Solapur University, Solapur

M.Sc. Bioinformatics
Part II
(New Credit Based Semester pattern)
Syllabus
w. e. f. June 2014

SEMESTER – III THEORY			
Paper	**Title**	**Credits**	**Total Marks**
Binf-301	Biological Database Management System	4	100
Binf-302	Advanced Biophysical Techniques	4	100
Binf-303	Computational Structure Biology and Drug designing	4	100
Binf-304	Research Methodology in Bioinformatics	4	100
SEMESTER – III PRACTICALS			
BinfPr-305	Biological Database Management System and Advanced Biophysical Techniques	4	100
BinfPr-306	Computational Structure Biology and Drug designing and Research Methodology in Bioinformatics	4	100
	Seminar		25
		TOTAL	**625**

SEMESTER – IV THEORY			
Paper	**Title**	**Credits**	**Total**
Binf-401	Biological Simulation and modeling	4	100
Binf-402	Biodiversity informatics and Intellectual Property Rights	4	100
Binf-403	Advanced Molecular biology	4	100
Binf-404	Emerging Areas of Bioinformatics	4	100
SEMESTER – IV PRACTICALS			
BinfPr-405	Biological Simulation and modeling, Biodiversity informatics and Intellectual Property Rights, Advanced Molecular biology and Emerging Areas of Bioinformatics.	4	100
BinfPr-406	Project dissertation and Viva Voce	4	100
	Seminar		25
		TOTAL	**625**

As per the credit system, the assessment of Theory paper of 100 marks weightage will be as:
70 marks theory assessment by University examination and 30 marks internal assessment by the Department. For internal assessment of candidate, periodical tests/seminars/ viva/oral / quiz etc. may be suitably adopted.

M. Sc. IN BIOINFORMATICS SYLLABUS

SEMESTER- III

Paper-Binf 301: BIOLOGICAL DATA BASE MANAGEMENT SYSTEM

(45L- 4 CREDITS)

Unit-I: Introduction to DBMS Architecture: Actors on scenes, worker behind the scene, database designing, data acquisition, data models, schemes, three schemes architecture, data-independence Data Modeling using E-R model Domains, Entity, attributes, tuples, conceptual design of company database, refining E-R design for company database, designing of various biological databases. **(10)**

Unit-II: Data mining: An overview of Data mining technology, classifications, clustering, data warehousing, Applications of Data mining, Access to Molecular biology data bases: Entrez, Sequence retrieval system, (SRS), Protein Identification Resources (PIR) and Bibliographic databases. **(5)**

Unit-III: Data Normalization for RDBMS: Introduction to RDBMS, Relational model concept, characteristics of relations, entity integrity, relational integrity and keys. Introduction, design, guidelines for relational schemes, semantic of attributes, Introduction to Normalization 1NF, 2NF, 3NF, BCNF, Introduction to relational algebra & calculus. **(15)**

Unit-IV: Overview of Oracle: Objectives, Introduction, Database Management Tools, The data dictionary, DBA, The utilities. Structures in Oracle, Physical structure, Data files, Control files, Logical structure. Introduction to SQL, Objectives, SQL Select Statements, Data Manipulation Statement, Data Definition Statements, Data Control Statements, Data query language, Basic SQL queries, more complex SQL queries, views in SQL. **(10)**

Unit -V: Basics of PL-SQL: Introduction to PL-SQL, syntax, commands & different querying types, applications in Bioinformatics by using PL-Block. **(5)**

References:

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

(45L-4 Credits)

Unit-I: Fundamentals of chemical bonding and non-bonding interactions: Electrovalent bond, stability of electrovalent bond. Covalent 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. (10)

Unit-II: Spectroscopy: Principles, Theory, Instrumentation and Application of UV-Visible, IR, FTIR, CD and ORD to macromolecules, Mass spectrometry; Introduction, different methods of ionization, MALDI-TOF, Analysis and application. NMR; Principles, Theory, Instrumentation and Application. (15)

Unit-III: Lasers: Introduction, basic working principle of lasers, types of lasers, importance and applications of lasers in biological studies (treatment and analysis). (5)

Unit-IV: X-ray crystallography: Early scientific history of crystals and X-rays, Principles, Theory, Instrumentation, Properties, sources of X-radiation, Application of X-rays to biology and medicine (diagnosis and molecular structure studies.). (5)

Unit-V: Microscopy: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM), Fluorescent Microscopy and Confocal Microscopy, Infra Red Microscopy and Raman Microscopy. (10)

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: COMPUTATIONAL STRUCTURE BIOLOGY AND DRUG DESIGNING

(45L- 4 CREDITS)

Unit -I: Introduction to Structural and Pathway Databases: structural data, exploring the structural databases such as 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, SCOP and CATH. Introduction to biological Pathway Databases. (9)

Unit -II: Structure Prediction Methods: Statistical methods of Chou-Fasman, Garnier-Osguthorpe-Robson method, Neural network method, Position specific scoring matrices, Motifs and domains, folds and protein folding. (9)

Unit -III: Homology Modeling: Introduction to homology modeling, Fold recognition and Threading, RNA structure prediction, architectures and topologies of protein and DNA using molecular visualization software, Structure validation. (6)

Unit -IV: Molecular interaction: Molecular interaction; protein-protein, protein-DNA, Protein-Lipid, Protein- Ligand, Protein-Carbohydrate, DNA-Drug interaction, Metalloproteins, Pi … Pi interactions, C-H…Pi interactions. (6)

Unit -V: Drug Discovery and Drug designing: Natural products, drugs, principles of drug development, Drug discovery, mutation in drug targets, automated drug design, structure based and ligand based drug design methods, combinatorial chemistry, high throughput screening (HTS), *in silico* ADMET properties, QSAR, developing lead library, DOCKING; introduction to docking method to generate new structure, tools and molecular docking programs-AUTODOCK, HEX, Drug metabolism; Cytochrome p450, pharmacodynamics and pharmacokinetics, clinical trials, FDA approval. (15)

Suggested Readings

1. Wilkins, M.R., Williams, K.L., Appel, R.D., Hochstrasser, D.F. (Editors) 1997
2. Proteome Research: New Frontiers in Functional Genomics. Springer Verlag Berlin Heidelberg.
3. Baxevanis, A.D. and Francis Ouellette, B.F. 2004 Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. Second Edition, Wiley.
4. Graur, D. and Li, W-H. 2000 Fundamentals of Molecular Evolution. Sinauer Ass.,USA.
5. Essential Bioinformatics, Jin Xiong
6. Rastogi S. C., Mendiratta. N., Rastogi. P. 2005 Bioinformatics methods and application, Genomics, Proteomics, and Drug Discovery.

Paper-Binf 304: RESEARCH METHODOLOGY IN BIOINFORMATICS

(45L- 4 CREDITS)

Unit-I: Research– Definition, Importance and Meaning of Research, Objectives of research, Characteristics of Research, Types of Research. 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. (15)

Unit-II: 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, Relevances, Limitations and Cautions. (10)

Unit-III: 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, Steps in drafting reports, editing the final draft, evaluating the final draft. (10)

Unit-IV: Thesis and Manuscript writing: Abstract, Introduction, Materials and Methods, Results and Discussion, Summary and Conclusion, References (IMRAD). Preparation of Manuscript; Author instructions, Methodology, modes of paper communication, criteria for publication.

(5)

Unit-V: Project Architecture: Introduction to Scientific papers and Journals, computer and internet application in Research. Presentation of a scientific Paper / Document: Preparation of Oral Presentation and Poster Presentation for conferences. Use of Audio-Visual aids in Presentation. (5)

Reference Books:

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

Practical Paper-Binf 305: Biological Data Base Management Systems and Advanced Biophysical techniques

(45L- 4 CREDITS)

1. Determination of absorption spectra of DNA.
2. Estimation of DNA by DPA method.
3. Estimation and Purity check of DNA using UV spectroscopy.
4. Estimation of RNA by Orcinol method.
5. Demonstration of FTIR.
6. Demonstration of Mass spectroscopy.
7. Practical based on "Data Definition Language"
8. By using DDL statements create table, modify table structure, drop table, rename table.
9. Practical based on "Data Manipulation Language"
10. Change the data within the database using SQL commands.
11. Data manipulation and updating of all or specific set of records in tables, viewing the attributes of table's column.
12. Perform queries using "Data Query Language"
13. Extracting the data out of the database using group function, min, max, order by clause, where clause, having clause.
14. Create a Biological table by defining constraints, like Primary Key, Foreign Key, Null and Unique constraints.
15. PL –SQL Programmes.
16. E-R Diagrams with reference to Biological Database.
17. Data mining studies and access with reference to Entrez, SRS.
18. Data mining studies and access with reference to UCSC, TIGR, EXPASY.

Practical Paper-Binf 306: Computational Structure Biology & Drug designing and Research Methodology. **(45L- 4 CREDITS)**

1. Accessing to Structural Databases and Data retrieval using RCSB PDB, CSA, PDBe, PDBeChem, PDBeFold, PDBeMotif, PdbSum.
2. Structural classification using CATH, SCOP resources.
3. Accessing biological pathway using KEGG, EMP and BIOCARTA.
4. Secondary structure prediction using SOPMA and GOR.
5. Fold recognition using 3DPSSM and Phyre
6. Homology modeling by SWISSMODEL, SPDBV and Modeller 9V2.
7. Model Validation using RAMPAGE or PRocheck.
8. Prediction of protein-protein, protein-DNA, protein-ligand interactions.
9. Developing protein interaction network.
10. Drugbank database
11. Chembank database
12. Design of ligands using ACD lab and Chemsketch.
13. Development of lead library and high throughput screening.
14. *In silico* ADMET Properties.
15. Docking studies using AUTODOCK and HEX.
16. Access to various scientific Journals and data retrieval.
17. Preparation of manuscript for publication.
18. Presentation of a scientific Paper / Document/Conference posters using power point.

M. Sc. IN BIOINFORMATICS SYLLABUS
SEMESTER- IV

Paper-Binf 401: BIOLOGICAL SIMULATION AND MODELING

(45L- 4 CREDITS)

Unit-I: Basics of Simulations: Introduction, general principles, models in simulations, quantum chemistry, Schrodinger equation, potential energy functions, energy minimization (global and local minima), molecular modeling methods. (10)

Unit-II: Molecular Mechanics: Definition, balls and springs, force fields; stretch, bend, torsion, etc, conformational search, full geometry optimization methods ZDO, MNDO, CNDO, NDDO, AMI, PM3, RMI, mechanics of biomacromolecules. (10)

Unit-III: Molecular Dynamics: Newton's equation for particles, Verlet and related algorithms, types of dynamics simulations; adiabatic, constant T, simulated annealing, molecular dynamics methodology, docking simulations, dynamics of biomacromolecules. (10)

Unit-IV: Introduction to Python: Introduction to python, working with data, program organization and functions, modules and libraries, classes and objects. (8)

Unit-V: Programming with Python: Python object system; inside the python object system, testing and debugging, iterators and generators, working with text, processors. (7)

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-4 CREDIT)

Unit-I: Introduction to Biodiversity Informatics: Global patterns of distribution of biodiversity, biomes, cause and consequences of biodiversity loss, species extinction, basic principles of taxonomy and phylogeny, modern taxonomical methods**.** (9)

Unit-II: Molecular Systematics: Molecular data types, generation and analysis, molecular databases, taxanomic database working group (TDWG), standards, compatibility and interoperability, botanical library and systematic databases, online biodiversity and ecosystem based database. (9)

Unit-III: Diversity of Life: Levels of biodiversity-genetic, species, community and landscape diversity, measurement methodologies and indices, hotspots of biodiversity, threats to biodiversity, conservation of biodiversity, Remote sensing and GIS, National, regional and global diversity information systems and networks. (9)

Unit-IV: Introduction to IPR and Patents: Intellectual property, Protection of Intellectual property, World organizations, forms of protection- patent, copyrig4ht, trademark, geographical indications, trade secrets. Criteria and procedure of patenting, patenting biological material. Patent procedure in India. Types of patenting, Patenting of biological materials with examples and case studies. (9)

Unit-V: Plant breeder's right: UPOV, Breeders exemption, Plant variety protection in India. Farmer's right, advantages and disadvantages of PBR**.** Technology transfer- Introduction, types of technology transfer and Indian scenario (9)

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-4 CREDITS)

Unit-I: PCR Techniques and Applications: Introduction to PCR, types of PCR; Real time PCR, Reverse transcription PCR , Multiplex-PCR, Designing of GSP, RAPD and 16s rRNA primers. *In vitro* amplification of DNA, DNA sequencing, Site Directed Mutagenesis; Introduction to SDM, Methodology and applications. (9)

Unit-II: rDNA Technology: Genomic library; Shotgun method, construction and screening of gene fragments, cDNA Library. 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. (9)

Unit-III: Molecular Markers and Applications: Restriction fragment length polymorphism (RFLP), Amplified fragment length polymorphism (AFLP), Random amplification of polymorphic DNA (RAPD), Simple sequence length polymorphism (SSLP), Variable number tandem repeat (VNTR), Microsatellite polymorphism or Simple sequence repeat (SSR), Single nucleotide polymorphism (SNP), Short tandem repeat (STR), DNA Finger printing and Microarray. (9)

Unit-IV: Protein Purification Techniques: Isolation, Production and Purification (Ultra filtration, Ammonium sulphate precipitation, Dialysis. Column chromatography; Ion exchange, Affinity, Gel filtration, HPLC and GLC. Electrophoresis; Basic principles of electrophoresis, SDS-PAGE, Native PAGE, IEF, 2D electrophoresis; Detecting proteins on gel, Electro blot, Image analysis, Digital imaging, Spot detection and quantification, Gel matching and Analysis. (9)

Unit-V: Protein Sequencing and Amino Acid Analysis: Different methods of protein sequencing, automated Protein sequencers and amino acid analyzers. Analysis of protein sequences using ExPasy Tools and peptide mass fingerprint analysis using MASCOT. (9)

Suggested Readings

1. Surzycki, S. 2000 Basic Techniques in Molecular Biology. Spring Verlag.
2. Celis, J.E., Cell Biology: A Laboratory Handbook 2nd Edition
3. 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- 4 CREDITS)

Unit-I: Chemoinformatics: Introduction to chemoinformatics, evolution and history of chemical information science, prospectus of chemoinformatics, chemical information source, chemical databases, chemical structure representation (1D, 2D and 3D structures), molecular file formats (SMILES, MOL, SDF, etc). (10)

Unit-II: Immunoinformatics: Bioinformatics strategies for better understanding of immune function, future of computational modelling and prediction systems in clinical immunology, immunoinformatics overview, immunoinformatics databases and tools (IMGT, IEDB, Epitome, etc), prediction of MHC class I and II, prediction of T and B cell epitopes, reverse vaccinology and *in silico* vaccine designing. (15)

Unit-III: Genome sequencing projects and applications: Introduction to various genome sequencing projects and their implications in human health and diseases. Genome data visualization using Ensemble and Mapviewer. (5)

Unit-IV: Nano Biotechnology: Introduction to nanoparticles, biological, chemical and mechanical synthesis of different nanoparticles, analysis of nanoparticles using UV-Visible spectroscopy, FTIR and NMR. Applications of nanoparticles. (8)

Unit-V: Pathology informatics: Introduction to pathology informatics, study of pathogen genomes (bacteria, fungi and viruses), databases, computational study of host–pathogen interactions (Animals and Plants). (7)

Suggested Readings

1. Gasteiger, 2003 Chemoinformatics A Text Book.
2. 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.
6. 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

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

(45L- 4 CREDITS)

1) Genostar tool.
2) Model building, energy minimization of biomolecules using simulation tools.
3) Model building of oligopeptides / oligonucleotides using Pymol and DS tools.
4) Geometry optimization of biomolecules using simulation tools.
5) Practicals based on Python.
6) Study of plant libraries – VPLANT.
7) Systematic databases and libraries - PLANTS
8) Study of Biodiversity database – GBIF.
9) Taxonomic database – TDWG.
10) A report on Intellectual Property Rights.
11) Isolation of Genomic DNA from different sources (soil & blood).
12) Isolation of total cellular RNA and quantification.
13) Isolation and purification of proteins.
14) Demonstration of Southern and Western blotting techniques.
15) Zymogram analysis by Native PAGE and Determination of molecular weight of proteins by SDS-PAGE.
16) PCR Amplification of a given gene and Gel electrophoresis.
17) Demonstration of DNA and protein sequencing (Visit to Institute).
18) Chemical structure representation using Marvin Sketch & Pubchem.
19) A brief introduction to ISIS database with special emphasis on the storage of chemical in the database format.
20) Study of Immunoinformatics resource – IMGT.
21) Genome data analysis using Ensembl and Mapviewer.
22) Epitope prediction and vaccine designing.
23) Synthesis of nanoparticles by chemical and biological methods.

Practical Paper Binf 406: PROJECT DISSERTATION AND VIVA VOCE

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