## M. Tech. Bioinformatics Semester III

| S. No. | Subject code | Subject | Credits | Periods | | | Evaluation Scheme | | | | Subject Total |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Theory | | L | T | P | CT | TA | Total | ESE | |
| 1 | MTBI 301 | Computer Aided Drug Design | 4 | 3 | 1 | 0 | 30 | 20 | 50 | 100 | 150 |
| 2 | MTBI 302 | Elective I | 4 | 3 | 1 | 0 | 30 | 20 | 50 | 100 | 150 |
| 3 | MTBI 303 | Elective II | 4 | 3 | 1 | 0 | 30 | 20 | 50 | 100 | 150 |
| 4 | MTBI 304 | Mini Project | 4 | 0 | 0 | 4 | 30 | 20 | 50 | 100 | 150 |
| 5 | MTBI 305S | Seminar | 2 | 0 | 0 | 2 | 15 | 10 | 25 | 50 | 75 |
| 6 | MTBI 306P | Computer Aided Drug Design Lab | 2 | 0 | 0 | 2 | 15 | 10 | 25 | 50 | 75 |
| | | Total | 20 | 9 | 3 | 4 | 120 | 80 | 200 | 550 | 750 |

### Elective I

**MTBI 302A: Applied Genomics**

**MTBI 302B: Protein Informatics**

### Elective II

**MTBI 303A: Computational and System Biology**

**MTBI 303B: Chemoinformatics and Pharmacogenomics**

### MTBI 301

**COMPUTER AIDED DRUG DESIGN**

w.e.f. Session 2014-15

| L | T | P |
|---|---|---|
| 3 | 1 | 0 |

**Unit 1:** **[8]**

Drug Discovery Pipeline: Strategies to identify possible drug targets, Validation and Druggability of targets, Discovery of Lead compounds, Optimization of Lead compounds to Candidate drugs, Clinical Trials and its applications.

**Unit 2:** **[8]**

Potential Drug Targets: Family of G-Protein Coupled receptors (GPCRs), Ion Channels: Molecular structure and significance; Aquaporins as Drug Targets, DNA as anti-cancer targets.

**Unit 3:** **[8]**

Structure based Drug Design: Molecular Docking- principles and concepts, Representation of molecules, Searching and Scoring of potential solutions, Special aspects of docking: protein flexibility and water molecules. Common Docking programs: AUTODOCK, GOLD.

**Unit 4:** **[8]**

Ligand based Drug Design: Quantitative Structure Activity Relationship (QSAR) – principles and concepts, Statistical Methods used in QSAR analyses, Pharmacophore Modeling: Criteria for satisfactory pharmacophore model, Basics of Hip Hop and Hypogen Model, Applications of pharamacophore model.

**Unit 5:** **[8]**

Pharmacokinetic analyses of Drugs: Quantitative Structure Property Relationship (QSPR) studies – important parameters and significance, ADME- TOX studies, Concept of Drug-likeliness and its applicability.

**References:**


1. Andrew R.Leach, Molecular Modelling Principles and applications, Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach", Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" Wiley-Liss Publishers.

**APPLIED GENOMICS**

w.e.f. Session 2014-15

| L | T | P |
|---|---|---|
| 3 | 1 | 0 |

**Unit 1:** **[8]**

Definition of genome, Genome Map: Types of Genome maps and their uses, High and low-resolution map, Polymorphic markers: LINEs, SINEs, RFLP, SNP; Types of maps: Cytogenetic map, Linkage map, Transcript map, Physical map.

**Unit 2:** **[8]**

DNA sequencing: Sanger's method and Maxam Gilbert method; Large scale genome sequencing strategies: Shot gun sequencing, Clone contig approach, Brief overview of Human Genome Project (HGP) and Rice Genome Project, OMIM–Online Mendelian Inheritance in man. Comparative Genomics: Purpose and Methods of comparison, Comparison at nucleotide level, breakpoints level, gene cluster level, ontological comparison, phylogenetic comparison; Applications of Comparative Genomics.

**Unit 3:** **[8]**

Structural genomics (SG): Basic principles, approaches for target selection. Functional genomics: application of sequence based and structure-based approaches to assignment of gene functions, e.g. sequence comparison, structure analysis (especially active sites, binding sites) and comparison, pattern identification, etc.; Use of various derived databases in function assignment.

**Unit 4:** **[8]**

Genome Annotation: Structural annotation - Various approaches for gene prediction in the case of prokaryotes and eukaryotes, ORF Finder, GenScan, Prediction of promoter sequences and splice sites, Evaluation of gene prediction methods.

**Unit 5:** **[8]**

Gene Expression and Microarray data Analysis: Exploring the microarray data set, Spatial images of microarray data, Statistics of the microarrays, Scatter plots of microarray data; Clustering gene expression profiles, Principal component analysis (PCA), Self-Organizing Maps (SOM), Bioinformatics tools for Microarray data analyses.

**References:**


1. O'Reilly, "Developing Bioinformatics Computer Skills".
2. Griffiths JF, "An Introduction to Generic Analysis".
3. Hunter L, "Artificial Intelligence & Molecular Biology".
4. Baxevanis AD, "Bioinformatics: A practical Guide to the analysis of genes and proteins".
5. Stephen A., David K, Womble D, "Introduction to Bioinformatics: A Theoretical and Practical Approach".
6. Brown TA, "Gene Cloning and DNA Analysis".

**MTBI 302B**
**PROTEIN INFORMATICS**
w.e.f. Session 2014-15

| L | T | P |
|---|---|---|
| 3 | 1 | 0 |

**Unit 1:** **[8]**
Overview of Amino acids, Secondary, Tertiary and Quaternary structure of proteins, Motifs and Domain, Significance of Leucine zipper and Zing finger, Principles of classification of proteins based on structural features: CATH and SCOP, Structural databases: PDB and MMDB, Concept of Folds and its databases.

**Unit 2:** **[8]**
Introduction to principles and applications of UV-Visible, Fluorescent Spectroscopy, and CD spectroscopy to stereochemistry of proteins and nucleic acids. Basic concepts of NMR, ESR and Mass Spectrometry and their significance in structural biology.

**Unit 3:** **[8]**
Basic applications of Chromatography and Electrophoresis techniques in isolating, separating and purifying protein molecules. X-ray diffraction studies: Principles of X-Ray, the unit cell & space group, Bragg's law; Protein structure Determination by X-ray crystallography.

**Unit 4:** **[8]**
Proteomics: an introduction; Study of transcriptome and proteome; Concept of protein-protein interactions and their databases such as DIP. Tools for analysis of protein protein interactions: PPI server. Protein arrays: basic principles; bioinformatics-based tools for analysis of proteomics data, ExPASy Proteomics server, STRING 9.0.

**Unit 5:** **[8]**
Concepts of Protein Folding and Stability: Hierarchical model, Energy funnel model, Assisted folding using Molecular Chaperons, Levinthal paradox, Simulation and Molecular dynamics stability studies of protein structures.

**References:**


1. K.P.Murphy, Protein structure, stability and folding, Humana press.
2. Arthur M.Lesk, Introduction to protein architechcture, Oxford University Press.
3. A.McPherson, Introduction to Macromolecular Crystallography, John wiley Publications.
4. Carl Branden and John Tooze and Carl Brandon Introduction to Protein Structure, John Garland, Publication Inc.
5. N.Gautham Bioinformatics, Narosa publications. ISBN-13: 9781842653005
6. Vasantha Pattabhai and N.Gautham Biophysics, Narosa Publishers ISBN 1-4020-0218-1.

**MTBI 303A**
**COMPUTATIONAL AND SYSTEM BIOLOGY**
w.e.f. Session 2014-15

| L | T | P |
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| 3 | 1 | 0 |

**Unit 1:** **[8]**
Basic Terminology & Principles – The Biology – Modeling – Properties of Models - Advantages of Computational Modeling - Typical Aspects of Biological Systems and Corresponding Models - Network Versus Elements – Modularity- Robustness and Sensitivity - Data integration – Living Science - The human genome landscape - Genetic regulation and disease – Differential Gene expression & Developmental Biology.

**Unit 2:** **[8]**
Computer-based Information Retrieval and Examination – Systems Biology Databases and Tools on the Internet- Gene Ontology – Reactome - TRANSFAC and EPD - Genome Matrix - Modeling Tools - Modeling and Visualization- Mathematica and Matlab – Gepasi - E-Cell – PyBioS - Systems Biology Workbench – Cell Designer, Data Formats - Systems Biology Markup Language - MathML.

**Unit 3:** **[8]**
Simulation and pathways: - Whole-cell: Principle and levels of simulation – Virtual Erythrocytes, Pathological analysis. Flux Balance Analysis – metabolomics- and enzymes, Gene Networks: basic concepts, computational model such transcription networks basic concepts.

**Unit 4:** **[8]**
Robustness and optimality in Biology: – model and integral feedback-signaling/bifunctional enzymes. Perfect robustness- Role and its measurement-the biochemical paradigm-the genetic paradigm- the systems paradigm. Linking models and measurement-concepts- calibration and identification –Data Vs Metadata

**Unit 5:** **[8]**
Design of Circuits and Databases: Introduction-, databases KEGG and EMP; MetaCyc and AraCyc .Expression databases and various databases related to systems biology. Optional design of gene circuits I: cost and benefit: gene circuits II selection of regulation. Stochasticity in gene expression.

**References:**


1. Uri Alon An Introduction to Systems Biology-Design principles of Biological circuits, Chapman and Hall/CRC Taylor francis group. ISBN 1-58488-642-0.
2. L. AlberghinaH.V.westerhoff. Systems Biology: Definitions and perspectives. Springer ISBN 978 3-540-74269-2.
3. A.Kriete, R.Eils Computational systems biology, Academic press.ISBN 0-12-088786-X.
4. E.Klipp ,R.Herwig, A.Kowlad, C.Wierling and H.Lehrach Systems Biology in practice: Concepts, Implementation and applications. ISBN 10-3-527-31078-9.

**MTBI 303B**
**CHEMOINFORMATICS AND PHARMACOGENOMICS**
w.e.f. Session 2014-15

| L | T | P |
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| 3 | 1 | 0 |

**Unit 1:** **[8]**
Role of computers in chemical research, Introduction to Chemoinformatics, Representation and manipulation of 2D and 3D molecular structures, Chemical Databases - Design, Storage & Retrieval methods, Overview of PubChem and ChEBI databases.

**Unit 2:** **[8]**
Reaction and Metabolic pathway databases: KEGG, EMP, Concepts and need of Combinatorial chemistry and Library design - Diversed and focused Libraries, Design strategies for Combinatorial library.

**Unit 3:** **[8]**
Design and Analysis of High-throughput screening, Virtual Screening, Common tools for Virtual screening, Prediction of ADME-TOX properties of chemical compounds, Chemoinformatics tools for drug discovery.

**Unit 4:** **[8]**
Pharmacogenomics: History and overview, Concept of Genomic medicine: current status and application in various diseases. Role of SNP's in pharmacogenomics and case study, Construction and application of Genomic library.

**Unit 5:** **[8]**
Pharmacogenomics and drug design: Need for protein structure information, Mutation in drug targets, Insilico drug design of small molecules at genetic level, Drug metabolism: Role of cytochromes P450; The genetics of drug metabolism and pharmacogenomics. Challenges of Pharmacogenomics.

**References:**


1. Wilkins, M.R., Williams, K.L., Appel, R.D., Hochstrasser, D.F. (Editors), Proteome Research: New Frontiers in Functional Genomics, Springer Verlag Berlin Heidelberg.
2. Baxevanis, A.D. and Francis Ouellette, B.F., Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins.
3. Graur, D. and Li, W-H. Fundamentals of Molecular Evolution. Sinauer Ass., USA.
4. Stephen Krawetz-Bioinformatics for systems Biology.
5. Joseph Seckback and Eitan Rubin-New Avenues in Bioinformatics.
6. Yan and Qing-Pharmacogenomics in Drug Discovery and Development

**MTBI 306P**
**COMPUTER AIDED DRUG DESIGN LAB**
w.e.f. Session 2014-15

| L | T | P |
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1. To retrieve the protein structures form PDB and perform its energy minimization studies by applying suitable force fields.
2. To visualize and comment on the active sites of the retrieved protein structures using Accelrys Discovery studio visualizer.
3. To identify the ligand binding sites in the protein molecules using Q-site Finder.
4. To retrieve the chemical compounds from the PubChem database in the sdf format and convert it into suitable pdb, asn and mol format using Open Babel.
5. To perform the protein-ligand docking experiments using AutoDock Tools and draw out important inferences.
6. To perform the protein-protein docking experiments using Z-DOCK server and draw out important inferences.
7. To check the Drug-Likeliness properties of the given chemical compound using Lipinski's Rule of Five.
8. To carry out the Insilico toxicity studies of the given chemical compound and draw out the important inferences.

**References:**


1. Andrew R.Leach, Molecular Modelling Principles and applications, Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach", Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers.