# M.Sc. SYSTEMS BIOLOGY AND BIOINFORMATICS FOR THE ACADEMIC SESSION 2016-2017

**SEMMER I**

<table>
<thead>
<tr>
<th>PAPER CODE</th>
<th>PAPER</th>
<th>MARKS</th>
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</thead>
<tbody>
<tr>
<td>MSBB101</td>
<td>Biophysical Chemistry of Biomacromolecules</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB102</td>
<td>Metabolomics and Metabolic Pathway Engineering</td>
<td>100*</td>
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<tr>
<td>MSBB103</td>
<td>Basic Concepts in Mathematics</td>
<td>100*</td>
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<tr>
<td></td>
<td>(For students with Biology Background)</td>
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<tr>
<td>MSBB104</td>
<td>Basic Concepts in Biology</td>
<td>100*</td>
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<tr>
<td></td>
<td>(For students with Non-Biology Background)</td>
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<tr>
<td>MSBB105</td>
<td>Biostatistics</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB106</td>
<td>Data Management and Biological Databases</td>
<td>100*</td>
</tr>
<tr>
<td>Practical 110</td>
<td>Based on MSBB101</td>
<td>25*</td>
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<tr>
<td>Practical 120</td>
<td>Based on MSBB102</td>
<td>25*</td>
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<tr>
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<td>TOTAL</td>
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*Internal Assessment based on house tests = 20, End Semester theory examination = 80
#Internal Assessment = 5, End Semester Practical examination = 20

**SEMMER II**

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<tr>
<th>PAPER CODE</th>
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<tbody>
<tr>
<td>MSBB201</td>
<td>Spectroscopic Methods in Structural Biology</td>
<td>100*</td>
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<tr>
<td>MSBB202</td>
<td>Genomics and recombinant DNA technology</td>
<td>100*</td>
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<tr>
<td>MSBB203</td>
<td>Computational Methods of Sequence Analysis and</td>
<td>100*</td>
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<td></td>
<td>Biomacromolecular informatics</td>
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<tr>
<td>MSBB204</td>
<td>Programming in C++ and PERL</td>
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<td>Practical210</td>
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<td>Practical240</td>
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<tr>
<td>Seminar</td>
<td>On (i) (a) Data bases and Bioinformatics tools on</td>
<td>50+50 = 100</td>
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<tr>
<td></td>
<td>the internet (b) Modeling tools—Visualization</td>
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<tr>
<td></td>
<td>and genome matrix (c) Solving of structures</td>
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<tr>
<td></td>
<td>using different softwares (ii) Journal Club</td>
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*Internal Assessment based on house tests = 20, End Semester theory examination = 80
#Internal Assessment = 5, End Semester Practical examination = 20
M.Sc. SYSTEMS BIOLOGY AND BIOINFORMATICS
FOR THE ACADEMIC SESSION 2016-2017

**SEMESTER III**

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<th>PAPER CODE</th>
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<tr>
<td>MSBB301</td>
<td>Computation Cell Biology I</td>
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<tr>
<td>MSBB302</td>
<td>Systems Biology</td>
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<tr>
<td>MSBB303</td>
<td>Proteomics and Systems Biology</td>
<td>100*</td>
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<tr>
<td>MSBB304</td>
<td>Molecular Modeling and Computer aided Drug Design</td>
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<td>Practical310</td>
<td>Based on MSBB301</td>
<td>25#</td>
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<td>Practical320</td>
<td>Based on MSBB302</td>
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<td>Practical340</td>
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<td>Seminar</td>
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*Internal Assessment based on house tests = 20, End Semester theory examination = 80

#Internal Assessment = 5, End Semester Practical examination = 20

**SEMESTER IV**

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<tr>
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<tr>
<td>MSBB401</td>
<td>Computation Cell Biology II</td>
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<tr>
<td>MSBB402</td>
<td>Chemoinformatics</td>
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<td>MSBB403</td>
<td>Advance Bioinformatics and Nanotechnology</td>
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<tr>
<td></td>
<td>Project Work and Oral Presentation</td>
<td>200+100 = 300</td>
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SEMESTER I

MSBB101 - BIOPHYSICAL CHEMISTRY OF BIOMACROMOLECULES

Maximum Marks- 100
Lectures 45

Objective
This paper covers the physical properties of biological macromolecules and the physical techniques used to study them. Thorough understanding of the structural characteristics of macromolecules is the most fundamental part of systems biology and bioinformatics.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I


UNIT II

Conformational stability: Biomacromolecules in Solution, Principles of ionization equilibrium ionization of side chains; Conformational equilibria in proteins. Two state model of protein stability. Chemical denaturation and stabilization, surface denaturation.

Structure of Nucleic acids: Ionization equilibria of nucleosides and nucleotides, Composition of nucleic acid, Chargaff’s rules in DNA, RNA base compositions. Primary structure, covalent chain structure, secondary structure inferences from RNA sequence comparisons, sequence information and analysis of structure and function.

UNIT III

Structure of Polysaccharides: Polysaccharide chains, sequence analysis of polysaccharides, 2° and 3° structure of polysaccharide chains, conformations of starch, glycogen, pectins, cellulose and chitin. Study of glycoproteins, associated glycans, neoglycans.
Glycomics: Features of glycomics- glycobiology; Glycomic databases and servers; Glycomics-genetic, proteoglycomic and chemoglycomicapproaches; Glycochip.

UNIT IV

Molecular distribution and statistical thermodynamics: Binding of small molecules by polymer, identical and independent sites model, Multiple Equilibria, Single-Site Binding, Multiple-Site Binding: General, Equivalent Sites, Nonequivalent Sites, Allosterism and Cooperativity. The random walk, Helix coil transitions in proteins, statistical thermodynamics. Organizational levels of biomacromolecule structure.


References books: -

Additional Reference Books:-

Practical110

1. Introduction to Nucleic acid and protein databases: GeneBank, EMBL, DDBJ, SWISSPORT, INTERPRO, And UNIPORT.
2. Introduction to Structural databases: PDB, PDBsum, NDB etc. RNA databases: RNA Base, SCOR. lipid databases: LIPIDAT.
3. Glycosuite database, SWEETDB
Objective
The central metabolic pathways would be covered in detail so that the students can understand how individual enzymes work in concert to perform complicated biochemical reactions, with special stress on enzymes kinetics and regulation. Further, signal transduction cascades will be introduced along with brief introduction to methods of metabolic analysis and metabolic pathway engineering would be done.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Introduction to Omics: Systems Biology, metabolomics, metabolonomics, Techniques to study omics.

UNIT II
Amino Acid synthesis, degradation, urea cycle, Fatty acid synthesis and degradation, FAS complex, Ketone bodies and their importance and Nucleic acid synthesis, degradation, Salvage pathway, Diseases associated with disturbances in metabolic pathways.

UNIT III
Enzymes and Enzyme kinetics: Activation energy and reaction coordinate, catalytic mechanisms, Basic equations of enzyme kinetics: steady state kinetics, significance of Michaelis-Menton parameters, graphical representation of data, inhibition, non-productive binding, $K_{cat}/K_{m}$, competing substrates, Reversibility, Energy substrate complementarity and the use of binding energy in catalysis: Utilization of E-S binding energy in catalysis, evolution of maximum rate, and molecular mechanisms for the utilization of binding energy. Conformational change, allosteric regulation: positive cooperativity, mechanisms of allosteric interactions and cooperativity, regulation of metabolic pathways by regulation of enzyme: phosphokinase and glycogen phosphorylase, Zymogens, Mechanism of Serine proteases-Trypsinogen, Chymotrypsin and ATCase.

UNIT IV
References books: -

Practical120

1. To carry out query retrieval using BRENDAN.
2. To study the services provided by KEGG database.
3. To study services provided by KEGG LIGAND databases.
4. To study Eco Cyc (Encyclopedia of E. coli) k-12 MG 1655 genes and metabolism.
5. To study services provides by Meta Cyc.
6. To study motif search for E.colitrp A.

MSBB103 – BASIC CONCEPTS IN MATHEMATICS
(For Students with Biology Background)

Maximum Marks- 100
Lectures 45

Objective

To introduce students of Biology to learn and apply the basic concepts of mathematics in Biological science for presentation and interpretation of data.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT – I


Calculus: Concept of limit and Continuity, Derivative of functions including exponential, logarithmic, trigonometric and algebraic functions. Monotonic functions, Maxima and Minima of a function.

UNIT-II

Integration: Various methods for computing integrals, Definite Integrals, Area under the curve, Trapezoidal Rule.

UNIT-III

Matrices: Definition, addition, subtraction, multiplication, transpose, inverse of a matrix, rank of a matrix solutions of simultaneous equations. Eigen values and Eigen vectors, Applications of Cayley Hamilton Theorem.
Vectors. Vector addition, subtraction, products of two vectors (dot product and cross product), scalar triple product, vector triple product.

UNIT-IV

Numerical methods: Curve fitting and interpolation, Solution of algebraic and transcendental equations (by using Bisection method and Newton-Raphson method).
Trigonometry and Analytical Geometry: De Moivre’s theorem, Equation of a Straight line, slope of a line, Angle between two lines.

Reference Books:
1. Basic Mathematics by Serge A. Lang. Springer Publisher. 1988

MSBB104 – BASIC CONCEPTS IN BIOLOGY
(For Students with Non-Biology Background)

Maximum Marks- 100
Lectures 45

Objective
It introduces the students of Non-Biology background to the concepts of biological sciences which are integral understanding and application of Bioinformatics.

Instructions for paper setters:
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.
UNIT - I

Cell Structure and Function


Microbes: Kingdom monera, protista, and fungi- characteristic features of the groups and their importance.

UNIT – II

Introduction to Genetics, Ecology, Origin of life and Evolution
Eukaryotic Chromosome Structure Organization, Histones, Nucleosomes, Organization of Genes and Noncoding DNA, Higher Levels of Chromatin Organization, Cell cycle, Mitosis and meiosis - Process, phases and comparison, Mutations and sources of mutations - Spontaneous mutations and Induced mutations.

UNIT – III

Animal system physiology
Blood and Circulation- Blood corpuscles, plasma function, blood groups. Endocrinology and reproduction- Endocrine glands, basic mechanism of hormone action, hormones and diseases.

Respiratory System- Comparison of respiration in different species, anatomical considerations, transport of gases, exchange of gases, waste elimination, neural and chemical regulation of respiration.

Excretory System- Comparative physiology of excretion, kidney, urine formation, urine concentration, waste elimination, micturition, regulation of water balance, blood volume, blood pressure, electrolyte balance, acid-base balance.

Digestive System- Digestion, absorption, energy balance, BMR.

UNIT – IV

Experimental Techniques
Chromatographic Techniques- Principles and Applications of Paper, TLC, Adsorption, Ion exchanges, Gel filtration, Affinity, GLC, HPLC

Electrophoretic Techniques- Polyacrylamide gel electrophoresis, SDS-PAGE, Agarose gel Electrophoresis Separation of Proteins. Lipoportins, Nucleic acids, Visualizing separated components- staining, Fluorescent techniques Isoelectric focusing, pulsed field electrophoresis

Ultra Centrifugation- Construction of preparative and analytical ultra centrifuge, Svedberg's constant, Sedimentation velocity and Sedimentation equilibrium

Reference Books:

Objective:
To introduce students to learn and apply the basic concepts of Biostatistics in Biological sciences for presentation and interpretation of data. To train students to use statistical software and handle large data sets.

Instructions for paper setters:
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT-I
Biostatistics: its meaning and objectives, measurement scales, Population and Samples. Frequency tables and their graphs. Measures of location, variability (box and whisker plot), Skewness and Kurtosis (Use of SPSS/R- package).
Probability: Intuitive concept of probability, conditional probability (Bayes’ theorem); Specificity, Sensitivity.

UNIT-II
Random variables: probability mass function, probability density function, distribution function, expectation and variance, moment generating function and probability function, Discrete Distributions: Binomial, Poisson, uniform, Geometric and negative binomial, Poisson Process. Continuous distributions: Normal, uniform, exponential, Gamma and Beta.

Correlation & Regression: Scatter diagram, Karl Pearson’s correlation and Spearman’s rank Correlation Coefficient, Simple and multiple regression (using SPSS only).

UNIT-III
Testing: Sampling, Distributions of sample mean, difference of means, sample proportion and difference of proportions, the basic idea of significance tests, Tests of hypothesis for the parameters of a normal distribution (two sample problems also) including testing for population proportions,
paired t-test, chi-square tests for association, Yates’ correction. Basic concepts of Analysis of Variance. One-way and two-way classification, Non-parametric: Sign-test, Wilcoxon Signed rank test, Mann-Whitney U-Statistic (Using SPSS).

UNIT-IV

Study Designs and Risk Assessment: Types of research and studies to be conducted in biological and clinical sciences, Experimental and Observational Studies, Different Phases of Clinical Trials, Designs of Fixed sample and Sequential Clinical Trials, Descriptive (cross-sectional and Longitudinal Studies), Analytical Studies: Case-control and Cohort Studies, Risk Assessment in Studies (Odds Ratio, Relative Risk, Attributable Risk etc.).

Reference Books:
7) Medical Statistics by PSS SundarRao and Richardson (2013)  

Practical 150

1. Measures of central tendency and dispersion  
2. Measures of Skewness and Kurtosis  
3. Histogram and Box-and –Whisker Plot  
4. Probability/conditional probability  
5. Problem solving related to various distributions  
6. Correlation & Regression  
7. Parametric tests  
8. Non-parametric tests
MSBB106 - DATA MANAGEMENT AND BIOLOGICAL DATABASES

Objective
This course aims to introduce to students the concept of database mining and management which is a fundamental part of bioinformatics. An overview of various biological databases along with their importance and knowledge discovery from these will also be covered.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I


UNIT II

Database System, architecture and Design: Data Models, Schemas bad instances, DBMS, Architecture and data independence, database languages, and classification of DBMS. Informal design guidelines for relation Schemas, Functional dependencies, normal forms based on primary keys, general definition of 2nd and 3rd normal forms, BCNF, need of further normalization.

UNIT III

Data mining: Definition, data mining and KDD, data mining on relational databases, data warehouses, transactional databases etc. Data mining functionalities, pattern mining. Association analysis, classification and prediction, cluster analysis and evolution analysis, data mining on biological data.

SQL overview, Modifying Data, Managing Constraints, Managing Views, User Access, Oracle Overview and Architecture, Managing Oracle, Control and Redo Log Files, Managing Tables, indexes and Constraints, Managing Users and Security, Introduction to Network Administration, Backup and Recovery Overview, Introduction to performance tuning.

UNIT IV

Introduction to Biological databases:
References books:
2) Jiawei Han, MichelineKamber, Data Mining Concepts and Techniques. Morgan Kaufman Publisher, 2001.
10) C.J. Date, Database Systems, Addison Wesley, 2000
11) Chip Dawes, Biju Thomas, Introduction to Oracle 9i SQL, BPB, 2002

Practical 160

Practical based on Biological databases
How to design a basic data structure for developing a database using SQL
How design and develop a model biological database with the help of SQL
How to perform high throughput biological data extraction using Data mining tools

SEMESTER II

MSBB201 - SPECTROSCOPIC METHODS IN STRUCTURAL BIOLOGY

Maximum Marks- 100
Lectures 45

Objective
The students would be exposed to various techniques of spectroscopy such as NMR, MS, IR and Raman along with X-ray diffraction to enable them to understand the importance of these techniques in structure elucidation of biomolecules.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I

NMR Spectroscopy: Basic concepts of NMR, theoretical treatment, chemical shift, coupling constant, instrumentation, FT, FFT. Modern techniques for structure elucidation, nuclear
overhauser effect, basic 2D spectroscopy, benefits of 2D NMR practical details of general 2D experiments (COSY, NOESY) ligand binding to macromolecules, molecular recognition, chemical exchange, \(^{13}\text{C}, \(^{19}\text{F}, \)^{31}\text{P} \) NMR spectroscopy, monitoring of cellular pH. Metabolism detail, compartmentation, pH gradient in tumor cells etc. Fluidity gradient in lipids, anisotropy \(^{31}\text{P} \) of resonance in membranes.

**UNIT II**

**ESR spin–labeling:** Information in ESR spectra, a reporter group technique, requirement of such a group, Nitro oxide, spin label probes and their molecular structures, anisotropy of the value order parameters, information obtained from ESR motion, polarity, biochemical data, orientation Intra-molecular distances etc. Applications of these concepts to (i) study structure and function of enzyme, i.e. lysozyme etc. (ii) conformational change of molecular artifact in trypsin, lipid spin labels in the biological membranes.

**UNIT III**

**Fluorescence:** Fluorescent probes, fluorescence lifetime and quenching studies; & application in proteins and membrane studies. Energy transfer for distance measurements in proteins & membranes. Fluorescence Dye-nucleic acid complexes.

**Circular Dichroism (CD), ORD:** Relationship between moral ellipticity of CD, comparison of CD and absorption spectra. Conformational dependence of CD helical structure, coupling between chromophore etc. Secondary and tertiary structures of peptides \(^{x} \) and proteins, effect of pH, temperature, organic solvents and neutral salts.

**Mass Spectroscopy:** Basic principles, analysis of amino acid sequence of peptides and proteins.

**UNIT IV**

**IR and Raman Spectroscopy:** Introduction to spectroscopy, principle, theory, instrumentation, vibrational modes and influencing factors, comparison of IR and Raman spectroscopy, Resonance Raman spectroscopy. Application in qualitative analysis with special emphasis on: peptide backbone conformation and microenvironment of protein side chains, peptide bond vibrations, conformation (\( \alpha \): helix, \( \beta \)-sheet, \( \beta \)-turns, random coils), Quantitative estimation of the structure from the amide I, II, III band intensity in ribonuclease A, lysozyme, IgG, poly L-Lys etc; Proteins containing disulphide links.

**X-Ray diffraction spectroscopy:** Basic principles crystallographic study of biomacromolecules (various steps), various electron density maps. Time-resolved X-ray crystallography, structural database.

**Reference Books:**

**Additional Reference Books:**
Practical

1. Demonstration of structure determination techniques like X-Ray crystallography.
2. Demonstration of structure elucidation of organic compounds & conformational analysis with NMR spectroscopy.
3. Demonstration of Fluorescent microscopy techniques.
4. Demonstration of how to study CD spectra data and their interpretation.
5. Demonstration of how to study IR spectra data, their interpretation and applications in molecular recognition.

MSBB202 – GENOMICS AND RECOMBINANT DNA TECHNOLOGY

Maximum Marks- 100
Lectures 45

Objective
The course covers the mechanism of DNA replication and repair in prokaryotes and eukaryotes along with various techniques and application of recombinant DNA technology.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I

Prokaryotic and Eukaryotic DNA replication- Polymerases, Telomeras, and Fidelity of replication; Mutation-Chemical mutagenesis and carcinogens; Recombination- mechanism, transposons; Repair- direct reversal of damage, nucleotide excision repair, SOS response and recombination repair. Control of prokaryotic and Eukaryotic gene expression.

UNIT II

Recombinant DNA technology- Restriction endonucleases, Chemical synthesis, sequencing and amplification of DNA. Plasmid cloning vectors, creating and screening a library, cloning DNA sequences that encode eukaryotic proteins, vectors for cloning large pieces of DNA, genetic transformation of prokaryotes, directed mutagenesis.

UNIT III

Genetic engineering of plants and animals-Methodology, applications, plants as bioreactors. Transgenic animals-methodology, applications, Knock-out animals, conditional control of gene expressions. Introduction of CRISPR-Cas systems for editing, regulating and targeting genomes.

UNIT IV

Molecular diagnostics of genetic disease (immunological, DNA), Therapeutic agents (Pharmaceutical-Interferons, Human growth hormones, TNF-α; Enzymes-DNAasel, α-Antitrypsin; Nucleic acids- Ribozymes, Chimeric RNA-DNA molecules), Vaccines (Subunit, attenuated and vector).
Reference Books:

Practical 220
1. Insilico Restriction map analysis
2. Study of various tools for nucleic acid sequence analysis and manipulation
3. Insilicoanalysis of cloning vectors generated.

MSBB203- COMPUTATIONAL METHODS OF SEQUENCE ANALYSIS AND BIOMACROMOLECULAR INFORMATICS

Maximum Marks- 100
Lectures 45

Objective
The students would be exposed to the basics concepts and methods of pair-wise, multiple sequence alignment along with molecular phylogenetics and gene, promoter prediction.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Pair Sequence alignment: Scoring matrices, PAM, BLOSUM, Local and global alignment concept, Dot matrix, sequence comparison, Dynamic programming, Needleman-Wunch algorithm, Smith-Waterman algorithm, statistics of alignment score.

UNIT II
Multiple sequence alignment: Scoring MSA, CLUSTALW, PILEUP, iterative methods of MSA, Data base searches for homologous sequences FASTA and BLAST, PSSM searching, HMM, PSI-BLAST and PHI-BLAST. Protein motifs and domain predication.

UNIT III
Molecular Phylogenetics: Evolutionary analysis relationship of phylogenetic analysis to sequence alignment genome complexity, concept of evolutionary trees, methods-maximum parsimony
method, distance methods, the maximum likelihood approach, sequence alignment based on evolutionary model, reliability of phylogenetic prediction, complications from phylogenetic analysis.

UNIT IV
MATLAB: Introduction, variables and Commands, Visualization with vectors and matrices, array operations, importing files, simple and multiple plots, basic fitting methods, built-in-function, writing functions, Statistical functions.

Reference Books: -

Additional Reference Books: -

Practical 230
1. Perform DOT BLOT analysis using MB DNA Analysis.
2. Perform Pair Sequence alignment using various types of BLAST and FASTA tools.
3. Perform multiple sequence alignment tools provided by NCBI and EBI.
4. Perform Phylogenetic analysis using CLUSTALW, PILEUP.
5. Matlab: Simple and Multiple plots
6. Basic Fitting methods
7. Statistical functions

MSBB204 -PROGRAMMING IN C++ and PERL

Maximum Marks- 100
Lectures 45

Objective
The objective of the course is to make students aware of the programming capabilities of C++ and Perl and enable them to understand and write programs in bioinformatics domain.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The
students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Basics of programming, algorithms, flowcharts, computer hardware, system software, application software, programming languages. An overview of procedure oriented and object oriented paradigm, their characteristics, concept of classes, objects, encapsulation, abstraction, inheritance, overloading, polymorphism.

UNIT II
Programming in C++: program development life cycle, building blocks of C++, identifiers, keywords, data types, operators, library functions, handling input and output, control statements: decision making statements, looping statements, jumping statements, arrays, functions, strings, recursion, pointers, dynamic memory management.

UNIT III
Programming in C++: Classes, objects, access specifiers, member functions, static members, friends of a class, constructors, destructors, operator overloading, type conversion, inheritance, polymorphism, virtual functions, exception handling, file handling.

UNIT IV
Perl: Basic syntax, I/O, variables, operators, control structures, regular expressions-pattern matching, file handling, subroutines, packages and modules, object-oriented Perl, CGI and Perl: static and dynamic pages, Perl and relational databases.

Reference Books:

Practical 240
1. Writing programs to understand and demonstrate the utility of following: control statements:
   - if, switch, while, do-while, for loop
2. Writing programs to understand and demonstrate the utility of following concepts:
   - Functions, Recursion, Arrays, Pointers, Structures
3. Writing programs to understand and demonstrate the utility of following object oriented concepts:
   - Classes and objects, encapsulation, abstraction, inheritance and its types, polymorphism and its types etc.
4. Writing programs to understand and demonstrate various data types and control statements in Perl
5. Writing programs to understand and demonstrate regular expressions and various pattern matching features of Perl
6. Reading and writing files using C++ and Perl constructs.
SEMESTER III
MSBB301 - COMPUTATION CELL BIOLOGY – I

Maximum Marks- 100
Lectures 45-50

Objective
This course of Computational cell biology aims to apply the mathematics of dynamical
systems with computer simulation techniques to study of various cellular transporters,
pumps and whole cell models.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3
hours. The question paper will have nine questions. The first question of 20 marks would be
compulsory having sub-parts covering the entire syllabus in the form of short and objective type
questions. Out of the remaining eight questions, two questions of 15 marks each and having at least
two parts would be set from each of the four units in which the syllabus has been divided. The
students would have to attempt one question from each unit, thus attempting five questions in all
including the compulsory question.

UNIT I
mechanisms- active and passive, facilitated diffusion. Channels and transporters- Glucose transporter
of erythrocytes, ABC-transporters, Aquaporins, Potassium channel, Sodium channel, Acetylcholine
receptor.

UNIT II
Dynamic Phenomena in Cells: Scope of Cellular Dynamics, Computational Modeling in Biology,
The role of Mathematics, Simple Molecular Switch, Introduction to Numerical Packages
Voltage Gated Ionic Currents: The Nernst Potential, The Resting Membrane Potential; The
Membrane Model- Equations for Membrane Electrical Behavior; Activation and Inactivation Gates-
Models of Voltage -Dependent Gating, The Voltage Clamp; Interacting Ion Channels-The Morris –
Lecar Model, Phase Plane and Stability Analysis, Oscillations, Type1 and Type II Spiking, Hodgkin-
Huxley Model.

UNIT III
Transporters and pumps: Passive transport; Transporter rates- Diagrammatic method, Rate of
Fast and Slow Time Scales: The Rapid Equilibrium Approximation, Asymptotic Analysis of Time
Scales, Glucose Dependent Insulin Secretion, Ligand Gated Channels, The Neuromuscular Junction,
The Inositol Triphosphate (IP3) receptor.

UNIT IV
Whole –Cell Models: Models of ER and PM Calcium Handling- Flux Balance Equations with Rapid
Buffering, Expressions for the Fluxes; Calcium Oscillations in the Bullfrog Sympathetic Ganglion
Neuron- Ryanodine Receptor Kinetics: The Keizer –Levine Model, Bullfrog Sympathetic Ganglion
Neuron Closed- Cell Model, Bullfrog Sympathetic Ganglion Neuron Open- Cell Model; The
Pituitary Gonadotroph- The ER Oscillator in a Closed Cell, Open -Cell Model with Constant
Calcium Influx, The Plasma Membrane Oscillator, Bursting Driven by ER in the Full Model; The
Pancreatic Beta Cell- Chay-Keizer Model, Chay –Keizer with an ER.
Reference Books-

Practical 310

1. To perform time course analysis using Copasi.
2. To perform the following using V-cell:-
   a. Creating reaction diagram of a bio model.
   b. Creating geometry for an image file.
   c. Structure making of a cell.
   d. Spatial analytical geometry using FRAP.
   e. Analysis of simulation results of concentration vs time plot.

MSBB302- SYSTEMS BIOLOGY

Maximum Marks- 100
Lectures 45-50

Objective
This course deals with introduction to the various ‘omics’ fields and DNA microarray technology. Further human genomics, gene therapy, mRNA and protein synthesis and engineering would be covered for better understanding of relation between genomics, transcriptomics and proteomics.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Microarrays-Basic Concepts: Concept of gene expression, Comparative Genomics; Making Microarrays-Spotted Microarrays, In situ synthesized oligonucleotide arrays; Affymetrix Technology, Inkjet array synthesis, Using Microarrays, Sample preparation and labeling, Hybridization, Washing, Image Acquisition, Computer design of oligonucleotide probes.

UNIT II
Microarray Image Processing: Image Formats, Feature Extraction, Normalisation, Measuring and Quantifying Microarray Variability-Analysis of Differentially Expressed Genes, Experiments using SMD/GEO.
Use of EST database-Unigene, Primer design, Restriction mapping, SNP database.

UNIT III

**Human Molecular genetics:** Genetic mapping of human chromosomes, detection of mutations in human genes, determining gene function, human gene therapy, pro-drug activation therapy.

UNIT IV

**Proteomics and the Proteome:** RNA synthesis and splicing, Protein synthesis, Protein Engineering; Protein traffic in cells: Protein sorting and signal sequences and their study using bioinformatics tools.

Reference Books-

Practical 320
1. To study the Microarray Databases.
2. Interpretation of results of SMD and their applications
3. To study the EST databases.
4. To study the SNP databases.
5. To study REBASE –the restriction enzyme database.

MSBB303- PROTEOMICS AND SYSTEMS BIOLOGY

Maximum Marks- 100
Lectures 45-50

Objective

*The course covers protein secondary and tertiary structure prediction and RNA structure prediction. Techniques for high throughput study of proteome expression, function, mining, protein-protein interaction and protein network mapping would also be covered.*

Instructions for paper setters

The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The
students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I

Protein structural Informatics: Protein structure visualization, comparison and classification, Secondary structure prediction methods: GOR, PHD, PSIPRED. Protein tertiary structure prediction, Fold recognition and threading, Homology modeling, Ab initio prediction of protein structure.

UNIT II

Gene and promoter prediction: Gene prediction in prokaryotic genomes, Gene prediction in eukaryotes, evaluation of gene prediction methods, promoter prediction in E.coli, and promoter prediction in eukaryotes.
RNA structure prediction using thermodynamic parameters and partition function, Online prediction tools.

UNIT III

Investigation of Proteome expression and function: 2-D gel electrophoresis, High throughput protein Crystallography, activity based probe, nonsense suppression mutagenesis and applications of these techniques. Protein chip: Introduction of protein chip, how to design, comparison of antibody and protein chips, protein delivery system, probe detection methods, functional class of protein chips, other analytical chips, Application of protein chips activity based probe, nonsense suppression mutagenesis.

UNIT IV

Applications of Proteomics: Mining proteomes, multidimensional peptide chromatography and LC-Tandem MS analysis, LC-MS and isotope tags; identifying protein-protein interactions and protein complexes by MS analysis, immunoprecipitations, bait and reverse bait, multiprotein-nucleic acid complexes, protein network mapping; mapping protein modifications from MS data, Integrating sequest and SALSA; new directions in Proteomics, micro and nanoscale instrumentation.

Reference Books-

Practical 330
1. Secondary structure prediction using GOR, PSIPRED, PHD.
2. To perform comparative gene prediction using various tools.
3. To study the RNA structure prediction softwares.
4. To study RNA databases- mirBase.
**Objective**
The students would be exposed to the concepts, algorithms and drug design techniques, with focal points being modeling and analysis of protein ligand complexes by database searching, docking, de novo design; quantitative assessment of binding interaction in terms of free energy calculation and scoring functions and the development of pharmacophores and analog design.

**Instructions for paper setters**
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

**UNIT I**
**Introduction to Molecular Modeling:** Types of models, Coordinate systems: Cartesian Coordinates & Internal Coordinates, Potential energy surface. Molecular Graphics Surfaces - vdw, molecular surface, accessible surface, Areas of application. Drawbacks of mechanical models as compared to graphical models.

**Molecular Mechanics:** The molecular potential energy function, Force field: The empirical force field, Sources of force field data, examples of important force fields.

**UNIT II**
**Energy Minimization:** First derivative techniques: steepest descent and conjugate gradients, Second derivative techniques: Hessian matrix and Newton-Raphson, Global optimization (simulated annealing, Tabu search, genetic algorithms).

**Molecular Dynamics:** Introduction, Molecular Dynamics using simple models. Dynamics with continuous potentials. Constant temperature and constant dynamics. Conformation searching, Systematic search.

**UNIT III**
**Conformational Analysis:** Systematic methods, Random search methods, Distance geometry.

**Solvation:** Brief comparison of different solvation methods, Periodic boundary conditions.

**Analog Based Drug Design:** Introduction to QSAR, lead module, linear and nonlinear modeled equations, biological activities, physicochemical parameter and molecular descriptors, molecular modeling in drug discovery.

**UNIT IV**
**Structure Based Drug Design:** 3D pharmacophores, molecular docking, De novo Ligand design, Free energies and solvation, electrostatic and non-electrostatic contribution to free energies.
Further Applications on the Design of New Molecules: 3D data base searching and virtual screening. Sources of data, molecular similarity and similarity searching, combinatorial libraries – generation and utility.

Reference Books-

Practical 340
1. Perform molecular mechanism method using online force field softwares.
2. Perform Conformational Analysis studies.
3. Perform Analog Based Drug Design.
4. Perform Structure Based Drug Design.
5. Perform molecular docking using FlexX.

SEMESTER IV
MSBB401 - COMPUTATION CELL BIOLOGY – II

Maximum Marks- 100
Lectures 45-50

Objective
MATLAB and Bioinformatics (Toolbox) provides an integrated software environment for genome and proteome analysis. It also gives scientists / engineers a set of computational tools to solve problems and build applications in drug discovery, genetic engineering, and biological research along with topics from proteomics covering specific examples.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Overview of probability and distribution concepts, Stochastic Process: Introduction and specification of stochastic process. Markov chains, transition probability and transition probability matrix; Markov Chains with absorbing states and with no absorbing states.
UNIT II
Analysis of one DNA Sequence – Shotgun Sequencing, Modeling DNA, Long Repeats, r-Scan and Analysis of Patterns. Analysis of Multiple DNA or Protein Sequences – Two Sequences: Frequency Comparisons, Testing Similarity in Alignments, Protein Sequences and Substitution Matrices, BLOSUM and PAM Substitution Matrices (using MATLAB only).

UNIT III

UNIT IV

Reference Books-
4. MATLAB package. 1999

MSBB402- CHEMoinFORMATICS

Maximum Marks- 100
Lectures 45-50

Objective
Chemoinformatics has a wide application in the field of chemical sciences and drug design. The students would be taught computer representation of chemical structures, deriving 3-D pharmacophores, molecular descriptors, database searching using similarity principles, virtual screening and toxicity modeling.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Computer representation of 2 D & 3 D chemical structures: Graph theoretic representation, canonical representation, Connection tables and Linear Notation, SMILES coding; Structure and substructure searching, algorithms for sub-graph isomorphism, practical aspects of substructure searching
UNIT II
3D Pharmacophores and databases, Experimental 3D databases, Implementation of 3D databases searching, Methods to derive 3D pharmacophores, pharmacophore mapping using constrained systematic, clique, maximum likelihood and genetic algorithm methods. Theoretical 3D databases, structure generation programs, conformational search analysis, comparison and evaluation of search methods, Applications of 3D pharmacophore mapping, Novel use of databases such as PDTD.

UNIT III
Molecular descriptors, Descriptor calculated from the 2D and 3D structure, Data verification and manipulation. Computer models: Deriving a QSAR Equation, Designing a QSAR Experiment and similarity methods: similarity based on 2D finger printing, Similarity Coefficients, 3D similarity; Selecting compounds: cluster analysis and Analysis of High throughput screening data.

UNIT IV

Reference Books-

MSBB403- ADVANCE BIOINFORMATICS AND NANOTECHNOLOGY

Maximum Marks- 100
Lectures 45-50

Objective
The students would be exposed to specialized bioinformatics softwares and tools for studying structural and functional genomics and proteomics. The building blocks of systems biology models/circuits and nanotechnology in terms of tools and application would be covered.

Instructions for paper setters
The maximum marks of the end semester examination would be 80 and duration of the paper 3 hours. The question paper will have nine questions. The first question of 20 marks would be compulsory having sub-parts covering the entire syllabus in the form of short and objective type questions. Out of the remaining eight questions, two questions of 15 marks each and having at least two parts would be set from each of the four units in which the syllabus has been divided. The students would have to attempt one question from each unit, thus attempting five questions in all including the compulsory question.

UNIT I
Advance Bioinformatics: Genome mapping and Assembly programs- Phred, Phrap, EULER, ARACHNE, Genome Annotation-GeneQuiz, genome economy, Whole Genome Alignment- MUMmer, MAVID, Studying proteomics using Mascot, PSORT, InterPreTS, ADVICE. Proteome expression analysis using bioinformatics tools- Melanine, Analysis of PTM, protein sorting.
UNIT II


UNIT III

Introduction to Nanoscience and Nanotechnology: Advent of the nanomaterial, top down and bottom up approaches to building materials. Properties of nanomaterial - Chemical, mechanical, thermal, electrical and optical. Carbon nanotubes- properties, types, applications and defects. Tools for measuring and making nanostructures.

UNIT IV


Reference Books-

4) Introduction to Bioinformatics by A.M. Lesk. OUP India 2005.