M. Phil Bioinformatics

[Choice based Credit System (CBCS)]

Regulations, Description and Syllabus

[For those who join the Course in July 2019 and after]

DEPARTMENT OF BIOINFORMATICS

(UGC-Innovative, DST-FIST and PURSE Sponsored Department)

ALAGAPPA UNIVERSITY

(A State University Accredited with "A+" grade by NAAC (CGPA: 3.64) in the Third Cycle and Graded as Category-I University by MHRD-UGC)

KARAIKUDI-630 004, TAMIL NADU, INDIA

ALAGAPPA UNIVERSITY

(*A State University Accredited with 'A+' Grade by NAAC(CGPA:3.64)in the Third Cycle and Graded as Category-I University by MHRD-UGC)*

DEPARTMENT OF BIOINFORMATICS

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Objective

To make the students impart a great knowledge on worldly research and teaching qualities in Bioinformatics.

Curriculum

The study of M. Phil course of bioinformatics includes the advanced areas of development of new computational methods for studying Evolutionary Genomics, Computational approaches to Macromolecular structure, dynamics and simulation, Comparative evolutionary genomics, Drug design and discovery, Pharmacogenomics, Algorithm development, Data mining, and Prediction and analysis of structure etc.

Course Description

The Course extends for a period of one year under Semester Pattern (Two semesters). The major and recent advances in Bioinformatics and career in Research is the major prospective of this program.

Outcome

The course has been designed in a way to enable analytical and scientific facets of research methodology.

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COURSE STRUCTURE

S. No	Course Code	Name of the Course	Credits	Marks		
		SEMESTER – I		**Int.**	**Ext.**	**Total**
1.	505101	Research Methodology in Bioinformatics	4	25	75	100
2.	505102	Advanced Topics in Bioinformatics	4	25	75	100
3.	505103	General Skills in Science	4	25	75	100
SEMESTER – II						
4.	505104	Research Area Specialization	4	25	75	100
5	505999	Dissertation and Viva Voice	8	50	150	200
		Total	**24**			**600**

SEMESTER I

Paper I Research Methodology in Bioinformatics

Paper II Advanced Topics in Bioinformatics

Paper III General Skills in Science

The Semester I examinations will be conducted during November/December and Semester II will be in April/May every Academic year.

SEMESTER II

Paper IV Research Area Specialization

Paper V Dissertation and Viva Voice

Candidates should choose a research problem in his/her area of research and submit a dissertation with the results of his /her Research, carried out under the supervision of a recognized supervisor.

Courses offered to other Departments: Research Area Specialization

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[For those who joined the Course in July 2019 and after]

REGULATIONS

1. **Eligibility**

   Candidates for admission to Master of Philosophy (M. Phil) in Bioinformatics must have obtained 55% marks in M.Sc. Life Sciences (any branch) /Physics/Chemistry.

2. **Duration of the Course**

   The course period is of one year under Semester Pattern (two Semesters).

3. **Standards of Passing and award of Division.**

   a) The Minimum marks for passing in each theory paper / lab course is 50% of the marks prescribed for the theory paper/ lab course.

   b) A candidate who secure 50% - 59% of the aggregate marks prescribed for two semesters taken together, will be awarded **SECOND CLASS.**

   c) A candidates who secures 60% or more of the aggregate marks prescribed for two semesters taken together, will be awarded **FIRST CLASS.**

   d) Project shall be assessed by the two examiners, appointed by the University.

4. **Admission**

   Admission is based on Entrance Examination.

   i) A candidate can answer a maximum of 100 questions.

   ii) Duration of Examination will be two hours.

   iii) Government of Tamil Nadu/University norms may be followed for selection.

5. Attendance

Students must have earned 75% of attendance in each course for appearing for the examination. Students who have earned 74% to 70% of attendance to be applied for condonation in the prescribed form with the prescribed fee. Students who have earned 69% to 60% of attendance to be applied for condonation in the prescribed form with the prescribed fee along with the Medical Certificate.

Students who have below 60% of attendance are not eligible to appear for the examination. They shall re-do the semester(s) after completion of the programme.

6. Project

Each candidate shall be required to take up a Project Work; submit Project Report at the end of the second year. The Head of the Department shall assign the Guide who in turn will suggest the Project Work to the student in the beginning of the second year. One typed copy of the Project Report shall be submitted to the University through Head of the Department on or before the date fixed by the University.

The project report will be evaluated by an Internal Examiner and an External Examiner, nominated by the University. The candidate concerned will have to defend his project in a Viva– Voce examination.

7. **Examination Question Pattern**

Theory Courses:	**Max: 75 Marks**
Five questions (either or type) (One question from each Unit)	5 x 15= 75 marks
Project Viva-voce	

8. Fee structure

Fee for First Semester	Rs.7500/-
Fee for Second Semester	Rs.2500/-
Total Fee	Rs.10,000/-

Tuition Fees, Laboratory Fees, Special Fees and other fees is as prescribed by the University.

For Foreign Nationals opting for M.Phil programme the fees in **USD $ 300**

9. Objectives of the Program

i. To strengthen teaching and research environment as a bridge course for scholars to provide the forefront of guidance in the field of Structural Biology, Computational Biology and Pharmacogenomics.

ii. To identify and perform Cloning, Expression, Purification and Crystallization techniques in order to solve crucial putative targets using X-ray Crystallography.

iii. To develop a proficient Structural Bioinformatics knowledgebase that is intended to provide with novel information of several targets and molecular signaling pathways which will further increase the innovative solutions from the growing scientific research community.

iv. To produce a research student who gains the all-round knowledge of a specialization area with expertise and present a part of original research for a higher degree.

10. Outcomes of the Program

i. To comprehend the scope and concepts of Structural Biology, CADD, Structural Pharmacogenomics and Structural Bioinformatics that will provide a profound impact on Scientific research.

ii. To build libraries of therapeutic interests for screening purposes after the target of interest has been identified (Structural and Functional aspects) thereon to propose a lead molecule with modifications that could enrich the drug-likeness for human uses which tend to be specific based on molecular fingerprints of human.

iii. Key information for one's research purposes can be obtained from the knowledgebase that is built using structured programming languages

iv. To understand and review the relative effectiveness among the different methods and techniques in Structural Biology, Drug Discovery and Pharmacogenomics

SYLLABUS

SEMESTER – I

PAPER-I: 505101 RESEARCH METHODOLOGY IN BIOINFORMATICS

Program: **MPhil.,**	Semester: **I (2019-20)**
Course Title: **Research Methodology (505101)**	Class Time: 10-12 & 2-4 : Monday 11-12 & 3-4: Tuesday 10-12: Wednesday 10-11: Thursday 11-1: Friday
Name of the Course Teacher	**Prof. J. Jeyakanthan**
Mobile: **+91 - 97898 09245**	Email: **jjkanthan@gmail.com**
Name of the Course Teacher	**Dr. Sanjeev Kumar Singh**
Mobile: **+91 - 9894429800**	**skysanjeev@gmail.com**
Name of the Course Teacher	**Dr. M. Karthikeyan**
Mobile: **+91 - 94869 81874**	Email: **mkbioinformatics@gmail.com**
Name of the Course Teacher	**Dr. J. Joseph Sahayarayan**
Mobile: **+91 - 90475 64087**	Email: **bioinformaticsjoseph2015@gmail.com**
Name of Course Teacher	**Dr. P. Boomi**
Mobile: +91-9486031423	**Email : pboomi1983@gmail.com**
Name of the Course Teacher	**Dr. V.K. Langeswaran**
Mobile: **+91 - 98844 95511**	Email: **dr.langeswaran@gmail.com**

Course Brief:

The course is designed exclusively for the students who want to further continue their higher education and provides a platform to excel outstandingly in research. In addition, this course will focus on scopes, uses of biodiversity and including the importance of intellectual property rights so as to apply accordingly for the patents. This course provides elementary knowledge of mathematics and biostatistics, vectors, various types of graphs, vector algebra and calculus, how to use statistical methods such as measures of central tendency, measures of dispersion and regression analysis in Biological problems. Genomics and proteomics resources on the web, gene prediction methods and tools used for gene prediction, Various molecular docking and structure visualization tools will be introduced and in advanced mode. Students will be introduced to sequence analysis, phylogenetic tree construction methods and the tools used for phylogenetic analysis.

Reference/ Text Books

Text books:

1. Gromiha, M.M. (2010). Protein Bioinformatics: From Sequence to Function, Academic Press, First Edition.

Reference Books:

1. Zoe Lacroix and Terence Critchlow (2003). Bioinformatics - Managing Scientific Data. Morgan Kaufmann Publishers.
2. Bourne, P.E. and Weissig, H. (2003). Structural Bioinformatics. John-Wiley and sons.
3. Mount D. (2004). Bioinformatics: Sequence and Genome Analysis; Cold Spring Harbor Laboratory Press, New York.
4. Attwood KJ and Parry-Smith JD. (2005). Introduction to Bioinformatics. Pearson Education.
5. John Smith, H. (2006), Introduction to the principle of Drug design and action; 4th edition, Taylor & Francis, New York.
6. Sensen, C. W. (2007). Essentials of Genomics & Bioinformatics. Wiley-VCH.
7. Gibson G and Muse SV. (2009). A Primer of Genome Science. Sinauer Associates, Inc. Publishers. Third edition.
8. Isaev and Alexander Berlin. (2010). Introduction to mathematical methods in Bioinformatics. Springer.
9. Arthur M Lesk. (2013). Introduction to Bioinformatics, 2nd Edition. Oxford University Press, New Delhi.
10. Zar, J.H. (2014). Biostatistical Analysis, Pearson Education, Inc., Fifth edition.
11. Rick, N.G. (2015), DRUGS from Discovery to Approval; A John Wiley & sons, inc. publications, New Jersey.
12. Philip W. Grubb, (2016), Patents for chemicals, pharmaceuticals and biotechnology-Fundamentals of Global Law practices and strategy; 4th Edition, Oxford Univ. press.
13. Balaguruswamy E. (2017). Numerical Methods. TMH publications.
14. Nucleic Acids Research Journal Database Issues and Web-server issues (current and past issues) (http://nar.oxfordjournals.org/)

Course Objectives: To make the students

1. Learn the statistical techniques such as measures of standard deviation, measures of dispersion and regression analysis.

2. The knowledge of intellectual property rights and filing the patents.

3. Learn the various sequence and phylogenetic analysis methods.

4. How to utilize genome resources on the web.

5. Gene prediction methods and tools used for gene prediction.

Course Outcomes: The students shall be able to:

i. Applying statistical techniques for data analysis: measurement of standard deviation, dispersion and regression analysis.
ii. Understand intellectual property rights and patent profiling.
iii. Learn sequence analysis methods and tools used for gene prediction.
iv. Student will learn to draw chemical structures and the uses of molecular modeling tools and their applications.
v. Learn the concept of graphs, vector algebra and matrices.
vi. Phylogenetic tree construction and application of phylogenetic analysis in evolutionary studies

Grading System

< 50 Marks in all	50 < Your Marks < 60	60 < Your Marks < 75	Your Marks ≥ 75
Fail	II Class	I Class	Distinction

Assessment & Evaluation: Student evaluation is based on exams, assignments, reviews and seminar. The grade allocation is as follows:

Continuous Internal Assessment : 25 Marks		**End-Semester Exam: 75 Marks**
Two, 3 hour test for 75 marks and then is converted to 15 marks	Assignments, Reviews, Seminars and Cases, for 10 Marks	Three Hour examination for 75 Marks.

Attendance: Having good attendance record marks the student's sincerity and has an overall positive impact on his/her personality trait development. The students are asked to attend the classes on a regular note and those having a minimum scale of 70-75% attendance are eligible to take up the end-semester examinations as per the University norms.

Punctuality: It is the most important attribute to be followed and maintained by the student throughout his/her life which for sure will lead to the path of success. Students who arrive late by

10 mins after the attendance will be marked absent unless there is a valid reason (medical/ personal emergency) at the discretion of the Head of the Department.

Class Participation: A student's overall growth and personality development is based on his/her involvement in the class not just by mere presence but rather being interactive through questioning that will lead to propagation of ideas, initiation of thought-provoking process and much more that will provide a wholesome enriched classroom experience. Therefore, students are advised to be more attentive so that they learn from one another and develop quality-based knowledge.

Submission of Assignments: Assignments are given to students with just one motive to get more quantitative and qualitative knowledge insights into the assigned topic/chapter that will lead to preparation and completion of the assignment in a constructive manner here just the knowledge provided is not merely counted but also completion prior to proposed deadline will also have a check on the student's serious consideration of the assignments.

Presentation of Seminars: Apart from the assignments the concerned instructors also allocate the students with a topic or based on their interests to present seminar that will aid them built their confidence levels, command over English language to communicate with precision and fluently. In addition, the fellow students are encouraged to pose questions that will instigate interest and provide update in that particular topic besides the information presented helping them to prepare for their examinations that can be taken as added advantage for the students.

Preparedness: At the end of every class, the concerned instructor tells the students what will be taken in the next class using these details the students should be aware of the topics that will be covered in the upcoming lectures which actually enhance the student's capability to grasp the knowledge and concepts provided much efficiently.

Academic Dishonesty: This is an important aspect that every student should be aware of. Thus, the respective faculty members educate the students of possible means of academic malpractices (plagiarism, violation of copyrights and stealing the patented knowledge) and the following consequences that will make them more vigilant in their academic career.

Subject to change clause: Based on the requirement of student's feasibility and meeting the competitive demands of the discipline the syllabus courses will be re-structured and updated accordingly at the discretion of the Professor(s) and Board of studies chairman.

Important dates: Please note down the important dates and stick to the schedule

Test I	Test II	Assignment	Seminar
As per Academic Calendar		After Test-I	

Course Outline: Research methodology in Bioinformatics (4 Credits)

i. Scopes, types and uses of biodiversity, loss of biodiversity.

ii. Introduction to intellectual property rights, types and importance of intellectual property rights and patent filing.

iii. Trigonometric functions, series expansion, inverse and general values.

iv. Statistical methods: measures of central tendency and dispersion.

v. Concept of linear regression including regression line, regression equation and regression co-efficient.

vi. Sequence databases: GenBank, EMBOSS.

vii. DNA and Protein sequence analysis.

viii. Proteomic analysis tools: ExPASy proteomic tools, AnthePro, PSAAM, PSIPRED and ProteinVis

viii. Sequence alignment and phylogenetic tree construction. Tools used for phylogenetic tree construction PAUP and Phylip.

ix. Learning tools for primer analysis: NetPrimer and PerlPrimer.

x. Molecular visualization tools: RasMol, CN3D and Swiss-PdbViewer.

xi. Molecular docking tools: Hex, AutoDock and ArgusLab.

xii. Knowledge of genome databases on the web. TIGR database and webservers.

xiii. Understanding Human Genome Project and its applications.

More books for Reading and Referencing

Bioinformatics: Databases and Algorithms: 1st edition (2006) by N. Gautham Kannan. Alpha Science Publishers.
Text books of Biostatistics I (2005) by A. K. Sharma. Discovery Publishing House

Molecular modeling for beginners: 2nd edition (2008) by Alan Hinchliffe. Wiley publisher
Genome Analysis: Current procedures and Applications (2014) by Maria S. Poptsova. Caister Academic Press
Analysis of Phylogenetics and Evolution with R (2012) by Paradis, Emmanuel. Springer Publisher.
Genomes and what to make to them (2008). By Barry Barnes, John Dupre. University of Chicago Press Publisher

Course Schedule: Research Methodology in Bioinformatics (4 Credits)

Syllabus	Schedule
Unit 1: Research methodology: Choosing of research problem/relevance to society, literature survey, research manuscript preparation, Dissertation/thesis preparation, writing of research project proposal, Intellectual Property Rights: Introduction, types and importance of Intellectual Property Rights (IPR) and patents, Organization – GATT-TRIPS, IPRs and ownership of traditional knowledge – IPR impacts on biological research in India	**3 days**
Unit 2: Mathematics and Bio-statistics: Trigonometric Functions, Series Expansion, Inverse, General Values, Graphs,: Vector Algebra, Vector Calculus, Basic Computations. Data Representation, Measures of central tendency, Measures of Dispersion, Linear Correlation: Types, Methods of studying Correlation, Karl Pearson's Coefficient of Correlation, Linear Regression: Regression line, Regression Equations, Regression Coefficients, Chi squared distribution, Students t distribution and ANOVA.	**3 days**
Unit 3: Sequence Alignment and analysis: Nucleic acids, central dogma of molecular biology DNA sequence analysis: Entrez, GenBank, EMBOSS, Artemis R11, Sequencher, DNAuser, jambw, GENSCAN, Glimmer. Amino acids, peptide bond, Protein sequence analysis: ExPASy Proteomics tools, AnthePro, PSAAM, Osprey, WinPep, SubMito, ProteinVis, and PSIPRED, Sequence alignment and Phylogeny: NetPrimer, PerlPrimer, SimVector, CGView, BioEdit, BioCococa, Readseq, PAUP, Phylip, ClustalW, Microarray analysis, ScanAnalyze, Cluster.	**2 days**

Unit 4: Protein Structure prediction methods: Levels of protein structures, protein structure determination using X-ray crystallography, Ramachandran Plot, PDB. Homology modeling, Threading and *ab initio* method, Tools for Structure prediction; Protein structural visualization; Geometry optimization and Loop refinement; Structure validation tools etc.,	**2 days**
Unit 5: Genome Database and Resources: Sequence and structural resources for bioinformatics – Genome Databases – The Human Genome Project – Genetic disease and Genomics –Comprehensive Microbial Resource of TIGR - Databases and webservers (PAM, BLOSSUM, PFAM, Uniprot/Swissprot, PDB, SCOP, CATH, DALI, PDBSum), (CSD/CCDC).	**2 days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 days**

Assignment: Research methodology in Bioinformatics (505101)

1. Define intellectual property rights. Describe the types of intellectual property rights and its importance.
2. Define linear correlation. Discuss about the types and various methods for studying correlation.
3. Describe the DNA sequence analysis and proteomic tools.
4. Define phylogeny. Discuss about the tools used for phylogenetic analysis.
5. Describe the tools used for molecular docking studies and structure visualization tools.
6. Describe genomic database resources on the web.
7. Discuss about Human genome project, its applications and ethical issues related to human genome project.
8. Describe microarray analysis techniques and its applications.
9. Discuss about structural bioinformatics resources on the web.
10. Write short notes on any five of the following

    i) GENSCAN

    ii) ANOVA

    iii) Chi squared distribution

    iv) Measures of central tendency

    v) Biodiversity

PAPER-II: 505102 ADVANCED TOPICS IN BIOINFORMATICS

Program: **M.Phil.,**	Semester: **I (2019-20)**
Course Title and Code: **Advanced Topics in Bioinformatics (505102)**	Class Time: **12-1 & 4-5: Monday** **10-5: Tuesday** **2-3: Wednesday** **11-1: Thursday** **10-11: Friday**
Name of the Course Teacher	**Prof. J. Jeyakanthan**
Mobile: **+91 - 97898 09245**	Email: **jjkanthan@gmail.com**
Name of the Course Teacher	**Prof. Sanjeev Kumar Singh**
Mobile: **+91 - 98944 29800**	Email: **skysanjeev@gmail.com**
Name of the Course Teacher	**Dr. M. Karthikeyan**
Mobile: **+91 - 94869 81874**	Email: **mkbioinformatics@gmail.com**
Name of the Course Teacher	**Dr. J. Joseph Sahayarayan**
Mobile: **+91 - 90475 64087**	Email: **bioinformaticsjoseph2015@gmail.com**
Name of the Course Teacher	**Dr. V.K. Langeswaran**
Mobile: **+91 - 98844 95511**	Email: **dr.langeswaran@gmail.com**

Course Brief:

Advanced Topics in Bioinformatics course cover broad areas like Molecular Modeling, Drug Discovery, Genomic Mapping, and Protein-protein Interaction networks and Transcriptomics etc. It is an interdisciplinary field that tends to develop software tools for understanding the raw biological data. It also plays a role in the gene analysis, protein expression and regulation. At a more integrative level, it helps to analyze the biological pathways and networks that are an important part of Systems Biology. Bioinformatics has a vital role in describing the complexities of biological processes and structures. This course includes the basic idea like how bioinformatics is correlating with experimental findings. Network analysis seeks to understand the relationships within biological networks such as protein-protein interaction networks, creating and designing the databases, which are essential for bioinformatics research and applications. Designing new drugs by using bioinformatics tools have opened a new area of drug research and development using various computational methods like QSAR, Pharmacophore and Molecular Docking etc. It is intended for graduate students and researchers who want an overview of the field and information about the possibilities and challenges

presented at the interface between Biologist and Computer science. At the end of the course, the student will gain valuable knowledge about Molecular Modeling methods - tools, and interdisciplinary connections in the fields of Molecular Modeling, Genome mapping, Networking and drug discovery.

Reference/Text Books:

Text Books:

1. Roderick D.M. Page, Edward C. Holmes, (1998) "Molecular Evolution: A Phylogenetic Approach", Wiley-Blackwell; 1 edition, 1st Edition, ISBN-13: 978-0865428898.
2. Mount, D. (2004) "Bioinformatics: Sequence and Genome Analysis"; Cold Spring Harbor Laboratory Press, New York.
3. Sung W (2010) "Algorithms in Bioinformatics: A Practical Introduction" CRC press, ISBN: 9781420070330.
4. Lesk, A.M. (2014) "Introduction to Bioinformatics", Oxford University Press, UK, Fourth edition.
5. Ramsden, Jeremy, (2015) "Bioinformatics An Introduction" Springer.

References:

1. Sankoff, D. and Nadeau, J.H. (2000) "Comparative genomics: empirical and analytical approaches to gene order dynamics, map alignment and the evolution of gene families"; Netherlands, Kluwer Academic Publishers.
2. Sensen, C.W. (2002) "Essentials of Genomics and Bioinformatics"; Wiley-VCH Publishers, USA.
3. Pevsner, J. (2003) "Bioinformatics and Functional Genomics"; John Wiley and Sons, New Jersey, USA.
4. Mount, D. (2004) "Bioinformatics: Sequence and Genome Analysis"; Cold Spring Harbor Laboratory Press, New York.
5. Ole Lund, Nielsen, M., Lundegaard, C. Kesmir, C. and Brnak, S. (2005) "Immunological Bioinformatics"; The MIT press.
6. Jean-Michel, Cand Notredame, C. (2006) "Bioinformatics for Dummies"; John Wiley& Sons, Second Edition.
7. Kindreas D Batevanis, (2006) "Bioinformatics: A Practical Guide to the Analysis of Gene and Protein"; Wiley Inter Science, Singapore, 3rd Edition.
8. David Edward, (2007) "Plant Bioinformatics: Methods and Protocol"; Humana Press.

9. Geoffrey S. Ginsburg,Huntington F. Willard, (2009) “Essentials of Genomic and .Personalized Medicine”, Academic Press, 1st Edition
10. Baxevanis, A.D. and Francis Ouellellette, B.F. (2011) “Bioinformatics –a practical guide to the analysis of Genes and Proteins”; John Wiley & Sons, UK, Third Edition.
11. Hossein G. Gilani,Katia G. Samper, Reza Khodaparast Haghi, (2012) “Chemoinformatics: Advanced Control and Computational Techniques”; Apple Academic Press, First edition.
12. Dan Graur, (2015) “Molecular and Genome Evolution”, Sinauer Associates, 1st Edition.
13. Gretchen Kenney, (2016) "Bioinformatics: Principles and Analysis" Syrawood Publishing House USA.
14. Kayvan Najarian, Siamak Najarian, Shahriar Gharibzadeh, (2017) “Systems Biology and Bioinformatics: A Computational Approach”; CRC Press; 1 Edition, ISBN-13: 978-1138118034.

Course Objectives: To make the students:

i. Familiarize Bioinformatics methods for managing, analyzing and interpreting data.

ii. To create biological databases and network analysis will be helpful for inferring the underlying interaction of genes and gaining insights about the pathway structures with which the drug interacts.

iii. Understand and detect the molecular bases for diseases and designing a molecule.

iv. Understand the molecular modeling methods to investigate the structure, dynamics, biological and polymeric systems.

Course Outcomes: The students shall be able to

i. Transform raw data into meaningful information by applying computational techniques.
ii. Identify new, clinically relevant, molecular targets to the discovery of innovative drugs using computational methods.
iii. Read, understand and create biological databases and gene network/maps.
iv. Study the behavior and properties of molecular systems. Specifically, the techniques employed in the fields of computational biology and chemistry.
v. Study of RNA, in any of its forms and expression profiling, examines the expression level of mRNAs based on DNA microarray technology.
vi. Describe and understand the operation of complex biological systems and ultimately to

develop predictive models of human disease.
vii. Gain knowledge in computer simulations.

Teaching Methods: The mode of teaching of delivering the courses are as follows through these below mentioned methodologies:

- Delivering the lectures in the form of presentation using advanced technologies devices such as smart board.
- Video-conferencing for lectures that will be sought from experts belonging to overseas reputed institutions.
- Case-studies and Review questions.

Grading System

< 50 Marks in all	50 < Your Marks < 60	60 < Your Marks < 75	Your Marks ≥ 75
Fail	**II Class**	**I Class**	**Distinction**

Assessment & Evaluation: Student evaluation is based on exams, assignments, reviews and class participation. The grade allocation is as follows:

Continuous Internal Assessment : 25 Marks		**End-Semester Exam: 75 Marks**
3 hour test for 75 marks and then is converted to 15 marks.	Assignments, Reviews and Seminars for 10 Marks	Three Hour examination on for 75 Marks.

Attendance: Having good attendance record marks the student's sincerity and has an overall positive impact on his/her personality trait development. The students are asked to attend the classes on a regular note and those having a minimum scale of 70-75% attendance are eligible to take up the end-semester examinations as per the University norms.

Punctuality: It is the most important attribute to be followed and maintained by the student throughout his/her life which for sure will lead to the path of success. Students who arrive late by 10mins after the attendance will be marked absent unless there is a valid reason (medical/ personal emergency) at the discretion of the Head of the Department.

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will provide a wholesome enriched classroom experience. Therefore, students are advised to be more attentive so that they learn from one another and develop quality-based knowledge.

Submission of Assignments: Assignments are given to students with just one motive to get more quantitative and qualitative knowledge insights into the assigned topic/chapter that will lead to preparation and completion of the assignment in a constructive manner here just the knowledge provided is not merely counted but also completion prior to proposed deadline will also have a check on the student's serious consideration of the assignments.

Presentation of Seminars: Apart from the assignments the concerned instructors also allocate the students with a topic or based on their interests to present seminar that will aid them built their confidence levels, command over English language to communicate with precision and fluently. In addition, the fellow students are encouraged to pose questions that will instigate interest and provide update in that particular topic besides the information presented helping them to prepare for their examinations that can be taken as added advantage for the students.

Preparedness: At the end of every class, the concerned instructor tells the students what will be taken in the next class using these details the students should be aware of the topics that will be covered in the upcoming lectures which actually enhance the student's capability to grasp the knowledge and concepts provided much efficiently.

Academic Dishonesty: This is an important aspect that every student should be aware of. Thus, the respective faculty members educate the students of possible means of academic malpractices (plagiarism, violation of copyrights and stealing the patented knowledge) and the following consequences that will make them more vigilant in their academic career.

Subject to change clause: Based on the requirement of student's feasibility and meeting the competitive demands of the discipline the syllabus courses will be re-structured and updated accordingly at the discretion of the Professor(s) and Board of studies chairman.

Important dates: Please note down the important dates and stick to the schedule

CIA Test I	CIA Test II	Assignment	Seminar
As per Academic Calendar		After CIA Test-I	

Course Outline: Core: Advanced Topics in Bioinformatics (4 Credits)

i. Introduction to the concepts of Molecular Modeling.
ii. Features of molecular mechanics and force field for metals and inorganic systems.
iii. Bond structure and bending angles.
iv. Types of interaction involved in molecular mechanics and derivatives of molecular mechanics energy function.
v. Calculating thermodynamic properties using force field.
vi. Introduction to Molecular Dynamics Simulation Methods- Solvent effects and conformational changes.
vii. Application of energy minimization.
viii. Deriving the 3D pharmacophore.
ix. Techniques involved in structure-based methods for identifying lead compounds.
x. Applications of 3D Database searching and Docking.
xi. Detailed study of descriptors used in QSARs.
xii. Introduction to Genome Mapping- types, elements, comparative and uses.
xiii. Introduction to Genome projects, browsers, databases, NCBI and Ensemble.
xiv. Detailed study of Protein-Protein Interaction Networks, databases and software.
xv. Introduction to Transcriptomics/Metabolomics.
xvi. Microarray analysis and types.
xvii. Application of Microarray in Pharmacogenomics.
xviii. E-cell Applications.

More books for Reading and Referencing

Basic methods in Molecular Biology Leonard G.Davis, Mark D.Dibner, James F.Battery; **ISBN: 0-444-01082-3**
Molecular Modeling-Basic principles and Applicationns Second edition Hans-Dieter Holtje, Wolfgang Sippl, Didier Rognan and Gerd Folkers; **ISBN:3-527-30589-0**
Molecular Modelling- Principles and Applications Andrew R. Leach

Pharmacokinetics and Metabolism in Drug Design Dennis A. Smith,Han van de Waterbeemd and Don K. Walker; **ISBN: 3-527-30197-6**

Schedule: Core: Advanced Topics in Bioinformatics (4 Credits)

Syllabus	Schedule
Unit I: **Concepts of Molecular Modeling**: Features of molecular mechanics, force fields; Bond structure and bending angles – electrostatic, van der Waals and non-bonded interactions, hydrogen bonding in molecular mechanics; Derivatives of molecular mechanics energy function; Calculating thermodynamic properties using force field; Transferability of force field parameters, treatment of delocalized *pi* system; Force field for metals and inorganic systems – Application of energy minimization. Molecular Dynamics Simulation Methods – using simple models; continuous potentials; constant temperature; pressure and time-dependent properties. Solvent effects and Conformational changes in Molecular Dynamics simulation.	**3 days**
Unit II: **Pharmacoinformatics in Drug Discovery**: Deriving and using 3D pharmacophore; Molecular Docking; Structure and ligand based methods to identify lead compounds; *de novo* ligand design; Applications of 3D Database Searching and Docking, Structure Activity Relationship - QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of genetic algorithms, neural networks and principle components analysis in the QSAR equations. Tools: Hex, Auto dock, Argus lab. RasMol, CN3D, DTMM, Swiss-PdbViewer, gopenmol, StrukEd, JMVC	**3 days**
Unit-III: **Genome Mapping**: Introduction, Relationship between mapping and sequencing, Genome mapping elements, Types of maps, Comparative Maps, Uses of Mapping resources. Genomic databases: Introduction, Genome projects, Genome browsers, UCSC, NCBI, Ensemble.	**2 days**

Assignment: Genome projects, Genomic databases.	
Unit IV: **Protein-Protein Interaction Networks, databases and software**: DIP (Database of Interacting Proteins), PPI Server, BIND - Bimolecular Interaction Network Database, PIM – Hybrigenics, PathCalling Yeast Interaction Database, PROXiMATE - A database of mutant protein-protein complex thermodynamics and kinetics, PPA-Pred2-Protein-protein binding affinity prediction from amino acid sequence,MINT - a Molecular Interactions Database, GRID - The General Repository for Interaction Datasets, InterPreTS - protein interaction prediction through tertiary structure.	**2 days**
Unit V: Transcriptomics – Metabolomics - Microarray analysis – DNA Microarrays – Protein Microarrays – Gene / Protein expression- Application of Microarrays in Pharmacogenomics - Mass Spectrometry –Systems Biology – biochemical / metabolic networks – small world networks – E-cell – Applications- Immunoinformatics, Artificial Intelligence, Neural networks and SVM	**2 days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 days**

Assignment: Advanced Topics in Bioinformatics

1. Define force field and its types?
2. Explain various types of interaction between non-bonded atoms in protein?
3. Explain in detail drug discovery process?
4. Explain Structure Activity Relationship and its applications?
5. Explain the different types of Molecular Simulation methods?
6. Explain *de novo* ligand design technique?
7. Write the importance of Human genome project?
8. Derive the molecular mechanics energy function?
9. Define energy minimization in detail?
10. Explain the various Descriptors used in QSAR?

PAPER III: 505103 GENERAL SKILLS IN SCIENCE

Program: **M.Phil.,**	Semester: **I (2019-20)**
Course Title and Code: **General Skills in Science (505103)**	Class Time: **2-5 : Thursday** **2-4 : Friday**
Name of the Course Teacher	**Dr. J. Sujathamalini**
Mobile: **+91 - 04565 225210**	Email: malinikaran@yahoo.com
Name of the Course Teacher	**Dr. M. Natarajan**
Mobile: **+91 - 9944647554**	Email: **mnjkumar.natraj@gmail.com**
Name of the Course Teacher	**Dr. RM. Vidhyavathi**
Mobile: **+91 - 94448 35869**	Email: **vidhyamiss@gmail.com**

Course Brief:

This course is an ideal way to improve your ability to communicate effectively and have confidence in your use of English language. Our dynamic approach is to make students, learning engaging and fun as well as developing the reading, writing and listening skills. Overview of computer applications helps to manipulate, create, store and retrieve information to express ideas and communicate with others. This course was designed to encourage students effectively about how to write practical report, essay and literature review. Choosing the correct words and using right grammar skills. Overview of telephonic conversation like handling calls, leaving message and making request. It covers Pedagogical skills, Handling of practical classes. Overview of new technologies for teaching experiences and curriculum development. This helps more effective class and motivates the participation of students in the activities of the classroom.

Reference/Text Books:

TEXT BOOKS

1. Jim Boyce, (2003), Absolute beginner's guide to Microsoft office 2003; Que publishing.
2. Sangeeta Sharma et al., (2009) Communication Skills For Engineers And Scientists, Phi Learning Publishers, 1st Edition

REFERENCE BOOKS

1. Harry chambers, (2001), Communication skills for scientific and technical professional; Perseus.
2. Vijaya Kohli, (2003), How to teach science: a treatise on methodology of teaching physics, chemistry and biology; Published by Vivek Publishers.
3. Joseph, W. Habraken, (2004), Microsoft office 2003, all in one; Que publishing.

4. Ferguson, J.G. (2004), Communication skills; Ferguson Publishing Company.
5. Curtis Frye, (2004), Microsoft office Excel 2003 step by step; Microsoft press.
6. Guy Hart-D Eavis, (2007), How to do everything with Microsoft office word 2007; Mac Graw-Hill professional.
7. Louis Rosenblatt, (2010), Rethinking the Way We Teach Science: The Interplay of Content, Pedagogy, and the Nature of Science; Published by Taylor & Francis.
8. Elizabeth Arnold, Kathleen Underman Boggs, (2015), Interpersonal Relationships Professional Communication Skills for Nurses, Elsevier, 7th Edition
9. Alan Barker, (2016), Improve your communication skills Kogan page.

Course Objectives: To make the students:

i. Attain Knowledge about introduction to Operating systems, Computer architecture, Hardware, Languages and creating Email, Website.
ii. To understand the principles, classes and structure of C++ Programming.
iii. Introduce students with basic MS office application operations like creating, saving, closing, renaming and deleting a document.
iv. Gain knowledge in writing, communication, Telephone, carrier, academic listening skills.
v. Preparation of charts, models, projector/LCD presentations, album for handling classes.

Course Outcomes: The students shall be able to

i. Develop more effective English language communication skills
ii. Identifies hardware components, starts an application and create a document.
iii. Creates a simple slide show, recognizes the elements of a multi-media presentation.
iv. Understands the general structure of an email address
v. Use new technologies of teaching methods.
vi. Write scientific reports, note-making, journal paper, review etc.

Teaching Methods: The mode of teaching of delivering the courses are as follows through these below mentioned methodologies:

- Delivering the lectures in the form of presentation using advanced technologies devices such as smart board.
- Video-conferencing for lectures that will be sought from experts belonging to overseas reputed institutions.
- Case-studies and Review questions.

Grading System

< 50 Marks in all	50 < Your Marks < 60	60 < Your Marks < 75	Your Marks ≥ 75
Fail	**II Class**	**I Class**	**Distinction**

Assessment & Evaluation: Student evaluation is based on exams, assignments, quizzes and class participation. The grade allocation is as follows:

Continuous Internal Assessment : 100 Marks	
3 hour test for 85 marks	Assignments and Seminars for 15 Marks

Attendance: Having good attendance record marks the student's sincerity and has an overall positive impact on his/her personality trait development. The students are asked to attend the classes on a regular note and those having a minimum scale of 70-75% attendance are eligible to take up the end-semester examinations as per the University norms.

Punctuality: It is the most important attribute to be followed and maintained by the student throughout his/her life which for sure will lead to the path of success. Students who arrive late by 10mins after the attendance will be marked absent unless there is a valid reason (medical/ personal emergency) at the discretion of the Head of the Department.

Class Participation: A student's overall growth and personality development is based on his/her involvement in the class not just by mere presence but rather being interactive through questioning that will lead to propagation of ideas, initiation of thought-provoking process and much more that will provide a wholesome enriched classroom experience. Therefore, students are advised to be more attentive so that they learn from one another and develop quality-based knowledge.

Submission of Assignments: Assignments are given to students with just one motive to get more quantitative and qualitative knowledge insights into the assigned topic/chapter that will lead to preparation and completion of the assignment in a constructive manner here just the knowledge provided is not merely counted but also completion prior to proposed deadline will also have a check on the student's serious consideration of the assignments.

Presentation of Seminars: Apart from the assignments the concerned instructors also allocate the students with a topic or based on their interests to present seminar that will aid them built their confidence levels, command over English language to communicate with precision and fluently. In addition, the fellow students are encouraged to pose questions that will instigate interest and provide update in that particular topic besides the information presented helping them to prepare for their examinations that can be taken as added advantage for the students.

Preparedness: At the end of every class, the concerned instructor tells the students what will be taken in the next class using these details the students should be aware of the topics that will be covered in the upcoming lectures which actually enhance the student's capability to grasp the knowledge and concepts provided much efficiently.

Academic Dishonesty: This is an important aspect that every student should be aware of. Thus, the respective faculty members educate the students of possible means of academic malpractices (plagiarism, violation of copyrights and stealing the patented knowledge) and the following consequences that will make them more vigilant in their academic career.

Subject to change clause: Based on the requirement of student's feasibility and meeting the competitive demands of the discipline the syllabus courses will be re-structured and updated accordingly at the discretion of the Professor(s) and Board of studies chairman.

Important dates: Please note down the important dates and stick to the schedule

CIA Test I	**CIA Test II**	**Assignment**	**Seminar**
As per Academic Calendar		After CIA Test-I	

Course Outline: General Skills in Science Core: (4 Credits)

- Introduction to Computer Hardware, Architecture and software types.
- Introduction to operating system, Internet, website and E-mail.
- Types of operating system and translators.
- Overview of Integrated office applicants: Word, Excel, Access, Power point.
- Principle, classes and structure of C++ Programming.
- Written communication skills.
- Telephone skill, career skills, and presentation skills.
- Preparations of teaching materials like charts, models, write and draw on the blackboard, album preparation.
- New technologies on methodology of teaching and learning.
- Handling of practical classes.
- Theory and models of curriculum development.
- Planning of science library.

More books for Reading and Referencing

Hope J. Hartman, (2001), Metacpgnition in learning and instruction: theory, research and practice; springer
Acklen, L.et al, (1998) Microsoft office 97 professional Essentials; Prentice-Hall India.
Alan Barker, (2000), Improve your communication skills Kogan page.
Libby kumin, (2003), early communication skills for children with Down syndrome; wood fine house.

Schedule: Core: General Skills in Science Core (4 Credits)

Syllabus	Schedule
Unit I: **Communication Skills in English:** Understanding communication – greeting and introducing – making requests – asking for and giving permission – offering help – giving instruction and directions- art of small talk – participating in conversation – making a short formal speech –Describing the people, place, events and things. Telephone skill: understanding, handling calls, leaving message and making request. Written communication: report writing, note making - career skills: curriculum vitae and cover letters - Facing an interview and presentation skills – academic listening.	**5 days**
Unit II: **Introduction to Computers:** Computer Hardware: Input devices and media – magnetic device and media – output devices and media – storage device and media – computer architecture – system software: types, operating system and translators – Application software: types of language – application packages – integrated software – Introduction to operating system – Working with windows and office programs – Internet, Website and Email.	**5 days**
Unit-III: **Computer Operating Skills:** Starting a program and opening a document – saving and naming the document- create file and folders – deleting and un-deleting a document – closing a document – renaming and moving a document – finding a document- MS office: Word, Excel, Access, power point, outlook and integrated office applications –C	**5 days**

programming – Principles, classes and structure of C++ Programming.	
Unit IV: **Pedagogical Skill for Science Teachers:** Science Teacher: Qualification, teacher competencies and professional growth. Theory and models of curriculum development: Concept and Technical scientific models of curriculum development - planning a science library – Handling of practical classes. Educational technology and classroom pedagogy: Educational Technology – Concept, Emerging technologies- New technologies on methodology of teaching, learning experiences and curriculum development. Micro-teaching: Meaning, teaching, skill of stimulus variation, questioning, explanation, reacting, linking and benefits.	**5 days**
Unit V: **Practical Training:** Preparation of charts and models for handling classes of science teacher - Creating management documents e.g. Curriculum Plan, Time Table scheduling, Evaluation-Strategies etc – Learning to write and draw on the blackboard - Preparation of over head projector presentations - Preparation of power point/LCD presentations – Preparation of micro-teaching skills — Preparation of teaching materials – seminar classes for PG students- Preparation of album.	**5 days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 days**

Assignment - General Skills in Science Core (4 Credits)

1. Write about classes and structure of C++ programming?
2. Explain the architecture of computer hardware?
3. Write short note on Internet and Email?
4. Write about the Teaching methods?
5. Prepare a Curriculum Plan, Time table and evaluation?
6. Explain the theory and models of curriculum development?
7. Difference between blackboard and powerpoint presentation?
8. How to write a scientific report and review?
9. Explain the types of communication?

10. How to give a nice powerpoint presentation explain the steps?

II SEMESTER

PAPER IV: 505104 RESEARCH AREA SPECILIZATION

Program: **M.Phil.,**	Semester: **II (2016-2017)**
Course Title and Code: **Research Area Specialization (505104)**	Class Time: **10-1 : Tuesday** **10-12: Thursday**
Name of the Course Teacher	**Prof. J. Jeyakanthan**
Mobile: **+91 - 97898 09245**	Email: **jjkanthan@gmail.com**
Name of the Course Teacher	**Prof. Sanjeev Kumar Singh**
Mobile: **+91 - 98944 29800**	Email: **skysanjeev@gmail.com**
Name of the Course Teacher	**Dr. M. Karthikeyan**
Mobile: **+91 - 94869 81874**	Email: **mkbioinformatics@gmail.com**
Name of the Course Teacher	**Dr. J. Joseph Sahayarayan**
Mobile: **+91 - 90475 64087**	Email: **bioinformaticsjoseph2015@gmail.com**
Name of the Course Teacher	**Dr. V.K. Langeswaran**
Mobile: **+91 - 98844 95511**	Email: **dr.langeswaran@gmail.com**

Course Brief:

The Research area Specialization of M.Phil course in Bioinformatics includes a six months project work in the thrust areas of specialization which is broadly classified into six categories keeping in mind the number of faculties present. First, is the Structural Biology and Bio - Computing where Molecular Biology concepts such as Protein Cloning, Expression, Purification and Crystallization are performed to work on the isolation of the desired protein where the structural and functional characteristics that are yet to be explored. Hence, through X-ray Crystallography one can deduce the same and collect the insight details. Based on the inputs from the X-ray crystallographic studies the computer aided drug designing techniques such as screening, molecular dynamics simulation, quantum based approaches, structure based drug design, QSAR etc (Drug Discovery and Design, CADD & Structural Bioinformatics) are performed to identify suitable leads from commercial/natural sources for a disease – associated targets. Either way, leads identified by targeting the molecular fingerprints of an individual known as Personalized medicine (Pharmacogenomics & CADD) as this sought to be the most

preferred, selected and specific approaches by the Pharma related Industries to further validate the compounds with the aid of assay to estimate its inhibitory potential against that target conferring to life-threatening diseases such as cancer, TB, Diabetes, HIV, Inference of Vitamin D – Deficiency on population through genetic studies etc. Bioinformatics application in research highlights the usage and importance of Next generation Sequencing (NGS), CRISPR cas9 technology, Artificial Intelligence and Machine Learning approaches. Role of these advanced technologies in healthcare and medical research are studies in the field of imaging and medical health records. Additionally, these collected inputs such as the availability of different targets in association in many pathways (cross-talk), established compounds based on experimental evidences either commercially or from natural sources (Isolation from plants that is claimed to have therapeutic significance) are well collected, documented and maintained in the form of databases and also the information that are collected from several sources are also included. Thus, the scholars can frame their thesis based on these areas mentioned above along with updated working of methodologies within the stipulated period of time.

Reference(s)/Text Books:

Textbook

1. F. C. Phillips "An Introduction to Crystallography" Cambridge
2. Stroud R, "Computational and Structural Approaches to Drug Discovery ligand- Protein", Royal Society of Chemistry, Acc. No. 100217
3. Allinger LN, "Molecular Structure : Understanding Steric And Electronic Effects From Molecular Mechanics", Springer,
4. R. P.W. Scott, (1995) "Techniques and Practice of Chromatography", Vol-70, CRC Press.
5. Robert Lanza, Robert Langer, Joseph Vacanti, (2013) "Principles of Tissue Engineering" (4^{th} Edition).
6. Young Min Kwon, Steven C. Ricke, (2011) "High-Throughput Next Generation Sequencing: Methods and Applications". Springer Protocols.
7. S.J. Russell, Peter Norvig, (2015) "Artificial Intelligence-A Modern Approach", 3^{rd} edition, Pearson

REFERENCE BOOKS

1. M.P. Sepe (1997) "Thermal Analysis of Polymers", iSmithers Rapra Publishing

2. Mount, D. (2004), Bioinformatics: Sequence and Genome Analysis; Cold Spring Harbor Laboratory Press, New York.
3. Pevzner, P.A. (2004), Computational Molecular Biology; Prentice Hall of India Ltd, New Delhi
4. Kindreas D Batevanis, (2006) "Bioinformatics: A Practical Guide to the Analysis of Gene and Protein"; Wiley Inter Science, Singapore, 3rd Edition.
5. David Edward, (2007) "Plant Bioinformatics" Humana Press, 1st Edition, ISBN: 9781588296535
6. Vlachakis D (2007) "An Introduction to Molecular Modelling, from Theory to Application", **ISBN**- 978-0615176062.
7. Ramachandran KI (2008) "Computational Chemistry and Molecular Modeling: Principles and Applications", Springer, ISBN- 978-3-540-77304-7.
8. Christopher Hammond (2009)"The Basics of crystallography and diffraction" Oxford.
9. W. Boyes, (2009) "Instrumentation Reference Book", Butterworth-Heinemann, Fourth Edition.
10. Bernhard Rupp (2010)"Biomolecular crystallography: Principles, practice and application to structural biology" Garland Science.
11. Kukol (2010) "Molecular Modeling of Proteins", Humana Press, ISBN- 978-1617378126.
12. Martin M. Zdanowicz, (2010), Concepts in Pharmacogenomics, American society of Health-system pharmacists, Behtesda, MD.
13. Baxevanis, A.D. and Francis Ouellellette, B.F. (2011) "Bioinformatics –a practical guide to the analysis of Genes and Proteins"; John Wiley & Sons, UK, Third Edition.
14. P.J. Haines, (2012) "Thermal Methods of Analysis: Principles, Applications and Problems", Springer Science & Business Media.
15. Michael R. Green, Joseph Sambrook, (2012) "Molecular cloning: a laboratory manual"; Cold Spring Harbor, N.Y.: Cold Spring Harbor Laboratory Press, 4th Edition.
16. Arthur Lesk, (2013) "Introduction to Bioinformatics"; OUP Oxford; 4 Edition, ISBN-13: 978-0199651566.
17. Dmitri I. Svergun (2013) "Small angle X-Ray and neutron scattering from solutions of biological macromolecules" Oxford.
18. Federico Innocenti *et al*, (2013), Pharmacogenomics: Methods and Protocols - Totowa, N.J. Humana Press, Springer Press, 2nd Edition.

19. Michael M. Cox, Michael O'Donnell, Jennifer Duodena, (2015) "Molecular Biology: Principles and Practice Hardcover"; WH Freeman; 1st Edition.
20. David Sadava, David Hillis, H Heller (2016) "Life: The Science of Biology"; WH Freeman; ISBN-13: 978-1319126575
21. David L. Nelson, Michael, (2017) "Lehninger Principles of Biochemistry: International Edition, WH Freeman, 7th Edition, ISBN: 9781319108243, 1319108245
22. H S Chawla, (2017), "Introduction to Plant Biotechnology"; CRC Press; 3 Edition, ISBN-13: 978-1138407671.
23. Carlo combi, "Artificial Intelligence in Medicine", Elsevier.
24. Xinkun Wang, (2016). "Next-Generation Sequencing Data Analysis" CRC Press. Apple Academic Press Inc.

Course Objectives: To make the students:

i. Knowledge of several growth techniques of crystals in different mediums and to be aware of several physical, chemical and environmental factors that could affect the growth of crystals.

ii. Comprehend with precision of various phase solving methods such as direct methods, molecular replacement and with the use of heavy atom derivatives that surfaces usually in small/macromolecular crystallization.

iii. Provide knowledge about model building methods and structure refinement using various crystallographic software(s) and also to be aware in analyzing the protein structures deposited in databases such as CCDC and PDB.

iv. To facilitate the students to be furnished about the concepts of bioinformatics to be implemented in drug design and development, methodologies to find new lead candidate to treat disease.

v. To brief out the clear concepts on the bond angle, bond stretching, bond distance and role on the different types of bonds in interactions which helps to gain enormous knowledge about the structure of protein.

vi. The influence of recombinant DNA technology on modern biotechnology

vii. Biotechnology encompassing the exploitation of natural as well as engineered microorganisms and that designing an industrial scale-process requires special additional consideration.

viii. To understand the recent technologies in the development of Bioinformatics.

ix. Updating the various types of biomedical application from these techniques

x. Explain the basic principles of a wide range of modern analytical methods.

Course Outcomes: The students shall be able to

i. To offer new insights on the improved methods available for isolation, purification, and stabilization of native and modified proteins.
ii. Define electron density maps and choose the proper algorithms for structure refinement. Use specific crystallographic software for structure visualization and refinement. Validate the final structures.
iii. Explicate about interactions that modulate protein-protein complexes (small-molecule, nucleic acids, biomolecules) which later on can be designed as therapeutic markers
iv. The capacity to pertain the ideas of identifying and validating the target, structure and ligand based methods, modelling of the target – small molecule interaction, Molecular dynamics simulation, Structure activity relationships, Quantum and Molecular mechanics.
v. They will find it easy for the understanding of the Molecular Dynamics simulation using the simple models, continuous potentials at constant temperature and pressure
vi. Explain the principles/steps required for cloning, PCR, sequencing, RT-PCR and blotting techniques.
vii. Use bioinformatics to search a genome database, annotate the structure of a gene, find mutations in it, identify encoded proteins, compare protein sequences and propose gene/protein functions.
viii. Will be able to study the importance of chromatography and thermal analysis.
ix. Will be able to find the materials properties and progress of chemical reactions
x. Will be able to separation of individual chemical substance
xi. The students will gain application knowledge from the recent development in biomedical research.

Teaching Methods: The mode of teaching of delivering the courses are as follows through these below mentioned methodologies:

- Delivering the lectures in the form of presentation using advanced technologies devices such as smart board.
- Video-conferencing for lectures that will be sought from experts belonging to overseas reputed institutions
- Case-studies and Review questions

Grading System

< 50 Marks in all	50 < Your Marks < 60	60 < Your Marks < 75	Your Marks ≥ 75
Fail	**II Class**	**I Class**	**Distinction**

Assessment & Evaluation: Student evaluation is based on exams, assignments, seminars, reviews and class participation. The grade allocation is as follows:

Continuous Internal Assessment : 25 Marks		**End-Semester Exam: 75 Marks**
3 hour test for 75 marks and then is converted to 15 marks	Assignments, Reviews and Seminars, for 10 Marks	Three Hour examination for 75 Marks.

Attendance: Having good attendance record marks the student's sincerity and has an overall positive impact on his/her personality trait development. The students are asked to attend the classes on a regular note and those having a minimum scale of 70-75% attendance are eligible to take up the end-semester examinations as per the University norms.

Punctuality: It is the most important attribute to be followed and maintained by the student throughout his/her life which for sure will lead to the path of success. Students who arrive late by 10mins after the attendance has been taken will be marked absent unless there is a valid reason (medical/ personal emergency) at the discretion of the Head of the Department.

Class Participation: A student's overall growth and personality development is based on his/her involvement in the class not just by mere presence but rather being interactive through questioning that will lead to propagation of ideas, initiation of thought-provoking process and much more that will provide a wholesome enriched classroom experience. Therefore, students are advised to be more attentive so that they learn from one another and develop quality-based knowledge.

Submission of Assignments: Assignments are given to students with just one motive to get more quantitative and qualitative knowledge insights into the assigned topic/chapter that will lead to preparation and completion of the assignment in a constructive manner here just the knowledge provided is not merely counted but also completion prior to proposed deadline will also have a check on the student's serious consideration of the assignments.

Presentation of Seminars: Apart from the assignments the concerned instructors also allocate the students with a topic or based on their interests to present seminar that will aid them built their confidence levels, command over English language to communicate with precision and fluently. In addition, the fellow students are encouraged to pose questions that will instigate interest and

provide update in that particular topic besides the information presented helping them to prepare for their examinations that can be taken as added advantage for the students.

Preparedness: At the end of every class, the concerned instructor tells the students what will be taken in the next class using these details the students should be aware of the topics that will be covered in the upcoming lectures which actually enhance the student's capability to grasp the knowledge and concepts provided much efficiently.

Academic Dishonesty: This is an important aspect that every student should be aware of. Thus, the respective faculty members educate the students of possible means of academic malpractices (plagiarism, violation of copyrights and stealing the patented knowledge) and the following consequences that will make them more vigilant in their academic career.

Subject to change clause: Based on the requirement of student's feasibility and meeting the competitive demands of the discipline the syllabus courses will be re-structured and updated accordingly at the discretion of the Professor(s) and Board of studies chairman.

Important dates: Please note down the important dates and stick to the schedule

CIA Test I	**II CIA Test**	**Assignment**	**Seminar**
As per Academic Calendar		After CIA Test-I	

Course Outline: Research Methodology (Small and Macromolecular X-ray Crystallography (4 credits)

- **Small molecular X-ray crystallography:** include Crystal growth and its techniques, Crystallization of synthetic compounds - X-ray data collection and direct methods to refine the structure.
- **Macromolecular X-ray crystallography:** include structure and function of different classes of proteins, cloning, expression, purification, crystallization, data collection and structure solution/ determination.
- Tools for model building and refinement.
- Structural data repositories: Protein Data Bank, Electron Microscopy Data Bank.
- Tools and resources for protein analysis and classification: Pfam, CATH, SCOP, InterPro, PDBeFold, ProFunc.

Pharmaceutical Chemistry: Modern Pharmaceutical Techniques

- This unit offers a general and theory background of instrumental techniques, which can be providing basic knowledge of pharmaceutical chemistry.
- Moreover it demonstrates the properties of respective resulting material which are utilized in pharmaceutical application.

Molecular Modeling and Structural Bioinformatics

- Target identification and validation, optimization and validation, Structure and ligand based drug design, Modelling of target small molecule interactions. Molecular docking, lead optimization, types of Molecular docking, docking algorithms, Structure based docking, de novo ligand design.
- Molecular simulations, Structure activity relationships, QSAR and QSPRs, QSAR methodology, Descriptors used in QSARs. Use of Genetic algorithm, neural networks.

Pharmacogenomics

- Overview of basic principles and present status of pharmacogenetics.
- Basic concepts about genetics diseases, mode of inheritance, population genetics concepts involved in Pharmacogenetics.
- Detailed concepts of individualized medicine.
- Role of Bioinformatics in Pharmacogenomics.
- Classical and non-Classical Pharmacogenomics, Advantage, Limitations and Ethical issues of Pharmacogenomics.

Tissue Engineering

- Construction principles and uses of gene/chromosome libraries (human, animal and plant gene libraries), restriction fragment length polymorphism (RFLP).
- Cloning and expression of mammalian and plant genes in bacteria and the use of *in vitro* and site-directed mutagenesis to change the sequences.
- Next Generation Sequencing, Artificial Intelligence, Machine Languages and CRISPR cas9 technologies.
- Bioinformatics application in Imaging, Tele-health and Electronic health records.

More books for Reading and Referencing

M. M. Woolfson, An introduction to X-ray crystallography; 2nd Edition.
Jan Drenth, Principles of Protein X-ray Crystallography; Springer- Verlag, New York.
Marcus Frederick Charles Ladd, Rex Alfred Palmer, Structure determination by X-ray

crystallography; 4th Edition.
Dennis W. Bennett, Understanding Single-Crystal X-ray Crystallography
Combinatorial Library Design and Evaluation: Principles, Software, Tools, Applications in Drug Discovery – Arup Ghose, Vellerkad Viswanadhan Publisher: CRC Press, 2001. **ISBN: 0-8247-0487-8**
3D QSAR in Drug Design: Recent Advances – Hugo Kubinyi, Gerd Folkers, Yvonne C. Martin Publisher: Springer Science & Business Media. ISBN: 0-306-46858-1
Molecular Modeling Basics - Jan H. Jensen Publisher: CRC Press, 2010. **ISBN 978-1420075267**
Pharmacogenomics Methods and Protocols - Totowa, N.J. Humana Press (2005) by Federico Innocenti.
Concepts in Pharmacogenomics by Martin M. Zdanowicz .
Mantel. S. H, Mathews. J. A, Mickee. R.A. (1985) "An Introduction to Genetic Engineering in Plants" Blackwell Scientific Publishers, London.
R.A. Dixon and R.A. Gonzales (Eds). (1994) "Plant Cell Culture: A Practical Approach" Second edition. Oxford University Press. Oxford.
Chromatography: Fundamentals and applications of chromatography and related differential migration methods - Part A: Fundamentals and techniques E. Heftmann; **ISBN: 0080472249, 9780080472249**
Introduction to Thermal Analysis: Techniques and Applications Michael Ewart Brown; **ISBN: 1402002114, 9781402002113**

Course Schedule: Core: Research Area Specialization (4 Credits)

Syllabus	Schedule

Unit I: **Small and Macromolecular X-ray Crystallography:** X-ray generation, synchrotron radiation and applications, unit cell, atomic scattering factor and structure factor, phase problem –methods of its solution – electron density function, anomalous scattering, intensity data collection and reduction, direct method of solving a small molecule, refinement of crystal structure, hydrogen bonding. Protein purification and crystallization methods, data collection and data reduction, protein structure determination-molecular replacement technique (MR); multiple isomorphous replacement method (MIR); multi wavelength anomalous diffraction method (MAD), Single wavelength anomalous diffraction method (SAD), Calculation and interpretation of electron density map, protein structure refinement and validation method (Ramachandran Plot).	**3 days**
Unit-II **Pharmaceutical Chemistry: Modern Pharmaceutical Techniques** Basic principle and theory of advanced Spectroscopy techniques such as UV-Vis, FT-IR, XRD, Mass spectrometry and NMR. Chromatography techniques- Principles, chromatographic parameters, factors affecting and applications of TLC, Column chromatography, Paper chromatography, Ion exchange chromatography and High pressure liquid chromatography. Introduction and application of various thermal methods TGA/DTA and DSC.	**5 Days**
Unit III : **Molecular Modeling and Drug Design:** Drug discovery process, Role of Bioinformatics in drug design, Target identification and validation, lead optimization and validation, Structure and ligand based drug design, Modeling of target-small molecule interactions, Molecular Simulations, Protein modeling. **Structure Activity Relationship** - QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations.	**5 Days**
Unit-IV **Pharmacogenomics:** Overview; Present status and Basic Principles of Pharmacogenetics, Basic concepts	**5 Days**

about genetics diseases, mode of inheritance, population genetics concepts involved in Pharmacogenetics, Concepts of individualized medicine; Pharmacogenomics of genetic diseases e.g.hypertension and Cancer, role of bioinformatics in Pharmacogenomics; Approaches to Pharmacogenomics studies; Classical and non-Classical Pharmacogenomics, Advantage, Limitations and Ethical issues of Pharmacogenomics.	
Unit – V **Tissue Engineering:** Cell and Tissue Biology, Different types of tissues, Biomaterials and their utility in Tissue Engineering, Drug & Growth factor Delivery. Application Bioinformatics: Introduction to Next generation sequencing (NGS), Application of NGS in Bioinformatics: Emergence of Next generation sequencing, Illumina Genome Analyzer and prominent techniques and methods. Drawbacks of NGS, NGS File formats, & applications. Artificial Intelligence and Machine Learning Languages. Introduction and their role in healthcare and medicine - Imaging, Telehealth, and Electronic Health Records. Bioinformatics tools and their application to CRISPR Cas9 technology	**5 Days**
CIA Tests, Seminars, Presentations, Reviews Assignments, Journal club and Career Guidance.	**5 days**

Assignment & Seminar Research Area Specialization (505104)

1. X-ray and its properties; X-ray generation diffraction and its applications.
2. Structure factor, Electron density calculations and phase problem.
3. Point group, Space group, Crystal systems and Symmetry.
4. Synchrotron radiation and its implications in structure determination.
5. NMR- Introduction and general aspects of structure determination.
6. Drug discovery process and role of Bioinformatics in drug design.
7. Modelling of target-small molecular interactions with Molecular simulations.
8. Drug discovery process and role of Bioinformatics in drug design.
9. Structure activity relationship – QSAR, QSPR and descriptors in QSAR
10. Genetic Algorithms, Neural networks and Principle component analysis in the QSAR equations.
11. Write about the basic concepts on genetic diseases.
12. Describe the mode of inheritance.

13. Discuss about the concepts of individualized medicine.
14. Explain the classical and non-classical Pharmacogenomics.
15. What are the advantage, limitations and ethical issues of Pharmacogenomics.
16. Describe theory and instrumentation of scanning calorimetry and micro calorimetry
17. Write shot notes on thermal analysis.
18. Explain the detail about the thin layer and column chromatography

PAPER V: 505999 DISSERTATION AND VIVA-VOCE

Program: **M.Phil.,**	Semester: **II (2016-17)**
Course Title and Code: **Dissertation (50599)** **8 Credits**	Class Time: **10 - 5** **From January to June**
Name of the Course Teacher	**Prof. J. Jeyakanthan**
Mobile: **+91 - 97898 09245**	Email: **jjkanthan@gmail.com**
Name of the Course Teacher	**Prof. Sanjeev Kumar Singh**
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Major Research Areas

- Small and Macro molecule X-ray Crystallography.
- 3D Quantitative Structure - Activity Relationship (3D-QSAR).
- Human Molecular Genetics.
- Pharmacogenomics.
- Cheminformatics.
- Quantum Pharmacology.
- Computer Aided Drug Designing (CADD).

- Structural Bioinformatics
- Data mining, Data warehousing and Networking.
- Plant tissue Culture, Genetic Transformation, Plant Molecular Biology, Virology and Plant Pathology.
- Molecular Oncology, Pharmacology and Environmental Toxicology.

Course Brief:

The study of M.Phil course in Bioinformatics includes a six months project work in the thrust areas of specialization which is broadly classified into six categories keeping in mind the number of faculties present. First, is the Structural Biology and Bio - Computing where Molecular Biology concepts such as Protein Cloning, Expression, Purification and Crystallization are performed to work on the isolation of the desired protein where the structural and functional characteristics that are yet to be explored. Hence, through X-ray Crystallography one can deduce the same and collect the insight details. Based on the inputs from the X-ray crustallographic studies the computer aided drug designing techniques such as screening, molecular dynamics simulation, quantum based approaches, structure based drug design, QSAR etc (Drug Discovery and Design, CADD & Structural Bioinformatics) are performed to identify suitable leads from commercial/natural sources for a disease – associated targets. Either way, leads identified by targeting the molecular fingerprints of an individual known as Personalized medicine (Pharmacogenomics & CADD) as this sought to be the most preferred, selected and specific approaches by the Pharma related Industries to further validate the compounds with the aid of assay to estimate its inhibitory potential against that target conferring to life-threatening diseases such as cancer, TB, Diabetes, HIV, Inference of Vitamin D – Deficiency on population through genetic studies, Implications of *Vibrio* species to the aquaculture residential species by the application of phage therapy. Additionally, these collected inputs such as the availability of different targets in association in many pathways (cross-talk), established compounds based on experimental evidences either commercially or from natural sources (Isolation from plants that is claimed to have therapeutic significance) is well collected, documented and maintained in the form of databases and also the information that are collected from several sources are also included. Thus, the scholars can frame their thesis based on these areas mentioned above along with updated working of methodologies within the stipulated period of time.

Reference/Text Books:

As per the area of study taken

Course Objectives: To make the students:

i. To strengthen teaching and research environment as a bridge course for scholars to provide the forefront of guidance in the field of Structural Biology, Computational biology and Pharmacogenomics.

ii. To identify and perform Cloning, Expression, Purification and Crystallization techniques in order to solve crucial putative drug targets using X-ray Crystallography

iii. To develop a healthy and proficient Structural Bioinformatics knowledgebase that is intended to provide with novel information of several targets and molecular signaling pathways which will further increase the innovative solutions from the growing scientific research community.

iv. To produce a research student to gain the good all-round knowledge of a specialization area with expert skills and present a part of original research for a higher degree.

Course Outcomes: The student shall be able to:

i. To comprehend the scope and concepts of Structural Biology, CADD, Structural Pharmacogenomics and Structural Bioinformatics that will provide a profound impact on scientific research.

ii. To build libraries of therapeutic interests for screening purposes after the target of interest has been identified (structural and functional aspects) thereon to propose a lead molecule with modifications that could enrich the drug-likeness for human use which tend to be specific based on molecular fingerprints of human.

iii. Key information for one's research purposes can be obtained from the knowledgebase that is built using structured programming languages.

iv. To understand and review the relative effectiveness among the different methods and techniques in Structural biology, Drug discovery and Pharmacogenomics.

Teaching Methods:

- Literature review, analysis and data collection
- Case-studies and Review questions
- Allowed for interaction with Research scholars
- Daily guidance and monitoring the work flow
- Presentation

Grading System

< 50 Marks in all	50 < Marks < 60	60 < Marks < 75	Marks ≥ 75
Fail	**II Class**	**I Class**	**Distinction**

Assessment & Evaluation: Student evaluation is based on the target work, presentation, observation and results. The grade allocation is as follows:

Continuous Internal Assessment : 50 Marks	**End-Semester Exam: 150 Marks**
Project work regular update for 50 Marks	Project work presentation by PowerPoint followed by viva-voce and evaluation of the thesis - 150 Marks.

Attendance: Having good attendance record marks the student's sincerity and has an overall positive impact on his/her personality trait development. The students are asked to attend the classes on a regular note and those having a minimum scale of 70-75% attendance are eligible to take up the end-semester examinations as per the University norms.