Chhatrapati ShahuJi Maharaj University, Kanpur

Revised scheme & syllabus for Advanced Post Graduate Diploma Bioinformatics

Course Curriculum:

Semester	Paper code	Subject/Paper	Credit Hours/ L-T-P	70% External	30% Internal	Total 100%
Semester I	MBI101. A/B	Mathematics & Statistics/ Cell & Molecular Biology	3-1-0	Theory	Theory	100
	MBI 102.	Data Structure & Database Management	3-1-4	Theory	Practical	100
	MBI 103.	Introduction to Programming	3-1-4	Theory	Practical	100
	MBI 104.	Computational Biology	3-1-3	Theory	Practical	100
	MBI 105.	Data Mining using R	3-1-3	Theory	Practical	100
	PBI 106	Technical Communication, Research and IPR	3-1-4	Theory	Theory	100
Semester II	MBI201.	Genomics & Transcriptomics	3-1-2	Theory	Practical	100
	MBI 202.	Metagenomics & Immunoinformatics	3-1-2	Theory	Practical	100
	MBI 203.	Programming using Perl & Python	3-1-4	Theory	Practical	100
	MBI 204.	Protein Design & Engineering	3-1-2	Theory	Theory	100
	MBI 205. PBI205A/ PBI-205B	Elective 1-Computer Aided Drug Design , Elective 2-Systems Biology & Metabolomics	3-1-4	Theory	Practical	100
	PBI 206	Project/Dissertation	0-3-6	Practical	Practical	100

Syllabus is designed and prepared by following members (Experts) of Board of Studies (BOS), Bioinformatics, CSJM University, and Kanpur under the supervision of Prof. R Sankar Ramakrishnan

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I SEMESTER

PBI 101A. Mathematics & Statistics

Unit 1. Matrices: Operations on Matrices, determinants, Adjoint, Inverse of a matrix, Cramer's rule. 3d Geometry: Equation of line in space, Vectors: Definition, Addition, Dot product, Cross product.

Unit 2. Differentiation: Derivatives of important functions (Formulae), sum rule, product rule, Quotient rule, Chain rule.

Unit 3. Integration: Indefinite integrals as anti-derivatives. Integration of sum of two functions, Product rule, quotient rule.

Unit 4. Set Theory, ~~quotient rule~~ basic sets, Ordered pair, Power sets and products, Relations and functions, Cardinality of set.

Unit 5. Permutation and combination., Probability, Random variables, binomial, Poisson and normal distributions.

Unit 6. Sampling distribution; Difference between parametric and non-parametric statistics; Confidence Interval; Errors; Levels of significance; Sampling Technique, Concept of population and sample.

Unit 7. Chi square Test, t test, Analysis of variance; Regression and Correlation

Programming in C for correlation and regression, standard deviation, testing of hypothesis etc. using standard package like SPSS and R package

Text Books and References:

Mathematics
1. G.B.Thomas and R.L.Finney : Calculus and Analytical Geometry, 9th edition, Pearson Educaion.
2. B.S. Grewal, Higher Engineering Mathematics, Khanna Publishers, 2005 Modern Biology
3. Ewens, W.J. and Grant, 2001 Statistical Methods in Bioinformatics: An Introduction. Springer-Verlag.
4. Warren J.J., Ewens Warren, Ewens Gregory Grant, Statistical Methods in Bioinformatics: An Introduction, Springer-Verlag.
5. Ayers, F. , Matrices and Vectors, Schaum .

Statistics
1. Statistical Methods in Bioinformatics: An Introduction by W. Evans & G. Grant, Springer, 2001
2. First course in Probability by Sheldon Ross, Prentice-Hall (India), 2001
3. Larson, H.J., Introduction to Probability Theory and Statistical Inference, John Wiley & Sons.
4. Goon, A.M., Gupta, M.K. and Dasgupta B.: Fundamental of Statistics - Vol. 1, The World Press Pvt. Ltd.
5. Devore, J.L., 2002 Probability and Statistics, 5th edition, Thomson Asia.

6. Hoel, Port and Stone, Introduction to Statistics.
7. Miller & Freund: Probability and Statistics for Engineers, 7th Edition.
8. Chung, Kai Lai, Elementry Probability Theory with Statistical Processes (Student Edition) Springer International
9. Angela Dean & Daniel Voss (2006). Design and Analysis of Experiments, Springer Verlag
10. Campbell M.J, Machin D. & Walters S.J (2007). Medical Statistics – A Text Book for the Health Sciences, Wiley.
11. Das M.N. & Giri N.C. (2006). Design and Analysis of Experiments, New Age Publications
12. Cochran, W.G. (2002). Sampling Techniques. Wiley Des Raj and Chandhok (1998). Sampling Theory, Narosa.
13. Murthy, M.N. (1967). Sampling Theory and Methods. Statistical Publishing Company, Calcutta.
14. Feller, W., An Introduction to Probability: Theory and its Applications, Wiley Eastern Limited.

PBI 101B. Cell and Molecular Biology

Unit 1. Structure of cell & Tissues; Cell-cell communication; Introduction to genome biology: Genome as the store house of information, DNA as the carrier of encoded messages; Organization and regulations of genes in prokaryotes and eukaryotes.

Unit 2. Intra-cellular transmission of genetic message and their cellular translation; Selective transmission of genetic messages- regulation of gene expression; logic of building body plans- developmental translation of encoded messages

Unit 3. Introduction to molecular and cellular biology from an engineering perspective. DNA sequencing methods, strategies for genome sequencing, Gene mapping methods: Linkage maps, tetrad analysis, mapping with molecular markers, mapping by using somatic cell hybrids, FISH, development of mapping population in plants.

Unit 4. DNA fingerprinting; Southern and northern blotting; In-situ hybridization Methods for analysis of gene expression at RNA and protein level, large scale expression, such as micro array based techniques. Isolation, separation and analysis of carbohydrate and lipid molecules RFLP, RAPD and AFLP techniques.

Unit 5. Generation of genomic and cDNA libraries in plasmid, phage, cosmid, BAC and YAC vectors. In vitro mutagenesis and deletion techniques, gene knock out in bacterial and eukaryotic organisms. Transposons and gene targeting; DNA labeling; DNA sequencing; Polymerase chain reactions; Gene isolation; Gene cloning; Expression of cloned gene; Applications of genetic engineering in drug design and therapeutics, agriculture and livestock improvement.

Text Books and References:

1. Lewin 2004, Genes VIII. Pearson.
2. Gerald Karp 2002, Cell and Molecular Biology. John Wiley.
3. Lodish et. al. 2004, Molecular Cell Biology. Freeman.
4. Molecular Biology of the Cell, by Alberts et al (4th edition or later), Garland Sciences, New York
5. Pollard & Earnshaw 2002, Cell Biology. Saunders.
6. Tobin & Morcel 1997, Asking about Cells. Saunders.
7. Watson et. al. 2004, Molecular Biology of the Gene. Pearson.
8. An Introduction to Genetic Engineering, Desmond S.T. Nicholl, third Edition.

9.

PBI 102. Data Structure and Database Management

Unit 1. Basic Concepts and algorithmic mathematical notations, Introduction to algorithm analysis for Time and Space requirements, (a)Arrays and Linked lists (b) Stacks and Queues, Searching Techniques

Unit 2. Hashing, Dynamic (c) Trees: Definition and basic concepts, Binary search trees and their usage, Basic concepts of Indexing , Graphs: Definition and Representations of graphs, Depth-first search, Breadth-first search, Dynamic programming algorithm, Sorting algorithms, Divide and Conquer, Introduction to Greedy algorithms.

Unit 3. Databases, ER-model, Relational model (relational algebra, tuple calculus), Database design (integrity constraints, normal forms), Query languages (SQL), Transactions and concurrency control, Introduction to Biological databases,

Unit 4. Relational database design: Normalisation - 1NF, 2NF and 3NF. File structures (sequential files, indexing, B trees), Indexing and Hashing. Security of databases. Design example on a popular RDBMS package.

Practical/Lab Data Structure
1. C Programming on operation on data structre.
2. Implementation of Searching and sorting algorithm using C.

Lab/Database Practical

1. Learning SQL commands and development of database.
2. Defining data structure for building a database.
3. Managing database objects within a database.
4. Normalization of tables in databases.
5. Manipulation of the data.

Text Books and References:

1. AV Aho, J Hopcroft, JD Ullman, Data Structures and Algorithms, Addison Wesley, 1983.
2. TH Cormen, CF Leiserson, RL Rivest, C Stein, Introduction to Algorithms, 3rd Ed., MIT Press, 2009.3. AV Aho, J
3. Hopcroft, JD Ullman, The Design and Analysis of Algorithms, AddisonWesley, 1974.
4. MT Goodrich, R Tamassia, DM Mount, Data Structures and Algorithms in Java, 5th Ed., Wiley, 2010. (Equivalent book in C also exists.)
5. Y. Langsam, M.J. Augenstein and A.M. Tenenbaum, Data Structure Using C and C++. Second Edition, Pearson education 2nd edition 2002.
6. John R. Husband – Schaum outline Data structure with C++, McGraw Hill
7. Design and Analysis of algorithms, David M Mount, University of Maryland 2003.
8. Ralph Kimball, "The Data Warehouse Lifecycle Tool Kit", John Wiley.
9. H GarciaMolina, JD Ullman and Widom, Database Systems: The Complete Book,2nd Ed., PrenticeHall, 2008.
10. A Silberschatz, H Korth and S Sudarshan, Database System Concepts, 6th Ed., McGrawHill, 2010.
11. R Elmasri, S Navathe, Fundamentals of Database Systems, 6th edition, AddisonWesley, 2010.4. R Ramakrishnan, J Gehrke, Database Management Systems, 3rd Ed., McGrawHill, 2002.
12. Introduction to Data Structure, Schaum series.
13. Introduction toAlgorithm3rd Edition by cormen, thomas h.|author; Leiserson, Charles E.|author; Rivest, Ronald

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PBI 103. Introduction to Programming

Unit 1. History of Computers, Basic concepts of Computers, system software, application software, database concept, number system, Basic UNIX Concepts and Vi – Editor, Learning OS Commands, Exposure to Windows environment, Practice of UNIX commands and Vi editor, Writing simple shell script.

Unit 2. Problem identification, analyzing requirements, research existing and alternative solutions, analyzing solutions quantitatively, synthesizing and evaluating data, prototyping, and testing.

Unit 3. Introduction to C: Basic Programming concepts, Program structure in C, Variables and Constants, Data types, Basics of Algorithm, Pseudocode and Flowcharts, Introduction to data structures.

Unit 4: C Programming: Practicing programs to get exposure to basic data types, algebraic expressions, sequential, conditional and loop constructs, control statements. Input, Output Formatting, Control structures, arrays, string, functions, structures, pointers and basic file handling.

Unit 5. Array string, function, structure, pointer, Input output file handle, Web technologies: HTML, XML, basic concepts of client-server computing, Basics of client server computing, data communication and computer networks.

Lab/Practical: Programming in C language

1. Program to carry out basic arithmetic operations (+,-,*, /, %), Integer division, Digit reversing
2. Program to find whether a given number is prime or not
3. Program to find the biggest of 2/3 numbers
4. Program to print a series of odd/even numbers or Determining if a number is +ve / -ve /
5. Program to find factorial of an integer with or without using recursion
6. Program to check whether a string is palindrome or not
7. Arrange a series of numbers/strings in ascending/descending order
8. Sum of first n numbers, given n numbers
9. Program for matrix addition, Substation, matrix multiplication
10. Program for string copying and String concatenation and File copying
11. Table generation for n, a^b, sine series, cosine series, ^nC_r , Pascal Triangle, Factors of a number,

Text Books and References:

1. A Balanced Introduction to Computer science by David Reed, PE, 2000.
2. Introduction to Computing Systems: From Bits to Gates to C and Beyond. Yale N. Patt and Sanjay J. Patel. Prentice Hall India, 1999
3. Programming with C, K.R.Venugopal & Sudeep R. Prasad, Tata McGraw Hill
4. Programming in C, Herbert Schildt, THM, Fifth Edition, 2002
5. C How to program, Deitel & Deitel, Pearson Edition, Third Edition, 2001
6. Programming in C, Denis Ritchie, THM, Fourth Edition, 2000
7. Programming in C, Schaum Series, 3rd edition
8. The 'C' Programming, Denis Ritchi (PHI)
9. Programming in C, Venugopal (TMH)
10. Programming in C, Balaguruswami (TMH)

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PBI 104. Computational Biology

Unit.1 Basic concepts: Sequence similarity, identity and homology, definitions of homologues, orthologues, paralogues, Introduction to Sequence analysis programs and structure prediction programs, Sequence assembly and finishing methods, Introduction to Genome and Genomic mapping, complexity of genome, Fragmentation of Genome. Primers design, mapping algorithms.

Unit 2. Scoring matrices: Basic concept of a scoring matrix, Matrices for nucleic acid and proteins sequences, BLAST and FASTA, PAM and BLOSUM matrices derivation, principles based on which these matrices are derived. Computation of various parameters using proteomics tools at the ExPASy server and EMBOSS

Unit 3. Pairwise sequence alignments: Basic concepts of sequence alignment: local and global alignments, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments, gap penalties, use of pairwise alignments for analysis of Nucleic acid and protein sequences and interpretation of results.

Unit 4. Multiple sequence alignments (MSA): The need for MSA, basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW and PileUp and their application for sequence analysis, concept of dendrogram, phylogram and cladogram, whole genome alignments: understanding significance. Use of HMM-based Algorithm for MSA (e.g. SAM method)

Unit 5. Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, various types of pattern representations viz. consensus, regular expression (Prosite-type) and sequence profiles; profile-based database searches using PSI-BLAST, MEME, PHI-BLAST, SCanProsite and PRATT, Algorithms for generation of sequence profiles: Profile Analysis method of Gribskov, HMMer, PSI-BLAST

Unit 6. Basic concepts in systematics, taxonomy and phylogeny; molecular evolution; nature of data, Phylogenetic tree analysis algorithms, Probabilistic models and associated algorithms such as Probabilistic models, Bayesian inference algorithm, Bootstrapping methods, use of tools such as PHYLIP, MEGA, PAUP Analysis of regulatory RNA's: Databases and tools.

Practical/Lab

1. Pair-wise global alignments of protein and DNA sequences using Needleman-Wunsch algorithm & interpretation of results to deduce homology between the sequences, use of scoring matrices
2. Pair-wise local alignments of protein and DNA sequences using Smith-Waterman algorithm and interpretation of results
3. Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences
2. Database (homology) searches using different versions of FASTA & interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences.
3. Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLUSTAL. Interpretation of results to identify conserved and variable regions and correlate them with physico-chemical & structural properties.
4. Profile-based database searches using PSI-BLAST, analysis and interpretation of profile-based searches. Conserved Motif search using MEME, PHI-BLAST

Text Books and References:

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Bioinformatics

1. Developing Bioinformatics Computer Skills by C. Gibas and P. Jam beck, 0' Reilly (2001)*
2. An Introduction to Bioinformatics Algorithms, Neil C Jones & Pavel A. Pevzner, Ane Books, 2005.
3. Bioinformatics: Sequence and Genome Analysis, David W Mount , 2nd Edition, cold Spring Harbor Press
4. Introduction to Computational Molecular Biology , Setubal and Meidanis, Thomson, 2003.
5. Introduction to Mathematical Method in Bioinformatics, Alexcender Isaev, Springer Universitext, 2004.
6. Biological Sequence Analysis Probablistc Models of Proteins and Nucleic Acid, R. Durbin, Eady, A. Krogh and Mitchison, Cambridge University Press, 1998.
7. Essential Bioinformatics-Jin Xiong, Cambridge University Press
8. Introduction to Bioinformatics – Attwood & Parry-Smith, Pearson Education
9. Bioinformatics- A beginner's guide by Jean-Michel Claverie, John Wiley & Sons.

PBI 105. Data Mining   using R

Unit 1. Data Mining: Basics, Architecture for Data Mining, Data Preprocessing, Data Integration and Transformation. Data mining techniques, KDP (Knowledge Discovery Process). Data Mining & Machine Learning methods: Clustering, Feature selection, Classification, Correlation analysis, Supervised and Unsupervised learning with regression etc.

Unit 2. Introduction to distributed database processing, Introduction to Fuzzy logic, Neural network, cognitive models. Application and Challenges of Data Mining in Bioinformatics.

Unit 3.   Introduction to Data analysis using R- Basics of R Language, Statistical models in R, Statistical techniques applied using R, Graphical analysis techniques. Practical examples/case studies. Tools for big data analytics in bioinformatics, GWAS, pathway analysis.
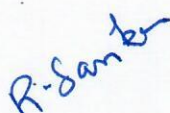
Unit 4. Bioimage Processing and Basics of computer assisted medical imaging, basics of computer assisted medical decision making.

Practical
   1. Implementation of data mining algorithms using R package
   2. Big data & Machine learning tools: Spark & SparkML , H2O , Azure ML
   3. Use of Hadoop and Hadoop related tools, MapReduce, Pig and HIVE for big data analytics
   4. Microarrays and Gene Expression (differentially expressed) data analysis by R
   5. Cluster Analysis of microarray information
   6. Analysis of NGS data R and bioconductor
   7. Analysis of Transcriptome data by R and Bioconductors packages

Text Books and References:
   1. J. Han, M. Kamber, "Data Mining: Concepts and Techniques", Harcourt India / Morgan Kauffman
   2. P. Ponnian, "Data Warehousing Fundamentals", John Wiley.
   3. M.H.Dunham, "Data Mining Introductory & Advanced Topics", Pearson Education.
   4. Ralph Kimball, "The Data Warehouse Lifecycle Tool Kit", John Wiley.
   5. H GarciaMolina, JD Ullman and Widom, Database Systems: The Complete Book,2nd Ed., PrenticeHall, 2008.
   6. A Silberschatz, H Korth and S Sudarshan, Database System Concepts, 6th Ed., McGrawHill, 2010.

7. R Elmasri, S Navathe, Fundamentals of Database Systems, 6th edition, AddisonWesley, 2010.4. R Ramakrishnan, J Gehrke, Database Management Systems, 3rd Ed., McGrawHill, 2002.

PBI 106. Technical Communication, Research & IPR (Practical based course)

Unit 1. Critical reasoning and verbal deduction. Numerical Ability: Numerical computation, numerical estimation, numerical reasoning and data interpretation.

Unit 2. Basics of Technical Communication: Technical Communication: features; Distinction between General and Technical communication; Constituents of Technical Written Communication: Technical Terms; Paragraph-Text Readings, Mechanics of writing, Forms of Technical Communication: Letters. Reports: Types; Significance; Structure, Style & Writing of Reports and Proposal; Significance.

Unit 3. Presentation Strategies: Defining Purpose; Audience & Locale; Organizing Contents; Preparing, Outline, Seminar, workshop and Conference.

Unit 4. Research, Scientific research, Format of Project Report, Thesis, Research Article, Review Article and their writing

Unit 5. Ethics and Technology: Intellectual property rights, patenting, Entrepreneurship development, Risk Assessment and Management Information Security. IPR issues in Biotechnology and Bioinformatics, impacts of IT on language & culture localization issues – Unicode – IT and regional languages, Integrated Practice Management Systems, Various IPR laws Copyright and Patents.

Text Books and References:
1. Improve Your Writing ed. V.N. Arora and Laxmi Chandra, Oxford Univ. Press, New Delhi.
2. Technical Communication – Principles and Practices by Meenakshi Raman & Sangeeta Sharma, Oxford Univ. Press 2007, New Delhi.
3. Effective Technical Communication by Barun K. Mitra, Oxford Univ. Press, 2006, New Delhi
4. Developing Communication Skills by Krishna Mohan, Meera Banerji- Macmillan India Ltd. Delhi.
5. Manual of Practical Communication by L.U.B. Pandey & R.P. Singh; A.I.T.B.S. Publications India Ltd.; Krishan Nagar, Delhi.
6. The Language of Literature and Science by A.Huxley
7. Core refere1. AnithaRao and BhanejiRao, "Intellectual Property rights: A primer", Eastern Book Company.
8. Rowena Murray, "How to Write a Thesis", Tata McGraw Hill Education Pvt. Ltd.
9. C.R.Kothari, "Research Methodology, New Age Publishers
10. Jeffrey A. Lee, "The scientific endeavor: a primer on scientific principles and practice", Benjamin Cummings.
11. Robert A. Day, "How to Write and Publish a Scientific Paper", Cambridge University Press.
12. Dr. Marlene Caroseli, "Quick Wits: 50 Activities for Developing Critical Thinking Skills", Ane Books.
13. Gregory Bassham, William Irwin, Henry Nardone and james Wallace, "Critical Thinking: A Student's Introduction", Tata McGraw Hill education Pvt. Ltd.
14. Rhonda Abrams and Julie Vallone," Winning Presentation in a Day", PHI Pvt Ltd. 6. Weisberg, R., "Creativity - Beyond the Myth of Genius", W.H. Freeman and Company, New York, 1993.

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II SEMESTER

PBI 201. Genomics & Transcriptomics

Unit 1. Identification of alternatively spliced genes; Transcription binding sites, Identification of genes in prokaryotes and eukaryotes. Promoter identification.

Unit 2. Introduction; The impact of Genomics on biological research; Identification of a large set of genes involved in a biological process; High throughput expression analysis; Genome wide search for interacting partners; Sequence variations and disease susceptibility.Genome wide annotation methods, identification analysis of various genome.

Unit 3. Comparative genomics: Basic concepts and applications, MegaBlast algorithms, PipMaker, AVID, Vista, MUMmer, applications of suffix tree in comparative genomics, synteny and gene order comparisons, Comparative genomics databases: Clusters of Orthologous Groups (COGs), Ensembl

Unit 4. 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, use of SNPs for identification of genetic traits, Gene/Protein function prediction using Machine learning tools:, supervised/unsupervised learning, Neural network, SVM etc

Unit 5. Microarray data analysis, Principle of NGS technology, Next Generation Sequencing Methods, Workflows for various NGS experiments, Various file formats such as SAM, VCF, BED, ChIP-seq, Binary Alignment/Map (BAM) format.

Unit 6. Transcriptomics Types of RNAs and the respective roles in cells. Transcriptome and techniques used for transcriptomics; microarray and RNA-seq. Impact of transcriptomics on biology, volume of data produced and important repositories. Comparing transcriptomics with genomics and proteomics

Lab/Practical

1. Searching for particular gene from Biological Databases, Genome Databases, Viral Genomes, Archeal and Bacterial Genomes, Eukaryotic genomes with special reference to model organisms (Yeast, Drosophila, *C. elegans*, Rat, Mouse) Human, plants such as Arabidopsis thaliana, Rice, etc.
2. Retrieving protein and nucleic acid sequences, structures, ESTsequences, SNP data using database browsers and genome browsers.
3. Gene sequence analysis : Prediction of ORF's, transcription factor binding site and promoters
4. Prediction of gene features, codon usage and RNA fold analysis.
5. Phylogenetic analysis of gene orthologs and paralogs: Prediction of conserved motif.
6. Micro array data analysis using online tools.
7. Prediction of splice sites using-SIN-4, spidey, BLAT etc.

Text Books & References

1. Gupta, PK (2004) Biotechnology and Genomics, Rastogi Publications, Meerut, India (ISBN: 81-7133-676-0)
2. Stuart M. Brown "Next-Generation DNA Sequencing Informatics", Cold Spring Harbor Laboratory Press
3. Genomics: the science and technology behind human genome project, Cantor and Smith
4. Pevnezer, "Bioinformatics and Functional Genomics", John Wiley.

5. Genomics, Proteomics and Bioinformatics. A. Malcolm Campbell & Laurie J. Heyer, CSHL
6. Press and Benjamin Cummings.Current Protocols in Bioinformatics, Edited by A.D. Baxevanis et al, Wiley Publishers.2005
7. Bioinformatics by David W. Mount, Cold Spring Harbor Laboratory Press. 2001
8. Fundamental concepts of Bioinformatics by D.E. Krane and M.L Raymer, Pearson Education. 2003

PBI 202. Metagenomics & Immunoinformatics

Unit 1. Metagenomics and Population genomics Overview of metagenomics principles, microbial and ecological aspects underlying metagenomic experiments, applications and limitations of metagenomics, differences between metagenomics and single-cell genomics. Definition and principle of population genomics, difference between metagenomics and population genomics, applications of population genomics.

Unit 2. Metagenomics, study of environmental effects on gene expression and biodiversity. Metagenomics: Concept, Approaches for metagenome analysis & ecological inference, QIIME pipeline for microbial community, SeqEnv: annotating sequences with environmental information; Introduction to shotgun metagenomics, Read based metagenomic profiling & analysis; Taxonomic classification and clustering of contigs.

Unit 3. Immunoinformatics overview, Reverse vaccinology, Rational Vaccine design o Evolution and escape due to variations, Immunoinformatics databases & tools, Molecular interactions, Specificity, characterization; Sequential and conformational epitopes, MHC- peptide HLA: nomenclature, HLA-peptide interactions & matrices

Unit 4. Epitope prediction algorithms: B-cell epitope predictions using sequence-based approaches o B-cell epitope predictions using structure-based approaches, T-cell epitope prediction methods, Epitope Predictions;

Unit 5. Predicting Peptide-MHC Binding using Profiles, Machine Learning Techniques for MHC Binders, Methods for Predicting T-Cell Epitopes, MHC-Class I and II Binding Affinity. MHC–Molecular Affinity and QSAR Models, Nonlinear Predictive Modelling of MHC Class II–Peptide Binding using Bayesian, Neural Networks; Vaccine design, Codon optimization, application of genetic engineering in vaccine design. Vaccine design: Pipeline & workflows o Prediction of immunogenicity, Case studies: Hepatitis B
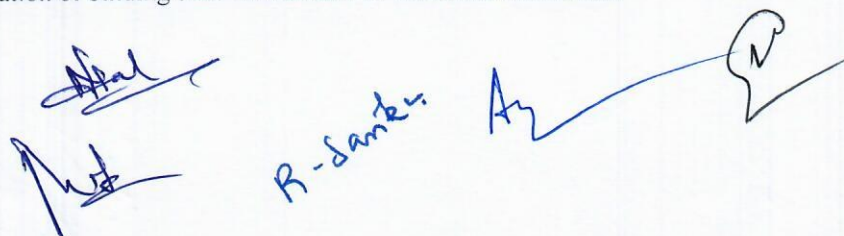
Lab/ Practicals

Metagenomics

1. Metagenoomic analysis using Megan
2. Searching in MGRast,IMG, WebMG,EBI

Prediction of Antigenic properties and Epitopes

1. Prediction of structural features of antibodies using computational tools
2. Retrieval of sequence & structure of Immunoglobulin in databases.
3. Study of Antibody sequence and structure: visualisation of structure & mapping CDRs on structure
4. Study of variable and constant domains
5. Characterization of binding sites on the basis of molecular interaction

6. Sequence analysis to study conserved regions and variable regions.
7. Prediction of conformational epitopes
8. Prediction of cytotoxic and helper T cell epitopes
9. Prediction of immunogenicity for vaccine design: Combination of MHC and Proteasome predictions
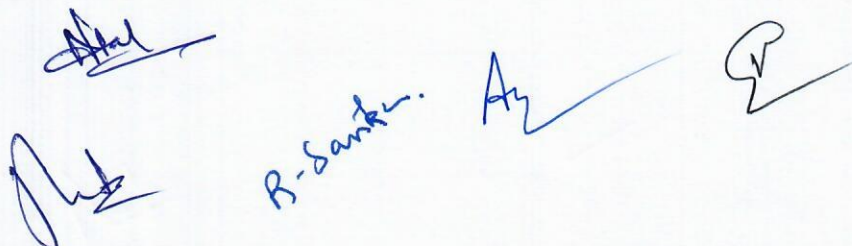
Vaccine Design

1. Screening of Antigenic protein using vaccine databases.
2. Study of model organisms.
3. Data base searching using MHCDB
4. Epitope prediction using NetMHC .
5. Mapping and identification of Epitopes
6. Codon optimisation of reverse translated sequence.
7. Study of open reading frame.

Text Books & References

1. Emily D. Aulicino, "Genetic Genealogy: The Basics and Beyond" 4. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
2. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
3. Lorenz, P and Eck, J (2005) Metagenomics and Industrial Applications, Nat. Rev. Micrbiol., Vol 3, pp. 510-516.
4. Đ Handelsman, J (2004) Metagenomics: Application of Genomics to Uncultured Microorganisms, Microbiol. Mol. Biol. Rev., Vol 68-4, pp. 669-685.
5. Đ Riesenfeld, CS, Schloss, PD, Handelsman, J (2004) Metagenomics: Genomic analysis of Microbial Communities, Annu. Rev. Genet.,
6. Flower Darren R. Bioinformatics for Vaccinology Publisher: UK, John Wiley & Sons Inc. 2008.
7. Flower Darren R. Immunoinformatics: Predicting Immunogenicity In Silico Publisher: New Jersey,Humana Press. 2007.
8. Kindt, Thomas J.,Osborne Barbara A.Goldsby Richard A. Kuby Immunology 6th Edition. Publisher:New York, W. H. Freeman. 2007. ISBN: 9780716785903.
9. Lund Ole , Nielsen Morten , Lundegaard Claus, Kesmir Can, Brunak SÃ¸ren. Immunological Bioinformatics. Publishesr: London, MIT PRess 2005 ISBN: 0262122804.
10. Foundation Novartis.Immunoinformatics: Bioinformatic Strategies for Better Understanding of Immune Function. Publisher: Chichester,John Wiley & Sons Inc. 2003. ISBN: 0470853565.
11. Roitt Ivan, Delves Peter. Roitt's Essential Immunology 10th Edition.Publisher: Canada,Blackwell. 2001, ISBN: 0632059028.

Metagenomicss

1. Emily D. Aulicino, "Genetic Genealogy: The Basics and Beyond" 4. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
2. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
3. Lorenz, P and Eck, J (2005) Metagenomics and Industrial Applications, Nat. Rev. Micrbiol., Vol 3, pp. 510-516.
4. Đ Handelsman, J (2004) Metagenomics: Application of Genomics to Uncultured Microorganisms, Microbiol. Mol. Biol. Rev., Vol 68-4, pp. 669-685.
5. Đ Riesenfeld, CS, Schloss, PD, Handelsman, J (2004) Metagenomics: Genomic analysis of Microbial Communities, Annu. Rev. Genet.

Chhatrapati ShahuJi Maharaj University, Kanpur

Revised scheme & syllabus for Advanced Post Graduate Diploma Bioinformatics

PBI 203.
Programming using Perl & Python

Unit 1. Introduction: An Introduction to Perl, The Perl Interpreter, How the Perl Interpreter Works, Variables and Data Types: Perl Variables, Scalar Values, Variable Definition, Special Variables. Arrays and Hashes: Arrays, Array Manipulation, Hashes Control Structures, Comparisons, Conditional statements, Loops, Operators, Subroutines: Creating a Subroutine, Arguments, Passing Arguments with References, String Manipulation: Array-Based Character Manipulation, Regular Expressions, Patterns

Unit 2. Input and Output: Program Parameters, File I/O (File handles, Working with Files, Built-in File, Handles, File Safety, The Input Operator, Binary I/O). Object oriented Perl: Introduction to modules and Packages, Objects creation Bioperl : Introduction, Installation procedures, Architecture, Uses of bioperl, Class, Method, Method overriding, Inheritance, Perl Database access.

Unit 3. Introduction to Python, Python features, Python Environment, Basic syntax, variables, function and method, operators, conditional statements, Looping, control statements, List, Tuple, string manipulation, Dictionaries, python standard Library. Modules, Input-Output, Exception handling

Unit 4. OOPs Concept: Class and object, Attributes, Inheritance, Overloading, Overriding, Data hiding, Regular expression, CGI, Database, Networking multithreading, GUI

Practical/Lab

1. Data storage and manipulation using array and hashes

2. Programming to implement conditional statement.
3. Programming to implement different types of Loops.
4. Programming to implement different types (eight) of operators.
5. Use of subroutines and references in programming.
6. Searching of patterns in sequences.
7. Programs to read and analyze DNA and Protein sequences in different file formats.
8. File handling to manage input/output.
9. Programming to predict genome annotation.
10. Programs to read and analyze PDB structure files
11. Scripts to automate other standalone Bioinformatics software.
12. Simple Programming to create class, method and initialise an object using Python programming..
13. Python Programming to inherit the class from base class.
14. Python Programming to perform operations on data structures.

Text Books and references:

1. Beginning Perl for Bioinformatics, James Tisdall, 2001, O'Reilly & Associates, (2001) Learning Perl, 3rd Edition.
2. Mastering Perl for Bioinformatics"James Tisdall, 2003, O'Reilly & Associates, (2001) Learning Perl, 3rd Edition.
3. Perl programming for Bioinformatics Bal, H.P.. Publisher: Tata McGraw-Hill New Delhi.
4. Bioinformatics, Biocomputing and Perl: an Introduction to bioinformatics computing skills and practice, Moorhouse Michael, Barry Paul.. Publisher: John Wiley and Sons, 2004
5. Curtis Jamison D. Perl programming for biologists. Publisher: John Wiley & sons, inc., 2003
6. Genomic Perl; *R.A. Dwyer*; Cambridge University Press, 2003.
7. Perl tutorial ,Tutorial point,.www.tutorialpoint.com

8. Python for Data Analysis: Data Wrangling with Pandas, NumPy, and IPython by Wes McKinney
9. Python Essential Reference (4th Edition) by David Beazley

PBI 204. Protein engineering and Design

Unit 1. Principles of protein structure; anatomy of proteins – Hierarchical organization of protein structure -Internal coordinates of proteins; Internal, Cartesian and distance coordinate representations of protein structures. Theory, Conformation of proteins (Ramachandran plot, secondary structure, domains, motif and folds). Stability of proteins stabilizing interactions (Van der Waals, electrostatic, hydrogen bonding, hydrophobic interaction, etc.). Classification of Three Dimensional Structures in Brookhaven Protein Data Bank (HSSP, SCOP, FSSP, CATH)

Unit 2. Fundamentals of the methods for 3D structure prediction (sequence similarity/identity of target proteins of known structure, Homology Modeling, Structural Alignment Methods, Structure superposition, Structure – structure alignment tool, DALI, CE, VAST, TM-align, Visualization and comparison of 3D structures of proteins, nucleic acids, rRNA. functional implications of protein domains, fold recognition, threading approaches, and ab-initio structure prediction methods.

Unit 3. Protein design: Principles of Protein Folding, Dynamics and Structural Evolution. Elementary ideas of bonding and structure, stereochemistry; Random, site directed mutagenesis; Strategies to alter catalytic efficiency; structure prediction and modeling proteins, Molecular graphics in protein engineering; and Dynamics.

Unit 4. Biomolecular Simulation: Computer simulation as a powerful research tool, atomic force field models, MD algorithm, numerical integration of equations of motion, ergodic hypothesis, long range interactions, microcanonical ensemble, NVT, NPT ensembles, limitations of MD simulation, simulation quality analysis, event analysis, time and size limitations, QM/MM techniques, steered MD simulation, free energy methods, examples of simulations on conformational changes in protein and inhibitor binding to proteins. Calculation of conformational energy for bio-macromolecules, Simulation of molecular mechanics and dynamics and free energy changes, Molecular Simulation, Molecular dynamics.
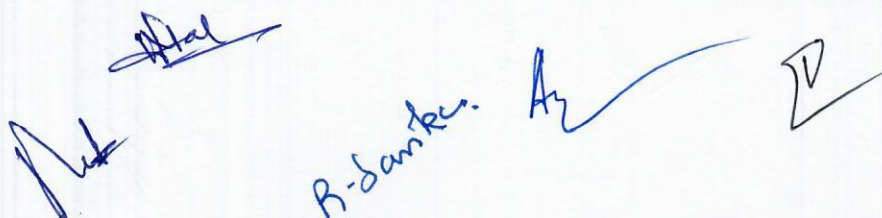
Lab/Practicals

A. Prediction of gene/protein for the selection of target and template protein (model)

1. Collection of Protein sequences related to specific biological activity from NCBI/SWISSPROT & UniProtKB to select Model protein and target protein
2. Pair-wise global alignments of protein and gene/ protein sequences using BLAST/FASTA & interpretation of results to deduce homology between the sequences, use of scoring matrices
3. Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences for the selection of plant protein, to modify protein using protein engineering approaches.
4. Database (homology) searches using different versions of FASTA & interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences.
5. Pattern searching using ScanProsite and PRATT

B. Protein Designing

1. Searching for a particular protein and its folds in Structural and Related Databases:PDB, NDB, CCSD, Prosite, PRODOM, Pfam, PRINTS, CATH, SCOP, DSSP, FSSP, DALI

2. Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLUSTAL W. Interpretation of MSA to identify conserved and variable regions which can be analysed for physico-chemical & structural properties in order to identify the residues which can be modified in plant proteins.
3. Visualization of structures: Search for modification sites (active site) to alter catalytic efficiency of protein

C. Modeling

1. Modeling protein structure using modeling tool Geno3D.
2. **3-D structure visualization and simulation:** Visualization of structures using Pymol Rasmol or SPDBV or CHIME or VMD
3. Structure analysis and validation: Pdbsum, Whatcheck, Procheck, Verify3D , Critical Assessment of Structure Prediction (CASP) Structures of oligomeric proteins and study of interaction interfaces, DALI, CE, VAST TM-align, Visualization and comparison of 3D structures of proteins
4. Visualization and comparison of 3D structures of proteins, nucleic acids, rRNA
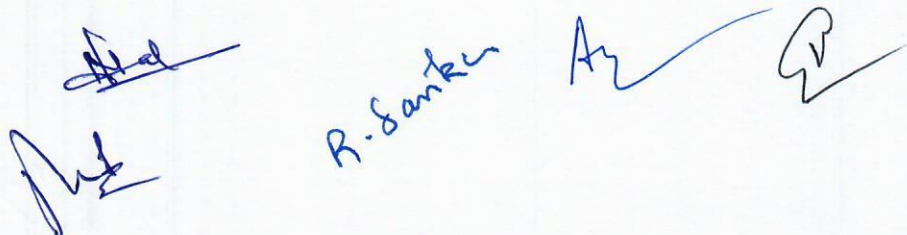
D. Simulation

1. Simulation of protein structure to analyse conformation of modelled protein using Desmond.

Text Books and References:

1. Molecular Modelling: Principle and Applications, Andrew R. Leach, Longman Singapore Publisher, 1999.
2. The Molecules of Life: Physical and Chemical Principles. John. Kurian, Boyana Konforti and D.Wemmer Garland Science, New York 2013
3. Introduction to Protein Structure. Carl Branden & John Tooze, Garland Science
4. Biochemistry by L. Stryer. Publishers : W.H. Freeman and Company(4th Edition)
5. Structural bioinformatics; P. E. Bourne and J. Gu. 2 nd Edition. John Wiley and Sons. 2009.
6. Bioinformatics vol:2: Structure, function & applications; J. M. Keith Humana Press. 2008.
7. An Introduction to Bioinformatics Algorithms, Neil C Jones & Pavel A. Pevzner, Ane Books, 2005.
8. Introduction to Computational Molecular Biology, Setubal and Meidanis, Thomson, 2003.
9. Biological Sequence Analysis Probablistc Models of Proteins and Nucleic Acid, R. Durbin, Eady, A. Krogh and Mitchison, Cambridge University Press, 1998.
10. Introduction to Mathematical Method in Bioinformatics, Alexcender Isaev, Springer Universitext,
11. Bioinformatics: From Genome to Drugs (Vol. I and II), Thomas Lengaue, Wiley- VCH, 2000.
12. Structural bioinformatics: An algorithmic approach; F. J.Burkowski. CRC Press. 2008.
13. Computational molecular biology: an introduction; P. Clote and R. Backofen, Wiley & Sons, 2000.

Elective 1

PBI 205A. Computer Aided Drug Design

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Unit 1. Introduction to drug discovery, drug discovery pipeline, Role of Bioinformatics in drug design, Aspect for new drug like safety, effectiveness, stability, solubility, synthetic feasibility and novelty and patent issue. Introduction to Retrometabolic drug design.

Unit 2. Enzyme Kinetics, line weaver plot for competitive and non-competitive inhibition, IC50, ED50, Therapeutic index, LD50, Lipinsiki Rule and Jorgensen Rule-of-Three. Pharmacokinetics: *In silico* prediction ADMET properties for Drug Molecules, Pharmacodynamics, Pharmacogenetics. Reactions of drugs and approaches for toxicity predictions.

Unit 3. Target identification and validation and lead optimization, Different systems for representing chemical structure of small molecules like SMILES etc Generation of 3D coordinates of small molecules, Structure-based drug design: Identification and Analysis of Binding sites and scoring function, Ligand based drug design, Pharmacophore modeling and mapping. Docking Concepts, Scoring functions, Software tools for Docking.

Unit 4. Structure Activity Relationship: Introduction to QSAR, QSPR, Various Descriptors used in QSARs: Electronics; Topology; Quantum Chemical based Descriptors. Regression Analysis, The Significance and Validity of QSAR Regression Equations, Partial Least Squares (PLS) Analysis, Multi Linear Regression Analysis. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations. Efficient search for drug candidates in chemical databases-library design and virtual screening, combinatorial library, automated synthesis. Pre-clinical and Clinical Testing.

Unit 5. Traditinal medicine system, Natural compounds, tribal medicines, ethno biology and traditional medicinal plants, their scope, folk herbal medicines, Ethnobotany, Databases and IT resources on traditional medicines.

Practical/Lab

Modelling

1. Drawing chemical structures by using the ChemSketch/ChemDraw software.
2. Protein-ligand docking by using the HEX program.
3. Protein-protein and Protein-Drug docking by using the open source docking software.
4. Virtual screening of ligands by using the open source software program.
5. QSAR modelling.
6. Molecular Dynamic Simulation using Desmond.
7. Database searching for traditional and ethno medicines.
8. Prediction of chemical compounds which is found in natural medicines.

Text Books and References:

1. Bioinformatics: From Genome to Drugs (Vol. I and II), Thomas Lengaue, Wiley- VCH, 2000.
2. The Molecules of Life: Physical and Chemical Principles. John. Kurian, Boyana Konforti and D.Wemmer Garland Science, New York 2013
3. Novartis Foundation, J. Craig Venter. From Genome to Therapy: Integrating New Technologies with Drug Development - No. 229. Publisher: Wiley; 1 edition, 2000.
4. Wyler David J. Modern Parasite Biology: Cellular, Immunological, and Molecular Aspects. Publisher: New York, W H Freeman & Co. 1990.
5. Burger's Medicinal Chemistry and Drug Discovery (Vol I to Vol IV) by Donald J Abraham, Wiley Inter-science

6. Computer-Aided Drug Design: Methods and Applications by Thomas J. Perun, Catherine Lamb Propst, Taylor & Francis
7. Rational Drug Design: Novel Methodology and Practical Applications (ACS Symposium Series) by Abby L. Parrill (Editor), M. Rami Reddy (Editor) American Chemical Society; Second Enlarged ed. edition (1 April 1999)

Elective 2
PBI 205B. Systems Biology & Metabolomics

Unit 1. Basic properties of network, Adjacency matrix, bipartite network. Random vs. Scale free network: power laws, hubs, ultra-small property, degree exponent and the Barabasi-Albert model. Degree correlations, Network topology.

Unit 2. Introduction to systems biology. Properties of Biological network, Concept of signal transduction network, Gene regulatory network and metabolic networks. Intercellular network: Neuronal networks, Network motifs, Network medicine, Disease Networks.
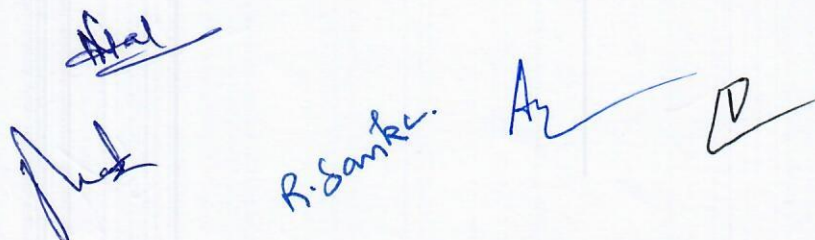
Unit 3. Systematic Determination of Biological Network Topology: Nonintegral Connectivity Method (NICM), Storing, Searching, and Disseminating Experimental Proteomics Data, Representing and Analyzing Biochemical Networks using BioMaze. Genome scale metabolic reconstruction, Self-organizing maps and Connectivity maps.

Unit 4. Metabolomics: pathways determinations and analysis. Technologies in metabolomics. Metabolic network Simulation: Mass/Flux balance analysis, Extreme Pathways, Elementary mode analysis, Minimal metabolic behaviors (MMBs), Dynamic simulation and parameter estimation, Synthetic Accessibility. Metabolic pathways resources: KEGG, Biocarta, MetaCyc BioCyc, Biogrid, String, Ingenuity Pathways Knowledge Base, EMP, AraCyc, MAPman , Biomodels, Human metabolome database.

Unit 5. Synthetic Biology: Introduction to synthetic biology Computational tools in synthetic Biology, Applications in synthetic biology.

Lab/Practical

1. File Formats for Pathways: Gene Ontology, PSIMI, CellML, BioPAX , CSML/CSO, SBML Models and MathSBML.
2. Enzyme Nomenclature and Classification, Compounds and Reactions databases: LIGAND - Biochemical Compounds and Reactions, ENZYME - Enzymes, BRENDA - Comprehensive Enzyme Information System
3. Numerical simulation of regulatory pathways and pharmacokinetics data.
4. Browse& search metabolic pathway databases: KEGG, EcoCyc and MetaCyc, EMP, Malaria Parasite Metabolic Pathways, Boehringer Mannheim - Biochemical Pathways.
5. Prokaryotes Vs Eukaryotes – single cell Vs multi cell species biology from a modeling. Rational Metabolic engineering design.
6. Interaction networks: Databases and visualization exercise
7. Structural and topological properties of biochemical networks SBML Models and MathSBML, CellDesigner: A Graphical Biological Network Editor and Workbench Interfacing Simulator, Systems Biology Workbench (SBW), Setting up Genome scale models
8. Computations of phenotypes and interpretation using genome scale models.
9. Cell Illustrator, Cellular Simulation: Towards a Virtual Biological Laboratory
10. Visualization of Integrated models of biomolecular interaction networks by cytoscape
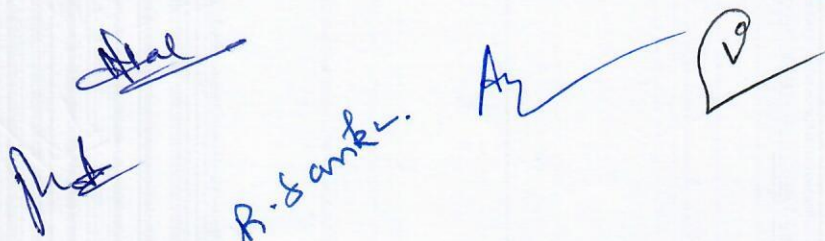
Text Books & References:

1. Bjo Rn H. Junker , Falk Schreiber. Analysis of Biological Networks. 2008. John Wiley & Sons, Inc., Hoboken, New Jersey
2. Choi Sangdun. Introduction to Systems Biology. Humana Press Inc. Totowa, New Jersey.2007. ISBN: 978-1-58829-706-8
3. Klipp Edda, Liebermeister Wolfram, Wierling Christoph, Kowald Axel, Lehrach Hans, Herwig Ralf. Systems Biology: A Textbook. Publisher: Germany, Wiley-VCH. 2009. ISBN: 9783527318742.
4. Uri Alon, An Introduction to Systems Biology: Design Principles of Biological Circuits, Chapman & Hall/CRC Press, Mathematical and Computational Biology, 2nd edition, 2006.
5. Alterovitz Gil, Ramoni Marco F. Systems Bioinformatics: An Engineering Case Based Approach. Publisher: Boston, Artech House Publishers. 2007. ISBN: 9781596931244.
6. Palsson Bernhard O. Systems Biology: Properties of Reconstructed Networks. Publisher: New York, Cambridge University Press. 2007. ISBN: 9780521859035.
7. Stephanopoulos Gregory N., Aristidou Aristos A., Nielsen Jens. Metabolic Engineering: Principles and Methodologies. Publisher: New Delhi, Reed Elsevier, India Pvt. Ltd. 2006. ISBN: 9788131203330.
8. Pengcheng Fu, Sven Panke, Systems Biology and Synthetic Biology. Wiley InterScience. 2009
9. E.Klipp R.Herwig, A.Kowlad, C.Wierling and H.Lehrach. Systems Biology in practice: Concepts, Implementation and applications by, Wiley InterScience. 2005
10. Huimin Zhao, Synthetic Biology: Tools and Applications. Elsevier, 2013.

PBI 206. Project Work / Dissertation (practical based course)

The Postgraduate project provides students with an opportunity to undertake research in bioinformatics. A wide variety of projects are offered each year in such diverse areas as microarray analysis, structure prediction, mining biomedical texts and genome analysis. Every student is expected to carry out computational work such as designing a database, or writing programs to analyse biological data or analysis of data to provide useful prediction for future research. Sometimes students suggest projects of their own that we are able support. Some of the following areas Systems Biology & Metabolomics, Molecular Modelling & Protein Engineering, Immunoinformatics , Pharmacogenomic, Metagenomics Analysis of Microarray Data, Database development, Data mining and tool development using computational algorithm and other Data mining algorithm.

Students will have to present seminar in a series of presentation and submit the report and review article on one of the following topic

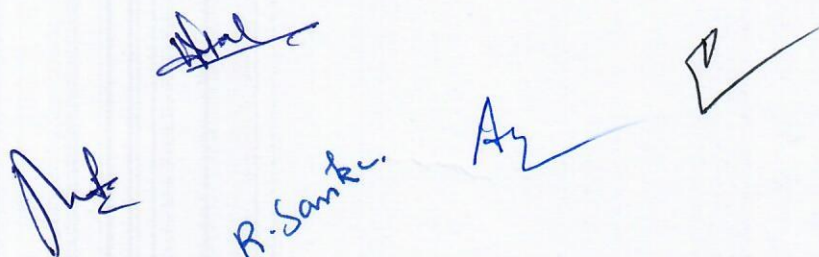| S.N.	Topic of seminar	Number of Presentations
Seminar I	Molecular Modelling & Protein Engineering	10
Seminar II	Microarray & NGS data Analysis	10
Seminar III	Database development & Software Engineering	10
Seminar IV	Data mining using R/MATLAB	10
Seminar V	Immunoinformatics & Vaccine design	10
Seminar VI	Pharmacogenomic & Metagenomics	10

Seminar VII	Systems Biology & Metabolomics,	10	
Seminar VIII	Computer Aided Drug Design	10	
Seminar IX	Agri-iformatics & Geoinformatics	10	
Seminar X	Medical Informatics	10	

Student will have to submit a draft of project report for internal assessment (shall be evaluated by the project supervisor) and final copy of project report for external evaluation (shall be evaluated by external examiner) based on six (6) month project work/dissertation (January to June) in final semester. Each student must present project work in series of presentations with the progress report for internal assessment (10% presentation+ 20% first draft of project report) and one final presentation/viva for external evaluation (40% second draft copy of project report+20% presentation of work +10% query/viva).

(1) **Internal Assessment (30%):** Regular Review of monthly progress report and project report by supervisor (20 marks) and presentation (10 marks)

(2) **External Evaluation (70%):** Review of Project Report by External examiner, which must be awarded on the basis of

(a) Scientific Reporting Standards (10)
(b) Lack of Plagiarism, Citing Literature (10)
(c) Work done (10)
(d) Results & Discussion (10)
(e) Presentation Skills (20 marks)
(f) Viva (10 marks)