	Microbial Identification and	5 hours

	Characterization	
Bacterial genome characterisation and dynamics- Sequence alignments to Phylogenetic relationships- Prediction of Genes in prokaryotic genomes- Prediction of Operons, Regulons, transcription signals and Biological pathways- Detection of Viruses using NGS - Reverse vaccinology: from genome to vaccine, Microbial genomics for antibiotic target discovery.		
Unit-III	**Microbial Genome Sequencing and Characterization**	**6 hours**
Genome sequence analysis- Sequence assembly, Annotation of genomes from sequence to functional annotation, Atlas visualisation of genome-wide information - Comparative genomics and metagenomics- Genome-wide gene expression analyses- Representational display analysis of genome comparisons - Whole genome phylogenetic analysis.		
Unit-IV	**16s rRNA based metagenome profiling**	**6 hours**
16S rRNA microbiome – study design - Sample collection, extraction and library prep - 16S rRNA bioinformatics pipelines- Reads quality and processing - Normalization- - Hierarchical clustering- Taxonomic classification and profiling of bacterial communities - Downstream analysis in R - phyloseq, NMF, vegan, metagenomeSeq, micropan: an R-package for microbial pan-genomics.		
Unit-V	**Whole Metagenome profiling**	**6 hours**
Metagenome sequencing: Cloning the metagenome, Preprocessing of raw sequence data, Downstream sequence analysis – community analysis in R, Shotgun sequencing - Sequencing errors and Diversity estimates, Functional and Pathway annotation- MetaCyc, BioCyc and KEGG, Genomic approaches to study Human microbiome – CRISPR-CAS9/TN-seq.		
	Total Lecture hours	**30 hours**
References		
1	Wren, B Dorrell, N, Functional Microbial Genomics: Methods in Microbiology, Academic Press Inc, 2002.	
2	Streit, Wolfgang, Daniel, Rolf (Eds.) Metagenomics, Methods and Protocols, Springer, 2010.	
3	Fraser C.M., Read T. and Nelson K.E. (2004) Microbial Genomes, Springer.	
4	Norman Grossblatt, (Ed), The new science of metagenomics, National Academic Press, Washington, 2007.	
5	https://nptel.ac.in/courses/102/103/102103015/	
Course Designed By: Dr. V. Hemamalini		

MEDICAL CODING





Course Timeline: 30 Hrs

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Course Code	502VAC010	Medical Coding	L	T	P	C
Core/Elective/Supportive		Value-Added Course		-	-	
Pre-requisite		Basic Knowledge in Life Science	Syllabus Version		2020-23	

Course Objectives:

The main objectives of this course are to:

4. Identify the attributes needed to become a successful medical coder.
5. Understand the guidelines for coding physiologic conditions involving different organ systems
6. Assign diagnosis and procedure codes using the ICD-10 coding manual.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Understand the layout and purpose of the ICD-10-CM coding manual.
2	Apply the guidelines of ICD-10-CM to code physiologic and pathologic conditions of different organ systems.
3	Evaluate the purpose of CPT manual and national level codes (HCPCS).
4	Analyze the difference between Inpatient and outpatient codes.
5	Use ICD-10-CM to assign codes for medical diagnoses.

Unit-I	Introduction to Medical Coding	6 hours

Purpose of Medical Coding, Types of codes and Types of payers. - NCD, LCD, ABN and HIPAA. Medical terminology.

Unit-II	International Classification of Diseases (ICD)	6 hours

Structure of International Classification of Diseases(ICD), steps to Find ICD 10 CM Code, ICD 10 CM Official Guidelines, Symbols and Conventions, ICD-10 outpatient coding and reporting guidelines, Z-codes. Official instructional notations in the ICD-10-CM. Guidelines for coding physiologic and pathologic conditions involving different organ systems with case study.		
Unit-III	**Current Procedural Terminology (CPT)**	**6 hours**
Sections of CPT manual, CPT guidelines, CPT code formats, Category I, II, III codes, CPT Conventions and Iconography, Modifiers. Case study.		
Unit-IV	**Healthcare Common Procedure Coding System (HCPCS)**	**6 hours**
Introduction to HCPCS manual, levels of HCPCS codes, Groupings of HCBCS codes (A, B, C, D, E, G, H, J, K, L, M, P, Q, R, S, T, or V). Case study.		
Unit-V	**Inpatient Coding**	**6 hours**
Difference between inpatient and outpatient coding, selection of principal diagnosis, reporting additional diagnosis, present on admission. Development of ICD-10-PCS. Case study.		
Total Lecture Hours		**30 hours**

References

1	Senthamarai Selvi and Dhanalakshmi, "Essentials of Bioinformatics and Basics of Medical Coding", Ryan Publication.
2	Buck's Step-by-Step Medical Coding. Elsevier.
3.	Sandra L. Johnson and Robin Linker, "Understanding Medical Coding: A Comprehensive Guide", AAPC publication
4.	ICD-10-CM 2022: The Complete Official Codebook With Guidelines (ICD-10-CM The Complete Official Codebook), American Medical Association publication.
5.	https://www.velocityhc.com/wp-content/uploads/2019/09/Step-by-Step-Medical-Coding-2017-Edition-E-Book.pdf

Synthetic Organic Chemistry

Course Timeline: 30 Hrs

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Course Code	502VAC011	**Synthetic Organic Chemistry**	**L**	**T**	**P**	**C**
Core/Elective/Supportive		**Value Added Course**				
Pre-requisite		**Basic Knowledge in Organic Chemistry**	**Syllabus Version**		**2021-2022**	

Course Objectives:

1. To introduce the concept of organic chemistry including their strength of acid and base, stability, resonance etc.
2. Be able to gain the knowledge about oxidation and redox reaction.
3. To attain the skill in basic reaction mechanism of aromatic and aliphatic substitution reaction.
4. The student will learn about various essential characterization techniques.
5. To make students understand the important feature of organic molecules in biology

Expected Course Outcomes:

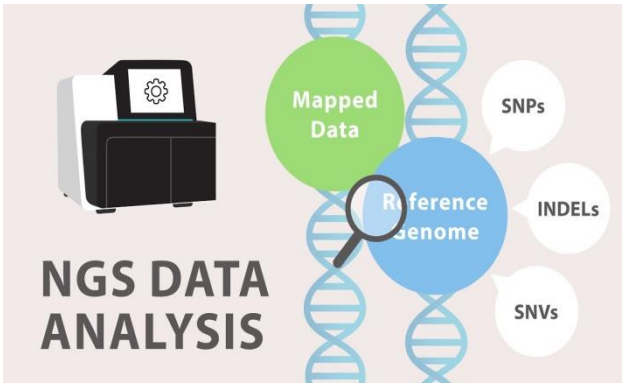
1.	Pave the way of the students to understand the basic knowledge of organic chemistry
2	Students will be able to explore how to know the oxidation and redox reaction.
3	Students will have a solid foundation in the basics of organic reaction and mechanism
4	To be able to explain and interpretation of results from different analytical techniques.
5.	The students would have evaluate and create structure and function of biological molecules

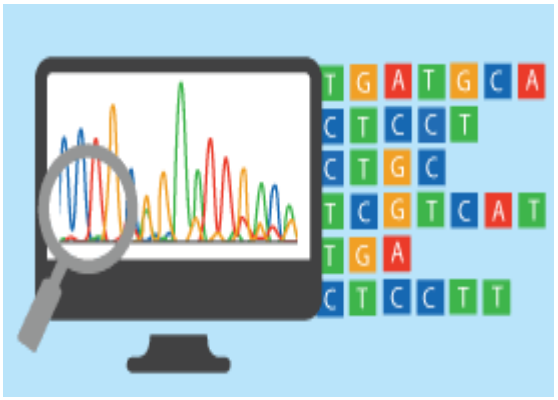
UNIT-I	**General Organic Chemistry**	**6 hours**

Inductive Effect, Acidic Strength, Basic Strength, Localised and Delocalised Electrons, Stability of Resonating Structure, Hyper Conjugation, Stability of Alkene and Heat of Hydrogenation,

Electromeric Effect and Tautomerism.		
UNIT-II	**Redox reactions**	**6 hours**
Concept of oxidation and oxidation, redox reactions oxidation number, balancing redox reactions in terms of loss and gain of electron and change in oxidation numbers.		
UNIT-III	**Reaction Mechanism**	**6 hours**
Reaction intermediates and stability of free radicals, carbenes, nitrenes, carbanions and carbocations. **Aromatic substitution reactions:** Electrophilic, Nucleophilic substitution of SN1 and SN2 mechanisms. **Aliphatic substitution reactions:** Electrophilic, Nucleophilic substitution of SE1 and SE2 mechanisms.		
Unit-IV	**Characterization techniques**	**6 hours**
UV-Vis spectroscopy: Basic principle and instrumentation, chromophores, solvent effect, Wood ward-Fieser rules. **Infrared spectroscopy:** Basic principle and instrumentation, molecular vibrations, finger-print region. **NMR Spectroscopy**: Chemical shift, spin-spin coupling, spin decoupling, factors influencing coupling constant 'J', instrumentation and application of proton NMR.		
Unit-V	**Organic molecules in Biology**	**6 hours**
Explain the biological molecules are organic compounds, Types of primary biological molecules, Fats, Steroids, Coenzymes: Structure and biological functions of coenzyme A, thiamine NAD+, NADP+, FMN, FAD, lipoic acid and Vitamin B12.		
Total Lecture		**30 hours**
References:		
1	Advanced organic chemistry by Jerry March (4th Edition) Wiley Eastern	
2	Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc. Graw Hill and Kogakush.	
3	Michael Edenborough, "Organic Reaction Mechanisms: A Step by Step Approach, 2nd Ed., Publisher-CRC, (1998)	
4	P. S. Kalsi, "Spectroscopy of Organic Compound", 6th Ed., Publisher-New Age International, (2007)	
5	Jag Mohan, "Organic Spectroscopy: Principles and Applications" Publisher-CRC, (2004)	
6	K.P. Media," Text Book of Biochemistry", Publisher-Krishna Prakashan Media, (ISBN-8185842655, 9788185842653)	

NEXT GENERATION SEQUENCING DATA ANALYTICS





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Course Code	**502VAC012**	**Next Generation SequencingData Analytics**	**L**	**T**	**P**	**C**
Core/Elective/Supportive		**Value-Added Course**		**-**		
Pre-requisite		**Basic Knowledge in olecular Biology/ ShellScripting and Computational Biology**	**Syllabus Version**		**2020-23**	

Course Objectives:

The main objectives of this course are to:

1. Comprehensive understanding of underlying principles of different pipelines, methods and technology involved in NGS that generates massive amounts of DNA or RNA sequencing data.
2. To comprehend Genome assembly, Genetic variations, Functional and comparative genomics employing DNAseq.
3. To outline and compute the transcriptome in any biological sample and identify the differential gene expression through RNAseq.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Download the NGS data from various NGS Data sources using SRA toolkitand clean the data using various software.
2	Perform RNA-seq workflow denovo and reference-based transcriptomeanalysis and their Visualization using R programming.
3	Perform DNA seq workflow which facilitates Genome Assembly analysis, variant calling, Genotype calling and Annotation
4	Have a detailed knowledge of all the tools used and file generated in theaforementioned steps

5	Have hands-on experience on various Pipelines involved in DNAseq andRNA seq.

Unit-I	**History and Evolution of sequencing**	**6 hours**
Different generation Sequencing technologies, Human Genome Project, different NGS platforms, Introduction to NGS technologies: DNA-seq, RNA-seq, ChIP-seq, Hi-seq,MI- Seq		
Unit-II	**Preparation and Pre-processing**	**6 hours**
Library Preparation methods, Sequencing methods, Data formats, Phred quality score, Different Tools for trimming the reads, NGS Data sources, SRA toolkit		
Unit-III	**Gene Prediction and Differential Gene expression**	**6 hours**
Gene prediction methods, RNA-seq workflow, Data analysis and Visualization using R, GO Annotation Gene Enrichment Analysis, Pathway analysis		
Unit-IV	**Whole Genome Sequencing**	**6 hours**
Introduction to DNA assembly, Whole genome and whole exome variant calling pipeline, Variant annotation tools- VCF file and its Visualization tools- Qualimap, IgV, Application of variant calling.		
Unit-V	**Single cell RNA sequencing and Metagenomics**	**6 hours**
Single cell RNA seq, Seurat pipeline, PCA, clustering, Metagenomics- Amplicon Sequencing, Whole genome Metagenomics, Sequence based Metagenomics Analysis; Function based Metagenomics Analysis		
Total Lecture		**30 hours**

References

1.	M. J. Bach; The Design of the UNIX Operating System; Pearson Education India, 1st edition,
2.	R. Durbin; Biological sequence analysis; Cambridge University Press, 1998.
3.	N. Gautham; Bioinformatics: Databases and Algorithms; Alpha Science, 2006.
4.	H. Schildt; C – The Complete Reference; McGraw Hill Education, 4th edition, 2017.
5.	References Papers for different Pipelines: DNA seq https://link.springer.com/article/10.1007/s00439-012-1213- zTux 1 https://www.nature.com/articles/nprot.2012.016 Tux 2 https://www.nature.com/articles/nprot.2016.095. Trinity https://www.nature.com/articles/nprot.2013.084.Sc- RNA https://www.singlecellcourse.org/