

VISVESVARAYA TECHNOLOGICAL UNIVERSITY, BELAGAVI
CHOICE BASED CREDIT SYSTEM (CBCS)
SCHEME OF TEACHING AND EXAMINATION 2015-2016
VISVESVARAYA TECHNOLOGICAL UNIVERSITY, BELGAUM
CHOICE BASED CREDIT SYSTEM (CBCS)
SCHEME OF TEACHING AND EXAMINATION 2016-2017
M.Tech. in -BIOINFORMATICS

I Semester

CREDIT BASED

Subject Code	Name of the Subject	Teaching hours/week		Duration of Exam in Hours	Marks for		Total Marks	CREDITS
		Lecture	Practical / Field Work / Assignment		I.A.	Exam		
16BBI11/16 BBT11/16B BC11	NUMERICAL METHODS AND BIOSTATISTICS	4	-	3	20	80	100	4
16BBI12/16 BBT12/16B BC12	CONCEPTS IN BIOTECHNOLOGY	4	--	3	20	80	100	4
16BBI13	ESSENTIAL BIOINFORMATICS	4	--	3	20	80	100	4
16BBI14	JAVA AND WEB BASED TOOLS	4		3				
16BBI15X	ELECTIVE – 1	3	--	3	20	80	100	3
16BBIL16	BIOINFORMATICS LAB	--	3	3	20	80	100	2
16BBI17	SEMINAR	--	3	--	100	--	100	1
Total		19	6	18	220	480	700	22

ELECTIVES	
16BBI151	Biomolecular Structure Interaction and Dynamics
16BBI152	Genomics and Proteomics
16BBI153	BIOPERL & PYTHON
16BBI154	Microarray Data Analysis

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II Semester

CREDIT BASED

Subject Code	Name of the Subject	Teaching hours/week		Duration of Exam in Hours	Marks for		Total Marks	CREDITS
		Lecture	Practical / Field Work / Assignment/ Tutorials		I.A.	Exam		
16BBI21	NGS Informatics and High Performance Computing	4	--	3	20	80	100	4
16BBI22	Computational Systems Biology	4	--	3	20	80	100	4
16BBI23	Advance DBMS	4	--	3	20	80	100	4
16BBI24	Chemoinformatics and Computational Medicinal Chemistry	4	--	3	20	80	100	4
16BBI25X	ELECTIVE 2	3	--	3	20	80	100	3
16BBIL26	Modelling And Stimulation Lab	--	3	3	20	80	100	2
16BBI27	SEMINAR	--	3	--	100	--	100	1
Total		19	6	18	220	480	700	22

ELECTIVE – 2	
16BBI251	Protein Engineering & Design
16BBI252	Data warehousing and data mining
16BBI253	Artificial Intelligence & Neural Networks
16BBI254	Metabolic Engineering

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III Semester:

Course Code	Subject	No. of Hrs./Week		Duration of the Exam in Hours	Marks for		Total Marks	CREDITS
		Lecture	Practical / Field Work		I.A.	Exam		
16XX31	Seminar/Presentation on Internship (8 weeks from the commencement of 3 rd semester)	-	-	-	25		25	20
16XX32	Report on Internship .	-	-	-	25		25	
16XX33	Evaluation and Viva on Internship				50	50	100	
16XX34	Evaluation of Project Phase: I	-	-	-	50		50	1
	Total	-	-	-	150		200	21

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IV Semester

CREDIT BASED

Subject Code	Subject	No. of Hrs./Week		Duration of Exam in Hours	Marks for		Total Marks	CREDITS
		Lecture	Field Work / Assignment / Tutorials		I.A.	Exam		
16BBI41	RESEARCH METHODOLOGY, BIOSAFETY AND IPR	4	--	3	20	80	100	4
16BBI42X	COURSE ELECTIVE – 3	3	--	3	20	80	100	3
16BBI43	Evaluation of Project Phase-II	-	-	-	50	-	50	3
16BBI44	Evaluation of Project Work and Viva-voce.	-	-	3	-	100+100	200	10
Total		7		09	90	360	450	20
Grand Total (I to IV Sem.) : 2050 Marks; 85 Credits								

COURSE ELECTIVE –3	
16BBI421	PROJECT MANAGEMENT
16BBI422	Health Informatics
16BBI423	Computer-Aided Drug Discovery
16BBI424	Entrepreneur Development

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I SEMESTER

NUMERICAL METHODS & BIOSTATISTICS			
Subject Code	16BBT11/16BBC11/16IB11	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03
CREDITS 04			
<p>Course objectives : The course will enables the students</p> <ul style="list-style-type: none"> • To develop skills towards the design & analysis of statistical experiments • Use appropriate numerical and statistical methods to analyze and interpret data • Demonstrate effective use of these tools in problem solving and analysis 			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
Introduction to statistics and study design: Introduction to statistics, data, variables, types of data, tabular, graphical and pictorial representation of data. Significance of statistics to biological problems, experimental studies; randomized controlled studies, historically controlled studies, cross over, factorial design, cluster design, randomized; complete, block, stratified design, biases, analysis and interpretation.		10	L1,L2,L3, L4
MODULE –2			
Descriptive statistics and Observational study design: Types of variables, measure of spread, logarithmic transformations, multivariate data. Basics of study design, cohort studies, case-control studies, outcomes, odd ratio and relative risks. Principles of statistical inference: Parameter estimation, hypothesis testing. Statistical inference on categorical variables; categorical data, binomial distribution, normal distribution, sample size estimation		10	L1, L2,L3,L4
MODULE – 3			
Comparison of means: Test statistics; t-test, F distribution, independent and dependent sample comparison, Wilcoxon Signed Rank Test, Wilcoxon-Mann-Whitney Test, ANOVA. Correlation and simple linear regression: Introduction, Karl Pearson correlation coefficient,		10	L2, L3,L4

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Spearman Rank correlation coefficient, simple linear regression, regression model fit, inferences from the regression model, ANOVA tables for regression. Multiple linear regression and linear models: Introduction, Multiple linear regression model, ANOVA table for multiple linear regression model, assessing model fit, polynomials and interactions. One-way and Two-way ANOVA tables, F-tests. Algorithm and implementation using numerical methods with case studies.		
MODULE – 4		
Design and analysis of experiments: Random block design, multiple sources of variation, correlated data and random effects regression, model fitting. Completely randomized design, stratified design. Biological study designs. Optimization strategies with case studies.	10	L3, L4, L5
MODULE – 5		
Statistics in microarray, genome mapping and bioinformatics: Types of microarray, objectives of the study, experimental designs for micro array studies, microarray analysis, interpretation, validation and microarray informatics. Genome mapping, discrete sequence matching, programs for mapping sequences with case studies.	10	L3, L4, L5
<p>Course outcomes: After studying this course, students will be able to:</p> <ul style="list-style-type: none"> • Demonstrate strong basics in statistics and numerical analysis, • foundation to tackle live problems in various spheres of bioscience and bioengineering • Study and design various statistical problems 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Problem Analysis. • Design / development of solutions. • Modern Tool Usage 		
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions. • Each full question consists of 16 marks • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT BOOKS</p> <ol style="list-style-type: none"> 1. Alvin E. Lewis, Biostatistics, McGraw-Hill Professional Publishing, 2013. 2. J.D. Lee and T.D. Lee. Statistics and Numerical Methods in BASIC for Biologists, Van Nostrand Reinhold Company, 1982. 3. T.P. Chapman, Statistical Analysis of Gene Expression Microarray Data, CRC, 2003. 		

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REFERENCE BOOKS

1. Wolfgang Boehm and Hartmut Prautzsch, Numerical Methods, CRC Press, 1993.
2. John F. Monahan. Numerical Methods of Statistics (Cambridge Series in Statistical and Probabilistic Mathematics), Cambridge University Press, 2011.
3. Joe D. Hoffman. Numerical Methods for Engineers and Scientists, CRC Press, 2nd Edition, 2001.
4. Warren J. Ewens Gregory Grant, Statistical Methods in Bioinformatics: An Introduction (Statistics for Biology and Health), Springer, 2005

CONCEPTS IN BIOTECHNOLOGY

Subject Code	16BBI12/16BBT12/16BBC12	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03

CREDITS 04

Course objectives : The course will enables the student:

- Appreciate the Basic concepts and apply the knowledge to Biotechnological problems
- Use these skills towards the design & analysis of life science experiments
- Demonstrate effective use of these tools and techniques in solving problems relevant for society

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
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MODULE – 1

Introduction to Biology; Macromolecules; Carbon chemistry; Proteins: Structure, folding, catalysis; Nucleic acids: DNA & RNA; storage and transfer of genetic information; Lipids: membranes, structure & function; Carbohydrate chemistry, energy storage, building blocks.	10	L1, L2,L3
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MODULE –2

Cell Structure: Eukaryotic and Prokaryotic cells, plant and animal cells, structure of nucleus, mitochondria, ribosomes, Golgi bodies, lysosomes, endoplasmic reticulum, chloroplast, vacuoles; Cell cycle and cell division: Different phases of cell cycle, cell division: Mitosis and meiosis. Mendelian law of inheritance: Monohybrid and dihybrid inheritance, law of segregation and independent assortment; Gene Interaction; Multiple alleles, supplementary and complementary genes, epistasis. Identification of genetic material: classical experiments; chromosome structure and organization, chemical composition of chromatin, structural organization of nucleosomes, heterochromatin, polytene and	10	L1, L2,L3,L4
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lamp-brush chromosomes, human chromosomes, chromosomal disorders.		
MODULE – 3		
Scope and History of microbiology, Introduction to the structure and functions of microorganism: Bacteria, Viruses, Fungi and Protozoan's. Microscopy and microbial techniques: Study of microscopes; sterilization techniques: Heat, steam, Radiation, Filtration and chemical methods; Pure culture techniques: Serial Dilution, Streak, Spread, Pour Plate. Immune System, Innate and adaptive immunity, antigens and antibodies; types of immune response, hypersensitivity. Humoral immunity: B-lymphocytes, Immunoglobulin classes, Major Histocompatibility Complex (MHC). Cell mediated immunity. Thymus derived lymphocytes (T-cells), Antigen presenting cells (APC); Immunity to infection, Cytokines.	10	L1, L2, L3, L4
MODULE – 4		
Scope of agricultural biotechnology, Role of Micorbes in agriculture, Biopesticides, Bio fertilizers (Nitrogen fixing microbes), GM crops. Plant metabolic engineering and industrial products: Molecular farming for the production of industrial enzymes, biodegradable plastics, antibodies, edible vaccines. Metabolic engineering of plants for the production of fatty acids, industrial oils, flavonoids etc. Basic aspects of Food & Nutrition.	10	L3, L4, L5, L6.
MODULE – 5		
Industrially important Microorganisms, Preservation techniques, Different media for fermentation, basic structure of fermentor and different types. Types of fermentation processes (surface, submerged, and solid state) and their products (ethanol, citric acid, lactic acid, enzymes, antibiotics) Biological treatment of waste water, primary, secondary and tertiary treatments. Bio indicators, Bioremediation of xenobiotic compounds, Bioleaching of minerals from ores, Bio-sorption of toxic metals. Solid waste management. Biofuel production from agricultural wastes.	10	L3, L4, L5, L6.
<p>Course outcomes: After completion of the course, students will be</p> <ul style="list-style-type: none"> • Demonstrate strong basics in principles of biotechnology. • Demonstrate strong basics in biotechnology and numerical analysis, 		

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Graduate Attributes (as per NBA)

- Problem Analysis
- Design / development of solutions.
- Societal and Environmental concern

Question Paper Pattern:

- The question paper will have ten questions
- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) form each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT BOOKS

1. De Robertis EDP and De Robertis Jr. EMF, Cell and Molecular Biology, Wippincott Williams and Wiilkins publisher, 2001.
2. Strickburger M W, Principles of Genetics, 3rd edition, Prentice Hall Publication, India, 2011.
3. Prescott and Dunn, Industrial Microbiology, Macmillian, 1982.
4. Ashim K Chakravarthy, Immunology & Immunotechnology, Oxford University Press, 2006.

REFERENCE BOOKS

1. Gardner, Simmonns and Snustad, Principles of Genetics, 8th edition, 2005.
2. P S Verma, V R Agarwal, Cell Biology, Genetics, Evolution and Ecology, New Publisher Delhi, 2007.
3. K. Lindsey and M.G.K. Jones, Plant biotechnology in Agriculture, Prentice hall, New Jersey. 1989.
4. Munnecke DM, Johnson LM and others, Biodegradation and Detoxification of Environmental Pollutants CRC Press, 1982

ESSENTIAL OF BIOINFORMATICS

Subject Code	16BBI13	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03

CREDITS 04

Course objectives :

- The objective of this course is to make students learn basic concepts of bioinformatics and the importance of biological databases and tools.

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MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		
Bioinformatics & Biological Databases: Introduction to Bioinformatics, Goals, Scope, Applications in biological science and medicine and Limitations,a) Sequence Databases b) Structure Databases c) Special Databases and applications: Genome, Microarray, Metabolic pathway, motif, multiple sequence alignment and domain databases. Mapping databases – genome wide maps. Chromosome specific human maps. Applications of these databases. Database Similarity Searching: Unique Requirements of Database Searching. Heuristic Databasesearching, Basic Local Alignment Search Tool (BLAST), FASTA, Comparison of FASTA and BLAST, Database Searching with the Smith–Waterman Method.	10	L1,L2,L5
MODULE –2		
Sequence Alignment: Evolutionary basis, Homology vs Similarity, Similarity vs Identity. Types of Sequence alignment - Pairwise and Multiple sequence alignment, Alignment algorithms, Scoring matrices, Statistical significance of sequence alignment. Multiple Sequence Alignment: Scoring function, Exhaustive algorithms, Heuristic algorithms, Practical issues. Profiles and Hidden Markov Models: Position-Specific scoring matrices, Profiles, Markov Model and Hidden Markov Model.	10	L3,L4,L5
MODULE – 3		
Prediction Motifs and Domains: Motif and Domain databases, Identification of Motifs and Domains in Multiple Sequence Alignment using Regular expressions, Motif and Domain Databases statistical models, Protein Family databases, Motif Discovery in unaligned sequences. Sequence logos. Gene and Promoter Prediction: Promoter and Regulatory elements in Prokaryotes and Eukaryotes. Promoter and Regulatory element prediction – algorithms. Gene prediction. Gene prediction in Prokaryotes and Eukaryotes. Categories of Gene Prediction Programs. Prediction algorithms. Discussions with case studies.	10	L5,L6
MODULE – 4		

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<p>Predictive Methods: Predictive methods using Nucleic acid sequence – DNA framework, Masking of repetitive DNA, predicting RNA secondary structure, Finding RNA genes, Detection offunctional sites and Codon bias in the DNA. Predictive methods using protein sequence – Protein identity and Physical properties. Structure prediction - Prediction of secondary structure of protein, Antigenic sites, Active sites, Folding classes, specialized structures and Tertiary structures. Discussions with case studies. Concepts involved in insilico Primer Designing and developing Restriction Maps.</p>	10	L5,L6
MODULE – 5		
<p>Molecular Phylogenetic: Phylogenetics Basics. Molecular Evolution and Molecular Phylogenetics - Terminology, Gene Phylogeny vs Species Phylogeny, Forms of Tree Representation. Phylogenetic Tree Construction Methods and Programs - Distance-Based Methods, Character-Based Methods. Phylogenetic Tree evaluation methods. Phylogenetic analysis software and algorithms. Bootstrap methods.</p>	10	L4,L5
<p>Course outcomes:</p> <ul style="list-style-type: none"> • Understanding the importance of different biological databases. • Students will be able to use the different software's and tools. 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Problem Analysis • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage 		
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) form each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT BOOKS</p> <ol style="list-style-type: none"> 1. Essential Bioinformatics by Jin Xiong, Cambridge University Press, 2006. 2. Essentials of Drug Designing by V. Kothekar, DHRUV Publications, 2005. 3. Systems Biology: Applications and Perspectives by Bringmann, Springer, 2007. 4. Bioinformatics and Molecular Evolution by Paul G. Higgs, Teresa K. Attwood, Blackwell, 2005. 5. Bioinformatics Basics: Applications in Biological Science and Medicine by Lukas, 2005. 		

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6. Bioinformatics - The Machine Learning Approach, Pierre Baldi and Søren Brunak, 2001.

REFERENCE BOOKS

7. Current Protocols in Bioinformatics by Andreas D. Baxevanis, Published by Wiley, 2003
 8. Bioinformatics: Sequence and Genome Analysis By David Mount, 2004
 9. Andreas D Baxevanis, B. F Francis Ouellette. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. III Edition. Wiley John & sons, 2005.
 10. Introduction to Bioinformatics: Anna Tremont, CRC Press, Taylor & Francis, 2006.
 11. Introduction to Bioinformatics: Arthur Lesk, III edition, Oxford Publications.2009.
 12. Stan Tsai. An introduction to computational Biochemistry. Wiley John & sons, inc., publication, 2002.

JAVA AND WEB BASED TOOLS

Subject Code	16BBI14	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03

CREDITS 04

Course objectives :

The objective of this course is to make students learn about developing life science oriented web based tools and their use in bioinformatics.

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		
Introduction to Java: Java and Java applications. Java Development Kit (JDK). Byte Code, JVM; Object-oriented programming. Simple Java programs. Data types and Tokens: Boolean variables, int, long, char, operators, arrays, white spaces, literals, assigning values. Creating and destroying objects. Access specifiers. Operators and Expressions: Arithmetic Operators, Bitwise operators, Relational operators, Assignment Operator, The ? Operator; Operator Precedence. Logical expression. Type casting, Strings. Control Statements: Selection statements, iteration statements, Jump Statements.	10	L2,L5

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MODULE –2		
Classes, Inheritance, Exceptions: Classes. Classes in Java - Declaring a class, Class name, Super classes, Constructors. Creating instances of class. Inner classes. Inheritance: Simple, multiple, and multilevel inheritance; Overriding, overloading. Exception handling: Exception handling in Java. Multi-Threaded Programming: Multi Programming: Extending threads; Implementing runnable. Synchronization, Changing state of the thread. Bounded buffer problems, Read-write problem, Producer-Consumer problems. Event Handling: Two event handling mechanisms, Delegation event model, Event classes; Sources of events; Event listener interfaces. Delegation event model; Adapter classes; Inner classes.	10	L3,L5,L6
MODULE – 3		
Applets: The Applet Class: Two types of Applets, Applet basics, Applet Architecture, An Applet skeleton; The HTML APPLET tag; Passing parameters to Applets, Simple Applet display methods; Requesting repainting; Using the Status Window. <code>getDocumentbase()</code> and <code>getCodebase()</code> ; <code>ApletContext</code> and <code>showDocument()</code> ; The <code>AudioClip</code> Interface; The <code>AppletStub</code> Interface; Drawing Lines; Drawing Other Stuff; Color; Mouse Input; Keyboard Input and Output to the Console. Threads and Animation, Backbuffers, Graphics, and Painting; Clocks. Playing with text: Introduction to 2D arrays and hyperlinks, 3D Graphics - Basic classes.	10	L4,L5
MODULE – 4		
Java 2 Enterprise Edition Overview, Database Access: Overview of J2EE and J2SE. The Concept of JDBC; JDBC Driver Types; JDBC Packages; A Brief Overview of the JDBC process; Database Connection; Associating the JDBC/ODBC Bridge with the Database; Statement Objects;ResultSet; Transaction Processing; Metadata, Data types; Exceptions.	10	L3,L5
MODULE – 5		

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<p>Servlets: Background; The Life Cycle of a Servlet; Using Tomcat for Servlet Development; Simple Servlet; The Servlet API. The Javax.servlet Package. Reading Servlet Parameter, Javax.servlet.http package, Handling HTTP Requests and Responses. Cookies and Session Tracking.</p>	10	L2,L5
<p>Course outcomes: . Students will gain knowledge about various web based tools and their applications.</p>		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Problem Analysis • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage 		
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) form each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT BOOKS</p> <ol style="list-style-type: none"> 1. Java - The Complete Reference, 7th Edition by Herbert Schildt, Tata McGraw Hill, 2007. 2. J2EE - The Complete Reference by Jim Keogh, Tata McGraw Hill, 2007. 3. Java 2D Graphics by Jonathan Knudsen, O'Reilly, 1999. 4. Introduction to JAVA Programming, 6th Edition by Y. Daniel Liang, Pearson Education, 2007. 		
<p>REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. The J2EE Tutorial, 2nd Edition by Stephanie Bodoff et al, Pearson Education, 2004. 2. Introduction to Java Programming Comprehensive Version (7th Edition) by Y. Daniel Liang, Pearson Prentice Hall – Publisher, 2010. 3. Java foundations by Todd Grealier, John Wiley and Sons, 2004. 		

BIOMOLECULAR MODELING & SIMULATION			
Subject Code	16BBI151	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80
Total number of lecture hours	40	Exam Hours	03
CREDITS 03			

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Course objectives : The objective of this course is to make students learn basic concepts of structural features of proteins, the modeling tools and their use in modern biology.		
MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		
Biomolecular Structure and Modeling: Historical Perspective, Introduction to Molecular Modeling, Roots of Molecular modeling in Molecular mechanics. Introduction to X-Ray crystallography and NMR spectroscopy. Introduction to PDB and 3D Structure data, Structure of PDB and other 3D Structure record. Protein Structure Hierarchy: Structure Hierarchy. Helices – Classic α -Helix and π Helices, Left-Handed α -Helix and Collagen Helix. β -Sheets - Turns and Loops. Supersecondary and Tertiary structure. Complex 3D Networks. Classes in Protein Architecture – Folds, α -Class, Bundles, Folded leaves, Hairpin arrays. β -Class folds, Anti-parallel β domains, parallel and Anti-parallel Combinations. α/β and $\alpha+\beta$ -Class, α/β Barrels, Open twisted α/β folds, Leucine-rich α/β folds. $\alpha+\beta$ folds. Quaternary structure. Discussions with case studies.	08	L4,L5
MODULE –2		
Force Fields: Formulation of the Model and Energy, Quantifying Characteristic Motions, Complex Biomolecular Spectra, Spectra as force constant sources, In-Plane and Out-of-Plane Bending. Bond Length Potentials - Harmonic term, Morse term, Cubic and Quadratic terms. Bond Angle Potentials - Harmonic and Trigonometric terms, Cross bond stretch / Angle bend terms. Torsional potentials - Origin of rotational barriers, Fourier terms, Torsional parameter Assignment, Improper torsion, Cross dihedral/Bond angle, Dihedral terms. Van der Waals potentials. Rapidly decaying potential. Parameter fitting from experiment. Two parameter calculation protocols. Coulomb potential - Coulomb's Law. Slowly decaying potential, Dielectric function and Partial charges. Discussions with case studies.	08	L2,L3,L4,L6
MODULE – 3		

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<p>Molecular modeling: Modeling basics. Generation of 3D Coordinates Crystal data, Fragment libraries, and conversion of 2D Structural data into 3D form. Force fields, and Geometry optimization. Energy minimizing procedures - Use of Charges, Solvent effects and Quantum Mechanical methods. Computational tools for Molecular modeling. Methods of Conformational analysis - Systematic search procedures, Monte Carlo and molecular dynamics methods. Determining features of proteins - Interaction potential, Molecular electrostatic potential, molecular interaction fields, Properties on molecular surface and Pharmacophore identification.</p>	08	L2,L3,L4,L6
MODULE – 4		
<p>3D QSAR Methods. Comparative protein modeling – Conformational properties of protein structure, Types of secondary structural elements, Homologous proteins. Procedures for sequence Alignments, Determination and generation of structurally conserved regions, Construction of structurally variable regions, Side-Chain modeling, Secondary structure prediction, Threading methods. Optimization and Validation of Protein Models with suitable case studies. Computation of the Free Energy: Free energy calculations in Biological Systems - Drug design, Signal transduction, Peptide folding, Membrane protein association, Numerical methods for calculating the potential of mean force, Replica-Exchange-Based Free-Energy Methods.</p>	08	L2,L3,L4,L6
MODULE – 5		
<p>Membrane Protein Simulations: Membrane proteins and their importance, Membrane protein environments <i>in vivo</i> and <i>in vitro</i>. Modeling a complex environment - Simulation methods for membranes, Membrane protein systems, Complex solvents, Detergent micelles, Lipid bilayers, Self-Assembly and Complex systems. Modeling and Simulation of Allosteric regulation in enzymes - Discussions with case studies. Electrostatics and Enhanced Solvation Models: Implicit solvent electrostatics in Biomolecular Simulation, New distributed multipole methods. Quantum mechanical principles and applications to force field development with case studies.</p>	08	L2,L5,L6

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Course outcomes:

Students will learn about structural features of proteins.
 Students will gain insights into the various tools used for modeling of small molecules, lipids and proteins.

Graduate Attributes (as per NBA)

- Problem Analysis
- Design / Development of Solutions
- Conduct investigations of Complex Computing Problems
- Modern Tool Usage
- Computational knowledge

Question Paper Pattern:

- The question paper will have ten questions
- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) form each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT BOOKS

1. Molecular Modeling by Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, GerdFolkers, 2008.
2. Modeling of Bimolecular Structures and Mechanisms by Alberte Pullman, Joshua Jortner, 1995.
3. Mathematical Approaches to Biomolecular Structure and Dynamics by Jill P. Mesirov, Klaus Schulten, De Witt L. Sumners, 1996.
4. Foundations of Molecular Modeling and Simulation by Peter T. Cummings, Phillip R. Westmorland, Brice Carnahan, Published by American Institute of Chemical Engineers, 2001.
5. New Algorithms for Macromolecular Simulation by Timothy J. Barth, Michael Griebel, David E.Keyes, Risto M. Nieminen, Dirk Roose, Tamar Schlick, Published by Springer, 2006.

REFERENCE BOOKS

1. Nicolas Claude Cohen, Guidbook on molecular modeling in drug design Academic Press. Elsevier, 1996.
2. Tamar Schlick. Molecular Modeling and Simulation: An Interdisciplinary Guide: An Interdisciplinary Guide. Second Edition, Springer. 2010.
- 3, Tamar Schlick, Innovations in Biomolecular Modeling and Simulations, Volume 2, RSC Publishing. 2012.

GENOMICS AND PROTEOMICS

Subject Code	16BBI152	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80

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Total number of lecture hours	40	Exam Hours	03
CREDITS 03			
Course objectives : <ul style="list-style-type: none"> • For understanding of genome organization, gene regulations and its basis in cell biology and in all organisms. 			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
Introduction: Introduction to Genomics & Proteomics. Structure, Organization and features of Prokaryotic & Eukaryotic genomes. C-values of eukaryotic genomes - coding, noncoding and repetitive sequences. Organisation of genome within nucleus, mitochondria and chloroplast. Genome mapping: Genetic and physical mapping. Polymorphisms. Molecular markers – RFLP, AFLP, RAPD, SCAR, SNP, ISSR, and Protein markers – Allozymes and Isozymes, Telomerase. FISH – DNA amplification markers and Cancer biomarkers.		08	L1,L2,L3
MODULE –2			
Genome sequences databases and Genome annotation: : Extrinsic, Intrinsic (Signals and Content), Conservative information used in gene prediction. Frameworks for Information integration – Exon chaining. Generative models: Hidden Markov Models, Discriminative learning and Combiners. Evaluation of Gene prediction methods – Basic tools, Systematic evaluation and Community experiments (GASP, EGASP and NGASP). and Gene Ontology. Functional annotation of Proteins: Introduction, Protein sequence databases, UniProt		08	L1,L3,L4
MODULE – 3			
UniProtKB – Sequence curation, Sequence annotation, Functional annotation, annotation of protein structure, post-translational modification, protein-protein interactions and pathways, annotation of human sequences and diseases in UniProt and UniProtKB. Protein family classification for functional annotation – Protein signature methods and Databases, InterPro, InterProScan for sequence classification and functional annotation. Annotation from Genes and		08	L1,L2,L5

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Protein to Genome and Proteome		
MODULE – 4		
Genome Sequencing: Recent developments and next generation sequencing, ultra-highthroughput DNA Sequencing using Microarray technology. Genome sequencing projects on <i>H. Influenzae</i> , <i>E. coli</i> , <i>Orizasativum</i> and <i>Neem</i> . Human-genome project. Raw genome sequence data, Gene variation and associated diseases, diagnostic genes and drug targets. Genotyping-DNA Chips. Comparative and Functional Genomics: Studies with model systems such as Yeast, <i>Drosophila</i> , <i>C. elegans</i> , <i>Arabidopsis</i> . Approaches to analyze global gene expression – transcriptome, Serial Analysis of Gene Expression (SAGE), Expressed Sequence Tags (ESTs), Massively Parallel Signature Sequencing (MPSS), microarray and its applications, gene tagging.	08	L1,L2,L3,L4
MODULE – 5		
Proteomics: Scope, Experimental methods for studying proteomics, methods of protein isolation, purification and quantification. Methods for large scale synthesis of proteins. Applications of peptides in biology. Analysis of proteome – High throughput screening – Yeast two hybrid system and Protein chips, engineering novel proteins, Mass Spectroscopy based protein expression and post-translational modification analysis. Bioinformatics analysis – clustering methods. Analysis of proteome functional information.	08	L1,L3,L4,L5
<p>Course outcomes: Students will learn about genome organization, gene regulation & their role in biology of cell. Students will gain knowledge about protein and role in biology.</p>		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Problem Analysis • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Life-long Learning 		
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) form each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from 		

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each module.

TEXT BOOKS

1. Pharmacogenomics by Werner Kalow, Urs A. Meyer, Rachel F. Tyndale, Informa Healthcare, 2005.
2. Statistical and Computational Pharmacogenomics (Interdisciplinary Statistics) by Rongling Wu, Min Lin, Chapman & Hall/CRC, 2008.
3. Genes VIII by Benjamin Lewis, Jones and Bartlett Publisher, 2006.
4. Genomics and Proteomics by Sándor Suhai, Springer, 2000.
5. Modern genome annotation: the BioSapiens Network by Dmitrij Frishman, Alfonso Valencia, Springer, 2008.
6. Discovering genomics, proteomics and bioinformatics by A. Malcolm Campbell, Laurie J. Heyer, Published by Pearson/Benjamin Cummings, 2006.

REFERENCE BOOKS

7. Bioinformatics Genomics, and Proteomics by Ann Batiza, Ann Finney Batiza, Published by Chelsea House Publishers, 2005.
8. Plant Genomics and Proteomics by: Christopher A. Cullis, Wiley-Liss 2004.
9. Stephen R. Pennington, Michael J. Dunn. Proteomics: From Protein Sequence to Function. Garland Science, 2001
10. Darius M. Dziuda. Data Mining for Genomics and Proteomics: Analysis of Gene and Protein Expression Data. John Wiley & Sons, 2010.
11. Christopher A. Cullis. Plant Genomics & Proteomics, John Wiley & Sons, 2004.
12. Ann Finney Batiza Bioinformatics, Genomics, and Proteomics: Getting the Big Picture, Infobase Publishing, 2006.

BIOPERL AND PYTHON

Subject Code	16BBI153	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80
Total number of lecture hours	40	Exam Hours	03

CREDITS 03

Course objectives :

The objective of this course is to make students learn about various algorithms that are used in developing softwares. It will help in learning various softwares used in modern biology.

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		

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<p>Basics of Perl. Introduction to BioPerl and BioPerl Objects - Brief descriptions (Seq, PrimarySeq, LocatableSeq, RelSegment, LiveSeq, LargeSeq, RichSeq, SeqWithQuality, SeqI), Location objects, Interface objects and Implementation objects. Sequence Representation: Representing large sequences (LargeSeq), Representing changing sequences (LiveSeq). Accessing Sequence data - Using Bioperl: Accessing sequence data from local and remote databases, Accessing remote databases (Bio::DB::GenBank, etc), Indexing and accessing local databases (Bio::Index::* ,bp_index.pl, bp_fetch.pl, Bio::DB::*). Sequence and Alignment format Interconversion - Transforming sequence files (SeqIO), Transforming alignment files (AlignIO). Performing Sequence analysis – Global alignment, Local alignment, Multiple sequence alignment, Parsing BLAST alignment report and Parsing multiple sequence alignment.</p>	<p align="center">08</p>	<p align="center">L1,L3,L5</p>
<p>MODULE –2</p>		
<p>Introduction to python. Python basics – Variables, Operators, Data types and Assignments. Statements – Input/output statements, flow control - IF...THEN...ELSE, SWITCH, FOR, MAP, FILTER and WHILE, goto statements. Names, Functions and Modules. Object Oriented Programming in Python: Introduction to object oriented programming in python. Classes and objects. Inheritance, Polymorphism. Constructors and Destructors.</p>	<p align="center">08</p>	<p align="center">L2,L3,L4</p>
<p>MODULE – 3</p>		
<p>Exception handling Biopython Bioinformatics: Parsing DNA data files, Image manipulation, Sequence analysis – Sequence alignment (pair wise and multiple sequence alignment), Dynamic Programming, Detecting tandem repeats and generating Hidden Marko Models, Simulation of EST Clustering. Data mining – Text mining, Simulating Genetic algorithm. Analysis of Microarray data – Spot finding and Measurement.</p>	<p align="center">08</p>	<p align="center">L2,L3,L4</p>
<p>MODULE – 4</p>		
<p>Introduction to the NCBI C++ Toolkit: Introduction to C++ modules - CORELIB, ALGORITHM,CGI, CONNECT, CTOOL, DBAPI, GUI, HTML, OBJECT MANAGER, SERIAL and UTIL module. C++ Toolkit Library Reference: CORELIB Module - Writing simple applications, Namespaces,</p>	<p align="center">08</p>	<p align="center">L1,L2,L3,L4</p>

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<p>CNcbiRegistry Class, Portable Stream Wrappers. Working with diagnostic streams - Debug Macros, Handling exceptions, CObject and CRef Classes and Atomic counters. Executing commands and Spawning processes using CExec class, working with files and directories using CFile and CDir, Input /Output utility class.</p>		
<p>MODULE – 5</p>		
<p>Overview of the R language: Defining the R project, Obtaining R, Generating R codes, Scripts, Text editors for R, Graphical User Interfaces (GUIs) for R, Packages. 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. Manipulating objects in 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).</p>	<p>08</p>	<p>L2,L3,L4,L5</p>
<p>Course outcomes:</p> <ul style="list-style-type: none"> • Students will learn about various algorithms used in software development. • Students will gain knowledge about various softwares and their applications 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Computational knowledge • Problem Analysis • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Professional Ethics • Life-long Learning 		
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) form each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		

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TEXT BOOKS

1. Java Foundations by John Lewis, Peter Joseph DePasquale, Joseph Chase, Joe Chase, Addison-Wesley, 2010.
2. Perl Programming for Biologists by D. Curtis Jamison, Wiley-IEEE, 2003.
3. Bioinformatics Programming Using Python by Mitchell L Model, O'Reilly Media, Inc., 2009.
4. Alain F. Zuur, Elena N. Ieno, and Erik Meesters. A Beginner's Guide to R. Use R. Springer, 2009.
5. Florian Hahne, Wolfgang Huber, Robert Gentleman, Seth Falcon. Bioconductor case studies. Springer, 2008
6. Robert Gentleman. Bioinformatics with R. Chapman & Hall/CRC, Boca Raton, FL, 2008.
7. Robert Gentleman. R Programming for Bioinformatics. Computer Science & Data Analysis. Chapman & Hall/CRC, Boca Raton, FL, 2008.
8. Peter Dalgaard. Introductory Statistics with R. Springer, 2nd edition, 2008.
9. Python for Bioinformatics (Chapman & Hall/CRC), Sebastian Bassi, 2009.

REFERENCE BOOKS

10. BioJava: A Programming Guide by Kaladhar D S V G K, 2012.11.
- 11 Python for bioinformatics by Jason M. Kinser, Jones & Bartlett Learning, 2009.
12. Mastering Perl for Bioinformatics by James T Tisdall, 2007.
13. D. Curtis Jamison. Perl Programming for Biologists, John Wiley & Sons, 2003
14. James Tisdall. Mastering Perl for Bioinformatics, O'Reilly Media, Inc, 2003.

MICROARRAY DATA ANALYSIS

Subject Code	16BBI154	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80
Total number of lecture hours	40	Exam Hours	03

CREDITS 03

Course objectives :

- **For understanding of genome organization, gene regulations and its basis in cell biology and in all organisms. To understand the implications and applications in modern biology**

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		

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Introduction to Biochip and Microarray Construction: Basics of Biochips and Microarray Technology, Biochip technologies. Types of Biochips - DNA Microarrays, Oligonucleotide, cDNA and genomic microarrays, Integrated biochip system. Biochip versus gel-based methods. Limitations of biochip technology	08	L1,L2,L3
MODULE -2		
Biochip construction -Mega10ne technology for fluid microarrays, Microarray labels, Microarray scanners, Microarray robotics. Microfluidics systems, Chips and Mass Spectrometry. Electrical detection methods for microarrays.	08	L1,L2,L3
MODULE - 3		
Applications of Biochips - Tissue Chip, RNA Chip, Protein Chip Technology, Glycochips, Biochip assays, Combination of microarray and biosensor technology. Microarray Data analysis: Introduction, Image Acquisition and Analysis, Detection of differential gene expression. Pathway analysis tools. Data validation.	08	L2L3L4
MODULE - 4		
Genomic Signal Processing: Introduction, Mathematical models, and Modeling DNA Microarray data - Singular Value Decomposition algorithm. Online Analysis of Microarray Data Using Artificial Neural Networks	08	L2L3L4
MODULE - 5		
DNA Computing: Introduction, Junctions, other shapes, Biochips and large-scale structures. Strand algebras for DNA computing – Introduction, Strand Algebras. Discussion of Robinson and Kallenbach's methods for designing DNA shapes, DNA cube, computing with DNA, Electrical analogies for biological circuits, Challenges, Future Trends. Discussions with case studies	08	L2L3L4L5
<p>Course outcomes: Students will gain insights into the methods used to analyse and interpret the microarray data.</p> <p>Students will learn the applications of DNA chips and microarray technology in modern biology.</p>		

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<p>Graduate Attributes (as per NBA) Computational knowledge Problem Analysis Design / Development of Solutions Conduct investigations of Complex Computing Problems Modern Tool Usage Life-long Learning</p>
<p>Question Paper Pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) form each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module.
<p>TEXT BOOKS 1 Biochips and Microarrays – Technology and Commercial Potential Published by: Informa Global Pharmaceuticals and Health Care. 2 Functional Protein Microarrays in Drug Discovery by Paul F. Predki, CRC Press – Publisher 3 DNA Computing: 15th International Meeting on DNA Computing, DNA 15, Fayetteville, AR,USA, June 8-11, 2009, Springer, 2009.</p>
<p>REFERENCE BOOKS 4 DNA Arrays: Technology and Experimental Strategies by Grigorenko, E.V (ed), CRC Press, 2002. 5 Wan-Li Xing, Jing Cheng. Biochips: Technology and Applications, Springer. 2003. 6 Richard Twyman, Principles of Proteomics, 2nd Edition, Garland Science, 2013</p>

ADVANCED BIOINFORMATICS LAB			
Subject Code	16BBIL16	IA Marks	20
No. of Lab Hrs./ Week :	03	Exam Marks	80
		Exam Hours	03
CREDITS 02			
Course objectives : The objective of this course is to make the students learn about developing bench skills through lab exercises, oriented towards utilizing various web based tools for bioinformatics projects.			
Sl.NO	Experiment	REVISED BLOOM'S TAXONOMY (RBT) LEVEL	
1	Sequence retrieval from nucleic acid and protein databases.	L3	

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2	Retrieval of information about structure, bioassay chemical compounds (such as Drugs and naturally occurring compounds).	L4
3	Retrieval of information about physical and Chemical properties of chemical compounds (such as Drugs and naturally occurring compounds).	L4
4	Gene sequence assembly and contig mapping and identification of Gene.	L3
5	Primer and Promoter design for a given sequences	L3
6	Sequence searches using FASTA and BLAST, and Phylogenetic analysis.	L4
7	Prediction of secondary structure for given protein and RNA sequences.	L3
8	Retrieval of protein structure from PDB and its visualization and modification.	L4
9	Prediction of 3D structure of unknown protein sequence.	L3
10	Prediction of protein-protein interactions.	L3
11	EST clustering and EST mapping, and Genome annotation	L3
12	Microarray data analysis- normalization, clustering.	L4
13	Study of Profiles, Patterns and PSSMs	L4

Course outcomes:

Students would learn to appreciate the various algorithms used for diverse exercises.
 Students would gain knowledge about various softwares and their multitude of applications.

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Graduate Attributes (as per NBA)

- Problem analysis
- Design / Development of solutions
- Modern tool usage
- Communication
- Life-long learning

Conduct of Practical Examination:

1. All laboratory experiments are to be included for practical examination.
2. Students are allowed to pick one experiment from the lot.
3. Strictly follow the instructions as printed on the cover page of answer script for breakup of marks.
4. Change of experiment is allowed only once and 15% Marks allotted to the procedure part to be made zero.

TEXT/REFERENCE BOOKS

1. ESSENTIALS OF BIOINFORMATICS, Jin Xinog, Texas A & M University, Cambridge University press.
2. Analytical Tools for DNA, Genes & Genomes: by Arseni Markoff, New Age.
3. DISCOVERING GENOMICS, PROTEOMICS & BIOINFORMATICS BY A M CAMPBELL & L J HEYER, PEARSON EDUCATION.
4. Fundamental Concepts of Bioinformatics by D E Krane & M L Raymer, Pearson. Computational methods in Molecular Biology. S.L.Salzberg, D B Searls, S Kasif, Elsevier.
5. BIOINFORMATICS – METHODS AND APPLICATIONS: GENOMICS,

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PROTEOMICS AND DRUG DISCOVERY BY S C RASTOGI, N MENDIRATTA
 & P RASTOGI, PHI.

6. Introduction to Bioinformatics by Arthur Lesk, Oxford Publications.
7. Structural Bioinformatics by Philip E Bourne, John Wiley & Sons

II SEMESTER

NGS INFORMATICS AND HPC IN BIOINFORMATICS			
Subject Code	16BBI21	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03
CREDITS: 04			
Course objectives : To introduce students to NGS and HPC applications in Bioinformatics. It will add a cutting edge advantage to know these techniques.			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
Introduction to Sequencing technology: Sequencing platforms, Chemistry of difference sequencing platforms, Advantages and disadvantages of the platforms, Need of Hybrid platforms. Base calling algorithms, Base quality, phred values, Reads quality checks, Interpretations from quality checks. Adapter and primer contamination. Processing reads using clipping of reads-Advantages and disadvantages of processing of reads. BWA and Bowtie Alignment programs, Burrows wheeler algorithm. Reference indexing and Alignment.		10	L2 L3
MODULE –2			

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<p>Building from source, the bowtie aligner, the -n alignment mode, the -v alignment mode, Reporting Modes, Paired-end Alignment, Color space Alignment, Color space reads, Building a color space index, Decoding color space alignments, Paired-end color space alignment, Performance Tuning, SAM and BAM format. Artifacts in alignment programs.</p> <p>Assembly-Denovo assembler, Debrunj graph theory, error removing, bubbles and sorts, contigs and scaffolds, Calculation N50 and its importance in assessing assembly, Quality checks for assembly, MIRA, Columbus, Velvet.</p>	10	L2, L3
MODULE – 3		
<p>Overview of NGS Application-Human Exome sequencing, Transcriptome sequencing, chip Sequencing, smallRNA sequencing, Methylome sequencing, RAD Sequencing and RRL sequencing.</p> <p>Big Data analytics-Introduction of Cloud computing, Hadoop architecture. MIKE2.0 , Multiple layer architecture, Distributed Parallel architecture , NGS data analysis using Hadoop,</p>	10	L3, L4
MODULE – 4		
<p>HPC overview and programming prerequisite- Applications of High performance Computing in the field of Bioinformatics. Introduction to Linux operating system, Basic commands used in HPC cluster, Major components and its functions in HPC Cluster- head node, login node, interactive node, compute node, I/O node, HPC Data Storage, Serial and parallel batch jobs and scripting to run processes in parallel. Molecular dynamics and use of VMD Software's and tools used to access HPC cluster with examples</p>	10	L3 L4
MODULE – 5		
<p>Tools and Techniques for high through put data analysis in HPC- Conversion of SRA files and FASTQC analysis using HPC – Command and tools required, result interpretation. Comparison of the results from different tools. Trimming of Adapter contamination from the Sequence reads using HPC – commands and tools required, interpretation of results, Comparison of output from different tools. Alignment of the Raw Sequence reads by various alignment algorithms using HPC cluster followed by analysis of the obtained output. Variant scanning in the Aligned reads using VARSCAN – examples of</p>	10	L5, L6

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<p>practical application of the process and the tool - case studies. Using Velvet to generate maps and indexes for transcriptome data. Performing BLAST using HPC cluster – interpretation of the results.</p>		
<p>Course outcomes: After going through this course the student will be able to:</p> <ol style="list-style-type: none"> 1. Understand the basic knowledge of Next Generation Sequencing. 2. Analyze and apply the appropriate tools and techniques to perform high throughput data analysis. 3. Design high throughput data analysis tools 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Computational knowledge • Problem Analysis • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Individual and Team Work 		
<p>Question Paper Pattern:</p> <p>The question paper will have ten questions.</p> <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT /REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. Review of "Next-generation DNA sequencing informatics" by Stuart M. Brown 2013. Cold Spring Harbor Laboratory Press, Cold Spring Harbor: New York. 256. ISBN-10: 1936113872. 2. Bioinformatics for High Throughput Sequencing By Naiara Rodríguez-Ezpeleta, Michael Hackenberg, Ana M. Aransay. ISBN-13: 9781461407812. 3. High-Throughput Next Generation Sequencing Methods and Applications Series: Young Min Kwon, Steven C. Ricke ISBN: 978-1-61779-088-1 (Print) 978-1-61779-089-8. 4. DNA Sequencing III: Dealing With Difficult Templates by: Jan Kieleczawa publisher: Jones & Bartlett Learning, published: 2008-04-04 ASIN: 076374297X ISBN: 978-0-12645-750-6 		

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COMPUTATIONAL SYSTEMS BIOLOGY			
Subject Code	16BBI22	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03
CREDITS: 04			
Course objectives : The objective of this course is to make students learn about concepts of modeling of biological processes and their representation.			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
Introduction to Systems Biology: Scope, Applications. Concepts, implementation and application. Databases for Systems Biology, Mass Spectrometry and systems Biology. Bioinformatics databases supporting systems biology approaches.		10	L1, L3
MODULE –2			
Network Models and Applications: Natural Language Processing and Ontology enhanced Biomedical data mining, text mining. Integrated Imaging Informatics - ntegrin, centroid, cell culture. Standard platforms and applications - metabolic control analysis, glycolysis, metabolic network, Michaelis-Menten kinetics, and flux balance analysis. Signal Transduction - phosphorylation, Jak-Stat pathway, MAP kinase. Biological Processes - mitochondria, cyclin, Cdc2. Modeling of Gene Expression - lactose, lac operon, tRNA. Analysis of Gene Expression Data - support vector machines, cDNA microarray. Evolution and Self organization - hypercycle, quasispecies model, self-replication. Reconstruction of metabolic network from Genome Information.		10	L4, L5,L6
MODULE – 3			

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Integrated Regulatory and Metabolic Models - Phosphorylation, Gene expression, and Metabolites. Estimation Modeling and Simulation - Circadian rhythms, Petri net, mRNA. Deterministic - Circadian rhythms, mRNA, Circadian oscillations. Multi scale representations of Cells and Emerging Phenotypes - Gene Regulatory Networks, attractor, and Boolean functions. Mathematical models and Optimization methods for De Novo Protein design. Global Gene expression assays. Mapping Genotype - Phenotype relationship in cellular networks.	10	L3, L4, L5
MODULE – 4		
Multiscale representations of cells and Emerging phenotypes: Multistability and Multicellularity. Spatio-Temporal systems biology, Interactomics, Cytomics – from cell state to predictive medicine.	10	L4,L5
MODULE – 5		
Modeling Tools: SBML, MathMLCellML, Petri Nets and Bioinformatics with case studies.	10	L3
<p>Course outcomes: After going through this course the student will be able to:</p> <ul style="list-style-type: none"> • learn about modeling and simulation of various biological processes using bioinformatics tools. • gain knowledge about importance of modeling and simulation of biological processes. 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Life-long Learning 		
<p>Question Paper Pattern: The question paper will have ten questions.</p> <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT /REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. Computational Systems Biology by Andres Kriete, Roland Eils. Academic Press, 2006. 2. Systems Biology by Andrzej K. Konopka, CRC, 2006. 3. Systems biology in practice: concepts, implementation and application by Edda Klipp, Wiley-VCH, 2005. 4. Systems Biology by Isidore Rigoutsos, G. Stephanopoulos, Published by Oxford 		

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University Press US, 2006.

5. Theoretical Models in Biology by Glenn Rowe, Oxford University Press – Publisher, 2004.
6. Transactions on Computational Systems Biology I by Corrado Priami, Springer – Publisher, 2009.
7. Systems Biology by Fred C. Booger, H.V. Westerhoff, Elsevier – Publisher, 2007.
8. Sangdun Choi. Introduction to Systems Biology, Humana Press. 2007.
9. Michael G. Katze. Systems Biology. Springer, 2013.
10. Konopka A.K. Systems Biology: Principles, Methods, and Concepts. CRC Press, Taylor & Francis. 2007.
11. Robert A. Meyers. Systems Biology, Wiley Blackwell. 2012.

ADVANCED DBMS			
Subject Code	16BBI23	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03
CREDITS: 04			
Course objectives :			
The objective of this course is to make students learn about concepts of databases, database management data warehousing and security.			
MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL	
MODULE – 1			
Overview: PL/SQL – Introduction to PL/SQL – Declare, begin statements, Variables, Control Structure, PL/SQL Transactions – Save point, Cursor, PL/SQL Database Objects – Procedures, Functions, Packages, Triggers. Programmatic SQL – Embedded SQL, Dynamic SQL, and ODBC Standard.	10	L1 L2	
MODULE –2			

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<p>Transaction processing and concurrency control: Definition of Transaction and ACID properties. Transaction Processing - Transaction-processing monitors, transactional workflows, main-memory databases, real-time transaction systems, long-duration transactions, transaction management in multi-databases. Concurrency Control – Locks, Optimistic Concurrency Control (Backward and Forward validations), Timestamping Concurrency Control.</p>	10	L4, L5
MODULE – 3		
<p>Object-based databases and xml: Object-based databases – Complex data types, structured types and inheritance in SQL, table inheritance, array and multiset types in SQL, object identity and reference types in SQL, implementing O-R features, Persistent programming languages. OO vs OR. XML – Structure of XML, Document Schema, Querying and Transformation, API in XML, XML applications.</p>	10	L3, L6
MODULE – 4		
<p>Data warehousing: Introduction to Data Warehousing – Concepts, Benefits and Problems, DW Architecture – Operational Data, load manager, meta data, DW Data flows – inflow, upflow, meta flow, DW tools and technologies – Extraction, cleansing and transformation tools, DW DBMS, admin and management tools, data marts – reasons and issues, Data Warehousing using Oracle. Data Warehousing Design – Designing, Dimensionality modeling, Design methodology, DW design using Oracle. Olap and data mining: On-line Analytical Processing – OLAP Benchmarks, applications, benefits, tools, categories, extensions to SQL, Data mining introduction, techniques, predictive modeling, tools. Data mining algorithms – Apriori, Decision tree, k-means, Bayesian classifier.</p>	10	L2, L3
MODULE – 5		
<p>Database security: Security and integrity threats, Defence mechanisms, Statistical database auditing & control. Security issue based on granting/revoking of privileges, Introduction to statistical database security. PL/SQL Security – Locks – Implicit locking, types and levels of locks, explicit locking, Oracles' named Exception Handlers.</p>	10	L1 L2 L3 L4 L5

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Course outcomes: After going through this course the student will be able to:

learn about structure of databases and different types of databases.
 gain knowledge about database management, warehousing and security related issues.

Graduate Attributes (as per NBA)

Computational knowledge
 Problem Analysis
 Design / Development of Solutions
 Conduct investigations of Complex Computing Problems
 Modern Tool Usage
 Life-long Learning

Question Paper Pattern:

The question paper will have ten questions.

- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) from each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT /REFERENCE BOOKS

1. Advanced DBMS by RiniChakrabarti, ShilbhadraDasgupta, Wiley.
2. AviSilberschatz, Henry F. Korth, S. Sudarshan, Database System Concepts, McGraw-Hill.
3. C. J. Date, An Introduction to Database Systems, Addison-Wesley Longman Publishing Co.
4. Advance Database Management System by ArihantKhicha, Neeti Kapoor.

CHEMOINFORMATICS & COMPUTATIONAL MEDICINAL CHEMISTRY

Subject Code	16BBT24	IA Marks	20
Number of Lecture Hrs./Week	4	Exam Marks	80
Total number of lecture hours	50	Exam Hours	3
CREDITS:04			
Course objectives :			
The objective of this course is to make students learn about importance of chemoinformatics in drug discovery and their use in modern biology			
MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL	

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MODULE – 1		
Introduction to Chemoinformatics: Fundamental concepts - molecular descriptors and chemical spaces, chemical spaces and molecular similarity, modification and simplification of chemical spaces. Compound classification and selection – cluster analysis, partitioning, support vectors machines. Predicting reactivity of biologically important molecules, combining screening and structure - 'SAR by NMR', computer storage of chemical information, data formats, OLE, XML, web design and delivery. Representing intermolecular forces: <i>ab initio</i> potentials, statistical potentials, force fields, molecular mechanics.	10	L2, L5
MODULE –2		
Chemoinformatics Databases: Compound availability databases, SAR databases, chemical reaction databases, patent databases and other compound and drug discover databases. Database search methods: Chemical indexing, Proximity searching, 2D and 3D Structure and Substructure searching. Similarity Searching: Structural queries and Graphs, Pharmacophores, Fingerprints. Topological analysis. Machine learning methods for similarity search – Generic and Neural networks. Library design – Diverse libraries, Diversity estimation, Multi-objective design and Focused libraries.	10	L3,L4,L6
MODULE – 3		
Computational Models: Introduction, Historical Overview, Deriving a QSAR Equation. Simple and Multiple Linear Regression. Designing a QSAR "Experiment". Principal Components Regression, Partial Least Squares. Molecular Field Analysis and Partial Least Squares. Quantitative Structure-Activity Relationship Analysis: Model building, Model evaluation, 3DQSAR, 4D-QSAR. Methods of QSAR analysis - Monte Carlo methods, Simulated annealing, Molecular dynamics and Probabilistic methods. Virtual screening and Compound filtering.	10	L4, L6
MODULE – 4		
Virtual Screening: Introduction. "Drug-Likeness" and Compound filters. Structure-based virtual screening and Prediction of ADMET Properties. Discussions with case studies. Combinatorial Chemistry and Library Design: Introduction. Diverse and Focused libraries. Library	10	L3, L6

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enumeration. Combinatorial library design strategies. Discussions with case studies.		
MODULE – 5		
Interaction of ‘receptors’ with agonists and antagonists. Receptor structure prediction methods. Enzyme kinetics and Interaction of enzymes with inhibitors (competitive, non-competitive). Drug discovery pipeline. Optimization of lead compound, SAR (structure-activity relationships), Physicochemical and ADME properties of drugs and Prodrugs. QSAR (Quantitative structure activity relationships), Combinatorial synthesis. Case studies (e.g. G-coupled protein receptor agonists and antagonists, antibacterial agents etc).	10	L2, L4
<p>Course outcomes: After going through this course the student will be able to:</p> <ul style="list-style-type: none"> • learn about various chemoinformatics databases and their importance in drugdiscovery process. • gain knowledge about chemistry of medicinal compounds. 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Computational knowledge • Problem Analysis • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Life-long Learning • Professional Ethics • Innovation and Entrepreneurship 		
<p>Question Paper Pattern:</p> <p>The question paper will have ten questions.</p> <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT /REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. Chemoinformatics: Theory, Practice, & Products by Barry A. Bunin, Jürgen Bajorath, Brian Siesel, Guillermo Morales, 2005. 2. Statistical and Computational Pharmacogenomics (Interdisciplinary Statistics) by Rongling Wu, Min Linen, Chapman & Hall/CRC, 2008. 3. An Introduction to Chemoinformatics by Andrew R. Leach, Valerie J. Gillet, Springer, 2007. 4. Chemoinformatics: Theory, Practice, & Products by Barry A. Bunin, Jürgen Bajorath, 		

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Brian Siesel, Guillermo Morales, Royal Society of Chemistry, 2006.

5. Chemoinformatics Approaches to Virtual Screening by Alexandre Varnek, Alex Tropsha. Royal Society of Chemistry, 2008.
6. Chemoinformatics by Johann Gasteiger Wiley-VCH, 2003.
7. "An introduction to medicinal chemistry", 5th edition, G. L. Patrick, Oxford University Press, New York.
8. Young D. C., Computational Drug Design: A Guide for Computational and Medicinal Chemists, John Wiley & Sons, 2009.
9. Peter Bladon, John E. Gorton, Robert B. Hammond. Molecular Modelling: Computational Chemistry Demystified. RSC Publishing, 2012.
10. Lee Banting, Tim Clark, David E. Thurston, Drug Design Strategies: Computational Techniques and Applications. RSC Publishing, 2012

PROTEIN ENGINEERING & DESIGN			
Subject Code	16BBT251	IA Marks	20
Number of Lecture Hrs./Week	3	Exam Marks	80
Total number of lecture hours	40	Exam Hours	3
CREDITS:03			
Course objectives : The objective of this course is to make students learn about concepts of engineering of proteins using various techniques for the biological applications.			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
Amino acids (the students should be thorough with three and single letter codes) and their molecular properties (size, solubility, charge, pKa), Chemical reactivity in relation to posttranslational modification (involving amino, carboxyl, hydroxyl, thiol, imidazole groups) and peptide synthesis. Primary structure: peptide mapping, peptide sequencing - automated Edman method and Mass Spectrometry.		8	L2 L3
MODULE –2			

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<p>High-throughput protein sequencing setup Secondary structure: Alpha, beta and loop structures and methods to determine Super-secondary structure: Alpha-turn-alpha, beta-turn beta(hairpin), beta-sheets, alpha-beta-alpha, topology diagrams, up and down & TIM barrel structures nucleotide binding folds.</p> <p>Sites Tertiary structure: Domains, denaturation and renaturation, protein folding pathways, overview of methods to determine 3D structures, Interaction with electromagnetic radiation (radio, micro, infrared, visible, ultraviolet, X-ray) and elucidation of protein structure. Quaternary associations: Modular nature, formation of complexes.</p>	8	L3,L4
MODULE – 3		
<p>Overview of protein structure, PDB, structure based classification, databases, visualization tools, structure alignment, domain architecture databases, protein-ligand interactions. Covalent, Ionic, Hydrogen, Coordinate, hydrophobic and Vander walls interactions in protein structure.</p> <p>Bioinformatics Approaches: Secondary structure prediction and determination of motifs, profiles, patterns, fingerprints, super secondary structures, prediction of substrate binding sites, tertiary structure, quaternary structure, methods to determine tertiary and quaternary structure, posttranslational modification.</p>	8	L2, L3
MODULE – 4		
<p>Methods of protein isolation, purification and quantification; large scale synthesis of engineered proteins, design and synthesis of peptides; methods of detection and analysis of proteins.</p> <p>Protein database analysis, methods to alter primary structure of proteins, examples of engineered proteins, protein design, principles and examples. Advantages and purpose, overview of methods, underlying principles with specific examples: thermal stability T4-lysozyme, recombinant insulin to reduce aggregation and inactivation, <i>de novo</i> protein design.</p>	8	L3, L4
MODULE – 5		
<p>DNA-binding proteins: prokaryotic transcription factors, Helix-turn-Helix motif in DNA binding, Trp repressor, Eukaryotic transcription factors, Zn fingers, helix-turn helix motifs in homeodomain, Leucine zippers, Membrane proteins: General characteristics, Trans-membrane segments, prediction, bacteriorhodopsin and Photosynthetic reaction center.</p> <p>Immunoglobulins: IgG Light chain and heavy chain</p>	8	L2, L4

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architecture, abzymes and Enzymes: Serine proteases, understanding catalytic design by engineering trypsin, chymotrypsin and elastase, substrate-assisted catalysis other commercial applications.		
Course outcomes: After going through this course the student will be able to: <ul style="list-style-type: none"> • learn about proteins and engineering of proteins for biological applications. • gain knowledge about isolation of proteins, examples of important proteins that are used for engineering. 		
Graduate Attributes (as per NBA) <ul style="list-style-type: none"> • Computational knowledge • Problem Analysis • Design / Development of Solutions • Modern Tool Usage • Life-long Learning • Professional Ethics 		
Question Paper Pattern: The question paper will have ten questions. <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
TEXT /REFERENCE BOOKS <ol style="list-style-type: none"> 1. Moody P.C.E and A.J Wilkinson. Protein Engineering, IRL Press, Oxford University Press. 2. Protein Science by Arthur M Lesk, Oxford University Press. 3. Protein Structure by Creighton, Oxford University Press. 4. Introduction of protein structure by Branden C and Tooze R., Garland. 5. The molecular modeling perspective in drug design by N Claude Cohen, Academic Press. 6. Bioinformatics Methods & Applications: Genomics, Proteomics & Drug Discovery, S C Rastogi, N Mendiratta & P Rastogi, PHI. 7. Young D. C., Computational Drug Design: A Guide for Computational and Medicinal Chemists, John Wiley & Sons, 2009. 8. Jeffrey L. Cleland, Charles S. Craik. Protein engineering: principles and practice, 		

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Wiley-Liss,1996.

9. Paul R. Carey. Protein Engineering and Design, Academic Press Inc., 1996.

10. In Silico Lead Discovery. Maria A. Miteva, Bentham Books, 2011.

11. Kenneth M. Merz, Jr, Dagmar Ringe, Charles H. Reynolds. Drug Design: Structure- and Ligand-Based Approaches, Cambridge University Press, 2010

DATA WAREHOUSING & DATA MINING

Subject Code	16BBT252	IA Marks	20
Number of Lecture Hrs./Week	3	Exam Marks	80
Total number of lecture hours	40	Exam Hours	3

CREDITS:03

Course objectives :

The objective of this course is to make students learn about concepts of data warehousing and issues related with data warehouse design. Students will also learn about concepts of data mining, algorithms and evaluation of data mining results.

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
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MODULE – 1

Introduction to Data Warehousing: Heterogeneous information, Integration problem. Warehouse architecture. Data warehousing, Warehouse vs DBMS. Aggregations: SQL and Aggregations, Aggregation functions and Grouping.
 Data Warehouse Models and OLAP Operations: Decision support; Data Marts, OLAP vs OLTP. Multi-Dimensional data model. Dimensional Modelling. ROLAP vs MOLAP; Star and snowflake schemas; the MOLAP cube; roll-up, slicing, and pivoting

10

L2, L4

MODULE –2

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Issues in Data Warehouse Design: Design issues - Monitoring, Wrappers, Integration, Data cleaning, Data loading, Materialised views, Warehouse maintenance, OLAP servers and Metadata. Building Data Warehouses: Conceptual data modeling, Entity-Relationship (ER) modeling and Dimension modeling. Data warehouse design using ER approach. Aspects of building data warehouses.	08	L3,L5
MODULE – 3		
Introducing Data Mining: KDD Process, Problems and Techniques, Data Mining Applications, Prospects for the Technology. CRISP-DM Methodology: Approach, Objectives, Documents, Structure, Binding to Contexts, Phases, Task, and Outputs. Data Mining Inputs and Outputs: Concepts, Instances, Attributes. Kinds of Learning, Kinds of Attributes and Preparing Inputs. Knowledge representations - Decision tables and Decision trees, Classification rules, Association rules, Regression trees & Model trees and Instance-Level representations.	08	L2, L4
MODULE – 4		
Data Mining Algorithms: One-R, Naïve Bayes Classifier, Decision trees, Decision rules, Association Rules, Regression, K-Nearest Neighbour Classifiers.	08	L2 L3 L4
MODULE – 5		
Evaluating Data Mining Results: Issues in Evaluation; Training and Testing Principles; Error Measures, Holdout, Cross Validation. Comparing Algorithms; Taking costs into account and Trade-Offs in the Confusion Matrix.	08	L5, L6
<p>Course outcomes: After going through this course the student will be able to:</p> <ul style="list-style-type: none"> • learn about data warehouse design and concepts of data warehousing. • gain knowledge about data mining algorithms and evaluation of data mining results. 		
<p>Graduate Attributes (as per NBA) Computational knowledge Problem Analysis Design / Development of Solutions Conduct investigations of Complex Computing Problems Modern Tool Usage Individual and Team Work Innovation and Entrepreneurship</p>		

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Question Paper Pattern:

The question paper will have ten questions.

- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) from each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT /REFERENCE BOOKS

1. Fundamentals of Data Warehouses by M. Jarke, M. Lenzerini, Y. Vassiliou, P. Vassiliadis (ed.), Springer-Verlag, 1999.
2. The Data Warehouse Toolkit by Ralph Kimball, Wiley 1996.
3. Data Mining: Practical Machine Learning Tools and Techniques with Java Implementations by I. Witten and E. Frank, Morgan Kaufman, 1999.
4. Data Mining: Concepts and Techniques by J. Han and M. Kamber, Morgan Kaufman, 2000.
5. Principles of Data Mining by D. Hand, H. Mannila and P. Smyth., MIT Press, 2001.
6. Data Mining: Introductory and Advanced Topic by M. H. Dunham, Prentice Hall, 2003.
7. Intelligent Data Warehousing by Zhengxin Chen, CRC Press, 2002.
8. Heuristics and optimization for knowledge discovery by Ruhul A. Sarker, Hussein A. Abbass, Charles Sinclair Newton, Charles Newton. Idea Group Inc (IGI), 2002.

ARTIFICIAL INTELLIGENCE & NEURAL NETWORKS

Subject Code	16BBT253	IA Marks	20
Number of Lecture Hrs./Week	3	Exam Marks	80
Total number of lecture hours	40	Exam Hours	3

CREDITS:03

Course objectives :

The objective of this course is to make students learn about concepts of artificial intelligence and applications of artificial intelligence in bioinformatics.

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MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1		
Introduction to Artificial Intelligence: Introduction to Artificial Intelligence, Problems, Approaches and tools for Artificial Intelligence. Introduction to search, Search algorithms, Heuristic search methods, Optimal search strategies. Use of graphs in Bioinformatics. Grammers, Languages and Automata. Current Techniques of Artificial Intelligence: Probabilistic approaches: Introduction to probability, Bayes' theorem, Bayesian networks and Markov networks.	08	L1, L2
MODULE –2		
Classification methods: Nearest Neighbour method, Nearest Neighbour approach for secondary structure protein folding prediction, Clustering and Advanced clustering techniques. Identification Trees - Gain criterion, Over fitting and Pruning. Nearest Neighbour and Clustering Approaches for Bioinformatics.	8	L3,L4
MODULE – 3		
Applications: Genetic programming, Neural Networks for the study of Gene-Gene interactions. Artificial neural networks for reducing the dimensionality of expression data. Cancer classification with Microarray data using Support Vector Mechanics. Prototype based recognition of splice sites. Analysis of Large-Scale mRNA expression data sets by genetic algorithms. Artificial Immune Systems in Bioinformatics. Evolutionary algorithms for the protein folding problem. Considering Stem-Loops as sequence signals for finding Ribosomal RNA genes. Assisting cancer diagnosis.	8	L3, L6
MODULE – 4		
Neural Networks: Methods and Applications. Application of Neural Networks to Bioinformatics. Genetic algorithms and Genetic programming: Single-Objective Genetic algorithm, Multi-Objective Genetic algorithm. Applications of Genetic algorithms to Bioinformatics. Genetic programming – Method, Applications, Guidelines and Bioinformatics applications. Boolean Networks, Bayesian Networks and Fuzzy Neural	8	L2, L3

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Networks with case studies.		
MODULE – 5		
Applications of Neural Networks: Introduction, Modeling gene regulatory networks. QSAR and structure prediction with case studies	8	L3
<p>Course outcomes: After going through this course the student will be able to:</p> <ul style="list-style-type: none"> • learn about concepts of artificial intelligence and their applications in bioinformatics. • gain knowledge about neural networks applications of neural networks in bioinformatics. 		
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Computational knowledge • Problem Analysis • Design / Development of Solutions • Conduct investigations of Complex Computing Problems • Modern Tool Usage • Individual and Team Work • Innovation and Entrepreneurship 		
<p>Question Paper Pattern: The question paper will have ten questions.</p> <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		
<p>TEXT /REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. Artificial Intelligence Methods and Tools for Systems Biology by Werner Dubitzky, Francisco Azuaje, Published by Springer, 2005. 2. Intelligent Bioinformatics: The Application of Artificial Intelligence Techniques to Bioinformatics Problems by Edward Keedwell, Ajit Narayanan, published by John Wiley and Sons, 2005. 3. Computational Intelligence in Bioinformatics by Arpad Kelemen, Ajith Abraham, Yuehui Chen, SpringerLink (Online service) Published by Springer, 2008. 4. Computational Intelligence in Biomedicine and Bioinformatics: Current Trends and Applications by Tomasz G. Smolinski, Mariofanna G. Milanova, Aboul Ella Hassanien Published by Springer, 2008. 		

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5. Artificial Intelligence: A Modern Approach by Stuart Jonathan Russell, Peter Norvig, John F. Canny, Published by Prentice Hall, 2003.
6. Stuart Jonathan Russell, Peter Norvig. Artificial Intelligence: A Modern Approach, Prentice Hall, 2010.
7. Zheng Rong Yang. Machine Learning Approaches to Bioinformatics. World Scientific, 2010
8. Suranjan Panigrahi, K. C. Ting. Artificial intelligence for biology and agriculture. Kluwer Academic Press, 1998.
9. Edward Keedwell, Ajit Narayanan. Intelligent Bioinformatics: The Application of Artificial Intelligence Techniques to Bioinformatics Problems, John Wiley & Sons, 2005

METABOLIC ENGINEERING			
Subject Code	16BBT254	IA Marks	20
Number of Lecture Hrs./Week	3	Exam Marks	80
Total number of lecture hours	40	Exam Hours	3
CREDITS:03			
Course objectives : The objective of this course is to make students <ul style="list-style-type: none"> • Explore the importance of metabolic engineering in relation to cellular reaction • Analyse the strategy for product enhancement and yield along with metabolic flux. 			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			

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Introduction to Cellular Metabolism: Metabolic engineering and its multidisciplinary nature; Review of cellular metabolism; Models for cellular reactions; Material balances and data consistency-Block box model, elemental balances, heat balance and analysis.	8	L1, L2, L3
MODULE – 2		
Regulation of Metabolic Pathways: Regulation of enzyme activity- Reversible and irreversible inhibition systems, regulation of enzyme concentration- Control of transcription and translation. Global control: Regulation at whole cell level- regulation of metabolic networks.	8	L1, L2, L3
MODULE – 3		
Metabolic Pathway Manipulations: Enhancement of product yield and productivity- Ethanol, Amino acids and Solvents. Extension of substrate- Sucrose utilization and pentose metabolism for ethanol production. Product spectrum and novel products- Antibiotics, Polyketides, Vitamins, Biological pigments. Improvements of cellular properties- Nitrogen metabolism, Oxygen utilization, Overflow metabolism and genetic stability maintenance. Xenobiotics degradation of Polychlorinated Biphenyls (PCBs) and Benzene, Toluene, p-Xylene Mixtures (BTX).	8	L1, L2, L3
MODULE – 4		
Metabolic Flux Analysis: Methods for determination of metabolic fluxes by isotope labeling- Fractional label enrichment, complete enumeration of TCA cycle metabolite isotopomers from labeled pyruvate and acetate. Applications of metabolic flux analysis: Amino acid production by Glutamic acid bacteria and mammalian cell cultures. Flux analysis of metabolic networks- Bottomup Approach, Top-Down Approach.	8	L1, L2, L3, L4
MODULE – 5		
Metabolic Control Analysis (MCA): MCA theorems, determination of flux control coefficient. MCA of linear and branched pathways. Theory of large deviations.	8	L1, L2, L3, L4
Course outcomes: After going through this course the student will be able to: <ul style="list-style-type: none"> • utilize the knowledge of cellular metabolic pathway and regulation to enhance the yield. 		
Graduate Attributes (as per NBA) <ul style="list-style-type: none"> • Problem Analysis • Modern tool usage • Professional ethics 		

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- Societal and Environmental Concerns

Question Paper Pattern:

The question paper will have ten questions.

- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) from each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT /REFERENCE BOOKS

1. Gregory N. Stephanopoulos, Aristos A. Aristidou and Jens Nielsen. Metabolic engineering –Principles and Methodologies. Academic press, USA 1998.
2. Nestor V. Torres and Eberhard O. Voit, Pathway analysis and optimization in metabolic, Cambridge University Press, 2002.
3. Shuler M.L. and F. Kargi. Bioprocess engineering basic concepts, 2ndEdn, Prentice Hall, 2001.
4. Cortassa s., Aon, M.A., Lglesias, A.A., and L LyodD. An introduction and metabolic and cellular Engineering. World scientific publications Pvt ltd. Singapore. 2002.

MODELING & SIMULATIONS LAB

Subject Code	16BBIL26	IA Marks	20
No. of Lab Hrs./ Week :	3	Exam Marks	80
		Exam Hours	3

Course objectives :

The objective of this course is to make the students learn about developing bench skills through lab exercises, oriented towards utilizing various web based tools for bioinformatics projects.

Sl.NO	Experiment	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
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1	Homology Modeling of Receptors	L3
2	Docking of small molecules into Receptors active sites.	L4
3	Modeling Protein-Protein Interactions	L3
4	Modeling mutations and Single Nucleotide Polymorphisms	L3
5	Modeling Nanopores for Sequencing DNA	L3
6	Simulation of lipid bilayer.	L4
7	Simulation of Water Permeation through Nanotubes	L3
8	Simulation of "Forcing Substrates through Channels"	L4
9	Design of polymeric membranes - modeling and simulation diffusion studies of small gas molecules in polymeric materials.	L3
10	Virtual sequencing (base calling, Sequence assembly, Mapping assembly, Contig mapping)	L3
11	Analysis of NGS (next generation sequencing) data	L3
12	Genome annotation and Comparative Genomics studies	L3

Course outcomes:

At the end of the course the graduates should be able to:

- learn to appreciate the various algorithms used for diverse exercises.
- gain knowledge about various softwares and their multitude of applications.

Graduate Attributes (as per NBA)

- Problem analysis
- Design / Development of solutions
- Modern tool usage
- Communication
- Life-long learning

Conduct of Practical Examination:

1. All laboratory experiments are to be included for practical examination.
2. Students are allowed to pick one experiment from the lot.
3. Strictly follow the instructions as printed on the cover page of answer script for breakup of marks.
4. Change of experiment is allowed only once and 15% Marks allotted to the procedure part to be made zero.

TEXT/REFERENCE BOOKS

1. Molecular Modeling by Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers, 2008.
2. Modeling of Bimolecular Structures and Mechanisms by Alberte Pullman, Joshua Jortner, 1995.
3. Mathematical Approaches to Biomolecular Structure and Dynamics by Jill P. Mesirov, Klaus Schulten, De Witt L. Sumners, 1996.
4. Foundations of Molecular Modeling and Simulation by Peter T. Cummings, Phillip R. Westmorland, Brice Carnahan, Published by American Institute of Chemical Engineers, 2001.
5. New Algorithms for Macromolecular Simulation by Timothy J. Barth, Michael Griebel, David E. Keyes, Risto M. Nieminen, Dirk Roose, Tamar Schlick, Published

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by Springer, 2006.

6. Nicolas Claude Cohen, Guidbook on molecular modeling in drug design Academic Press., Elsevier, 1996.
7. Tamar Schlick. Molecular Modeling and Simulation: An Interdisciplinary Guide: An Interdisciplinary Guide. Second Edition, Springer. 2010.
8. Tamar Schlick, Innovations in Biomolecular Modeling and Simulations, Volume 2, RSC Publishing. 2012.

SEMESTER III

16BBI31- 16BBI34 INTERNSHIP / PROJECT WORK
(PROJECT I PHASE EVALUATION)

IV SEMESTER

RESEARCH METHODOLOGY, BIOSAFETY & IPR			
Subject Code	16BBT41/16BBC41/16BBI41/16IB41	IA Marks	20
Number of Lecture Hrs./Week	04	Exam Marks	80
Total number of lecture hours	50	Exam Hours	03
CREDITS 04			
Course objectives : The course will enable the students: <ul style="list-style-type: none"> • To understand and apply different methodologies of scientific research • To appreciate the Basic concepts of IPR • To apply the principles of biosafety guidelines in biotech practices 			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
CONCEPT OF RESEARCH: Types & classification, steps involved. Identification of the research question, hypotheses, and justification for the topic Literature Collection: Review of literature, review process and bibliography, research/discriminative reading, consulting source material, Research Objectives and hypothesis, Research Design : detailed discussion of the conceptualization and operationalization of variables. Research method and materials, Research action. Data collection and analysis plan:		10	L1, L2,L3

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<p>data gathering – thorough description of methods of data gathering and sources.; Analytical techniques – detailed discussion of data gathering and analytical methods, including explanation of their suitability of these techniques compared with others and any possible problems arising from the methods selected; application and execution of analytical techniques and interpretations of findings. Format for manuscript writing, documentation, organization of reference material, bibliography, end note etc to be discussed with case studies. Research budget and resources.</p>		
MODULE –2		
<p>INTRODUCTION TO INTELLECTUAL PROPERTY: Types of IP: Patents, Trademarks, Copyright & Related Rights, Issues related to plagiarism in research, copyright laws, acknowledging the sources etc to be discussed with case studies. Basics of Patents and Concept of Prior Art; Introduction to Patents; Types of patent applications: Ordinary, PCT, Conventional, Divisional and Patent of Addition; Specifications: Provisional and complete; Forms and fees Invention in context of “prior art”; Patent databases; Searching International Databases; Country-wise patent searches (USPTO, esp@cenet(EPO), PATENTScope(WIPO), IPO, etc.)</p>	10	L2,L3,L4
MODULE – 3		
<p>Industrial Design, Traditional Knowledge, Geographical Indications, Protection of GMOs IP as a factor in R&D; IPs of relevance to Biotechnology and few Case Studies. Patent filing procedures; National & PCT filing procedure; Time frame and cost; Status of the patent applications filed; Precautions while patenting – disclosure/non-disclosure; Financial assistance for patenting - introduction to existing schemes Patent licensing and agreement Patent infringement- meaning, scope, litigation, case studies.</p>	10	L3,L4
MODULE – 4		
<p>BIOSAFETY: Introduction & historical background; Primary Containment for Biohazards; Biosafety Levels for Microbes, Plants & Animals; Biosafety guidelines - Government of India; Definition of GMOs & LMOs: RCGM, GEAC etc. for GMO applications in food and agriculture; Environmental release of GMOs; Risk Analysis; Risk Assessment; Risk management and communication. Roles of Institutional Biosafety Committees</p>	10	L2, L3, L4
MODULE – 5		
<p>History, broad account & latest amendments (if any) of the provisions of :- Indian Patent Act 1970 & recent amendments, GATT & TRIPS Agreement, Madrid Agreement, Hague Agreement, WIPO Treaties, Budapest Treaty, PCT.</p>	10	L2, L3, L4, L5

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<p>Course outcomes: After studying this course, students will be able to:</p> <ul style="list-style-type: none"> • Demonstrate strong basics in principles of Research methodology, IPR and biosafety issues
<p>Graduate Attributes (as per NBA)</p> <ul style="list-style-type: none"> • Problem Analysis • Design / development of solutions. • Professional Ethics
<p>Question Paper Pattern: The question paper will have ten questions.</p> <ul style="list-style-type: none"> • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module.
<p>TEXT BOOKS</p> <ol style="list-style-type: none"> 1. C R Kothari Research Methodology, New Age International (P) Ltd. 2008 . 2. Wayne Goddard, Stuart Melville Research Methodology: An Introduction: Juta and Company Ltd, 2004 3. P. Hambleton, J. Melling, T. T. Salusbury Biosafety in industrial biotechnology – Springer 4. M. K. Sateesh. Bioethics and Biosafety By IK International 2008
<p>REFERENCE BOOKS</p> <ol style="list-style-type: none"> 1. D K Bhattacharyya, Research Methodology By Excel Publisher Publishing Co. Pvt. Ltd., 2007 2. Kankanala C., Genetic Patent Law & Strategy 1st Edition, Manupatra Information Solution Pvt. 2007 3. BAREACT Indian Patent Acts & Rules, Universal Law 1970

PROJECT MANAGEMENT			
Subject Code	16BBI421	IA Marks	20
Number of Lecture Hours/Week	03	Exam Marks	80
Total Number of Lecture Hours	40	Exam Hours	03
CREDITS – 03			
<p>Course objectives: The course will enable the students</p> <ul style="list-style-type: none"> • To Appreciate the Basic concepts of Project management • To understand and apply the different principles of project management methodologies. • To learn the translation of Proof-of-concepts to product realization, and product life cycles, marketing, IPs, regulatory affairs etc 			
Modules		Teaching Hours	Revised Bloom's Taxonomy (RBT) Level
MODULE -1			

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<p>PROJECT PLANNING: scope – problem statement – project goals – objectives – success criteria –assumptions – risks – obstacles – approval process – projects and strategic planning. Project implementation – project resource requirements – types of resources – men –materials finance. Case studies.</p>	08 Hours	L1, L2,L3
MODULE -2		
<p>PROJECT MANAGEMENT : Introduction – Meaning – nature and characteristics of Management, Scope and functional areas of Management – Management as a Science, Art or Profession Management & Administration – Roles of Management, Levels of Management, Development of Management Thought – Early Management Approaches – Modern Management Approaches.</p>	08 Hours	L2, L3, L4
MODULE -3		
<p>PLANNING: Nature, importance and purpose of planning, process objectives – Types of plans (Meaning only) – Decision making – Importance of planning – steps in planning & planning premises – Hierarchy of plans.</p>	08 Hours	L2, L3, L4
MODULE -4		
<p>ORGANIZING AND STAFFING: Nature and purpose of organization - Principles of organization – Types of organization - Departmentation – Committees – Centralization Vs decentralization of authority and responsibility – Span of control – MBO and MBE (Meaning only) Nature and importance of Staffing – Process of Selection & Recruitment (in brief).</p>	08 Hours	L2, L3, L4
MODULE -5		
<p>DIRECTING & CONTROLLING: Meaning and nature of directing-Leadership styles, Motivation Theories, Communication – Meaning and importance – Coordination, meaning and importance and Techniques of Coordination. Meaning and steps in controlling – Essentials of a sound control system –Methods of establishing control.</p>	08 Hours	L3, L4, L5
<p>Course outcomes: After studying this course, students will be able to:</p> <ul style="list-style-type: none"> • Demonstrate strong basics in principles and applications of Project Management 		
<p>Graduate Attributes (as per NBA):</p> <ul style="list-style-type: none"> • Problem Analysis • Design / development of solutions. • Innovation and Entrepreneurship • Professional Ethics • Individual and Team Work 		
<p>Question paper pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions. • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. 		

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- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT BOOKS

1. Beenet P Lientz, Kathyn, Project Management – for 2 1st Century- Academic Press, 1995
2. Martin Grossmann Entrepreneurship in Biotechnology: managing for growth from start-up to initial public offering. Verlag. Springer-2003
3. Holger Patzelt and Thomas Brenner. Handbook of Bioentrepreneurship By Springer 2008
4. Graham Dutfield, IPR, Trade and Biodiversity, Earthscan publications, 2000

REFERENCE BOOKS:

1. Damian Hine, John Kapeleris. Innovation and entrepreneurship in biotechnology, an international prospective. By Edward Elgar Publishing. 2006
2. P. S. Teng. Bioscience entrepreneurship in Asia: creating value with biology. By World scientific publishing. Co. Pte. Ltd. 2008
3. A.K. Singh. Entrepreneurship Development and Management by Firewall Media, 2006
4. Ramachandran, Entrepreneurship Development by. Tata McGraw-Hill Education, 2008

HEALTH INFORMATICS			
Subject Code	16BBI422	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80
Total number of lecture hours	40	Exam Hours	03
CREDITS 03			
Course objectives : The objective of this course is to make students learn about concepts of health informatics, tools and techniques used in health informatics. This course will also give insights into Applications IT in health informatics to help humans.			
MODULES		TEACHING HOURS	REVISED BLOOM'S TAXONOMY (RBT) LEVEL
MODULE – 1			
An introduction to Health care informatics: An interaction between health care and information systems. Acquisition, storage, retrieval, and use of information in health and biomedicine. Tools and techniques. Information systems in Medicine, Dentistry, Nursing,surgery and diagnosis. Future prospects.		08	L2, L3, L5

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MODULE –2		
Building blocks of Health care informatics: Standards, types of standards. Modeling –principles of modeling for healthcare. Architecture of Health care system – models, subsystems, packages and components. Modeling framework for health care. generic health care information model. Unified modeling language. Modeling methodologies in healthcare systems. Databases, types, and applications. Database Architecture; ANSI/SPARC three tier architecture. Data warehousing; architecture.	08	L1,L2,L3
MODULE – 3		
Tools and techniques in Health Informatics: Introduction, conditions for telemedicine development, applications, access techniques in telecare and Internet technologies in medical systems: Requirement of Medical systems in the internet environment, internet medical architectures, and internet based telemedical services, next generation point of care information systems, internet access technologies in Telecare Wireless communication technologies. Electronic Health records (HER): Challenges in clinical care, characteristics of good EHR, Generic EHR representation, EHR Standards and Scope of the HER.	08	L2,L4,L5
MODULE – 4		
Decision support systems and Telematic networks in Medicine: Decision support systems, knowledge based and Expert based. Probabilistic and Logical decision systems. Transport layer in telematics networks, health digital data standards, E-health networks services.	08	L2,L3,L4
MODULE – 5		
Applications of IT in hearing and chronic problems: Methodology of hearing screening, computer aided adjustment of hearing aids, diagnosis, tinnitus treatment. Application of IT to diagnose chronic conditions patient-centered symptom monitoring. Computer aided techniques in Medicine: Laproscopic surgery navigation, Intraoperative imaging, multimodal imaging, Biosignal processing and algorithms. Biosignal databases.	08	L2,L3,L4

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COURSE OUTCOMES

Students will gain knowledge about concepts and building blocks of health informatics
 ii. Students will learn about tools and techniques used in health informatics.
 iii. Students will gain insights into the applications of IT in health informatics.

Question paper pattern:

- The question paper will have ten questions.
- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) from each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

Graduate Attributes (as per the NBA)

Conduct investigations of Complex Computing Problems
 Professional Ethics
 Communication Efficiency
 Individual and Team Work
 Innovation and Entrepreneurship

TEXT BOOKS/REFERENCE BOOKS

- 1 Naakesh A. Dewan, John Luo, Nancy M. Lorenz. Information Technology Essentials for Behavioral Health Clinicians, 2010.
2. Krzysztof Zielinski, MariuszDuplaga. Technology Solutions for Healthcare, 2006.
3. Moya Conrick, Health Informatics, 2006.
4. Frank Sullivan, Jeremy Wyatt. ABC of Health Informatics, 2009

COMPUTER-AIDED DRUG DISCOVERY

Subject Code	16BBI423	IA Marks	20
Number of Lecture Hrs./Week	03	Exam Marks	80
Total number of lecture hours	40	Exam Hours	03

CREDITS 03

Course objectives :

The objective of this course is to make students learn about concepts of drug design process, methods used for the drug design and role of bioinformatics in drug discovery.

MODULES	TEACHING HOURS	REVISED BLOOM'S TAXONOMY
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		(RBT) LEVEL
MODULE – 1		
Drug Design Process: Drug design - Compound searching, Target Identification, ADMET Studies and Study of drug resistance. Drug design process for a known protein target – Structure based drug design process, finding initial hits, Compound refinement, ADMET Studies and Study of drug resistance. Drug design process for unknown protein target – Ligand based drug design process, finding initial hits, Compound refinement, ADMET Studies and Study of drug resistance. Compound Library Design: Target library vs diverse libraries, Non-Enumerative techniques, Drug likeliness and Synthetic accessibility, Analyzing diversity and Spanning known chemistries. Compound selection techniques.	08	L1,L2,L3
MODULE –2		
Homology Modeling and Drug Design: Structure Generation, Retrieval, Structure Visualization. Homology modeling - Constructing an initial model, Refining the model, Manipulating the model, Navigation of the model. Model evaluation – Model evaluation techniques, Concept of energy minimization and Energy minimization techniques. Conformation generation, Deriving bioactive conformations, Molecular superposition and alignment, deriving the Pharmacophoric pattern, receptor mapping and estimating biological activities. Molecular Mimicry and Chemical Intuition- important key and the role of the Molecular Modeling, limitations of Chemical Intuition.	08	L1,L2,L3
MODULE – 3		
Molecular Mechanics and Docking: Introduction to Molecular mechanics, Force fields for drug design. Study of protein folding: Algorithms, Conformation analysis. Quantum Mechanics in Drug Design: Quantum Mechanics algorithms in Drug design - Modeling Systems with metal atoms, computing reaction paths and computing spectra. Docking: Introduction, Search algorithms, Scoring functions, Docking Process – Protein Preparation, Building the ligand, setting the bounding box, running the docking calculations. Molecular docking	08	L1,L2,L3,L4

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softwares and their utilities in drug design.		
MODULE – 4		
Building the Pharmacophore Models: Components of Pharmacophore model, creating a Pharmacophore model from active compounds, Creating Pharmacophore model from Active site and Searching compound databases. QSAR: Conventional QSAR vs 3D-QSAR, QSAR Process, Molecular descriptors, Automated QSAR Programs. 3D-QSAR – 3D-QSAR Process. ADMET Studies: Oral bioavailability of compound, Finding Drug Half life in the Blood stream, Blood- Brain Barrier permeability and Toxicity studies.	08	L1,L2,L4,L5
MODULE – 5		
Computer-Assisted Drug Discovery: Drug Discovery and Development process, New Lead Discovery Strategies. Composition of Drug Discovery teams, Current Practice of CADD in the Pharmaceutical industry, Management structures of CADD groups, Contributions and achievements of CADD groups, Limitations of CADD support, Inherent Limitations of CADD support. State of Current Computational Models, Software and Hardware constraints	08	L,L3,L4,L5
<p>Course outcomes: Students will gain knowledge about drug design process and methods and tools used for the drug discovery. Students will learn about the computer-assisted drug discovery and various tools used.</p>		
<p>Graduate Attributes (as per NBA) Computational knowledge Problem Analysis Design / Development of Solutions Conduct investigations of Complex Computing Problems Life-long Learning</p>		
<p>Question paper pattern:</p> <ul style="list-style-type: none"> • The question paper will have ten questions. • Each full question consists of 16 marks. • There will be 2 full questions (with a maximum of four sub questions) from each module. • Each full question will have sub questions covering all the topics under a module. • The students will have to answer 5 full questions, selecting one full question from each module. 		

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TEXT BOOKS

- 1 Cancer Drug Design and Discovery by Stephen Neidle, Academic Press – Publisher, 2008.
2. Bioinformatics Technologies by Yi-Ping Phoebe Chen, Springer – Publisher, 2005.
3. Textbook of drug design and discovery by PovlKrogsgaard-Larsen, Tommy Liljefors, Ulf Madsen, Published by Taylor & Francis, 2002.
4. Computational Drug Design: A Guide for Computational and Medicinal Chemists by D. C. Young, Wiley-Interscience, 2009.
5. Moody P.C.E and A.J. Wilkinson. Protein Engineering, IRL Press, Oxford University Press.
6. Protein Science by Arthur M Lesk, Oxford University Press

REFERENCE BOOKS

- 7 The Molecular Modeling Perspective in Drug Design by N Claude Cohen, Academic Press.
8. Bioinformatics Methods & Applications: Genomics, Proteomics & Drug Discovery by SC Rastogi, N Mendiratta& P Rastogi, PHI.
9. Drug Discovery Strategies and Methods by AlexandrosMakriyannis, Diane Biegel, Marcel Dekker, 2004.
10. Modern Methods of Drug Discovery by Alexander Hillisch, Rolf Hilgenfeld, Birkhäuser, 2003.
11. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry by Charles Owens Wilson, John H. Block, Ole Gisvold, John Marlowe Beale, Lippincott Williams & Wilkins, 2010.
12. Structure- based drug design by Veerapandian, PandiVeerapandian, Marcel Dekker, 1997.
13. 3D QSAR in Drug Design by Hugo Kubinyi, GerdFolkers, Yvonne Connolly Martin, Springer – Publisher, 1998.

ENTREPRENEUR DEVELOPMENT

Subject Code	16BBI424/16BBT42 4/16BBC424	IA Marks	20
Number of Lecture Hours/Week	03	Exam Marks	80
Total Number of Lecture Hours	40	Exam Hours	03

CREDITS – 03

Course objectives: The course will enables the students

- Appreciate the Basic concepts of entrepreneur development
- Apply the proof-of-concepts to Large scale and Entrepreneurship opportunities

Modules	Teaching Hours	Revised Bloom's Taxonomy (RBT) Level
MODULE -1		
ENTREPRENEURSHIP-ENTERPRISE: Conceptual issues. Entrepreneurship vs. Management. Roles and functions of Entrepreneur in relation to the enterprise and in relation	08 Hours	L1, L2,L3

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to the economy. Entrepreneurship is an interactive process between the individual and the environment. Small business as seedbed of Entrepreneurship. Entrepreneur competencies, Entrepreneur motivation, performance and rewards.		
MODULE -2		
OPPORTUNITY SCOUTING AND IDEA GENERATION: Role of creativity and innovation and business research. Sources of business ideas. Entrepreneur opportunities in contemporary business environment, for example opportunities in net-work marketing, franchising, business process outsourcing in the early 21 century. The process of setting up a small business: Preliminary screening and aspects of the detailed study of the feasibility of the business idea and financing/non-financing support agencies to familiarize themselves with the policies/programs and procedures and the available schemes. Preparation of Project Report and Report on Experiential Learning of successful and unsuccessful entrepreneurs	08 Hours	L2,L3,L4
MODULE -3		
MANAGEMENT ROLES AND FUNCTIONS IN A SMALL BUSINESS: Designing and re-designing business process, location, layout, operations planning and control. Basic awareness on the issues impinging on quality, productivity and environment. Managing business growth. The pros and cons of alternative growth options: internal expansion, acquisitions and mergers, integration and diversification. Crisis in business growth.	08 Hours	L2, L3,L4
MODULE -4		
PRINCIPLES OF DOUBLE-ENTRY BOOK-KEEPING: Journal entries, cash-book, pass book, and Bank Reconciliation Statement, ledger accounts, trail balance and preparation of final accounts: Trading and Profit and Loss Account; Balance-sheet. Brief introduction to Single-Entry system of record keeping. Sources of risk/venture capital, fixed capital, working capital and a basic awareness of financial services such as leasing and factoring.	08 Hours	L2, L3, L4
MODULE -5		
ISSUES IN SMALL BUSINESS MARKETING: The concept and application of product life cycle, advertising and publicity, sales and distribution management. The idea of consortium marketing, competitive bidding/tender marketing, negotiating with principal customers. The contemporary perspectives on Infrastructure Development, Product and Procurement Reservation, Marketing Assistance, Subsidies and other Fiscal and Monetary Incentives. National state level and grass-root level financial and non-financial institutions in support of small business development.	08 Hours	L3, L4, L5
Course outcomes: After studying this course, students will be able to: <ul style="list-style-type: none"> • Demonstrate strong basics in entrepreneurship • Demonstrate the ability to manage industrial projects and develop products 		
Graduate Attributes (as per NBA):		

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- Problem Analysis
- Design / development of solutions.
- Innovation and Entrepreneurship

Question paper pattern:

- The question paper will have ten questions.
- Each full question consists of 16 marks.
- There will be 2 full questions (with a maximum of four sub questions) from each module.
- Each full question will have sub questions covering all the topics under a module.
- The students will have to answer 5 full questions, selecting one full question from each module.

TEXT BOOKS

1. Brandt, Steven C., "The 10 Commandments for Building a Growth Company",
1. Macmillan Business Books, Delhi, 3rd Ed., 1977.
2. Bhide, Amar V., "The Origin and Evolution of New Business", Oxford University Press
York, 2000.
3. Dollinger M.J., "Entrepreneurship strategies and Resources", Pearson Education, New
Delhi, 3rd Ed., 2006.
4. Desai, Vasant Dr., "Management of small scale enterprises", Himalaya Publishing House,
5. Taneja, Gupta, "Entrepreneur Development New Venture Creation", Galgotia Publ
Company, 2nd Ed., 2001.

Reference Books:

1. Patel, V.G., "The Seven Business Crises and How to Beat Them", TMH, 1995.
2. SIDBI Report on Small Scale Industries Sector [latest edition]
3. Verma, J.C., and Gурpal Singh, "Small Business and Industry-A Handbook for Entrepreneurs",
New Delhi, 2002.
4. Manohar, "Entrepreneurship & Management", Wiley India, 2012.