ALAGAPPAUNIVERSITY
Syllabus for Ph.D. Bioinformatics

S. No	CourseCode	Nameof the Course	Marks		
			Int.	Ext.	Total
1.	Paper–I(15611)	ResearchMethodology	25	75	100
2.	Paper-II(15612)	Proteomicsand Cheminformatics	25	75	100
3	Paper-III	StructuralBiologyandBio-Computing (15613) **OR** MolecularmodelingandStructural Bioinformatics (15613 B) **OR** Pharmacogenomics and Phylogenetics(15613C) **OR** Bio-Computing and Computational Biology: Algorithms, Database and Tools (15613D) **OR** Functional Plant Genomics and Next-Generation Sequencing Analysis (15613E) **OR** Nanomaterials and Its Biomedical Applications (15613F)	25	75	100

ALAGAPPAUNIVERSITY, KARAIKUDI
Department:BIOINFORMATICS
Course Depiction

PAPER–IRESEARCHMETHODOLOGY

Program: **PhD.,**	Semester: **One year**
Course Title: **Research Methodology (15611)**	Class Time: **Basedontheconvenience,the concerned faculty can take classes during the working hours including Saturdays.**
Name of the CourseTeacher	**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 dockingandstructurevisualizationtoolswillbeintroduced andinadvancedmode.Studentswill beintroducedtosequenceanalysis,phylogenetictreeconstructionmethodsandthetoolsusedfor phylogenetic analysis.

Reference/Text Books

1. KrishnamurthyKV.(2003).AnadvancedTextbookonBiodiversity-principleand practice. Oxford & IBH publishing Co. Pvt. Ltd.
2. BalaguruswamyE. (2008).Numerical Methods.TMH publications.
3. Isaev and Alexander Berlin. (2004). Introduction to mathematical methods in bioinformatics. Springer.
4. MurrayJD.(1989).Mathematical Biology. Springer Verlag.
5. SegalL.(1980).Mathematical Models in Molecular and Cellular Biology.Cambridge University Press.
6. ZarJH.(1984).Bio Statistical Methods. Prentice Hall International Edition, USA.
7. MountD. (2004).Bioinformatics:Sequence andGenome Analysis;ColdSpring Harbor Laboratory Press, New York.
8. ChristophW.Sensen.(2002).EssentialsofgenomicsandProteomics.Wiley-VCH.
9. DubeyRC. (1993). Atext book of Biotechnology.S. Chand & company Ltd, New Delhi.
10. GibsonGandMuseSV.(2002).APrimerofGenomeScience.SinauerAssociates,Inc. Publishers.
11. BournePE and WeissigH.(2003). StructuralBioinformatics. John-Wileyand sons.
12. ArthurMLesk.(2005).IntroductiontoBioinformatics,2nd Edition.OxfordUniversity Press, New Delhi.

13. AttwoodKJandParry-SmithJD.(2005).IntroductiontoBioinformatics.PearsonEducation.
14. Baxevanis AD and Francis Ouellellette BF. (1998). Bioinformatics- a practicalguide tothe analysis of Genes and Proteins. John Wiley & Sons, UK.
15. ZoeLacroixandTerenceCritchlow(2003).Bioinformatics-ManagingScientificData. Morgan Kaufmann Publishers.
16. Nucleic Acids Research Journal Database Issues and Web-server issues (current and pastissues) (http://nar.oxfordjournals.org/)

CourseObjectives: To makethe students
1. Learn the statistical techniques such as measures of standard deviation, measures of dispersion and regression analysis.
2. Theknowledgeof intellectual propertyrights and filingthe patents.
3. Learnthevarioussequenceandphylogeneticanalysis methods.
4. Howtoutilizegenome resourcesontheweb.
5. Genepredictionmethodsandtoolsusedforgeneprediction.

CourseOutcomes: Thestudents shallbeable to:

i.Applyingstatisticaltechniquesfordataanalysis:measurementofstandarddeviation, dispersionandregressionanalysis.
ii.Understandintellectualpropertyrightsandpatent profiling.
iii.Learnsequenceanalysismethodsandtoolsusedforgeneprediction.
iv.Studentwilllearntodrawchemicalstructuresandtheusesofmolecularmodeling tools andtheirapplications.
v.Learntheconceptof graphs,vector algebraandmatrices.
vi.Phylogenetictreeconstructionandapplicationofphylogenetic analysisin evolutionarystudies

Grading System

<50 Marksin all	50 <YourMarks <60	60 <YourMarks <75	YourMarks≥75
Fail	IIClass	IClass	Distinction

Assessment&Evaluation: Studentevaluationisbasedonexams,assignments,andseminar.The grade allocation is as follows:

ContinuousInternalAssessment:25Marks		**End-Semester Exam: 75 Marks**
3 hour test for 75 marks and then is convertedto15 marks	Assignments,SeminarsandCases, for 10 Marks	ThreeHourexaminationfor75 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 theclasses 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 preparefor 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.

AcademicDishonesty: Thisisanimportant aspectthateverystudentshouldbeawareof.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.

Importantdates: Please notedowntheimportant datesandsticktotheschedule

TestI	TestII	Assignment	Seminar
AsperAcademic Calendar		AfterTest-I	

CourseOutline:Researchmethodology

i. Scopes,typesandusesofbiodiversity,lossofbiodiversity.

ii. Introductiontointellectualpropertyrights,typesandimportanceofintellectualpropertyrights and patent filing.

iii. Trigonometricfunctions,seriesexpansion,inverseand general values.

iv. Statisticalmethods:measuresofcentraltendencyanddispersion.

v. Conceptoflinearregressionincludingregressionline,regressionequationandregression co-efficient.

vi. Sequence data bases: Gen Bank, EMBOSS.

vii. DNAandProteinsequence analysis.

viii. Proteomic analysis tools: ExPASyproteomictools,AnthePro,PSAAM,PSIPREDand ProteinVis

viii. Sequencealignmentandphylogenetictreeconstruction.Toolsusedfor phylogenetic tree construction PAUP and Phylip.

ix. Learningtoolsforprimeranalysis:NetPrimerandPerlPrimer.

x. Molecularvisualizationtools:RasMol,CN3Dand Swiss-PdbViewer.

xi. Moleculardockingtools: Hex,AutoDockand ArgusLab.

xii. Knowledgeof genomedatabasesontheweb. TIGRdatabaseandwebservers.

xiii. UnderstandingHuman GenomeProject andits applications.

Morebooks forReading and Referencing

Bioinformatics:DatabasesandAlgorithms:1st edition (2006)byN. GauthamKannan. Alpha SciencePublishers.
Textbooks ofBiostatisticsI(2005)byA.K.Sharma. DiscoveryPublishing House
Molecularmodelingfor beginners: 2nd edition (2008) byAlan Hinchliffe.Wileypublisher
GenomeAnalysis:Current proceduresandApplications(2014)byMaria S.Poptsova. Caister AcademicPress
AnalysisofPhylogenetics andEvolutionwith R(2012)byParadis,Emmanuel. Springer Publisher.
Genomesand what to maketo them (2008). ByBarryBarnes, John Dupre.University of ChicagoPress Publisher

CourseSchedule:ResearchMethodology

Syllabus	Schedule
Unit 1: Biodiversity: Scope, types, values and uses, Loss of biodiversity, Biodiversity and Biotechnology; Intellectual Property Rights: Introduction, typesand importance of Intellectual Property Rights (IPR) and patents, Organization – GATT-TRIPS,IPRsandownershipoftraditionalknowledge–IPRimpactson biologicalresearchin 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,KarlPearson'sCoefficientofCorrelation,LinearRegression: Regression line, Regression Equations, Regression Coefficients, Chi squared distribution, Students t distribution and ANOVA.	**22 days**
Unit 3: Sequence analysis:DNAsequence analysis:Entrez,GenBank,EMBOSS, ArtemisR11,Sequencher,DNAuser,jambw,GENSCAN,Glimmer.Protein sequenceanalysis: ExPASyProteomicstools,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,Microarrayanalysis**:**ChemSketch,ChemDraw,BKChem,ScanAnalyze, Cluster	**22 days**
Unit 5: Genome Database and Resources: Sequence and structural resources for bioinformatics – Genome Databases – The Human Genome Project – Genetic diseaseandGenomics–ComprehensiveMicrobialResourceofTIGR-Databases andwebservers.	**22 days**
Tests,Seminars,Presentations,Reviews,Assignments,JournalclubandCareer Guidance.	**5 days**

Assignment:Researchmethodology

1. Define intellectual property rights. Describe the types of intellectual property rights and itsimportance.
2. Definelinearcorrelation.Discussaboutthetypesandvariousmethodsforstudying correlation.
3. DescribetheDNAsequenceanalysisandproteomictools.
4. Definephylogeny.Discussaboutthetoolsusedforphylogenetic analysis.
5. Describethetools used formoleculardockingstudies andstructurevisualization tools.
6. Describegenomicdatabaseresourcesontheweb.
7. DiscussaboutHumangenomeproject,itsapplicationsandethicalissuesrelatedtohuman genome project.
8. Describemicroarrayanalysistechniquesandits applications.
9. Discussaboutstructuralbioinformatics resourcesontheweb.
10. Writeshort notes on anyfiveof the following

i) GENSCAN
ii) ANOVA
iii) Chisquareddistribution
iv) Measuresofcentraltendency
v) Biodiversity

=-=-=

PAPER–IIPROTEOMICSAND CHEMOINFORMATICS

Program:**PhD.,**	Semester: **One year**
Course Title: **Proteomics and chemoinformatics(15612)**	ClassTime:**Basedontheconvenience,the concernedfacultycantakeclassesduringthe working hours including Saturdays.**
NameofCourse 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/TextBooks

1. LehningerA. (1987).PrinciplesofBiochemistry. CBSPublishers,NewDelhi.
2. GeraldReed.(1993).EnzymesinFoodProcessing.Academic presses.
3. BrandenCandToozeR.(1993). Introductiontoproteinstructure.Garland.
4. JamesMLee.(1992).BiochemicalEngineering. PrenticeHall.
5. AshokPandey.(2005).EnzymeTechnology.Springer-VerlagNewYorkInc.
6. Trevor Palmer and Philip Bonner. (2007). Enzymes: BiochemistryBiotechnology, Clinical chemistry. Horwood publication.
7. Andrew R Leach and Valerie J. Gillet. (2007). Introduction to Chemoinformatics. Springer publications.
8. FrankJensen.(1999).IntroductiontoComputationalChemistry.JohnWiley&SonsLtd.
9. JohannGasteigerandThomasEngel.(2003).Cheminformatics.WILEY-VCHVerlagGmbh& Co, KgaA, Weinheim.
10. VyasSPandKharRK.(2002).TargetedandControlledDrugDiscovery.1stedn,CBS Publisher and distributors (New Delhi).
11. ThomasLangauer.(2002).BioinformaticsfromGenometoDrug.WILEY-VCHVerlagGmbh& co, KgaA, Weinheim.
12. AndrewR.Leach(2001).MolecularModeling–PrinciplesandApplications.Second Edition, Prentice Hall, USA
13. Fenniri,H.(2000).CombinatorialChemistry–Apracticalapproach.OxfordUniversity Press, UK.
14. Lednicer, D. (1998). Strategies for Organic Drug Discovery Synthesis and Design. Wiley International Publishers.
15. Gordon,E.M.andKerwin,J.F.(1998).Combinatorialchemistryandmoleculardiversityin drug discovery. Wiley-Liss Publishers.

16. Swatz,M.E.(2000).AnalyticaltechniquesinCombinatorialChemistry.MarcelDekker Publishers.

CourseObjectives: To makethe students

1. Understandingorganizationofproteinstructureandmethodsforproteinstructure determination.
2. Knowledgeof threedimensional structureof proteins.
3. Applicationofchemoinformaticsin drugdesigning.
4. Pharmacokineticsactionofdrugsonhumanbody.
5. Conceptofmolecular mechanicsenergyfunctionandapplication ofenergyminimization.
6. Moleculermodelingindrugdiscoveryand drug designing tools.

CourseOutcomes: Thestudents shallbeable to:

i. Learn the organization of protein structure and methods of protein structure determination
ii.Understandingconformationsofproteinandmultienzymecomplex
iii.Distinguishthevarioustypesofdescriptorsthatdescribethetopologyofacompoundin ordertoapplyquantumbased approaches tothebiological system
iv.Knowledgeofmoleculardescriptors andcalculationofphysicalandchemical data
v.Novel approaches ofdrugdesigningandpharmacokinetics action ofdrugon human body
vi.Aptlychoosethe appropriateforcefieldtosimulate abiological complex
vii.Feasibilitytoperformdrugdesignandproceedtopharmacological testing/analysis

Grading System

<50 Marksin all	50 <YourMarks <60	60 <YourMarks <75	YourMarks≥75
Fail	IIClass	IClass	Distinction

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

ContinuousInternalAssessment:25Marks		**End-SemesterExam:75Marks**
3hourtestfor75 marksandthenis converted to 15 marks	AssignmentsandSeminars,Cases, for 10 Marks	ThreeHourexaminationofor75Marks.

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 theclasses 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 validreason (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 preparefor 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.

AcademicDishonesty: Thisisanimportant aspectthateverystudentshouldbeawareof.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.

Importantdates: Please note downtheimportantdatesandsticktotheschedule

TestI	**TestII**	**Assignment**	**Seminar**
AsperAcademic Calendar		AfterTest-I	

CourseOutline:Proteomics andChemoinformatics

i. Organizationofproteinstructure

ii. Methodsforthedeterminationofthreedimensionalstructureof protein

iii. Posttranslationalmodificationsanditsimportance.

iv. Enzymesubstrate complex

v. Applicationofchemoinformaticsdrugdiscovery

vi. 2Dand3Dstructureofchemicalcompounds.

vii. Representationofchemicalreactions

viii. Moleculardescriptorsanditsvarioustypes.

ix. Novelapproachesin drugdesigning.

x. Pharmacokineticsactionofdrugonhumanbody.

xi. Moleculardynamicssimulationmethods.

xii. Applicationofenergyminimization

xiii. Molecularmodeling indrugdiscovery.

xiv. Structureactivityrelationship.

Morebooks forReading and Referencing

Proteinstructureandfunction (2005)byDavidWhitford. WileyPublisher
Enzymefunctionality:Design:Engineeringandscreening(2003)byAllan Svendsen.CRC Publisher
Chemoinformatics(2003) byJohann Gasteiger and Thomas Engel. WileyPublisher
Drugdesign: Structureand ligand based approaches(2010)byKenneth MMerz, Jr,Dagmar Ringe,Charles H.Reynolds.CmabridgeUniversitypress Publisher
MolecularmodelingforBeginners: 2nd edition (2008)byAlan Hinchliffe.WileyPublisher
BasicsPharmacokineticsandPharmacodynamics:AnintegratedTextbookandcomputer simulations (2011)bySaraE,Rosenbaum. Wiley Publisher

CourseSchedule:Proteomicsandchemoinformatics

Syllabus	Schedule
Unit-I Proteinsstructure:Organizationofproteinstructure,Methodsinprotein structuredetermination,factorsdeterminingstabilityofproteins,determinationof 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–flexibilityandconformationalmobilityofproteins–interactions betweennon bondedatoms – bindingenergiesofproteins.	**22 Days**
Unit-III Introduction, history and applications of cheminformatics; Representation ofchemicalcompounds,manipulationsin2Dand3Dstructuresofchemical compounds,representationofchemicalreactions,moleculardescriptors,calculations of physical and chemical data, calculations of structural deciphers.	**22 days**
Unit-IV Developmentofdrug,druglifecycle,drugdevelopmenttimelines,stages of drug discovery, strategic issues in drug discovery, emerging approaches to drugdesign and discovery, drug	**22 days**

metabolism physicochemical properties,	
pharmacokinetic actionof drugonhuman 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**,**DrugDesigningRelatedApplications**:**MolecularSimulations,MolecularModeling inDrugDiscovery**,**StructureActivityRelationship**,**Drugdesigningsoftwares.	**22 days**
Tests,Seminars,Presentations, Reviews,Assignments,JournalclubandCareer Guidance.	**5 days**

Assignment:PROTEOMICSAND CHEMINFORMATICS

1. Determinationofthreedimensionalstructureof protein
2. Performingmoleculardynamicssimulation
3. Drawing2D and3Dstructureof chemical compounds
4. Predictingposttranslationalmodificationof protein.
5. Performingenergyminimization ofthemolecule.

=-=-=

PAPER –III AREA OF SPECIALIZATION

STRUCTURALBIOLOGY&BIO-COMPUTING

Program:**PhD.,**	Semester: **One year**
Course Title: **Structural biology & Bio-Computing (15613)**	ClassTime:**Basedontheconvenience,the concernedfacultycantakeclassesduring the working hours including Saturdays.**
NameofCourse 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 crystallographytechniques 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/TextBooks

1. Woolfson MM. (1997). An introduction to X-ray crystallography, 2nd Edition, Cambridge University Press.
2. GiacovazzoAC,MonacoHL,ArtioliGandViterboD.(2002).Fundamentalsof Crystallography. Oxford University Press.
3. Stout GH and JensenLH. (1989). X-ray Structure Determination. Macmillan PublishingCo., Inc., New York.
4. DennisWBennett.(2010).UnderstandingSingle-CrystalX-RayCrystallography.WILEY-VCH VerlagGmbh&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. JanDrenth.(1994).PrinciplesofProteinX-rayCrystallography.Springer-Verlag,New York.
7. Leon Aand LeonM.(1999).IntroductiontoComputers.VikasPublishingHouse.
8. Hayes.(1998).ComputerArchitectureandOrganization.TataMcGraw Hill.
9. PattersonandHennessey(1999).ComputerOrganizationandDesign".TheHardware /Softwareinterface.HarcourtAsiaMorganKaufmann.
10. Cormen,TH,LeisersonCEandRivestRL.(2001).IntroductiontoAlgorithms.3rdEd, Association of American Publishers.
11. GuigoRedandGusfieldDEd.(2002).Algorithmsinbioinformatics.Springer-Verlag, Berlin.
12. Kanetkar.(2002).Let UsC.BPBPublications.
13. PatrickNaughtonandHerbertSchildt.(1999)Java2:TheCompleteReference. Osborne/McGraw-Hill.

14. Randal LSchwartz,TomPhoenixandO-Reilly.(2001).LearningPerl.O'ReillyMedia.
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.GalgotiaBooks Pvt. Ltd.

CourseObjectives: To makethe 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 symmetrythat 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. Awareof several solvingmethods 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.

CourseOutcomes: Thestudents shallbeable to:

i.Designtheprocessstepsleadingtodeterminationofcrystalstructuresofsmallandmacro molecules.
ii.Definewhatacrystalisanddescribethedifferencesinpropertiesofmolecularandmacro molecularcrystals.
iii.Explainthedifferencesbetweencrystallizationofsmallmoleculesandmacromolecules; choosepropermethodsforprotein crystallization.
iv.Characterizemethodsofphaseproblemsolvingandchoosepropermethodsformolecularand macromolecularstructures.
v.Defineelectrondensitymapsandchoosetheproperalgorithmsforstructurerefinement.Use specific crystallographic software for structure visualization and refinement.Validate the finalstructures.
vi. Explicate about interactionsthat modulate protein-protein complexes(small-molecule, nucleic acids,biomolecules)whichlater oncanbedesignedastherapeuticmarkers
vii. Learntheconceptofcomputernetworking
viii.Writingcodesforbiologicaldata analysis.

Grading System

<50 Marksin all	50 <YourMarks <60	60 <YourMarks <75	YourMarks≥75
Fail	IIClass	IClass	Distinction

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

ContinuousInternalAssessment:25Marks		**End-Semester Exam: 75 Marks**
3 hour test for 75 marks and then is convertedto15 marks	Assignments, Seminars, Reviews, Cases, for 10 Marks	ThreeHourexaminationfor75 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 theclasses 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 preparefor 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.

AcademicDishonesty: Thisisanimportant aspectthateverystudentshouldbeawareof.Thus,the respectivefacultymemberseducatethestudentsofpossiblemeansofacademicmalpractices

(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.

Importantdates: Please notedowntheimportant datesandsticktotheschedule

TestI	TestII	Assignment	Seminar
AsperAcademic Calendar		AfterTest-I	

CourseOutline:Structural biology&Bio-computing

- X-raygeneration,Synchrotronradiationand applications.
- Introductiontounitcell,lattices,planesandcrystalsystems.
- X-rayscatteringand diffraction.
- ConceptofelectrondensitymapsandFouriertransform.
- Diffractionbycrystals, Lorenz andpolarizationfactor.
- Smalland MacroMolecule X-raycrystallography.
- Isolationandpurification ofprotein.
- Crystallizationmethods,intensitydata collection,reductionandphaseproblem.
- Knowledgeofworkingofcomputer,generationofcomputerandtypesofmodern computers.
- Conceptofcomputernetworkinganddatasecurity.
- Knowledgeofworkingon different operatingsystems (Windows/Unix/Linux).
- Programminglanguages (C,Perl,and Java).
- Conceptofrelationaldatabasemanagementsystem(RDBMS).
- Array,functionsanddatastructures.

Morebooks forReading and Referencing

An Introduction toX-rayCrystallography:2nd edition(1997)byMichael M.Woolfson. Cambridge UniversityPress Publisher
X-rayCrystallography2nd edition (2015)byWilliam Clegg. OxfordUniversityPress
Basicconcepts ofX-raydiffraction(2014) byEmillZolotoyabko. Wileypublisher.
Isolationand purificationof proteins(2003)byRajniHatti-kaul, BoMattiasson. CRC Publisher
Basicsof computerNetworking(2012) byRobertazzi,Thomas.Springer Publisher
ProgrammingPerl: 4th edition(2012)byTom Chrisiansen,brian d foy,Larrywall and Jon orwant.O'ReillyMediaPublisher.

CourseSchedule:Structuralbiology&Bio-computing

Syllabus	Schedule
Unit-I Elementary Crystallography: X-ray generation; Synchrotron radiation and applications; unit cell, Lattices, Planes, Crystal systems, stereographic projection of pointgroups,spacegroups,Symmetryelements,isogonalsymmetrygroupsand reciprocallattice.Crystalsandgrowingcrystalsproperties,X-raydiffraction,Laue	**25 days**

equations, Bragg Law, reciprocal lattice and application to geometrical crystallography.	
Unit-IIX-ray Scattering and Diffraction: Atomic scattering factor, diffraction by a space lattice, structure factor equation, electron density and Fourier series, Fourier Transformandcrystaldiffraction,diffractionbyrealcrystals,Lorentzand polarizationfactor,primaryandsecondaryextinctions	**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, Interpretationofresults,bondlengths,bondangles,torsionangles,thermalmotion analysisandInteractions, ValidationmethodsandStructureanalysis.	**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,JournalclubandCareer Guidance.	**5 days**

Assignment&Seminar Structuralbiology&Bio-computing

1. Describethemethodsusedforcrystalstructure determination.
2. Discussaboutmethodsof proteinisolationand variousproteinpurification techniques.
3. Define electron density maps.Describe the calculation and interpretationof electron densitymaps. Write in brief about least squares techniques in refinement.
4. Describemacromolecularstructuredeterminationmethods and theirvalidation.
5. DefineX-raygeneration.Describesynchrotron radiationanditsapplications.
6. Discussabout variousX-rayscatteringtechniques.
7. Discussaboutvariousgenerationsofcomputers.Writeinbriefabouttypesofmodern computers.
8. Describedifferenttypesofoperatingsystemandtheirfeatures.
9. Discussaboutthefeaturesofprogramminglanguages:C,PerlandJava.
10. Writeshort noteson the following
    i) BraggLaw
    ii) FourierTransform
    iii) RDBMS
    iv) X-raydiffraction
    v) datastructures

=-=-=

MOLECULARMODELINGANDSTRUCTURALBIOINFORMATICS

Program:**Ph.D.,**	Semester: **Oneyear**
CourseTitle:**MolecularModelingand Structural Bioinformatics (15613 B)**	ClassTime:**Basedontheconvenience, the concerned faculty can take classes during the working hours including Saturdays.**
NameofCourse Teacher	**Dr.SanjeevKumarSingh**
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-novoligand 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 modellingmethods. It also serves as a introduction of molecular modeling to the students which could provide strong basic knowledge as well.

Reference/TextBooks:

1. Leach,A.R.(2001)“MolecularModeling–PrinciplesandApplications”;Second Edition, Prentice Hall, USA
2. Fenniri, H. (2000) “Combinatorial Chemistry – A practical approach”, Oxford University Press, UK.
3. Xiang,ZandRoy,A.“Schaum'sOutlineofComputerGraphics”;PlastockSecond Edition, Mc-Graw Hill, USA.

4. Johann,G.(2003)Chemoinformatics:ATextbook,Wiley,John&Son,ISBN-13: 9783527306817
5. Lednicer,D.(1998)“StrategiesforOrganicDrugDiscoverySynthesisandDesign”; Wiley International Publishers.
6. Gordon, E.M. and Kerwin, J.F. (1998) “Combinatorial chemistry and molecular diversity in drug discovery”; Wiley-Liss Publishers.

CourseObjectives: To makethe students:

i. To help the students to be familiar about the concepts of bioinformatics to be implemented in drug design and development.

ii. Tofindnewtargetstotreatdisease;mechanismofdrugdesigning

iii. Tomakethestudentsunderstandtheconceptofmolecularmodeling,mechanicsand interactions

iv. Toprovideclearconceptsonbondangle,bondstretching,bonddistanceandroleon different types of bonds in interactions

v. Toacquiretheknowledgeabouttheproteinstructurepredictionandconformationalchanges throughout the simulation

vi. To provide brief idea of receptor and receptor-ligand complex, inhibition and inactivation of enzyme, receptor theories

vii. Toprovidetheabundantknowledgeaboutthestructuralandchemicalfeaturesofthe receptor and the ligand compounds.

CourseOutcomes: Thestudents shallbeable to:

i.Thestudentwouldbeabletoidentifythestepsfordesigningnewdrugs,target identification and validation
ii. They would acquire the capacity to apply the ideas of atomic displacement, Quantum andMolecularMechanics,bondedinteractions,hydrogenbondingsanditssignificancein the application of drug development
iii.Theywouldbeabletoexecuteproteinstructurepredictionandwouldbeabletopredict the derivatives of the molecular mechanics energy function
iv.TheywillfinditeasyfortheunderstandingoftheMolecularDynamicssimulation using the simple models, continuous potentials at constant temperature and pressure
v.Theywillbeverycapabletopresentthedockingstrategiesbasedontheligand,receptor and de novo ligand design.

vi.Understandingofthecombinatorialchemistryandlibrarydesign,virtualscreeningand compound filtering.
vii.Theywouldbeabletounderstandthetheoryofinhibitionandinactivationofenzymes, drug deactivation and susceptibility

TeachingMethods:Themode ofteachingis based on the followinglearning activities:

- LecturescoveringthetheoreticalpartwillbedeliveredusingPowerPointpresentations.
- A set of laboratory exercises to analyze biological problems using softwares and tools to develop student's interests in scientific discovery.
- Casestudiesininformatics-basedresearch.

Grading System

<50 Marksin all	50<Obtained Marks <60	60<Obtained Marks <75	ObtainedMarks≥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:

ContinuousInternalAssessment:25Marks		**End-SemesterExam:75Marks**
Two, 3 hour test for 75 marks and is converted to 15 marks	Assignments and Seminarsfor10Marks	ThreeHourexaminationonthe 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 of70-75%attendanceareonlyqualified to writetheirend-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 throughquestioning 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 conceptsfordeeperunderstandingofthesubject.Therefore,eachstudentwillbeallocatedtwoassignments 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.

Importantdates: Scheduleddatesforthevariousactivitiesrelatedtothe course

TestI	TestII	Assignment	Seminar
AsperAcademic Calendar		AfterTest-I	

CourseOutline:MolecularModelingandStructuralBioinformatics

1. Drug discovery process, Role of Bioinformatics in drug design, Target identification and validation, lead optimization and validation, Structure-based drug design and ligandbased drug design.
2. Modellingofprotein andtarget-smallmoleculeinteractions,Molecularsimulations
3. Quantum mechanics and Molecular Mechanics, Potential energy, van der Waalsand 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. Varioous 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 predictionand application in drug discovery, QSAR methodology, Electronic Topology, Quantum chemical based Descriptors.
9. Genetic algorithms, Neural networks and Principle component analysis in QSARequation

Morebooks forReading and Referencing

Computationalmethodsindrugdesign **FredE.Cohen,WalterHamiltonMoos** Publisher:ESCOMScience, 1993.
MolecularModellingfor Beginners -**Alan Hinchliffe** Publisher:JohnWiley&SonsInc,2008.ISBN:978-0470513149
Combinatorial Library Design and Evaluation: Principles, Software, Tools, Applications in Drug Discovery – **Arup Ghose, VellerkadViswanadhan** Publisher:CRCPress,2001.ISBN:0-8247-0487-8
MolecularModelingBasics-**Jan H. Jensen** Publisher:CRCPress,2010.ISBN978-1420075267
3D QSAR in Drug Design: Recent Advances – **Hugo Kubinyi, GerdFolkers, Yvonne C.Martin** Publisher:SpringerScience&BusinessMedia. ISBN:0-306-46858-1
ComputationalChemistryandMolecularModeling-**K.I.Ramachandran,GopakumarDeepa, Krishnan Namboori** Publisher:Springer–VerlagBerlinHeidelberg.ISBN:978-3540773023

CourseSchedule:MolecularModellingandStructuralBioinformatics

Syllabus	Schedule
Unit-I Molecular Modelling in Drug Discovery: Drug discovery process, Role of Bioinformaics in drug design, Methods of computer aided drug design,ligand design methods, drug design approaches, Target identification and validation,leadoptimizationandvalidation,Structureandligandbaseddrug design, modelling of target-small molecule interactions, Molecular simulations. Protein Modelling	**14 Days**
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 inmolecularmechanics;Derivativesofmolecularmechanicsenergyfunction; Application ofenergyminimization	**10 Days**
Unit-III MolecularDynamicssimulationmethods–MolecularDynamicsusing	**16 Days**

simple models; Molecular Dynamics with continuous potentials and at constant temperature and pressure; Time – dependent properties; Solvent effectsinMolecularDynamics;ConformationalchangesfromMolecular Dynamicssimulationand 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 identificationandValidation,leadidentification,optimizationandvalidation. Combinatorial chemistry and library design, virtual screening, drug likeness and compound filtering, Absorption, distribution, metabolism, excretion and toxicity(ADMET)propertyprediction,computerbasedtoolsfordrug 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.UseofGeneticAlgorithms,NeuralNetworksandPrincipleComponents AnalysisintheQSARequations	**18 Days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 days**

Assignment:MolecularModelingandStructural Bioinformatics

1. RoleofBioinformatics indrugdesign
2. StructureBasedDrugDesign
3. Coordinate System
4. Quantum Mechanics
5. Energyconcept and itsimportancein drugaction
6. Pharmacophorehypothesis
7. ADMEcalculation
8. SolventeffectsinMolecularDynamics
9. Applicationof3D DatabasesearchinginMolecular Docking
10. Receptortheoriesanddrugaction

=-=-=

PHARMACOGENOMICSAND PHYLOGENETICS

Program:**Ph.D.**	Semester: **One year**
CourseTitleand Code: **PharmacogenomicsAndPhylogenetics (15613C)**	ClassTime:**Basedontheconvenience,the concernedfacultycantakeclassesduringthe working hours including Saturdays.**
Nameofthe CourseTeacher	**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/TextBooks:

1. Mount,D.(2004)"Bioinformatics:SequenceandGenomeAnalysis";ColdSpringHarbor Laboratory Press, New York.
2. Baxevanis,A.D.andFrancisOuellellette,B.F.(1998)"Bioinformatics–apractical guide to the analysis of Genes and Proteins"; John Wiley & Sons, UK.
3. Richard,J.R.(2003)"AnalysisofGenesand Genomes";WileyPublications.
4. Falconer,D.S., Mackay, T.F.C.,(1996)"Introduction to QuantitativeGenetics".Pearson Education Ltd, 4thEd.
5. PankhurstRJ.(1991).Practicaltaxonomiccomputing.ColumbiaUniversityPress.
6. Lednicer,D.(1998).StrategiesforOrganicDrugDiscoverySynthesisandDesign.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. Tounderstand how individualization ofdrugtherapybased on aperson's geneticmakeup can optimize the effectiveness of that therapy while reducing unwanted drug effects.

Course Outcomes:

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.

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 andtoxicity, adverse drug reactions and drug-drug interactions
iv.UnderstandingofthebasicsofPharmacogenomicswillenablestudentstobetter understand and manage the new genomics based tools as they become available as wellas make best treatment choices.

Teaching Methods: Themode of teachingof deliveringthe 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 overseasreputed institutions
- Case-studiesandReview questions

Grading System

<50Marksinall	50<YourMarks <60	60 <YourMarks <75	YourMarks≥75
Fail	**II Class**	**I Class**	**Distinction**

Assessment&Evaluation: Studentevaluationisbasedonexams,assignments,reviews,and class participation. The grade allocation is as follows:

ContinuousInternalAssessment:25Marks		**End-SemesterExam:75Marks**
Two, 3 hour test for 75 marks and thenisconverted to 15 marks	Assignments, Seminars, Reviews, Cases for 10 Marks	ThreeHourexaminationonthe 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 theclasses 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 preparefor 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.

AcademicDishonesty: Thisisanimportant aspectthateverystudentshouldbeawareof.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.

Importantdates: Please notedowntheimportant datesandsticktotheschedule

TestI	**TestII**	**Assignment**	**Seminar**
AsperAcademic Calendar		AfterTest I	

CourseOutline:Pharmacogenomics andPhylogenetics

- Basicconceptsofpharmacogenomicsandgeneticsdiseases.
- Pharmacogenomicsnecessityin drugdesigning.
- ThePharmacogeneticsandPharmacogenomicsknowledgeBase.
- Polymorphismsandtheir importanceindrugdesigning.
- CYP2D6,CYP2C19in drugmetabolism.
- StructuralinfluenceintheDrugresponse.
- Cellculturetechniquesandgoodlaboratorypracticetomaintainthevariouscelllinesand chemicals, *In vitro* and *in vivo* drug Discovery.
- Predictionofstructuralchangesamongsequencesbythe influenceof polymorphisms.
- Toolsforpharmacogenomicanalysis.Pharmacokinetics(PK),Pharmacodynamics (PD).

- TargetStructureoptimization,Validation,leadidentification,ADME prediction.
- Synthesis,assay,andclinicaltrialsfortheidentificationofnoveldrug.
- BasicconceptsinSystematics,TaxonomyandPhylogeny.
- ConceptsinMolecularEvolution.

Morebooks forReading and Referencing

MolecularanalysisandGenomediscovery;JohnWilley&Sons,Ltd.(2004)byRapley,R.& Harbron,S.
Comparativegenomics:empiricalandanalyticalapproachestogeneorderdynamics,mapalignmentandtheevolutionofgenefamilies";Netherlands,KluwerAcademicPublishers. (2000)bySankoff, D. &Nadeau, J.H.

CourseSchedule:Core:PharmacogenomicsandPhylogenetics

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;conceptsofindividualizedmedicine;howpharmacogenomicsaims 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,AssociationStudiesinPharmacogenomics,Studyon industriesdevelopingpharmacogenomic 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 UsingOligoMicroarrays,RocheAmpliChip,HaploChIP:AnInVivo 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 –Nucleicacidstructures-Basicconceptsandmodeofinheritanceofgenetics diseases, population genetics.Transcription: Initiation-Promoter and enhancers, Elongation, Termination and RNA Processing, Prokaryotic and Eukaryotictranslation. Regulation geneexpression: LacOperon.Cell culture techniquesandgoodlaboratorypracticetomaintainthevariouscelllinesand chemicals, Invitroandin vivodrugDiscovery.	22 days
UnitV:Phylogenetics:BasicconceptsinSystematics,Taxonomyand Phylogeny:Speciesconcept,kingdomtospecies,thefivekingdoms,	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;Stepsinconstructingatree,Consensus(strict,semi-strict,Adams, majorityrule).	
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 days**

Assignment&Seminar:PharmacogenomicsandPhylogenetics

I. ObjectivetypeQuestions.Choosethecorrector mostcorrectalternatives

1. Potentialoutcomesofpharmacogeneticresearchincludeallthefollowingexcept
   - A) lowerincidenceofadversedrugeffects.
   - B) newdrugdevelopment.
   - C) higherhealthcarecosts.
   - D) improvedtreatmentoutcomes.
   - E) pretreatmentscreeningforgenetic polymorphisms.
2. Themost commonlyoccurringvariant in the human genome is
   - A) tandem-repeatpolymorphism.
   - B) prematurestopcodon.
   - C) nucleotidebase insertion.
   - D) single-nucleotidepolymorphism.
   - E) defectivegenesplicing.
3. Geneticvariations in drugtargets maycontributeto which drugproperty?
   - A) Bioavailability
   - B) Half-life
   - C) Racialdifferencesinresponse
   - D) Peak-doseareaunderthe curve
   - E) Entryinto the central nervous system
4. CYP2D6polymorphismcan affect:
   - A) drug efficacy.
   - B) drugtoxicity.
   - C) druginteractionpotential.
   - D) drugdelivery.
   - E) a,b,and c.

II. Writeshort notes forthefollowingquestions

5. Explainthe role ofBioinformatics in Pharmacogenomics.
6. Whatispolymorphism?andexplain itsimportanceindrugtargeting.
7. PrepareaGlossaryfor any25 Cypenzymes involved in Pharmacogenomics.
8. Howpharmacogenomics aimsto improvedrugefficacyand toxicity?
9. Explainabout SingleNucleotide Polymorphismand itsrole in Pharmacogenomics.
10. Describepersonalizedmedicineanditsimportance

BIO-COMPUTING AND COMPUTATIONAL BIOLOGY: ALGORITHMS, DATABASES AND TOOLS

Program: **Ph.D.**	Semester: **One Year**
Course Title: Bio computing and Computational Biology: Algorithms, Database and Tools	Class Time: **Based on the convenience, the concerned faculty can take classes during the working hours, including Saturdays.**
Name of Course Teacher	**Dr. RM. Vidhyavathi**
Mobile: **+91 – 94448 35869**	Email:**vidhyavathirm@alagappauniversity.ac.in**

Course Brief:

The course is designed to provide doctoral scholars with an advanced and integrated understanding of computational approaches used to analyse biological systems through algorithms, databases, and bioinformatics tools. The course focuses on the systematic interpretation of biological information across multiple levels, including genomic sequences, protein structures, functional annotations, and evolutionary relationships. Emphasis is placed on understanding the computational foundations of sequence analysis, including pairwise and multiple sequence alignment algorithms, heuristic similarity searching methods such as BLAST, and the use of scoring matrices and statistical significance measures for biological interpretation. The course provides comprehensive knowledge of biological databases, including primary, secondary, and integrated resources such as NCBI, UniProt, Ensembl, KEGG, and the Protein Data Bank, with a focus on data retrieval, annotation, and cross-referencing of biological entities. It further introduces core computational methods used in comparative genomics, conserved motif detection, phylogenetic tree construction, and functional inference from sequence and evolutionary patterns. A detailed overview of structural bioinformatics is included, covering protein structure representation, molecular visualization, homology modelling concepts, and structure validation tools. The course also introduces applied computational techniques such as binding site prediction, molecular docking, and the fundamentals of molecular dynamics simulation, highlighting their role in drug discovery and protein–ligand interaction studies. Overall, the course equips students with strong theoretical foundations, practical tool-based competence, and critical analytical skills required to design reproducible computational workflows, interpret bioinformatics outputs, and address real biological research problems, thereby preparing them for independent research careers in computational biology, genomics, and bioinformatics-driven biomedical research.

Reference/Textbooks:

1. A Biologists Guide to Principles and Techniques of Practical Biochemistry, K Wilson & KH Goulding, ELBS Editon, 1986
2. David Mount. “Bioinformatics: Sequence and Genome Analysis” 2nd edition, cold spring harbor laboratory.
3. Hector C Keun. “NMR-based Metabolomics”, 2018, Royal Society of Chemistry Glick, B.R. and Pasternak J.J. Molecular Biotechnology.ASM Press, Washington DC.2003.
4. JinXiong– Essential Bioinformatics – Cambridge University Press – 2006 (1st Edition).
5. Lesk, A. M – Introduction to Bioinformatics – Oxford University Press – 2003 (1st Edition).
6. Baldi, P., Brunak, S – Bioinformatics, The Machine Learning Approach – MIT press – 2008 (2nd Edition).
7. Daniel C. Liebler Introduction to Proteomics tools for the New Biology – 2002

Course Objectives: The course aims to enable students to:

i.) Understand the scope, applications, and limitations of bioinformatics and computational biology in life science research.

ii.) Develop skills to cross-link gene, protein, and structural information across databases.

iii.) Understand and apply global and local alignment algorithms (Needleman–Wunsch, Smith–Waterman).

iv.) Understand and Identify conserved regions, motifs, and functional domains from MSA outputs.

v.) Understand protein structure organization and explore structure databases (PDB).

vi.) Apply computational tools such as binding site prediction, molecular docking, and basic molecular dynamics concepts in biological research.

Course Outcomes: After successful completion of the course, students will be able to:

i.) Apply computational biology principles to analyze biological sequence, structure, and functional datasets.
ii.) Retrieve, curate, and interpret biological information using major databases such as NCBI, UniProt, Ensembl, and PDB.
iii.) Implement and compare core bioinformatics algorithms including sequence alignment, similarity searching, and multiple sequence alignment.
iv.) Construct and interpret phylogenetic relationships using appropriate evolutionary models and tree-building tools.
v.) Analyze protein structures and functional features using molecular visualization, structure validation, and docking tools.
vi.) Design independent computational biology workflows integrating algorithms, databases, and software tools for real biological research problems.

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

- Lectures using PowerPoint presentations and research articles
- Case studies based on recent biological systems through algorithms, databases, and bioinformatics tools
- Journal club discussions and student-led seminars
- Hands-on demonstrations and data analysis workflows (where applicable)

Grading System

< 50 Marks in all	50 < Obtained Marks < 60	60 < Obtained Marks < 75	Obtained Marks ≥ 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-hourtests for 75 marksand 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:Bio-Computing and Computational Biology: Algorithms, Databases and Tools

1. Introduction to Bio-Computing and Computational Biology: scope and applications; biological data types (DNA, RNA, protein, metabolomics); role of computation in modern life sciences; overview of major bioinformatics problems.
2. Biological Databases and Data Retrieval: primary and secondary databases; NCBI, GenBank, RefSeq, UniProt, Ensembl; PDB and structural repositories; database searching, annotation, accession systems, and data integration.
3. Sequence Formats and Bioinformatics File Handling: FASTA, FASTQ, GenBank, GFF/GTF, SAM/BAM, VCF; quality scores; preprocessing and basic scripting for biological datasets; data cleaning and reproducibility.
4. Pairwise Sequence Alignment Algorithms: global and local alignment principles; Needleman–Wunsch and Smith–Waterman algorithms; scoring matrices (PAM, BLOSUM); gap penalties; alignment evaluation and interpretation.
5. Multiple Sequence Alignment (MSA) and Comparative Genomics: progressive and iterative MSA approaches; Clustal Omega, MUSCLE, MAFFT; conserved motif detection; orthologues vs paralogs; functional inference from alignments.
6. Heuristic Search Algorithms and Similarity Tools: BLAST and FASTA algorithms; E-value and bit score interpretation; sensitivity vs speed trade-offs; database indexing; PSI-BLAST and profile-based searches.
7. Phylogenetic Analysis and Evolutionary Algorithms: phylogenetic tree concepts; distance-based and character-based methods; Neighbor-Joining, Maximum Parsimony, Maximum Likelihood; bootstrap analysis; visualization and interpretation tools.

8. Protein Structure Bioinformatics and Molecular Visualization: protein structure levels; structure databases; homology modeling concepts; structure validation; molecular visualization tools (PyMOL, Chimera); structural comparison and RMSD.
9. Computational Tools for Functional Genomics: gene prediction methods; motif finding; transcriptomics and RNA-Seq basics; differential expression analysis overview; functional enrichment (GO, KEGG) and pathway analysis tools.
10. Molecular Docking, Simulation Tools and Systems Biology Overview: ligand–protein docking principles; binding site prediction; docking software (Auto Dock, PyRx, Glide overview); molecular dynamics basics; network biology and pathway modeling tools.

Course Schedule:Bio-Computing and Computational Biology: Algorithms, Databases and Tools

Syllabus	Schedule
Unit -I 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, Web designing, Basics, functions, arrays, data structure and modules/classes, Biological Algorithms Development, RDBMS.	**14 Days**
Unit -II Molecular Docking and Lead optimization: Molecular Docking; Types of Molecular Docking, docking algorithms and programs, Strategy for target identification and Validation, lead identification, Optimization and Validation. Virtual Screening, drug likeness and compound filtering, Absorption, distribution, metabolism, excretion and toxicity (ADMET) property prediction, computer-based tools for drug design.	**16 Days**
Unit -III DNA data bank: EMBL nucleotide sequence data bank – GenBank – DDBJ. Enzyme databases – cloning vector data bases, BLAST, FASTA, algorithm to analysis sequence data. Pairwise alignment and multiple alignment of nucleic acids and protein sequences, CLUSTAL W.	**14 Days**
Unit -IV Proteins: Protein structure - primary, secondary, tertiary and quaternary, globular, fibrous proteins, Ramachandran plot. Three-dimensional structure and confirmation using physical methods – ORD, CD, ESR, PAGE, SDS-PAGE, diagonal electrophoresis. DNA-protein interactions; DNA-drug interactions	**18 Days**
Unit -V Proteomics: Introduction and scope of proteomics; Protein separation techniques: ion exchange, size-exclusion and affinity chromatography; Electrophoresis techniques- Polyacrylamide gel electrophoresis, 1D and 2D gel electrophoresis, isoelectrofocusing. Fundamentals of mass spectrometry [basic theory, ionization techniques and mass analysers, electrospray ionization (ESI)] and matrix adsorption laser dissociation ionization (MALDI).	**18 Days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 Days**

Assignment:Bio-Computing and Computational Biology: Algorithms, Databases and Tools

1. Comparative Study of Global and Local Alignment Algorithms (Needleman–Wunsch vs Smith–Waterman)
2. How BLAST Works: Heuristic Algorithm, E-value, and Sensitivity vs Speed Trade-off

3. Exploring Biological Databases: Data Retrieval, Annotation, and Cross-Linking of Gene–Protein–Structure Information
4. MSA-Based Phylogenetic Tree Construction Using Clustal Omega / MUSCLE and MEGA
5. Protein Structure Modeling: Homology Modeling, AlphaFold Predictions, and Structure Validation Tools (Ramachandran, Verify3D)
6. Ligand Screening and Molecular Docking Pipeline: Target Selection, Ligand Preparation, Docking, and Binding Site Analysis

FUNCTIONAL PLANT GENOMICS AND NEXT-GENERATION SEQUENCING ANALYSIS

Program: **Ph.D.**	Semester: **One Year**
Course Title: **Functional Plant Genomics and Next-Generation Sequencing Analysis**	Class Time: **Based on the convenience, the concerned faculty can take classes during the working hours, including Saturdays.**
Name of Course Teacher	**Dr. J. Joseph Sahayarayan**
Mobile: **+91 – 90475 64087**	Email: **josephj@alagappauniversity.ac.in**

Course Brief:

The course is designed to provide doctoral scholars with an advanced and integrated understanding of plant biological systems through the application of functional genomics and high-throughput sequencing technologies. The course focuses on elucidating the molecular mechanisms underlying plant growth, development, adaptation, and interactions with biotic and abiotic environments by integrating plant–plant, plant–microbe, plant–fungal, and plant–pollinator interactions at genomic and regulatory levels. Emphasis is placed on plant secondary metabolism, defence responses, stress tolerance mechanisms, and the regulatory roles of signalling peptides and small RNAs. The course provides comprehensive knowledge of plant genomics and genetic engineering, including gene transformation technologies, vector systems, and selectable marker development. It further introduces plant synthetic biology and targeted genome editing approaches such as ZFN, TALEN, and CRISPR–Cas systems for precise functional validation and crop improvement. A detailed overview of next-generation sequencing platforms, including second-, third-, and fourth-generation sequencing technologies such as SMRT and nanopore sequencing, is covered along with their applications in whole-genome sequencing, transcriptomics, epigenomics, metagenomics, and DNA–protein interaction studies. Overall, the course equips students with the theoretical foundation, analytical competence, and critical research skills required to design, execute, and interpret genomics-driven plant research, thereby preparing them for independent research careers in plant genomics, biotechnology, and systems biology.

Reference/Textbooks:

1. Gloria Coruzzi, Rodrigo Gutirrez (2009) Plant systems Biology Annual Plant Reviews, Volume 35, Wiley Blackwell.
2. Heribert Hert (2009) Plant Stress Physiology From genomics to system biology, Wiley Blackwell.
3. Stuart M. Brown (2013) Next-generation DNA sequencing Informatics by, Cold Spring Harbor Laboratory.
4. Brown, S.M. ed., (2015) Next-generation DNA sequencing informatics. New York, NY: Cold Spring Harbor Laboratory Press.
5. C. Neal Stewart Jr. (2016) Plant biotechnology and genetics principles, techniques, and applications.
6. Stewart Jr, C.N. ed., (2025) Plant biotechnology and genetics: principles, techniques, and applications. John Wiley & Sons.
7. Shui Quing Ye. Chapman and Hall (2016) Big Data Analysis for Bioinformatics and Biomedical Discoveries, CRC Press.

Course Objectives: The course aims to enable students to:

vii.) Understand plant–plant, plant–microbe, plant–fungal, and plant–pollinator interactions at the molecular and genomic levels.

viii.) Explain molecular mechanisms underlying plant adaptation, defence, and stress tolerance.

ix.) Gain in-depth knowledge of plant genomics and genetic engineering technologies.

x.) Learn principles and applications of plant synthetic biology and genome editing tools.

xi.) Understand next-generation sequencing platforms and their applications in plant systems biology.

xii.) Develop the ability to analyze and interpret large-scale genomics and sequencing data for functional studies.

Course Outcomes: After successful completion of the course, students will be able to:

vii.) Analyze functional interactions in plant systems using genomics approaches.
viii.) Interpret biosynthetic and regulatory pathways involved in plant secondary metabolism.
ix.) Apply concepts of plant genetic engineering and genome editing in research.
x.) Select appropriate NGS platforms for plant genomics, transcriptomics, epigenomics, and metagenomics studies.
xi.) Critically evaluate high-throughput sequencing data and relate it to plant function and adaptation.
xii.) Design independent research problems integrating functional genomics and NGS tools.

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

- Lectures using PowerPoint presentations and research articles
- Case studies based on recent plant genomics and NGS research
- Journal club discussions and student-led seminars
- Hands-on demonstrations and data analysis workflows (where applicable)

Grading System

< 50 Marks in all	50 < Obtained Marks < 60	60 < Obtained Marks < 75	Obtained Marks ≥ 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-hourtests for 75 marksand 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:Functional Plant Genomics and Next-Generation Sequencing Analysis

11. Plant–plant interactions: competitive, non-competitive and complementary interactions; plant–microbe interactions; plant–fungus interactions; plant–pollinator interactions and their molecular and ecological significance.
12. Molecular mechanisms of plant adaptation; plant secondary metabolism; biosynthetic and regulatory pathways; plant defense systems including plant defensins, phenylpropanoids, jasmonates and aromatic alkaloids.
13. Abiotic stress tolerance mechanisms in plants; stress-induced peptides; small signaling peptides; role of small RNAs in plant development, defense and stress responses.
14. Overview of plant genomics and functional genomics; principles of plant genetic engineering; gene transformation technologies; vector systems for plant transformation; direct transformation of regenerable explants and development of selectable and reporter marker systems.
15. Plant synthetic biology and its applications; targeted plant genome editing approaches including Zinc Finger Nucleases (ZFN), Transcription Activator-Like Effector Nucleases (TALEN) and CRISPR–Cas systems.
16. Whole-genome sequencing and analysis in plant systems; exome sequencing; transcriptome sequencing (RNA-Seq) and functional interpretation of gene expression data.
17. Analysis of DNA–protein interactions using ChIP-Seq; epigenomics and DNA methylation analysis; regulatory mechanisms controlling gene expression in plants.
18. Metagenomics and metatranscriptomics approaches in plant-associated microbial communities and their relevance to plant health and productivity.

19. Introduction to next generation sequencing technologies; second-generation sequencing platforms including pyrosequencing, reversible dye-terminator sequencing, emulsion PCR-based sequencing and ion semiconductor sequencing (Ion Torrent).
20. Third-generation sequencing technologies including Single Molecule Real-Time (SMRT) sequencing; fourth-generation nanopore-based sequencing; comparative analysis of sequencing platforms and their applications in functional plant genomics research.

Course Schedule:Functional Plant Genomics and Next-Generation Sequencing Analysis

Syllabus	Schedule
Unit -I Plant Interactions: Modes- Competitive, Non-competitive and Complementary. Plant to microbe interactions, plant to fungus interactions, and plant to pollinators interactions.	**14 Days**
Unit -IIMolecular mechanism in plant adaptation: Plant secondary metabolism, Biosynthetic and regulatory pathway. Plant defensins- defensive phenyl propanoids, jasmonates, aromatic alkaloids. Abiotic stress tolerance-induced peptides, small signalling peptides and the role of small RNAs.	**16 Days**
Unit -III Plant Genomics: Overview on the genetic engineering of plants, development in gene transformation technologies, methods to utilize these vectors for the direct transformation of regenerable explants and development of selectable markers.	**14 Days**
Unit -IVPlant Synthetic Biology and its biological applications: Targeted plant genome editing - gene editing, ZFN, TALEN and CRISPR. Whole-genome sequencing, Exome sequencing, Transcriptome sequencing, DNA-Protein Interactions (CHIP-Seq), Epigenomics and DNA methylation analysis, Metagenome analysis.	**18 Days**
Unit -V Next Generation Sequence in plant system: Introduction to NGS, Second-generation DNA sequencing: Pyrosequencing, Reversible Dye-Terminator Sequencing, Emulsion PCR approach with small magnetic beads, Ion semiconductor sequencing, Ion torrent, Third-generation DNA sequencing: Single molecule real time (SMRT) sequencing, Fourth-generation nanopore-based sequencing.	**18 Days**
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	**5 Days**

Assignment:Functional Plant Genomics and Next-Generation Sequencing Analysis

7. Functional genomics approaches in plant biology.
8. Role of secondary metabolites in plant defense.
9. Applications of CRISPR–Cas in crop improvement.
10. RNA-Seq analysis in plant stress biology.
11. Epigenetic regulation of gene expression in plants.
12. Comparative analysis of NGS platforms for plant genomics.

ALAGAPPA UNIVERSITY, KARAIKUDI
Department: BIOINFORMATICS
Course Depiction
PAPER –III NANOMATERIALS AND ITS BIOMEDICAL APPLICATIONS

Program:Ph.D.,	Semester:**One Year**
CourseTitle**:** **Nanomaterials And Its Biomedical Applications (156303)**	ClassTime:**Based on the convenience, the concerned faculty can take classes during the working hours including Saturdays**.
NameofCourseTeachers	**Dr.P. Boomi**
Mobile:**+91-9486031423**	E-mail:**boomip@alagappauniversity.ac.in**

CourseBrief:

This course introduces the fundamentals and applications of nanoscience and nanotechnology, covering the classification and properties of nanomaterials, including zero-, one-, two-, and three-dimensional systems, quantum dots, and semiconducting nanoparticles. It addresses conventional and green synthesis methods such as sol–gel, solvothermal, co-precipitation, phytosynthesis, and microbial synthesis. Scholars gain knowledge of key characterization techniques including UV–Visible spectroscopy, FTIR, XRD, NMR, SEM, TEM, and EDAX. The course emphasizes nano-based drug delivery systems and biomedical nanotechnology, focusing on diagnostics, antibacterial and anticancer applications, cellular uptake mechanisms, nanotoxicology, and emerging clinical areas, supported by seminars, assessments, and career guidance.

Course Objective:

i. To provide fundamental knowledge of nanoscience and nanotechnology, including the synthesis, properties, and characterization of nanomaterials.

ii. To develop an understanding of nano-enabled biomedical applications, particularly in drug delivery, diagnostics, and therapeutic interventions.

Course Outcome:

1. Explain the principles of nanoscience, classify nanomaterials based on dimensionality, and relate size-dependent properties to their applications.
2. Apply conventional and green synthesis methods to design nanomaterials suitable for biomedical and technological uses.
3. Analyse and interpret data from major nanomaterial characterization techniques such as spectroscopy, diffraction, and electron microscopy.
4. Evaluate nano-based drug delivery systems and biomedical nanotechnology applications with respect to targeting strategies, therapeutic efficacy, and safety considerations.

TeachingMethods:Themodeofteachingisbasedonthefollowinglearningactivities:

- LecturescoveringthetheoreticalpartwillbedeliveredusingPowerPointpresentations.
- Asetoflaboratoryexercisestoanalyzebiologicalproblemsusingsoftwareandtoolstodevelopstudent'sinterests inscientificdiscovery.

Grading System

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

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

Continuous Internal Assessment: 25 Marks		**End-Semester Exam: 75 Marks**
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: The students are expected to attend the classes regularly, since regularattendance is essential to gain academic achievement. As per the University norms, thestudents having a minimum scale of 70-75% attendance are only qualified to write theirend-semesterexaminations.

Punctuality: Punctuality is the most important quality for the student to be followed andmaintained to achieve success. Students who arrive late by 10 mins to the class withoutany 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 consentbytheHeadoftheDepartment.

Class Participation:A student's overallgrowth and personality development is basedonhis/herinvolvementintheclassnotjustbymerepresencebutratherbeinginteractivethroughquestioningthatwilllead topropagationofideas,initiationofthought-provoking practiceand muchmorethatwillprovideawholesomeenrichedclassroom experience. When students participate, they learn from one another and gaintheirknowledge better.

Submission of Assignment: Assignments are given to students in order to apply theconceptsfordeeperunderstandingofthesubject.Therefore,eachstudentwillbeallocated two assignments for the course,covering the entire topic.Students will begivendeadlinetosubmittheassignmentbythecourseinstructorandgoodpreparationofassignmentwillhelpthestudentsfortheirfinalexams.

Presentation of Seminar: Apart from the assignments, students are supposed to give anoral presentation during the class seminar hours in their assigned topic. The concernedinstructorwillencouragetheparticipantstoaskvalidquestionsduringseminarpresentation in order to put up their confidence levels and communication skills. Inaddition,studentswillbeabletogaininformationandcanbeupdatedintheircourse.

Preparedness: At the end of every class, the concerned instructor conveys the studentsaboutthedetailsthatwillbehandledinthenextclasstoincreasethestudent's awarenessrelatedtothe topics.

AcademicDishonesty: Academicdishonestyisacompletelyunacceptablemodeofconduct and every student should be

aware of this important aspect. Thus, the respectivefacultymemberseducatethestudentsofpossiblemeansofacademicmalpractices(plagiarism,violationofcopyrightsandstealingthepatentedknowledge)andthefollowingconsequencesthatwillmakethemmorevigilantintheiracademic career.

Subject to change clause: Depending upon the requirement of student's possibility, thecourse syllabus will be re-structured and updated accordingly at the discretion of theProfessor(s)andBoard ofstudies chairperson.

Importantdates: Scheduleddatesforthevariousactivitiesrelatedtothecourse

TestI	TestII	Assignment	Seminar
AsperAcademicCalendar		AfterTest I	

CourseOutline:Core:IntroductiontoBioinformatics

- Introduction to nanoscience and nanotechnology: scope, definitions, and interdisciplinary nature
- Classification of nanomaterials: zero-, one-, two-, and three-dimensional nanostructures
- Size-dependent properties of nanomaterials, quantum effects, and structure–property relationships
- Chemical synthesis methods: sol–gel, solvothermal, co-precipitation, hydrolysis, ultrasonication, and sonochemical techniques
- Green synthesis approaches: phytosynthesis using plant extracts and microbial synthesis using bacteria, fungi, algae, yeast, and actinomycetes
- Bulk nanomaterials and nanocomposites: preparation methods and applications
- Characterization techniques: UV–Visible spectroscopy, FTIR, NMR, mass spectrometry, XRD, thermal analysis, SEM, TEM, and EDAX
- Fundamentals of nano-based drug delivery systems: polymers, lipids, metals, dendrimers, and self-assembled nanoparticles.
- Drug targeting strategies and controlled release mechanisms for site-specific delivery
- Biomedical nanotechnology applications: diagnostics, antibacterial and anticancer studies, cellular uptake mechanisms, nanotoxicology, and emerging clinical fields

MorebooksforReadingandReferencing:

Introduction to Nanotechnology - Charles P.Poole, Frank J. Owens, Wiley – India, 2009.
Nanostructures and Nanomaterials synthesis, properties and applications - Guozhong Gao, Imperial College Press, London, 2004.
Fundamentals of Nanotechnology, Hornyak, G. Louis, Tibbals, H. F., Dutta, Joydeep, CRC Press, 2009
Nanomaterials: Synthesis, properties and applications. Edited by A. S. Edelstein and R. C. Cammarata, Institute of Physics Publishing, Bristol, UK 1996. xix, 596 pp., hardcover, ISBN 07503-0358-1

Tyagi, A.K., Roy, Mainak, Kulshreshtha, S.K., and Banerjee, S., Advanced Techniques for Materials Characterization, Materials Science Foundation's (monograph series), Volumes 49 – 51, (2009)
Impedance Spectroscopy: Theory, Experiment, and Applications, E. Barsoukov and J. Ross Macdonald (Editors) (2000) John Wiley & Sons (P) Ltd.
Wachtman, J.B., Kalman, Z.H., Characterization of Materials, Butterworth Heinemann, (1993).
Li, Lin, Ashok Kumar Materials Characterization Techniques Sam Zhang; CRC Press, (2008).
Nanotechnology and Drug Delivery Volume one and two: Nanoplatforms in Drug Delivery, Jose L. Arias, CRC press
C. Kumar, Nanomaterials for medical diagnosis and therapy, Wiley –VCH, 2007, USA

Course Schedule: Core: Nanomaterials and Its Biomedical Applications

Syllabus	Schedule
Unit-I:Introduction to Nano Science and Technology: Definition of nanomaterials-Zero-, One-, Two- and three- dimensional structure-size control of metal nanoparticles and properties of nanomaterials- Quantum Dots shell structures-nonporous materials- semiconducting nanoparticles-emergence and challenges of nanoscience and nanotechnology.	22 days
Unit-II:Synthesis of Nanomaterials: Chemical method: Sol-gel technique-solvothermal methods-control of grain size-co-precipitation hydrolysis-Ultra sonication-Sono chemical method-bulk and nano composite materials- colloidal precipitation template process. Greener method: Phyto-synthesis (Plant extract) and Microbial synthesis (Fungi, Bacteria, Algae, Yeast and actinomycetes).	22 days
Unit-III:Characterization Techniques: Instrumentation and applications of UV-Vis Spectroscopy, Infrared Spectroscopy, Nuclear magnetic resonance spectroscopy, Mass spectroscopy, X-ray Diffraction, FTIR, Thermal Analysis, Scanning Electron Microscopy and Transmission Electron Microscopy with EDAX.	22 days
Unit-IV:Nano drug Delivery: Definition of drug delivery-polymers and lipids-based drug delivery system- metal nanoparticles-based drug delivery system-self assembled nanoparticles-based drug delivery- dendrimers based drug delivery- drug targeting strategies for site specific drug delivery- time and rate-controlled drug delivery.	22 days
Unit-V:Biomedical Nanotechnology: Introduction to biomedical nanotechnology-Nanotechnology in diagnostic application-In vitro and In vivo methods of antibacterial, anticancer and wound healing properties using nanomaterials- Cellular uptake mechanisms of Nanomaterials-Nanotoxicology, Nanoneurology –Nanocardiology, Nano-Orthopedics, Nano-Ophthalmology.	22 days
Tests, Seminars, Presentations, Reviews, Assignments, Journal club and Career Guidance.	5 days

Assignment&Seminar- IntroductiontoBioinformatics

1. Classification of nanomaterials and their size-dependent physicochemical properties
2. Quantum dots: synthesis, optical properties, and applications in diagnostics
3. Comparison of chemical and green synthesis methods for metal nanoparticles
4. Role of plant extracts in phytosynthesis of nanoparticles and their biomedical relevance

5. Microbial synthesis of nanoparticles using bacteria, fungi, and algae: mechanisms and challenges
6. Principles and applications of X-ray diffraction and electron microscopy in nanomaterial characterization
7. Polymer- and lipid-based nano drug delivery systems: advantages and limitations
8. Metal nanoparticle-based drug delivery and toxicity considerations
9. Cellular uptake mechanisms of nanomaterials and factors influencing bio-distribution
10. Emerging trends in biomedical nanotechnology: nanotoxicology, nanoneurology, and nanocardiology.

DISSERTATION

Program:**PhD.,**	Semester:**period 3 -7 years**
CourseTitle:**Dissertation**	ClassTime:**Depending upon the time taken in completion of the research work (period 3-7 years).**
Nameofthe CourseTeacher	**Prof.J.Jeyakanthan**
Mobile: **+91-97898 09245**	Email:jjeyakanthan@alagappauniversity.ac.in
Nameofthe CourseTeacher	**Prof.Sanjeev Kumar Singh**
Mobile: **+91-98944 29800**	Email: sksingh@alagappauniversity.ac.in
Nameofthe CourseTeacher	**Dr.M.Karthikeyan**
Mobile: **+91-94869 81874**	Email: karthikeyanm@alagappauniversity.ac.in
Nameofthe CourseTeacher	**Dr.RM.Vidhyavathi**
Mobile: **+91-94448 35869**	Email: vidhyavathirm@alagappauniversity.ac.in
Nameofthe CourseTeacher	**Dr.J.JosephSahayarayan**
Mobile: **+91-90475 64087**	Email: josephj@alagappauniversity.ac.in
Name of the Course Teacher	**Dr.P. Boomi**
Mobile: **+91-9486031423**	Email: boomip@alagappauniversity.ac.in

MajorResearchAreas

- Smalland Macromolecule X-rayCrystallography.
- 3DQuantitativeStructure-ActivityRelationship(3D-QSAR).
- HumanMolecularGenetics.
- Pharmacogenomics.
- Cheminformatics.
- Quantum Pharmacology.
- ComputerAidedDrugDesigning(CADD).
- Datamining,DatawarehousingandNetworking.
- PlanttissueCulture,GeneticTransformation,PlantMolecularBiology,Virologyand Plant Pathology.
- MolecularOncology,PharmacologyandEnvironmental 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 Biologyand 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-rayCrystallographyonecandeducethe sameandcollectthe insightdetailsbasedonthese 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, InferenceofVitaminD –Deficiencyonpopulationthroughgeneticstudies, Implicationsof *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)/TextBooks:

Asper thetaken areaof specialization

CourseObjectives: To makethe 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 identifyits 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. Haveacquired knowledgein various formsofcancer associatedin health implications

CourseOutcomes: Thestudents shallbeable to

i.Researchon crystallizationandthe development ofnewmethodsforcrystalmanipulationthat couldleadtonovelstructuredeterminationthatwouldhaveimmediatecontributiontothe establishedstructuralresearchcommunities.
ii.Developpotentialleadsofdesiredtherapeuticindicesthatcouldbeobtainedfrom computationalcombinatorialscreeningandalsothetechniquesoftheidentificationprocessare evolvingand keepingupwiththechangeis muchappreciated.

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 modificationsthatcouldenrichthedrug-likenessforhumanusewhichtendtobespecificbased onmolecularfingerprintsofhuman.
iv.Keyinformationforone'sresearchpurposescanbeobtainedfromtheknowledgebasethatis builtusingstructuredprogramminglanguages.
v.Propose,planandmanagewelldefinedresearchanddesignprojectsinvolvingateamof individualsfollowedbyreasonedinterpretationandcriticallyassessexistingtheoriesand modelswithinhis fieldof specialization.
vi.Familiarwiththepublicationprocessofscientificresultsandbeabletoselectthe appropriatepublicationoutletsforarticlesreportingontheir researchwork.

=-=-=