Integrated Programme in Bioinformatics

Courses of study, Schemes of Examinations & Syllabi (Choice Based Credit System)



# **DEPARTMENT OF BIOTECHNOLOGY & BIOINFORMATICS**

BISHOP HEBER COLLEGE (Autonomous) (Reaccredited with 'A' Grade (CGPA – 3.58/4.0) by the NAAC & Identified as College of Excellence by the UGC) DST – FIST Sponsored College & DBT Star College TIRUCHIRAPPALLI – 620 017 TAMIL NADU, INDIA

2016 – 2017

# Integrated Programme in Bioinformatics

Parts of the Curriculum	No. of Courses	Credits		
Part – I : Language	4	12		
Part – II : English	4	12		
Part – III				
Major				
Core	18	90		
Core Practical	13	31		
Elective	7	31		
Allied	6	22		
Group Project	1	5		
Project	1	6		
Part – IV				
SBEC	3	6		
NMEC	3	6		
VLOC	2	4		
Env. Studies	1	2		
SBC	1	1		
Part – V				
Extension Activities	1	1		
Gender Studies	1	1		
Total	66	230		

# Structure of the Curriculum

							Marka			
Se	m t Course		code	Course title	Prereq	Hrs/	Credit	CIA	FSA	Total
			COUC	ப்பில் செய்யுள், இலக்கிய வரலாறு,		week	3	UA	LJA	iotal
	1	Tamil I/*	U15TM1L1	உரைநடை,மொழிப்பயிற்சியும் படைப்பாக்கமும்		6	3	25	75	100
	II	English I	U16EGNL1	English Communication Skills-I		6	3	40	60	100
		Core I	I16BI101	Introduction to Computers and Bioinformatics		4	4	25	75	100
		Core Prac. I	I16BI1P1	Introduction to Computers Lab		3	2	40	60	100
		Allied I	I16BI1Y1	Cell Biology		4	4	25	75	100
		Allied Prac.l	I16BIYP1	Cell Biology and Biochemistry Lab		3	-	-	-	-
		Env. Stud	U16EST11	Environmental Studies		2	2	25	75	100
	IV	VLOC	U14VL1:1/ U14VL1:2	RI/MI		2	2	25	75	100
	1	Tamil II /*	U15TM2L2	செய்யுள், இலக்கிய வரலாறு, சிறுகதைத்திரட்டு, மொரிப்பயில்கி & படைப்பாச்சும்		6	3	25	75	100
		English II	U16EGNL2	English Communication Skills – II		6	3	40	60	100
		Core II	I16BI202	Computational Biologyand Sequence Analysis	I16BI101	6	6	25	75	100
		Core Prac. II	I16BI2P2	Introduction to Bioinformatics Lab		3	2	40	60	100
		Allied II	I16BI2Y2	Biochemistry		4	4	25	75	100
		Allied prac.l	I16BIYP1	Cell Biology and Biochemistry Lab		3	3	40	60	100
	IV	SBEC I	I16BI2S1	General Chemistry		2	2	25	75	100
		Tamil III/*	U15TM3L3	செய்யுள் - காப்பியங்கள், இலக்கிய வரலாறு, நாவல், மொழிப்பயிற்சி		6	3	25	75	100
		English III	U16EGNL3	English for Competitive Examinations		6	3	40	60	100
		Core III	I14BI303	Programming in C		6	6	25	75	100
	ш	Core Prac. III	116BI3P3	Programming in C Lab		3	2	40	60	100
		Allied III	116BI3Y3	Microbiology		4	4	25	75	100
		Allied Prac.ll	I16BIYP2	Microbiology and Genetic Engineering Lab		3	-	I	-	-
	IV	NMECI		To be selected from courses offered by other departments		2	2	25/ 40	75/ 60	100
	I	Tamil IV/*	U15TM4L4	செய்யுள் - நாடகம், இலக்கிய வரலாறு, மொழிப்பயிற்சி		5	3	25	75	100
		English IV	U16EGNL4	English through Literature		5	3	40	60	100
		Core IV	I16BI404	Basic Mathematics		6	5	25	75	100
		Core prac. IV	116BI4P4	Programming in Sci Lab		3	2	40	60	100
N/		Allied IV	I16BI4Y4	Molecular Biologyand Genetic Engineering		4	4	25	75	100
		Allied prac.ll	I16BIYP2	Microbiologyand Genetic engineering Lab		3	3	40	60	100
		NMECII		To be selected from courses offered by other departments		2	2	25/ 40	75/ 60	100
	IV	SBC	U16LFS41	Life Skills		2	1	100		100
	V	Extension Activities	U16ET A41				1	-	-	-

# M.Sc Bioinformatics (Five year integrated Course) (For the students admitted from the year 2016 onwards)

Som	Dort	Cou	***	Course	Course title	Prerequisi	uisi Hrs/ Cr		Marks		
Sem	Part	Cou	rse	code	Course lille	tes	week	ts	CIA	ESA	Total
		Core V		I16BI505	Structural Bioinformatics and Medicinal Chemistry		6	5	25	75	100
		Core V	l	I16BI506	Programming in PERL and BioPERL		6	5	25	75	100
		Core Pr	ac. V	116BI5P5	Advanced Bioinformatics Lab-I		3	2	40	60	100
V		Core Pr	ac. VI	116BI5P6	Programming in PERL and BioPERL Lab		3	2	40	60	100
v		Elective	ective I I13BI5:1/		Biophysics/Database & tools for		5	5	25	75	100
				I13BI5:2	Bioinformatics						
		Elective	ell	113BI5:3/	Biostatistics & Numerical Methods/ I16BI		5	5	25	75	100
				113BI5:4	International matrix International biological constraints International constraint <						
		SBEC		114BI5S2	Applied Bioinformatics		2	2	25	75	100
	Ш	Core V	ll	I16BI607	Introduction to DBMS and SQL		5	5	25	75	100
		Core V		I16BI608	Molecular Modeling and Drug design	I16BI505	5	5	25	75	100
		Core P VII	rac.	I16BI6P7	Introduction to DBMS and SQL Lab		3	2	40	60	100
VI		Core P VIII	rac.	I16BI6P8	Advanced Bioinformatics Lab-II		3	2	40	60	100
		Elective	e III	113BI6:1/	Biodiversity Informatics/		6	5	25	75	100
				113BI6:2	Immunoinformatics						
		Core P	roject	113BI6PJ			6	5	-	-	100
	IV	IV SBEC III 116BI5S3		I16BI5S3	Comprehensive practice for Bioinformatics competitive examination	Part III of Sem I-VI	2	2	25	75	100
	V		U16GST6	Genderstudies			1	20	80	100	
	Total						140			4300	
					Possible exit point with Under Graduate	Degree					
Sem	Co	Course Course code Course title			Prerequisi	Hrs/	Credi	<u> </u>	/larks		
	Cara	IV			Coll and Malagular Biology		week	ts		ESA	Total
	Core	IX	I13BI	709	Jell and Molecular Biology	110BH Y I, 115BH VA	5 5		25	15	100
	Core	Core X I17BI710		710	Programming in C++ and JAVA	113Bi414	5	5	25	75	100
	Core XI I13BI		711	Bioinformatics Databases and Tools	113BI5:2	5	5	25	75	100	
VII	Core Prac. I13BI		7P5	Programming in JAVA Lab		5	3	40	60	100	
	Core Prac. I13BI		7P6	Bioinformatics databases and Tools Lab		5	3	40	60	100	
	Elect	ive IV	113BI 113BI	7:1/ 7:2	Proteins - Structure and functions/Molecular Interactions	I16BI505	5	4	25	75	100
	Core XII I13Bl		812	Agorithm for Computational Biology	I16BI202	5	5	25	75	100	
	Core XIII  17BI		117BI	813	Probability and Biomathematics	I16BI404, I13BI5:3	5	5	25	75	100
VIII	Core	XIV	113BI	814	Molecular Modeling and Drug Designing	116Bi505, 116Bi608	5	5	25	75	100
	Core XI	Prac	117BI	8P7	Computational Biology, Biostatistics using R and Drug Designing Lab		5	3	40	60	100
	Elective V 117BI8			8:1/ 8:2	Basics of Next Generation Sequencing Herbal Medicine	I16BI202	4	4	25	75	100

Som	Course	Course Course title P		Prerequisi	Hrs/	Cre		Mark	s
Sem	Course	code	Course true	tes	week	dits	CIA	ESA	Total
VIII	NMEC III		To be selected from courses offered by other departments		4	2	25/ 40	75/ 60	100
	VLOC	P17VL1:1/ P17VL1:2	RI/MI		2	2	25	75	100
	Core XV	I17BI915	Genomics and Proteomics	I13BI711	5	5	25	75	100
IX	Core XVI	I13BI916	Advances in Structural Bioinformatics	16B 505,  16B 608,  13B 814	5	5	25	75	100
	Core XVII	I17BI917	Programming in Python		5	5	25	75	100
	Core PracXII	113BI9P8	Advances in Structural Bioinformatics Lab		5	3	40	60	100
	Core Prac XIII	117BI9P9	Programming in Python Lab		5	3	40	60	100
	Elective VI	113Bl9:1/ 113Bl9:2	Cheminformatics/Biodiversity, Bioethics and IPR		5	4	25	75	100
	Core XVIII	I17BIX18	Pharmacoinformatics		5	4	25	75	100
х	Elective VII	I17BIX:1/ I17BIX:2	Advanced Applied Bioinformatics / Bioinformatics in Biodiversity, Agriculture, Medicine and Environment	I14BI5S2	5	4	25	75	100
	Project	I13BIXPJ	Project		-	6	-	-	100
				230			6500		

#### SBEC- Skill Based Elective Course VLOC- Value added Life Oriented Course CIA- Continuous Internal Assessment

#### NMEC- Non Major Elective Course SBC- Skill Based Course ESA- End Semester Assessment

* Other Languages	Hindi	Sanskrit	French		Hindi	Sanskrit	French
Semesterl	U14HD1L1	U15SK1L1	U14FR1L1	Semester III	U14HD3L3	U15SK3L3	U14FR3L3
Semester II	U14HD2L2	U15SK2L2	U14FR2L2	Semester IV	U14HD4L4	U15SK4L4	U14FR4L4

# CORE I : INTRODUCTION TO COMPUTERS AND BIOINFORMATICS

Semester : I Credits : 4 Course Code: I16BI101 Total Hrs :60

## **General Objectives**

- 1. To understand the basic principles of computers and bioinformatics.
- 2. To become familiar with existing resources for computational analysis of biological data.

#### Unit I Introduction to computers

Introduction to Computers - Need for programming in Life sciences - Characteristics of Computers -Evolution of computers - computer generations - classification of computers - Basic computer organization - Hardware - Input Devices - Output devices - memory - Introduction of operating systems - Windows - Unix/Linux(Basic concepts only) -Application software - MS office.

#### Unit II Computer software and internet

Computer software - Types of software - software development steps - Internet evolution - Basic Internet terminology - getting connected to internet applications - Internet usage - Browsers - Internet explorer - Mozilla - search engines - Email.

#### Unit III- Bioinformatics

Overview- Definition and History; Milestones in Bioinformatics Methods in Bioinformatics - Goals - Scope - Applications - Limitations - New themes - Useful Bioinformatics web sites.

#### Unit IV-Databases

Introduction to database - Primary and Secondary databases - Nucleotide Sequence databases and Database formats - Protein sequence databases- GenPep - RefSeq - Uniprot - UniParc - Uniprot knowledgebase.

#### Unit V-Composite and Secondary database

Composite protein sequence databases - NRDB -OWL - MIPSX - Swiss prot and TrEMBL - Secondary database-Prosite - Prints - Blocks - Profiles - Pfam - Identify - Composite protein pattern databases-Structure classification databases-SCOP - CATH - PDBsum

#### Text Books

- 1. Rajaraman V, Fundamentals of Computers, 6<sup>th</sup> Edition, Prentice Hall India Pvt., Limited, 2003. (Unit-I P.No, 1-81, 191-218, 249-264)
- 2. Anita Goel, Computer Fundamentals, Pearson Publications, 2010. (Unit-I P.No. 1-87, 131-150, 307-422)
- 3. uwf.edu/clemley/cgs1570w/notes/ (Unit-II)

- 4. JinXiong, Essential Bioinformatics, Cambridge University Press, 2006. (Unit-III P.No 1-8)
- 5. Andreas D.Baxevanis, B.F. Francis Ouellette, Bioinformatics A practical guide to the analysis of genes and proteins, Wiley Interscience, 2000 (Unit-IVP.No 4-21)
- 6. Attwood T.K and Parry Smith D.J, Introduction to Bioinformatics, Pearson Education Ltd., New Delhi, 2003. (Unit-V P.No 43-65)

- 1. Peter Norton, Introduction to computers sixth edition, Tata McGraw, Hill pub.Co.Ltd., New Delhi ,2006.
- 2. Sinha PK, Computer fundamentals, 2<sup>nd</sup> Edition, BPB New Delhi, 1992.
- 3. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, NewDelhi, 2003.
- 4. David W mount, Bioinformatics: Sequence and genome analysis, 2<sup>nd</sup> edition, CBS publishers, New Delhi, 2004.
- 5. ManjuBansal, Basic Bioinformatics, Atlantic publishers & distributors, 2009.

# CORE PRAC I: INTRODUCTION TO COMPUTERS LAB

Semester : I Credits : 2 Course Code: I16BI1P1 Total Hrs :45

#### **General Objective**

To understand the basics of computers and its operations.

#### **Fundamentals of Computer Practical**

1. Dos commands File Commands, Miscellaneous Commands

#### Windows

- 2. Creating folder, cut, copy, paste, managing file and folder in windows.
- 3. Arrange icons, set display properties
- 4. File Searching

## **MS-Word**

- 5. Creating & Editing Document, Formatting Document
- 6. Use of Auto text, Autocorrect, Spelling and Grammar Tool, Word Count.
- 7. Page Formatting, Page Border, Background,
- 8. Practice of Printing, page setup etc.
- 9. Design a document for Genbank and PDB format.

# **MS-Excel**

- 10. Creating & Editing Worksheet and File Handling
- 11. Use Formulas and Functions
- 12. Calculation of the given Amino acid composition and average
- 13. Preparation of Charts

#### **MS-Powerpoint**

- 14. Creating, Manipulating & Enhancing Slides,
- 15. Inserting Organizational Charts, Excel Charts
- 16. Using Word Art
- 17. Putting Animations and Sounds
- 18. Inserting Animated Pictures
- 19. Inserting Recorded Sound Effect

# ALLIED I : CELL BIOLOGY

Semester : I Credits : 4 Course Code: I16BI1Y1 Total Hrs :60

#### **General Objective**

To understand the basics of structure and function of cellular organelles and components, and the functional interaction of the cell with its microenvironment.

#### Unit I Basic concepts of Microscopy

The cell -basis of life-Cells under the microscope-Light & Electron microscopy-Types-Advanced features and mechanism.

#### Unit II Ultrastructure and classification of cell

Classification of cell types - organization of prokaryotic and eukaryotic cells - Ultrastructure of cells (Images only) -comparison of microbial - plant and animal cells

## Unit III Cell composition and permeability

Cell - composition and biological significance -proteins - lipids - carbohydrates and nucleic acids -cell transport -active - passive - diffusion - osmosis and ion transport.

#### Unit IV Organelles and membrane

Cell membrane - models -unit membrane and fluid mosaic models -cytosol - nucleus - mitochondria - cytoskeleton - microtubules - Golgi complex - Endoplasmic reticulum - Chloroplast - Vacuoles - Ribosomes and lysosomes.

#### Unit V Cell Division and Cell Cycle

Cell Division - mitosis and meiosis - regulation - steps in cell cycle and control of cell cycle - cell death and senescence.

# Text Books

- 1. Stephen R. Bolsover ,JeremyS.Hyams, Elizabeth A. Shephard, Hugh A.White ,Claudia G.Wiedemann. Cell biology. A short course John Wiley & Sons Publications, New Jersey.2003.(Unit I-pgs.1-9; Unit II-pgs.11-15 Unit IV-pgs.51-61; Unit V-pgs.401-410).
- 2. Bruce Alberts, Dennis Bray, Karen Hopkins, Alexander Johnson, Julian Lewis. Essential cell biology, Garland Science, Newyork .2003. (Unit III-pgs.389-414:Unit V-pgs.637-646).

- 1. De RobertisE.D.P and De. RobertisE.M.F., Cell and Molecular Biology, 8<sup>th</sup> edition, Lippincott Williams and Wilkins Publisher, India, 2005.
- 2. Cooper G.M and Hausman R.E. The Cell A molecular Approach, 4<sup>th</sup>edition, Sinauer Associates Inc. USA, 2007.
- 3. Lodish H, Berk A, Zipursky S.L, Matsudair P, Baltimore D and Darnell J., Molecular Cell Biology, 4th Edition., W.H Freeman and company, USA, 2000.
- 4. Verma PS and Agarwal VK, Cell Biology, Genetics, Molecular Biology, Evolution and Ecology, S. Chand & Co, New Delhi, 2005.
- 5. Bruce Alberts, Dennis Bray, Karen Hopkin, Alexander Johnson, Julian twis, Martin Ratt, Krith Roberts and Peter walter, Essential Cell Biology, Garland Science Publications, Newyork, 2004.

# CORE II: COMPUTATIONAL BIOLOGY AND SEQUENCE ANALYSIS

Semester : II Credits : 6 Course Code: I16BI202 Total Hrs :90

## **General Objective**

To acquire information from biological databases by using computational approaches to analyze this information and to interpret the results as a guide to experiments in Biology

## Unit I -Sequence alignment

Pairwise Sequence alignment- Evolutionary basis - Homology vs similarity vs identity - Methods in Global and local alignment - Alignment algorithms- Dot matrix method - dynamic programming global alignment-GAP - dynamic programming Local alignment-SIM - SSEARCH -LALIGN - Introduction to Scoring matrix. Database similarity searching - Heuristic database searching-BLAST - FASTA - Statistical significance - Comparison of FASTA and BLAST.

#### Unit II - Multiple sequence alignment

Introduction to Multiple sequence alignment - Scoring function - Exhaustive algorithms - Heuristic algorithms-Progressive alignment method-iterative alignment - Block-based alignment. Profile and Hidden Markov models-PSSM - Profiles-PSI-BLAST - introduction to Markov model - HMM - Protein Motif and Domain prediction - Protein family databases. Phylogenetics Basics.

#### Unit III Protein structure alignment

Protein 3D structure comparison and alignment -structure superposition -RMSD -structure alignment methods -DALI - SSAP - CE -multiple structure alignment.

#### **Unit IV Structure Prediction**

Protein secondary structure prediction -Chou -Fasman - Garnier -Osguthorpe -Robson(GOR) methods -Neural network concepts and secondary structure prediction -amphipathic helix prediction -trans membrane structure prediction.

#### Unit V Probablistic approaches(Qualitative approach)

Fragment assembly -genome sequence assembly -gene finding methods: content and signal methods - analysis and prediction of regulatory regions -probabilistic models: Markov chain -random walk -Hidden Markov models -Gene identification and other applications.

#### Text Book

JinXiong, Essential Bioinformatics, Cambridge University Press,2006. (Unit I Page no 31-61; Unit II Page no 63-91; 127-132, Unit-III P.No. 190-195, Unit-IV P.No. 200-211, Unit-V P.No. 243-250).

- 1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003.
- 2. David W.Mount.Bioinformatics: Sequence and genome analysis. Cold Spring Harbour Laboratory Press, New York, 2001.
- 3. Rastogi S.C NamithaMendiratta, ParagRastogi. Bioinformatics,concepts, Skills, application CBS publishers&distributors, New Delhi, 2004.
- 4. Andreas D. Baxevanis , B. F. Francis Ouellette, Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, 3<sup>rd</sup> Edition, 2005

# CORE PRAC II: INTRODUCTION TO BIOINFORMATICS LAB

Semester : II Credits: 2 Course Code: I16BI2P2 Total Hrs :45

#### **General Objective**

To have profound knowledge in Bioinformatics and its applications in molecular biology, chemistry, physics and other disciplines.

- 1. Nucleotide Sequence databases NCBI EMBL
  - DDBJ
- 2. Protein sequence databases PIR Swiss-Prot
- 3. Secondary database Prosite Prints Blocks Profiles Pfam Identify
- 4. Structure classification databases SCOP, CATH, PDBsum
- 5. Database formats ReadSeq
- 6. Protein sequence analysis :ExPASY Aminoacid composition Peptide mass SOPMA
- 7. Pubmed
- 8. OMIM
- 9. Pairwise alignment Global and local alignment, Dot matrix method,
- 10. Database searching- BLAST, FASTA,
- 11. Multiple Sequence Alignment-ClustalX

# ALLIED II: BIOCHEMISTRY

Semester : II Credits : 4 Course Code: I16BI2Y2 Total Hrs :60

#### **General Objectives**

- 1. To know the biological phenomena at the molecular level.
- 2. To understand the fundamental chemical principles that governs complex biological systems.

## Unit I: Basic Molecules of Life

Water –Properties of water; pH – Measurement; Determination of pKa-(Henderson Harsel Balch Equation); Buffer actions (strong and weak acids) and Biological buffer systems.

#### Unit II: Carbohydrates

Classification of Carbohydrates; Monosaccharides- Properties and Classification; Monosaccharides-Glucose and Fructose; Oligosaccharides- Classification; Sucrose and Lactose; Polysaccharides: Homopolysaccharides – Starch and Glycogen; Heteropolysaccharides – Heparin and Agar-agar; Functions of Carbohydrates.

## Unit III: Proteins

Structure - Classification - Physical and Chemical Properties of Proteins; Configuration of Proteinsprimary - secondary - tertiary and quaternary structure; Biological functions of proteins.

#### Unit IV: Lipids

Classification and properties of lipids; Simple lipids-Fats and Oils; Compound lipids-Phospholipids and Glycolipids; Derived lipids- Steroids and Carotenoids; Biological importance of lipids.

#### Unit V: Nucleic Acids and Vitamins

Nucleic Acids- Types of DNA and RNA; Composition, structure and functions of nucleic acids. Vitamins-Deficiencies of Vitamins- Fat soluble-A, D, E & K and Water soluble- B & C.

# Text Books

- 1. Arumugam N., Dulsy Fatima, L.M.Narayanan, R.P.Meyyan, K.Nallasingam and S.Prasannakumar. Biochemistry. 5<sup>th</sup> Edition, Saras Publication, 2014.
- 2. Jain J.L., Sunjay Jain and Nitin Jain. Fundamentals of Biochemistry, 5<sup>th</sup> Edition, S. Chand and Company Ltd., New Delhi, 2010.

- 1. Berg J.M., Tymoczko, J.L., Stryer, L. Biochemistry, 7<sup>th</sup> Edition. W.H.Freeman, USA, 2010.
- 2. Campbell M.K., Farrell, S.O. Biochemistry, 6<sup>th</sup> Edition. Brooks Cole Publishing Company, USA, 2007.
- 3. Mathews C. K., Van Holde, K.E., Ahern, K.G. Biochemistry, 3<sup>rd</sup> Edition. Addison Wesley, USA, 2000.
- 4. Voet D., Voet, J.G. and Pratt, C.W. Principles of Biochemistry, 3<sup>rd</sup> Edition. John Wiley & Sons, USA, 2008.
- 5. Zubay G.L. Biochemistry, 7<sup>th</sup> Edition. William C Brown Publishers, NewYork, 1995.
- 6. Nelson D.L., Cox, M.M. Lehninger Principles of Biochemistry, 5<sup>th</sup> Edition. W.H Freeman and Company, USA, 2008.

# ALLIED PRAC I: CELL BIOLOGY AND BIOCHEMISTRY LAB

Semester : I/II Credits : 3 Course Code: I16BIYP1 Total Hrs :45

## **General Objectives**

- 1. To apply the practical approaches that synchronize with the theoretical concepts.
- 2. To handle the instruments effectively.

## A. Cell Biology

- 1. Mitosis in onion root tips
- 2. Barr body staining from buccal epithelial cells
- 3. Preparation of giant /polytene chromosomes from chironomous larvae.
- 4. DNA isolation from Buccal cells

## B. Biochemistry

- 1. Preparation of solutions
- 2. Colorimetry verification of Beer Lambert's law
- 3. Estimation of glucose by anthrone method
- 4. Estimation of protein by Bradford method
- 5. Chromatography Paper and Thin Layer

#### **Reference Books**

- 1 Rajan, S, Experimental Procedures in Life Sciences. Anjanaa Book House, 2010
- 2. Karp, G, Cell and Molecular Biology: Concepts and Experiments. 6th Edition. John Wiley & Sons. Inc.,2010.

# SBEC-I GENERAL CHEMISTRY

Semester :II Credits: 2 Course Code: I16BI2S1 Total Hrs :30

#### **General Objectives**

- 1. To impart knowledge in chemistry and to understand the types of chemical bonding.
- 2. To learn different kinds of polar effects operating in the organic molecule and to study the chemical equilibrium and kinetics of chemical reaction.

#### UNIT I Fundamentals of atomic and molecular orbitals

Theory of atomic and molecular orbitals - Linear combination of atomic orbitals .Shape of orbitals and hybridization. VSEPR Theory- CH<sub>4</sub>, NH3,H<sub>2</sub>O,PCI<sub>5</sub> and BF<sub>3</sub>.

#### UNIT II Fundamentals of chemical bonding and non-bonding interactions

Electrovalent bond - Factors influencing the stability of electrovalent bond. Co -valent bond – partial ionic character of co-valent bonds. Co-ordination bond - Vander Waals forces. Theories of hydrogen bonding and types of hydrogen bonding with examples of RCOOH - ROH - Salicylaldehyde - amides and proteins.

## **UNIT III Principles of Bioenergetics**

Free energy - laws of thermodynamics; endergonic and exergonic reactions. Role of high energy phosphates in metabolism - metabolic pathways (anabolism -catabolism).

#### UNIT IV Chemical Kinetics

Rate - rate law - order and molecularity of a chemical reaction. Rate constant equation for I and II order equation. Factors affecting rate of reactions.

#### Unit V Receptor Drug Action

Forces involved in Drug Receptor Complex : Covalent bonds-Electrostatic or ionic interactions-Hydrogen bonds-Charge transfer complexes-Dispersion Forces (Vander waals)

#### Text Books

- 1. ArunBahl and S. Bahl; A text book of Organic chemistry, Chand and company pvt Ltd;2006 (Unit-I)
- 2. Puri, Sharma, Kalia, Principles of inorganic chemistry, Milestone publisher, India, 2012.(Unit-I,II)
- 3. JainJ.L.; Sunjay Jain and Nitin Jain, Fundamentals of Bio Chemistry, 6<sup>th</sup> edition, S. Chand and company pvt Ltd. 2008. (Unit –III)
- 4. ArunBahl, Bahl.B.S and G.D.Tuli ; Essentials of physical chemistry; S. Chand and company pvt Ltd;2006. (Unit –IV)
- 5. Ahulwalia.V.K and Madhu Chopra, Medicinal Chemistry, Any Books India, 2008. (Unit-V)

- 1. Bahl.A and Bahl. .S, A text book of organic chemistry, Chand & Company pvt ltd., 2006.
- 2. Atkins. P, Paula, IX edition, Physical Chemistry, oxford Publications, 2010.
- Fisher.J, Arnold.J.R.P, Instant notes in chemistry for Biologists,2<sup>nd</sup> Edition, Taylor & Francis,1999.
- 4. Mukherji. S.M, Singh. S.P, Reaction Mechanism in Organic Chemistry, Macmillan, 1984.

# CORE III: PROGRAMMING IN C

Semester :III Credits : 6 Course Code: I14BI303 Total Hrs :90

#### General Objective

To know the fundamentals of programming techniques namely: (a) Sequence of execution (b) Selection of blocks to be executed (c) Repetition of execution, with the help of C programming language.

#### Unit –I Introduction to C

Introduction - Character Set - C Tokens - Keywords and identifiers - Constants - Variables and Data types - Declaration of variables - Declaration of Storage Class - Assigning values to variables - Operators and expressions - Data Input and Output operations.

#### Unit-II Decision making and looping

Introduction - Decision Making with If statement - Simple IF statement - IF...Else statement - Nesting of IF...Else Statement - The ELSE IF Ladder - switch statements - GOTO Statement. Decision making and looping - The WHILE statement - DO statement - FOR Statement - Arrays - Character Arrays and strings.

#### Unit-III Functions

Introduction - Need for User-defined functions - Element of User-Definition of functions - Return values and their types - Function Calls - Function declaration - Category of function - Nesting of Functions - Recursion.

#### Unit IV Data Types

User defined data types in C. Structures -Declaring structures and Accessing members -Array of structures - Structure within structure.Unions.File operations -open - close - reading and writing - Random access files.Linked list -Preprocessor directives -Macros -Command line arguments.

#### Unit V Operating systems

Introduction to operating systems -MS windows commands - UNIX -basic commands -General purpose - file handling - vi editor & environment - Linux -basic commands. Internet browsers -Net scape - Mozilla - Internet Explorer. HTML -XML -web page design tools -CGI -bin scripts -Linking -Text Formatting -Adding Images -Tables -Frames - web pages.

#### Text Books

- 1. Balagurusamy E, Programming in ANSI C, 4E, The McGraw-Hill Companies. 2000 (Unit I P.No. 23-38; 52-98; Unit II P.No.114-250; Unit III P.No.262-295, Unit-IV, P.No. 317-331, 335-337, 389-405, 411-421, 444-450)
- 2. Lister.A, Fundamentals of Operating Systems, 1993. (Unit-V P.No. 1-6, 9-15)
- 3. Achyut S Godbole, Operating Systems, 2<sup>nd</sup> Edition, 2008. (Unit V P.No. 555-606, 653-663)

# 4. Spark Forme, HTML: Basics – Professional (Unit-V ) **References**

- 1. Byron S. Gottfried, Schaum's outline of Theory and Problems of Programming with C,TataMcGraw,Hill,New Delhi,1991.
- 2. BrainW.Kernighan and Dennis. M.Ritche, The C Programming Language, Second Edition, Printice, Hall of India, 1988.
- 3. Parthasarathy S, Essentials Of Computer Programming in C for Life Science, AneBooks,NEW DELHI,2008.
- 4. SumitabhaDas, UNIX Concepts and Applications, 3rdEdition, TataMcGraw-Hill, New Delhi, 2003.
- 5. Thomas A. Powell, HTML&XHTML, The Complete Reference,4<sup>th</sup>Edition, TataMcGraw,Hill,New Delhi,2007.

# CORE PRAC: III. PROGRAMMING IN C LAB

Semester : III Credits : 2 Course Code: I16BI3P3 Total Hrs :45

#### **General Objective**

To know the basics of programming in C and to apply the concepts in real world applications.

#### List of Practicals

- 1. Find the pH of a solution given the concentration of H+ (or) OH- ions
- 2. Compute the area and the circumference of the circle
- 3. Compute the volume of a cylinder and cone
- 4. Convert the given Fahrenheit value to centigrade scale (or vice versa)
- 5. Compute the relative centrifugal force using r\_max (in cm) and rpm value
- 6. Compute the rpm value using r\_max (in cm) and RCF value
- 7. Find the biggest of three given numbers using if-else statement
- 8. Compute all possible roots of quadratic equation using if-else statement
- 9. Find the molecular weight of a DNA with n base pairs in length
- 10. Find the molecular weight of a given dephosphorylated oligonucleotide sequence
- 11. Find the molecular weight of a given DNA sequence, after checking for phosphorylation
- 12. Find the sum of n natural numbers
- 13. Compute the sum of n odd numbers
- 14. Find the factorial of a given integer number
- 15. Compute the nature of the solution based on the pH value using switch case statement.
- 16. Determine the percentage of a,t,g,c in the given sequence
- 17. Calculating the reverse complement in the given sequence
- 18. Searching for MOTIF in the given sequence
- 19. Swap two numbers using pointers
- 20. Convert the RNA sequence into DNA sequence using text file

# ALLIED III: MICROBIOLOGY

Semester :III Credits : 4 Course Code: I16BI3Y3 Total Hrs :60

## **General Objective**

To have an exposure to microbiology and to comprehend the impact of microbes in human welfare.

#### Unit I Introduction to microbiology

Scope & History of microbiology - characterization - classification – Bacteria-3 Kingdom - 5 Kingdom concepts

#### Unit II Microorganisms - Cultivation and maintenance

Morphology of Bacteria - cultivation - preservation of culture - growth - growth curve. Measurements of growth & factors affecting growth.

#### Unit III Control of microorganisms

Control of organisms by physical agents - chemical agents - chemotherapeutic agents (Penicillin - Streptomycin -Tetracyclin).

#### Unitl V Environmental & Industrial uses

Extremophiles - thermophiles& methanogens. Alcohol production & penicillin production by bacteria & Yeast.

#### Unit V Microbial Diseases

Water borne (cholera) - food borne (typhoid) - air borne (pneumonia). Fungal- Dermatitis -Viral disease-HIV.

#### Text Books

- 1. Rajan.S, Essential of Microbiology, Anjana Book house publishers, First edition, 2015. (Unit-I & II)
- 2. Maheshwari, D.K, Dubey, R.C. A Textbook Of Microbiology by S.Chand & Company Ltd New Delhi, 2013.(Unit-III)
- 3. Arora, D.R. Textbook of Microbiology, CBS, 5<sup>th</sup> Edition ,2016 (Unit-IV)
- 4. Jayaram Paniker, C.K, Jaypee Brothers Medical Publishers Private Limited; 7 edition, 2013.(Unit-V)

#### Reference

1. Prescott, Harley and Klein's Microbiology 8<sup>th</sup>edition (Willey, Sherwood, Woolverton),2002.

# CORE IV: BASIC MATHEMATICS

Semester :IV Credits : 5 Course Code: I16BI404 Total Hrs :90

#### General Objective

To comprehend the basics of mathematics and to understand statistical methods to analyze biological data from DNA to the biological processes of healthcare systems.

#### Unit I Matrices and determinants

Matrix: Algebra of Matrix – Determinants and its properties – Co-factor of Determinants–Adjoint -Inverse – Solution of system of linear equations by matrix inversion method –Rank of a Matrix – Consistency of a system of linear equations – Cramer's rule

#### Unit II Vector Algebra

Definition – algebraic properties – scalar multiplication – properties – position vector – resolution of a vector in two and three dimensions – direction cosines and direction ratios – Scalar Product – Angle between two vectors – Vector product – Applications – Bond length – Bond angle Torsion angles calculations

#### Unit III Differential Calculus

Functions – Limit of a function – fundamental results - Important limits – Continuity of a function – Concept of Differentiation – Derivatives – Differentiation techniques – Product rule, quotient rule, chain rule, inverse functions, method of substitution, parametric functions

#### Unit IV Differential Calculus – Applications I

Derivative as a rate measure – rate of change – velocity – acceleration – related rates – Derivative as a measure of slope – tangent, normal and angle between curves

#### Unit V Differential Calculus - Applications II

Maxima and minima – mean value theorem (statements only) – Taylor's and Maclaurin's series - L'Hopital's Rule – Stationary points – increasing – decreasing – maxima, minima, concavity, convexity, points of inflexion

- 1. Erwin Kreysig, Engineering Mathematics, 7<sup>th</sup> Edition, John Wiley, USA, 2001.
- 2. Narayanan S and Manicavachagam Pillay TK, Calculus, Vol.I, S.Viswanathan Publ. Pvt. Ltd., Chennai, 1982.

# CORE PRAC IV: PROGRAMMING IN SCI LAB

Semester :IV Credits : 2 Course Code: I16BI4P4 Total Hrs:45

# **General Objective**

To apply the mathematical concepts for solving biological problems with the help of Scilab.

- 1). Basic commands
- 2). If Statement
- 3). Branching- Switch statement
- 4). Integral Calculator
- 5). Processing biological sequences

# ALLIED IV: MOLECULAR BIOLOGY & GENETIC ENGINEERING

Semester :IV Credits : 4 Course Code: I16BI4Y4 Total Hrs :60

## General Objective

To understand the importance of the central dogma of molecular biology in life.

## Unit I Introduction to Molecular Biology

DNA replication: Various modes of replication. Mechanisms of prokaryotic and Eukaryotic DNA replication. Properties of DNA polymerases - Synthesis of Leading and lagging strands DNA Repair: Photo -reactivation - excision repair - post replication repair - SOS repair etc.

#### Unit II Transcription

RNA polymerase in prokaryotes - its molecular composition - role of each component of RNA polymerase - mechanism of transcription - Eukaryotic transcription Regulation of gene expression in prokaryotes: Transcriptional control; enzyme induction and repression - constitutive synthesis of enzymes and catabolite repression. The lac-operon. The trp-operon.

#### Unit III Translation

The genetic code.Prokaryotic and Eukaryotic Translation. Modification of RNA : 5' – CAP formation - 3 – end processing polyadenylation - Splicing - Editing - Nuclear export of mRNA & mRNA stability

#### Unit IV Recombinant DNA

History and scope of recombinant DNA technology - DNA modifying enzymes.

#### Unit V Cloning and expression vectors:

Characteristics of cloning and expression vectors; plasmid - phages - and cosmid vectors - multipurpose cloning vectors - shuttle vectors - bacterial - yeast - plant and mammalian expression vectors. BACs and YACs.DNA cloning strategies Preparation of genomic and cDNA libraries.

# Text Books

- 1. Gupta. P.K. Cell and Molecular biology. Rastogi Publications, India. 2005. (UNIT I-III)
- 2. Sathyanarayana U, Biochemistry, 3rd Édition. New Central Book Agency(p) Ltd, 1999. (UNIT I-III)
- 3. Jogdand, S.N., Gene biotechnology. Himalaya Publishing House. 2009. (UNIT IV-V)

- 1. Roodney Boyer, Concepts in Biochemistry, Brooks/Cole Publishing Co. 1st Edition, 1999.
- 2. Bernard R, Glick and Jack J. Pastermack, Molecular Biotechnology: Principles and Applications of Recombinant DNA. American Society Microbiology Edition: 3<sup>rd</sup>, (2003).
- 3. Brown TA, Gene Cloning, Published by Blackwell Science, 7<sup>th</sup>Edition. 2001.
- 4. Primrose SB and RW, Principles of Gene Manipulation, Old, Published by Blackwell, 6<sup>th</sup>Edition, 2002.
- 5. Maniatis T, Molecular Cloning. A. Laboratory Manual. CSH Lab. N.Y. (1989).

# ALLIED PRAC II: MICROBIOLOGY AND GENETIC ENGINEERING LAB

Semester :III/IV Credits : 3 Course Code: I16BIYP2 Total Hrs :45

#### General Objective

To comprehend and analyze the microbes that are involved in human welfare by using basic microbiology and genetic engineering laboratory techniques.

# A. Microbiology

- 1. Simple staining
- 2. Gram staining
- 3. Pure culture techniques, streak, spread, pour, plate

#### **B.** Genetic Engineering

- 1. Isolation of Genomic DNA and Quantization of DNA
- 2. Isolation of bacterial plasmid DNA
- 3. Agarose gel electrophoresis of DNA
- 4. Restriction digestion of DNA with one restriction enzyme
- 5. Southern blot hybridization with non-radioactive probe (Demo)

# CORE V:STRUCTURAL BIOINFORMATICS AND MEDICINAL CHEMISTRY

Semester :V Credits : 5 Course Code: I16BI505 Total Hrs :90

#### General Objective

To understand the concepts of molecular modelling, quantum mechanics and molecular mechanics pertaining to drug discovery.

## Unit I Introduction (Basic Concept Only)

Bioinformatics and structural bioinformatics - Definition - fundamentals of protein structure - fundamentals of DNA &RNA structure - computational aspects of high throughput Crystallographic macromolecular structure determination - Macromolecular structure determination by NMR Spectroscopy - Electron Microscopy - and Molecular visualization.

#### Unit II Data representation - Structural Databases and Validation Servers

PDB Format - Structural Databases: PDB - NDB - SCOP Database - CATH domain structure database - Other structure based database: CSD - PDBsum - MolProt - PubChem - ChEMBL - ZINC Database -ChemBank. Structure Validation Servers: SAVES- Ramachandran Plot - WHAT\_IF server - ProSA -Naccess

#### Unit III Methods of Protein Structure Prediction and Visualization

Fold Recognition Method (Threading) - Ab-initio Method - Homology Modeling - CASP and CAFASP. Secondary structure assignments - identifying structural domains in proteins. Visualization tools: PyMol - SPDBV - Chimera.

#### Unit IV Basics of Medicinal Chemistry

Basics and properties of small molecules: Physiochemical & Biological. Other properties influence small molecules: Lipinski rule of 5 - ADMET properties - Pharmacophore - Ames Mutagenicity - QSAR - 3D QSAR.

#### Unit V Drug target principles & Molecular visualization

Drug action that affects the structure of cell membranes and walls - receptors and messengers; chemical nature of the binding of ligands to receptors - structure and classification of receptors - general mode of action - ligand-response relationships - ligand-receptor theories - drug action and design. Enzymes: active site and catalytic action - regulation of enzyme activity - specific nature of enzyme action - mechanism of enzyme action - enzyme kinetics - enzyme inhibitors - transition state inhibitors - enzyme and drug design - examples of drugs used as enzyme inhibitors - enzymes and drug resistance.

# Text Books

- 1. JinXiong, Essential Bioinformatics, Cambridge University Press 2006.
- 2. Manju Bansal, Basic Bioinformatics, Atlantic publishers & distributors, 2009
- 3. Harisha.S, Fundamentals of Bioinformatics, 2007.

- 1. Phillip E. Brurne, HelgeWeissig, Structural Bioinformatics, A John Wiely& Sons Publications, 2011
- 2. David M, Bioinformatics: Sequence and Genome analysis, Cold Spring Harbor Laboratory, 2004.
- 3. JinXiong. Essential Bioinformatics. Cambridge University Press 2006
- 4. Rastogi RS, Bioinformatics: Concepts, Skills & Applications, Eastern Economy Edition 2008.
- 5. Thomas Hamelrcyck, Mardia KV, Bayesian methods in Structural Bioinformatics, Springer 2012.
- 6. Johann Gasteiger, Chemoinformatics: A Textbook, Thomas Engel 2006.

# CORE VI: PROGRAMMING IN PERL AND BIOPERL

Semester :V Credits : 5 Course Code: I16BI506 Total Hrs :90

#### General Objective

To know the basics of programming in Perl and to apply the concepts in real world applications.

## Unit I Introduction to PERL

Introduction to PERL - Variable Types - Data types - operators - control structures - lists and Arrays - Subroutines - Hash functions - other useful functions - Regular expressions.

#### Unit II PERL variables

Basic Input output - special variable @ ARGV - Command live Arguments - File Handles and Tests - Directory Operations - CGI Programming: GET and Post Methods; PERL graphics.

#### UNIT III Control Statements

Perl control statements – control structures – if statements – if-else – if-elsif – if-elsif-else – while loop – until loop –unless for loop – for each loop – scoping of variables.

#### Unit IV Pattern Matching

Manipulation of strings - Regular expressions - Pattern, Matching Operators - Standard Modules -Subroutines - Using system command - Important functions (split, index, substr, chomp, length, reverse, shift, sort)

#### Unit V BIOPERL

Introduction to BIOPERL - BIOPERL objects - implementation of Bioinformatics algorithms for searching and matching in PERL - BLAST parsing - handling PDB files - sequence retrieval - alignments.

#### **Text Books**

- 1. Simon Cozens, Peter Wainwright, Beginning Perl, Wrox Press, 2000.(Unit I-IV)
- 2. https://www.perl.org/books/beginning-perl/ (Unit I-IV)
- 3. James Tisdall, Beginning Perl for Bioinformatics, O'Reilly Media, Inc., 2001(Unit-V)

- 1. Wall, L, Christiansen. Tand Orwant, J. Programming Perl, 3<sup>rd</sup>Edition, O'Reilly, 2000.
- 2. Tisdall.J, Mastering Perl for Bioinformatics, O'Reilly, 2003.
- 3. Rex A. Dwyer, Genomic PERL, Cambridge Univ. Press, UK, 2003.
- 4. Harshawardhan P. Bal, PERL programming for Bioinformatics, Tata McGraw-Hill, NewDelhi, 2003.
- 5. htrtp://bioperl.org

# CORE PRAC V: ADVANCED BIOINFORMATICS LAB-I

Semester :V Credits :2 Course Code: I16BI5P5 Total Hrs :45

# **General Objective**

To understand the basics of Bioinformatics and its applications in sequence analysis, phylogeny and structure visualization.

- 1. ExPASy proteomics tools
- 2. Sequence similarity searching (NCBI BLAST)
- 3. Multiple sequence alignment (Clustal)
- 4. Molecular phylogeny (PHYLIP).
- 5. Gene prediction (using GenScan, GeneMark).
- 6. Sequence analysis using EMBOSS.
- 7. Sequence Manipulation -NEB cutter, RevComPlement, Expasy Translator, NCBI ORF finder.
- 8. Protein Structure retrieval using PDB,MMDB, NDB, CCSD.
- 9. Molecular visualization, RasMol, Cn3D, SPDBV.

# CORE PRAC VI: PROGRAMMING IN PERL AND BIOPERL LAB

Semester :V Credits : 2 Course Code: I16BI5P6 Total Hrs :45

# **General Objective**

To apply the programming concepts for solving biological problems with the help of Perl.

- 1. Concatenating DNA
- 2. Transcription DNA to RNA
- 3. Calculate the reverse complement of a strand of DNA
- 4. Searching for Motif
- 5. Determining frequency of nucleotide in a text file
- 6. Mutation of given DNA sequence
- 7. Translating DNA into Proteins
- 8. Translate a DNA sequence in all six reading frames
- 9. Extract annotation and sequence from GenBank file
- 10. Extract sequence chains from PDB file

# **ELECTIVE I: BIOPHYSICS**

Semester :V Credits : 5 Course Code: I13BI5:1 Total Hrs :75

#### **General Objectives**

- 1. To have an insight in the biophysical techniques
- 2. To analyze protein molecules.

## Unit I Laws of Physics and Chemistry

Introduction - Quantum Mechanics- The Electronic Structure of Atoms -Molecular Orbitals and Covalent Bonds-Molecular Interactions-Strong interactions -Weak interactions -Stereochemistry and Chirality - Entropy -Enthalpy -The free energy of a system.

#### Unit II Biophysical Techniques

Chromotography-Introduction, Principles, Process and Applications of Thin layer chromatography, Column chromatography -lon exchange and Affinity Chromatography, HPLC. Introduction to Electrophoresis, Uni Directional and 2D Electrophoresis, introduction UV Visible spectroscopy, Introduction NMR and MALDI-TOF.

#### Unit III X-ray crystallography

Crystal and symmetries -Crystal system - Point groups and space group - growth of crystal of Biological molecule - X-ray diffraction - X-ray data collection - Structure solution - refinement of the structure.

#### Unit IV NMR Spectroscopy

Introduction to NMR - Basic principle of NMR - NMR Theory and experiments - classical description of NMR - NMR parameter - Nuclear Overhauser Effect - NMR applications in the field of Medicine.

#### Unit V Molecular structure and modeling

Introduction- Nucleic acid structure - Protein structure. Generating the model - Building the protein structure and nucleic acid structure - displaying and altering the generated model - optimizing the model

#### Text Book

1. VasanthaPattabhi and N.Gautham, Biophysics, Narosa Publishing house, 2002. (Unit I-V)

- 1. Thomas. E. Creighton, Proteins Structures and Molecular Properties Freeman and Company, 1993.
- 2. Cantor and Schimmel, Biophysical Chemistry Part II Techniques for the study of biological structure and function, Freeman and Company,2003.
- 3. Thomas M Devlin, Textbook of Biochemistry, Wiley LISS Fifth edition, 2010.
- 4. Stephen Neidle, Nucleic Acid Structure and Recognition, Oxford University Press, 2002.
- 5. Leonard Banaszak, Foundations of Structural Biology, Academic Press, 2000.
- 6. Philip E. Bourne, Structural Bioinformatics, John Wiley & sons, 2011.

# ELECTIVE I: DATABASE AND TOOLS FOR BIOINFORMATICS

Semester : V Credits : 5 Course Code: I13BI5:2 Total Hrs :75

#### **General Objective**

To have an in depth knowledge of Bioinformatics resources that helps in analyzing biological problems to provide better solutions.

## Unit I

Database-Repositories for high throughput genomic sequences: EST, STS GSS ; Genome Databases at NCBI, EBI, TIGR, SANGER – Viral Genomes.

#### Unit II

Archeal and Bacterial Genomes Database; Eukaryotic genomes with special reference to model organisms, Yeast, Drosophila, *C. elegans*, Rat, Mouse, Human, plants such as *Arabidopsis thaliana*, Rice.

#### Unit III

Protein derived databases-InterPro, Prosite, Pfam, ProDom; Structure: FSSP, DSSP. Databases of structure-based classification; CATH and SCOP

#### Unit IV

Introduction structural database, Protein Visualization tools-Rasmol-SwissPDBviewer-Chime, Cn3D. Tools used for homology modeling.

#### Unit V

Principle and Application Drug designing; Tools used for computational Drug Design - Target Selection; Active site prediction; Small molecule building-Chemsketch, SMILES; Docking using gemdock.

#### Text Books

- 1. JinXiong, Essential Bioinformatics, Cambridge University Press, 2006.
- 2. Bioinformatics: Databases and Algorithms, N. Gautham, Narosa Publishing House. 2005

- 1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003.
- 2. Higgins, D and Taylor.W (Eds), Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi, 2000.
- 3. Durbin.R,Eddy. S.R,Krogh.A and Mitchison.G, Biological Sequence Analysis, Cambridge Univ. Press, Cambridge, UK, 1998.
- 4. Gibson.G&Muse.S.V, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002.

- 5. Baxevanis.A and Ouellette.B.F, Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005.
- 6. Campbell.A.M&Heyer.L.J, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003.
- 7. Creighton.T.E, Protein Function A Practical Approach, Oxford university press, 2004.
# ELECTIVE II: BIOSTATISTICS AND NUMERICAL METHODS

Semester :V Credits : 5 Course Code: I13BI5:3 Total Hrs :75

## **General Objective**

To understand the computational, mathematical and statistical approaches to analyze biological data involving in biological processes.

## Unit I Numerical Measures

Review of types and frequency distribution- Graphical representation of data - Measures of central tendency – mean, median, Mode –Measures of Dispersion- range, interquartile range, Variance and Standard deviation, Coefficient of Variation and Applications. (Problems only, Derivations not included.)

#### Unit II Correlation and Regression

The two way scatter plot- Pearson's correlation coefficient- spearman's rank correlation coefficient. Regression concepts-the population regression line- the method of least squares- inference for regression coefficients – inference for predicted values. (Problems only, Derivations not included.)

#### Unit III Probability

Events and Probability- Conditional probability- Baye's Theorem. Probability distribution- Binomial Distribution. (Problems only, Derivations not included.)

## Unit IV Numerical Integration

Introduction – A general quadrature formula for equidistant ordinates (or Newton-cote's formula) – The Trapezoidal rule - Simpson's one third rule - Simpson's three eighths rule. (Problems only, Derivations not included.)

## Unit V Numerical Solutions for Ordinary Differential Equations

Solution by Euler's Methods- Modified Euler's method-second order Runge-kutta method for first order ordinary differential equations - fourth order Runge-kutta method for first order ordinary differential equations. (Problems only, Derivations not included.)

## Textbooks

- 1. Pranab Kumar Banerjee, Introduction to Biostatistics, S.Chand & Company Ltd.2006 Unit-I, Unit-II, Unit-III only).
- 2. Kandasamy.P, Thikagavathy.K, Gunavathy.K, Numerical Methods, S.Chand & Company Ltd. 2003 (Unit-IV, Unit-V only).

- 1. Veer Bala Rastogi, Fundamentals of Biostatistics, Ane Books India. 2007
- 2. Sastry.S.S, Introductory Methods of Numerical Analysis, 2001.

# ELECTIVE II: RESEARCH METHODOLOGY

Semester : V Credits : 5 Course Code: I13BI5:4 Total Hrs :75

## **General Objective**

To understand the basics of research methodology and research ethics that helps to find better solutions for biological problems.

## Unit I Introduction

Objectives and types of research, Motivation and objectives – Research methods & Methodology. Types of research – Descriptive & Analytical, Applied & Fundamental, Quantitative, Qualitative, Conceptual, Empirical.

## Unit II Research Formulation

Defining and formulating the research problem - Selecting the problem - Necessity of defining the problem - Importance of literature review in defining a problem - Literature review - Primary and secondary sources - Development of working hypothesis.

## Unit III Research design and methods

Research design – Basic Principles- Need of research design, Features of good design, Important concepts relating to research design, Developing a research plan - Exploration, Description, Diagnosis, Experimentation. Determining experimental and sample designs.

## Unit IV Reporting and thesis writing

Structure and components of scientific reports - Types of report - Technical reports and thesis – Significance - Different steps in the preparation - Layout - structure and Language of typical reports – Illustrations and tables - Bibliography - referencing and footnotes.

## Unit V Application of results and ethics

Environmental impacts - Ethical issues - ethical committees - Commercialisation - Copy right - royalty - Intellectual property rights - and patent law - Trade Related aspects of Intellectual Property Rights - Reproduction of published material - Plagiarism - Citation and acknowledgement - Reproducibility and accountability.

## Textbook

1. Kothari, C.R., Research Methodology: Methods and Techniques. New Age International, 1990.

- 1. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., An introduction to Research Methodology, RBSA Publishers, 2002.
- 2. Kothari, C.R., Research Methodology: Methods and Techniques. New Age International, 1990.
- 3. Sinha, S.C. and Dhiman, A.K., Research Methodology, EssEss Publications, 2002.

# SBEC II: APPLIED BIOINFORMATICS

Semester :V Credits : 2 Course Code: I14BI5S2 Total Hrs :30

# General Objective

To understand the potential applications of bioinformatics in various life sciences studies. .

# Unit I

Commercial bioinformatics - Survey of bioinformatics companies in India and abroad –Economics prospects - pharma informatics - combinatorial chemistry - HT screening – in silico screening - from lead to commercialization.

## Unit II

Pharmacokinetics and Pharmacodynamics - Human genetic variations - alleles - Types of Polymorphisms - SNP's at structural and functional level. Personalized Medicine and ethical issues in pharmacogenomics - Case study of Pharmacogenomics and Pharmacogenomic markers in Schizophrenia - Alcoholism & Neurodegenerative diseases.

# Unit III

Microarray Bioinformatics: Concept of gene expression, Types of microarrays - Making Microarrays - Spotted Microarrays, Insitu synthesized Oligonucleotide arrays, Affymetrix technology, Using Microarrays

## Unit IV

Cheminformatics - Toxicogenomics - Clinomics - Ayurinformatics - Mitochondrionics - Metabolomics - Transcriptomics - Next generation Sequencing.

## Unit V

Introduction to Research Methodology-Research design – Basic Principles- Need of research design, Features of good design, important concepts relating to research design, Developing a research plan. IPR Awareness-Copyrights and Patents, IPR for Soft Wares and Life forms, IPR Laws in India, Patent Amendment -2005 and its impact, Economic benefits of IPR protection, Ethical Issues of Genetic Engineering.

## Textbooks

- 1. Online Material (Unit-I & IV)
- Rastogi,S.C. Parag Rastogi, Namita, Bioinformatics Methods And Applications: Genomics Proteomics And Drug Discovery, 3<sup>rd</sup> Edition, 2008. (Unit-II P.No. 322-340, Unit-III P.No. 191-220)
- 3. Kothari, C.R. Research Methodology: Methods and Techniques, 2009 (Unit-V)

- 1. Brown, T.A, Genomes, 2nd Edition, BIOS Scientific Publishers, Ltd., Oxford, UK, 2002.
- 2. Baxevanis D and Ouellette BFF, Bioinformatics: A practical guide to the analysis of genes and proteins (3rd Ed), John Wiley & Sons, Inc., 2005.
- 3. Sensen CW, 2002. Essentials of Genomics and Bioinformatics, Wiley-VCH.
- 4. Jenson, O.N., in Proteomics. A Trends Guide (eds Black Stock, Co- and Mann), Elsevier Science, London, 1998.
- 5. Pennington, S.R and Dunn.M.J, Proteomics, Viva Books Pvt. Ltd., New Delhi, 2002.
- 6. Subbaram,N.R What everyone should know about patents, 2nd Edition, Pharma Book Syndicate, Hyderabad, 2006.
- 7. Philip W.Grubb, Patents for Chemicals, Pharmaceuticals and Biotechnology-Fundamentals of Global Law practices and strategy, 4th Edition, Oxford University Press, 2006.
- 8. Dubey, R.C, A Textbook of Biotechnology, S.Chand& Company, 1993.
- 9. Ben Mepham, Bioethics-an Introduction for the biosciences, Oxford University Press, 2005.

# CORE VII: INTRODUCTION TO DBMS & SQL

Semester :VI Credits : 5 Course Code: I16BI607 Total Hrs :75

# **General Objective**

To comprehend Database concepts and management of the data in the field of bioinformatics.

# Unit I

Introduction – History of database systems - Database system applications – Database systems vs File systems – View of data: Data abstraction – Instances and Schemas – Database users and administrators - Transaction management – Database system structure – Advantages and disadvantages

# Unit II

Database Models: Basic concepts and structure of Entity relationship data model, Relational data model, Object-oriented data model, Object-relational data model, Network data model and Hierarchical data model . Integrity and security – Normalization – Constraints - Indexing and Hashing

# Unit III

SQL basics – SQL languages: DDL, DML, TCL, DCL and non-procedural languages – MySQL data types, operators and functions – Working with databases and tables – working with data – Joins – Sub queries – Transactions. Introduction to PL/SQL - simple PL/SQL programs.

## Unit IV

Managing scientific data: Introduction – Challenges faced in the integration of biological information – Data management and data integration in bioinformatics – Issues to address while designing a biological information system

## Unit V

SRS: An integration platform for databanks and analysis tools in bioinformatics - The Kleisli query system as a backbone for bioinformatics data integration and analysis

## Text Books

- 1. Abraham Silberchatz, Henry F. Korth, S. Sudharshan, Database System Concepts (5<sup>th</sup> Edition), McGraw Hill, 2002(Unit I,II).
- 2. Bipin C. Desai, An introduction to database systems, Galgotia publications pvt. Ltd., New Delhi, 2003(Unit I, II).
- 3. VikramVaswani, The Complete Reference MySQL, Tata McGraw-Hill, New Delhi, 2002 (Unit III).
- 4. Zoe Lacroix and Ternce Critchlow, Bioinformatics Managing Scientific Data, Morgan Kaufmann publishers, 2003(Units IV, V).

- 1. James Martin, Principles of Database management, Prentice Hall of India, 1976.
- 2. James Martin, Computer database organization, Prentice Hall of India, 1977.
- 3. Peter Rob Carlos Coronel, Database systems, design, implementation & management, Course technology, 2000.
- 4. Database systems A practical approach to design, implementation and management, Thomas Cannolly and Carolyn Begg, Pearson Education, 2002.

# CORE VIII: MOLECULAR MODELING AND DRUG DESIGN

Semester :VI Credits : 5 Course Code: I16BI608 Total Hrs :75

# General Objectives

- 1. To understand the critical relationship among biomolecular structure, function and force field models.
- 2. To analyze Modelling, drug/receptor interactions in detail by molecular mechanics, molecular dynamics, simulations and homology modeling.

# Unit I Introduction to Molecular Modeling

Introduction - Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature

# Unit II Force Fields

Fields - Bond Stretching - Angle Bending - Introduction to Non-bonded Interactions - Electrostatic Interactions - Van der Waals Interactions - Hydrogen Bonding in Molecular Mechanics -Force Field Models for the Simulation of Liquid Water.

# Unit III Energy Minimisation and Computer Simulation:

Minimisation and Related Methods for Exploring the Energy Surface - Non-Derivative method, 1st and 2nd order minimisation methods - Computer Simulation Methods - Simple Thermodynamic Properties and Phase Space - Boundaries -

# Unit IV Molecular Dynamics & Monte Carlo Simulation:

Molecular Dynamics Simulation Methods - Molecular Dynamics Using Simple Models - Molecular Dynamics with Continuous Potentials - Molecular Dynamics at Constant Temperature and Pressure - Molecular Modeling software: BIOSUITE

## Unit V Structure Prediction and Drug Design

Structure Prediction - Introduction to Comparative Modeling. Sequence Alignment. Constructing and Evaluating a Comparative Model. Predicting Protein Structures by 'Threading', Molecular Docking, AUTODOCK and HEX. Structure based De Novo Ligand design, Drug Discovery – Chemo informatics – QSAR.

## Textbooks

- 1. Bioinformatics Methods And Applications: Genomics Proteomics And Drug Discovery, Rastogi,S.C. Parag Rastogi, N. Mendiratta, 4<sup>th</sup> Edition.2008.
- 2. Bioinformatics: Principles and Applications, Zhumur Ghosh, Bibekanand Mallick, Oxford Press. 2015.

- 1. Andrew Leach, Molecular Modeling: Principles and Applications (2<sup>nd</sup> Edition), Addison Wesley Longman, Essex, England, 1996.
- 2. Alan Hinchliffe, Modeling Molecular Structures, 2<sup>nd</sup> Edition, John, Wiley, 2000.
- 3. Alan Hinchliffe, Molecular Modeling for Beginners, John, Wiley, 2003.
- 4. Cohen(Ed.), Guide Book on Molecular Modeling in Drug Design, Academic Press, San Diego, 1996.
- 5. Frenkel D and Smith B, Understanding Molecular Simulations. From Algorithms to Applications, Academic Press, samdiego, California, 1996.
- 6. Rauter C and Horn K, X,ray crystallography and drug design, Elsevier, 1984.
- 7. Kalos and P.A Whitlock, Monte Carlo Methods, John Wiley & Sons, New York, 1986.
- 8. McCammon JA and Harvey SC. Dynamics of Proteins and Nucleic Acids. Cambridge University Press, Cambridge, 1987.

# CORE PRAC VII: INTRODUCTION TO DBMS & SQL LAB

Semester :VI Credits : 2 Course Code: I16BI6P7 Total Hrs :45

# **General Objective**

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To create and analyze the biological databases with the help of DBMS and SQL.

- 1. Data definition language
  - Create table
    - Alter table
  - Drop table
- 2. Data manipulation language
  - Insert
  - Delete
  - Update
  - Select
    - Distict
- 3. Single row functions
  - Char
  - Numeric
  - Data functions
- 4. Group functions
  - Group
  - Union

# CORE PRAC VIII: ADVANCED BIOINFORMATICS LAB-II

Semester :VI Credits : 2 Course Code: I16BI6P8 Total Hrs :45

# **General Objective**

To know the basic modeling and docking techniques to explore biological phenomena at the molecular level.

- 1. Homology Modeling using SPDBV/MODELLER, Model structure refinement, Model Validation.
- 2. Identifying fold of proteins
- Use of threading servers: Phyre, SwissPDBetc.,
- 3. Energy minimisation & geometry optimization for proteins & peptides
- 4. Building of small molecule, using CHEMDRAW.
- 5. Docking using iGEMDOCK and HEX.
- 6. ADME Property prediction-MedChem Designer
- 7. Post Docking Analysis-Pose View

# ELECTIVE III: BIODIVERSITY INFORMATICS

Semester :VI Credits : 5 Course Code: I13BI6:1 Total Hrs :90

## **General Objective**

To comprehend the digitized biodiversity data resource available nationally and internationally and to utilize the same effectively and to conserve biodiversity.

# Unit I Biological Diversity of life

Methods for species identification & classification - Information needs in biodiversity assessments and inventorying programmes - Role of information technology in distributing biodiversity information.

## **Unit II Introduction to Biodiversity Informatics**

Assessing - analyzing and documenting biodiversity - Morphological and molecular characterization of biodiversity -Introduction to biodiversity database: endangered animals - endemism and Red data books - Biodiversity registers.

## Unit III Biodiversity Information System

Designing information systems to support biodiversity conservation Networks for distributing information - Distributed Databases and Web -Accessible Resources.

## Unit IV Tools for Biodiversity Informatics

Software for identification of Assessing existing biodiversity databases on the world -wideweb - Probabilistic and deterministic identification - Delta - MicroIS - AVIS - ICTV.

## Unit V Global Biodiversity System

Global biodiversity information system -Overview of the UNEP/GEF biodiversity data management project (BDM) –CBD and bioethics -General agreement on trade and traffics.

# Text Books

1. Krishnamurthy, An Advanced Textbook On Biodiversity: Principles And Practice, Oxford and IBH Publishing, 2004.

## Web Resource

- 1. www.Biodiv.org
- 2. www.wri.org/wri/biodiv/
- 3. www.wcmc.org.uk

- 1. Global Biodiversity: Status of the Earth's Living Resources. Water Conservation Monitoring Centre, Chapman & Hall, London. 1992
- 2. Forey PL, Humphries CJ and VaneWright RI, Systematics and Conservation Evaluation, (eds), Clarendon press, Oxford.1994.
- 3. Hawkswoth, D.I, Biodiversity: Measurement &Estimation (Ed.), Hapman&Hall, London, 1995.
- 4. Cnhos, DAL, Canhos VP and Kirsop BE, Alice, A Biodiversity database system. Alice software partnership. Linking Mechanisms for biodiversity information, Tropical foundation, Tropical Foundation, Campinas, Brazil, 1994.
- UhlirPF. The public international law of civilian remote sensing: an overview. In: Mink, P.D. (ed), American Enter price, the law, and the commercial use of spece, Vol II. National Legal Center for the public interest, Washington, Dc. 1980.
- 6. Heywood VH, WatsonRT, Global Biodiversity Assessment.Published for the United Nations Environment programme, Cambridge University press, Cambridge, 1995.
- 7. Shanmughavel P, Bioinformatics Applications in Forestry, VDM Verlag, Germany. 2010.

# ELECTIVE III: IMMUNOINFORMATICS

Semester :VI Credits : 5 Course Code: I13BI6:2 Total Hrs :90

#### **General Objectives**

- 1. To understand the basics of immune system and immune power.
- 2. To understand the techniques and tools that enhance to provide solutions for various infections and diseases.

## Unit I Immune systems and Systems biology

Innate and adaptive immunity in vertebrates - Antigen processing and presentation. Antibodies: Immunoglobulins - Immunoglobulin classes and subclasses - CDR and LDR regions and sequence numbering - Immunogenetics - Hybridoma technology: applications and engineering - Humanization of antibodies by design.

#### Unit II Membrane receptors for antigen

The B-cell surface receptor for antigen (BCR) - The Tcell surface receptor for antigen (TCR) - Antigen recognition diversity - the major histocompatibility complex (MHC). Contemporary challenges to the immune system: Infectious diseases - clustering of infectious disease organisms - autoimmune diseases. Epitopes: Affinity Maturation - Recognition of Antigen by B cells - Neutralizing Antibody - Prediction of epitopes.

## Unit III Vaccine design

Categories of vaccines - Polytope vaccines - Therapeutic vaccines - Evolution and escape due to variations. HLA - immunogenomics and viral bioinformatics - generating data for databases - the peptide repertoire of HLA molecules - HLA nomenclature and IMGT/HLA sequence database.

## Unit IV Mathematical models

Reverse immunology and approaches in computer aided vaccine design - Viral bioinformatics: computational views of host and pathogen. MHC polymorphism: Causes of MHC polymorphism - MHC super types

## Unit V Browsing and searching immunological databases

Immunoglobulin: sequence and structure - Databases of epitopes. Antibody: Antibody numbering - Prediction of 3D structure using homology modeling - Sequence analysis in immunology: Alignments - Molecular evolution and phylogeny - Prediction of functional features of biological sequences.

- 1. Ole Lund, Morten Nielsen, Claus Lundegaard, Can Kesmir, and Soren Brnak, Immunological Bioinformatics, The MIT press, 2005.
- 2. Immunoinformatics: Bioinformatics Strategies for Better Understanding of Immune Function, Wiley; 1<sup>st</sup> Edition, 2003.
- 3. Ivan M. Roitt and Peter J. Delves, Essential Immunology, Wiley-Blackwell ,2011

Project

Sem. VI Total Hrs. : 90 Code : I13BI6PJ Credits : 5

# SBEC III: COMPREHENSIVE PRACTICE FOR BIOINFORMATICS COMPETITIVE EXAMINATION

Semester :VI Credits : 2 Course Code: I16BI5S3 Total Hrs :30

# **General Objectives**

To understand and apply the interdisciplinary skill to clear competitive examinations.

# Unit I

Introduction to computers - Evolution of computers - computer generations - classification of computers - Basic computer organization - Introduction of operating systems - Computer software and internet - Programming in C - Perl. Database - DBMS - SQL.

# Unit II

Bioinformatics - Overview- Definition and History; Milestones in Bioinformatics. Biological database - Primary - Secondary - Structure - Specialized - Sequence alignment - Structure Alignment - Structure prediction. Phylogenetic analysis.

# Unit III

Basic concepts of Microscopy - Ultrastructure and classification of cell - Cell composition and permeability - Organelles and membrane - Cell Division and Cell Cycle - Basics of molecular structure of proteins & Carbohydrates - Chemistry of lipids - Major metabolic pathways - Enzymology - Introduction to microbiology - Microorganisms - Cultivation and maintenance - Control of microorganisms - Environmental & Industrial uses - Microbial Diseases - Introduction to Molecular Biology - Transcription - Translation - Recombinant DNA - Cloning and expression vectors.

## Unit IV

Basic mathematics – matrices and determinants - Vector algebra – Differential Calculus - Differential calculus - Numerical measures - Correlation and regression - Probability - Numerical integration - Numerical solutions for ordinary differential equations.

## Unit V

Structural bioinformatics - Data representation and Database - PDB Format -mmCIF format and other dataformat - PDB - Nucleic acid Database - Other structure based database - Comparative features - structure and functional assignment & Protein Interaction - Drug target principles & Molecular visualization.

- 1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003.
- 2. Higgins.D and Taylor.W (Eds), Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi, 2000.
- 3. Durbin, R. Eddy. S. R, Krogh. A and Mitchison. G, Biological Sequence Analysis, Cambridge Univ. Press, Cambridge, UK, 1998.
- 4. Gibson.G&Muse.S.V, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002.
- 5. Baxevanis.A and Ouellette, B.F. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005.
- 6. Campbell.A.M&Heyer, L.J, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003.
- 7. Tsai.C.S, An Introduction to Computational Biochemistry, Wiley-Liss, New York, 2002.
- 8. Creighton.T.E, Protein Function A Practical Approach, Oxford university press, 2004.
- 9. Pennington. S.J &Dunn.M.J, Proteomics from protein sequence to function, BIOS Scientific Publishers, 2002.
- 10. Andrew Leach, Molecular modeling: Principles and Applications (2<sup>nd</sup> Edition), Addison Wesley Longman, Essex, England, 1996.
- 11. Erwin Kreysig, Engineering Mathematics, 7<sup>th</sup>Edition, John Wiley, USA, 2001.
- 12. Narayanan S and Manicavachagam Pillay TK, Calculus, Vol.I, S.Viswanathan Publ. Pvt. Ltd., Chennai, 1982.

UG -	Non I	Major	Elect	ive Co	urses	(NMEC)
(Offe	red to	Stud	ents	of othe	r Disc	iplines)

Sem.	Course	Code	Title	Hrs./	Credite	Marks		
				week	oreuns	CIA	ESA	TOTAL
Ш	NMEC I	113BI3E1	BASIC BIOINFORMATICS	2	2	25	75	100
IV	NMEC - II	113BI4E2	BASIC STRUCTURAL BIOINFORMATICS	2	2	25	75	100

# NMEC-I: BASIC BIOINFORMATICS

Semester : III Credits : 2 Course Code: I13BI3E1 Total Hrs : 30

# **General Objective**

To understand the basic concepts and application of Bioinformatics and to know the basics of protein structure prediction and functions and also various tools for analysis of proteins.

## Unit I

Introduction to Bioinformatics - History - scope and applications. Research Areas of Bioinformatics - Pharmaceutical - Bioinformatics industries and Institutions in India & Worldwide.

#### Unit II

Biological Databases: Nature and diversity of data - classification and importance of Biological Databases - Nucleic Acid databases-Primary Sequence Databases and secondary sequence Databases - NCBI - Protein databases-sequence and structure - databases (Primary and secondary)

#### Unit III

Literature Databases-Pubmed - Disease Databases-KEGG disease - Microbiological databases-UNIQEM - Genome Databases-Human Genome NCBI - GOLD and other specialized Databases.

## Unit IV

Pairwise Alignment - Local and Global Alignment concept -Needleman wunsch method and Smith waterman method - Fasta and Blast - Multiple Sequence Alignment-Clustal W.

#### Unit V

Visualization of structure using Rasmol or SPDBViewer or CHIME - Basic concept in molecular modeling; different type of computer representations of molecules.

## Text Books

- 1. JinXiong, Essential Bioinformatics, Cambridge University Press 2006. (Unit-II P.No 10-18, Unit-IV P.No.31-48, 63-71, Unit-V P.No 187-190)
- 2. Manju Bansal, Basic Bioinformatics, Atlantic publishers & distributors, 2009. (Unit-I P.No.1-8, Unit-III P.No. 66-70, 48-56, 224-228)

- 1. David M, Bioinformatics: Sequence and Genome analysis, Cold Spring Harbor Laboratory, 2004.
- 2. Rastogi RS, Bioinformatics: Concepts, Skills & Applications, Eastern Economy Edition 2008.

# NMEC II : BASIC STRUCTURAL BIOINFORMATICS

Semester : IV Credits : 2 Course Code: I13BI4E2 Total Hrs :30

# **General Objective**

To understand the structural information of protein and analyze the functions of protein through three dimension structure.

# Unit I

Defining bioinformatics & Structural bioinformatics - Fundamentals of protein structure-fundamentals of DNA & RNA structure - Organization of structural bioinformatics - Role of structural bioinformatics in Systems biology.

# Unit II

Protein structure Databases- PDB, MMDB, Protein structure visualization software- RASMOL - SwissPDBviewer.

# Unit III

Protein structure alignment-Tools used for protein structure alignment- Maxcluster-DaliServer

# Unit IV

Protein 3D Structure Prediction by computation Methods-Homology Modeling – Fold Recognition Methods- ab *initio* methods-Structure Validation.

## Unit V

Application of structural Bioinformatics-structure based drug design-Tools used for structure bases drug design-ADME properties.

# Text Books

- 1. Philip E. Bourne, Helge Weissig, Structural Bioinformatics, John Wiley & Sons, 2003. (Unit-I, Chapter 1,2,3)
- 2. JinXiong. Essential Bioinformatics. Cambridge University Press 2006(Unit-II P.No.182-186, 187-190, Unit-III P.No. 190-195, Unit-IV P.No. 214-228)
- 3. Rastogi,S.C. Parag Rastogi, N. Mendiratta, 4<sup>th</sup> Edition. 2009 (Unit-V)

- 1. David M, Bioinformatics: Sequence and Genome analysis, Cold Spring Harbor Laboratory, 2004.
- 2. Branden and J. Tooze, Introduction to Protein Structure, Garland Publishing Inc., New York., 1999.

# UG – Skill Based Courses (SBC)

Sem.	Course	Code	Title	Hrs. Credi	Credite	Marks		
					Greatis	CIA	ESA	TOTAL
IV	SBC-I	U16LFS41	Life Skills	2	1	100	-	100

# LIFE SKILLS

Semester IV Total Hrs : 30 Course code: U16LFS41 Credit 1

# **General Objectives :**

- 1. To acquire skills and abilities for adaptive and positive behavior that helps to deal effectively with the demands and challenges of everyday life.
- 2. To develop creative, communicative and critical thinking skills necessary for employability

# Unit I Basics of Communication skills & Effective Communication

Features of Communication – Process of Communication Verbal, nonverbal, Body Language – Postures & Etiquette –Listening & speaking Skills- Communication Barriers – Listening & speaking Skills.

# Unit II Personal Effectiveness

Maslow's theory – Self-esteem- Role Conflict – Intra & Inter personal Skills – Efficiency Vs effectiveness – Team Building – Emotional Intelligence & Quotient

# Unit III Interview Skills

Types of Interviews – Resume Formats & preparation - Cover letters – Simple rules to face interviews – Dos &Don'ts in a an Interview – Telephonic Interview and Etiquette - Group Discussions – Types – Methods – Ingredients and Tips for a Successful Group Discussion.

# Unit IV Test of Reasoning & Numerical Ability

- A. Numerical Ability: Problems related to Average Percentage Profit /Loss Simple & Compound Interest- Time & Work Boats & Streams etc.
- B. Logical reasoning: Logical Detection Nonverbal reasoning Problems related to seating arrangements Relationship model Assertion & Reasoning etc.
- C. Online Tests: Aptitude Logical Reasoning Problem Solving –Time management in Online tests- Online tests on Language skills- Aptitude and technical rounds

## Unit V Outbound Learning

Physical, Mental, and emotional exercises

## Texts for Reference:

- 1. Barun.K.Mitra, Personality Development and Soft Skills, 6<sup>th</sup> edition, Oxford University press Noida 2012.
- 2. M.Sarada, The complete Guide to Resume Writing, Sterling Publishers Pvt Ltd, New Delhi 2012.
- 3. Gloria J.Galances& Katherine Adams,Effective Group Disscussions,Theory & practice,12<sup>th</sup> Edition, Tata McGrawHillpvt Ltd 2012.
- 4. Francis Soundararaj, Basics of Communication in English, SoftSkills for Listening Speaking, Reading& Writing, Macmillan Publishers India Ltd. 2013.

# Scheme of Evaluation

	Total	100 Marks
7.	OBL Observation / Work book	40 Marks
6.	Team Work	10 Marks
5.	Group Discussion	10 Marks
4.	Online test 1( aptitude)	10 Marks
3.	Numerical Ability Test	10 Marks
2.	Resume	10 Marks
1.	EQ test	10 Marks

# CORE IX: CELL AND MOLECULAR BIOLOGY

Semester : VII Credits : 5 Course Code I13BI709 Total Hours :75

# **General Objectives**

- 1. To understand the concept of cell and its activity.
- 2. To know the internal structure and organization of cells.
- 3. To know genetics, gene expression and its regulation

# Unit I Basics of Cell and Organelles

Discovery-Cell theory-Prokaryotes & Eukaryotes- Cellular Organelles: Structure, Organization and Functions of Plasma membrane, Nucleus & nucleolus, Mitochondria, ER-rough and smooth, Ribosomes, Golgi apparatus, Plastids, Vacuoles, Lysosomes, Peroxisomes and Microbodies. Cell junction.

# Unit II Cell Cycle and Signaling

Overview, Structure and Organization of Microtubules and Microfilaments-Cell movement. Cell Division: Cell Cycle-Regulation of Cell Cycle- Cell signaling- (adrenalin receptors, acetylcholine receptors, insulin receptors) Programmed Cell Death. Transformation, Transduction and Conjugation, Recombination -Generalized and Site specific in bacteria- Holiday model.

## Unit III Overview of genetic material

Structure of DNA and RNA- Composition, Types and Functions, Replication mechanisms - Enzymes involved in replication. Mutation: Origin and Classification - Types- Molecular Mechanism of Mutation-Detection of DNA damage at molecular level, Ames test, cytogenetic analysis in mammalian cells - in vitro and in vivo- Host mediated assay- DNA repair and recombination mechanisms. Transposons and transposable elements- Mechanism of transposition.

## Unit IV Transcription and RNA Processing

Transcription in Prokaryotes and Eukaryotes -Post transcriptional modifications. Genetic code and Translation: Features of genetic code -Deciphering of the codon- Translation in Prokaryotes and Eukaryotes- Post translation modifications- Protein targeting.

## Unit V Regulation of Gene Expression

Cistron, muton and recon -exons and introns. Regulation of gene expression in prokaryotes and eukaryotes -positive and negative control in prokaryotes - Operon models(Lac,Tryp,Ara) - Spatial and Temporal regulation of eukaryotic genes, mi RNA, si RNA, Micro-satellites.

## Text Book

1. Geoffrey M Cooper, Robert E Hausman. "The Cell-A Molecular Approach", Third Edition ,ASM Press, Washington, 2004.

- 1. Harvey Lodish*et al.* "Molecular Cell Biology", W.H.Freeman& Company, New York, Fourth Edition, 2002.
- 2. Gerald Karp. "Cell and Molecular Biology", Third edition, John Wiley & Sons, New York, 2001.
- 3. Alberts *et al.* "Essential Cell Biology: An Introduction to the Molecular Biology of the Cell", Second edition. Garland Science Taylor& Francis Group, New York. 2003.
- 4. Benjamin A.Pierce "Genetics-A Conceptual Approach" W.H.Freeman& Company, New York, Second Edition, 2006.

# CORE X: PROGRAMMING IN C++ AND JAVA

Semester : VII Credits : 5 Course Code I17BI710 Total Hrs :75

# **General Objectives**

- To comprehend the fundamentals of programming techniques such as
- (a) Sequence of execution
- (b) Selection of blocks to be executed
- (c) Repetition of execution, with the help of C++ and Java programming language

#### Unit I

Basic Concepts of Procedure-Oriented Programming, Object-Oriented Programming – Tokens, Keywords, Identifiers and Constants – Basic Data Types – Variables – Operators in C++ - Expressions, Control Structures

#### Unit II

Classes and Objects – Specifying a Class, Creating Objects, Accessing Class Members, Defining Member functions – Arrays within a class, Static Data Members and Functions, Arrays of Objects, Friendly Functions, Returning Objects

## Unit III

Java Features – Difference between Java and C++ - Java and Internet, Web browsers – Java Environment, Java Development Kit (JDK), Application Programming Interface (API), Java Runtime Environment – Java Program Structure – Java Tokens – Java Statements – Java Virtual Machine (JVM) – Command Line Arguments – Constants, Variables, Data Types, Operators and Expressions

## Unit IV

Decision Making and Branching, Looping – Classes, Objects and Methods - Arrays, Strings and Vectors – Wrapper Classes – Enumerated Types – Annotations – Interfaces, Defining Interfaces, Extending Interfaces and Implementing Interfaces, Accessing Interface variables – Packages

## Unit V

Multithreaded Programming – Managing Errors and Exceptions, Types of Errors, Exceptions, Exception Handling, Catch and Final statements – Applet Programming, Applet Life Cycle, Creating and Executing Applets, Running the Applets – Graphics Programming; Drawing Line, Rectangle, Circles, Eclipse, Arcs, Line Graphs, Bar Graphs and Polygons

# Text Books

- 1. Balagurusamy, E, Programming with Java, Tata McGraw Hill Education Pvt Ltd, 5<sup>th</sup> Edition, 2015
- 2. Balagurusamy, E, Object Oriented Programming with C++, Tata McGraw Hill Education Pvt Ltd, 5<sup>th</sup> Edition, 2011
- 3. Patric Naughton and Herbert Schildt, Java 2 Complete Reference, TMH, 1999
- 4. Somasundaram, K, Programming in Java 2, Jaico Publishing House, 2008

- 1. Eckel Bruce, Thinking in Java for Java SE5/6, Pearson, 4<sup>th</sup> Edition, 2013
- 2. Herbert Schildt, Java A Beginners Guide (4th Ed.,), Tata McGraw Education Pvt Ltd, 2007
- 3. Horstmann, C.S, Computing Concepts with Java 2 Essentionals(2<sup>nd</sup> Ed), John Wiley Publishers, 2000

# CORE XI: BIOINFORMATICS DATABASES & TOOLS

Semester :VII Credits : 5 Course Code I13BI711 Total Hrs :75

# General Objective

To understand the information from biological databases and tools by using computational approaches to analyze this information.

## Unit I Biological Database

Introduction to Biological databases, Types database, Relational Databases, Object oriented databases, Biological Databases, Primary Databases- GenBank, EMBL, DDBJ,PIR, Swiss Prot, Secondary Databases, Specialized Databases Literature Databases, PubMed, OMIM.

#### Unit II Mapping Databases

Introduction to Mapping databases, relationship between mapping and sequencing, Genomic map elements-DNA Markers, Polymorphic Markers, DNA clones, Genomic annotations. Types of Maps-Cytogenetic Maps, Genetic Linkage Maps, Physical Maps, STS content Maps, Clone-based maps, Radiation Hybrid Maps, Sequence based Maps

#### Unit III Genome Databases

Introduction to Genome Database, eGenome, LDB2000, Gene Integration Resources, GeneCards and GeneLoc, Genelynx, euGenes, AceView, Comparative Maps. Mouse Genome informatics Database, Rat Genome Database, UCSC, Ensembl.

## Unit IV Predictive methods using protein Sequences

Introduction-Predictive features of individual residues- Secondary structure prediction-Prediction methods-PHDacc and PROfacc-Jpred. Transmembrane segments-Prediction methods-TopPred, PHDhtm, ProfTMB, SOSUI, TMHMM and DAS. Predicting Function-Annotation transfer-Motifs and patterns-Methods-PROSITE, Pfam, InterPro and BLOCKS. Subcellular Localization-Prediction Methods-PSORT, SUBLOC, TargetP and LOC3D.Functional Class-Prediction methods-EUCLID and ProtFun.

## Unit V Protein structure prediction and analysis, Pathway and Molecular Interaction Databases

Introduction-Protein structure databases-Other structure databases-MSD, MMDB, PDBSum, TargetDB. Visualizing Proteins-Three-Dimensional visualization packages. Protein structure prediction-homology modeling-threading-Ab initio prediction. Protein structure evaluation-DSSP-PROCHECK-VADAR-Verify3D. Protein structure comparison. Pathway and Molecular Interaction Databases-Primarily molecular Interaction Databases-BIND, DIP, GRID, HPRD, IntAct, MINT. Primarily Metabolic Pathway Databases-EcoCyc, KEGG.

# Text Book

1. Baxevanis, A.D. and Francis Ouellellette, Bioinformatics a Practical Guide to the Analysis of Genes and Proteins, B.F., Wiley India Pvt Ltd 2009.

- 1. Mount D. Bioinformatics : Sequence and Genome Analysis, Cold Spring Harbor Laboratory Press, New York.2004.
- 2. Teresa K. Attwood, David J. Parry-Smith. Introduction to bioinformatics, Pearson Education, 1999.

# CORE PRAC IX : LABORATORY COURSE: PROGRAMMING IN JAVA

Semester :VII Credits: 3 Course Code I13BI7P5 Total Hrs :75

# **General Objectives**

To know the basics of programming in JAVA and to apply the concepts in bioinformatics applications.

- 1. Transcription to DNA to RNA sequence.
- 2. Calculate rotations per minute [ rpm =  $1000 \sqrt{\text{RCF} / 11.17\text{r}}$  ]
- 3. Create amino acid dictionary using switch construct
- Identify the glucose level in blood using if ,else if construct [The glucose level is identified by <70 – hypoglycemia, 70-180 hyperglycemia, > 180 diabetics]
- 5. Identify the type of two peptides using nested if [peptide length is < 8 small, poly otherwise ]
- 6. Count the number of base characters entered among n characters using loop
- 7. Implement stack operation
- 8. Count the number of positive, negative and zero energy molecules stored in an array
- 9. Find the transpose of the given matrix using two dimensional array
- 10. To calculate pH value for a given [OH-] concentration [ pH = -log10(OH-) ]
- 11. Draw a line in different pattern using user defined function
- 12. Write a user defined function to illustrate the storage class of the variables
- 13. Count the number of gaps in the given sequence using user defined function
- 14. Sort n names
- 15. Align two sequences
- 16. Count the number of motif in the given sequence
- 17. Swap two numbers using pointers
- 18. Process the organism details using structure

# CORE PRAC X: LABORATORY COURSE: BIOINFORMATICS DATABASES AND TOOLS

Semester : VII Credits :3 Course Code I13BI7P6 Total Hrs : 75

# General Objective

To apply the knowledge of computational approaches for analyzing the information from biological databases

- 1. Bioinformatics Resources : NCBI-Mapping Databases, EBI, DDBJ, RCSB, ExPASy
- 2. Open access bibliographic resources and literature databases
  - a. PubMed
  - b. BioMed Central
  - c. Public Library of Sciences (PloS)
  - d. CiteXplore.
  - e. OMIM/OMIA
  - f. Citation matcher
- 3. Bioinformatics Resources at the species level
  - a. ICTV Database
  - b. AVIS
  - c. VirGen
- 4. SRS of Biological Databases
  - a. Nucleotide/ Genome Databases.
  - b. Protein Sequence Database.
  - c. Structure databases.
  - d. Protein Pattern Databases
- 5. Sequence databases
  - a. Protein sequence databases: Uniprot-KB: SWISS-PROT, TrEMBL, UniParc;
  - b. Repositories for high throughput genomic sequences: EST, STS, GSS.
  - c. Genome Databases at NCBI, EBI, TIGR, SANGER
- 6. Structure Databases: PDB, NDB, PubChem, ChemBank, FSSP, DSSP
- 7. Derived Databases: InterPro, Prosite, Pfam, ProDom
- 8. Sequence file formats: GenBank, FASTA, GCG, MSF.
- 9. Protein and nucleic acid properties: Proteomics tools at the ExPASy server, and EMBOSS

# ELEC IV: PROTEINS – STRUCTURE AND FUNCTIONS

Semester :VII Credits :4 Course Code I13BI7:1 Total Hrs :75

# **General Objective**

To know the advanced level of structural and functionality of the proteins.

## Unit I

Building blocks, hierarchical representation of proteins: primary, secondary, tertiary and quaternary structure. Structural classification of proteins, structural databases

## Unit II

Computation and representation of solvent accessibility, residue – residue contacts, contact potentials, cation –  $\pi$  interactions, free energy calculations, protein parameters, protein structure comparison.

#### Unit III

Introduction, protein identification and characterization, structure analysis and prediction, substructure: motifs, profiles, patterns and fingerprint search, methods of structure prediction: sequence based, Ab Initio approach, 2D-Structure prediction.

## Unit IV

Structure function relationship - Tools for studying structure function relationship. Protein evolution - phylogenic tree, convergent and divergent trees, sequence analysis, comparison matrix, Dot matrix and substitution matrix. Protein turnover: Ubiquitination, proteasome and protein degradation.

## Unit V

Coenzymes and cofactors-Concept of prosthetic group, apoenzyme, holoenzyme, enzyme, Coenzyme.Vitamins as coenzymes: sources, requirements, functions and deficiency symptoms of water soluble vitamins. Structure and biochemical role, Assay of vitamins. Cofactors: Role of trace elements, their bound forms in biological systems and in enzyme structure and function.

## Text Book

1. Micheal Gromiha, M. Protein Bioinformatics: From sequence to function, Academic Press, 2011.

- 1. Gregory A. Petsko, Dagmar Ringe, Protein Structure and Function, New Science Press, 2004.
- 2. David Whitford, Proteins: Structure and Function, Wiley, 2005.
- 3. Daniel John Rigden, From Protein Structure to Function with Bioinformatics. Springer, 2009.
- 4. Engelbert Buxbaum, Fundamentals of Protein Structure and Function, Springer, 2007.

# ELEC IV :MOLECULAR INTERACTIONS

Semester :VII Credits :4 Course Code I13BI7:2 Total Hrs :75

# **General Objective**

To know the biophysical level of interactions in between the atoms of carbohydrates, proteins and lipids.

# Unit I

Fundamentals of atomic and molecular orbitals: Theory of atomic and molecular orbitals; Linear combination of atomic orbitals; Quantitative treatment of valency bond theory and molecular orbital theory; Resonance structures; -bonds and -bonds.

## Unit II

Fundamentals of chemical bonding and non-bonding interactions: Electrovalent bond, stability of electrovalent bond. Covalent bond – partial ionic character of covalent bonds. Shape of orbitals and hybridization. Co-ordination bond, Vander Waals forces; Metallic bond. Molecular geometry- VSEPR Theory.

# Unit III

Folding pathways: Principles of protein folding, role of chaperons, hydrophobic interactions, electrostatic interactions, non-bonded interactions. Beta turns, gamma turns, types of helices, Disulphide Bridge.

## Unit IV

Molecular interactions: protein-protein, protein-DNA, DNA-Drug, Protein-Lipid, Protein-Ligand, Protein-Carbohydrate interaction, Metalloprotein. Pi ... Pi interactions, C-H...Pi interactions.

## Unit V

Spectroscopy: Principle, Theory, Instrumentation and Application of UV, IR, NMR and Circular dichroism (CD) to macro molecules. Stereochemistry of proteins and nucleic acids.

## Text Books

VasanthaPattabhi, N. Gautham, Biophysics, Narosa publishing house, 2002.

- 1. Albert cotton, F. Chemical Application of Group Theory. John Wiley and Sons, Inc. New York, 1971.
- 2. Spice, J. E. Chemical Bonding and Structure. Pergamon Press Ltd., Headington Hill Hall, Oxford, 1964
- 3. Winter, M.J.Chemical Bonding. Oxford University Press, Inc., New York, 1996.
- 4. Ernest Eliel. Stereochemistry of carbon compounds, Prentice Hall, 1996.
- 5. Shanmughavel, P. Principles of Bioinformatics, Pointer Publishers, Jaipur, India, 2005.

# CORE XII:ALGORITHM FOR COMPUTATIONAL BIOLOGY

Semester :VIII Credits : 5 Course Code I13BI812 Total Hrs :75

## General Objective

To know the Algorithmics in Computational Biology to solve protein sequence, protein evolution and protein structural problems typically encountered in molecular biology research.

## Unit I Sequence alignment

Sequence Analysis : Similarity vs Homology, Homologs, hetrologs, analogs, orthologs, paralogs, xenologs, , significance of an alignment, Dot matrices and hash coding, Dynamic programming in sequence alignment. BLAST and FASTA.

## Unit II Multiple alignment

Goals of MSA, Scoring of MSA, Progressive or hierarchical alignment, Substitution matrices, Evolutionary models, PAM and BLOSUM substitution matrices, Gap penalties. Introduction Phylogenetic tree - Distance matrix methods-UPGMA, NJ, Maximum parsimony, Maximum likelihood

## Unit III Protein and DNA sequence analysis

Pattern representing and characterization, Deterministic pattern, Probabilistic patterns, Pattern characterization, pattern discovery and sequence classification in proteins-general methods for proteins, Hidden Markov models, Gene discovery- gene discovery using HMM-GenMark, ANN-GRAIL, Fourier analysis-GeneScan.

## Unit IV Molecular Structures

Experimental structure determination techniques-X-ray crystallography, NMR, Electron microscopy, Visualisation and representation of molecular structures, Geometrical analysis of structure-Structure comparison.

## Unit V Protein structure prediction and folding

Introduction-prediction accuracy, statistical techniques-CF algorithm, GOR, Neural Network in secondary structure prediction-PHD, Nearest neighbour methods-PREDATOR, NNSSP, Consensus methods-JPRED, NPS, Protein tertiary structure prediction, Protein folding.

## Text Books

1. Gautham N, Bioinformatics Database and Algorithms, Narosa publishing House. 2009.

- 1. David W Mount, Bioinformatics : Sequence and Genome Analysis , Cold Spring Harbor Laboratory Press, New York.2004.
- 2. Baxevanis, A.D. and Francis Ouellellette B.F, Bioinformatics –a Practical Guide to the Analysis of Genes and Proteins, Wiley India Pvt Ltd .2009.

# CORE XIII : PROBABILITY AND BIOMATHEMATICS

Semester : VIII Credits : 5 Course Code I17BI813 Total Hrs :75

# **General Objective**

To apply mathematical and statistical approaches for analyzing biological data, from DNA to the biological processes in healthcare systems.

# Unit I

Set theory, Probability theory - Conditional probability, Baye's theorem

# Unit II

Random variable, Distribution – Binomial distribution, Poisson distribution and Normal distribution

# Unit III

Sampling techniques - t-test, Chi-Square test, ANOVA test - Derivative function with Examples

# Unit IV

Differential Equations – Types, Order, Degree, Linear and Non-linear differential equations – Delay differential equations; Mathematical modeling of biological problems, initial value problems, Boundary value problems.

## Unit V

Models – Growth and Decay model – Lead in mammals model – Pharmacokinetics Non-linear Models – Conduction of Action potential model – Two variable action potential system model – Enzyme kinetics model – HIV infection model – Parasitic disease model

## Text Books

- 1. Zar, J.H., Biostatistical Analysis, Pearson Education (Singapore) Pte Ltd, 4<sup>th</sup> Edition, 1999
- 2. George F.Simmons, Differential Equations with applications and historical notes, Mcgraw-Hill Publishers, 2<sup>nd</sup> Edition, 2003
- 3. Kapur. J.K, Mathematical Models, Wiley Eastern Limited, Reprint 2013.

# CORE XIV :MOLECULAR MODELING AND DRUG DESIGNING

Semester :VIII Credits : 5 Course Code I13BI814 Total Hrs :75

## General Objective

To understand the comparative modeling, QSAR studies, drug/receptor interactions in detail by molecular mechanics, molecular dynamics simulations.

# Unit I Protein Modeling

Introduction, methods of protein modeling: homology and comparative modeling. Model refinement, Evaluation of the model, threading and fold recognition, Ab Initio / De novo method.

# Unit II Drug Discovery: Technologies and Strategies

Introduction, area influencing drug discovery, important parameters in drug discovery, drug discovery technologies, Target discovery strategy, identification of possible drug targets, target validation.

# Unit III Virtual Screening and Computer-Aided Drug Design (CADD)

Introduction, virtual high-throughput in silico screening, drug designing approaches, computer-aided drug designing methods, ADME-Tox property predictions, GPCRs as drug targets, aquaporins as targets for drug discovery.

## Unit IV Small Molecules

Introduction - generation of 3D coordinates- computational tools for geometry optimization - conformational analysis - molecular interaction potential -, building a pharmacophore model - SAR and QSAR techniques in drug design - 3D QSAR methods and analysis.

## **Unit V Simulation and Statistical Protocols**

Introduction - Monte Carlo methods - molecular dynamics - energy minimization - leading molecular dynamics simulation packages - Markov chain and Hidden Markov Model. Application of Viterbi algorithm - application of HMM to specific problem and advantages.

## Text Books

- 1. Rastogi,S.C. Parag Rastogi, N. Mendiratta. Bioinformatics Methods and Applications: Genomics Proteomics And Drug Discovery, 4<sup>th</sup> Edition, Prentice-Hall of India (Private), Limited, 2013.
- 2. Zhumur Ghosh, Bibekanand Mallick. Bioinformatics: Principles and Applications, Oxford Press, 2012.
- 3. Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, and Gerd Folkers, Molecular Modeling: Basic Principles and Applications, 2<sup>nd</sup> Edition, Wiley, 2003.

- 1. Andrew Leach, Molecular modeling: Principles and Applications (2<sup>nd</sup> Edition), Addison Wesley Longman, Essex, England, 1996.
- 2. Alan Hinchliffe, Modeling Molecular Structures, 2<sup>nd</sup> Edition, John, Wiley, 2000.
- 3. Alan Hinchliffe, Molecular Modeling for Beginners, John, Wiley, 2003.
- 4. Cohen, N. Guide Book on Molecular Modeling in Drug Design, Academic Press, San Diego, 1996.
- 5. Frenkel D and Smith B, Understanding Molecular Simulations. From Algorithms to Applications, Academic Press, samdiego, California, 1996.
- 6. Rauter C and Horn K, X,ray crystallography and drug design, Elsevier, 1984.
- 7. Kalos, M. and Whitlock, P.A. Monte Carlo Methods, John Wiley & Sons, New York, 1986.
- 8. McCammon JA and Harvey SC. Dynamics of Proteins and Nucleic Acids. Cambridge University Press, Cambridge,1987.
## CORE PRAC XI: COMPUTATIONAL BIOLOGY, BIOSTATISTICS USING R AND DRUG DESIGNING LAB

Semester :VIII Credits :3 Course Code: I17BI8P7 Total Hrs :75

## General Objective

To apply the Biostatical and Algorithmic approaches in bioinformatics for solving various biological problems through Computational Biology.

- 1. Pair wise alignment:
  - i. Global Alignment
  - ii. Local Alignment
  - a. Search tools against Databases:
  - i. BLAST
  - ii. FASTA
- 2. Multiple sequence alignment:
  - a. Clustal
  - b. Dialign
  - c. Multalign
- 3. Sequence patterns and profiles:
  - a. generation of sequence profiles
  - i. PSI-BLAST
  - b. derivation of and searching sequence patterns:
  - i. MeMe,
  - ii. PHI-BLAST
  - iii. SCanProsite
  - iv. PRATT
- 4. Protein motif and domain analysis:
  - a. MEME/MAST
  - b. eMotif
  - c. InterproScan
  - d. ProSite
  - e. ProDom
  - f. Pfam
- 5. Phylogenetic analysis MEGA, PAUP, PHYLIP
- 6. Drawing chemical structure using ChemSketch.
- 7. Conversion of 2D to 3D: Open Babel
- 8. Molecular Docking: AUTODOCK
- 9. Post Docking Analysis: LIGPLOT. PoseView.

## **Biostatistics**

- Calculation of measures of central tendency Calculation of measures of dispersion 1.
- 2.
- 3.
- Graphical display of data Analysing data using tables 4.
- Binomial distribution 5.
- Normal distribution 6.
- 7. Poisson distribution
- 8. One sample t-test
- One-way between groups ANOVA 9.
- 10. Bivariate correlation
- 11. Rank correlation
- Regression 12.

## ELECTIVE V : BASICS OF NEXT GENERATION SEQUENCING

Semester :VIII Credits : 4 Course Code 117BI8:1 Total Hrs :60

#### General Objective

To understand the basic principles of next generation sequencing technology. This includes basic biological applications, basics in data processing, statistical and informatics theories in data analysis, advantages, limitations and assumptions of different methodologies and biological interpretation of the results.

#### Unit-I

What is NGS - Platform overview - Biological applications - Basic concepts - Recent scientific breakthroughs using NGS technology - Analysis workflow - Sequence quality evaluation - Alignment theories - Data formats, Data visualization

#### Unit -II

What is genetic variations, States of the genetic research for complex disease prior to high throughput sequencing - NGS and genetics of complex disease (etiology) - NGS and personal genome sequencing - Experimental considerations- Whole genome sequencing - Target sequencing - Pool sequencing

#### Unit -III

Sequencing mappability, Refined alignment, Base quality recalibration, Variants identification for Diploid genome, Pooled DNA sequencing, Cancer genome, Variation recalibration, Pair-ends – identifying structure variants

#### Unit -IV

Exome sequencing in FIA and PD- DNA-seq III- Prioritizing genetic variants- Non-synonymous variants (SIFT- PolyPhen)- Synonymous variants- Regulatory variants- Statistical methods on rare variants-Biological theories on RNA-seq experiments- Major scientific advance using RNA-seq- Alignment-Gene expression analysis

#### Unit -V

Transcript variation- Allele-specific expression- RNA editing- smRNA- ChIP-seq I Introduction-Biological theories on ChIP-seq analysis- DNA methylation- Statistical considerations & Bioinformatics tools- Histone modification- Experimental approaches & Statistical considerations-. Hidden Markov model annotating histone marks

#### Text Books

- 1. David W Mount, Bioinformatics : Sequence and Genome Analysis, Cold Spring Harbor Laboratory Press, New York.2004.
- Baxevanis, A.D. and Francis Ouellette B.F, Bioinformatics A Practical Guide to the Analysis of Genes and Proteins, Wiley India Pvt Ltd .2009.

## ELECTIVE V : HERBAL MEDICINE

Semester : VIII Credits : 4 Course Code 113BI8:2 Total Hrs :60

#### **General Objectives**

To analyze herbal research and contribute to the current herbal literature

#### Unit I

Evolution of conscious use of plants in the management of health and disease – The Alma – Ata Declaration – The World Health Organization (WHO) – The need for the study of herbals and herbal medicine: Rescue and Preservation of traditional medicinal knowledge and herbals - Understanding the potential and option values of hitherto unknown/ yet to be evaluated herbals - Understanding mode of action- synthesis and designing of herbal drugs - Pharmacodynamics - Improvement of drugs.

#### Unit II

Systems of Medicine – Evolution of systems of medicine – Allopathy – Alternative and complementary medicinal stems – Ayurveda : dimensions- encyclopaedic source texts- eight chikitsas- philosophical and theoretical bases- The Ayurvedic Pharmacopoeia and Materia Medica- Principles and strategies of ayurvedic treatment- types of therapies and treatment methods- current research trends.

#### Unit III

The Siddha system of medicine : dimension- source texts- philosophical and theoretical bases- Siddha Pharmacopoeia and Materia Medica- Principles and strategies of treatment- current research trends – The Unani- Chinese- Tibetan- Babylonian and Egyptian Systems of medicine – Homeopathy.

#### Unit IV

Naturopathy- Aromotherapy-Bach's flower remedies- Tribal medicine- Faith healing- Religious beliefs-Ethnotherapeutics and Ethnopharmacology – Concept of Holistic medicine – Common herbals and herbal medicines of India.

#### Unit V

Economic value of herbals and herbal drugs- wealth of Indian and World herbals- standardization and preservation of herbal drugs. Drug adulteration- identification and substitutions- Identification- cultivation and micropropagation of herbals- biotechnological exploitation- Databases on herbals and herbal drugs.

- 1. GuhabakshiD.N., Sensarma and Pal D.C., A lexicon of medicinal plants in India. Nayaprokash publications. 1999.
- 2. ChopraR.N., NayarS.L.and Chopral.C., Glossary of Indian medicinal plants. C.S.I.R, New Delhi. 1956.
- 3. Rajiv K.Sinha. Ethnobotany The Renaissance of Traditional Herbal Medicine. INA SHREE publishers. 1996.

- 4. Kanny, Lall, Dey and Raj Bahadur, The indigenous drugs of India, International Book Distributers, 1984.
- 5. Agnes Arber, Herbal plants and Drugs. Mangal Deep Publications. 1999.
- 6. WagnerH. and Wolff P., New Natural products and Plant drugs with Pharmacological, Biological(or) therapeutical activity. Springer, New Delhi. 1979.
- 7. SivarajanV.V. and Balachandran Indra, Ayurvedic drugs and their plant source. Oxford IBH publishing Co. 1994
- 8. Miller, Light and Miller, Bryan, Ayurveda and Aromatherapy. Banarsidass, Delhi. 1988.
- 9. Anne Green, Principles of Ayurveda. Thorsons, London. 2000.

## CORE XV : GENOMICS AND PROTEOMICS

Semester : IX Credits : 5 Course Code I17BI915 Total Hrs :75

#### General Objective

To understand the advanced level of genomes and their expressions from structure to functional level.

#### Unit I

Genome Sequencing: Sequencing genomes-methodology- chain termination method- chemical degradation methods- shotgun sequencing and assembly of contiguous DNA sequence-Gene Database-OMIM-dbGaP

#### Unit II

Genomic Mapping: Different types of genome maps and their uses- genetic and physical mapping techniques-Map resources -Practical uses of genome maps-Map Viewer- Genetic markers-RFLP - Miniand Micro satellite- STS and EST- RAPD- AFLP- SNPs. RFLP Database -uniSTS --dbEST -dbSNP-SNPSTR.

#### Unit III

Gene Expressions and Microarrays: Characteristics of human-genome sequence repeats- transposable elements- gene structure and pseudogenes- gene order- clustering of genes- composite genes-Differential gene expression- Analyzing gene expression—DNA microarray-design- analysisvisualization of data-Tools for microarray analysis- MADAM-Gene Expression Omnibus -spot finder-Applications of Microarrays.

#### Unit IV

2D Gel electrophoresis – protein digestion techniques –Mass spectrometry for protein and peptide analysis – protein identification by peptide mass finger printing – peptide sequence analysis by Tandem Mass Spectrometry – Protein identification with Tandem Mass Spectrometry.

#### Unit V

Protein-protein interaction mapping – experimental – yeast two hybrid system – surface Plasmon resonance biosensor analysis – Protein-protein interaction mapping – computation. Protein expression profiling – protein arrays and protein chip.

- 1. Brown TA. genomes, John Wiley & sons (Asia) Pvt. Ltd, Singapore, 2002.
- 2. Charles R. Cantor, Cassandra L. smith, genomics the science and technology behind the human genome project, John Wiley & SONS (Asia) Pvt. Ltd. Singapore, 1999.
- 3. Primrose and Twyman. principles of genome analysis. Blackwell publishing, Oxford. 2003.

- 4. Gibsona and Muse, A primer of genome science. Sinauer Associates Inc. publisher, Sunderlands, New York. 2003.
- 5. DovStekal ,Microarray Bioinformatics, Cambridge University Press, Cambridge. 2003.
- 6. Liebler, Introduction to Proteomics, Tools For new biology, Humana Press, New Jersey. 2001
- 7. Richard P. Simpson, proteins and proteomics. A Laboratory Manual. Cold Spring Harbor Laboratory Press, New York. 2004.
- 8. Reiner Westermeier, Tom Naven, proteomics in practice. Wiley-VCH, Weinheim.2002.
- 9. Permington S and MJ Dun, proteomics from protein sequence to Function. Bios. Scientific Pub.Ltd. Oxford. 2002.
- 10. Philip E. Bourne, Helge weissig., Structural Bioinfomatics. John wiley& Sons (Asia), Singapore. 2003.

## CORE XVI: ADVANCES IN STRUCTURAL BIOINFORMATICS

Semester : IX Credits : 5 Course Code I13BI916 Total Hrs :75

## General Objective

To comprehend the advanced level with molecular modelling, molecular dynamics simulation and molecular mechanics pertaining to drug discovery.

#### Unit I

Structural biology and structural databases:Nucleic acid structures- RNA folding- RNA loopsconformational study. Various ribose ring conformations- ribose-ring puckering. Protein-protein interactions- protein ligand interactions. DNA-binding proteins- RNA-binding proteins. Ramachandran plot- 3-dimensional structures of membrane proteins- importance of 310 helix and loops- biophysical aspects of proteins and nucleic acids. Structural databases: - Protein Data bank (PDB)- Nucleic Acid Data Bank (NDB)- Molecular modeling Data Bank (MMDB). Secondary structure- three-dimensional structure prediction- protein folding and functional sites- protein folding classes.

#### Unit II

Protein structure prediction:Protein Structure Prediction:- Homology modeling- prediction of protein structure from sequences- functional sites. Protein folding problem- protein folding classes- protein identification and characterization:-AACompldent- Tagldent- PepIdent and Multildent- PROSEARCH-PepSea- PepMAPPER- FindPept- Predicting transmembrane helices- Primary structure analysis and prediction- Secondary structure analysis and prediction- motifs- profiles- patterns and fingerprints search. Methods of sequence based protein prediction.

#### Unit III

Molecular Modeling :Molecular modeling:-Introduction- force field- quantum chemistry- Schrödinger equation- potential energy functions. Energy minimization- local and global minima- saddle point-gridsearch.Various approximations; LCAO- HF- semi-empirical calculations; single point calculations-full-geometry optimization methods- ZDO- MNDO- CNDO- NDDO- AM1- PM3- RM1.Conformational search-Z-matrix- docking- molecular modeling packages.

#### Unit IV

Molecular mechanics:-Definition- balls and springs- force fields- bond-stretching- bond-bendingdihedral motions- out of plane angle potential- non-bonded interaction. Derivative methods:- First-order methods; Steepest descent- conjugate gradient- Second order methods; Newton-Raphson method.

#### Unit V

Molecular dynamics: Molecular dynamics: -Introduction- Newton's equation of motion- equilibrium pointradial distribution function- pair correlation functions- MD methodology- periodic box- algorithm for time dependence; leapfrog algorithm- Verlet algorithm- Boltzman velocity- time steps- duration of the MD run. Starting structure- analysis of MD job- uses in drug designing- ligand protein interactions. **References** 

- 1. Phillip E. Brurne, HelgeWeissig, Structural Bioinformatics, A John Wiely& Sons Publications, 2011.
- 2. David M, Bioinformatics: Sequence and Genome analysis, Cold Spring Harbor Laboratory, 2004.
- 3. Rastogi RS, Bioinformatics: Concepts, Skills & Applications, Eastern Economy Edition 2008.
- 4. Thomas Hamelrcyck, Mardia KV, Bayesian methods in Structural Bioinformatics, Springer 2012.
- 5. Andrew Leach, Molecular modeling: Principles and Applications (2<sup>nd</sup> Edition), Addison Wesley Longman, Essex, England, 1996.
- 6. Frenkel D and Smith B, Understanding Molecular Simulations. From Algorithms to Applications, Academic Press, samdiego, California, 1996.
- 7. McCammon JA and Harvey SC. Dynamics of Proteins and Nucleic Acids. Cambridge University Press, Cambridge,1987.

## CORE XVII : PROGRAMMING IN PYTHON

Semester : IX Credits : 5 Course Code I17BI917 Total Hrs :75

#### General Objective

To know the fundamentals of programming techniques such as (a) Sequence of execution (b) Selection of blocks to be executed (c) Repetition of execution, with the help of Python programming language

#### Unit I

Introduction to Digital Computer – Von Neumann Concepts, Storage – Programming Languages, Translators – Hardware and Software, Operating Systems; Problem Solving Strategies – Problem Analysis, Algorithms, Flow Charts

#### Unit II

Introduction to Python – Python Comments, Identifiers, Keywords, Variables, Standard Data Types, Operators – Statement and Expression, String Operations, Boolean Expressions – Control Statements, Iteration-while Statement; Input from Keyboard

#### Unit III

Functions - Built-in Functions, Compositions of Functions, User Defined Functions – Parameters and Arguments, Function Calls, The return Statement – Recursive Function – Anonymous Functions – Strings - Lists

#### Unit IV

Tuples and Dictionaries – Files, Text Files, Directories – Exceptions, Exceptions with Arguments, User-Defined Exceptions

#### Unit V

Object-oriented Programming – OOP Overview – Class Definition, Creating Objects, Objects as Arguments, Objects as Return Values – Built-in Class Attributes, Inheritance, Method Overriding – Data Encapsulation – Data Hiding

#### Text Books

- 1. Balagurusamy, E, Introduction to Computing and Problem Solving using Python, Tata McGraw Hill Education Pvt Ltd, Ist Edition, 2016
- 2. Lutz Mark, Learning Python, O'Reilly, 5<sup>th</sup> Edition, 2015
- 3. Lutz Mark, Programming Python, O'Reilly, 4<sup>th</sup> Edition, 2013

#### Reference

1. McKinney Wes, Python for Data Analysis, O'Reilly, 1st Edition, 2013

## CORE PRAC XII : LABORATORY COURSE- ADVANCES IN STRUCTURAL BIOINFORMATICS LAB

Semester : IX Credits :3 Course Code I13BI9P8 Total Hrs :75

## **General Objectives**

To know the advanced modeling, docking and post-docking techniques to explore biological phenomena at the molecular level.

- 1. Genome annotation using GenSAS Genome Sequence Annotation Server
- 2. Viral ORF prediction using genome Viral Genome ORF Reader (VIGOR)
- 3. Conserved Domain prediction
- 4. Prediction of Expressed Sequence Tags
- 5. Model building of nucleic acid, protein and organic molecules using the ISIS draw.
- 6. Model building of organic molecules using the ChemSketch, CHEMDRAW.
- 7. Three dimensional structure prediction by using MODELLER.
- 8. Chemical structure retrieval from Zinc and NCI database.
- 9. Energy calculation of the biomolecules using molecular mechanics and quantum mechanics. (Argus lab).
- 10. Molecular Docking of protein and ligand by AUTODOCK, HEX.

## CORE PRAC XIII: PROGRAMMING IN PYTHON LAB

Semester : IX Credits :3 Course Code I17BI9P9 Total Hrs :75

## **General Objective**

To apply the basic programming concepts for solving real time problems with the help of Python.

- 1. Write a Python program to check largest among the given three numbers.
- 2. Write a Python program to check the input year is a leap year or not.
- 3. Write a Python program to print prime numbers for a user provided ranges.
- 4. Write a Python function to display Fibonacci sequence using recursion.
- 5. Write a Python function to display factors of the given numbers.
- 6. Write a Python function to find the sum of "n" natural numbers using recursion.
- 7. Write a Python program to find the duplicate characters in a given string.
- 8. Write a Python program to check whether the string is a palindrome or not.
- 9. Write a Python program to add two matrices.
- 10. Write a Python program to demonstrate string functions and operations.
- 11. Write a Python program for list functions and operations.
- 12. Write a Python program to print a tuple whose values are even numbers in the given tuple.
- 13. Write a Python program to catch a Divide-by-Zero exception.
- 14. Write a Python program to write data in a file for both write and append modes.
- 15. Write a Python program that defines the class name Employee, define any two sub-classes using Employee.
- 16. Write a Python program to demonstrate inheritance and method overriding.

#### **ELECTIVE VI : CHEMINFORMATICS**

Semester : IX Credits :4 Course Code I13BI9:1 Total Hrs :75

#### **General Objective**

To understand the different methods of cheminformatics with particular emphasis on applications including modern drug discovery

#### Unit I

Introduction to cheminformatics- Evolution of cheminformatics- History of chemical information science-Use of cheminformatics- Prospectus of cheminformatics- History of medicinal chemistry. Prodrugs and soft drugs- Drug targets- Drug solubility- Natural resources of lead compounds- Pharmacokinetics & drug metabolism. Biological testing and bioassays- Preclinical testing and clinical trial- Synthesis-Patenting and manufacture

#### Unit II

Modern Combinatorial Chemistry & Chemical Information Sources Combinatorial Chemistry Technologies & Libraries- Solution Phase Synthesis- High-Throughput Synthesis and Screening-Combinatorial Libraries- Analytical Methods- Biopanning- Peptide Display Libraries: design and Construction Chemical Literature- Chemical Information Searches- Chemical Information Sources-Chemical Name and Formula Searching.

#### Unit III

Cheminformatics: Database Design & their Management Chemical Database Design- Bio Catalysts Database- The MOS Database- The Failed Reaction Database-Protecting Groups Database- Solid-Phase Synthesis Database.

#### Unit IV

Introduction: - Natural product- Drugs; principles of drug Development. Bioinformatics in drug development- Chemoinformatics and Pharmacoinformatics. Applications of Drug Discovery and In-Silico Drug Designing-Area influencing drug discovery; Molecular Biology- pharmacogenomics and pharmacoproteomics.

#### Unit V

Drug Design and Discovery: Contour of Drugs- Development of New Drugs- chemical & physiochemical parameters in Drug design- Design of enzyme inhibitors- Drug metabolism- Structure Based drug Designing- Drug Discovery- computation techniques in drug design process.

- 1. And rew R. Leach, Valerie J. Gillet, An Introduction to Chemoinformatics 2008
- 2. Mannhold, Raimund, Chemoinformatics in Drug Discovery (Methods and Principles in Medicinal Chemistry)Wiley-VCH Verlag publication. 2007.
- 3. Johann Gasteiger, Thomas Engel, Chemoinformatics: A Textbook, 2005
- 4. Lisa B. English, Combinatorial Library Methods and Protocols Humana Press Inc, Volume:201, 2002.
- 5. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006.
- 6. Prasad R.K., Quantum chemistry , Halsted Press, 2002.

## ELECTIVE VI : BIODIVERSITY, BIOETHICS AND IPR

Semester : IX Credits :4 Course Code I13BI9:2 Total Hrs :75

#### **General Objective**

To understand the basics of Biodiversity and Bioethics to comprehend intellectual property rights

#### Unit I

Introduction to biodiversity – levels of biodiversity –values of biodiversity – loss of biodiversity – Species concept – Classification and systematics: biological nomenclature – biological classification; Biodiversity conservation: *in situ* and *ex situ* - Magnitude and distribution of biodiversity - wild life biology – conservation strategies – measures of biodiversity – biodiversity in India and global level – biodiversity hot spots.

#### Unit II

Introduction to ethics/bioethics – Framework for ethical decision making; biotechnology and ethics – biotechnology in agriculture and environment: benefits and risks – benefits and risks of genetic engineering – ethical aspects of genetic testing – ethical aspects relating to use of genetic information – genetic engineering and biowarfare.

#### Unit III

Ethical implications of cloning: Reproductive cloning , therapeutic cloning ; Ethical, legal and socioeconomic aspects of gene therapy, germ line, somatic, embryonic and adult stem cell research - GM crops and GMO's – biotechnology and biopiracy – ELSI of human genome project.

#### Unit IV

Introduction to biosafety – biosafety issues in biotechnology – risk assessment and risk management – safety protocols: risk groups – biosafety levels – biosafety guidelines and regulations (National and International) – operation of biosafety guidelines and regulations – types of biosafety containments.

#### Unit V

Introduction to intellectual property and intellectual property rights – types: patents, copy rights, trade marks, design rights, geographical indications – importance of IPR – patentable and non-patentable – patenting life – legal protection of biotechnological inventions – world intellectual property rights organization (WIPO).

- 1. Jose Cibelli, Robert P. lanza, Keith H. S. Campbell, Michael D.West, Principles of cloning, Academic Press, 2002.
- 2. Shaleesha AS.Bioethics,WisdomEducationalservicepublications,Chennai, IstEdition, 2008.
- 3. JeyakumarV, Professionalethics and Humanvalues, Anuradha Publications, Chennai, 2006.
- 4. Lewis Vaughn, Bioethics: Principles, Issues, and Cases, Oxford University Press, IstEdition, 2009.
- 5. Thomas A. Shannonand Nicholas J. Kockler, An Introduction to Bioethics, Paulist Pr, 4<sup>th</sup> Edition, 2009.

## CORE XVIII : PHARMACOINFORMATICS

Semester : X Credits :4 Course Code I17BIX18 Total Hrs :75

## **General Objective**

To know the techniques and tools that assist in providing solution for various infections and diseases.

#### Unit I

Introduction to pharmacogenomics- pharmacodynamics- pharmacokinetics- toxicokinetics and ADME properties- process of drug development-clinical trials phase I, II and III. Physiological drug distribution of protein binding: physiological factors- drug distribution- clinical pharmacodynamics- clinical pharmacokinetics and toxicokinetics.

#### Unit II

Drug concentration- nature of cell membrane- physiological factors related to drug absorption-drugs across cell membrane- route of drug administration- oral absorbtion and gastro intestinal tract absorption. Metabolic changes of drugs and related organic compounds: General pathways- sites of drug biotransformation- oxidative biotransformation- reductive reactions- hydrolytic reactions- conjugation reactions- factors affecting drug metabolism.

## Unit III

Factors affecting variability in drug response-drug metabolism-Ayugenomics (integration of Ayurveda & genomics)- genetic analysis of human variation-Microsatellite for studying genetic variation-Ayugenomics for human population. Microarray in herbal drug research- Pharmacodynamics-Pharmacogenomics and Pharmacognosy.

#### Unit IV

Analyzing databases for Metabolic Pathways (WIT- KEGG- PathDB- BIOCARTA- PathCase-PharmGKB). Metabolic and Cellular simulation: Gepasi- XPP- Virtual cell. Reconstruction of metabolic pathways (Biocyc- ASGARD).

#### UNITV

Pharmacogenomics in the treatment of cancer- neurodegenerative diseases- cardiovascular diseases. Pharmacogenomics in pharmaceutical industry- Ethical issues related to Pharmacogenomics-Pharmacogenomics and ethanopharmacology- Benefits of Pharmacogenomics.

- 1. Block J.H. and Beale Jr.J.M.. Organic medicinal and Pharmaceutical chemistry. Lippincott Williams and Wilkins, New York.2004
- 2. Patwaradhan.B.. Drug discovery and development. New India publishing agency, New Delhi.2007
- 3. ShargelL.and Yu.A.B.C. Applied Biopharmaceutics and Pharmacology. McGraw-Hill, New York.1999
- 4. BrownD.M.. Drug delivery systems in Cancer therapy. Humana press, Totowa, New Jersey.2004.
- 5. Rothstein, Pharmacogenomics: Social, ethical and clinical dimensions, Wiley Less. 2005
- 6. JinXiong. Essential Bioinformatics. Cambridge University Press. 2000

## ELECTIVE VII : ADVANCED APPLIED BIOINFORMATICS

Semester : X Credits :4 Course Code I17BIX:1 Total Hrs :75

#### General Objective

To understand and analyze the applications of Bioinformatics with focus to the broad scope of Bioinformatics in different fields.

Unit I

Profile analysis – Expression profile analysis of cells, Mining data from Yeast. Microarray and genome wide expression analysis: transcriptomes, proteome: Genomics in medicine, disease monitoring, profile for therapeutic molecular targeting.

#### Unit II

Reconstruction of pathways and annotation – Reconstructing metabolic pathways from sequence and function information in microbial species; statistical profiling and function annotation of genomes with a microbial genome as an example.

#### UNITIII

Drug Designing Related Applications – Finding new drug targets to treat diseases – Pharmacophore identification - Structure based drug design – Molecular Simulations.

#### Unit IV

Systems Biology - objectives of Systems Biology, Strategies relating to *In silico* Modeling of biological processes, Metabolic Networks, Signal Transduction Pathways, Gene Expression Patterns. E-cell and V-cell Simulations and Applications.

#### Unit V

Commercial Bioinformatics - Definition of Bioinformatics company. Genome Technology: high throughput sequencing and assembly. Diagnostic drug discovery and genomics. Pharmacogenomics and its application. SNPs and their applications. Proteomics in medicine, Toxicology.

- 1. Hunt S.P. and Livesey, F.J. Functional Genomics a practical approach, Oxford University Press, UK. 2000.
- 2. Wilkins, M.R., Wiliams, K.L., Appel, R.D. and Hochstrasser, D.F. "Proteome Research: New frontiers in Functional Genomics", Springer Verlag, New York, USA. 1997.
- 3. Witten, I.H. and Frank, E. "Data mining: Practical Machine Learning Tools and Techniques", Morgan Kauffman Publishers, USA. 2005.

# ELECTIVE VII : BIOINFORMATICS IN BIODIVERSITY, AGRICULTURE, MEDICINE AND ENVIRONMENT

Semester : X Credits:4 Course Code I17BIX:2 Total Hours :75

## **General Objectives**

To understand and analyze the applications of Bioinformatics with focus to the broad scope of Bioinformatics in the field of agriculture, medicine and environment.

#### Unit I

Diversity: Biodiversity Scope, Types, Values and Uses of Biodiversity, Loss of biodiversity, Biotechnology information: Management and Communication, Libraries, Bibliographies, Periodicals, Databases, Distribution of biodiversity information, Metadatabases, Virtual libraries, Special interest networks, Biodiversity Application Software – CD-ROMs and Diskettes.

#### Unit II

Agriculture: Crops: Comparative genomes of plant and model plants, Insect resistance, Improve nutritional quality, Grow drought resistant crops in poorer soils, Biodiversity of Indian medicinal plants.

#### Unit III

Medicine: Gene therapy - Fundamentals of gene therapy, Gene therapy present and future, clinical trials. Applications of Bioinformatics in cancer detection, Drug targets, Human genome diversity.

#### Unit IV

Environment: Waste cleanup: Superbugs and their concept, Microbes and Climate change, Alternative energy sources and Fuel cells. Biotechnological applications of microbes, Antibiotic resistance, Forensic analysis of microbes, the reality of bioweapon, Metagenomics.

#### Unit V

Synthetic Biology: Introduction, definition and Basics, Synthetic Oligonucleotide/DNA-based, RNAbased, Peptide-based and polyketide Technologies and Applications, Technologies and Applications of Directed Evolution and Microbial Engineering.

- 1. Lukas, K., Buehler, Hooman, H. Rashidi. Bioinformatics Basics: Applications in Biological Science and Medicine, CRC Press.2000.
- 2. Krishnamurthy, K.V. An advanced Textbook on Biodiversity principle and practice, Oxford & IBH publishing Co. Pvt. Ltd.2003.
- 3. FulekarM.H. Bioinformatics: Applications in Life and Environmental Sciences, Springer, 2009.
- 4. Pramod Tandon, Yash P Abrol and Suman Kumaria, Biodiversity and its Significance, I. K. International Publishing House Pvt. Ltd.2007.

## PG - Non Major Elective Course (NMEC) (For the candidates admitted from the year 2016 onwards) (Offered to Students of other Disciplines)

Sem.	Course	Code	Title	Hrs./ week	Credits	Marks		
						CIA	ESA	TOTAL
Ш	NMEC	116BI8E3	DATABASES AND SEQUENCE ANALYSIS	4	2	25	75	100

## NMEC-III DATABASES AND SEQUENCE ANALYSIS

Semester : II Credits : 2 Course Code I16BI8E3 Total Hrs :60

## **General Objective**

To understand the basic concepts and application of Bioinformatics databases and sequence analysis.

#### Unit I

Introduction to Bioinformatics, Biological Databases and Data formats, Nomenclature of nucleotides and amino acids, Application of Bioinformatics.

#### Unit II

Introduction to sequence alignment, PAM - BLOSUM, Local and Global alignment, Needleman-wunsch algorithm, Smith-waterman algorithm, Multiple sequence alignment, FASTA, BLAST.

#### Unit III

Evolutionary analysis, Cladistic, and Phenetic methods, Clustering methods, Rooted and Unrooted tree representation.

#### Unit IV

Gene finding methods, Gene prediction methods, Repeat sequence finder.

#### Unit V

Structure prediction methods: Chou-Fasman/GOR method, Neural Network, Threading and Fold recognition, Modeling.

#### **Text Books**

- 1. Attwood T.K and Parry Smith D.J, Introduction to Bioinformatics, Pearson Education Ltd., New Delhi, 2004.
- 2. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, NewDelhi ,2003.
- 3. Manju Bansal, Basic Bioinformatics, Atlantic publishers & distributors, 2009.

- 1. David. W. Mount: Bioinformatics Sequence and Genome Analysis, Cold spring Harbor Lab. NY.USA, 2001
- 2. BrownT.A,Genomes, Taylor and Francis Group.2001.