FACULTY OF SCIENCE

SYLLABI

FOR

M.Sc. SYSTEM BIOLOGY AND BIOINFORMATICS
(SEMESTER SYSTEM)

1ST TO 4TH SEMESTER

EXAMINATIONS 2011 - 2012

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# M.Sc. System Biology and Bioinformatics

**For the Academic Session 2011-2012**

**Duration:** IV Semesters

## Semester I

<table>
<thead>
<tr>
<th>Paper Code</th>
<th>Paper</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSBB101</td>
<td>Biophysical Chemistry of Biomacromolecules</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB102</td>
<td>Metabolomes and Metabolic Pathway Engineering</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB103</td>
<td>Biomathematics and Biostatistics</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB104</td>
<td>Data Management, Data Mining and Biological and Structural 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>
<td>Practical 130</td>
<td>Based on MSBB103</td>
<td>25*</td>
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<tr>
<td>Practical 140</td>
<td>Based on MSBB104</td>
<td>25*</td>
</tr>
<tr>
<td>Seminar</td>
<td>(i) Experimental Techniques (ii) Immunology</td>
<td>50+50=100</td>
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**Total:** 600

*Internal Assessment based on house tests = 20; End Semester theory examination = 80

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

## Semester II

<table>
<thead>
<tr>
<th>Paper Code</th>
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<tbody>
<tr>
<td>MSBB201</td>
<td>Spectroscopic Methods in Structural Biology</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB202</td>
<td>Genomics and recombinant DNA technology</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB203</td>
<td>Computational Methods of Sequence Analysis and Biomacromolecular informatics</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB204</td>
<td>Computer programming in C, C++, BioPerl and Java</td>
<td>100*</td>
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<tr>
<td>Practical 210</td>
<td>Based on MSBB201</td>
<td>25*</td>
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<tr>
<td>Practical 220</td>
<td>Based on MSBB202</td>
<td>25*</td>
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<tr>
<td>Practical 230</td>
<td>Based on MSBB203</td>
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<tr>
<td>Practical 240</td>
<td>Based on MSBB204</td>
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<tr>
<td>Seminar</td>
<td>(i) (a) Data bases and Bioinformatics tools on the internet (b) Modeling tools-Visualization and genome matrix (c) Solving of structures using different softwares (ii) Journal club</td>
<td>50+50=100</td>
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**Total:** 600

*Internal Assessment based on house tests = 20; End Semester theory examination = 80

# Internal Assessment = 5; End Semester Practical examination = 20
### SEMESTER III

<table>
<thead>
<tr>
<th>PAPER CODE</th>
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<tr>
<td>MSBB301</td>
<td>Computation Cell Biology I</td>
<td>100*</td>
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<tr>
<td>MSBB302</td>
<td>System Biology</td>
<td>100*</td>
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<tr>
<td>MSBB303</td>
<td>Proteomics and System Biology</td>
<td>100*</td>
</tr>
<tr>
<td>MSBB304</td>
<td>Molecular Modeling and Computer aided Drug Design</td>
<td>100*</td>
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<tr>
<td>Practical 310</td>
<td>Based on MSBB301</td>
<td>25#</td>
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<td>Practical 320</td>
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<td>Practical 330</td>
<td>Based on MSBB303</td>
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<tr>
<td>Practical 340</td>
<td>Based on MSBB304</td>
<td>25#</td>
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<tr>
<td>Seminar</td>
<td>On (i) (a) AMBER &amp; Molecular dynamics</td>
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<td></td>
<td>(b) E-cell</td>
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<td></td>
<td>(c) Py Bio-S</td>
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<tr>
<td></td>
<td>(d) System Biology benchworks</td>
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<tr>
<td></td>
<td>(ii) Journal Club</td>
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<td></td>
<td><strong>TOTAL</strong></td>
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</table>

*Internal Assessment based on house tests = 20, End Semester theory examination = 80
#Internal Assessment = 5, End Semester Practical examination = 60

### SEMESTER IV

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<tr>
<th>PAPER CODE</th>
<th>PAPER</th>
<th>MARKS</th>
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</thead>
<tbody>
<tr>
<td>MSBB401</td>
<td>Computation Cell Biology II</td>
<td>100*</td>
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<tr>
<td>MSBB402</td>
<td>Chemoinformatics</td>
<td>100*</td>
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<tr>
<td>MSBB403</td>
<td>Advance Bioinformatics and Nanotechnology</td>
<td>100*</td>
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<tr>
<td></td>
<td>Project work and Oral Presentation</td>
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<tr>
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</table>

*Internal Assessment based on house tests = 20, End Semester theory examination = 80
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
Conformational analysis and forces that determine protein structure: Basic problems of protein structure, Polypeptide chain geometries, estimates of potential energy, results of potential energy calculations, hydrogen bonding, hydrophobic interactions and water as universal solvent in biological systems. Disruption of hydrophobic interactions by urea, ionic interactions, hydrophobic versus ionic interactions, disulfide bonds. Ways of Pairing N-half cystines, formation of specific disulfide links, prediction of protein structure.


UNIT II
Conformational stability: 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, Chargaffe’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 chemoglycomic approaches; Glycochip.

UNIT IV
Molecular distribution and statistical thermodynamics: Binding of small molecules by polymer, identical and independent sites model, nearest interaction and statistical weight* cooperative binding, anti-cooperative binding and excluded side binding. The random walk, Helix coil transitions in proteins, statistical thermodynamics. Organizational levels of biomacromolecule structure.


References books: -

Additional Reference Books:-

Practical 110

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. Carbohydrate and lipid databases: GlycosuitDB, PDB2linucs, LIPIDAT.
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 reaction, 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
Overview of major metabolic pathways- Glycolysis, Kreb’s cycle, oxidative phosphorylation, Amino Acid, Fatty Acid and Nucleotide metabolism, their control and integration.

UNIT II
Enzymes and Enzyme kinetics: Activation energy and reaction coordinate, catalytic mechanisms, Basic equations of enzyme kinetics: steady state kinetics, significance of Michaelis-Menten parameters, graphical representation of data, inhibition, non-productive binding, $K_{cat}/K_m$, compelling substrates, Reversibility, Haldane equation, Breakdown of Michaelis-Menten equation, Multi-substrate systems.
Conformational change, allosteric regulation: positive cooperativity, mechanisms of allosteric interactions and cooperativity, negative cooperativity and half-of the site reactivity, Quantitative analysis of cooperativity (Hill’s equation), Molecular mechanism of cooperative binding to hemoglobin, regulation of metabolic pathways, control of enzymes: phosphokinase and glycogen phosphorylase.
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.

UNIT III

UNIT IV
Metabolic networks. Applications: Identifying biomarkers and therapeutic targets in CNS, Targeted drug design.

References books:

Practical 120
1. To study the services provided by KEGG and Glycolytic pathway.
2. To study services provided by KEGG LIGAND databases.
3. To study computational tools provided by ligand databases.
4. To study motif search for E.coli trp A.
5. To study Eco Cyc (Encyclopedia of E. coli) k-12 MG 1655 genes and metabolism.
6. To study services provides by Meta Cyc and TCA Cycle.
7. To carry out the query retrieval using Meta Cyc.
8. To study the services and resources provided by EMP.
9. To carry out query retrieval using BRENDA.

MSBB103 - BIOMATHEMATICS AND BIOSTATISTICS

Maximum Marks- 100
Lectures 45

Objective
To introduce students to learn and apply the basic concepts of Biomathematics and 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
Co-ordinate Geometry: Line, circle, parabola, hyperbola and sphere
Function: Definition, domain, range, classification, graphs of functions, sum, difference, products, quotients and composition of functions, some standard functions
Calculus: Limits, Continuity, Differentiability, and basic concepts of integration.
Vector Differential: Level surfaces, parametric representation of curves and surfaces, limit, continuity and differentiability of vector functions, gradient of a scalar field, directional derivative, divergence and curl of a vector field
UNIT-II
Matrices: Definition, addition, subtraction, multiplication, transpose, determinant and inverse of a matrix, solutions of simultaneous equations.
Differential Equation: Introduction to ordinary and partial differential equation
Numerical methods: Curve fitting and interpolation

UNIT-III
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 package).
Probability: Intuitive concept of probability, conditional probability (Bayes’ theorem); Specificity, Sensitivity; relative risk, odds ratio.
Random variables: Discrete and Continuous random variables, probability mass function, probability density function, distribution function, expectation and variance, moment generating and probability generating functions.
Correlation and regression: Scatter diagram, Karl Pearson’s and Spearman’s rank Correlation Coefficient, Simple and multiple regression (using SPSS only).

UNIT-IV
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.
Analysis of variance (ANOVA): one-way and two-way classification, Non-parametric: Sign-test, Wilcoxon Signed rank test, Mann-Whitney U-Statistic (Using SPSS).

References
9) Alan Agreti: Categorical data Analysis, 1990

Practical 130
Practicals will be based on Topics of Biostatistics, using SPSS/STATISTICA Softwares.
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
Introduction: Characteristics of Data base approach, Database users, Intended uses of databases, Implication of database approach. Data warehousing and data capture-type and kinds of databases e.g. PUBMED and MEDLINE. Database system concepts and architecture, Data Models, Schemas bad instances, DBMS, Architecture and data independence, database languages, and classification of DBMS.

UNIT II
Database Design: Informal design guidelines for relation Schemas, Functional dependencies, normal forms based on primary keys, general definition of 2\textsuperscript{nd} and 3\textsuperscript{rd} normal forms, BCNF, need of further normalization.

Data modeling using ER diagram, ER model concepts, notation for ER diagrams. The relational model, relational model concepts, relational model constraints, introduction to relational algebra.

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.

UNIT IV
Introduction to Biological databases:

References books:
2) Jiawei Han, Micheline Kamber, Data Mining Concepts and Techniques. Morgan Kaufmann Publisher, 2001.

**Practical 140**

Practical based on Biological databases and Data mining.
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, the information in NMR, Modern techniques for structure elucidation. FT and FFT. Nuclear Overhauser effect. Basic 2D spectroscopy, benefits of 2D NMR, Practical details of general 2D experiments (COSY, NOESY). Ligand binding to macromolecules, chemical exchange $^{31}$P NMR spectroscopy, monitoring of cellular pH. Metabolism detail, compartmentation, pH gradient in tumor cells etc. Fluidity gradient in lipids, anisotropy $^{31}$P of resonance in membranes.

UNIT II
ESR spin–labelling: 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 Intramolecular 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


Mass Spectroscopy: Basic principles, analysis of amino acid sequence of peptides.
UNIT IV
**IR and Raman Spectroscopy:** Introduction, comparison of IR and Raman spectroscopy, peptide backbone conformation and microenvironment of protein side chains, peptide bond vibrations, conformation (α: helix, β-sheet, β- 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; Resonance Raman spectroscopy.

**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 210**
1. Demonstration of structure determination techniques like X-Ray crystallography & NMR.
2. Demonstration of Fluorescent microscopy techniques.
3. Demonstration of how to study CD spectra data and their interpretation.
4. Demonstration of how to study IR spectra data and their interpretation.
5. Demonstration of how to study X-Ray diffraction data and their interpretation.

**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, Telomerase, 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. Chemical synthesis, sequencing and amplification of DNA.

UNIT II

Recombinant DNA technology- Restriction endonucleases, 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 prokaryotics, directed mutagenesis.

UNIT III

Genetic engineering of plants and animals - Methodology, applications, plants as bioreactors. Transgenic animals-methodology, applications, Knock-out animals, transgenic models for Alzheimer’s disease and conditional control of gene expressions and cell death.

UNIT IV


Reference Books: -

Practical 220

1. Designing PCR primers insilico.
2. insilico Restriction map analysis
3. Study of various tools for nucleic acid sequence analysis and manipulation
4. insilico analysis of cloning vectors generated.
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 prediction.

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
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.

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. Perform Gene prediction using tools provided by EBI.

MSBB204 - COMPUTER PROGRAMMING IN C, C++ & BIOPERL

Objective
The students would be covering programming languages C, C++ and Bioperl for better understanding and application to bioinformatics algorithms/programs.

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
Principles of Computing, Computer hardware, system software, and Applications software.

UNIT II

UNIT III

UNIT IV

Reference Books:
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
Fundamentals of cell biology: Membrane structure and introduction to different types of channels and transport mechanisms. Mathematical biology (dynamical systems, phase plane, elementary bifurcations)


Theories of Protein Folding

UNIT II

UNIT III

**UNIT IV**


**Reference Books-**

**Practical 310**
1. Demonstration of Computational modeling showing functionality of the mammalian cells.
2. Demonstration of E-cell.
3. Demonstration of Neuron cell model.

**MSBB302- SYSTEM 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

Introduction: To understand the gradual maturation of Genomics and Proteomics into Biology *insilico*. Convergence of Genomics, Proteomics, Transcriptomics and Metabolomics into Phenomics.

**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 MAGIC.

**Creative Bioinformatics:** Novel use of databases such as PDTD, Pharmacophore building, use of EST database-Unigene, Primer design, Restriction mapping, SAGE, SNP database, Target identification, Epitope identification.

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 and SNP databases.
4. To study PDTD and TarFishDocking and their importance in disease.
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
Proteome Informatics I: Proteomics and the New Biology, Protein structure visualization, comparison and classification, Secondary structure prediction methods: First, second, third and fourth generation methods like FASMAN, GOR, LIM, PHD, PSIPRED, JPRED, SOPM. Neural network models, nearest neighbor methods, Hidden Markov model.

UNIT II
Proteome Informatics II: Protein tertiary structure prediction, 3-D structure modeling, sequence similarity and alignment, structure similarity and overlap, Fold recognition and threading, Homology modeling, Ab initio prediction of protein structure, solvation, on-line protein structure prediction, protein-protein interactions. RNA structure prediction.

UNIT III
Investigation of Proteome expression and function: 2-D gel electrophoresis, Proteome analysis by MS, Analysis of posttranslational modifications by MS, High throughput protein Crystallography, protein-protein interactions by two-hybrids assay, protein chip, activity based probe, nonsense suppression mutagenesis.

UNIT IV
Applications of Proteomics: Mining proteomes, 2D-SDS-PAGE and MALDI-TOF-MS, multidimensional peptide chromatography and LC-Tandem MS analysis; compararive proteomics with 2D gels, 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, Protein Arrays/protein chips.

Reference Books-

Practical 330

1. Protein structure visualization using Rasmol and its features.
2. Protein structure visualization using Cn3D and its features.
3. To study the importance of VAST tool.
4. Secondary structure prediction using GOR and PSIPRED
5. To study the RNA structure prediction softwares.

MSBB304- MOLECULAR MODELING AND COMPUTER AIDED DRUG DESIGN

Maximum Marks- 100
Lectures 45-50

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 Modelling: Introduction to Molecular Modelling. What are models used for? Areas of application – Single molecule calculation, assemblies of molecules. Reaction of the molecules. Drawbacks of mechanical models as compared to graphical models. Co-ordinate systems Two Matrix, potential Energy surface.

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

UNIT II
**Molecular Dynamics:** Introduction, Molecular Dynamics using simple models. Dynamics with continuous potentials. Constant temperature and constant dynamics. Conformation searching, Systematic search. Applications to protein folding.

**UNIT III**

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

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

**UNIT IV**

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

**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.
OBJECTIVE

Introduction to Stochastic Processes, analysis of DNA or Protein Sequences will help the students 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


UNIT II

Analysis of one DNA Sequence – Shotgun Sequencing, Modeling DNA, Long Repeats, r-Scans 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.

UNIT III

Protein-protein Interaction networks-----Protein chip technology, String and Bind databases


UNIT IV

Structures of protein complexes-- GroEL/ES complexes and subcellular structures (location proteomics) and biomolecular association and binding.

REFERENCE BOOKS-
4. MATLAB package.
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 2D & 3D chemical structures: Graph theoretic representation, canonical representation, Connection tables and Linear Notation, SMILES coding; Structure and substructure searching.

UNIT II
3D Pharmacophores and databases, Experimental 3D databases, Implementation of 3D databases searching, Methods to derive 3D pharmacophores, Theoretical 3D databases, Applications.

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-
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: Euler, ARACHNE, GeneQuiz, Phred, Phrap, MUMmer, ProSplicer, MAVID, Swaap for Genome assembly, annotations & comparison. Studying proteomics using Mascot, SVM, PSORT, InterPreTS, ADVICE. Concepts of Systems and Synthetic Biology, Properties of models- Robustness, Redundancy, Control, Modular Design, Model development and Assignment, system state, steady states, variables, parameters & constants.

UNIT II


UNIT III

Introduction to Nanoscience and Nanotechnology: Underlying physical principles of 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.

UNIT IV

The basic tools of nanotechnology: Tools for measuring and making nanostructures -Scanning probe microscopy and near-field optics; electron and ion-based microscopy and manipulation; Molecular synthesis, polymerization etc. Nanoscale biostructures Overview of self-assembly and its potential applications, self healing, smart materials, biosensors etc. Biomedical applications. Societal Aspects of Nanotechnology: Regulations, Implications on health and environment.

Reference Books-

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