

DEPARTMENT OF BIOCHEMISTRY
FACULTY OF ARTS, SCIENCE AND HUMANITIES
KARPAGAM ACADEMY OF HIGHER EDUCATION
(Deemed to be University, Established Under Section 3 of UGC Act 1956)
Eachanari PO, Coimbatore – 641 021, India.

M.Phil / Ph.D– BIOINFORMATICS
(Effective from the academic year 2018 - 2019 and onwards)

PREAMBLE

- The degree of Master of Philosophy [M.Phil] /Doctor of Philosophy (Ph.D) is awarded to a candidate who has submitted a thesis on the basis of original and independent research in any biochemistry field of research.
- This makes a contribution to the advancement of knowledge, which can be useful to the society.

DEPARTMENT OF BIOINFORMATICS
FACULTY OF ARTS, SCIENCE AND HUMANITIES
RESEARCH PROGRAM – M.Phil / PhD in Bioinformatics
(2018–2019 and onwards)

Course code	Name of the course	Instruction hours / week	credits	Maximum Marks (100)
18RBI101	Research Methodology and Pedagogy	4	4	100
18RBI201	Advanced Techniques in Bioinformatics	4	4	100
18RBI301A	Drug Discovery and Modeling	4	4	100
18RBI301B	Advanced Bioinformatics			
18RBI301C	Biochematics			
Program Total		12	12	300

Instruction hours/week: L: 4 T: 0 P: 0**Marks: 100****End Semester Exam: 3 Hours****UNIT I: Research Methodology**

Introduction; Definition; Objectives of research; Types of research; Research approaches; Significance of research; Research methods; Research process; Criteria of good research; Problem encountered by researchers in India; Need for research design: Features of good design; Important concepts relating to design; Different research designs; Basic principles of experimental design. Writing a Research proposal for financial assistance from National and International funding agencies.

UNIT II: Computational Biology

Computer hardware – Hardware components – input and output devices. Secondary storage devices – Operating Systems: need and usage, Evolution of operating systems, functions. MS DOS, DOS, LINUX, Basic Internal and external commands for each OS. Networking – Advantages of network, types of networks, Data warehouses and Data marts Data mining. Biological Databases- Sequence databases-Nucleic acid and protein sequence databases, GenBank, DDBJ, EMBL, Swiss-Prot and PIR. Structural databases-PDB and MMDB. Motif database-PROSITE, CATH and SCOP. Genome and Proteome databases.

UNIT III: Algorithms and Protein Structure Analysis

Algorithms: Protein and Nucleic acid sequence Algorithms: Sequence Databases, Use of the algorithms BLAST, Multiple sequence alignments and Clustering algorithms. Phylogeny: Evolutionary trees; Biological networks: Pathway analysis.

Protein structure analysis: Protein structure databases; Protein structure comparison; Fold recognition; 3D-1D Profiles; Threading and Comparative structure modeling.

UNIT IV: Scientific writing

Scientific writing – writing methodology, results & discussion, presentation. Correlation & regression, Sampling distribution – Students t test. Experimental design – CRD, RBD. Analysis of experimental results – ANOVA and its interpretation. Duncan's Multiple Range Test.

UNIT V: Pedagogical methods in higher education

Objectives and role of higher education- Important characteristics of an effective lecture- Quality teaching and learning- lecture preparation- characteristics of instructional design- Methods of teaching and learning: Large group- Technique – lecture, seminar, symposium, team teaching, project, small group technique- simulation, role playing demonstration, Brain storing, Case discussion, and assignment, methods of evaluation- self evaluation, student evaluation,

diagnostic testing and remedial teaching- question banking- electronic media in education:- 'e' learning researches- web based learning.

SUGGESTED READING

1. Andrews D. Baxevanis and BF. Francis Ouellette, (2004) Bioinformatics-A Practical guide to the Analysis of Genes and Proteins, 2nd Edition, A John Wiley & Sons Publishers
2. Bharihoke (2009). Fundamentals of Information Technology, Excel Books India, 3rd Edition Paperback.
3. David W.Mount, (2003) Bioinformatics-Sequence and Genome Analysis, CBS, Publishers.
4. Gupta S.P (2008), Statistical Methods. Sultan and Sons Company, New Delhi.
5. Gupta S.C., and Kapoor V.K (2004) Fundamentals of Mathematical Statistics, Sultan and Sons Company, New Delhi.
6. Ian Korf, Mark Xandell & Joseph Bedell, (2003) BLAST (O'REILLY), SPD Private Ltd. Ignacimuthu.S, 2005. Basic Bioinformatics, Narosa Publishing House, Chennai.
7. Kothari C.R, (2004), Research Methodology - Methods and Techniques, New Age International (P) Ltd. New Delhi
8. Rastogi S.C, Namitha Mendiratta and Parag Rastogi.,2004. Bioinformatics – Concepts, Skills, Applications.CBS Publishers & Distributors, New Delhi.

Instruction hours/week: L: 4 T: 0 P: 0**Marks: 100****End Semester Exam: 3 Hours****UNIT I: Elements of C Programming, Perl and Visual Basic**

C Programming: Variables, Data types, Operators, Statements, Loops-Simple programs using Loops, Arrays-Integer arrays, Character arrays, Programs using arrays. Introduction to Functions - Programs using functions, Introduction to Pointers, Files: Defining & Opening a file, closing a file, Input/Output operations on files.

Perl: Introduction to Perl, I/O variables, Control Statement and Regression

Visual Basic: Introduction and Purpose of Database, Introduction to Visual Basic Function in VB, Controls, Data connectivity using DAO.

UNIT II: High throughput Technology

High throughput genome and Protein sequencing, Genome and Proteome assembly; DNA and Protein micro arrays, Gene and Protein expression data sets. Micro array techniques- Types of micorarrays-Designing a microarray experiment-Microarray Technology in Treating Disease

UNIT III: Proteomics

Introduction to Proteomics – The Proteome – Mining proteomes- Bridging Genomics and Proteomics- Proteomics and the new biology. Application of proteome analysis- drug development and toxicology, Pharmaceutical Applications – Proteomics in drug Discovery in human - phage antibodies as tools- Glycobiology and Proteomics- In plant genetics and breeding

UNIT IV: Genomics

Genome annotation – traditional routes of gene identification – detecting open-reading frames – software programs for finding genes - Identifying the function of a new gene – gene ontology – overview of comparative genomics – Protein structural genomics – introduction – determining gene function by sequence comparison and through conserved protein structure

UNIT V: Applications of Bioinformatics

Agriculture, Molecular biology, Environment, Biotechnology, Neurobiology, Drug Designing, Biomedical genome medicines.

SUGGESTED READING

1. Balagurusamy E. (2011), Programming in ANSI C, 5th Edition, Tata McGraw Hill Publication.

2. Dan Graur and Wen-Hsiung Li. (2000). Fundamentals of Molecular Evolution, , II Ed., Sinauer Associates, INC
3. Plenum Publication, Campell, Discovering Genomics, Proteomics and Bioinformatics Yashwant Kanetkar (2006), Let us "C", 12th Edition- BPB Publications.
4. Primrose and. Twyman R.M (2005) Principles of Genome analysis and Genomics – Blackwell Publishing.
5. Roderic D. M. Page, Edward C. (2009) Holmes Molecular evolution, A phylogenetic approach, John Wiley & Sons, Publications.
6. Sahai S. (2000) Genomics and Proteomics, Functional and Computational Aspects,

UNIT I: Introduction to drugs

Introduction- Basics of combinatorial chemistry and natural product libraries-chemical parameters in drug design pro drugs and soft drugs-physiochemical parameters in drug design – structure based drug design-Microarray and drug discovery.

UNIT II: Drug design

Homology modeling –Molecular modeling using computers-CADD, protein-ligand docking in drug design –vaccine development through bioinformatics.

UNIT III: Target of drug

Target discovery-Target validation-Assay development-High through screening-Lead optimization-Drug substrate manufacture-Development of new drugs.

UNIT IV: Clinical trial

Candidate drug nomination-clinical trial-Investigational new drug application-FDA, patenting and formulations-Marketing.

UNIT-V: Tools used for drug docking

Determination of active site and hot spots, Receptor-Ligand interactions, Pharmacophore Identification (Catalyst, DISCO, GASP), Denovo drug designing (Group Build, Gen Star). Tools used for docking (DOCK, FLEX, GLIDE, SLIDE, GOLD, SURFLEX).

SUGGESTED READING

1. Campbell A. M. and L. J. Heyer, 2003. Discovering Genomics, Proteomics & Bioinformatics, CSHL Press,
2. Creighton T.E., 2004. Protein Function A Practical Approach, Oxford University press, UK
3. Richard B. Silverman, (2014) The Organic Chemistry of Drug Design and Drug Action, 3rd Edition, Academic Press.USA.

4. Stuart M. Brown (2002) Essentials of Medical Genomics, John Wiley & Sons. UK
5. Thomas Lengauer (Ed). (2001) Bioinformatics - From Genomes to Drugs, Wiley-VCH Germany.
6. Tsai, C.S. 2002 An Introduction to Computational Biochemistry, Wiley-Liss, New York.
7. Vogel H. (2007), Drug Discovery and Evaluation: Pharmacological Assays, Springer Science & Business Media Publications.
8. Wu-Pong Susanna, Rojanasakul, Youngyut (2010) Biopharmaceutical Drug Design and Development, Molecular Modeling-Principles and application. 2nd Edition, Springer Science & Business Media Publications.
9. Young DC. (2009), Computational Drug Design: A Guide for Computational and Medicinal Chemists. John Wiley & Sons Publications.

WEB SOURCES

1. www.healthtech.com/2002/sbd
2. www.sdsc.edu/~wilfred/genome/lectures/lab_6.html
3. www.ncbi.nlm.nih.gov/entrez/query/febi/db-genome
4. www.sanger.ac.uk/projects/microbes

Instruction hours/week: L: 4 T: 0 P: 0**Marks: 100
End Semester Exam: 3 Hours****UNIT I: Structural Bioinformatics**

Structural features of Biomolecules – Techniques used to determine structure of biomolecules – geometrical parameters – potential energy surfaces molecular graphics – hardware and software requirements – internet – mathematical concepts.

UNIT II: Structural Bioinformatics Approaches

Protein stability and folding – SCOP – DALI Assignment of protein structures to genomes – Determining gene function through conserved protein structure – prediction of protein function – approaches to protein structural genomics.

UNIT III: Pharmacogenomics and Toxicogenomics

Definition of pharmacogenomics and toxicogenomics – case study in cancer – safety metabolisms pharmacology – exploitative toxicology, pre clinical toxicology, pharmacokinetics and metabolism.

UNIT IV: Nutrigenomics

Nutritional genetics – Nutritional genomics – Genetic nutrition – gene director nutrition with reference to diabetes cardiovascular disease and obesity and neurogenomics – short notes on herbal informatics (Medicinal Foods)

UNIT V: Chemogenomics and Metagenomics

Definition – Effects of Chemical on genes – delayed mutation – Interaction of molecules (Small & Big) with DNA intercalation. Application of Metagenomics to cultured and uncultured microorganisms.

SUGGESTED READING

1. David.W.Mount, 2001. Bioinformatics – Sequence and Genome Analyses, 1st Edition Cold Spring Harbor Laboratory Press, New York, USA.
2. Hamadeh, H. K and C.A.Afshari, 2004. Toxicogenomics: Principles and Applications Wiley – Liss, NJ, USA

3. Jacoby, E.,2005. Chemo genomics- Knowledge – Based Approaches to Drug Discovery, Word Scientific, Singapore.
4. Rimbach, G, J. Fuchs and L. Packer, 2005. Nutrigenomics, CRC. Press, Australia.
5. Rothstein, M.A., 2003. Pharmacogenomics, Willey – Liss, NJ, USA
6. Westhead, D.R., J.H. Parish, and R.M Twyman.,2003. Instant Notes Series – Bioinformatics, 1st Edition, Viva Books Private Ltd, New Delhi.

WEB LINKS

1. www.healthtech.com/2002/sbd/
2. <http://speedy.emb-heidelberg.de/gtsp/>
<http://www.chemsoc.org/exemplarchem/entris/2002/gram/index.html>

Instruction hours/week: L: 4 T: 0 P: 0

Marks: 100
End Semester Exam: 3 Hours

UNIT I: Isolation and Purification of Protein & Bio-active compounds- Techniques

Extraction (soxhlet and cold percolation), Isolation of Alkaloids, Flavonoids and Terpenoids Protein extraction from Plants, Animals and Microorganism. Purification: Native gel, Chromatographic methods (Column, Preparative TLC, HPLC, HPTLC, Ion exchange, Gas Chromatography, Gel filtration, Affinity).

UNIT II: Structure elucidation of Protein and Bioactive compounds

FT-IR, UV, Crystallization, NMR, MASS, CHN analysis, X-ray diffraction, 2-D Electrophoresis, Structure prediction methods: Prediction of secondary structure – Chou-Fasman, Garnier-Osguthorpe-Robson (GOR) methods. Homology Modeling – Fold Recognition Methods – *ab initio* methods –Rosetta – CASP — transmembrane structure prediction – solvent accessibility calculations and prediction. Structure prediction tools: Modeler, 3-D- PSSM, PHD, PSIPRED, JPRED

UNIT III: Macromolecular Modelling

Software tools for modeling bio-molecules. Molecular electrostatic potentials, charge analyses. Protein conformations, folding and mutation through modeling-design of ligands for known macro molecular target sites. Computer representations of molecules, chemical databases and 2D substructure searching, 3D database searching, deriving and using Three-dimensional pharmacophores, sources of data from 3D database.

UNIT IV: Advances in drug design methodologies

Biomolecular structure, Lipinski's rule, Structure activity relationship (SAR), Pharmacokinetics, Pharmacophoric pattern, ADME Properties, quantitative structure activity relationship. Use of genetic algorithms and principle component analysis in the QSAR equations.

UNIT V: Docking

Docking-Rigid and Flexible Structure-based drug design and induced fit for all classes of targets- Theories of enzyme inhibition - Enzyme Inhibition strategies.- Enzyme inhibition as a tool for drug development –Examples. Finding new drug targets to treat disease- strategies for target identification and lead design Screening technology and Informatics for natural products drug discovery. The drug development process, the practice and limitations of Computer assisted drug discovery process.

SUGGESTED READING

1. Alan L. Harvey, 1998. *Advances in Drug Discovery Techniques*, John Wiley & Sons, New York.
2. Arup K Ghose, 2001. *Combinatorial Library Design and Evaluation*, Marcel Dekker Publishers, New York.
3. Alan Hinchliffe. 2003. *Molecular Modelling for Beginners*, John-Wiley and Sons New York.
4. Andrew R. Leach., 2001. *Molecular Modeling; Principles and Applications*, Prentice Hall Publications, New Delhi.
5. Chatwal. G.R and Sham Anand., 2015. *Instrumental Methods of Chemical Analysis*, 5th edition, Himalaya Publishing House Pvt. Ltd, Mumbai.
6. Kothekar.V, 2005. *Essential of Drug Designing* 2nd Edition, Academic Press, New York.
7. Sujatha VB, B.A.Nagasampagi, S. Meenakshi (2014) *Natural Products-Chemistry and applications*. Second reprint. NK Mehra for Narosa Publishing House Pvt Ltd, New Delhi.
8. Williams D.M. and I. Fleming., 1990. *Spectroscopic Methods in Organic Chemistry*. Forth Edition. Tata - McGrawHill, New Delhi.