

**DEPARTMENT OF COMPUTATIONAL BIOLOGY AND
BIOINFORMATICS**

UNIVERSITY OF KERALA



**M.PHIL PROGRAMME IN COMPUTER AIDED DRUG DESIGN
SYLLABUS**

Under credit and semester system w. e. f. 2016 admissions

**DEPARTMENT OF COMPUTATIONAL BIOLOGY AND BIOINFORMATICS
UNIVERSITY OF KERALA**

SYLLABUS

M. Phil. PROGRAMME IN COMPUTER AIDED DRUG DESIGN

PROGRAMME OBJECTIVES

- *To impart relevant scientific knowledge that underpins various concepts in Computer Aided Drug Design.*
- *To expose students to popular genomic and proteomic databases and to impart knowledge and skills in processing and analyzing these data.*
- *To impart state of the art generic knowledge about diseases and drugs from theoretical, practical and commercial viewpoints.*
- *To impart knowledge and skills in molecular modelling and docking.*

STRUCTURE OF THE PROGRAMME

Semester No.	Course code	Name of the course	Number of Credits
I	BIN -711 (II)	Research Methodology	4
	BIN -712 (II)	Introduction to Bioinformatics	4
	BIN -713 (II)	Advanced Topics in CADD	4
	BIN -714 (II)	CADD and Molecular Biology Lab	4
	BIN -715 (II)	Applied Mathematics & Scientific Computing	0
	BIN -716 (II)	Introduction to Informatics (E)	0
	BIN -717 (II)	Introduction to Biosciences (E)	0
II	BIN -721 (II)	Dissertation	20
		TOTAL CREDITS	36

Semester : I
Course Code : BIN 711 (II)
Course Title : RESEARCH METHODOLOGY
Credits : 4

AIM: To expose students to creative and critical thinking skills as relevant to a scientific research and innovation process and introduce the student to current professional issues in research process and allied areas.

COURSE OBJECTIVES:

- To develop an in-depth understanding of the scientific method and research process management.
- To trigger the creativity of students
- To temper research attitudes and skills
- To create awareness about current issues related to research management and ethics

COURSE CONTENT

Module I: Creativity, Innovation & Thinking Skills: Various views on creativity; characteristic features of creativity; stimulating creativity; obstructions to creativity; creativity & innovation, creativity & craft; *Thinking skills:* critical thinking, logical thinking – inductive & deductive logic – common logical fallacies; *Problem solving strategies*, Visual thinking- Mind mapping; Lateral thinking.

Module II: Research and Scientific Method: Various outlooks on Research; Types of research: pure versus applied, incremental versus innovative, qualitative versus quantitative; *Philosophy of science*; the scientific method, evolution & philosophy, falsifiability, the research process –creative question –hypothesis – planning and designing of experiments – critical analysis – sources of errors and minimization.

Module III: Publishing Science: Formats of a science research paper – the IMRAD format – objectives of each section – reference citing styles; Proof reading & editing; Authorship models; Publication process -Peer review – single/double blind and open; Open Access publications and other emerging trends in scientific communication; case study of designing and conducting experiments, paper writing and peer review, Making effective multimedia and poster presentations, Writing research proposal, Major funding agencies.

Module-IV: Information Literacy Skills: Learning about Learning- multiple intelligences- learning styles; Active reading, listening and comprehension skills; Advanced internet search skills –Google scholar and scopus; Current awareness: TOC alerts, DB alerts, popular journals in Computational Biology & Bioinformatics (brief overview of their scope). Journal Indexing and Scientometrics, Bibliometrics and webometrics – impact factors –h, h-b and g indices – pitfalls in interpreting impact; Ethics – its role in scientific research and academics. Fabrication, falsification and plagiarism, Introduction to Latex, Reference management tools: diigo, zotero, mind manager, endnote; Plagiarism- URKUND, Turnitin, Social Media in research.

Module V: Professional Issues: IPR: Intellectual property Vs physical property, Types of IP, Copylefts, copyrights and patents; Argument for and against patenting, Current issues in IPR: Brief overview of IPR laws in India, IPR of software and life forms; Protection of

traditional knowledge; Product Vs Process, Patent amendment of 2005 and its impact. – International administration of IP, Profile of key Bioinformatics/ CB/ Industries. Job opportunities in CB/BI skill profiles. Nature of Ethics as an academic discipline- Normative ethics- Meta ethics- Ethics in Science and Technology- Environmental ethics- Cyber ethics- Bioethics (Abortion, Euthanasia, surrogacy, cloning etc.)- Ethical codes- Human values and attitudes.

ASSESSMENT

End-Semester Assessment (100 marks):

3 hour written exam consisting of 30% short answer questions, 40% descriptive questions and 30% long essay questions.

REFERENCES:

- Ahuja, Virendra Kumar. *Law Relating to Intellectual Property Rights*. LexisNexis Butterworths, 2007.
- Buzan, Tony. *Mind maps at work*. Thorsons, 2004.
- Bouchoux, Deborah E. *Intellectual property: The law of trademarks, copyrights, patents, and trade secrets*. Cengage Learning, 2012.
- Buzan, Tony. *The power of creative intelligence*. HarperCollins UK, 2001.
- De Bono, Edward. *How to have creative ideas: 62 exercises to develop the mind*. Random House, 2007.
- Gastel, Barbara, and Robert A. Day. *How to write and publish a scientific paper*. ABC-CLIO, 2016.
- Katz, Michael Jay. *From research to manuscript: a guide to scientific writing*. Springer Science & Business Media, 2009.
- Lee, Jeffrey A. *The scientific endeavor: A primer on scientific principles and practice*. Benjamin-Cummings Publishing Company, 2000.
- Lester, James D. *Research Paper Handbook: Your Complete Guide*. Good Year Books, 2005.
- Murray, Rowena. *How to write a thesis*. McGraw-Hill Education (UK), 2011.
- Piscitelli, Steve. *Study skills: Do I really need this stuff?*. Pearson Higher Ed, 2012.
- Ramkumar, Mu. *Intellectual Property Rights Demystified*. New India Publishing, 2008.
- Robert Allen. *Boost your creativity*. Pavilion Books, 2005.

ADDITIONAL REFERENCES

- Abrams, Rhonda. *“Winning presentation in a day: get it done right, get it done fast”*. Planning Shop, 2005.
- Bassham, Gregory. *“Critical thinking: A student’s introduction”*. Tata McGraw Hill Education Pvt. Ltd, 2011.
- Friedland, Andrew J., and Carol L. Folt. *“Writing successful science proposals”*. Yale University Press, 2009.
- Kitchin, Rob, and Duncan Fuller. *“The academic’s guide to publishing”*. Sage, 2005.
- Mak, Don K., Angela T. Mak, and Anthony B. Mak. *“Solving everyday problems with the scientific method: thinking like a scientist”*. 2009.
- Mark Barness. *“Time to Think”*. Westland Ltd, 2000. Syllabus of M. Phil CADD (2016 onwards)
- Marlene Caroseli. *“Quick Wits: 50 Activities for Developing Critical Thinking Skills”*. Ane Books, 2004.
- Meredith, Dennis. *“Explaining research: How to reach key audiences to advance your work”*. OUP USA, 2010.
- Oech, Roger von. *“A whack on the side of the head: How to unlock your mind for innovation”*. Fine

communications, 2001.

- Petre, Marian, and Gordon Rugg. *"The unwritten rules of PhD research."* McGraw-Hill Education (UK), 2010.
- Sloane, Paul. *"The Leader's Guide to Lateral Thinking Skills: Unlock the Creativity and Innovation in You and Your Team."* Kogan Page Publishers, 2017.

MOOC COURSES

- Ignite Your Everyday Creativity: <https://www.coursera.org/learn/ignite-creativity>
- Learning How to Learn: <https://www.coursera.org/learn/learning-how-to-learn/outline>

Semester : I
Course Code : BIN 712 (II)
Course Title : INTRODUCTION TO BIOINFORMATICS
Credits : 4

AIM: To introduce the students to the sequence-level understanding of genomics and allied areas and to familiarize the related data bases, tools and important problems.

COURSE OBJECTIVES:

- To impart knowledge and skills in basic Molecular Biology, Genomics, sequencing informatics
- To familiarize the concept of phylogenetics, proteomics and allied areas in Bioinformatics.

COURSE CONTENT

Module I: Composition of DNA- (Chargaff's Rule), String view of DNA, Reading frames +1, +2, +3 and -1, -2, -3, ORFs, sense/coding and anti-sense/template strands, codon-genetic code, gene expression- Transcription, translation; microsatellite, minisatellite, tandem and inverted repeats, SNPs, Basic file formats, TIGR, BLAST & FASTA file formats, Sequence Data Bases, detailed study of GenBank of NCBI- typical Gen Bank (DDBJ+EMBL) entry for DNA and RNA. Basic gene statistics-base counts, word (n- mer) frequencies, sequence logos, sequence chromatograms, sequence profiles, Codon usage bias, Genome annotation- gene finding, splice site recognition, transcription factor binding site identification, RNA structure prediction.

Module II: Sequencing Informatics, History of DNA sequencing- Maxam and Gilbert, Sangers method, Sequence alignments: Pair-wise sequence alignment, Need of Scoring schemes- Penalizing gaps; Scoring matrices for amino acid sequence alignment, PAM Probability matrix and Log odds matrix; BLOSUM, Dot-plot visualization; Needleman-Wunch algorithm effect of scoring schemes- e values, bit scores and sensitivity specificity; BLAST and FASTA, Smith- Waterman algorithm for local alignment; Multiple sequence alignment, SP measure- n dimensional dynamic programming, Tools for local, global and MSA : Clustal W, Muscle, Toffee.

Module III: Molecular Phylogenetics: concepts of similarity homologous, orthologous and paralogous sequences, Concept of phylogenetics - Basic terminology-taxa, taxonomy, clade, root, leaf, node graph & tree, dendrogram, cladogram, rooted tree, unrooted tree, scaled trees-Molecular clock hypothesis, Distance based methods-UPGMA, NJ algorithm, Character based methods-Maximum parsimony methods. Validating phylogenetic trees – jack knifing and bootstrapping, Tree calibration, Application of Phylogenetic trees, Study of Phylip, NJ plot, Clustal X and other popular software.

Module IV: Protein Structure: Interatomic forces and protein structure; covalent interaction, hydrogen bonds, hydrophobic and hydrophilic interaction, charge/dipole interaction, Vander waals forces, steric interaction. Primary structure; 20 amino acids as structural units, peptide bonds, proteins as polypeptides. Secondary structure; Alpha

helices, Beta sheets and turns, Backbone flexibility- Φ and ψ - Properties of amino acids- Hydrophobicity, EIIP, Molecular weight, α and β propensities. Tertiary and quaternary structures, protein folding, protein domains, Ramachandran plot and its significance.

Module V: Proteomic Tools & Databases: Protein visualization tools- Swiss PDB Viewer, Pymol. Sequence manipulation suite. Protein databases: UniProtKB/Swiss-Prot, PDB, SCOP & CATH, ProDom, PFAM; Chou Fasman method- $p(a)$, $p(b)$ and $p(\text{turn})$ propensities, Garnier Osguthorpe and Robson(GOR) method, Threading, Homology modeling, CASP, *ab-initio* prediction, Introduction to proteomic tools: Phyre, JPred, 3DPSSM, 123D, Modeller, Procheck, ITASSER; Prediction of function. Introduction to molecular docking, conformational energy calculation.

Module VI: Overview of Genome Sequencing, Next generation DNA sequencing Informatics, Introduction to NGS technology, advantages, limitations and applications, Different methods of NGS technology:- Genomics- Whole genome sequencing, Exome sequencing, Transcriptomics- RNA sequencing, NGS Data analysis -Data formats, Data handling, Quality checking, preprocessing, Basic concepts about data alignment and genome assembly, BWA, Bowtie, Genome/Exome Variant calling, VCF Genome Browsers, Epigenomics- MeDIP, ChIPSeq; Application of NGS in Clinical diagnosis.

ASSESSMENT

End-Semester Assessment (100 marks):

3 hour written exam consisting of 30% short answer questions, 40% descriptive questions and 30% long essay questions.

REFERENCES

- Agostino, Michael. *Practical bioinformatics*. Garland Science, 2012.
- Aoyama, Yukiya, and Jun Nakano. *Rs/6000 sp: Practical MPI programming*. Poughkeepsie, New York: IBM, 1999.
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- Bergeron, Bryan P. *Bioinformatics computing*. Prentice Hall Professional, 2003.
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- Lesk, Arthur. *Introduction to genomics*. Oxford University Press, 2017.

- Lewin, Benjamin, et al. *Lewin's genes X*. Vol. 10. Jones & Bartlett Learning, 2011.
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- Orengo C, Jones D. T., & Thornton J. M., *Bioinformatics: Genes, proteins and computers*. Garland Science, 2012
- Pierce, Benjamin A. *Genetics: A conceptual approach*. Macmillan, 2012.
- Ramsden, Jeremy. *Bioinformatics: an introduction*. Vol. 21. Springer, 2015.
- Rastogi, S. C., Parag Rastogi, and Namita Mendiratta. *Bioinformatics Methods and Applications: Genomics Proteomics and Drug Discovery 3Rd Ed*. PHI Learning Pvt. Ltd., 2013.
- Snustad, D. P. Simmons, M. J. Jenkins, J. B. & Crow J. F. *Principles of genetics*. John Wiley, 2000.
- Supratim Choudhari, *Bioinformatics for Beginners*, Elsevier, 2014.
- Tropp, Burton E. *Molecular Biology*. Jones & Bartlett Publishers, 2012.
- Xiong, Jin. *Essential bioinformatics*. Cambridge University Press, 2006.
- Zvelebil, M., and J. O. Baum. *Understanding Bioinformatics, Holdsworth*. Diss. D., ed. (Garland Science, Taylor & Francis Group, LLC, an informa business), 2008.

ADDITIONAL REFERENCES

- BED Tools: <https://code.google.com/p/bedtools/>
- Bowtie: [http:// http://bowtie-bio.sourceforge.net/index.shtml](http://http://bowtie-bio.sourceforge.net/index.shtml)
- DESeq: <http://bioconductor.org/packages/release/bioc/html/DESeq.html>
- DEXSeq: [http:// http://bioconductor.org/packages/release/bioc/html/DEXSeq.html](http://http://bioconductor.org/packages/release/bioc/html/DEXSeq.html)
- HTSeq-count: [http:// http://www.huber.embl.de/users/anders/HTSeq/doc/count.html](http://http://www.huber.embl.de/users/anders/HTSeq/doc/count.html)
- <http://159.226.149.45/kizsjzx/hpc/mpc-course.pdf>
- <http://spectrum.ieee.org/biomedical/devices/the-dna-data-deluge>
- <http://www.ensembl.org/>
- <http://www.enterisetech.com/2014/04/11/genome-researchers-battling-data-storage-bottlenecks/>
- <https://www.encodeproject.org/>
- IGV genome browser: <http://www.broadinstitute.org/igv/>
- MACS: [http:// http://liulab.dfci.harvard.edu/MACS/index.html](http://http://liulab.dfci.harvard.edu/MACS/index.html)
- PeakAnalyzer: <http://www.ebi.ac.uk/research/bertone/software#peakanalyzer>
- Sam Tools: [http:// http://samtools.sourceforge.net/](http://http://samtools.sourceforge.net/)
- UCSC Tools: <http://hgdownload.cse.ucsc.edu/admin/exe/>

MOOC COURSES

- Bioinformatics algorithms (Part 1), conducted by University of California San Diego. <https://www.coursera.org/course/bioinformatics>
- Bioinformatics methods I, conducted by University of Toronto. [https:// www.Coursera.org/course/bioinfomethods1](https://www.Coursera.org/course/bioinfomethods1)
- Bioinformatics: introduction and methods conducted by Peking University. <https://www.coursera.org/course/pkubioinfo>
- <https://bigdatacourse.appspot.com/course>
- <https://bigdatauniversity.com/courses>

Semester : I
Course Code : BIN 713 (II)
Course Title : ADVANCED TOPICS IN CADD
Credits : 4

AIM: To expose the student to current and emerging areas and techniques in CADD and allied areas so as to prepare them to take up problem solving in frontier areas.

COURSE OBJECTIVES:

- To impart knowledge and skills in Molecular docking, modeling
- To introduce the basic concepts in Chemoinformatics, Pharmacogenomics, Immunoinformatics
- To familiarize the basic concepts in systems and synthetic Biology

COURSE CONTENT

Module I: Molecular docking & Modeling: Mechanics of docking- search algorithm- Genetic algorithm, Monte Carlo method, Incremental construction, simulated annealing; and search space, - Scoring functions: Major scoring functions- Shape & Chemical Complementary Scores, Empirical Scoring, Force Field Scoring, Knowledge-based Scoring, Consensus Scoring, structure based and ligand based approaches for drug design, Docking tools- Argus Lab, Autodock, History of molecular modeling, mechanical, graphical & computational models, molecular surface, molecular properties, interactions, Protein modeling and engineering. Molecular Dynamics: Energy calculations, force fields, AMBER and CHARMM. Various constraints, Molecular Dynamics Simulations, Tools including NAMD and Gromacs.

Module II: Chemoinformatics: Medicinal chemistry, combinatorial chemistry. Chemogenomics & chemogenetics, applications of chemogenomics in drug discovery. Chemistry of target drug interactions, chemical descriptors. Chemogenomic approaches of target prediction, adverse drug reaction prediction, and chemical databases.

Module III: Immunoinformatics: Basic concepts of immunology, active and passive immunity, antigen and antibodies, monoclonal antibodies. Tissues and cells of immune system- lymphoid organs, B & T lymphocytes, monocytes. Humoral & cell mediated immunity, immunoglobulins, Major Histo-compatibility Complex. Immune response. Immunological memory, Vaccination, auto immunity, immunodeficiency, AIDS, Cancer immunity and immunotherapy. Computational immunology: MHC peptides- structure and interactions, QSAR- based predictions of epitopes, epitope modification, epitope mapping tools, Allergenicity prediction, Vaccine design, systems immunology.

Module IV: Pharmacogenomics: Introduction to pharmacogenomics, Pharmacokinetics, pharmacodynamics, drug metabolism, drug interaction and its action, Genetic marker- SNP and its drug response, non-genetic markers, Concept of P4/ Personalized medicine; Inter-individual variability, factors affecting drug response, personal genomics, design of drugs less prone to variations, common genetic variants affecting drug response. Dose - response relationships.

Module V: Systems and Synthetic Biology: Introduction to systems biology, concept of a system, properties of biological systems, self-organization, emergence and emergent property, feedback, abstraction, modularity; Introduction to biological networks, types of biological networks: GRN, PPIN, Metabolic pathways, signaling pathways; Network motifs, Modeling of Biological networks: what is a model? Overview of modeling approaches, Advantages of computational modeling of biological systems. Introduction to synthetic biology, systems biology v/s synthetic biology, Abstraction hierarchy: sequence, parts, device, systems, biobricks, Registry of Standard Biological Parts, oscillators, toggle switch, SBML, BioPAX, SBGN, software and tools for systems and synthetic biology, applications of synthetic biology.

ASSESSMENT

End-Semester Assessment (100 marks):

3 hour written exam consisting of 30% short answer questions, 40% descriptive questions and 30% long essay questions.

REFERENCES

- Alon, Uri. *"An introduction to Systems Biology: design principles of biological circuits."* CRC press, 2006.
- Appasani, Krishnarao, ed. *"Genome-wide association studies: From polymorphism to personalized medicine."* Cambridge University Press, 2015.
- Cohen, N. Claude, ed. *"Guidebook on molecular modeling in drug design."* Academic Press, 1996.
- Edda Klipp, Wolfram Liebermeister, Christoph Wierling, Axel Kowald, Hans Lehrach and Ralf Herwig, *"Systems Biology,"* Wiley-Blackwell.
- Flower, Darren R., *"Bioinformatics for Vaccinology"* Willey-Blackwell.
- Flower, Darren R., ed. *"Immunoinformatics: Predicting immunogenicity in silico."* Springer Science & Business Media, 2007.
- Hanson, James R. *"Chemistry and Medicines: An Introductory Text"* Royal Society of Chemistry, 2011.
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- Khudyakov, Yury E., ed. *"Medicinal protein engineering."* CRC Press, 2008
- Kubinyi, Hugo. *"Chemogenomics in drug discovery."* Chemical Genomics 2006.
- Lam, Yui-Wing Francis, and Larisa H. Cavallari, eds. *"Pharmacogenomics: Challenges and Opportunities in Therapeutic Implementation."* Academic Press, 2013.
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- Zhou, Xiaobo, and Stephen TC Wong. *"Computational Systems Bioinformatics â Methods and Biomedical Applications."* World Scientific Publishing Co Inc, 2008.

Semester : I
Course Code : BIN 714 (II)
Course Title : CADD AND MOLECULAR BIOLOGY LAB
Credits : 4

AIM: To give hands on exposure to students in basic wet-lab and informatics lab techniques covered in various courses in this programme.

COURSE OBJECTIVES:

- To familiarize students with basic wet laboratory concepts and techniques.
- To give an overview about basic Microbiology and Molecular Biology concept.
- To understand the basic Bioinformatics databases and algorithms used in Computational Biology.
- To give an overview about structural proteomics and Computer Aided Drug Design.

COURSE CONTENT

Module I: Laboratory safety guidelines, equipment handling, Preparation of buffers, reagents and media: simple media, special media.

Module II: Basic experimental concepts in Microbiology, Sterilization: dry heat, moist heat, Radiation, chemical treatment, Isolation of bacteria from different samples: soil, water and air, Microscopic examination of bacteria by simple and differential staining, bacterial colony characterization, Biochemical characterization of bacterial colonies, Antibiotic sensitivity test, Bacterial growth curve, Decontamination of microbial culture. Differential staining of blood, Blood typing, chromosome preparation: mitosis- Onion root tip.

Module III: Facilitating access from various Bioinformatics databases: NCBI, PDB, SWISS PROT, Pfam etc., and pairwise sequence alignment using BLAST, multiple sequence alignment tools- Clustal X, Clustal Omega, Phylogenetic Analysis – Mega.

Module IV: Extraction of DNA and protein, quantification of DNA and protein, Separation techniques- chromatographic methods- paper, column, thin layer, Electrophoresis- Agarose gel electrophoresis, Poly acrylamide gel electrophoresis, Polymerase chain Reaction, Extraction of plant metabolites.

Module V: Experiments in Genomics and structural proteomics-ORF finder, Genscan Pymol, Rasmol, Argus Lab, Modeling tools, Discovery studio, protein dynamics study.

ASSESSMENT:

End-Semester Assessment (100 marks):

3 hour examination consisting of 30% for major experiments , 40% for minor experiments, 10% for lab report and 20% for course viva voce.

REFERENCES:

- Aneja, K. R. "*Laboratory Manual of Microbiology and Biotechnology.*" Scientific International, 2014.

- Claverie, Jean-Michel, and Cedric Notredame. "*Bioinformatics for dummies.*" John Wiley & Sons, 2011.
- Jayaraman, J. "*Laboratory manual in biochemistry.*" Wiley Eastern, 1981.
- Miller, J. H. "*Experiments in molecular genetics.*" 1992
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- Winfrey, Michael R. "*Unraveling DNA: molecular biology for the laboratory.*" Benjamin-Cummings Publishing Company, 1997.

ADDITIONAL REFERENCES:

- <http://www.ncbi.nlm.nih.gov/education/tutorials/>
- <http://www.ncbi.nlm.nih.gov/books/NBK143764/>

Semester : I
Course Code : BIN 715 (II)
Course Title : APPLIED MATHEMATICS AND SCIENTIFIC COMPUTING
Credits : 0

AIM: The course serves to provide basic overview of Mathematical concepts of Applied Mathematics relevant to Bioinformatics and introduce the use of scientific computing tools, aimed at students from non -technical background

COURSE OBJECTIVES:

- To revive basic concepts in mathematics studied so far
- To reinforce fundamental concepts of higher mathematics through Scilab exercises
- To introduce basic algebra and calculus
- To introduce probability and allied areas
- To understand the use of statistical methods in analyzing biological data

COURSE CONTENT

Module I: Number systems, real numbers, rational numbers and complex numbers (basic operations only), solving equations- first-order equations, quadratic equations, simultaneous linear equations, introduction to vectors and matrices: scalars & vectors, addition, subtraction, dot, cross & scalar triple products basic operations, inverse of a matrix, solution of simultaneous equation by using matrix, Eigen value, Eigen vector (basic concepts using 2*2 matrix only). Scilab: basic environment, data types, variables, operators, built-in functions and user defined function, matrix processing, tool box overview

Module II: Functions, inverse functions, exponentials and logs, e-to represent natural growth and decay, circles and angles, straight lines, angles, area and volume, Pythagoras' theorem, basic trigonometric functions: sine and cosine, sinusoidal oscillations, amplitude, frequency and phase of sinusoidal oscillation, damped oscillations, waves, Fourier series- basic introduction only, introduction to trigonometric Scilab functions

Module III: Differentiation: slope of a straight line, average and instantaneous rates of change, slope of a curve, differentiating simple expressions, differentiating a sum of two functions, maximum and minimum points, points of inflexion, sketching graphs integration: the area under a curve, integration as reverse process of differentiation, integrating simple expressions, definite and indefinite integrals, introduction to differential calculus and integration Scilab tool box

Module IV: Statistics and Probability : importance of data handling, continuous and discrete data, pie charts and column graphs, histograms, sample mean, variance and standard deviation, median, range and interquartile range, covariance and correlation probability: permutation and combination, definition of probability, basic problems, conditional probability, Bayes theorem- intro only probability distributions- binomial, Poisson and normal distribution, probability mass functions of distributions, Familiarization of statistical toolbox

Module V: Statistical inference and Graph theory: Interpreting confidence intervals, hypothesis testing using test statistics, hypothesis test when the population variance is estimated (t tests), Pearson's chi-square test for goodness-of-fit for categorical data. Graph terminology: edges, vertices, loop, path, circuit, bridge, Euler's path; graph representation: adjacency matrix, incident matrix. Graphs: null, complete, regular, bipartite and complete bipartite

Module VI: Flexi Module: Biological modeling: Differential equations: modeling changing systems, classifying differential equations, solving differential equations, separation of variables, writing population growth and decline using differential equation, modeling and simulation of biological reaction, basics of analysis of biological networks by using graph theory

REFERENCES:

- Griffiths, Dawn. *"Head First Statistics: A Brain-Friendly Guide."* O'Reilly Media Inc, 2008.
- Hsu, Hwei P. *"Schaum's outline of theory and problems of probability, random variables, and random processes."* McGraw-Hill, 1997.
- Isaev, Alexander. *"Introduction to mathematical methods in bioinformatics."* Springer Science & Business Media, 2006.
- Jenny Olive, *Maths -A self-study guide.* Cambridge University Press, 2000.
- McKillup, Steve. *"Statistics explained: an introductory guide for life scientists."* Cambridge University Press, 2011.
- Rao, PSS Sundar, and J. Richard. *"Introduction to biostatistics and research methods."* PHI Learning Pvt. Ltd., 2012.
- Stewart, James. *"Calculus: early transcendentals".* Cengage Learning, 2010.

Semester : I
Course Code : BIN 716 (II)
Course Title : INTRODUCTION TO INFORMATICS (E)
Credits : 0

AIM: This course is aimed at students with non-IT background, to enable them to understand basic concepts and acquire moderate skills in selected computing tools/systems.

COURSE OBJECTIVES:

- To review the basic concepts in the field of Informatics and basic programming
- To enable the students to understand basic concepts and acquire moderate skills in selected computing tools/systems
- To give an overview of Programming languages and Web Programming

COURSE CONTENT

Module-I Review of IT Fundamentals: Social and Ethical aspects of IT; Data, information, knowledge; Introduction to Hardware (CPU, memory, storage, etc.); Role of IT in Bioinformatics; Introduction to problem solving: algorithms, flow charts; Introduction to networking: Types of networks, world wide web; distributed computing; *Introduction to Programming:* Elements of classical programming- Syntax and Semantics; Primitives: Data types, built-in data, built-in functions; combination: Setting Expressions, Operators, Control structures, Subroutines; Abstraction: Naming Variables, Data and procedure abstraction; Capturing common patterns: Object oriented concept, classes, objects, Inheritance; Execution environment: Tools, interpreter, compiler, Debugger, Executable files.

Module-II Overview of classic Programming languages & Web programming: *Basics of C:* Basic data types, writing a subroutine in C; *Basics of C++:* Basic datatypes, writing a subroutine in C ++, Basic Object Oriented concepts in C++; *Overview of Java:* JVM, Running a simple program in Java; *Basic Web Programming:* Introduction in to HTML5, Basic tags, Creating web pages & forms with basic tags; Styling Web pages with basic CSS3; *Making Dynamic web pages with JavaScript:* Basic Datatypes & Operators, Writing basic JavaScript programs for HTML pages.

Module-III Scripting Languages for Bioinformatics-I: *Python:* Python environment, IDLE, Core Containers, Basic Operators & Control Structures, File Handling, Creating Modules & Packages, Regular Expressions, Basic Object Oriented concepts, CGI programming, Database connectivity, Bio-Python.

Module-IV Scripting Languages for Bioinformatics-II: *Perl:* Perl environment, Datatypes, Basic Operators & Control Structures, File Handling, Basic string manipulations using built-in functions, Regular Expressions, CGI programming, Database connectivity, Bio-Perl.

REFERENCES:

- Allen Downey et.al. "*Learning with Python*". Dreamtech Press, 2015.
- Ananthi Sheshasayi. "*Programming Language C with Practicals*". Margham Publishers, 2012.
- Arbuckle, Daniel. "*Python Testing: Beginner's Guide*." Packt Publishing Ltd, 2010.

- Babu, A. Chandra, and T. Joshva Devadas. *"Programming with C++."* Alpha Science International, 2009.
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- An introduction to interactive programming in Python, conducted by Rice University <https://www.coursera.org/course/interactivepython>.
- Dive into Python <http://www.diveintopython3.net/>
- Google's Python Class <https://developers.google.com/edu/python/?hl=de-DE&csw=1>
- <http://learn.perl.org/tutorials/>
- http://www.bioperl.org/wiki/BioPerl_Tutorial
- <http://www.ebi.ac.uk/~lehvasla/bioperl/BioperlOverview.html>
- <https://www.perl.org/books/beginning-perl/>
- <https://www.perl.org/books/beginning-perl/>
- Learn Python the Hard Way <http://learnpythonthehardway.org/book/>

MOOC COURSES

- Learn/logic-introduction: <https://www.coursera.org/learn/logic-introduction>
- Computer-fundamentals: <https://www.coursera.org/specializations/computer-fundamentals>
- Python Programming: <https://www.coursera.org/specializations/python>
- Programming for everybody (Python), conducted by University of Michigan. <https://www.coursera.org/course/pythonlearn>.

Semester : I
Course Code : BIN 717 (II)
Course Title : INTRODUCTION TO BIOSCIENCES (E)
Credits : 0

AIM: To give a bird's eye view of Bioscience and to introduce basics of Biotechnology with specific reference to their application in Bioinformatics, aimed at students from non- life-science background

COURSE OBJECTIVES:

- To introduce students to basic concepts and theories in the field of biosciences
- To give an overview about basic Molecular Biology concept
- To introduce the concepts I Biotechnology and various techniques rDNA technology

COURSE CONTENT

Module I: Basics of Biology: Characteristics of Life; Levels of organization in nature: from atoms to biosphere; Different Kingdoms; Branches of Biology; Cell Biology: Cell as the structural and functional unit of life, Cell theory, Structural components of a cell, Types of cells, Comparison between plant and animal cells, Evolution: Evolution at molecular level, Mutations Cell division.

Module II: Basics of Biochemistry: Biomolecules and its properties; Acids and bases; Other small molecules: sugars , fatty acids, amino acids, nucleotides; Macromolecules: Monomer, Polymer, Carbohydrates, Lipids, Proteins, Nucleic acids; Cofactors and vitamins.

Module III: Basics of Genetics: Definition and scope of genetics, Inheritance of acquired characters, Genotype and phenotype, Mendel's principles, Multiple alleles-definition; Flow of genetic information, Gene structure, Expression and regulation

Module IV: Basics of Biotechnology: What is Biotechnology, Recombinant DNA technology, Putting new genes into cells, Genetic engineering, Gene cloning Vs Animal cloning, PCR, DNA probes, DNA finger printing, gene therapy.

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Semester : II
Course Code : BIN 721 (II)
Course Title : DISSERTATION
Credits : 20

AIM: To expose students to international project practices, through a real-life project work under time and deliverable constraints, applying the knowledge acquired through various courses, aiming at some original work.

COURSE OBJECTIVES:

- Students are required to carry out a 4-6 month individual project and submit a dissertation embodying the findings of the same.
- Being an M. Phil level dissertation, some original work is expected. The dissertation shall be evaluated by an external examiner as public viva voce and open to all faculty members of the Department, research scholars and interested experts/researchers/students.
- The project work is to be done preferably in an external organization of repute such as national R and D institutions or global IT/BT companies.
- Students should maintain Lab Note Books; with one page brief report for each day. Lab note books shall form a component for evaluation and shall be presented to the external examiner, if demanded.
- Internal evaluation shall be based on project progress reports submitted on a monthly basis. Along with it, a student peer review should also be given.
- Students are expected to spend a minimum of clear 8 hours per day, ideally 10-12 hours.
- Students are required to (i) give a handwritten anti-plagiarism statement and (ii) submit a verification report from URKUND, recommended by UGC. Plagiarism will not be condoned on whatever excuse. Overlap of less than 10% (excluding) shall be considered as unavoidable.

COURSE CONTENT:

Students need to solve an independent problem in Bioinformatics/Computer Aided Drug Design or allied areas, which involves 6 months of intellectual activity including documentation. The students are required to make a 20 min presentation of the project which will be evaluated by an external examiner.

The Viva shall, in addition to evaluation of project work, also attempt to gauge overall professional development of the student and also the generic subject awareness and knowledge of the student. **Appendix I** - describes project practices and evaluation components.

APPENDIX- I
DOCKETS INDICATING VARIOUS PHASES OF PROJECT MANAGEMENT

PART-A: PROJECT PLANNING DOCKET

1. Name of the Student:
2. What broad area would you like to work?
3. List five areas of your interest:
4. State your understanding of how an M. Phil project is different from a MSc. project.
5. What are the general objectives of a Project work?
6. List 5 skill sets you have in relation to your project work?
7. List three Institution and guides in consideration. (Summary of their work that interests you (attach as appendix if lengthy), Skill sets required, Constraints, Name of Guide, His/her current area of work, Full Address.;
8. Does the institution have date/ skill/ fee or other constraints? Briefly note
9. In case of institutions other than DCBB, please mention logistics like a. Arrangements for stay b. Living Expenditure and/or Fees (affordable?) c. Support from family. Mention 3 Key advantages of doing project in the concerned institution and three challenges that you envisage.
10. Do you plan for a publication? Mention (title of the paper, one target journal).
11. How many hours of work /day are you prepared to put in during the project? How will you raise so many hours? What changes will you make in your current routine?
12. Have you read any past M. Phil? Give a brief summary of it and add 3 critical observations.
13. Key resource persons you would like to consult regarding your project.
14. Your choice of (i) Internal supervisor and (ii) Assistant supervisor.
15. Remarks by Project advisory Committee.

PART-B: PROJECT PROGRESS REPORTING DOCKET

Regular documentation is required to ensure that meaningful monitoring and management of project work is carried out. This docket to be submitted thrice during project period. You are also encouraged to record key discussions and minute them as appendix.

1	Name of Student:
2	Name(s) of Guide(s):
3	No. of weeks elapsed after beginning of the project:
4	List 2 keywords to describe the project:
5	List couple of papers published in journals which directly relate to the area of proposed work.
6	List 2 areas of basic knowledge that are directly related to the project work.
7	List 2 tools/ skills required to do the project.
8	List 2 prominent researchers in the field who are currently active in the area.
9	List 2 journals in which papers of this area are appearing
10	List some books which deal with basics of your project area.
11	List 2 upcoming conferences you would like to attend.
12	List 2 strengths you have to do this project
13	List 2 areas of weakness in doing this project (also say how you propose to overcome them)
14	List a possible title of paper that you could publish on your project.

15	List 2 possible titles of your thesis.
16	List the possible titles of your thesis chapters.
17	List 2 challenges you are facing:
18	List 2 deliverables of your project.
19	Write in one sentence the up to date Synopsis of your project.
20	Write in one paragraph (4-5 sentences), the up to date Synopsis of your project.
21	Attach hand out / print out of the following PPTs. i) 1 slide PPT describing your project (This should capture the essence of the work in compact graphics). ii) 10 slide PPT describing your project.
22	What are your major achievements in the reporting period?
23	What are your immediate milestones and estimated dates to reach them?
24	Papers read in the last month with a 2-3 sentence comment in your own words and also mentioning the open questions identified.
25	Lectures / Conferences / Training attended with 2-3 sentence summary/outcome.
26	Write an appreciation of your work during last month.
27	Write a criticism of your work during last month.
28	Describe your recent library usage. Key subject books you read; Key non-subject books you read; Key online resources you read:
29	Is there any query you would like to make to your supervisor?
30	What are some of the issues (intellectual as well as otherwise) you face in project? (Also mention personal circumstances which prevent full output.)
31	Rate your motivation level now: Poor/Average/Good /Very Good/Excellent.
32	Is there some specific query/request that you wish to make to your guide?
RATING OF PROGRESS (in percentage) Your Own Rating of Progress since the last report, Guide's Rating of Progress since the last report, Your own Rating of Total Progress , Guide's Rating of Total Progress .	

PART-C: FORM FOR STUDENT PEER REVIEW OF PROJECTS

Your Name:
Title of project you are reviewing:
Name of Project student:
Give 5 positive aspects of the project:
Give 5 aspects that need improvement:
Do you find the quantum of work comparable to your own? YES/NO
Do you find the quantum of references compared to your own? YES/NO
What are your suggestions for enhancing the quality of work?
Are there books/web resources/journal papers/persons that you would like to suggest to the project student for drawing knowledge?

PART- D: INTERIM REVIEW REPORTS BY INTERNAL SUPERVISOR

Name:	Date:
Title of Project	
Quick Remarks (Scale of 5/4/3/2/1/0)	
Satisfactory Progress:	
Technical correctness of methodology:	
Sufficient use of knowledge resources (References):	
Good library usage:	
Good work habits:	
Satisfactory maintenance of lab Note Book:	
Student Peer Review and use:	
Satisfactory Attendance:	
Remarks on Technical Progress of Work:	
General Advices on bettering project work	
Specific reply to questions, if any, raised by student in Progress Report	
Any 'To-Do' before Next Review:	

**PART-E: MPHIL FINAL EVALUATION REPORT
PAGE-1: DATA TO BE FILLED-IN BY STUDENT**

1. Name of Student
2. Title of Thesis
3. Supervisors:
4. Total no. of pages in Dissertation.....
5. No of pages of the final chapter (Conclusions and future work).....
6. Total no of references.....No of journal cited.....
7. Have you taken peer reviews from other students? YES/NO
8. Give three key achievements in your project work.
9. Give three weak aspects of project work and dissertation
10. If you were asked to say in one sentence, the abstract of your project, what would you say?
11. What were the unanswered questions you identified at the end of the project?
12. Have you attended any seminar/conferences? Give details
13. Have you ensured that every sentence in your dissertation is your own? YES/NO Have you cited any long paragraph as such with/without giving references? YES/NO Are all images, table, etc. your own, or sources cited clearly? YES/NO Have you spell checked the whole dissertation? YES/NO Have you verified the format of the dissertation based on instructions? YES/NO Have you separately checked the punctuation and formatting, including reference section? YES/NO
Dated Signature
Enclosures to be provided by students <i>1. One page synopsis including key references, 2. Lab Notebook. 3. Three project progress reports and corresponding assistant supervisors review report, 4 Peer review reports by fellow students.</i>

MPHIL FINAL EVALUATION REPORT

PAGE-2: TO BE FILLED IN BY EXAMINERS

(2-6 TO BE FILLED IN BY BOTH EXAMINERS AND AVERAGE AWARDED)

Name	
Register Number	
EVALUATION COMPONENTS & SUB COMPONENTS (Weightage out of 100 in brackets)	GRADE A-Outstanding, B-Excellent, C-Good, D-Average, E-Below, F-Fail.
1. PROJECT MANAGEMENT (15) (To be given by internal Supervisor)	
Lab Note Book is regular & detailed (5)	A/B/C/D/E/F
Detailed & Precise Progress Reports (5)	A/B/C/D/E/F
Regular Peer Review/Supervisor review & Action (5)	A/B/C/D/E/F
2.PROJECT REPORTING (10)	
Scientific Reporting Standards, Formatting (5)	A/B/C/D/E/F
Avoidance of Plagiarism, Citing Practice(5)	A/B/C/D/E/F
3. TECHNICAL WORK (40)	
Quantum of work (10)	A/B/C/D/E/F
Meetings Objectives (10)	A/B/C/D/E/F
Demonstration of Results (10)	A/B/C/D/E/F
Originality (Some originality in work is mandatory) (10)	A/B/C/D/E/F
4.SCHOLARSHIP (15)	
Critical Analysis in concluding chapter (5)	A/B/C/D/E/F
Contextualizing the work (5)	A/B/C/D/E/F
Knowledge as demonstrated in Viva (5)	A/B/C/D/E/F
5. COMMUNICATION SKILLS (10)	
Presentation Skills in Viva (5)	A/B/C/D/E/F
Use of language in Dissertation (5)	A/B/C/D/E/F
6. OVERALL IMPRESSION (10)	A/B/C/D/E/F
Total Marks (out of 100*)	

Internal Examiner

External Examiner

*Converting Grades to Marks

MAX	A	B	C	D	E	F
5	5	4	3	2	1	0
10	10	8	7	5	3	1