

**ALAGAPPA UNIVERSITY**  
**Syllabus for M.Phil Bioinformatics**  
 [Choice Based Credit System (CBCS)]

S. No	Course Code	Name of the Course	Credits	Marks		
				Int.	Ext.	Total
<b>SEMESTER – I</b>						
1.	505101	Research Methodology	6	25	75	100
2.	505102	Advances in Bioinformatics	6	25	75	100
3.	505103	General Skills in Science	6	100	-	100
<b>SEMESTER – II</b>						
4.	505104	Research Area Specialization	6	25	75	100
5	505999	Dissertation and Viva Voice	12	50	150	200
		<b>Total Marks</b>	<b>36</b>			<b>600</b>

**SEMESTER – I**  
**ALAGAPPA UNIVERSITY, KARAIKUDI**  
**DEPARTMENT: BIOINFORMATICS**

*Course Depiction*

Program: <b>MPhil.,</b>	Semester: <b>I (2016-17)</b>
Course Title: <b>Research Methodology (505101)</b>	Class Time: <b>10-11 &amp; 12-1 : Wednesday</b> <b>11-12 : Thursday</b>
Name of the Course Teacher	<b>Dr. M. Karthikeyan</b>
Mobile: <b>+91 - 94869 81874</b>	Email: <b>mkbioinformatics@gmail.com</b>
Name of the Course Teacher	<b>Dr. RM. Vidhyavathi</b>
Mobile: <b>+91 - 94448 35869</b>	Email: <b>vidhyamiss@gmail.com</b>
Name of the Course Teacher	<b>Dr. J. Joseph Sahayarayan</b>
Mobile: <b>+91 - 90475 64087</b>	Email: <b>bioinformaticsjoseph2015@gmail.com</b>

**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**

1. Krishnamurthy KV. (2003). An advanced Textbook on Biodiversity - principle and practice. Oxford & IBH publishing Co. Pvt. Ltd.
2. Balaguruswamy E. (2008). Numerical Methods. TMH publications.

3. Isaev and Alexander Berlin. (2004). Introduction to mathematical methods in bioinformatics. Springer.
4. Murray JD. (1989). Mathematical Biology. Springer Verlag.
5. Segal L. (1980). Mathematical Models in Molecular and Cellular Biology. Cambridge University Press.
6. Zar JH. (1984). Bio Statistical Methods. Prentice Hall International Edition, USA.
7. Mount D. (2004). Bioinformatics: Sequence and Genome Analysis; Cold Spring Harbor Laboratory Press, New York.
8. Christoph W. Sensen. (2002). Essentials of genomics and Proteomics. Wiley-VCH.
9. Dubey RC. (1993). A text book of Biotechnology. S.Chand & company Ltd, New Delhi.
10. Gibson G and Muse SV. (2002). A Primer of Genome Science. Sinauer Associates, Inc. Publishers.
11. Bourne PE and Weissig H. (2003). Structural Bioinformatics. John-Wiley and sons.
12. Arthur M Lesk. (2005). Introduction to Bioinformatics, 2<sup>nd</sup> Edition. Oxford University Press, New Delhi.
13. Attwood KJ and Parry-Smith JD. (2005). Introduction to Bioinformatics. Pearson Education.
14. Baxevanis AD and Francis Ouellette BF. (1998). Bioinformatics - a practical guide to the analysis of Genes and Proteins. John Wiley & Sons, UK.
15. Zoe Lacroix and Terence Critchlow (2003). Bioinformatics - Managing Scientific Data. Morgan Kaufmann Publishers.
16. 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 $\geq$ 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 (6 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: 1<sup>st</sup> 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: 2 <sup>nd</sup> 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 (6 Credits)

Syllabus	Schedule
<b>Unit 1:</b> Biodiversity: Scope, types, values and uses, Loss of biodiversity, Biodiversity and Biotechnology; 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	<b>3 days</b>
<b>Unit 2:</b> Mathematics and Bio-statistics: Trigonometric Functions, Series Expansion, Inverse, General Values, Graphs, Vector & Matrices: Vector Algebra, Vector Calculus, Basic Computations, Matrices. 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.	<b>3 days</b>
<b>Unit 3:</b> Sequence analysis: DNA sequence analysis: Entrez, GenBank, EMBOSS, Artemis R11, Sequencher, DNAuser, jambw, GENSCAN, Glimmer. Protein sequence analysis: ExPASy Proteomics tools, AnthePro, PSAAM, Osprey, WinPep, SubMito, ProteinVis, and PSIPRED.	<b>2 days</b>
<b>Unit 4:</b> Sequence alignment and Phylogeny: NetPrimer, PerlPrimer, SimVector, CGView, BioEdit, BioCococa, Readseq, PAUP, Phylip. Hex, Auto dock, Argus lab. RasMol, CN3D, DTMM, Swiss-PdbViewer, gopenmol, StrukEd, JMVC. Chemical drawing, Microarray analysis: ChemSketch, ChemDraw, BK Chem, ScanAnalyze,	<b>2 days</b>

Cluster	
<b>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.</b>	<b>2 days</b>
<b>Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.</b>	<b>5 days</b>

**Assignment: Research methodology (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

Program: <b>M.Phil.,</b>	Semester: <b>I (2016-17)</b>
Course Title and Code: <b>Advances in Bioinformatics (505102)</b>	Class Time: <b>12-1: Tuesday</b> <b>11-12: Wednesday</b> <b>10-11: Thursday</b> <b>10-12: Friday</b>
Name of the Course Teacher	<b>Prof. J. Jeyakanthan</b>
Mobile: +91 - 97898 09245	Email: <b>jjkanthan@gmail.com</b>
Name of the Course Teacher	<b>Prof. Sanjeev Kumar Singh</b>
Mobile: <b>+91 - 98944 29800</b>	Email: <b>skysanjeev@gmail.com</b>
Name of the Course Teacher	<b>Dr. M. Karthikeyan</b>
Mobile: <b>+91 - 94869 81874</b>	Email: <b>mkbioinformatics@gmail.com</b>
Name of the Course Teacher	<b>Dr. J. Joseph Sahayarayan</b>
Mobile: <b>+91 - 90475 64087</b>	Email: <b>bioinformaticsjoseph2015@gmail.com</b>
Name of the Course Teacher	<b>Dr. V.K. Langeswaran</b>
Mobile: <b>+91 - 98844 95511</b>	Email: <b>dr.langeswaran@gmail.com</b>

### Course Brief:

Advances 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:**

1. Graur, D. and Li W.H. Fundamentals of Molecular Evolution; 2<sup>nd</sup> Edition, Sinauer Associates.
2. Page, R. D. M. and Holmes, E.C. (1998), Molecular Evolution a Phylogenetic Approach; Blackwell Scientific.
3. Mount, D. (2004), Bioinformatics: Sequence and Genome Analysis; Cold Spring Harbor Laboratory Press, New York.
4. Pevzner, P.A. (2004), Computational Molecular Biology; Prentice Hall of India Ltd, New Delhi
5. Pevsner, J. (2003), Bioinformatics and Functional Genomics; John Wiley and Sons, New Jersey, USA.
6. Sensen, C.W. (2002), Essentials of Genomics and Bioinformatics; Wiley-VCH Publishers, USA
7. 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.

**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 $\geq$ 75
<b>Fail</b>	<b>II Class</b>	<b>I Class</b>	<b>Distinction</b>

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

<b>Continuous Internal Assessment : 25 Marks</b>		<b>End-Semester Exam: 75 Marks</b>
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.

**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.

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**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: Advances in Bioinformatics (6 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 Applications 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: Advances in Bioinformatics (6 Credits)

Syllabus	Schedule
<b>Unit I: Concepts of Molecular Modeling</b> – 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.	<b>3 days</b>

<p><b>Unit II: Pharmacoinformatics in Drug Discovery</b> – Deriving and using 3D pharmacophore; Molecular Docking; Structure-based methods to identify lead compounds; <i>de novo</i> 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.</p>	<p><b>3 days</b></p>
<p><b>Unit-III: Genomic Mapping:</b> Introduction, Relationship between mapping and sequencing, Genomic mapping elements, Types of maps, Comparative Maps, Uses of Mapping resources. Genomic databases: Introduction, Genome projects, Genome browsers, UCSC, NCBI, Ensemble.</p>	<p><b>2 days</b></p>
<p><b>Unit IV: Protein-Protein Interaction Networks, databases and software:</b> DIP (Database of Interacting Proteins), PPI Server, BIND - Bimolecular Interaction Network Database, PIM – Hybrigenics, PathCalling Yeast Interaction Database, MINT - a Molecular Interactions Database, GRID - The General Repository for Interaction Datasets, InterPreTS - protein interaction prediction through tertiary structure.</p>	<p><b>2 days</b></p>
<p><b>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</b></p>	<p><b>2 days</b></p>
<p><b>Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.</b></p>	<p><b>5 days</b></p>

**Assignment: Advances 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?

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ALU - DBI

Program: <b>M.Phil.,</b>	Semester: <b>I (2016-17)</b>
Course Title and Code: <b>General Skills in Science (505103)</b>	Class Time: <b>2-5 : Thursday</b> <b>2-4 : Friday</b>
Name of the Course Teacher	<b>Dr. J. Sujathamalini</b>
Mobile: <b>+91 - 04565 225210</b>	Email: malinikaran@yahoo.com
Name of the Course Teacher	<b>Dr. M. Natarajan</b>
Mobile: <b>+91 - 9944647554</b>	Email: <b>mnjkumar.natraj@gmail.com</b>
Name of the Course Teacher	<b>Dr. RM. Vidhyavathi</b>
Mobile: <b>+91 - 94448 35869</b>	Email: <b>vidhyamiss@gmail.com</b>

### **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:**

1. Joseph, W. Habraken, (2004), Microsoft office 2003, all in one; Que publishing.
2. Curtis Frye, (2004), Microsoft office Excel 2003 step by step; Microsoft press.
3. Greg Harvey, (2006), Microsoft office Excel 2007 for dummies; For Dummies,
4. Guy Hart-D Eavis, (2007), How to do everything with Microsoft office word 2007; Mac Graw-Hill professional.
5. Jim Boyce, (2003), Absolute beginner's guide to Microsoft office 2003; Que publishing.
6. Benny Raphael, Smith, F.C. (2003), Fundamentals of computer- aided engineering; John wiley &sons.

7. Dietel, An introduction to operating system; Addison Wesley.
8. Ravi Sethi, Principles of Programming Languages; Addison Wesley.
9. Balagurusamy, E. (1995), C++ programming; Tata Mc Graw Hill, New Delhi.
10. Gottfried, B.S. (1990), Theory and programming with C; Mc Graw Hill publishers, New York.

**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:

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**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: (6 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 applications: 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), Metacognition 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 (6 Credits)

Syllabus	Schedule
<b>Unit I: Introduction to Computers:</b> 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.	<b>5 days</b>
<b>Unit II: Computer Operating Skills:</b> Starting a program and opening a document – saving and naming the document- create file and folders – deleting and undeleting 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 programming – Principles, classes and structure of C++ Programming.	<b>5 days</b>
<b>Unit-III: Communication Skills in English:</b> 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	<b>5 days</b>

communication: report writing, note making - career skills: curriculum vitae and cover letters - Facing an interview and presentation skills – academic listening.	
<b>Unit IV: Pedagogical Skill for Science Teachers:</b> 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.	<b>5 days</b>
<b>Unit V: Practical Training:</b> 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.	<b>5 days</b>
<b>Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.</b>	<b>5 days</b>

#### **Assignment - General Skills in Science Core (6 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?

ALU - DBI

## SEMESTER –II

Program: <b>M.Phil.,</b>	Semester: <b>II (2016-2017)</b>
Course Title and Code: <b>Research Area Specialization (505104)</b>	Class Time: <b>10-1 : Wednesday 10-11: Thursday</b>
Name of the Course Teacher	<b>Prof. J. Jeyakanthan</b>
Mobile: <b>+91 - 97898 09245</b>	Email: <b>jjkanthan@gmail.com</b>
Name of the Course Teacher	<b>Prof. Sanjeev Kumar Singh</b>
Mobile: <b>+91 - 98944 29800</b>	Email: <b>skysanjeev@gmail.com</b>
Name of the Course Teacher	<b>Dr. M. Karthikeyan</b>
Mobile: <b>+91 - 94869 81874</b>	Email: <b>mkbioinformatics@gmail.com</b>
Name of the Course Teacher	<b>Dr. RM. Vidhyavathi</b>
Mobile: <b>+91 - 94448 35869</b>	Email: <b>vidhyamiss@gmail.com</b>
Name of the Course Teacher	<b>Dr. J. Joseph Sahayarayan</b>
Mobile: <b>+91 - 90475 64087</b>	Email: <b>bioinformaticsjoseph2015@gmail.com</b>
Name of the Course Teacher	<b>Dr. V.K. Langeswaran</b>
Mobile: <b>+91 - 98844 95511</b>	Email: <b>dr.langeswaran@gmail.com</b>

### 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 these inputs computational studies 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(s)/Text Books:**

1. Bourne, P. E. & Weissig, H. (2003) “Structural bioinformatics”; Wiley-Liss, 2003.
2. Giacovazzo, C. (2002) “Fundamentals of crystallography”; Oxford [u.a.]: Oxford Univ.Press.
3. Banaszak, L. J.(2000) “Foundations of Structural Biology”; Academic Press
4. Leach, A. R. (2001) “Molecular Modeling – Principles and Applications”; Second Edition, Prentice Hall, USA
5. Lednicer, D. (1998) “Strategies for Organic Drug Discovery Synthesis and Design”; Wiley International Publishers.
6. Richard, J.R. (2003) “Analysis of Genes and Genomes”; Wiley Publications.
7. Falconer, D.S., Mackay, T.F.C., (1996) “Introduction to Quantitative Genetics”. Pearson Education Ltd, 4<sup>th</sup> Ed.
8. Baxevanis, A.D. and Francis Ouellette, B.F. (1998) “Bioinformatics – a practical guide to the analysis of Genes and Proteins”; John Wiley & Sons, UK.
9. Dodds J.H. (2004) “Plant Genetic Engineering” Cambridge University Press, Cambridge.
10. Grierson and S.V. Convey. (1984) “Plant Molecular Biology” Blackie and Son, New York.
11. Bernard R Glick and J. J. Pasternak (Eds). (1998) “Molecular Biotechnology: Principle and Applications of Recombinant DNA technology” ASM Press, Washington, D.C.

**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. Explain which properties can be measured by these techniques
- ix. Updating the various types of pharmaceutical 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. iWill be able to separation of individual chemical substance

**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 $\geq$ 75
<b>Fail</b>	<b>II Class</b>	<b>I Class</b>	<b>Distinction</b>

**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 (6 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.

#### **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.

### **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.

### **More books for Reading and Referencing**

M. M. Woolfson, An introduction to X-ray crystallography; 2 <sup>nd</sup> 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; 4 <sup>th</sup> 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
<b>Pharmacogenomics Methods and Protocols</b> - Totowa, N.J. Humana Press (2005) by Federico Innocenti.
<b>Concepts in Pharmacogenomics</b> 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 (6 Credits)**

Syllabus	Schedule
<p><b>Unit I: Small and Macromolecular X-ray Crystallography:</b> 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)</p>	<p><b>3 days</b></p>

<p><b>Unit-II</b></p> <p>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.</p>	<p><b>5 Days</b></p>
<p><b>Unit III : Pharmacogenomics:</b></p> <p>Overview; Present status and Basic Principles of Pharmacogenetics, Basic concepts 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.</p>	<p><b>5 Days</b></p>
<p><b>Unit-IV Tissue Engineering</b></p> <p>Identification of Bacteria, Fungi and Viruses and its types, Isolation, Purification and Culture Techniques, Production of Transgenic Plants, Molecular Markers, Photochemistry: Primary and Secondary Metabolic Products of Plants, Biosynthesis of Secondary Metabolites, Therapeutic, Pharmaceuticals, Antioxidants, Anti- Bacterial, Anti- Fungal and Anti- Insect, Protein Modeling, Gene Prediction applications.</p>	<p><b>5 Days</b></p>
<p><b>Unit – V Pharmaceutical Chemistry: Modern Pharmaceutical Techniques</b></p> <p>Principles, separation and applications of Thin layer chromatography, Column chromatography, Paper chromatography, Ion exchange chromatography, Counter current chromatography, High pressure liquid chromatography and electrophoresis. Introduction to various thermal methods of analysis, basic principle and theory; differential thermal analysis and differential scanning calorimetry and micro calorimetry</p>	<p><b>5 Days</b></p>
<p><b>CIA Tests, Seminars, Presentations, Reviews Assignments, Journal club and Career Guidance.</b></p>	<p><b>5 days</b></p>

### **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

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Program: <b>M.Phil.,</b>	Semester: <b>II (2016-17)</b>
Course Title and Code: <b>Dissertation (50599)</b> <b>12 Credits</b>	Class Time: <b>10 - 5</b> <b>From January to June</b>
Name of the Course Teacher	<b>Prof. J. Jeyakanthan</b>
Mobile: <b>+91 - 97898 09245</b>	Email: <b>jjkanthan@gmail.com</b>
Name of the Course Teacher	<b>Prof. Sanjeev Kumar Singh</b>
Mobile: <b>+91 - 98944 29800</b>	Email: <b>skysanjeev@gmail.com</b>
Name of the Course Teacher	<b>Dr. M. Karthikeyan</b>
Mobile: <b>+91 - 94869 81874</b>	Email: <b>mkbioinformatics@gmail.com</b>
Name of the Course Teacher	<b>Dr. RM. Vidhyavathi</b>
Mobile: <b>+91 - 94448 35869</b>	Email: <b>vidhyamiss@gmail.com</b>
Name of the Course Teacher	<b>Dr. J. Joseph Sahayarayan</b>
Mobile: <b>+91 - 90475 64087</b>	Email: <b>bioinformaticsjoseph2015@gmail.com</b>
Name of the Course Teacher	<b>Dr. V.K. Langeswaran</b>
Mobile: <b>+91 - 98844 95511</b>	Email: <b>dr.langeswaran@gmail.com</b>

### 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).
- 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 these inputs computational studies 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 $\geq$ 75
<b>Fail</b>	<b>II Class</b>	<b>I Class</b>	<b>Distinction</b>

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

<b>Continuous Internal Assessment : 50 Marks</b>	<b>End-Semester Exam: 150 Marks</b>
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.

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