BANASTHALI VIDYAPITH

Master of Science (Bioinformatics)

Curriculum Structure

First Semester Examination, December, 2020
Second Semester Examination, April/May,2021
Third Semester Examination, December, 2021
Fourth Semester Examination, April/May, 2022

BANASTHALI VIDYAPITH
P.O. BANASTHALI VIDYAPITH
(Rajasthan)-304022

July, 2020

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No. F. 9-6/81-U.3
Government of India
Ministry of Education and Culture
(Department of Education)

New Delhi, the 25th October, 1983

N O T I F I C A T I O N

In exercise of the powers conferred by Section 3 of the University Grants Commission Act, 1956 (3 of 1956) the Central Government, on the advice of the Commission, hereby declare that Banasthali Vidyapith, P. O. Banasthali Vidyapith, (Rajasthan) shall be deemed to be a University for the purpose of the aforesaid Act.

Sd/-
(M. R. Kolhatkar)
Joint Secretary of the Government of India

N O T I C E

Changes in Bye-laws/Syllabi and Books may from time to time be made by amendment or remaking, and a Candidate shall, except in so far as the Vidyapith determines otherwise, comply with any change that applies to years she has not completed at the time of change.

PROGRAMME EDUCATIONAL OBJECTIVES

The M.Sc. Bioinformatics programme aims for the holistic development of the students through the unique and innovative fivefold education ideology of Banasthali Vidyapith.

Bioinformatics is an interdisciplinary approach to study of biological processes including gene expression, protein modifications or interactions as well as the molecular evolution. The programme focuses on specific knowledge of computational biology and the associated academic disciplines including molecular cell biology, structural biology, mathematics and statistics, computer programming, drug designing, database management systems and genetic engineering. The program fulfills the requirements of the students to become familiar with basic and advanced concepts of the subject thus providing them the scientific background they need to find career opportunities in any related field of bioinformatics.

Main objectives of M.Sc. Bioinformatics programme are to:

- develop interdisciplinary approach for learning about the biological processes and their significance ranging fromsingle cell to multicellular system.
- enable students to solve complex biological questions by developing the the mathematical and computational skills.
- decipher the process of molecular evolution and phylogenetic reconstruction.
- develop understanding of organisms functioning at the molecular level of the gene, genome, cell.

- apply bioinformatics for biological database management, exploring behavior of the biomacromolecules and drug discovery programs.
- gain the ability to work as computational biophysicist, computational chemist in chemical biology projects, medical bioinformatician and evolutionary biologist.
- access the primary literature, recognize relevant works for a particular topic, and evaluate the scientific content of these works.
- demonstrate ability in the experimental and computational techniques and methods of analysis appropriate for their area of specialization within bioinformatics.

PROGRAMME OUTCOMES

PO1: Knowledge: Equipped with an in-depth knowledge in the area of basic and applied bioinformatics including molecular evolution, computational structural molecular biology, cell biology, computer programming and database management system. Enable them to specialize in one of the many branches of bioinformatics through dissertation work.

PO2: Planning abilities: Develop efficient planning abilities with time management, analytical and decisive skills to reach achievable goals.

PO3: Problem analysis: Devise and sustain logical thinking to tackle detailed problem-solving and analytical tasks associated with questions in core and applied bioinformatics.

PO4: Bioinformatics tool usage: Learn, select, and apply statistical, mathematical and computational tools of bioinformatics. Develop competence in the handling of research facilities and work in a laboratory environment, both individually and as a teammember.

PO5: Leadership skill: Develop leadership skills to work in a team and take initiative for fulfillment of professional and societal responsibilities.

PO6: Professional Identity: Understand, analyze and communicate the value of their professional roles in different research and development laboratories, information technology, pharmaceutical industries etc.

PO7: Communication: Develop skills used in reasoning and communication with scientific community and society.To synthesize information from literature and its communication in form of scientific papers, reports, poster and oral presentations.

PO8: The Bioinformatics and society: Contribute to society, in the realms of the agriculture, biological resource management, human and animal health well being.

PO9: Environment and sustainability: Development of efficient predictive bioinformatics methods for sustainable development conservation and preservation of biodiversity.

PO10: Life-long learning: Develop independent, critical and creative thinker who has a self-motivated passion for life-long learning.

Curriculum Structure

Master of Science (Bioinformatics)

First Year

Semester - I

Course Code		Course Name	L	T	P	C*
BIN	406	Biological Databases	4	0	0	4
BIO	407	Cell and Molecular Biology	4	0	0	4
BIO	426	Structural Biology	4	0	0	4
MATH	421	Introductory Mathematics	4	0	0	4
BIO	419L	Bioscience Lab-I	0	0	12	6
CS	443	Fundamentals of Computer and Programming	2	0	0	2
CS	443L	Fundamentals of Computer and Programming Lab	0	0	4	2
		Semester Total:	**18**	**0**	**16**	**26**

Semester - II

Course Code		Course Name	L	T	P	C*
BIN	404	Algorithms in Computational Biology	4	0	0	4
BIN	407	Sequence analysis and Phylogenetics	4	0	0	4
BT	408	Genetic Engineering	4	0	0	4
CS	418	Database Management Systems	4	0	0	4
CS	418L	Database Management Systems Lab	0	0	4	2
CS	446	Programming with Perl and R	4	0	0	4
CS	446L	Programming with Perl and R Lab	0	0	8	4
		Semester Total:	**20**	**0**	**12**	**26**

Second Year

Semester - III

Course Code	Course Name	L	T	P	C*
BIN 511	Biomolecular Modeling and Computational Drug Design	4	0	0	4
BIN 511L	Biomolecular Modeling and Computational Drug Design Lab	0	0	8	4
BT 545	Genomics and Proteomics	4	0	0	4
CS 538	Python Programming	4	0	0	4
CS 538L	Python Programming Lab	0	0	4	2
	Discipline Elective	4	0	0	4
	Open Elective	4	0	0	4
	Semester Total:	**20**	**0**	**12**	**26**

Semester - IV

Course Code	Course Name	L	T	P	C*
BIN 512D	Dissertation	0	0	48	24
	Reading Elective	0	0	4	2
	Semester Total:	**0**	**0**	**52**	**26**

List of Discipline Elective

Course Code	Course Name	L	T	P	C*
BIN 507	Mining and Warehousing of Biological Data	4	0	0	4
CS 530	Neural Networks	4	0	0	4
CS 512	Cloud Computing	4	0	0	4
BIN 513	Systems Biology	4	0	0	4
BIO 503	Fundamentals of Bioentrepreneurship	4	0	0	4
BIN 514	RNA Structure Function and Transcriptomics	4	0	0	4

List of Reading Elective

Course Code	Course Name	L	T	P	C*
BIN 601R	Chemoinformatics	0	0	4	2
BIN 602R	Immunoinformatics	0	0	4	2
BT 529R	Drug Discovery	0	0	4	2
BT 531R	Human Genetics and Diseases	0	0	4	2
BT 539R	Protein Engineering	0	0	4	2

*** L - Lecture hrs/week; T - Tutorial hrs/week; P-Project/Practical/Lab/All other non-classroom academic activities, etc. hrs/week; C - Credit Points of the Course**

Student can opt open (Generic) elective from any discipline of the Vidyapith with prior permission of respective heads and time table permitting.

Every Student shall also opt for:

Five Fold Education: Physical Education I, Physical Education II,

Five Fold Education: Aesthetic Education I, Aesthetic Education II,

Five Fold Education: Practical Education I, Practical Education II

one each semester

Five Fold Activities

Aesthetic Education I/II		Physical Education I/II	
BVFF 101	Classical Dance (Bharatnatyam)	BVFF 201	Aerobics
BVFF 102	Classical Dance (Kathak)	BVFF 202	Archery
BVFF 103	Classical Dance (Manipuri)	BVFF 203	Athletics
BVFF 104	Creative Art	BVFF 204	Badminton
BVFF 105	Folk Dance	BVFF 205	Basketball
BVFF 106	Music-Instrumental (Guitar)	BVFF 206	Cricket
BVFF 107	Music-Instrumental (Orchestra)	BVFF 207	Equestrian
BVFF 108	Music-Instrumental (Sarod)	BVFF 208	Flying - Flight Radio Telephone Operator's Licence (Restricted)
BVFF 109	Music-Instrumental (Sitar)	BVFF 209	Flying - Student Pilot's Licence
BVFF 110	Music-Instrumental (Tabla)	BVFF 229	Aeromodelling
BVFF 111	Music-Instrumental (Violin)	BVFF 210	Football
BVFF 112	Music-Vocal	BVFF 211	Gymnastics
BVFF 113	Theatre	BVFF 212	Handball
Practical Education I/II		BVFF 213	Hockey
BVFF 301	Banasthali Sewa Dal	BVFF 214	Judo
BVFF 302	Extension Programs for Women Empowerment	BVFF 215	Kabaddi
BVFF 303	FM Radio	BVFF 216	Karate - Do
BVFF 304	Informal Education	BVFF 217	Kho-Kho
BVFF 305	National Service Scheme	BVFF 218	Net Ball
BVFF 306	National Cadet Corps	BVFF 219	Rope Mallakhamb
		BVFF 220	Shooting
		BVFF 221	Soft Ball
		BVFF 222	Swimming
		BVFF 223	Table Tennis
		BVFF 224	Tennis
		BVFF 225	Throwball
		BVFF 226	Volleyball
		BVFF 227	Weight Training
		BVFF 228	Yoga

Every Student shall also opt for:
Five Fold Education: Physical Education I, Physical Education II,
Five Fold Education: Aesthetic Education I, Aesthetic Education II,
Five Fold Education: Practical Education I, Practical Education II
one each semester

Evaluation Scheme and Grading System

Continuous Assessment (CA) (Max. Marks)					End-Semester Assessment (ESA) (Max. Marks)	Grand Total (Max. Marks)
Assignment		Periodical Test		Total (CA)		
I	II	I	II			
10	10	10	10	40	60	100

In all theory, laboratory and other non classroom activities (project, dissertation, seminar, etc.), the Continuous and End-semester assessment will be of 40 and 60 marks respectively. However, for Reading Elective, only End semester exam of 100 marks will be held. Wherever desired, the detailed breakup of continuous assessment marks (40), for project, practical, dissertation, seminar, etc shall be announced by respective departments in respective student handouts.

Based on the cumulative performance in the continuous and end-semester assessments, the grade obtained by the student in each course shall be awarded. The classification of grades is as under:

Letter Grade	Grade Point	Narration
O	10	Outstanding
A+	9	Excellent
A	8	Very Good
B+	7	Good
B	6	Above Average
C+	5	Average
C	4	Below Average
D	3	Marginal
E	2	Exposed
NC	0	Not Cleared

Based on the obtained grades, the Semester Grade Point Average shall be computed as under:

$$SGPA = \frac{CC_1 * GP_1 + CC_2 * GP_2 + CC_3 * GP_3 + ---- + CC_n * GP_n}{CC_1 + CC_2 + CC_3 + ---- + CC_n} = \frac{\sum_{i=1}^{n} CC_i * GP_i}{\sum_{i=1}^{n} CC_i}$$

Where n is the number of courses (with letter grading) registered in the semester, CC_i are the course credits attached to the i^{th} course with letter grading and GP_i is the letter grade point obtained in the i^{th} course. The courses which are given Non-Letter Grades are not considered in the calculation of SGPA.

The Cumulative Grade Point Average (CGPA) at the end of each semester shall be computed as under:

$$CGPA = \frac{CC_1 * GP_1 + CC_2 * GP_2 + CC_3 * GP_3 + ----+ CC_n * GP_n}{CC_1 + CC_2 + CC_3 + ----+ CC_n} = \frac{\sum_{i=1}^{n} CC_i * GP_i}{\sum_{i=1}^{n} CC_i}$$

Where n is the number of all the courses (with letter grading) that a student has taken up to the previous semester.

Student shall be required to maintain a minimum of 4.00 CGPA at the end of each semester. If a student's CGPA remains below 4.00 in two consecutive semesters, then the student will be placed under probation and the case will be referred to Academic Performance Review Committee (APRC) which will decide the course load of the student for successive semester till the student comes out of the probationary clause.

To clear a course of a degree program, a student should obtain letter grade C and above. However, D/E grade in two/one of the courses throughout the UG/PG degree program respectively shall be deemed to have cleared the respective course(s). The excess of two/one D/E course(s) in UG/PG degree program shall become the backlog course(s) and the student will be required to repeat and clear them in successive semester(s) by obtaining grade C or above.

After successfully clearing all the courses of the degree program, the student shall be awarded division as per following table.

Division	CG
Distinction	7.50 and above
First Division	6.00 to 7.49
Second Division	5.00 to 5.99
Pass	4.00 to 4.99

CGPA to % Conversion Formula: % of Marks Obtained = CGPA * 10

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First Semester

BIN 406 Biological Databases

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- learn about different databases useful in biological studies
- understand the architecture of different sequence and structure database
- mine and analyze the biological information from different database

Section A

Bioinformatics Sequence Databases–Primary Databases- GenBank, EMBL, DDBJ.

Composite Databases- UniProt.

Secondary databases - Prosite, ProDom, Pfam, InterPro, gene ontology; sequence file formats:- GenBank, FASTA, PIR, ALN/ClustalW2.

Literature Databases- Open access and open sources, PubMed, PLoS, Biomed Central, NAR databases;

Bioinformatics Resources- NCBI, EBI, ExPASy.

Section B

Structure database – Primary structure databases - PDB, NDB, MMDB.

Secondary databases-Structural Classification of Proteins – SCOP, Class Architecture Topology Homology –CATH.

Specialized Databases – Viral genome database-ICTVdb; Microbial genome database-MBGD; Genome browsers- Ensembl, VEGA genome browser, NCBI-Genome Data viewer, KEGG, UCSC Genome Browser; Archeal Genomics, Eukaryotic genomes with special reference to model organisms-Yeast (SGD), Drosophila (FlyBase), C.elegans (WormBase), Mouse, Human (OMIM / OMIA), plants – Arabidopsis (TAIR).

Section C

Derived Databases- Catalytic Site Atlas –CSA; Databases of molecular functions /enzymatic catalysis databases - KEGG ENZYME database;

Protein-Protein interaction database - STRING; chemical structure database - Pubchem; gene expression database - GEO.

Database search engines – Text-based search engines (Entrez, DBGET /LinkDB). Sequence similarity based search engines (BLAST and FASTA). Motif-based search engines (Scan Prosite).

Proteomics tools- ExPASy server, EMBOSS.

Suggested Books

- Baxevanis, A.D. & Ouellette, B.F.F. (2004). Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins (3rd Ed.). John Wiley.
- Bosu, O. & Thukral, S.K.(2007). Bioinformatics: database, tools and algorithms (1st Ed.). Oxford University Press.

Suggested e-Resources:

- NCBI: https://www.ncbi.nlm.nih.gov/
- EBI: https://www.ebi.ac.uk/
- UNIPORT: https://www.uniprot.org/
- EXPASY: https://www.expasy.org/
- Biomed Central: https://www.biomedcentral.com/
- Databases Journal: https://academic.oup.com/database

BIO 407 Cell and Molecular Biology

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand membrane transport and cell signalling mechanisms.
- develop comprehensive understanding of endo-membrane system.
- understand the mechanism of DNA replication and gene expression in prokaryotes and eukaryotes

Section-A

Molecular structure and function of plasma membrane; Transport of ions and macromolecules; Pumps, carriers and channels; Membrane carbohydrates and their significance in cellular recognition; Cellular junctions and adhesions.

Endocytosis and exocytosis, clathrin coated vesicles, SNARE proteins.

Cell to cell signalling: autocrine, paracrine and endocrine stimulation.

Signaling via G-protein linked cellsurface receptors, adenylatecyclase system, inositol phosphate pathway, role of Ca^{2+} ions.

Signaling via enzyme-linked surface receptors, tyrosine kinases.

Steroid receptors.

Section-B

Protein sorting and targeting: Signal hypothesis, SRP, SRP Receptor, ER Resident proteins, ER chaperone proteins and their functions, glycosylation of proteins in ER.

Golgi apparatus, role in protein glycosylation and transport.

Lysosomes, intracellular digestion, sorting of lysosomal enzymes in Golgi, lysosomal storage diseases.

Transport of proteins into mitochondria and chloroplasts.

Cell Cycle and its regulation, apoptosis.

Section-C

Replication of genetic material in prokaryotes and eukaryotes: initiation, elongation and termination; Replication of single stranded circular DNA.

Prokaryotic transcription: Transcription units; RNA polymerase structure and assembly; Promotors; Rho-dependent and Rho-independent termination; Anti-termination.

Eukaryotic transcription: RNA polymerase structure and assembly; RNA polymerase I, II, III; eukaryotic promoters and enhancers; general transcription factors; TATA binding proteins (TBP) and TBP associated factors (TAF).

Post transcriptional modifications: processing of hnRNA, tRNA and rRNA; 5'-Cap formation; 3'-end processing and polyadenylation; Splicing; RNA editing; Nuclear export of mRNA; Catalytic RNA.

Genetic code, Isoaccepting tRNA; Translation: Translation machinery; initiation, elongation and termination; Co- and post-translational modifications.

Suggested Books:

- De Robertis, E.D.R., & De Robertis, E.M.F. (2017) *Cell and Molecular Biology*. Lippincott Williams & Wilkins.
- Hardin, J., Bertoni, G., & Lewis, K.J. (2011) *Becker's World of the Cell*. Pearson.
- Karp, G., Lwasa, J., & Larshall, W. (2015) *Cell and Molecular Biology: Concepts and Experiments*. John Wiley & Sons.
- Cooper, G., M., & Hausman, R., E. (2013) *The Cell :A Molecular Approach*. Sinauer Associates
- Lodish, H., Berk, A., Kaiser, C. A., Krieger, M., Bretsher, A., Ploegh, H., Amon, A., & Martin, K. C. (2007). *Molecular Cell Biology*. W.H.Freeman & Co Ltd.
- Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K., & Walter, P. (2007). *Molecular Biology of the Cell*. Garland Science.
- Freifelder , D. M. (1986). *Molecular Biology*. Jones & Bartlett Publishers.

Suggested e-Resources:

- **Cell Biology resources**: https://www.nature.com/scitable
- **Sorting and trafficking of proteins**:

  http://www.vcell.science/project/proteintrafficking
- **RNA editing**: study.com/academy/lesson/rna-editing-definition-processes. html

BIO 426 Structural Biology

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand the biophysical processes working at molecular level
- develop analytical understanding of macromolecular folding and interactions
- learn various techniques to study the biomolecular structures

Section A

Introduction to proteins:– Amino acids classification and their physicochemical properties.

Hierarchical organization of protein structures – primary, secondary, tertiary and quaternary structure of proteins.

Ramachandran Map. Motifs and domains.

Packing of protein structure Structures of oligomeric proteins and study of interaction interfaces

Base pairing in nucleic acids – Watson-Crick and Hoogstein; geometrical and structural properties of A, B, & Z DNA.

Secondary and Tertiary structures of RNA.

Section B

Principles and practices in Centrifugation, Chromatography and Electrophoresis for isolation & purification of biomacromolecules.

Circular Dichroism Spectroscopy.

X-Ray crystallography: Introduction, Bragg's law; Crystal system, Bravais Lattices, Space group, symmetry. Protein crystallization, Phase problem and its solutions. Calculation and analysis of electron density map.

Nuclear magnetic resonance: Introduction, chemical shift, NOE and coupling constant, spin – spin coupling and relaxation; 2D – NMR spectroscopy (COSY, NOESY).

Section C

Three dimensional structure comparison and classification of proteins (VAST, DALI).

Assignment of protein secondary structural elements; DSSP and STRIDE methods.

Various types of weak interactions and their roles in stabilizing the biomolecular structures and their interactions. Macromolecular interactions.

Protein-Protein, Protein – DNA and Protein – Ligand interactions

Suggested Books:

- Nelson, D.L. & Cox, M.M. (2017) *Lehninger's Principles of Biochemistry* (7th Ed.). W.H. Freeman.
- Schulz, G.E.& Schirmer, R.H. (1979). *Principles of Protein Structure*. Springer.
- Cantor, C.R. & Schimmel, P.R. (1980). *Biophysical Chemistry* (1st Ed.). W. H. Freeman.
- Wilson, K. & Walker, J. (2010). *Practical Biochemistry* (7th Ed.). Cambridge University Press
- Schwede, T. & Peitsch, M. (2008). *Computational Structural Biology: methods and applications*. World Scientific Press.

Suggested e-Resources:

- **X-ray crystallography**:

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1186895/

- **VAST**: https://structure.ncbi.nlm.nih.gov/Structure/VAST/vast.shtml
- **DALI**: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2896194/

MATH 421 Introductory Mathematics

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand the principles of algebra
- solve the complex biological problems using calculus methods
- develop a basic understanding of statistics and statistical distributions

Section A

Set Theory; Introduction to sets and elements, Universal, and empty sets, subsets. Venn diagrams, Set operations and algebra of sets, ordered sets, cartesian product of sets, Classes of sets, power sets and partition. Relations; product sets, equivalence relations, partial ordering relations.

Logarithms- Definition and laws regarding product, quotient, power and change of base.

Introduction to complex numbers; algebra of complex number, modulus and conjugate of a complex number.

Introduction to Matrix: types, Order and transpose of matrix. Operations on matrix; addition, subtraction, multiplication. Associative and distributive laws of matrix, Inverse of Matrix and matrix division; determinant of a matrix, Eigen values and Eigenvectors of matrix.

Section B

Differential Calculus- Derivative of a function, Concept of limit, Continuity, Differentiation, Maxima and Minima of a function.

Introduction to Partial Differentiation.

Integral Calculus: The Idea of the Integral, The Definite Integrals, Indefinite Integrals, Area under curve.

Trigonometric ratios, De Moivre's theorem.

The general equation of a Straight line, slope of a line, intercepts of a line, Angle between two lines, Intersection of two lines, The general equations of a Circle, Parabola, Ellipse, Hyperbola, Cylinder, Cone and Sphere.

Section C

Probability theory and probability distributions; Concepts of random experiment, sample space and events, definition of probability and some elementary results of probability.

Conditional probability and Bayes theorem.

Random variable, probability mass function and probability distribution function, cumulative distribution function, Binomial, Poisson and Normal(Gaussian) distribution.

Measures of central tendency- Mean, Median, Mode. Measures of dispersion- range, mean deviation, variance, standard deviation, skewness and kurtosis. Bivariate data: Correlation and regression analysis.

Suggested Books:

- Artin M. (2015) Algebra (2nd Ed.). Pearson Education.
- Aitken, M., Broadhurst, B. & Hladky, S. B. (2009). Mathematics for Biological Scientists. Garland Science.
- Thomas, G.B. (2013). Thomas Calculus (12th Ed.) Pearson education.
- Spiegel, M.R. & Stephens, L. J. (2014). Schaum's Outline Statistics (4th Ed.) McGraw-Hills Education.
- Spiegel, M., Schiller, J., Srinivasan, R.A.& Goswami, D. (2017). Schaum's Outline Probability *and Statistic* (3rd Ed.). McGraw-Hills Education.

BIO 419L Bioscience Lab -1

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**12**	**6**

Learning Outcome:

After successful completion of the course, students should be able to:

- gain hands-on experience in various biochemical assays used for quantification of fats, carbohydrate, protein and enzymes
- perform techniques for isolation of microbes, growth assessment, staining and antibiotic sensitivity
- access, retrieve, and analyze nucleotide and protein sequences using bioinformatics tools

ANALYTICAL TECHNIQUES

1. Demonstration: Working principle & applications of
2. Centrifuges (high speed refrigerated centrifuge & ultracentrifuge),
3. Fluorescence microscope.
4. Atomic absorption spectrophotometer,
5. HPLC, FPLC, GC-MS
6. Separation of amino acids by TLC and Paper Chromatography.

CELL AND MOLECULAR BIOLOGY

7. Study of different stages of mitosis (onion root tip) and meiosis (onion buds/grasshopper testis) and determine the mitotic index.
8. Separation of chloroplast by sucrose density gradient centrifugation

BIOCHEMISTRY

9. To prepare an Acetic-Na Acetate Buffer and validate the Henderson-Hasselbach equation.
10. Extraction of crude enzyme from germinating mung bean seeds.
11. Estimation of total protein content by Lowry's method
12. Separation of protein by SDS PAGE.
13. Estimation of acid phosphatase activity using standard curve of p-nitrophenol.
14. Purification of the crude enzyme extract (from Expt. 6) using ammonium sulphate precipitation and ion exchange/ affinity chromatography (demonstration).

15. Determination of kinetic properties (Km and Vmax values) of acid phosphatase.
16. Estimation of total carbohydrates using Anthrone method.
17. Estimation of reducing sugar by Nelson-Somogyi method.
18. Estimation of fats (cholesterol).

MICROBIOLOGY

19. Isolation and enumeration of microbes from soil and water.
20. Staining of selected bacterial and fungal strains
21. Estimation of bacterial growth by turbidometric method.
22. Antibiotic sensitivity test.
23. Estimation of infectivity titre of a virus sample using Plaque assay

BIOINFORMATICS

24. Database Search: Use and analysis of BLAST tool for protein and DNA sequences.
25. Molecular Evolution: Multiple sequence alignment and phylogenetic analysis. (Clustal X/ Mega/ Tree-View)
26. Structure Prediction: Protein secondary and tertiary structure prediction using online tools.
27. Molecular Visualization: Structural analysis of PDB entries for active and inactive states of protein (Pymol).

Suggested Books

- Aneja, K.R. (1996). Experiments in Microbiology, Plant Pathology, Tissue Culture and Mushroom Cultivation (II Ed.). New Delhi: Wishwa Prakashan.
- Cappuccino, J. G. & Sherman, N. (2014). Microbiology – A laboratory manual (10th ed). Pearson

Suggested e-Resources:

- **Harisha, S. Biotechnology procedures and experiments handbook**: http://site.iugaza.edu.ps/mwhindi/files/BIOTECHNOLOGY-PROCEDURES-AND-EXPERIMENTS-HANDBOOK.pdf
- **Introduction to biotechnology** : http://www.austincc.edu/awheeler/Files/BIOL%201414%20Fall%202020 11/BIOL1414_Lab%20Manual_Fall%202011.pdf

CS 443 Fundamentals of Computer and Programming

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**2**	**0**	**0**	**2**

Learning Outcome

After successful completion of the course, students should be able to:

- understand working of computation
- learn scientific computation techniques
- write simple programs to carry out bioinformatics analyses

Section A

Block diagram of computers, its components and functions. Data representation.

Boolean algebra, Basic defintions and theorems of boolean algebra, logic gates and circuits. Sum of products and product of sums, truth tables and Boolean functions.

History of computer evolution.

Concept of program, programming language, algorithms and flowcharts, compilers, interpreters.

Section B

Operating Systems: Unix, Linuxand Windows.

Basic Utilities commands. Pipe and Filters: Grep, SED, AWK, Shell scripting.

Introduction to HPC systems.

Communication technology; Network basics; LAN, WAN & MAN, Intranet, Wireless, and Internet services. Web Services; WWW, URL.

Section C

Introduction to MATLAB; understanding the MATLAB environment.

Data types in MATLAB; Local and Global variables in MATLAB.

Programming with MATLAB Relational and Logic operators, Control structure of MATLAB, conditional and Loops; Creating user – defined functions and function files.

2D and 3D graph plotting with MATLAB.

Introduction to Bioinformatics Toolbox.

Suggested Books:

- Sinha, P.K & Sinha, P. (2016). *Computer Fundamentals* (6th Ed.). BPB publication, New Delhi.
- Barret, D.G.(2016). *Linux Pocket Guide* (3rd Ed.). OReilly Media.
- Gilat, A. (2012). *MATLAB® An Introduction with Applications* (4rd Ed.). John Wiley and Sons.

Suggested e-Resources:

- Matlab tutorial: https://www.tutorialspoint.com/matlab/

CS 443L Fundamentals of Computer and Programming Lab

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**4**	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- write programs to analyze biological and statistical data.
- understand the working of Bioinformatics toolbox.
- perform data analysis with MatLab for biological problems.

1. MatLab working environment.
2. Constructing vectors and Matrices.
3. Diagrammatic representation of data by : Simple Bar, pie-diagrams, Histogram
4. File handling in MatLab.

5. Computation of :
   (i) Range, standard deviation, Mean deviation, Quartile deviation and coefficient of variation.
   (ii) Combined mean and combined standard deviation.
6. Introduction to Bioinformatics Toolbox.
7. Fitting of following curves by the method of least square:
   (i) Staight line
   (ii) Parabola
   (iii) Exponential curve
   (v) Power Curve
8. Computation of coefficient of correlation and rank correlation.
9. Fitting of regression lines.
10. Probability distributions curves :
    (i) binomial
    (ii) Poison and
    (iii) Normal Distribution.
11. Comparative studies of different database file formats: GenBank, FASTA and PIR.
12. Survey of various genomic, proteomic and evolutionary tools available at ExPasy server.
13. Study of Databases: Uniprot, Unigene, PDB and KEGG

Second Semester

BIN 404 Algorithms in Computational Biology

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- develop understanding on the efficiency and speed of computer algorithm
- understand the stochastic process and sampling methods
- learn the system optimization using computational tools

Section A

Algorithms and Data structures in Bioinformatics; Algorithms and complexity, Iterative and recursive algorithms, Fast versus slow algorithms, Big-O Notation, Algorithm design and analysis techniques, Greedy Algorithms, Randomized Algorithms, Divide-and-Conquer approach, Searching and Sorting algorithms, Linear and non-linear data structure, Stack, Queues, Linked list, Trees-Terminologies, Binary trees, Tree traversal (Pre-order, In-order, post-order).

Section B

Brute Force, Dynamic programming: Shortest Superstring Problem, Random Walk (1D & 2D), Markov chain; Hidden markov models – Forward, Backward, Viterbi and Baum – Welch algorithm. Population dynamics algorithms; Intraspecies, Interspecies, and Pre – Predator (two species Lotka – Voltera). Fibonacci series, golden ratio. Introduction to chaos and fractals; Lorenz equation. Random sampling; Monte Carlo, Metropolis algorithms.

Section C

Introduction to optimization problem, methods of optimization: Genetic algorithm, Particle – Swarm algorithm and Ant – colony optimization. Introduction to data clustering; definitions of distance, similarity, cluster, centre and modes. Measure of distances; Euclidean, Maximum, Mahalanobis and average. The EM Algorithm, Center-based Clustering

Algorithms; The k-means Algorithm. Hierarchical Clustering; Agglomerative clustering methods; Single link, complete link, group average, centroid and median methods.

Suggested Books:

- Jones, N.C. & Pevzner, P.A. (2000). An Introduction to Bioinformatics Algorithms. The MIT Press.
- Dediu, A. H., Hernández-Quiroz, F., Martín-Vide, C. &Rosenblueth, D.A. (2015). (Eds.)Algorithms for Computational Biology. Springer.
- Baxevanis, A.D., Davison, D.B., Page, R. D. M. & Petsko, G.A. (2004). Current Protocols in Bioinformatics. John Wiley & Sons Inc.
- Gibas, C. & Jambeck, P. (2001). Developing Bioinformatics Computer Skills. O'Reilly Media, Inc.,
- Parida, L. (2008). Pattern Discovery in Bioinformatics: Theory & Algorithms. Chapman and Hall/CRC.

Suggested e-Resources:

- **Bio-Informatics:Algorithms and Applications**: https://onlinecourses.nptel.ac.in/noc19_bt01/preview
- **Markovian Processes**: https://www.coursera.org/learn/dna-analysis

BIN 407 Sequence Analysis and Phylogenetics

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- learn to perform the biological sequence analysis
- identify similar sequences in the database
- understand the process of molecular evolution

Section A

Sequence Analysis – concepts of sequence similarity, Sequence identity vs homology. Definitions of homologues, orthologues, paralogues and xenologues. Basic methods of sequence analysis; Dot plot method,

sequence distance calculation (Hamming and Levinshtein), their merits and demerits. Scoring matrices: basic concept and construction of a scoring matrix; PAM and BLOSUM matrix and their derivatives. Pairwise sequence alignment: Global and Local alignment algorithms; gap penalties, ends free alignment. Statistical significance of alignment score.

Section B

Sequence-based database searches: algorithm of BLAST and FASTA and interpretation of results. Algorithms for generation of sequence profiles; profile-based database searches using PSI-BLAST, analysis and interpretation of profile-based searches. Multiple sequence alignments (MSA): the need for MSA. Theory and application of various approaches for MSA; progressive and hierarchical. Algorithm of CLUSTALW and PileUp and their application for sequence analysis.

Section C

The concept of evolutionary tree; types of phylogenetic trees (rooted vs. unrooted trees), Molecular Clock, Newick format of tree representation. Introduction to evolutionary models; Jukes Cantor and Kimura two parameter. Algorithms of Phylogenetic Tree Construction: UPGMA, Neighbor-Joining, Maximum Parsimony, Maximum likelihood, and Bayesian Inference. Statistical assessments of phylogenetic methods (Consistency, Efficiency, Robustness, & Computational speed). Evaluvation of phylogenetic tree: Bootstrapping, Randomized and jack-knifing methods.

Suggested Books:

- Mount, D.W. (2004). Bioinformatics: Sequence and Genome Analysis. (2nd Ed.). Cold Spring Harbor Press.
- Durbin, R., Eddy, S.R., Anders, K. & Graeme, M (2002). Biological Sequence Analysis: Probabilistic models of protein and Nucleic acids. Cambridge University Press.
- Nei M. & Kumar, S. (2004). Molecular Evolution and Phylogenetics. Oxford University Press.

Suggested e-Resources:

- **Sequence Analysis**: https://www.coursera.org/learn/undefined
- **Molecular Evolution**: https://www.ebi.ac.uk/training/online/course/introduction-phylogenetics

BT 408 Genetic Engineering

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	4	0	0	4

Learning Outcome:

After successful completion of the course, students should be able to:

- develop comprehensive understanding of gene manipulation techniques
- describe various cloning and expression vectors
- develop skills for primer designing, gene amplification and expression

Section-A

Basic concepts of DNA structure and properties, restriction enzymes, DNA ligase, Klenow enzyme, T4 DNA polymerase, Polynucleotide kinase, Alkaline phosphatase, Cohesive and blunt end ligation, Linkers, Adapters, Homopolymeric tailing, Labeling of DNA, Nick translation, Random priming, Radioactive and non-radioactive probes, Hybridization techniques, Northern, Southern and Colony Hybridization, Chromatin immunoprecipitation, DNA-Protein Interaction-Electromobility shift assay, DNaseI footprinting, Methyl interference assay, Isolation of genomic DNA from prokaryotes and eukaryotes, Isolation of Plasmid DNA and Bacteriophage DNA. Isolation of total RNA and mRNA.

Section-B

Plasmids, Bacteriophages, pBR322 and pUC series of vectors, M13 and P2 phage based vectors, High capacity vectors:Cosmids, phagemid, BAC, Animal and Plant virus based cloning vectors, Shuttle vectors, Expression vectors, pMal, GST, pET-based vectors, Constructions of libraries, cDNA and genomic libraries, cDNA and genomic cloning, Expression cloning, Jumping and hopping libraries, South-western and Far-western cloning, Protein-protein interactive cloning and Yeast two hybrid system, Phage display.

Section-C

Primer designing, Fidelity of thermostable enzymes, Types of PCR-multiplex, nested, reverse transcriptase, real time PCR, touchdown PCR,

hot start PCR, colony PCR, in situ PCR, cloning of PCR products, T-vectors, Principles in maximizing gene expression, Gene expression analyses, differential gene expression methods, Introduction of DNA into mammalian cells, transfection techniques

Suggested Books:

- Old, R. W., Primrose, S. B., & Twyman, R. M. (2001). Principles of GeneManipulation: an Introduction to Genetic Engineering. Oxford: Blackwell Scientific Publications
- TBrown, T. A. (2006). Genomes (3rd ed.). New York: Garland Science Pub
- Glick, B.R. & Pattern, C.L. (2017). Molecular Biotech: Principles and application of recombinant DNA(5th Ed.).ASM Press.
- Reece, R. J. (2004). Analysis of genes and genome. John Wiley and sons Ltd.
- Green, M. R., & Sambrook, J. (2012). Molecular Cloning: a Laboratory Manual. Cold Spring Harbor, NY: Cold Spring Harbor Laboratory Press.

Suggested e-Resources:

- **Genetic engineering – Basics, New Applications and Responsibilities** - http://library.umac.mo/ebooks/b28055287.pdf

CS 418 Database Management Systems

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand relational database systems
- calling, processing and optimizing the databases
- learn Mining of data from open access biological databases

Section A

Introduction: - Data base system concepts, Comparison between traditional file system and DBMS, Database Users, Data models, schemas and

instances, Data independence, 3-level architecture of DBMS, Overall data base structure. Data modeling using Entity Relationship Model: - ER model, mapping constraints, Concept of super key, candidate key, primary key, Generalization, aggregation, reducing ER diagrams to tables. Relational Data Model: concepts, integrity constraints, relational algebra, SQL queries.

Section B

Data Base design: - Functional Dependency and its types, normal forms: first, second, third and BCNF, multi-valued dependency, fourth normal form, join dependency and fifth normal form. Steps in database design. Transaction processing: Introduction, ACID properties, Concurrency control techniques: Locking techniques, Time stamping, Optimistic approach, Multi-version. Management of deadlocks, Query processing and optimization.

Section C

Recovery, Integrity and security of Databases. Distributed Database systems: Introduction, Fragmentation, Replication, Transparency, Consistency and Concurrency control, Homogeneous Vs Heterogeneous systems. Advanced topic in databases: temporal database, spatial database, data mining, data warehousing and its applications. Case studies using NCBI, SwissProt and PDB.

Suggested Books:

- Hanery, K. & Abraham, S. (1997). Database System Concepts. New York, Tata Mac- Graw Hill.
- Date, C. J. (1999). An Introduction to Database Systems(6th Ed.). Addison Wesley.
- Hanery, K. & Abraham, S. (1997). Database System Concepts. New York, Tata Mac-Graw Hill.
- Baxevanis, A.D. & Ouellette, B.F.F. (2004). Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins (3rd Ed.). John Wiley.
- Bayross, I. (2003). SQL, PL/SQL The Programming Language of Oracle (2nd Ed.). BPB New Delhi. 2003

Suggested E-Resources:

1. Data Base Management System

https://nptel.ac.in/courses/106105175/

2. Database Management Essentials by University of Colorado
   https://www.coursera.org/learn/database-management
3. Database System Concepts by Abraham Silberschatz, Henry F. Korth and S. Sudarshan
   https://kakeboksen.td.org.uit.no/Database%20System%20Concepts%206the%20edition.pdf

CS 418L Database Management Systems Lab

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**4**	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- create relational databases
- perform query calling form the databases
- execute databases management for biological purposes

1. Basic DDL commands (creat, drop, alter) with integrity constraints.
2. DML and DCL commands (Insert, Update, Delete, Select, Commit, Rollback)
3. Operators (Arithmatic, Logical, Relational etc.)
4. Assignment based on DDL and DML with conditions also join (Self join, inner join, outer join, equi join)
5. Complex queries (Retrieval of data from more than one table)

CS 446 Programming with Perl and R

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- learn Perl scripting for string manipulations.
- understand using the Perl modules.

- understand the environment of R and Bioconductors

Section A

Perl Data types: Scalar variables, scalar operations and functions, array variables, array representation, array operations and functions, hash variables and its representation, hash functions. Application of hashes to write genetic code and gene expression data. Perl regular expression: Concepts and use of regular expression for biological data. Metacharacters, Pattern-matching, Substitutions, Transliteration, split and join functions. Control Structure in Perl (Conditions and Loops).

Subroutines and its advantage, arguments, passing data to subroutines. Concept of file handling, opening, rading editing and closing a File. Directory handling: opening reading and closing a directory.

Section B

Bioperl: Introduction to Bioperl and its installation. Bioperl architecture: general classes, Sequences -Bio::Seq Class, sequence manipulation, alignments -AlignIO, Analysis -Blast, Databases- Database Classes. Introduction to common gateway interface module (CGI.pm), CGI program in Context, Perl and the Web.

Introduction to R language; R Objects and data structures – Variable classes, Vectors and matrices, Data frames and lists, Data sets included in R packages, Summarizing and exploring data, Reading data from external files, Storing data to external files, Creating and storing R workspaces. Flow Control in (Conditions and Loops).

Section C

Object Manipulating using R – Mathematical operations (recycling rules, propagation of names, dimensional attributes, NA handling), Basic matrix computation (element-wise multiplication, matrix multiplication, outer product, transpose, eigenvalues, eigenvectors), Textual operations, Basic graphics (high-level plotting, low-level plotting, interacting with graphics).

Introduction to Big data in Bioinformatics: Characteristics, data structures and data repositories; exploratory analysis of big data in R environment, Bioconductor, Microarray and next-generation sequencing (NGS) data analysis in R environment.

Suggested Books:

- Curtis, J. D. (2003). Perl programming for biologists. John Wiley & sons, inc
- Bal, H.P. (2003). Perl programming for Bioinformatics. Tata McGraw-Hill New Delhi.
- Gerrard, P. & Johnson, R.M. (2015). Mastering Scientific Computing with R. Packt Publishing, UK.
- Hahne, F. et al. (2008). Bioconductor case studies. Springer.
- Lewis, P.D. (2010). R for Medicine and Biology. Jones and Bartlett Series.
- Tisdall, J.D. (2001). Beginning Perl for bioinformatics. Shroff Publishers and distributors O'Reilly Media, Inc.
- Tisdall, J.D. (2003). Mastering Perl for bioinformatics. Shroff Publishers and distributors O'Reilly Media, Inc.

Suggested e-Resources:

- **Perl Programming**: https://www.learn-perl.org/
- **R Programming**: https://www.rstudio.com/online-learning/

CS 446L Programming with Perl and R Lab

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**8**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- write the Perl programs for string manipulations
- develop and use simple Perl modules
- use the bioconductor packages from R for statistical analyses of biological data

1. Use of various arithmetic and logical operators
2. Programming based on string manipulation (concatenation, splitting etc.)

3. Regular expression and its applications. Use of s/// and tr/// operators.
4. Pattern matching to locate and count motifs in a string.
5. Constructing arrays. addition and removal of elements from array, exploring array.
6. Use hashes in conversion of three letter code to one letter code and proteing translation.
7. Perl subroutines.
8. File handling, reading data from a file writing data to a file and editing a file.
9. Directory handling, make a directory, change present working directory, reading files from a directory.
10. Introduction to Perl modules, construction of simple module
11. Basic statistical analyses in R.
12. Using R for simple problems of molecular biology.
13. Use of Bioconductor for analyzing biological data.

Suggested Books:

- Wall L et al.; Programming Perl (2012, 4th Ed.) O'Reilly.
- Gerrard P and Johnson RM.; Mastering Scientific Computing with R (2015), Packt Publishing, UK.

Suggested e-Resources:

- **Perl Programming**: https://www.learn-perl.org/
- **R Programming**: https://www.rstudio.com/online-learning/

Third Semester

BIN 511 Biomolecular Modeling and Computational Drug Design

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome

After successful completion of the course the candidates should be able to:

- understand the principles of statistical thermodynamics
- develop understanding of principles of biomolecular modelling and simulations
- understand the computational methods for drug designing and development

Section – A

Basic Thermodynamics - The Laws of Thermodynamics, the Maxwell Relations, the Gibbs-Duhem Equation and Extensive Functions, Intensive Functions.Lagrangian Formulation, Hamiltonian Formulation and Canonical Transformations, Classical approach to Ensembles: Ensembles and Phase Space. Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium.

Section – B

Homology modeling, Protein Threading and abinitio methods. Introduction to Molecular mechanics. Optimization of modeled protein 3D structure. Energy minimization (steepest descent, conjugate gradient and Newton-Raphson methods). Molecular dynamics simulation: Equation of motion, integration schemes; Introduction to force fields, its popular variants; Ergodic Hypothesis, Ensembles (Canonical and Micro-Canonical) and their control in MD simulation, periodic boundary conditions and calculation of long range potentials (Particle – Mesh and Ewald summation methods). Potential energy surface: Convergence Criteria, Characterizing Stationary Points, Search for Transition States.

Section – C

Computational Drug design; Drug likeness: Lipinski's rules, ligand efficiency and lipophilic ligand efficiency. Molecular recognition: affinity determination, intermolecular binding free energy. Ligand based drug design: - pharmacophore, constrained systematic search and genetic algorithm. Structure based drug design: Molecular docking and virtual screening.

Introduction to QSPR and QSAR. Molecular descriptors used in QSAR studies: electronic; topological and quantum chemical. QSAR models: Free Wilson and Hansch equation. Statistical methods for QSAR modeling: regression, principle component and partial least squares analysis. Bioisosteres, Hammet substituent constant.

Suggested Books:

- Cramer, C. (2004) Essentials of Computational Chemistry (2nd Ed); John Wiley.
- Leach, A. R. (2001). Molecular Modeling-Principles and applications. Pearson Education.
- Thomas G. (2003) Fundamentals of Medicinal Chemistry; John Wiley.
- Alvarez J. and Shoichet B. (Ed.) (2004). Virtual Screening in Drug Discovery. Taylor and Francis.
- Kukol, A. (Ed.) (2015). Molecular Modeling of Proteins (2nd Ed.). Springer Nature. Young, D.C. (2009). Computational Drug Design. John Wiley.

Suggested e-Resources:

- **Statistical Mechanics**: https://onlinecourses.nptel.ac.in/noc19_ph06/preview
- **MD Simulation and SBDD**:

  https://nptel.ac.in/courses/103103036/13

  https://onlinecourses.nptel.ac.in/noc18_bt28/preview

BIN 511L Biomolecular Modeling and Computational Drug Design Lab

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**8**	**4**

Learning Outcome:

After successful completion of the course the candidates should be able to:

- model the 3D structure of the biomolecules
- carry out biomolecular interaction studies
- perform MD simulations to study the biomolecular dynamics

1. Molecular visualization tool (applications such as molecular interaction, Molecular surface visualization, electrostatics, H-bond calculation etc.)
2. Identification of different structural motifs in proteins.
3. Analysis of PDB (NMR and X-ray) structures (Quality of structure, analyzing molecular interactions, protein-ligand/protein-protein if any, from PDB).
4. Homology based protein structure prediction.
5. Quality estimation of modeled protein structure (ProCheck, PROSA, Verify 3D, Errat etc.).
6. Contact map based protein structure comparison.
7. Energy minimization based mutational analysis of proteins (using SwissPDB-Viewer).
8. Protein-Ligand docking Autodock and MGL Tools and Pharmacophore analysis.

BT 545 Genomics and Proteomics

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	4	0	0	4

Learning Outcome:

After successful completion of the course the candidates should be able to:

- understand the experimental methods available to study the genome and proteomes
- develop understanding of computational tools of genomics and proteomics
- learn next generation sequencing methods for genomics and transcriptomics

Section – A

Genomics – Introduction to genome and genomics; genetics vs genomics. DNA microarray; prepration, understanding of microarray data, normalizing microarray data, detecting differential gene expression, correlation of gene expression data to biological process and analysis tools. Gene Expression Omnibus (GEO). Genomics and Metagenomics – Large scale genome sequencing strategies. Genome assembly and annotation. Genome databases of Plants, animals and pathogens. Metagenomics: Gene networks: basic concepts, computational model such as Lambda receptor and lac operon. Prediction of genes, promoters, splice sites, regulatory regions: basic principles, application of methods to prokaryotic and eukaryotic genomes.

Section – B

Proteomics – Introduction to proteome and proteomics; protein chemistry vs proteomics. Analytical techniques of proteomics; working principles of 2D – gel electrophoresis, mass spectrometry with their merits and demerits. Mass spectrometers for protein and peptide sequencing; MALDI – TOF, Electospray Ionization coupled tendem Mass spectrometry.Tendem mass analyzer, triple quadrupole mass analyzer, ion – trap mass analyzer and FT – ion cyclotron resonance MS. Peptide Mass Fingerprinting.Sequencing the protein fragments: Scoring Algorithm for Spetral Analysis. Application of SALSA in amino acid – Motif searching.

Section – C

Next Generation sequencing & assembly: Elements of big data analysis, NGS Platforms based on pyrosequencing, sequencing by synthesis, emulsion PCR approach with small magnetic beads and single molecule real time (SMRT) sequencing; Genome assembly algorithms, De-novo assembly algorithms, Sequence Alignment formats: Sequence Alignment/Map (SAM) format, Binary Alignment/Map (BAM) format.Protein function prediction using Machine learning tools: supervised/unsupervised learning, Neural network, SVM. Protein-protein interactions: databases such as STRINGS, DIP, PPI server and tools for analysis of protein-protein interactions

Suggested Books:

- Brown, S.M. (2015). Next-generation DNA sequencing Informatics (2nd Ed.). Cold Spring Harbor Press.
- Liebler, D. C. (2001). Introduction to proteomics tools for the new biology. Humana Press.
- Lesk, A.M. (2015). Introduction to Genomics (2nd Ed). Oxford University Press.
- Pevsner, J. (2017). Bioinformatics and Functional Genomics (3rd Ed). John Wiley.
- Twyman, R.M. (2004). Principles of Proteomics; CBS Publishers.
- Thangadurai, D. & Sangeetha, J. (2015). Genomics and Proteomics: Principles, Technologies, and Applications. CRC Press.

Suggested e-Resources:

- **Proteomics**: https://nptel.ac.in/courses/102101055/4
- **Genomics**:

  https://edu.t-bio.info/course-category/omics/

  https://ocw.mit.edu/courses/biology/7-012-introduction-to-biology-fall-2004/video-lectures/lecture-25-genomics/

CS 538 Python Programming

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After the successful completion of course the candidates should be able to:

- understand the python programming environment
- learn using the python libraries
- learn file and directory handling in python

Section A

Python interpreter and interactive mode; values and types: int, float, boolean, string, and list; variables, expressions, statements, tuple assignment, precedence of operators, comments; modules and functions, function definition and use, flow of execution, parameters and arguments; Illustrative programs: exchange the values of two variables, circulate the values of n variables, distance between two points.

Section B

Conditionals: Boolean values and operators, conditional (if), alternative (if-else), chained conditional (if-elif-else); Iteration: state, while, for, break, continue, pass; Fruitful functions: return values, parameters, local and global scope, function composition, recursion; Strings: string slices, immutability, string functions and methods, string module; Lists as arrays. Illustrative programs: square root, gcd, exponentiation, sum an array of numbers, linear search, binary search.

Section C

Lists: list operations, list slices, list methods, list loop, mutability, aliasing, cloning lists, list parameters; Tuples: tuple assignment, tuple as return value; Dictionaries: operations and methods; advanced list processing – list comprehension; Illustrative programs: selection sort, insertion sort, mergesort, histogram. Files and exception: text files, reading and writing files, format operator; command line arguments, errors and exceptions, handling exceptions, modules, packages; Illustrative programs: word count, copy file.

Suggested Books:

- Sedgewick, R., Wayne, K. & Dondero R. (2015). Introduction to Programming in Python: An Inter-disciplinary Approach. Addison – Wesley Professional.
- Lambert, K.A. (2011). Fundamentals of Python: First Programs, Cengage Learning.
- Goodrich, M.T., Tamassia, R. & Goldwasser M.H. (2016). Data structure and Algorithms in Python. Wiley India Pvt.Ltd.
- Bassi, S. (2017). Python for Bioinformatics (2nd Ed.). Chapman and Hall/ CRC press.

Suggested e-Resources:

- **Python Tutorials**:

  https://www.tutorialspoint.com/execute_python_online.php

  https://onlinecourses.nptel.ac.in/noc16_cs11/preview

CS 538L Python Programming Lab

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**0**	**0**	**4**	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- write python programs for studying biological samples
- learn using python libraries
- perform data analysis in python

1. Introduction to variables and various arithmetic & logic operations.
2. Introduction to strings and lists
3. Conditionals and Loops in python.
4. Working with files and directories in python.
5. Working with Molecular biology problems such as transcription, translation, GC island identification.
6. Working with sequence analysis problems such as global alignment, local alignment Parsing Blast output etc.
7. Accessing biological databases with Python.

Discipline Electives

BIN 507 Mining and Warehousing of Biological Data

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course the candidates should be able to:

- understand the knowledge discovery from the databases
- categorizing the biological data based on various parameters
- learn to use data mining tools

Section A

Fundamentals of Data Mining – concept, definitions, why data mining, kind of data for data mining, knowledge discovery in databases (KDD), data mining functionalities, data mining primitives, classification of data mining systems, data mining techniques, major issues in data mining.

Data Preprocessing – Needs for preprocessing the data, data cleaning, data integration and transformation, data reduction, data discretization and concept hierarchy generation.

Data Warehousing – need, definitions, characteristics, data marts, metadata, operational versus analytical databases, data warehouse architecture, multi dimensional data model, schemas for multidimensional databases, introduction to DMQL, implementation of data warehouse, OLAP, OLTP, ROLAP, MOLAP, HOLAP.

Section B

Association Rules Mining – market basket analysis, apriori algorithm, FP-growth method, Mining Multilevel Association Rules from Transaction Databases, Mining Multidimensional Association Rules

Classification and Prediction – classification by decision tree induction, classification by back propagation, linear and non-linear regression, classifier accuracy.

Clustering – types of data in clustering, categorization of clustering methods, Major Clustering Methods (K-means, Hierarchal clustering, DBSCAN).

Section C

Mining Complex Types of Data - Spatial databases, multimedia databases, time-series and sequence data, text mining, web mining, trends in data mining, Introduction to various data mining tools (SAS Enterprise Miner 5.1, Oracle Data Mining, SPSS Clementine 8.5).

Biological databases, Application of data mining in DNA/protein sequence analysis, protein structure analysis, gene expression analysis, application of specific examples of designing biological databases, application of mining and warehousing in bioinformatics.

Suggested Books:

- Han, J., Kamber, M. & Pei, J. (2012). Data mining concept and technique (3rd Ed.). Elsevier.
- Chen, J.Y. & Lonardi, S. (Eds.) (2017). Biological Data Mining (1st Ed.). Chapman and Hall/CRC.
- Elayidom, M. S. (2014). Data Mining and Warehousing. Cengage Learning.
- Baxevanis, A.D. & Ouellette, B.F.F. (2004). Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins (3rd Ed.). John Wiley.
- Morey, D., Maybury, M. & Thuraisinghan, B. (Eds) (2002). Knowledge Management, Classic and Contemporary Works; The MIT Press.

Suggested e-Resources:

- **Data Mining**: https://nptel.ac.in/courses/106105174/
- **Data Mining**: Concepts and Techniques: https://hanj.cs.illinois.edu/bk3/bk3_slidesindex.htm

CS 530 Neural Networks

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand the concept of machine learning and soft computing
- understand the automated classification methods
- learn the basic theory of artificial intelligence

Section A

Introduction to Neural Networks, Models of a Neuron, Network architectures, feedback, learning process - error correction, learning, Hebbian, Competitive, Boltzman, Supervised and unsupervised learning, the perceptron model, Multilayer perceptrons.

Section B

Recurrent Networks, the Hopfield Network, the Boltzmann machine, its Markov Chain model, self organizing systems : Hebbian learning, Competitive learning.

Section C

Moduler Networks, associative Model, Stochastic Model, Temporal processing : Back propagation learning, real time recurrent networks.

VLSI implementations of Neural Networks : Design considerations, Neurocomputing hardware.

Suggested Books:

- Bishop, C.M. (1995). *Neural Networks For Pattern Recognition*. Oxford University Press.
- Fausett L.V. (2004). Fundamentals of neural networks. Pearson Education
- Gurney, K. (1997) An introduction to neural networks . CRC press.

Suggested e-Resources:

- **Introduction to Neural Networks**: http://www.cs.bham.ac.uk/~jxb/NN/

- **Neural Networks and Deep Learning**:
  https://www.coursera.org/learn/neural-networks-deep-learning

CS 512 Cloud Computing

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand virtualization of machines
- learn to use various cloud platforms
- understand the cloud based computation process

Section A

Introduction to Cloud Computing, Definition, Characteristics, Components, Administering & Monitoring cloud services, benefits and limitations, Deploy application over cloud, Cloud computing platforms: Infrastructure as service: Platform as Service: Google App Engine,

Introduction to Cloud Technologies, Study of Hypervisors, Compare SOAP and REST, Web services, AJAX and mashups-Web services: SOAP and REST, SOAP versus REST, AJAX: asynchronous 'rich' interfaces, Mashups: user interface services.

Section B

Virtualization Technology: Virtual machine technology, virtualization applications in enterprises, Pitfalls of virtualization, Multitenant software: Multi-entity support, Multi-schema approach, Multitenance using cloud data stores, Data access control for enterprise applications.

Data in the cloud: Relational databases, Cloud file systems: GFS and HDFS, Map-Reduce and extensions: Parallel computing.

Section C

Cloud security fundamentals, Vulnerability assessment tool for cloud, Privacy and Security in cloud, Cloud computing security architecture: Architectural Considerations- General Issues, Trusted Cloud computing, Secure Execution Environments and Communications, Micro-architectures; Identity Management and Access control Identity management, Access control, Autonomic Security

Cloud computing security challenges: Virtualization security management virtual threats, VM Security Recommendations, VM-Specific Security techniques, Secure Execution Environments and Communications in cloud. Issues in cloud computing, Implementing real time application over cloud platform.

Suggested Books:

- Puttini, R., Erl, T. & Mahmood, Z. (2013) Cloud Computing: Concepts, Technology & Architecture.
- Rittinghouse, J.W. & Ransome, J.F. (2010).Cloud Computing, Implementation, Management, and Security. CRC Press.
- Hurwitz, J., Bloor, R., Kanfman, M. & Halper, F. (2009) Cloud Computing for Dummies.Wiley India Edition.
- Rafaels, R. (2015). Cloud Computing from Beginning to End. Createspace Independent Publishing.

Suggested e-Resources:

- **Cloud Computing**:https://nptel.ac.in/courses/106105167/1
- **Cloud Computing Specialization**: https://www.coursera.org/specializations/cloud-computing

BIN 513 Systems Biology

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After the successful completion of course the candidates should be able to:

- understand the different types and properties of biological networks
- understand using the various databases of biological networks
- learn to model the metabolic processes

Section A

Introduction to Graph, forest & Network. Parameters of networks: degree of node, degree distribution and power law behaviour, shortest path, mean path, clustering coefficient, node centrality and network centrality. Types of networks: random, small world, scale-free networks, and Hierarchical networks. Robustness of a Network: Topological, Functional and dynamical robustness.

Section B

Introduction to biological networks, properties and importance of biological networks. Types of biological networks. Protein interaction network, Types of Protein-Protein interactions (PPI): Stable, Transient, Physical, and Genetic interactions. Prediction of Protein-Protein interactions: experimental and computational methods. Databases of biological networks (STRING, BioGRID, STITCH and KEEG), Designing of network circuitry (CYTOSCAPE), Network layouts.

Section C

Gene Regulatory network: Methods for regulatory network reconstruction, Boolean and Bayesian network model. Multi-layer hierarchical structure of regulatory networks.Metabolic Network, Signaling networks and their identification methods Methods in system Biology: Interaction based method, Construction based methods, and Mechanism based methods. Visual representations and notations for systems biology, Metabolic Pathway visualization and editing software (MyBioNet, MetaViz, Cytoscape). Future for system Biology. Synthetic biology and artificial gene circuits.

Suggested Books:

- Klipp, E., Liebermeister W., Wierling C., Kowald A. & Herwig R. (2016). Systems Biology: A Textbook. Wiley – Blackwell.
- Covert, M.W. (2014). Fundamental of Systems Biology: From Synthetic Circuits to Whole – Cell Models. CRC press.
- Helms, V. (2008). Principles of Computational Cell Biology. Wiley – Blackwell.
- Panchenko, A. & Przytycka T.M. (Ed.) (2008). Protein-protein Interactions and Networks: Identification, Computer Analysis, and Prediction. Springer – Verlag London.
- Vadyanathan, S., Harrigan G.G. & Goodacre R. (2005). Metabolome analyses: Strategies for Systems Biology. Springer – Verlag.
- Alon, U. (2006). An Introduction to Systems Biology: Design Principles of Biological Circuits. Chapman & Hall/CRC, Tailor & Francis.

Suggested e-Resources:

- **Network Biology**: https://www.coursera.org/learn/network-biology

- **System Biology**: https://www.coursera.org/learn/systems-biology
- **Synthetic Biology**: https://www.edx.org/course/principles-of-synthetic-biology

BIO 503 Fundamentals of Bioentrepreneurship

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand role of entrepreneurship in promoting innovation and wealth generation
- develop skills for writing business models for new ideas and market segments
- explain various financial, marketing, sales and legal issues associated with entrepreneurship

Section-A

Concept of entrepreneurship; Classification and types of entrepreneurship, Myths about entrepreneurship; Role of entrepreneurship in wealth building and creating an impact; Society, Technology and Entrepreneurship.

Creativity and Innovation; Types and forms of Innovation; Sources of innovative opportunity; Entrepreneurship as a career option.

Section-B

Introduction to the Design Thinking Process; Problem identification; Idea Generation; Value Proposition; Lean Canvas.

Identifying Customer Segments; Idea Validation; Developing Business Model; Sizing the opportunity; Building MVP; Concept of Start-up, Importance of Incubation.

Section-C

Financial and Non financial support: Revenue streams; Pricing and Costs; Sources of funds; Importance of project management.

Marketing and Sales: Positioning; Channels and Strategy; Sales Planning.

Team: Importance of teambuilding; Complementary skill sets.

Legal issues: Brief overview of- intellectual property rights, patents, trademarks, copy rights, trade secrets, licensing and GI.

Business Plan writing.

Policies and Initiatives to promote Entrepreneurship in India.

Suggested Books:

- Jain, P.C. (2001). Hand Book for New Entrepreneurs. UK: Oxford University Press.
- Hisrich R. D., Manimala M. J., Peters Michael P. & Shepherd D. A. Entrepreneurship (9th ed.). McGraw Hill Publication.
- Roy, R. (2011). Entrepreneurship (2nd ed.). UK: Oxford University Press.
- Drucker, P. (2015). Innovation and Entrepreneurship (1st ed.). Routledge Classics.
- Kotler, P & Keller, K.L. (2017).Marketing Management (15th ed.). Pearson Publications
- Desai, V. (2011) Dynamics of Entrepreneurial Development & Management (6t ed.). Mumbai: Himalaya Publishing House.
- Khanka, S.S. (2007) Entrepreneurial Development. New Delhi: S. Chand & Company Ltd.
- Mohanty, S K. (2005). Fundamentals of Entrepreneurship. EEE Prentice Hall India Learning Private Limited.
- Gupta C.B. & Srinivasan N.P. (2013). Entrepreneurship Development in India. Sultan Chand & Sons.
- Gupta A.K. (2016).Grassroots Innovations (Minds On the Margin Are Not Marginal Minds). Random House.
- Patzelt, H., &Bernner, T. (Eds.). (2008). Handbook of Bioentrepreneurship. Berlin, Germany: Springer.
- Robert, D. H., & Peters, M. P. (2002). Entrepreneurship. New York, USA: McGraw-Hill Education

- Shane, S. (2004). Academic Entrepreneurship: University Spinoffs and Wealth Creation. Northampton, M.A.: Edward Elgar

Suggested e-Resources:

- https://www.startupcommons.org/what-is-startup-ecosystem.html
- https://getproductmarketfit.com/how-to-select-test-to-get-market-validation-for-new-product-or-business-idea/
- https://www.coursera.org/learn/wharton-launching-startup
- https://www.coursera.org/learn/wharton-entrepreneurship-opportunity
- **Bioentrepreneurship**: www.birac.nic.in/webcontent/jk.pdf
- **Biotechnology and entrepreneurship**: http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.463.4354&rep=rep1&type=pdf
- **Accounts and Bioentrepreneur**: https://www.nature.com/bioent/2003/031101/full/bioent779.html
- **Bioentrepreneurship:** www.birac.nic.in/webcontent/jk.pdf

BIN 514 RNA Structure Function and Transcriptomics

Max. Marks : 100	**L**	**T**	**P**	**C**
(CA: 40 + ESA: 60)	**4**	**0**	**0**	**4**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand the structure and applications of various non-coding RNAs
- learn techniques of genome wide expression studies
- understand the usage of various online resources for transcriptomic studies

Section A

The biology, chemistry, structure and function of the RNA molecule in prokaryotic and eukaryotic systems including their viruses. Interaction between RNA molecules. Interaction between RNA and proteins. Interaction between RNA and small ligands. The role of RNA in an evolutionary perspective. Description of non coding RNA and their functions and possible mechanism of action. (SnRNA, SnoRNA, siRNA, miRNA, Catelytic RNA and Ribozymes).

Section B

Transcriptome and Transcriptomics; Genome Wide Gene Expression Analysis: Microarrays: experiments to annotation. Expressed sequence tags: EST Genration, EST Clustering importance in gene identification. Serial analysis of gene expression (SAGE), SAGE data and its importance. Tools for Transcriptomics and Transcriptome Analysis.

Section C

Database and web tools for ESTs project. Tissue Specific Transcriptomics and Expression Pattern Analysis. Transcriptional Regulation of Gene Expression in Prokaryotes and Eukaryotes. The Transcriptome Projects. Impact of Transcriptomics on functional genomics, Diseases and drug discovery, Evolutionary analyses and Pharmaceutical Research.

Suggested Books:

- Meister G. (2011), RNA Biology; Wiley – VCH.
- Gesteland, R. F., Cech, T & Atkins, J. (2005). The RNA World (3rd Ed.), CSHL – press.
- Wu J. (Ed.) (2016),Transcriptomics and Gene Regulation; Springer – Nature.
- Passos G.A. (Ed.) (2014). Transcriptomics in Health and Disease; Springer Publications.

Suggested e-Resources:

- **Genomics 1 - T-BioInfo in Education**: https://edu.t-bio.info/course-category/omics/
- **Non coding RNA**: https://www.nature.com/collections/sqtqxdnvdz
- **Epigenetics**: https://www.whatisepigenetics.com/non-coding-rna/

Fourth Semester

BIN512D: Dissertation

Max. Marks: 100	L	T	P	C
(CA: 40 + ESA: 60)	0	0	48	24

Learning Outcome:

After successful completion of the course student should be able to:

- develop working skills in organizations such as academic institutions, research laboratories and industries.
- plan and execute the research work for the given problem.
- lifelong learning from the experiences of research project.
- develop academic writing skills to present new findings in scientific journals.

Reading Elective

BIN 601R Chemoinformatics

Max. Marks : 100	**L**	**T**	**P**	**C**
ESA : 100	**0**	**0**	4	**2**

Learning Outcome:

On completion of this course, students should be able to:

- learn various computational methods used in chemical sciences.
- learn about different chemical databases and techniques.
- apply the chemoinformatics knowledge for drug discovery.

The informatics has influenced the fate of chemical sciences since last quarter of the 20th century, with evolution of computational methods such as combinatorial libraries, virtual screening and molecular modeling has led the medicinal chemists to speed up the drug discovery.

To store the data computational chemists uses different nomenclatures such as SMILES and variety of file formats like MOL, MOL2 and SDF. The entire chemical space has been maintained in various databases such as PUBCHEM, DRUGBANK, NCI and ZINC. Further, the details of chemical reactions and novelty of the chemical species are maintained at chemical abstract service (CAS).

Searching full or fragments of chemical structures involves pharmacophore methods, that forms the ground for ligand based drug discovery programs. The methods involve 3D searching of chemical space;

Predicting different physico-chemical properties, toxicity of compounds has been a challenging task since the inception of chemoinformatics.

Suggested Books:

- Leach A.R. Gillet V.J. (2007), An Introduction to Chemoinformatics. Springer Netherlands.
- Goodman J.M. (1998), Chemical Applications of Molecular Modelling, RSC Publications.
- Varnek A. (Ed.) (2017) Tutorials in Chemoinformatics. John Wiley and Sons Ltd.

➢ Bunin B.A., Siesel B., Morales G. & Bajorath J. (2007), Chemoinformatics: theory, practice and products. Springer Netherlands

Suggested e-Resources:

➢ **Chemoinformatics**

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6146447/

➢ **Databases and tools of medicinal chemistry**

https://core.ac.uk/download/pdf/82152489.pdf

BIN 602R Immunoinformatics

	L	T	P	C
Max. Marks : 100				
ESA : 100	**0**	**0**	4	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- develop an understanding of immunological informatics.
- learn about different databases of immunological importance.
- apply various bioinformatics tools for the study of immunological processes.

Immunology is a core biological science course that deals with the immunity, classification of Immunity, antigens, Immunoglobulins and biochemical processes in antigen – antibody reactions. The antigen representation is a challenging task to understand the antigen – antibody reactions, which are followed by th major histocompatibility complexes and variety of receptors such as T and B cell receptors. The immunology has played a great role in human health improvement by development of vaccines and organ transplantation. However, hyper-activation of immune system may result in the autoimmune disorders such as psoriasis.

The informatics is currently playing great role in immunological sciences such as by developing databases dbMHC, IMGT, IPD, SYFPEITHI, Bcipep etc.). Bioinformatics methods such as molecular modeling, Protein – Protein/Peptide interactions are routinely being used to understand the

Preptide-MHC Binding. Further the machine learning techniques are also being used to predict the MHC Binders, T-Cell Epitopes, MHC-Class I and II Binding Affinity.

Suggested Books:

- Punt J., Stranford S., Jones P. & Owens J.A. (2018), Kuby Immunology (8th Ed.); W.H. Freeman & Company.
- Roitt I.M. & Delves P.J. (2001) Roitt's Essential Immunology(10th Ed.) Blackwell Science Ltd.
- Flower D.R. (Ed.) (2007) Immunoinformatics: Predicting Immunogenicity in-silico. Humana Press: Methods in Molecular Biology.

Suggested e-Resources:

- **Immunoinformatics:**
  http://www.imgt.org/about/immunoinformatics.php

BT 529R Drug Discovery

	L	T	P	C
Max. Marks : 100				
ESA : 100	**0**	**0**	4	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand the role of synthetic chemistry in the development of pharmaceutical agents; and the modification of chemical structures to develop new drug molecules.
- develop an understanding of drug targets as a recognition site for pharmaceutical agents.
- apply the knowledge of pharmacogenomics and bioinformatics as for drug designing and discovery.

Modern drug discovery involves the identification of a target or drug lead using different techniques including molecular modeling, combinatorial libraries and high-throughput screening (HTS). Rational drug design is

based on the understanding of the three-dimensional structures and physicochemical properties of drugs and receptors. Knowledge of molecular mechanisms, molecular dynamics simulations and homology modeling is necessary for studying drug/receptor interactions. The different conformational sampling techniques, fitness functions used in molecular docking and computational receptor-based and ligand-based drug design approaches are mostly used to design compounds with improved biological activity in rational drug design. Quantitative drug design using QSAR models are used to correlate structural molecular properties (descriptors) with functions (i.e. physicochemical properties, biological activities, toxicity, etc.) of the compounds. Understanding the structure activity relationship between the 3D structure of a molecule and its biological activity may act as the basis for the prediction of compounds with improved biological activities. Different bio-analytical assays (LC/MS/MS, GC/MS and ELISA) could be developed further in support of *in vitro* and *in vivo* studies. Understanding the principles as well as an early characterization of drug toxicity, adsorption, distribution, metabolism and excretion (ADME) along with drug-drug interactions, plasma protein binding assays and metabolite profile studies helps in eliminating compounds with unacceptable pharmacokinetic characteristics, which is critical to successful drug discovery programs.

Suggested Books:

- Krogsgaard-Larsen et. al. (2016). Textbook of Drug Design and Discovery. 5th Edition. CRC Press.
- Satyanarayanajois, S. D. (2011). Drug Design and Discovery: Methods and Protocols. Humana Press.
- Rahman, A. U., Caldwell, G. W., and Choudhary, M. I. (2007). Frontiers in Drug Design and Discovery. Bentham Science publishers Limited.
- Dastmalchi, S. et. al. (2016). Methods and Algorithms for Molecular Docking-Based Drug Design and Discovery. IGI Global.

Suggested e-Resources:

- **Drug Discovery:**

https://www.studocu.com/en/document/university-of-leeds/drug-development-pre-clinical-to-practice/lecture-notes/lecture-i-drug-discovery-lecture-notes-lectures-1-8/615380/view

- **Peptide therapeutics:**
  https://www.sciencedirect.com/science/article/pii/S1359644614003997
- **Bio-analytical techniques:**
  https://www.pharmatutor.org/articles/bioanalytical-techniques-overview

BT 531R Human Genetics and Diseases

	L	T	P	C
Max. Marks : 100				
ESA : 100	**0**	**0**	4	**2**

Learning Outcome:

After successful completion of the course, students should be able to:

- understand hereditary and molecular genetics with a strong human disease perspective.
- describe genetic abnormalities underlying human disease and disorders
- develop understanding of biomedical research, genetic counseling, medicine and clinical genetics

Since the rediscovery of Mendel's work in 1900, investigations on the genetic nature of human traits have gained significant importance. Understanding the genetic basis behind human disease is one of the most important reasons to study human chromosome structure, human karyotype, banding techniques, chromosome identification and nomenclature (ISCN)**.** Classical genetics has considerable importance in constructing genetic hypothesis from pedigree data analysis in monogenetic traits, autosomal dominant, autosomal recessive, sex linked dominant, sex linked recessive and sex influenced traits. The impact of consanguinity in causing sex linked anomalies (haemophilia, colour blindness and Duchenne Muscular Dystrophy) has been observed in human population. Current knowledge on genetic variations across populations is applied to study human health and diseases which include chromosomal disorders, structural and numerical chromosomal anomalies (Klinefelter syndrome, Down's syndrome, Turner syndrome, Achondroplasia), inborn errors of metabolism (Phenylketonuria

(PKU), Alkaptonuria, Albinism, Galactosemia), haemoglobinopathies, Thalassemia syndromes, multifactorial disorders (diabetes, schizophrenia, huntington disease). Medical genetics involves ethical issues therefore serious discussion is required for prenatal/adult diagnosis of genetic disorders, medical ethics, risks and benefits, informed consent and right of choice.

Suggested Books:

- Human Molecular Genetics (2011) 4thed - Strachan T. & Read A., Garland Science
- An introduction to Human Molecular Genetics-Mechanism of Inherited Diseases (1999)-
- Pasternak J. Fitzgerald, Science Press
- Genetics in Medicine 7th Ed (2007) - Thompson and Thompson, Saunders

Suggested e-Resources:

- **Chromosome identification and nomenclature (ISCN):** http://www.cydas.org/Resources/ISCN_Discussion.html
- **Pedigree data analysis:**

  https://learn.genetics.utah.edu/content/disorders/
- **Genetic disorders:** https://www.genome.gov/10001204/specific-genetic-disorders/
- **Prenatal/ adult diagnosis of genetic disorders, medical ethics:**

  https://www.michiganallianceforfamilies.org/all/#sectionD

BT 539R Protein Engineering

Max. Marks : 100	L	T	P	C
ESA : 100	0	0	4	2

Learning Outcome:

After successful completion of the course, students should be able to:

- perform computational analysis of proteins.
- analyze and compare the protein sequence and structure for their functional annotations .
- explain applications of proteins for different industrial and academic purposes such as structure determination, organic synthesis and drug design.
- plan and execute the activity measurements of isolated proteins and characterize their purity and stability.

An introduction to protein engineering for developing proteins with desired functions. Various methods (rational design and directed evolution) of protein engineering are employed to manipulate the different features or characteristics (affinity, specificity and stability etc) of proteins. Engineering various physicochemical and biological properties (stability to changes in parameters as pH, temperature, amino acid sequence and aggregation propensities etc) of the proteins could be important in their use as protein drugs and/or catalysts in bioreactors. The insight into the fundamental understanding of the mechanisms and forces (Van der waals, electrostatic, hydrogen bonding, weakly polar interactions, and hydrophobic effects), by which protein stabilizes, will help in the formulation of protein based pharmaceuticals. Protein engineering with site-specifically incorporation of unnatural or non-canonical amino acids has been used to improve protein function for medical and industrial applications. Different computational approaches (sequence and 3D structure analysis, data mining, Ramachandran map etc) to protein engineering would help to address the requirements in order to find amino acid sequences that will optimize a desired property (physicochemical property and/or biological function) of a protein. Determination of the physicochemical properties of proteins using various spectroscopic methods (Far-UV and Near-UV CD, Fluorescence, UV absorbance and Optical rotatory dispersion) would further support the drug development process. Yeast surface display

(YSD)has become a valuable protein engineering tool for modifying the affinity, specificity, and stability of antibodies, as well as other proteins. YSD could be successfully used for protein epitope mapping, identification of protein-protein interactions, and uses of displayed proteins in industry and medicine. Developing vaccines and peptidomimetics will further allow the investigators to identify novel therapeutic leads for numerous unmet clinical needs.

Suggested Books:

- Walsh, G.(2014). Proteins: biochemistry and biotechnology, Second edition. Chichester, West Sussex: Wiley Blackwell.
- Creighton, T. E. (1997). Protein Structure: a Practical Approach, 2nd Edition. Oxford University press.
- Cleland, J. L., and Craik, C. S. (2006). Protein Engineering, Principles and Practice, Vol 7. Springer Netherlands.
- Mueller, K., and Arndt, K. (2006). Protein Engineering Protocols, 1st Edition. Humana Press.
- Robertson, D., and Noel, J. P. (2004). Protein Engineering Methods in Enzymology, Vol 388. Elsevier Academic Press.
- Kyte, J. (2006). Structure in Protein Chemistry, 2nd Edition. Garland publishers.
- Williamson, M. P. (2012). How proteins work. New York: Garland Science.

Suggested e-Resources:

- **Protein Engineering**: https://nptel.ac.in/courses/102103017/pdf/lecture%2022.pdf
- **Conformational stability of proteins**: https://www.khanacademy.org/test-prep/mcat/biomolecules/amino-acids-and-proteins1/v/conformational-stability-protein-folding-and-denaturation
- **Protein Engineering with Non-Natural Amino Acids:** https://library.umac.mo/ebooks/b2805488x.pdf

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