Solapur University, Solapur

**M.Sc. Bioinformatics
(Semester pattern)
Syllabus 2010- 2011**

Semester – III

Theory:

PAPER NO:

Binf 301 DBMS with reference to Biological Data	100
Binf 302: Advanced Biophysical techniques	100
Binf 303: Structural Biology & Pharmacogenomics	100
Binf 304: Research Methodology in Bioinformatics	100

Practical

BinfPr 305: DBMS Biological Data & Biophysical techniques.	100
BinfPr 306: Structural Biology, Pharmacogenomics and Research Methodology	100

Semester – IV

Theory

PAPER NO:

Binf 401: Simulation and Modeling for Biologists and Soft Computing	100
Binf 402: Biodiversity informatics and IPR	100
Binf 403: Advanced Molecular Biology	100
Binf 404: Emerging areas of Bioinformatics.	100

Practical:

BinfPr 405: Simulation, and Modeling for Biologists & Soft Computing Techniques, Advanced Molecular Biology.	100
BinfPr 406: Project dissertation & Viva voce.	100

M. Sc. IN BIOINFORMATICS SYLLABUS

SEMESTER- 3

Paper Binf 301: DATA BASE MANAGEMENT SYSTEM WITH REFERENCE TO BIOLOGICAL DATA   (45L)

SECTION-I BASIC CONCEPTS OF DBMS AND RDBMS

1) Introduction: Actors on the scene, workers behind the scene.   (2)

2) **Database System Concepts and Architecture:** Data models, Schemes, Instances and Database state. The three-scheme Architecture, Data independence, Database languages and Interfaces. (6)

3) Data Modeling using the Entity-Relationship Model: Conceptual data Models for database design Entities and Attributes, Initial conceptual design of the COMPANY Database, Relationships, Relationship Types, Tools and constraints, Weak Entity types, Refining the ER Design for the company database, proper naming of scheme constructions.   (6)

4) The relational data model: Relational Model Concepts, Domains, Attributes, Triply and Relations, Characteristics of Relations, Relation Model Notification, Relation constraints and Relational Database Schema, Entity Integrity, Relational Integrity and key, Relational algebra and Relational calculus. SQL: Data definition, constraints, basic SQL-queries, more complex SQL queries, views in SQL.   (6)

SECTION-II PROGRAMMING IN PL - SQL

1) Basics of PL – SQL: Introduction, Commands and different querying types   (3)

2) Functional Dependencies and Normalization for Relational Databases: Introduction, design guidelines for relational schemes, semantics of the attributes, reading the reluctant values in tuples. Functional dependencies, introduction to normalization INF, 2NF, 3NF, BCNF, Multivalued Dependencies and fourth normal form.   (7)

3) Data Mining: An overview of Data Mining Technology. Classification, Clustering, Data Warehousing, Applications of Data Mining. Access to Molecular Biology Data Bases: Entrez, Sequence Retrieval System SRS), Protein Identification Resource (PIR) and Bibliographic databases.   (5)

4) Overview of Oracle: Objectives, Introduction, Database Management Tools, The kernel, The data dictionary, DBA, The utilities. Structures in Oracle, Physical structure, Data files, Control files, Logical structure, Steps in processing SQL statements. Structured Query Language: Objectives, Introduction, SQL commands, Data manipulation Language, Data Definition Language, Data types, CREATE command, DROP command, ALTER Command, INSERT Command, SELECT command.   (10)

Suggested Readings

1.   Database System Concepts by Hanery Korth and Abraham Silberschatz, Tata Mac-Graw Hill.
2.   An Introduction to Database Systems by C.J. Date, Addison-Wesley.
3.   Database system organization by J.M. Martin, Princeton-Hall.
4.   Introduction to Database systems by J.M. Martin; Princeton-Hall.
5.   ORACLE: Power Objects Handbook by Bruce Kolste, David Peterson.
6.   Oracle 8 SQL Programming and Tuning by P. Cassidy, 1998.
7.   SQL, PL/SQL: the programming language of oracle by I. Bayross, Ed. 2, New Delhi. BPB Publications, 2002.
8.   Oracle SQL & PL/SQL Handbook: a guide for data administrators, developers, and business analysis (With CD) by J. Palinski, Delhi, Pearson Education, 2003.

9. Wiederhold, Database Design. McGraw Hill.
10. Miers, Relation Database. Computer Science Press.
11. The Complete Reference of PL-SQL, McGraw Hill

PAPER Binf 302: ADVANCED BIOPHYSICAL TECHNIQUES

SECTION 1: Fundamentals   (45L)

1) **Fundamentals of chemical bonding and non-bonding interactions**
   Electrovalent bond, stability of electrovalent bond. Co- valent bond – partial ionic
   character of co-valent bonds. Shape of orbitals and hybridization. Co-ordination bond,
   Vander Waals forces; Metallic bond and Electron density map and its interpretation.
                                                                                              (5)

2) **Spectroscopy:** Principles, Theory, Instrumentation and Application of UV/visible,
   IR, CD and ORD to macromolecules.   (10)

3) **Lasers:** Introduction, basic working principle of lasers, types of lasers, importance and
   applications of lasers in biological studies (treatment and analysis).   (5)
4) **X-rays:** Properties, sources of X-radiation, Application of X-rays to biology
   and medicine (diagnosis and molecular structure studies.).   (5)

SECTION 2: Instrumentation

1) **X-ray crystallography:** Principles, Theory, Instrumentation and Application.   (5)

2) **NMR**:   Principles, Theory, Instrumentation and Application.   (5)

3) **Mass spectrometry:** Introduction, different methods of ionization, MALDI-TOF, Analysis and
   application.   (5)

4) **Microscopy:** Scanning Electron Microscopy (SEM), Transmission Electron
   Microscopy (TEM), Fluorescent Microscopy And Confocal Microscopy.   (5)

Suggested Readings
1. Spice, J. E. 1964. Chemical Bonding and Structure. Pergamon Press Ltd., Headington
   Hill Hall, Oxford. 395 pp.
2. Jan Drenth Principles of Protein X-ray Crystallography (Springer Advanced Texts in
   Chemistry), Springer-Verlag Telos.
3. Lipson, H. and Steeple, H., Interpretation of X-Ray Powder Diffraction Patterns. St.
   Martin's Press.
4. Bovey, F,A., Mirau, P.A. and Gutowsky, H.S., Nuclear Magnetic Resonance
   Spectroscopy (2nd Edition). Academic Press.
5. Hallet, F.R., Stinson, R.H., Speight, P.A. and Graham, W.G., 2004 Physics for the
   Biological Science, Toronto: Nelson Can.
6. Yadav, L.D.S., Organic Spectroscopy (1st Edition). Springer.
7. Hollas, J.M., High Resolution Spectroscopy (2nd Edition). John Wiley & Sons.

PAPER Binf 303: STRUCTURAL BIOLOGY AND PHARMACOGENOMICS
SECTION 1: STRUCTURAL BIOLOGY   (45L)

1) **Introduction to Structural Databases:** Protein Data Bank (PDB) at RCSB, Catalytic Site Atlas (CSA), Homology Derived Structures of Proteins (HSSP), Protein Data Bank Europe (PDBe), PDBeChem, PDBeFold, PDBeMotiff, PDBeNMR, PDBsum.   (5)

2) **Protein Secondary Structure Prediction Methods**
Statistical Methods of Chou and Fasman, Garnier-Osguthorpe-Robson, Stereochemical Method of Lim and Neural Network Method, etc, Fold Recognition and Threading Methods Position Specific Scoring Matrices Repeat Finding and pattern Recognition   (5)

3) **Classification of Three Dimensional Structures of Proteins**
Structural Classes, Motifs, Folds and Domains, Classification of Three Dimensional Structures in Brookhaven Protein Data Bank (HSSP, SCOP, FSSP, CATH).   (5)

4) **Folding pathways:** Principles of protein folding, hydrophobic interactions, electrostatic interactions, non-bonded interactions. Beta turns, gamma turns, types of helices, disulphide-bridge. Protein Structure Prediction: Secondary and tertiary. Structural Alignment Methods, Homology Modeling. Proteome analysis and Prediction of epitopes.   (5)

SECTION II: Pharmacogenomics

1) **History and overview:** Historical perspectives, current view of Pharmacogenomics. Introduction to pathway Databases.   (3)

2) **Molecular interactions:** protein-protein, protein-DNA, DNA-Drug, Protein-Lipid, Protein- Ligand, Protein-Carbohydrate interaction, Metalloproteins, Pi … Pi interactions, C-H…Pi interactions.   (7)

3) **Pharmacogenomics and drug design:** Need for protein structure information, Drug Discovery, Mutation in drug targets, Insilco drug design of small molecules, automated drug design, structure based drug design, and ligand based drug design methods, challenges of pharmacogenomics.   (10)

4) **Drug metabolism:** Role of cytochromes P450; Elimination half-life; Toxicity screening. The genetics of drug metabolism. The genetics of therapeutic drug targets.   (5)

Suggested Readings

1. Wilkins, M.R., Williams, K.L., Appel, R.D., Hochstrasser, D.F. (Editors) 1997 Proteome Research: New Frontiers in Functional Genomics. Springer Verlag Berlin Heidelberg.
2. Baxevanis, A.D. and Francis Ouellette, B.F. 2004 Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. Second Edition, Wiley.
3. Graur, D. and Li, W-H. 2000 Fundamentals of Molecular Evolution. Sinauer Ass., USA.
4. Tisdall, D., 2003 Mastering Perl for Bioinformatics. O'Reilly.

Paper Binf 304: RESEARCH METHODOLOGY IN BIOINFORMATICS

SECTION I: Research Methodology   **(45L)**

1) **Research** – Definition, Importance and Meaning of Research, Objectives of research, Characteristics of Research, Types of Research.   (5)
2) **Steps in Research:** Identification, Selection and Formulation of Research Problem, Research Questions, Research Design, Formulation of Hypothesis, Review of Literature. Problems encountered by researchers in India.
(5)
3) **Sampling Techniques**: Sampling theory, Types of Sampling, Steps in Sampling, Sampling and Non-sampling error, Sample Size, Advantages and limitations of Sampling. Collection of Data: Primary Data, Meaning, Data Collection Methods, Secondary Data, Meaning, Relevance's, Limitations and Cautions.   (5)
4) **Parametric Tests:** Testing of significance Mean, Proportion, Variance and Correlation, Testing for Significance of Difference between Means, Proportions, Variances and Correlation Co efficient. Chi-square tests, ANOVA One way and two ways. Research Report: Types of Reports, Styles of reporting, Seeps in drafting reports, editing the final draft, evaluating the final draft.   (10)

SECTION II: Project Architecture

1) **Introduction:** Introduction to Scientific papers and Journals, computer and internet application in Research.   (2)
2) **Thesis Writing:** Abstract, Introduction, Materials and Methods, Results and Discussion, Summary and Conclusion. References.   (7)
3) **Presentation of a scientific Paper / Document:** Preparation of Oral Presentation, and Poster Presentation for conferences. Use of Audio-Visual aids in Presentation.
(8)
4) **Preparation of Manuscript:** Author instructions, Methodology, modes of paper communication, criteria for publication.   (3)

Reference Books:

1. **Statistical Methods by S.P. Gupta.**
2. **Research Methodology, Method and Techniques by C.R. Kothari or by Santosh Gupta.**

Practical Paper Binf 305: Data Base Management Systems With Reference to Biological Data and Advanced Biophysical techniques

(45L)

1. Determination of absorption spectra of DNA
2. Estimation of DNA by DPA method.
3. Determination of absorption Spectra of RNA
4. Estimation of RNA by orcinol method.
5. Study of denaturation & renaturation curves of DNA.
6. Determination of absorption spectra of proteins.
7. Demonstration of Mass spectrometry.
8. PL-SQL Programmes.
9. Relational Datamodel programmes.
10. ER-Diagrams
11. Data mining studies and access with reference to Entrez, SRS, ExPasy, Net Phos.
12. Data mining studies and access with reference to UCSC, TIGR, COG, GLIMMER.
13. Access to Expert Protein Analysis System (Expasy tools).

Practical Paper Binf 306: Structural Biology & Pharmacogenomics and Research Methodology. **(45L)**

1. Accessing to Structural Databases and Data retrieval.
2. Protein 3D structure studies using CATH, SCOP resources.
3. Homology modeling by Threader and Modeller 9V2.
4. Developing protein interaction network.
5. Developing Ligand specific pathway from protein interaction network.
6. Docking studies by Hex 4.5 and Auto Dock 4.0.
7. QSAR, Discovery Studio Gene or MDL tools, ChemX, CADD.
8. Drug target and vaccine identification
9. Determination of epitope for a given protein.
10. Drug Bank,
11. ChemBank,
12. ACD-Lab.
13. Access to various scientific Journals and data retrieval.
14. Preparation of manuscript for publication.
15. Presentation of a scientific Paper / Document/Conference posters using power point.

M. Sc. IN BIOINFORMATICS SYLLABUS
SEMESTER- 4
Paper Binf 401: SIMULATION AND MODELING FOR BIOLOGISTS AND SOFT COMPUTING TECHNIQUES.   (45L)

SECTION –I Simulation and Modeling for Biologists

1) **Basics of simulation:** Introduction, general principles; Statistical models in simulation.   (5)
2) **Queuing models:** Random numbers, Random-variate generation; Input modeling, verification and Validation of simulation models, output analysis, Monte-Carlo simulation method   (5)
3) **Biological Models:** Population models, Models for Biochemical reaction kinetics, Epidemic models, Vegetation growth models, Bacterial growth model and Artificial Intelligence.   (3)
4) **Introduction to Simulation soft wares:** Open source and Commercial categories Example: - genostar, SOAP, REST, Simulation Methods: Molecular dynamics methods, Monte Carlo methods, Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics: Simulated annealing procedure. Initial configuration, Periodic Boundary conditions, Solvent access, Equilibration, cutoffs, Problems and remedies.   (7)

SECTION- II Soft Computing Techniques

1) **Introduction to Genetic Algorithm:** Genetic Operators and Parameters, Genetic Algorithms in Problem Solving, Theoretical Foundations of Genetic Algorithms, Implementation issues.   (5)
2) **Neural Model and Network Architectures:** Perceptron Learning, Supervised Hebbian Learning, Back propagation, Associative Learning.   (5)
3) **Competitive Networks**, Hopfield Network, Computing with Neural Nets and Applications of Neural Network.   (5)
4) **Computational Chemistry**: Concepts of computational chemistry, Born-Oppenheimer approximations semi-empirical methods.   (5)

Reference Books:

[1] Robert A. Muenchen and Joseph M. Hilbe. *R for Stata Users*. Statistics and Computing. Springer, 2010. ISBN: 978-1-4419-1317-3.
[2] Rob Kabacoff. *R in Action*. Manning, 2010. | http://www.manning.com/kabacoff]

[3] Christian Robert and George Casella. *Introducing Monte Carlo Methods with R*. Use R. Springer, 2010. ISBN: 978-1-4419-1575-7.

Paper Binf 402: BIODIVERSITY INFORMATICS AND IPR

(45L)

SECTION-I Biodiversity Informatics

1) **Introduction:** Basic Principles of Taxonomy & Phylogeny and Modern Taxonomical Methods. (5)

2) **Molecular Systematic:** Molecular data types, generation and analysis, Botanical Library and Systematic Databases. (5)

3) **Diversity of Life:** Genetic, Species, Community and Landscape Diversity, Species Diversity: Measurement methodologies, Indices. (5)

4) **Biodiversity Informatics:** Databases, National, Regional and Global Diversity

   Information Systems and Networks. Online Biodiversity and Ecosystem based Databases. (10)

SECTION-II Intellectual Property Rights (IPR)

1) **Introduction-** Intellectual property, Protection of Intellectual property, World organizations, forms of protection- patent, copyright, trademark, geographical indications, trade secrets. (5)

2) **Patent-** Criteria and procedure of patenting, patenting biological material. Patent procedure in India. Types of patenting, Patenting of biological materials with examples and case studies. (8)

3) **Technology transfer:** Introduction, types of technology transfer and Indian scenario.

   (3)

4) **Plant breeder's right**- UPOV, Breeders exemption, Plant variety protection in India. Farmer's right, advantages and disadvantages of PBR. (8)

Suggested Readings

1. Recknagel, F. 2002 Ecological Informatics: Understanding Ecology by Biologically-Inspired Computation. Springer, New York.
2. Phillipson, J. 1972 Ecological Energetics, Edward Arnold.
3. Odum, E.P. 1983 Basic Ecology. Saunders International Edition, Japan.
4. Atkinson, P.M. and Tate, N.J.(Eds.) 1999 Advances in remote sensing and GIS analysis., Wiley, New York.
5. Gunther,O. 1998 Environmental Information Systems. Berlin, New York, Springer.
6. Pankhurst, R.J. 1981 Practical taxonomic computing. Cambridge University Press, Cambridge, U.K.
7. Judd, W.S., Campbell, C.S., Kellogg, E.A.,Stevens, P.F. and Donoghue, M.J.(2002) Plant Systematics: A Phylogenetic Approach, 2nd Ed., Sinauer Associates, Inc. Publishers, Sunderland, Masssachusetts, U.S.A.
8. Nordenstam, B., El Gazaly, G. and Kassas, M. 2000 Plant Systematics for 21st Century Portland Press Ltd.,London.

Paper Binf 403: ADVANCED MOLECULAR BIOLOGY
(45L)

SECTION-I Genomics

1) **PCR techniques and Application:** Introduction to PCR, types of PCR, Designing of GSP, RAPD and 16s rRNA primers. *In-vitro* amplification of DNA. (5)
2) **cDNA Library:** Shotgun method, Construction and screening gene fragments from cDNA Library. (2)
3) **Blotting Techniques:** Preparation of DNA and RNA Probes, Southern, Northern, Western and Southwestern blot technique. Hybridization techniques: Colony Hybridization, Plaque Hybridization, *in situ* hybridization, Autoradiography. (8)
4) **Molecular Diagnostics:** Restriction Fragment Length Polymorphism (RFLP), Amplified Fragment Length Polymorphism (AFLP), Random Amplified Polymorphic DNA (RAPD). DNA Finger printing and Microarray. (5)

SECTION-II Proteomics

1) **Protein purification Techniques:** Isolation, Production and Purification (Ultra filtration, Ammonium sulphate precipitation, Dialysis. Column chromatography: Ion exchange, Affinity, Gel filtration. HPLC and GLC). (10)
2) **Electrophoresis:** Basic principles of electrophoresis, SDS-PAGE, Native PAGE, IEF, 2D electrophoresis: First dimension criteria, second dimension criteria, Stabilization, Detecting protein on gel, Electro blot, Image analysis, Digital imaging, Spot detection and quantification, Gel matching and Analysis.

(8)

Protein sequencing and amino acid analysis: Different methods of protein sequencing, Automated Protein sequencers and amino acid analyzers. Analysis of protein sequences (ExPasy Tools) and peptide mass fingerprint using MASCOT

(5)

3) **Site Directed Mutagenesis:** Introduction to SDM, Methodology and Applications. (2)

Suggested Readings

1. Surzycki, S. 2000 Basic Techniques in Molecular Biology. Spring Verlag.
2. Celis, J.E., Cell Biology: A Laboratory Handbook 2nd Edition
2. Ninfa, A.J. and Ballou, D.P. 1998 Fundamental Laboratory Approaches for Biochemistry and Biotechnology.
4. Ausubel et. al. 2002 Short Protocols in Molecular Biology. Wiley.
5. Sambrook et. al. 2001 Molecular Cloning. CSHL.
6. Bartlett 2003 PCR Protocols: Methods in Molecular Biology, Vol. 226 2nd Edition.
7. Simpson, R.J. 2004 A Laboratory Mannual Purifying Proteins for Proteomics. Cold Spring Harbor Laboratory Press, New York.

Paper Binf 404: EMERGING AREAS OF BIOINFORMATICS (45L)

SECTION-I Chemoinformatics And Immunoinformatics

1) **Basics of Cheminformatics:** Introduction to Cheminformatics, Evolution of Cheminformatics, History of Chemical Information Science, Use of Cheminformatics, Prospectus of Cheminformatics.
(5)

2) **Medicinal Chemistry:** Prodrugs and Soft Drugs, Drug Targets, Drug Solubility, Natural Resources of Lead Compounds, Pharmacokinetics & Drug Metabolism, Biological Testing and Bioassays, Preclinical Testing and Clinical Trial, Synthesis. (5)

3) **Use of Bioinformatics in Immunology:** Bioinformatics strategies for better understanding of immune function, Future of computational modeling and prediction systems in clinical immunology, Role of Immunoinformatics in personalized medicine.
(5)

4) **Immunome Databases:** International immunogenetics information system. peptide repertoire in HLA molecules, HLA nomenclature and IMGT/HLA sequence databases. Viral bioinformatics-computational views of host and pathogen. (5)

SECTION-II Thrust Areas

1) Nano-Biotechnology and Nanoinformatics: Introduction to nanoparticles, synthesis and analysis of nanoparticles and its applications. (5)

2) Bioinformatics in agriculture: Introduction and Application of Remote Sensing and GIS (Geographical information system) for agriculture. (5)

3) Bioinformatics in forestry: Introduction and application of bioinformatics in forestry, Bio-Informatics in present scenario. (5)

4) **Genome Sequencing Projects and applications:** Introduction to various Genome Sequencing Projects and their implications in human health and diseases. (10)

Suggested Readings
1. Gasteiger, 2003 Chemoinformatics A Text Book.
3. Bujnicki, J.M. 2004 Practical Bioinformatics (Series: Nucleic Acids & Molecular Biology Vol. 15). Springer.
3. Hassan, A.S. 2004 Bioinformatics: Principles and Basic Internet. Trafford Publishing.
4. Kohane, I.S., Kho, A. and Buthe, A.J. 2002 Microarrays for an Integrative Genomics. Barnes & Noble, MIT Press.
5. Lengauer, T. et. al. 2001 Bioinformatics: From Genomes to Drugs. Wiley-VCH.
8. Tudor, I.O., Mannhold, R. Kubinyi, H. and Folkers, G. Chemo Informatics in Drug Discovery (Methods and Principles in Medicinal Chemistry).
7. Jensen, F. Introduction to Computational Chemistry. John Wiley & Sons
8. Stan Tsai, C. An Introduction to Computational Biochemistry 1st Edition. John Wiley & Sons. Inc.
9. Vyas, S.P. and Kohli, D.V. Methods in Biotechnology and Bioengineering.

Practical Paper Binf 405: Simulation and Modeling for Biologists and Soft Computing Techniques & Biodiversity and IPR and Advanced Molecular Biology & Emerging areas of Bioinformatics.

(45L)

1) VAST Alignment Algorithm
2) Study of open source simulation tools
3) Demonstration of Monte-Carlo method of Simulation algorithm.
4) Online neural network prediction.
5) GRAIL algorithm using EBI support.
6) Protein 3D structural simulation studies by 3D-PSSM.
7) Study of plant libraries and Systematic databases.
8) Biodiversity informatics and database studies.
9) Online Biodiversity and Ecosystem based Database studies.
10) A report on Intellectual Property Rights.
11) Isolation of Genomic DNA from different samples
12) Isolation of total cellular RNA and quantification.
13) Purification of proteins by chromatographic techniques.
14) Zymogram analysis by Native PAGE and Determination of molecular weight of proteins by SDS-PAGE.
15) PCR Amplification of a given gene.
16) Analysis of PCR product in Gel by Gel Documentation system
17) Demonstration of DNA and protein sequencing (Visit to Institute).
18) Introduction to chemoinformatics and immunoinformatics resources

Practical Paper Binf 406: PROJECT DESERTATION AND VIVA VOCE

Students have to begin their projects in 3rd Semester and submit the report in 4th Semester