

ALAGAPPA UNIVERSITY
Syllabus for Ph.D Bioinformatics

S. No	Course Code	Name of the Course	Marks		
			Int.	Ext.	Total
1.	Paper –I (15611)	Research Methodology	25	75	100
2.	Paper-II (15612)	Proteomics and Cheminformatics	25	75	100
3	Paper-III	Structural Biology and Bio-Computing (15613)	25	75	100
		OR			
		Molecular modeling and Structural Bioinformatics (15613 B)			
		OR			
		Pharmacogenomics and Phylogenetics (15613 C)			

ALAGAPPA UNIVERSITY, KARAİKUDI
Department: BIOINFORMATICS
Course Depiction

PAPER –I RESEARCH METHODOLOGY

Program: PhD.,	Semester: One year
Course Title: Research Methodology (15611)	Class Time: Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays.
Name of the Course Teacher	Prof. J. Jeyakanthan
Mobile: +91 - 97898 09245	Email: jjkanthan@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

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, 2nd 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, and seminar. 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, 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

- 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, EMBL, GenBank.
- 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 web servers.
- xiii. Understanding Human Genome Project and its applications.

More books for Reading and Referencing

Bioinformatics: Databases and Algorithms: 1 st 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 nd 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

Syllabus	Schedule
Unit 1: 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	25 days
Unit 2: 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.	22 days
Unit 3: 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.	22 days
Unit 4: 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, Cluster	22 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.	22 days
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment: Research methodology

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

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ALU - DBI

PAPER –II PROTEOMICS AND CHEMOINFORMATICS

Program: PhD.,	Semester : One year
Course Title: Proteomics and chemoinformatics (15612)	Class Time: Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays.
Name of Course Teacher	Prof. J. Jeyakanthan
Mobile: +91 - 97898 09245	Email : jjkanthan@gmail.com

Course Brief:

The course covers organization of protein structures and its importance during post - translation modification and methods for structure determination. Protein diversity concepts, formation of multi-enzyme complexes and its implications on binding energy. Discussion on chemoinformatics and its applications. Two dimensional and three-dimensional structures of chemical compounds. Knowledge of molecular descriptors and based on that calculation of physical and chemical data. Different stages and novel approaches to drug design and drug discovery. Drug metabolism and pharmacokinetics action of drugs on human body. Concept of molecular modeling and molecular mechanics. Discussion on structure activity relationship and drug designing tools.

Reference/Text Books

1. Lehninger A. (1987). Principles of Biochemistry. CBS Publishers, New Delhi.
2. Gerald Reed. (1993). Enzymes in Food Processing. Academic presses.
3. Branden C and Tooze R. (1993). Introduction to protein structure. Garland.
4. James M Lee. (1992). Biochemical Engineering. Prentice Hall.
5. Ashok Pandey. (2005). Enzyme Technology. Springer-Verlag New York Inc.
6. Trevor Palmer and Philip Bonner. (2007). Enzymes: Biochemistry Biotechnology, Clinical chemistry. Horwood publication.
7. Andrew R Leach and Valerie J. Gillet. (2007). Introduction to Chemoinformatics. Springer publications.
8. Frank Jensen. (1999). Introduction to Computational Chemistry. John Wiley & Sons Ltd.
9. Johann Gasteiger and Thomas Engel. (2003). Cheminformatics. WILEY-VCH Verlag GmbH & Co, KgaA, Weinheim.
10. Vyas SP and Khar RK. (2002). Targeted and Controlled Drug Discovery. 1st edn, CBS Publisher and distributors (New Delhi).
11. Thomas Langauer. (2002). Bioinformatics from Genome to Drug. WILEY-VCH Verlag GmbH & co, KgaA, Weinheim.
12. Andrew R. Leach (2001). Molecular Modeling – Principles and Applications. Second Edition, Prentice Hall, USA
13. Fenniri, H. (2000). Combinatorial Chemistry – A practical approach. Oxford University Press, UK.
14. Lednicer, D. (1998). Strategies for Organic Drug Discovery Synthesis and Design. Wiley International Publishers.
15. Gordon, E.M. and Kerwin, J.F. (1998). Combinatorial chemistry and molecular diversity in drug discovery. Wiley-Liss Publishers.

16. Swatz, M.E. (2000). Analytical techniques in Combinatorial Chemistry. Marcel Dekker Publishers.

Course Objectives: To make the students

1. Understanding organization of protein structure and methods for protein structure determination.
2. Knowledge of three dimensional structure of proteins.
3. Application of chemoinformatics in drug designing.
4. Pharmacokinetics action of drugs on human body.
5. Concept of molecular mechanics energy function and application of energy minimization.
6. Molecular modeling in drug discovery and drug designing tools.

Course Outcomes: The students shall be able to:

i. Learn the organization of protein structure and methods of protein structure determination
ii. Understanding conformations of protein and multienzyme complex
iii. Distinguish the various types of descriptors that describe the topology of a compound in order to apply quantum based approaches to the biological system
iv. Knowledge of molecular descriptors and calculation of physical and chemical data
v. Novel approaches of drug designing and pharmacokinetics action of drug on human body
vi. Aptly choose the appropriate force field to simulate a biological complex
vii. Feasibility to perform drug design and proceed to pharmacological testing/analysis

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 and seminar. 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 and Seminars, Cases, for 10 Marks	Three Hour examination o 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.

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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: Proteomics and Chemoinformatics

- i. Organization of protein structure
- ii. Methods for the determination of three dimensional structure of protein
- iii. Posttranslational modifications and its importance.
- iv. Enzyme substrate complex

- v. Application of chemoinformatics drug discovery
- vi. 2D and 3D structure of chemical compounds.
- vii. Representation of chemical reactions
- viii. Molecular descriptors and its various types.
- ix. Novel approaches in drug designing.
- x. Pharmacokinetics action of drug on human body.
- xi. Molecular dynamics simulation methods.
- xii. Application of energy minimization
- xiii. Molecular modeling in drug discovery.
- xiv. Structure activity relationship.

More books for Reading and Referencing

Protein structure and function (2005) by David Whitford. Wiley Publisher
Enzyme functionality: Design: Engineering and screening (2003) by Allan Svendsen. CRC Publisher
Chemoinformatics (2003) by Johann Gasteiger and Thomas Engel. Wiley Publisher
Drug design: Structure and ligand based approaches (2010) by Kenneth M Merz, Jr, Dagmar Ringe, Charles H. Reynolds. Cambridge University press Publisher
Molecular modeling for Beginners: 2 nd edition (2008) by Alan Hinchliffe. Wiley Publisher
Basics Pharmacokinetics and Pharmacodynamics: An integrated Textbook and computer simulations (2011) by Sara E, Rosenbaum. Wiley Publisher

Course Schedule: Proteomics and chemoinformatics

Syllabus	Schedule
Unit-I Proteins structure: Organization of protein structure, Methods in protein structure determination, factors determining stability of proteins, determination of protein folding and unfolding pathways, types and importance of post translational modification in proteins	25 Days
Unit-II Structure and conformation of proteins – three dimensional structure of proteins – protein diversity – multi enzyme complexes – enzyme-substrate complexes – flexibility and conformational mobility of proteins – interactions between non bonded atoms – binding energies of proteins.	22 Days
Unit-III Introduction, history and applications of cheminformatics; Representation of chemical compounds, manipulations in 2D and 3D structures of chemical compounds, representation of chemical reactions, molecular descriptors, calculations of physical and chemical data, calculations of structural decipherers.	22 days
Unit-IV Development of drug, drug life cycle, drug development time lines, stages of drug discovery, strategic issues in drug discovery, emerging approaches to drug design and discovery, drug metabolism physicochemical properties,	22 days

pharmacokinetic action of drug on human body.	
Unit-V Molecular Modeling and Drug Design: Concepts in Molecular Modeling, Molecular Mechanics, Derivatives of molecular mechanics energy function, Application of energy minimization, Molecular Dynamics Simulation Methods, Drug Designing Related Applications: Molecular Simulations, Molecular Modeling in Drug Discovery, Structure Activity Relationship, Drug designing softwares.	22 days
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment: PROTEOMICS AND CHEMINFORMATICS

1. Determination of three dimensional structure of protein
2. Performing molecular dynamics simulation
3. Drawing 2D and 3D structure of chemical compounds
4. Predicting posttranslational modification of protein.
5. Performing energy minimization of the molecule.

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PAPER –III AREA OF SPECIALIZATION

STRUCTURAL BIOLOGY & BIO-COMPUTING

Program: PhD.,	Semester : One year
Course Title: Structural biology & Bio-Computing (15613)	Class Time: Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays.
Name of Course Teacher	Prof. J. Jeyakanthan
Mobile: +91-9789809246	Email : jjkanthan@gmail.com

Course Brief:

The course is designed to make the research scholars learn of the basics of X-ray crystallography techniques and their application to solve crystal structures. The coursework covers X-ray generation resources, Synchrotron radiation and applications, scattering and diffraction, electron density and Fourier series. Scholars will learn about Macro molecule structure determination methods, Interpretation of electron density map Fourier refinement. The course includes discussion about types of modern computers, concept of computer networking and data storage devices. Students will learn different types of operating systems, programming languages (Perl, C, Java) and relational database management system (RDBMS).

Reference/Text Books

1. Woolfson MM. (1997). An introduction to X-ray crystallography, 2nd Edition, Cambridge University Press.
2. Giacovazzo AC, Monaco HL, Artioli G and Viterbo D. (2002). Fundamentals of Crystallography. Oxford University Press.
3. Stout GH and Jensen LH. (1989). X-ray Structure Determination. Macmillan Publishing Co., Inc., New York.
4. Dennis W Bennett. (2010). Understanding Single-Crystal X-Ray Crystallography. WILEY-VCH Verlag GmbH & Co, KGaA, Weinheim.
5. Marcus Frederick Charles Ladd, Rex Alfred Palmer. (2003). Structure determination by X-ray crystallography, 4th Edition, Kluwer Academic/Plenum Publishers, New York.
6. Jan Drenth. (1994). Principles of Protein X-ray Crystallography. Springer- Verlag, New York.
7. Leon A and Leon M. (1999). Introduction to Computers. Vikas Publishing House.
8. Hayes. (1998). Computer Architecture and Organization. Tata McGraw Hill.
9. Patterson and Hennessey (1999). Computer Organization and Design". The Hardware /Software interface. Harcourt Asia Morgan Kaufmann.
10. Cormen, TH, Leiserson CE and Rivest RL. (2001). Introduction to Algorithms. 3rd Ed, Association of American Publishers.
11. Guigo Red and Gusfield DEd. (2002). Algorithms in bioinformatics. Springer- Verlag, Berlin.
12. Kanetkar. (2002). Let Us C. BPB Publications.
13. Patrick Naughton and Herbert Schildt. (1999) Java 2: The Complete Reference. Osborne/McGraw-Hill.

14. Randal L Schwartz, Tom Phoenix and O-Reilly. (2001). Learning Perl. O'Reilly Media.
15. Sriram Srinivasan and O-Reilly. (1997). Advanced Perl Programming. 1st Edition O'Reilly Media.
16. Horowitz E and Sahani S. (1999). Fundamentals of Data structures. Galgotia Books Pvt. Ltd.

Course Objectives: To make the students

- i. Familiar of three-dimensionality aspects of the protein through X-ray Crystallography by enlightening them with underlying principles of crystal concepts.
- ii. Understand different crystal systems and symmetry that follows along with space groups to classify the crystals accordingly depending on their arrangement.
- iii. 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.
- iv. Aware of several solving methods to solve small/macromolecular structures and distinguish accordingly.
- v. 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.
- vi. 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.

Course Outcomes: The students shall be able to:

i. Design the process steps leading to determination of crystal structures of small and macro molecules.
ii. Define what a crystal is and describe the differences in properties of molecular and macro molecular crystals.
iii. Explain the differences between crystallization of small molecules and macromolecules; choose proper methods for protein crystallization.
iv. Characterize methods of phase problem solving and choose proper methods for molecular and macromolecular structures.
v. 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.
vi. Explicate about interactions that modulate protein-protein complexes (small-molecule, nucleic acids, biomolecules) which later on can be designed as therapeutic markers
vii. Learn the concept of computer networking
viii. Writing codes for biological data analysis.

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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: Structural biology & Bio-computing

- X-ray generation, Synchrotron radiation and applications.
- Introduction to unit cell, lattices, planes and crystal systems.
- X-ray scattering and diffraction.
- Concept of electron density maps and Fourier transform.
- Diffraction by crystals, Lorenz and polarization factor.
- Small and Macro Molecule X-ray crystallography.
- Isolation and purification of protein.
- Crystallization methods, intensity data collection, reduction and phase problem.
- Knowledge of working of computer, generation of computer and types of modern computers.
- Concept of computer networking and data security.
- Knowledge of working on different operating systems (Windows/Unix/Linux).
- Programming languages (C, Perl, and Java).
- Concept of relational database management system (RDBMS).
- Array, functions and data structures.

More books for Reading and Referencing

An Introduction to X-ray Crystallography: 2 nd edition (1997) by Michael M. Woolfson. Cambridge University Press Publisher
X-ray Crystallography 2 nd edition (2015) by William Clegg. Oxford University Press
Basic concepts of X-ray diffraction (2014) by Emill Zolotoyabko. Wiley publisher.
Isolation and purification of proteins (2003) by Rajni Hatti-kaul, Bo Mattiasson. CRC Publisher
Basics of computer Networking (2012) by Robertazzi, Thomas. Springer Publisher
Programming Perl: 4 th edition (2012) by Tom Chrisiansen, brian d foy, Larry wall and Jon orwant. O'Reilly Media Publisher.

Course Schedule: Structural biology & Bio-computing

Syllabus	Schedule
Unit-I Elementary Crystallography: X-ray generation; Synchrotron radiation and applications; unit cell, Lattices, Planes, Crystal systems, stereographic projection of point groups, space groups, Symmetry elements, isogonal symmetry groups and reciprocal lattice. Crystals and growing crystals properties, X-ray diffraction, Laue	25 days

equations, Bragg Law, reciprocal lattice and application to geometrical crystallography.	
Unit-II X-ray Scattering and Diffraction: Atomic scattering factor, diffraction by a space lattice, structure factor equation, electron density and Fourier series, Fourier Transform and crystal diffraction, diffraction by real crystals, Lorentz and polarization factor, primary and secondary extinctions	22 days
Unit-III Small and Macro Molecule X-ray Crystallography: Organic and Inorganic synthesis, Isolation and purification of protein, Crystallization methods, Intensity data collection, reduction, Phase problem, electron density function, Patterson methods, Structure solution, Calculation of electron density map, interpretation of electron density map Fourier refinement, Least squares techniques in refinement, Macro molecule structure determination methods and Structure refinement, Interpretation of results, bond lengths, bond angles, torsion angles, thermal motion analysis and Interactions, Validation methods and Structure analysis.	22 days
Unit-IV Computer Organization: Generation of Computers, Types of modern computers, Computer Storage, devices, memory, etc- Computer Networking, Internet, Data security, Introduction to Operating System (Windows/Unix/Linux) and software concept, Programming Language of C, Perl and JAVA and Web designing, Basics, functions, arrays, data structures and modules/classes, Biological Algorithms Development, RDBMS.	22 days
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment & Seminar Structural biology & Bio-computing

1. Describe the methods used for crystal structure determination.
2. Discuss about methods of protein isolation and various protein purification techniques.
3. Define electron density maps. Describe the calculation and interpretation of electron density maps. Write in brief about least squares techniques in refinement.
4. Describe macromolecular structure determination methods and their validation.
5. Define X-ray generation. Describe synchrotron radiation and its applications.
6. Discuss about various X-ray scattering techniques.
7. Discuss about various generations of computers. Write in brief about types of modern computers.
8. Describe different types of operating system and their features.
9. Discuss about the features of programming languages: C, Perl and Java.
10. Write short notes on the following
 - i) Bragg Law
 - ii) Fourier Transform
 - iii) RDBMS
 - iv) X-ray diffraction
 - v) data structures

MOLECULAR MODELING AND STRUCTURAL BIOINFORMATICS

Program: Ph.D.,	Semester : One year
Course Title: Molecular Modeling and Structural Bioinformatics (15613 B)	Class Time: Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays.
Name of Course Teacher	Dr. Sanjeev Kumar Singh
Mobile: +91 - 9894429800	Email : skysanjeev@gmail.com

Course Brief:

The course depicts the essential theory of molecular modeling and Structural bioinformatics. It gives a vast idea about the processes of drug discovery and also it reviews a vast range of topics including the concept of computer aided drug design; structure and ligand based methods, Molecular simulations, protein modelling, Ab initio structure modelling and Quantum and Molecular Mechanics, active site prediction, theories and molecules of drug to recognize drug like properties, Combinatorial molecular design, computer molecular dynamics simulation and changes in conformations, pharmacophore, lead identification and De-novo ligand design methods, molecular docking, QSAR, HTVS, Lipinski rule, ADME properties, energy concepts, Bond structure and bending angles, finding new drug targets to treat diseases; drug discovery and development. This course gives the detailed information on the recent advances and the limitations of the molecular modelling methods. It also serves as a introduction of molecular modeling to the students which could provide strong basic knowledge as well.

Reference/Text Books:

1. Leach, A. R. (2001) "Molecular Modeling – Principles and Applications"; Second Edition, Prentice Hall, USA
2. Fenniri, H. (2000) "Combinatorial Chemistry – A practical approach", Oxford University Press, UK.
3. Xiang, Z and Roy, A. "Schaum's Outline of Computer Graphics"; Plastock Second Edition, Mc -Graw Hill, USA.

4. Johann, G. (2003) Chemoinformatics: A Textbook, Wiley, John & Son, ISBN-13: 9783527306817
5. Lednicer, D. (1998) "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers.
6. Gordon, E.M. and Kerwin, J.F. (1998) "Combinatorial chemistry and molecular diversity in drug discovery"; Wiley-Liss Publishers.

Course Objectives: To make the students:

- i. To help the students to be familiar about the concepts of bioinformatics to be implemented in drug design and development.
- ii. To find new targets to treat disease; mechanism of drug designing
- iii. To make the students understand the concept of molecular modeling, mechanics and interactions
- iv. To provide clear concepts on bond angle, bond stretching, bond distance and role on different types of bonds in interactions
- v. To acquire the knowledge about the protein structure prediction and conformational changes throughout the simulation
- vi. To provide brief idea of receptor and receptor-ligand complex, inhibition and inactivation of enzyme, receptor theories
- vii. To provide the abundant knowledge about the structural and chemical features of the receptor and the ligand compounds.

Course Outcomes: The students shall be able to:

i. The student would be able to identify the steps for designing new drugs, target identification and validation
ii. They would acquire the capacity to apply the ideas of atomic displacement, Quantum and Molecular Mechanics, bonded interactions, hydrogen bondings and its significance in the application of drug development
iii. They would be able to execute protein structure prediction and would be able to predict the derivatives of the molecular mechanics energy function
iv. They will find it easy for the understanding of the Molecular Dynamics simulation using the simple models, continuous potentials at constant temperature and pressure

v. They will be very capable to present the docking strategies based on the ligand, receptor and de novo ligand design.

vi. Understanding of the combinatorial chemistry and library design, virtual screening and compound filtering.

vii. They would be able to understand the theory of inhibition and inactivation of enzymes, drug deactivation and susceptibility

Teaching Methods: The mode of teaching is based on the following learning activities:

- Lectures covering the theoretical part will be delivered using PowerPoint presentations.
- A set of laboratory exercises to analyze biological problems using softwares and tools to develop student's interests in scientific discovery.
- Case studies in informatics-based research.

Grading System

< 50 Marks in all	50 < Obtained Marks < 60	60 < Obtained Marks < 75	Obtained Marks \geq 75
Fail	II Class	I Class	Distinction

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

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

Attendance: The students are expected to attend the classes regularly, since regular attendance is essential to gain academic achievement. As per the University norms, the students having a minimum scale of 70-75% attendance are only qualified to write their end-semester examinations.

Punctuality: Punctuality is the most important quality for the student to be followed and maintained to achieve success. Students who arrive late by 10 mins to the class without any vital reason will be marked absent in the attendance register. On the other hand, valid excuse including personal or medical emergency is acceptable, with prior consent by 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 practice and much more that will provide a wholesome enriched classroom experience. When students participate, they learn from one another and gain their knowledge better.

Submission of Assignments: Assignments are given to students in order to apply the concepts for deeper understanding of the subject. Therefore, each student will be allocated two assignments for the course, covering the entire topic. Students will be given deadline to submit the assignment by the course instructor and good preparation of assignment will help the students for their final exams.

Presentation of Seminars: Apart from the assignments, students are supposed to give an oral presentation during the class seminar hours in their assigned topic. The concerned instructor will encourage the participants to ask valid questions during seminar presentation in order to put up their confidence levels and communication skills. In addition, students will be able to gain information and can be updated in their course.

Preparedness: At the end of every class, the concerned instructor conveys the students about the details that will be handled in the next class to increase the student's awareness related to the topics.

Academic Dishonesty: Academic dishonesty is a completely unacceptable mode of conduct and every student should be aware of this important aspect. 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: Depending upon the requirement of student's possibility, the course syllabus will be re-structured and updated accordingly at the discretion of the Professor(s) and Board of studies chairperson.

Important dates: Scheduled dates for the various activities related to the course

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

Course Outline: Molecular Modeling and Structural Bioinformatics

1. Drug discovery process, Role of Bioinformatics in drug design, Target identification and validation, lead optimization and validation, Structure-based drug design and ligand based drug design.
2. Modelling of protein and target-small molecule interactions, Molecular simulations
3. Quantum mechanics and Molecular Mechanics, Potential energy, van der Waals and non-bonded interactions, hydrogen bonding in Molecular mechanics, Features of molecular mechanics, derivatives of molecular mechanics energy function
4. Bond structure and bending angles, Electrostatic forces analysis, Molecular dynamics simulation methods with the help of simple models, continuous potential, Molecular dynamics simulation with the constant temperature and pressure, Solvent effects in Molecular dynamics. Conformation changes incorporation in Molecular dynamics.
5. Molecular docking, lead optimization, types of Molecular docking, docking algorithms, Structure based docking, de novo ligand design.
6. Various approaches of target identification, validation, lead identification, optimization and validation, Combinatorial chemistry and library design, Virtual screening
7. Drug likeness analysis, compound filtering, Absorption, distribution, metabolism, excretion and Toxicity (ADMET) property analysis
8. Pharmacophore and QSAR, Pharmacophore derivation, 3D pharmacophore prediction and application in drug discovery, QSAR methodology, Electronic Topology, Quantum chemical based Descriptors.
9. Genetic algorithms, Neural networks and Principle component analysis in QSAR equation

More books for Reading and Referencing

<p>Computational methods in drug design Fred E. Cohen, Walter Hamilton Moos Publisher: ESCOM Science, 1993.</p>
<p>Molecular Modelling for Beginners - Alan Hinchliffe Publisher: John Wiley & Sons Inc, 2008. ISBN: 978-0470513149</p>
<p>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</p>
<p>Molecular Modeling Basics - Jan H. Jensen Publisher: CRC Press, 2010. ISBN 978-1420075267</p>
<p>3D QSAR in Drug Design: Recent Advances – Hugo Kubinyi, Gerd Folkers, Yvonne C. Martin Publisher: Springer Science & Business Media. ISBN: 0-306-46858-1</p>
<p>Computational Chemistry and Molecular Modeling - K. I. Ramachandran, Gopakumar Deepa, Krishnan Namboori Publisher: Springer – Verlag Berlin Heidelberg. ISBN: 978-3540773023</p>

Course Schedule: Molecular Modelling and Structural Bioinformatics

Syllabus	Schedule
<p>Unit-I Molecular Modelling in Drug Discovery: Drug discovery process, Role of Bioinformatics in drug design, Methods of computer aided drug design, ligand design methods, drug design approaches, Target identification and validation, lead optimization and validation, Structure and ligand based drug design, modelling of target-small molecule interactions, Molecular simulations. Protein Modelling</p>	14 Days
<p>Unit-II Quantum Mechanics and Molecular Mechanics – 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; Application of energy minimization</p>	10 Days
<p>Unit-III Molecular Dynamics simulation methods – Molecular Dynamics using</p>	16 Days

simple models; Molecular Dynamics with continuous potentials and at constant temperature and pressure; Time – dependent properties; Solvent effects in Molecular Dynamics; Conformational changes from Molecular Dynamics simulation and application.	
Unit-IV Molecular Docking and lead optimization – Molecular Docking; Types of Molecular Docking, docking algorithms and programs, Structure-based methods to identify lead compounds; de novo ligand design; Applications of 3D Databases Searching and virtual Screening; Strategy for target identification and Validation, lead identification, optimization and validation. Combinatorial chemistry and library design, virtual screening, drug likeness and compound filtering, Absorption, distribution, metabolism, excretion and toxicity (ADMET) property prediction, computer based tools for drug design.	10 Days
Unit-V Pharmacophore and QSAR – Pharmacophore derivation, 3D pharmacophore prediction and application in drug discovery; 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	18 Days
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment: Molecular Modeling and Structural Bioinformatics

1. Role of Bioinformatics in drug design
2. Structure Based Drug Design
3. Coordinate System
4. Quantum Mechanics
5. Energy concept and its importance in drug action
6. Pharmacophore hypothesis
7. ADME calculation
8. Solvent effects in Molecular Dynamics
9. Application of 3D Database searching in Molecular Docking
10. Receptor theories and drug action

PHARMACOGENOMICS AND PHYLOGENETICS

Program: Ph.D.	Semester: One year
Course Title and Code: Pharmacogenomics And Phylogenetics (15613 C)	Class Time: Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays.
Name of the Course Teacher	Dr. M. Karthikeyan
Mobile: +91 - 9486981874	Email: mkbioinformatics@gmail.com

Course Brief:

The course will provide an introduction to the application of genetic and genomic methods to the study of drug response and the genetic basis for variation in that response. It will give students a broad perspective on the emergence of Pharmacogenomics as a new field and provide them with insight into the growing importance it will play in clinical therapeutics and future drug design. The biologists address questions relative to the evolutionary relationships among these sequences, as well as the evolutionary forces structuring biodiversity at different scales.

References/Text Books:

1. Mount, D. (2004) "Bioinformatics: Sequence and Genome Analysis"; Cold Spring Harbor Laboratory Press, New York.
2. Baxevanis, A.D. and Francis Ouellette, B.F. (1998) "Bioinformatics – a practical guide to the analysis of Genes and Proteins"; John Wiley & Sons, UK.
3. Richard, J.R. (2003) "Analysis of Genes and Genomes"; Wiley Publications.
4. Falconer, D.S., Mackay, T.F.C., (1996) "Introduction to Quantitative Genetics". Pearson Education Ltd, 4th Ed.
5. Pankhurst R.J. (1991). Practical taxonomic computing. Columbia University Press.
6. Lednicer, D. (1998). Strategies for Organic Drug Discovery Synthesis and Design. Wiley International Publishers.
7. Molecular Evolution a Phylogenetic Approach by R. D. M. Page and E.C. Holmes, Blackwell Scientific, 1998.

Course Objectives:

- i. To improve patient outcomes by maximizing efficacy and minimizing toxicity of drug therapy through research, teaching and service focused on genetically-guided drug therapy decision-making, drug discovery and drug development.
- ii. To understand how individualization of drug therapy based on a person's genetic makeup can optimize the effectiveness of that therapy while reducing unwanted drug effects.

Course Outcomes:

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| <ol style="list-style-type: none">i. The goal of the course is to give students an understanding of the principles of human genetics and genomics as they apply to improving the problems in drug therapy optimization and patient care. |
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ii. Students completing this course will gain an understanding of how genetic differences between individuals can impact the outcome of drug therapy in a positive and negative way.
iii. The genetic basis of variability in drug response can contribute to drug efficacy and toxicity, adverse drug reactions and drug-drug interactions
iv. Understanding of the basics of Pharmacogenomics will enable students to better understand and manage the new genomics based tools as they become available as well as make best treatment choices.

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
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
Two, 3 hour test for 75 marks and then is converted to 15 marks	Assignments, Seminars, Reviews, Cases for 10 Marks	Three Hour examination on the whole syllabus 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

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

Course Outline: Pharmacogenomics and Phylogenetics

- Basic concepts of pharmacogenomics and genetics diseases.
- Pharmacogenomics necessity in drug designing.
- The Pharmacogenetics and Pharmacogenomics knowledge Base.
- Polymorphisms and their importance in drug designing.
- CYP2D6, CYP2C19 in drug metabolism.
- Structural influence in the Drug response.
- Cell culture techniques and good laboratory practice to maintain the various cell lines and chemicals, *In vitro* and *in vivo* drug Discovery.
- Prediction of structural changes among sequences by the influence of polymorphisms.
- Tools for pharmacogenomic analysis. Pharmacokinetics (PK), Pharmacodynamics (PD).

- Target Structure optimization, Validation, lead identification, ADME prediction.
- Synthesis, assay, and clinical trials for the identification of novel drug.
- Basic concepts in Systematics, Taxonomy and Phylogeny.
- Concepts in Molecular Evolution.

More books for Reading and Referencing

Molecular analysis and Genome discovery; John Willey & Sons, Ltd. (2004) by Rapley, R. & Harbron, S.
Comparative genomics: empirical and analytical approaches to gene order dynamics, map alignment and the evolution of gene families”; Netherlands, Kluwer Academic Publishers. (2000) by Sankoff, D. & Nadeau, J.H.

Course Schedule: Core: Pharmacogenomics and Phylogenetics

Syllabus	Schedule
Unit 1: Pharmacogenomics: Overview, present status, Pharmacogenomics and Personalized medicine, Pharmacogenomics Case Study: example-Personalized anticoagulant therapy, role of bioinformatics in pharmacogenomics. Basic Principles; Approaches to pharmacogenomics studies; concepts of individualized medicine; how pharmacogenomics aims to improve drug efficacy and toxicity, genetics of drug metabolism, Limitation.	22 days
Unit II: The Pharmacogenetics and Pharmacogenomics knowledge Base, Systems for the Management of Pharmacogenomic Information, Ethnicity and Pharmacogenomics. Functional Analysis of Gene Variation: Human Genome and Genomic Applications, Genetic Polymorphism of Metabolic Reactions, SNPs, Association Studies in Pharmacogenomics, Study on industries developing pharmacogenomic research.	22 days
Unit III: Transfection Assays with Allele-Specific Constructs: Functional Analysis of UDP-Glucuronosyltransferase Variants, CYP2D6, CYP2C19 in drug metabolism, Snapshot of the Allele-Specific Variation in Human Gene Expression, Genome-Wide Analysis of Allele-Specific Gene Expression Using Oligo Microarrays, Roche Ampli Chip, HaploChIP: An In Vivo Assay. Association Studies in Pharmacogenomics, Pharmacogenomics of Cancer, Hypertension and Cardiovascular Diseases.	22 days
Unit IV: Human Genetics and Molecular biology: DNA as a genetic material – Nucleic acid structures- Basic concepts and mode of inheritance of genetics diseases, population genetics. Transcription: Initiation-Promoter and enhancers, Elongation, Termination and RNA Processing, Prokaryotic and Eukaryotic translation. Regulation gene expression: Lac Operon. Cell culture techniques and good laboratory practice to maintain the various cell lines and chemicals, In vitro and in vivo drug Discovery.	22 days
Unit V: Phylogenetics: Basic concepts in Systematics, Taxonomy and Phylogeny: Species concept, kingdom to species, the five kingdoms,	22 days

classical, phenetic and cladistic approaches. Taxonomic information on viruses, microbes, plants & animals. Concepts in Molecular Evolution. Phylogenetic representations, Definition and description, various types of trees; Steps in constructing a tree, Consensus (strict, semi-strict, Adams, majority rule).	
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment & Seminar: Pharmacogenomics and Phylogenetics

I. Objective type Questions. Choose the correct or most correct alternatives

1. Potential outcomes of pharmacogenetic research include all the following except

- A) lower incidence of adverse drug effects.
- B) new drug development.
- C) higher health care costs.
- D) improved treatment outcomes.
- E) pretreatment screening for genetic polymorphisms.

2. The most commonly occurring variant in the human genome is

- A) tandem-repeat polymorphism.
- B) premature stop codon.
- C) nucleotide base insertion.
- D) single-nucleotide polymorphism.
- E) defective gene splicing.

3. Genetic variations in drug targets may contribute to which drug property?

- A) Bioavailability
- B) Half-life
- C) Racial differences in response
- D) Peak-dose area under the curve
- E) Entry into the central nervous system

4. CYP2D6 polymorphism can affect:

- A) drug efficacy.
- B) drug toxicity.
- C) drug interaction potential.
- D) drug delivery.
- E) a, b, and c.

II. Write short notes for the following questions

5. Explain the role of Bioinformatics in Pharmacogenomics.

6. What is polymorphism? and explain its importance in drug targeting.

7. Prepare a Glossary for any 25 Cyp enzymes involved in Pharmacogenomics.

8. How pharmacogenomics aims to improve drug efficacy and toxicity?

9. Explain about Single Nucleotide Polymorphism and its role in Pharmacogenomics.

10. Describe personalized medicine and its importance

DISSERTATION

Program: PhD.,	Semester: period 3 - 7 years
Course Title: Dissertation	Class Time: Depending upon the time taken in completion of the research work (period 3 - 7 years).
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. RM. Vidhyavathi
Mobile: +91 - 94448 35869	Email: vidhyamiss@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

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:

At the end of the Ph.D course, the research scholars are advised to submit their thesis work mandatorily based on their mentor's area 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:

As per the taken area of specialization

Course Objectives: To make the scholars:

- i. Demonstrate and comprehend the knowledge underlying the central concepts (elucidation of protein – structure function) in the structural biology through theoretical and practical methodologies. Proteomics based research such as crystal and solution structure determination of bio - molecules.
- ii. Structure-based design of new molecules (Virtual Screening, QSAR, Application of Quantum mechanism in the macromolecule complex environment) that are vital to identify its therapeutic impacts by making a thorough detailed study on its atomistic structure make-up and its correlation with function delivered in biological process.
- iii. To study the impact of variations in human populations and their associated role in the onset of diseases with help of omics and genetics approach
- iv. To learn the concepts of data collection and storage in the form of databases with the help of Structured Query Programming Languages
- v. Concepts and methodologies involved in the isolation of therapeutic compounds from medicinally important plants
- vi. Have acquired knowledge in various forms of cancer associated in health implications

Course Outcomes: The students shall be able to

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| i. Research on crystallization and the development of new methods for crystal manipulation that could lead to novel structure determination that would have immediate contribution to the established structural research communities. |
| ii. Develop potential leads of desired therapeutic indices that could be obtained from computational combinatorial screening and also the techniques of the identification process are evolving and keeping up with the change is much appreciated. |

iii. 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.

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

v. Propose, plan and manage well defined research and design projects involving a team of individuals followed by reasoned interpretation and critically assess existing theories and models within his field of specialization.

vi. Familiar with the publication process of scientific results and be able to select the appropriate publication outlets for articles reporting on their research work.

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ALU - DBI