

**COURSES OF STUDIES**  
**I.M.SC.**  
**BIO-INFORMATICS**

**Admission Batch - 2023-24**



**Buxi Jagabandhu Bidyadhar Autonomous College**

**Bhubaneswar - 751014**

Accredited at the 'A' Level by

National Assessment and Accreditation Council (NAAC)

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## COURSE STRUCTURE

### FIRST YEAR, SEMESTER – I

Paper Code	Title of the Paper	Term End Marks	Internal Marks	Full Marks
101	Communicative English	80	20	100
102	(Introduction to Biology & Bioinformatics)	60	15	75
103	Practical P I (Introduction to Biology & Bioinformatics)	25	0	25
104	Chemistry	60	15	75
105	Practical (Chemistry)	25	0	25
<b>TOTAL</b>			<b>300</b>	

### FIRST YEAR, SEMESTER – II

Paper Code	Title of the Paper	Term End Marks	Internal Marks	Full Marks
201	Biochemistry & Molecular Biology	60	15	75
202	Practical (Biochemistry & Molecular Biology)	25	0	25
203	Chemistry	60	15	75
204	Practical (Chemistry)	25	0	25
205	Fundamentals of Bioinformatics-I	80	20	100
<b>TOTAL</b>			<b>300</b>	

### SECOND YEAR, SEMESTER – III

Paper Code	Title of the Paper	Term End Marks	Internal Marks	Full Marks
301	Mathematical & Statistical Foundation	60	15	75
302	Practical (Mathematical & Statistical Foundation )	25	0	25
303	Chemistry	60	15	75
304	Practical (Chemistry)	25	0	25
305	Fundamentals of Bioinformatics-II	80	20	100
<b>TOTAL</b>			<b>300</b>	

### SECOND YEAR, SEMESTER – IV

Paper Code	Title of the Paper	Term End Marks	Internal Marks	Full Marks
401	Microbiology & Immunology	60	15	75
402	Practical (Microbiology & Immunology)	25	0	25
403	Chemistry	60	15	75
404	Practical (Chemistry)	25	0	25
405	Environmental Studies	80	20	100
<b>TOTAL</b>			<b>300</b>	

### THIRD YEAR, SEMESTER – V

Paper Code	Title of the Paper	Term End Marks	Internal Marks	Full Marks
501	Genetic Engineering, Gene Sequencing & RDT	60	15	75
502	Bioinformatics Algorithm & programming	60	15	75
503	Practical Genetic Engineering, Gene Sequencing & RDT	50	0	50
504	Computational Techniques	80	20	100
<b>TOTAL</b>			<b>300</b>	

**THIRD YEAR, SEMESTER –VI**

<b>Paper Code</b>	<b>Title of the Paper</b>	<b>Term End Marks</b>	<b>Internal Marks</b>	<b>Full Marks</b>
601	Data Analysis & Molecular Modeling	60	0	60
602	Biomedical & Drug Designing	60	0	60
603	Practical Bioinformatics Algorithm & programming	40	0	40
604	Project	30	0	30
605	Seminar	10	0	10
606	I.S.C	80	20	100
		<b>TOTAL</b>	<b>300</b>	

**FOURTH YEAR, SEMESTER –VII**

<b>Paper Code</b>	<b>Title of the Paper</b>	<b>Term End Marks</b>	<b>Internal Marks</b>	<b>Full Marks</b>
701	Cell Biology & Genetics	80	20	100
702	Biochemistry of nucleic Acids & Proteins	80	20	100
703	Biophysics	80	20	100
704	Programming in C	80	20	100
705	Lab (Cell Biology, Biochemistry, C )	100	0	100
			<b>TOTAL</b>	<b>500</b>

**FOURTH YEAR, SEMESTER –VIII**

<b>Paper Code</b>	<b>Title of the Paper</b>	<b>Term End Marks</b>	<b>Internal Marks</b>	<b>Full Marks</b>
801	Molecular Biology & Genetic engineering	80	20	100
802	Comparative & Functional Genomics	80	20	100
803	Data Structure & Algorithms	80	20	100
804	Biological Database & Their Management	80	20	100
805	Practical-I on MB, GE, SMB, DSA	100	0	100
			<b>TOTAL</b>	<b>500</b>

**FIFTH YEAR, SEMESTER –IX**

<b>Paper Code</b>	<b>Title of the Paper</b>	<b>Term End Marks</b>	<b>Internal Marks</b>	<b>Full Marks</b>
901	Programming in PERL, C++ & Java	80	20	100
902	Computational Genomics,	80	20	100
903	Computational Proteomics	80	20	100
904	Molecular Evolution & Comparative Genomics	80	20	100
905	Lab on All Papers	100	0	100
			<b>TOTAL</b>	<b>500</b>

**FIFTH YEAR, SEMESTER –X**

<b>Paper Code</b>	<b>Title of the Paper</b>	<b>Term End Marks</b>	<b>Internal Marks</b>	<b>Full Marks</b>
1001	Advanced topics in Bioinformatics	80	20	100
1002	Neural Network and Genetic Algorithm	80	20	100
1003	Computer Aided Drug Design	80	20	100
1004	Project		0	100
1005	Presentation & Viva		0	100
			<b>TOTAL</b>	<b>500</b>

## DEPARTMENT OF IMSc. BIOINFORMATICS

### Programme Outcome:

To build in candidates a strong foundation in interdisciplinary sciences such as Computer Sciences and Biological Sciences, to develop accelerated and precise technologies for industrial problems, and prepare them for productive careers in fields of biotechnology, pharmaceutical, bioinformatics, Research, and healthcare industries

### Programme Specific Outcome:

Strengthening ongoing university research in the area of bioinformatics, in particular and life science in general. Further it will be helpful in creating an advanced research facility to carry out research in frontier areas of bioinformatics, biotechnology, and molecular modelling.

To address the challenges arising from the huge amount of genomic data and to overcome by analyzing and individualizing the corresponding drug responses towards appropriate drug specified dosages.

## IMSC BI 1<sup>st</sup> YEAR 1<sup>st</sup> SEMESTER

### AECC 1 - COMMUNICATIVE ENGLISH

CREDIT: 06

END SEMESTER: 80 MARKS

MID SEMESTER: 20 MARKS

#### UNIT- I

Communication in language: Communication: definition, types of communication and their process, Barriers to communication, its features, Writing skills - its features - how it differs from other language skills. How to put ideas together, identifying the logical development of ideas in piece writing

#### UNIT- II

Report writing-How to present facts clearly and logically. Standard formats for writing, writing paragraphs, Precis Writing, Preparation of abstract, technical documents.

#### UNIT- III

Reading skills – Reading to get main ideas, Reading to summarize, Reading to take and make notes. Meaning of Comprehension, Techniques of answering questions from unknown passages. Audio-visual aids for communication: Communicative/functional Grammar–Communicative use of structures, collocations

#### UNIT- IV

Speaking –Group discussion based on current topics. Group dynamics Paralinguistic communication-gestures, actions, body language Linguistic tools for better communication. Elementary Phonetics: Speech Sounds, consonance, vowels, stress and intonation.

#### TEXTBOOKS:

1. Technical communication by Raman and Sharma
  2. A Communicative Grammar of English By Geoffrey Leech and Jan Svartvik, Longman
  3. Oxford Guide to Writing and Speaking, OUP. By John Sealy
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4. Krishnaswamy, N. Modern English: A Book of Grammar Usage and Composition. Macmillan India Ltd, 2009. Print. (Module III & IV)
5. Murphy, Raymond. Essential English Grammar: A Self-Study Reference and Practice Book IMSC BI 1<sup>st</sup> YEAR 1<sup>st</sup> SEMESTER

## CORE PAPER - 1

### INTRODUCTION TO BASIC BIOLOGY & BIOINFORMATICS

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Basic Introduction to basic biology and their components used in research. The introduction of computers and computational biological systems.

#### Unit-I

Classification, Characteristics and Distribution of different groups of living Organisms. Introduction to genetics, Mendelian laws of inheritance, Sex determination, Chromosome – Structural and Numerical aberrations. Linkage, Crossing Over, Chromosomal Maps, Mutations, Chromosome and inheritance factors, Extra Chromosomal inheritance.

#### Unit-II

Molecular Basis of life, Structure of DNA & RNA, Prokaryotic and Eukaryotic replications of DNA. Protein & Amino Acid.

Protein synthesis Transcription initiation complex, Mitochondrial and Chloroplast RNA, Polymerases, Initiation and Transcription, Role of mRNA and tRNA in protein synthesis, Codon, Anticodon Interaction.

#### Unit-III

Ribosome structure, translation initiation in both Prokaryotes and Eukaryotes, Chain Elongation in Prokaryotes and Eukaryotes, Protein folding. Prokaryotic gene expression (lac, his, trp, catabolic repression), analysis and comparison between Prokaryotic and Eukaryotic 'Gene Expression'.

#### Unit- IV

Introduction to the Bioinformatics and its application in Basic Biology. Its Scope and opportunities. Genome analysis and sequencing, Mapping of Human Genome, Human Genome project, Future of Genome Research, its application and opportunities.

#### REFERENCE BOOKS:

1. Biology by Roberts
  2. Genetics by Gardner
  3. Molecular Biology by Robert. F. Weaver– McGraw Hill International Edition
  4. Text Book of Botany by A.C Dutta
  5. Text Book of Zoology by Vidyanthi
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## CORE 1 - PRACTICAL

CREDIT : 02

END SEMESTER : 25 MARKS

1. To study/verify Monohybrid Mendelion ratio dyChi-squareanalysis
2. Tostudy/verifyDihybridMendelion ratiobyChi-squareanalysis
3. Tostudy andidentifydifferentgroupsofhumanchromosomesbyKaryotypeanalysis
4. Qualitative analysisofProtein from different samples.
5. QualitativeanalysisofAminoacid.

## IMSC BI 1<sup>st</sup> YEAR 1<sup>st</sup> SEMESTER

### CORE PAPER - 2 FUNDAMENTALS OF COMPUTERS & THEIR APPLICATION IN LIFE SCIENCES

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Basic fundamentals of computers? Updating students about Basic skills used for programming?  
Includes Basic search engines used to biological research

#### 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 and output devices – CPU –memory – Software – Programming languages – Operating Systems - Number Systems – Decimal, Octal, Hexadecimal and Binary – Conversion to different number systems

#### 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 PROBLEM SOLVING AND OFFICE AUTOMATION

Planning the Computer Program – Purpose – Algorithm – Flow Charts – Pseudocode -Application Software Packages- Introduction to Office Packages – Word Processing, Spread Sheet, Presentations, Database (Basic Commands only)

#### UNIT -IV OPERATING SYSTEMS

Introduction to operating Systems - Windows Commands, UNIX / Linux - basic commands - General purpose, file handling, vi editor & environment. Internet resources for Life Sciences – Literature Databases - Biological Websites and Databases – NCBI – PubMed, Entrez – DNA sequence databases - Gen Bank, EMBL, DDBJ - Protein sequence databases - PIR, Swissprot, PDB.

#### BOOKS RECOMMENDED:

1. Peter Norton, Introduction to Computers 6th Edition, Tata McGraw-Hill Pub. Co.Ltd., New Delhi, 2006

2. Pradip Dey, Manas Ghosh, Computer Fundamentals and Programming in C, Oxford University Press, New Delhi, 2006.
3. Sumitabha Das, UNIX Concepts and Applications, 4th Edition, Tata McGraw-Hill, New Delhi, 2006.
4. Bioinformatics: Databases, Tools & Algorithms—Orpita Bosu and Simminder Kaur Thukral (Oxford Higher Education)

## CORE-2 PRACTICAL

CREDIT: 02

FULL MARKS: 25

1. Windows commands date, time, help, cls, echo, copy, del, dir, md, cd, rd, ren, more, path, sort, tree, dir, find, chkdsk, ver
2. Linux commands a) Working with the files and directories related commands date, who, man, cal, clear, echo, finger, cat, cp, ls, mv, rm, wc, chmod, pwd, mkdir, chdir, rmdir, ;. &&. b) Pipes and Filters sort, head, tail, grep, more, nl, cut, cmp, diff
3. Biological Databases: NCBI, UNIPROT, DDBJ, EMBL, PDB
4. Biological Search Engines: PubMed, Entrez
5. Sequence Retrieval Methods from NCBI, EMBL, PDB

# IMSC BI 1<sup>st</sup> YEAR 1<sup>st</sup> SEMESTER

## GENERAL ELECTIVE - 1

### CHEMISTRY

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Unit - I KINETIC THEORY OF GASES

Derivation of Kinetic equation, Deduction of gas laws, Avogadro's Hypothesis and law of diffusion of gases, gas constants, behaviour of real gases, Vander Wall's equation of state.

Colloids and Surface Chemistry: Types of colloids, methods of preparation, Dialysis, optical and electrical properties of colloids, Coagulation, peptisation. Absorption, Langmuir and Gibb's adsorption isotherm.

#### Unit - II ATOMIC STRUCTURE

Bohr's model of atom, Sommerfeld's modifications, wave nature of matter, deBroglie equation, Heisenberg's uncertainty principle, probability and orbital shapes, Quantum number, Aufbau's principle, Pauli's exclusion principle, Hund's rule, stability of half filled and fully filled orbitals.

#### Unit-III PERIODIC PROPERTIES & CHEMICAL BONDING

Atomic size, Atomic, Ionic and covalent radii, ionisation potential, electron affinity and electronegativity, Ionic bond, Lattice energy, Born-Haber Cycle, Fajan's rule, covalent bond, valence bond theory, its limitations. VSEPR theory, Hybridisation and shapes of simple molecules

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**Unit-IV DISTRIBUTION OF ELECTRONS IN ORGANIC COMPOUNDS**

Inductive effect, resonance, hyper-conjugation and steric effect. Conditions of resonance, planarity uncharged atomic skeleton, presence of electron donating and withdrawing groups. Influence of these effect on acidity, basicity and dipole moment. Carbocation, Carbanion structure and stability. Free radical. Carbenes, Nucleophile, electrophile and their reaction.

**GENERAL ELECTIVE 1: CHEMISTRY PRACTICAL**CREDIT: **02**END SEMESTER: **25** MARKS

1. Estimation of acetic acid in commercial vinegar using NaOH.
2. Determination of alkali content in Antacid tablets using HCL.
3. Estimation of Calcium content in chalk as calcium oxalate by permanganometry.
4. Estimation of hardness of water by EDTA.
5. Estimation of amount of  $\text{Na}_2\text{CO}_3$  and NaOH in a solution. IMSC BI 1<sup>st</sup> YEAR 2<sup>nd</sup> SEMESTER

**AECC - 2  
ENVIRONMENTAL SCIENCE**CREDIT: **06**END SEMESTER: **80** MARKSMID SEMESTER: **20** MARKS**Unit - I**

The Environment : The Atmosphere, Hydrosphere, Lithosphere, Biosphere, Ecology, Ecosystem, Biogeochemical Cycle (Carbon Cycle, Nitrogen Cycle), Environment Pollution : Air Pollution, Water Pollution, Soil Pollution, Radiation Pollution.

**Unit - II**

Population Ecology : Individuals, Species, Pollution, Community, Control Methods of Population, Urbanization and its effects on Society, Communicable Diseases and its Transmission, Non Communicable Diseases. Environment and human health, community health. Pollution and health, Occupation and health, Radiation and health, stress and health, Food and health

**Unit - III**

Bioremediation and Xenobiotics, Solid waste management, Industrial and urban waste management. Source, effect control measures. Role of individuals in preventing pollution, Disaster management, Environmental Movements in India : Grassroot Environmental movements in India, Role of women, Environmental Movements in Odisha, State Pollution Control Board, Central Pollution control Board.

**Unit - IV**

Natural Resources : Conservation of Natural Resources, Management and conservation of Wildlife, Soil Erosion and Conservation, Environmental Laws : Water Act, 1974, Air Act, 1981. The Wildlife (protection) Act, 1972, Environment Protection, 1986, Natural Disasters and their Management. Resettlement and Rehabilitation of people. Environmental education. Role of NGO' sin environmental protection

**RECOMMENDED BOOKS**

1. Environmental Biology and Toxicology – R.D. Sharma.
2. Fundamentals of Environmental Studies – S.N.Tripathy & S.Panda.
3. Environmental Economics – S. Sankaran
4. The Text Book of Environmental Studies– P.K Das, S.N.Gosh, D.K.Sarangi, S.P.Mohanty

**IMSC BI 1<sup>st</sup> YEAR 2<sup>nd</sup> SEMESTER****CORE PAPER – 3****BIOCHEMISTRY & MOLECULAR BIOLOGY**

CREDIT- 04

END SEMESTER THEORY: **60** MARKSMID SEMESTER THEORY: **15** MARKS**Course Outcome:**

Understanding the chemistry and reactivity of biomolecules? The research based on the Biochemical systems? The biology and research for the small biomolecules

**Unit–I**

Carbohydrates and lipids, their importance in cells. Proteins: Amino acids and peptides; primary, secondary, tertiary and quaternary structures; protein–protein interactions; sequence homology, functional and evolutionary relationships of proteins.

**Unit–II**

Nucleic acids: Bases, nucleotides, RNA and DNA. Different Structural from of DNA, denaturation and renaturation of DNA, protein-nucleicacid interactions.

**Unit–III**

Enzymes: Units of activity, coenzymes and metal cofactors, temperature and pH effects, Michaelis-Menten kinetics, active site and mechanism of enzyme action, isoenzymes, allosteric enzymes, Organization of metabolic systems: enzyme chains, multi enzyme complexes and multifunctional enzymes, regulatory enzymes and feedback control of metabolic pathways, energy charge.

**Unit–IV**

Carbohydrate metabolism: Glycolysis, gluconeogenesis, glycogenolysis and pentose phosphate pathway; hormonal control. TCA cycle and oxidative phosphorylation. Transamination and deamination of amino acids, urea cycle. Purine and pyrimidine biosynthesis.  $\beta$ -oxidation and biosynthesis of fatty acids

**Reference Books:**

1. Principles of Biochemistry–Lehninger
  2. Biochemistry–Satya Narayan
  3. Biochemistry–Stryer
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## CORE - 3 PRACTICAL

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. Qualitative Biochemical tests for carbohydrates-monosaccharides and polysaccharides.
2. Qualitative tests for lipids.
3. Estimation of catalase and peroxidase.
4. Preparation of standard curve of BSA by Biuret method.
5. Separation of amino acid by paper chromatography.
6. Viva-Voce

## IMSC BI 1st YEAR 2nd SEMESTER

### CORE PAPER - 4 PROGRAMMING IN C

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Basic programming language? Designed to update students with language and coding for biological systems

#### UNIT -I FUNDAMENTALS AND INPUT /OUTPUT STATEMENTS

History & Features of C – Character Set – Identifiers and Keywords – Data Types – Constants and Variables – Declaration of Variables and Constants – Symbolic Constants – Operators – arithmetic, unary, relational, logical, assignment and conditional operators – Hierarchy of operators – Input and output statements - character, string and formatted input and output

#### UNIT -II ARRAYS AND STRINGS

Arrays – one, two and multi-dimensional arrays – character arrays and strings comparison of strings – mathematical and string library functions – Control Statements – branching statements – if and switch statements – simple programs

#### UNIT -III CONTROL STATEMENTS

Control Statements – looping statements – while, do-while and for statements – goto statement – simple programs – sum of n natural numbers, sum of individual digits, ascending order, addition of matrices, alphabetical order, molecular weight and A+T & G+C content of DNA sequence

#### UNIT -IV FUNCTIONS

User Defined Functions in C – Defining and Accessing Functions – Passing Arguments – Function prototypes – scope and visibility of variables – simple programs – nPr, nCr, n!, swap two values. User defined data types in C – Structures – Declaring structures and Accessing members – Array of structures – Unions – Defining and Opening a File – Closing a File – Input/Output Operations on Files – simple programs

#### RECOMMENDED BOOKS:

1. S. Parthasarathy, Essentials of Programming in C for Life Sciences, Second Edition, Ane Books India, New Delhi, 2011.
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2. . E.Balagurusamy, Programming in ANSI C, Fourth Edition, Tata McGraw-Hill Publishing Company Limited, 2002.
3. Byron S. Gottfried, Schaum's Outline of Programming with C, McGraw-Hill Publications. 2006.

### CORE - 4 PRACTICAL

CREDIT- 04

END SEMESTER THEORY: 25 MARKS

1. a) Compute the relative centrifugal force using rmax (in cm) and rpm value  
b) Compute the rpm value using rmax (in cm) and RCF value  
c) Calculate sedimentation time (in hrs. & mins.) using clearing factor and sedimentation coefficient
2. a) Find the biggest of three given numbers using if-else statement  
b) Compute all possible roots of quadratic equation using if-else statement
3. a) Find the molecular weight of a given dephosphorylated oligonucleotide sequence  
b) Find the molecular weight of a given DNA sequence, after checking for phosphorylation
4. a) Find the sum of n natural numbers using while and for statements  
b) Compute the sum of n odd numbers using while statement  
c) Find the factorial of a given integer number using for statement
5. a) Compute the nature of the solution based on the pH value using switch –case statement  
b) Compute all possible roots of quadratic equation using switch – case statement

## IMSC BI 1<sup>st</sup> YEAR 2<sup>nd</sup> SEMESTER

### GENERAL ELECTIVE - 2 CHEMISTRY

CREDIT- 04

END SEMESTER THEORY: 60 MARKS  
MID SEMESTER THEORY: 15 MARKS

#### UNIT - I

**Homogeneous Equilibria** : Law of mass action, Le Chatelier's principle, their application to following systems.

- a) Manufacture of  $\text{NH}_3$  from  $\text{N}_2$  and  $\text{H}_2$
- b) Dissociation of  $\text{N}_2\text{O}_4$
- c) Dissociation of  $\text{PCl}_5$
- d) Hydrolysis of  $\text{CH}_3\text{COOC}_2\text{H}_5$

**Chemical Kinetics**: Order and molecularity of reaction, rate of zero order reaction, 1<sup>st</sup> and 2<sup>nd</sup> order reactions, Half life period, General methods for determining the order of reaction. Effects of extraneous conditions on reaction rates (Activated Complex).

#### UNIT - II

P-Block elements-Comparative study including diagonal relationship

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**Unit - III**

Aliphatic substitution reaction. SN<sup>1</sup> and SN<sup>2</sup> and SN<sup>i</sup> reaction: Kinetic, stereo chemical, structural environmental (solvent) aspects, Neighboring group Participation reaction with simple examples. SE, E<sup>1</sup>, E<sup>2</sup> (full term explanation with examples)

**Unit - IV**

StereoChemistry

**Conformational isomerism** : Concept of confirmation in ethane, n-Butane, Sawhorse, Newman and Fisher projection formula of molecule containing single bond, conformation of cyclohexane – axial and equatorial bonds, boat and chair conformation and their energies. Optical isomerism, concept of mirror image, enantiomers and dia-stereo-mers, D,L.notation, R.S.notations with chiral centre. Geometrical Isomerism.

**RECOMMENDED BOOKS:**

1. Organic Chemistry : Mukherjee, Singh & Kapoor
2. Organic Chemistry : Bhal & Bhal
3. Inorganic Chemistry : Puri & Sharma
4. Physical Chemistry : S.Glastone
5. Physical Chemistry : Puri, Sharma and Pathania

**GENERAL ELECTIVE – 2 PRACTICAL CHEMISTRY**

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. Mixture Analysis: Mixture Containing 4 radical (insoluble saltsexcluded) (Interfering radicals and Phosphate separation included)

**IMSC BI 2<sup>nd</sup> YEAR 3<sup>rd</sup> SEMESTER****SKILL ENHANCEMENT COURSE (SEC – I)  
CHEMOINFORMATICS**

CREDIT- 04

END SEMESTER THEORY: 80 MARKS

MID SEMESTER THEORY: 20 MARKS

**UNIT - I**

Introduction to cheminformatics, Evolution of cheminformatics, History of chemical information science, Use of cheminformatics, Prospectus of cheminformatics, History of medicinal chemistry. Role of Computers in Chemicals structures, SMILES, QSAR in Chemoinformatics.

**UNIT – II**

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, Complexes and chelating agents, Molecular modeling using computer.

**UNIT – III**

Combinatorial chemistry technologies & libraries. Solution phase synthesis, High-throughput synthesis and screening. Combinatorial libraries, Analytical methods, Biopanning. Peptide display

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libraries:- Design and construction, Chemical literature, Chemical information searches, Chemical information sources, Chemical name and formula searching, Analytical chemistry (Constitutional Chemistry), Chemical history, Biography, Directories, and industry sources.

#### UNIT – IV

Chemical Database Design. Bio Catalysts Database, The MOS Database, The Failed Reaction Database, Protecting Groups Database, Solid-Phase Synthesis Database Database concepts, structured query language, Design of chemical database, data abstraction, bio Catalysts Database, Reaction database, Failed reaction Database, Sequence Database, Spectra Database, Toxicology Database

#### RECOMMENDED BOOKS:

1. An Introduction to Chemoinformatics by Andrew R Leach, V J Gillet
2. Tutorials in Chemoinformatics by Alexandre Varnek (Editor)
3. Practical Chemoinformatics by Muthukumarasamy Karthikeyan, Renu Vyas IMSC BI 2<sup>nd</sup> YEAR 3<sup>rd</sup> SEMESTER

### CORE -5

## MATHEMATICAL & STATISTICAL FOUNDATION IN BIOINFORMATICS

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Application of biostatistical approaches in big data analysis? Use of statistical formulas in evaluating NGS and derive regressional analysis between the molecular calculations.

#### Unit - I

Sets:- Finite set, infinite set, null or void set, subset, Intervals; closed and open, universal set, operations of set. Relations and functions,

Matrices:-Types of matrices, properties of matrices, addition, subtraction of matrices, matrix, Multiplication, transpose and inverse and rank of matrices, solution of linear equations

#### Unit - II

Derivatives: Laws of derivatives of function, differential of all types of function, Function logarithmic, Exponential, Trigonometric, implicit and explicit functions.

#### Unitl - II

Counting principles, permutation & combination, binomial theorem, probability independent events, concept of expectation. Idea of population and sample, moment's skewness and kurtosis, concepts of random variable, Univariate distributions: Binomial, Poisson and Normal distribution. Their means and variances. Area under Normal curves.

#### Unitl - V

Basic principles of probability theory, Bayes theorem Normal distribution, statistical inference – Types of errors and levels of significance. Comparison of variance (F-test), small sample test, t-test for comparison of means, chi square test.

#### RECOMMENDED BOOKS:

1. Topics in Mathematics by G.Das and others.
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2. Theory of Matrices by B.S.Vatssa.
3. Statistical Methods and Concepts by M.N.Das (Wiley Eastern LTD.)
4. Statistical Methods by S.P. Gupta.

## CORE- 5 PRACTICAL

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. Calculation of different measures of central tendency, dispersion, skewness and kurtosis.
2. Calculation of Null Hypothesis using Chi Square Test, F Test and T test.
3. Fitting of 1<sup>st</sup>, 2<sup>nd</sup> degree polynomials and exponential curves.
4. Calculation of simple correlation and regression lines, rank correlation.

## IMSC BI 2<sup>nd</sup> YEAR 3<sup>rd</sup> SEMESTER

### CORE - 6

### COMPUTATIONAL BIOLOGY

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Computational Analysis of Biological Systems? Enables students to handle biological databases, tools and servers used at research

#### UNIT - I SEQUENCE ALIGNMENT ALGORITHMS

Definition of Sequence alignment – Local and Global alignment concepts – Methods for sequence alignment: Dot matrix – Scoring matrices: PAM and BLOSUM matrices, Dynamic programming – Needleman and Wunsch algorithm, Smith-Waterman algorithm–FASTA and BLAST programs – Statistics of alignment score – P value and E value.

#### UNIT - II MULTIPLE SEQUENCE ALIGNMENT

Multiple sequence alignment (MSA) – Methods of Multiple Sequence Alignment: Progressive alignment – Clustal W, T-Coffee, Iterative Method – DIALIGN – Blocks, patterns and Profiles.

#### UNIT - III PHYLOGENETIC ANALYSIS

**Phylogenetic tree:** Rooted and Unrooted – Methods for phylogenetic tree construction: Character (NJ) and Distance based methods (MP and ML) – Tree evaluation (Bootstrap)– lineage sorting, orthology, paralogy, xenology; “basal” lineages– crown vs. stem groups– Phylogram vs. cladogram.

#### UNIT - IV PROTEIN SECONDARY STRUCTURE PREDICTION

Protein Secondary structure prediction – Chou-Fasman , GOR methods (SOPMA) and Neural network concepts – Nearest Neighbour method – Transmembrane structure prediction. Online Analysis tools – PSIPRED and J-Pred

#### RECOMMENDED BOOKS:

1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi 2003.
  2. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001.
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3. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ (1998).
4. Rastogi, S. C., Mendiratta, N., & Rastogi, P. (2013). Bioinformatics: Methods And Applications: (Genomics, Proteomics and Drug Discovery). PHI Learning Pvt. Ltd

## CORE 6 PRACTICAL

CREDIT: **02**

END SEMESTER THEORY: **25** MARKS

1. To perform the dot matrix analysis using Dot matcher.
2. Analyze the sequence similarity of given sequence using BLAST tool.
3. To find the conserved /consensus region in the given sequence using MEME/Interpro.
4. To compute the primary feature of protein sequence using PROTPARAM
5. To perform the prediction of gene location for a given sequence using GENSCAN.
6. To perform phylogenetic analysis using MEGA.
7. To predict the Secondary structure by SOPMA

## IMSC BI 2<sup>nd</sup> YEAR 3<sup>rd</sup> SEMESTER

### CORE -7

#### OBJECT ORIENTED PROGRAMMING USING C++

CREDIT- **04**

END SEMESTER THEORY: **60** MARKS

MID SEMESTER THEORY: **15** MARKS

#### Course Outcome:

Advancement in Programming language? Application of programming languages in solving biological problems

#### UNIT- I PRINCIPLES OF OBJECT ORIENTED PROGRAMMING

Object Oriented Programming (OOP) – Introduction – Basic concepts – Classes, Objects, Data abstraction and encapsulation – Inheritance – Polymorphism – Dynamic Binding and Message Passing – Object oriented Languages – Applications.

#### UNIT- II INTRODUCTION TO C++

Introduction to C++ – History – Applications – Procedure-Oriented Programming – Object Oriented Programming versus Procedure-Oriented Programming – Structure of C++ Program. Tokens, expressions, keywords, Identifiers, constants, Operators, Data types – Standard input and output statements – Use of << and >> operators – Declaration of variables

#### UNIT - III CONTROL STATEMENTS & FUNCTIONS

Branching statements – if and switch statements– looping statements – while, do-while and for statements – goto statement – sample programs – Functions, Function prototype – Inline Functions – Default arguments – Function overloading – Sample Programs.

#### UNIT -IV CLASSES AND OBJECTS

Creating a class – Defining member functions – Creating objects – Accessing class member – Arrays within a class – Arrays of objects – Friend function – Local classes – Sample Programs.

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**RECOMMENDED BOOKS:**

1. E. Balaguruswamy, Object Oriented Programming with C++, 4th Edition, Tata McGraw Hill Publications, New Delhi, 2017.
2. Robert Lafore, Object Oriented Programming in C++, 4th Edition, Galgotia Publications, New Delhi, 2017.

**PRACTICAL CORE -7**

CREDIT- 02

END SEMESTER PRACTICAL: 25 MARKS

1. C++ Program to compute a DNA string
2. C++ program to compute the molecular weight of Macromolecules
3. C++ program to identify whether the string is DNA/RNA/ Aminoacids
4. C++ program to Reverse the given integer number and store it in a variable using do-while statement
5. C++ program to Compute the sum of individual digits up to a single digit of a given number
6. Reverse a given string of Sequence
7. Checking for palindrome of a given string of sequence
8. Program to identify a various promoter sequence in given sequence

**IMSC BI 2<sup>nd</sup> YEAR 3<sup>rd</sup> SEMESTER****GENERAL ELECTIVE -3  
CHEMISTRY**

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

**Unit-I Colligative Properties**

Osmotic pressure. Law of osmotic pressure, relative lowering of vapour pressure, lowering of freezing point and elevation of boiling point; Determination of molecular weight by these methods, Anomalous molecular weight of solutes due to dissociation and association.

**Unit-II Thermodynamics**

Thermo Chemistry Extensive and intensive properties of the system, state of a system, first law of thermo dynamics, enthalpy of chemical reaction Laws simple calculation based on them, spontaneous and non-spontaneous processes. Second Law of thermo dynamics: concept of free energy, entropy and thermodynamics criteria of equilibrium, effect of temperature and pressure on equilibrium, relation between equilibrium constant and free energy.

**Unit-III Chemistry of elements of first transition series**

Characteristic properties of d-block elements, properties of elements of 1<sup>st</sup> row transition series, relative stability of their oxidation states, coordination number and geometry. Coordination Compounds: Werner's coordination theory, nomenclature, isomerism in complexes.

**Unit-I-V**

Preparation properties and structure of diborane, boric acid, Borazenes, Silicones compounds.

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Organometallic Compounds, Grignard's reagent, preparation from alkyl bromide (principle only), synthetic uses (as carbonion precursor). Nomenclature, preparation from dihalides, Dieckmann's reaction and stability Bayer's strain theory.

**REFERENCE BOOKS:**

1. Physical Chemistry : Bhal & Tuli
2. Physical Chemistry : J.D. Lee
3. In-Organic Chemistry : Part-I–R.L. Dutta
4. Organic Chemistry : R.K. Bansal

**GENERAL ELECTIVE - 3 PRACTICAL CHEMISTRY**CREDIT: **02**END SEMESTER : **25** MARKS

1. Estimation of Ferrous and Ferric by dichromate method.
2. Estimation of copper using thiosulphate.
3. Estimation of Cu as CuSCN. (Gravimetry)
4. Estimation of Ni as Ni(DMG)<sub>2</sub> (Gravimetry)
5. Determination of specific reaction rate of hydrolysis of ester by titration method.
6. To study the distribution of I<sub>2</sub> between Water and CCl<sub>4</sub> OR Benzoic acid and between Benzene and Water.

**IMSC BI 2<sup>nd</sup> YEAR 4<sup>th</sup> SEMESTER****SKILL ENHANCEMENT COURSE (SEC -2)****IMMUNOINFORMATICS**CREDIT- **04**END SEMESTER THEORY: **80** MARKS  
MID SEMESTER THEORY: **20** MARKS**UNIT - I**

Innate and Adaptive Immunity: Cell types and processes involved, Anatomical and Physiological Barriers, Inflammation, Soluble molecules and Toll-like receptors, Innate Immune response and their recognition structures, Humoral and Cell mediated responses of immune system. Cells of Immune system: Lymphocytes, Mononuclear phagocytes, Antigen Presenting cells, polymorphs, Natural Killer cells, Granulocytes, Mast cells, Dendritic cells, Cluster designation (CD) and antigen specific receptors

**UNIT II**

IMGT & IEDB, BciPep, Epitome, CED, Ag-Ab database, Allergen Databases, Allergenicity Prediction. Major Histocompatibility Complex: Structure and functions of MHC class I and II, MHC polymorphism, MHC supertypes, MHC peptides Specificity, characterization, MHC peptide designing tool. HLA: nomenclature, HLA-peptide interactions, Antigen Processing in the MHC Class I Pathway, Processing of MHC Class II Epitopes, Sequential and Conformational Epitopes, Epitope Prediction algorithms - T cell, B cell epitope prediction tool.

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**UNIT III**

Rational vaccine design, Reverse vaccinology, Prediction of immunogenicity - Pipeline & workflows, Toxoid as vaccine, Conjugate vaccine, DNA vaccine, Recombinant vector vaccines, Personalised vaccination. Structure-based Vaccine design - tools and techniques, Antigenicity modification, Epitope replacement, germline targeting, Epitope focussing, hyperglycosylation, chimeric fusion, epitope scaffold, Conformational stabilization, multimeric scaffolding, stabilizing mutations, Antigen display and delivery platforms - multivalent display, co-display, immunomodulation, Genetic delivery

**UNIT IV**

Malignant transformation of cells, Oncogenes and cancer induction, Tumors of immune system, Tumor antigens, Tumor evasion of the immune system, Cancer immuno therapy. Secondary immuno deficiency in Immuno logical abnormalities associated with HIV infection, Discrete Models of HIV Infection, Simulation of HIV-1 Infection. Emerging and Re-emerging Infectious Diseases – Pathogens with antigenic variation, Modifying and Improving Biological Therapeutics, Computational Immunology

**RECOMMENDED BOOKS:**

1. Thomas J. Kindt , Barbara A. Osborne , Richard A. Goldsby , “ Kuby Immunology”, WH Freeman, Sixth Edition, 2006.
2. Rammensee, “Immuno informatics - Bioinformatics Strategies for better understanding of Immune Function”, Wiley, 2003.
3. Computational Immunology: Models and Tools by Josep Bassaganya-Riera

**IMSC BI 2<sup>nd</sup> YEAR 4<sup>th</sup> SEMESTER****CORE PAPER- 8****MICROBIOLOGY AND IMMUNOLOGY**

CREDIT- 04

END SEMESTER THEORY: **60** MARKSMID SEMESTER THEORY: **15** MARKS**Course Outcome:**

Understanding microbial research and metagenomics study ? Immunology and role of immune systems and immune molecules at human and medical research ? Structure of Immune systems and Immunoinformatics

**Unit - I**

**Viruses:** Morphology, Architecture, Nomenclature, Classification and symmetry, Structure of atypical plant (TMV), Animal (polio) and Bacterial (T4) Viruses; Bacteriophages (Lytic & lysogenic cycles). Bacteria: General idea about Arche bacteria, Eubacteria and Cyano bacteria, Structure of a typical bacterial cell, Bacterial recombination (transduction, transformation and conjugation)

**Unit - II**

Role of micro organisms in biogeochemical cycles of Nitrogen and Carbon. Biological nitrogenfixation with special reference to Rhizobium. Industrial application of micro organisms: Organic acids, alcohol, food processing, milk, anti biotics with reference to Streptomyces, biopesticides. Methods in Microbiology – staining, sterilization method culturemedia, pure culture methods, methods for population estimation, growth determination.

**Unit - III**

Immunology: Immunity, Immune system in Human: Active and Passive Immunity, Antigens, Antibodies, Classes of Immunoglobulins, Antigen – Antibody reaction, B-cells and T-cells and their role in immunity to infection, Major Histocompatibility Complexes (MHC)

**Unit - IV**

Immunity to infectious agents; Auto immunity. AIDS and other immuno deficiencies, Vaccines, Hybridoma Technology and Monoclonal antibodies, Gene Therapy.

**Reference Books :**

1. Microbiology by Pelczar, Chan & Krieg–Tata McGrawHill.
2. Textbook of Microbiology by Ananthanarayanan & Paniker
3. Microbiology– 7<sup>th</sup> edition (Prescott, Harley, Klein) by Willey, Sherwood, Woolverton.
4. Immunology by Nandini Shetty

**CORE – 8 PRACTICAL**

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. Sterilization and preparation of culture media.
2. Culture of bacteria from water and soil.
3. Identification and observation of bacteria by Gramstaining.
4. Preparation of Alcohol by Fermentation.
5. Determination of bacteria sensitivity to antibiotics.
6. Determination of Blood groups.

**IMSC BI 2<sup>nd</sup> YEAR 4<sup>th</sup> SEMESTER****CORE PAPER- 9****GENETIC ENGINEERING & GENOME SEQUENCING**

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

**Course Outcome:**

To understand role of biotechnology in Biological research and deriving the relationship with its computational studies ? Preparing pipelines to drive in the computational calculations in biological approaches and to understand the Genomics/Proteomics in it.

**Unit-I**

DNA as genetic material, Structure and Biological importance of DNA; Types of RNA and their structure; Replication of DNA. Genetic code, Central Dogma, Transcription, Translation, RNA editing, DNA repair

**Unit-II**

**Introduction:** Plasmids, pBR 322, PUC 9 bacteriophages: Cosmids, M13, Shuttle vectors and lambda of *E. coli*, Applications of genetic engineering in medicine, industry and agriculture.

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**Unit-III**

Enzymes for RDT: polymerase, restriction endo nucleases, ligases, Introduction of DNA in to living cells– Transformation and Transfection, Identification of recombinants.

**Unit-IV**

Techniques in Genetic Engineering: PCR, Gene Sequencing – Maxam Gilbert method & Sanger method, Electrophoresis, Southern and northern blotting techniques. Transgenic plants and animals, Gene therapy, Intellectual Property Rights, Bioethics.

**REFERENCE BOOKS**

1. Gene Cloning & DNA Analysis: An Introduction (T.A. Brown, Blackwell).
2. Principles of Gene Manipulation: An Introduction to Genetic Engineering (R.W. Old, & S.B. Primrose, Blackwell).
3. Molecular Biology, Genetic Engineering and Applications of Biotechnology (B.D. Singh, Kalyani Publishers)

**CORE PAPER- 9 PRACTICAL****CREDIT- 02****END SEMESTER THEORY: 25 MARKS**

1. Isolations of genomic DNA
2. Separation of Genomic DNA using electrophoresis
3. Local Alignment using SMITH WATERMANN Algorithm
4. Global Alignment using NEEDLEMANNWUNSCH Algorithm
5. Phylogenetic Tree Construction using UPGMA Method
6. Gene Prediction Tools

**IMSC BI 2<sup>nd</sup> YEAR 4<sup>th</sup> SEMESTER****CORE PAPER- 10****BIOINFORMATICS ALGORITHM AND PROGRAMMING****CREDIT- 04****END SEMESTER THEORY: 60 MARKS****MID SEMESTER THEORY: 15 MARKS****Course Outcome:**

Bioinformatics Algorithm & Programming ? Computational algorithmic studies to calculate various fields like sequence alignment, Force field calculations, simulations etc

**Unit-I Pairwise Sequence Alignment**

Similarity and Homology, Optimal Alignment, Global Alignment, Local Alignment, Similarity Search, Alignment Scoring Scheme, Hamming Distance, Unit Cost, Edit Operation, Similarity vs Distance, Gaps & Insertions, Gap Penalty, Gap Cost, Scoring Matrix, log odds Matrices, Substitution Matrices, Dot Plots, Identity Blocks, Dynamic Programming, Blossum Substitution Searching Matrix, PAM Matrices.

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## Unit-II Multiple Sequence Alignment

Local vs Global Multiple Alignment, Applications of Multiple Sequence Alignment, Mathematical Definition of Multiple Sequence Alignment, Multiple Sequence Alignment tools, Open Reading Frame (ORF), Gene Recognition, Machine Learning & Artificial Neural Networks, Hidden Markov Models.

## Unit-III Phylogenetics

Categories of Data, Evolutionary Models, Homology, Gene Trees Versus Species Trees, How to read a phylogenetic Tree, Components of tree, Methods for Tree Building, Character Based Method, Distance Methods, Bootstrap Values.

## Unit-IV Protein Structure

Nucleic Acids, DNA Structure, RNA Structure, Coding, Central Dogma, Protein Structure, Amino acid properties and Substitution, Levels of Protein Structure, Denaturation and Renaturation, Protein Secondary Structure Prediction Algorithms, Protein Database, Visualization Tools.

### RECOMMENDED BOOKS:

1. A Text Book of Bio-informatics-Singhal and Singhal (Pragati Prakashan)
2. Bioinformatics: Databases, Tools & Algorithms–Orpita Bosu and Simminder Kaur Thukral (Oxford Higher Education)
3. Biological Sequence analysis-David Mount

## CORE 10 PRACTICAL

CREDIT: 02

END SEMESTER: 25 MARKS

- (a) Use of CLUSTALW for Multiple Sequence Alignment tools.
- (b) Use of PYMOL & RASMOL Tool for Protein Prediction
- (c) Implementation of Protein Secondary Structure Prediction Tools & Algorithm
- (d) Phylogenetics Tree Construction using MEGA and PHYLIP
- (e) PHYRE Protein Structure prediction

## GENERAL ELECTIVE- 04

### CHEMISTRY

CREDIT- 04

END SEMESTER THEORY: 60 MARK

MID SEMESTER THEORY: 15 MARK

#### UNIT- I Electro Chemistry

Specific, Equivalent and molar conductance Kohlrausch's law of independent mobility of ions, variation of conductance with concentration for strong and weak electrolytes, application of conductance measurement, determination of solubility product, degree of dissociation of weak electrolytes, degree of hydrolysis of salts, conductometric titrations, Acids and Bases, Bronsted Lowry and Lewis concept of Acids and Bases.

#### UNIT- II Nuclear Chemistry

Binding energy, mass defect, Nuclear reactions induced by  ${}^1_1\text{H}$ ,  ${}^1_0\text{n}$ ,  ${}^2_1\text{D}$ ,  ${}^4_2\text{He}$  Nuclear Fission, Bohr's liquid drop model, fusion reaction, chain reaction, Nuclear reactor, **Zero group elements:**

Chemical properties of noble gases. Chemistry of Xenon, Structure and bonding in Xenon compounds

### UNIT- III Ester Chemistry

Esters containing active methylene group (Acetoacetic ester: Synthesis Claisen condensation) synthetic uses (alkane, ketone, acid,  $\alpha$ ,  $\beta$  unsaturated acid, structure of acetoacetic ester, keto-enol tautomerism. Malonic ester: Preparation and synthetic uses (alkane, ketone, acid).

### UNIT - IV Aromatic Compounds:

Aromaticity and anti aromaticity, Huckel's Rule and its application, electrophilic substitution reaction in aromatic compounds (Nitration, sulphonation, halogenation, Friedel – Crafts alkylation and acylation).

Phenols: Synthesis, Physical properties, Acidic character of phenols, Chemical reaction (Kolbe's reaction, Reimer-Tiemann reaction)

### RECOMMENDED BOOKS:

1. Physical Chemistry : Bhal & Tuli
2. Physical Chemistry : J.D. Lee
3. In-Organic Chemistry : Part-I–R.L. Dutta
4. Organic Chemistry : R.K. Bansal

## PRACTICAL GENERAL ELECTIVE- 04

CREDIT- 04

END SEMESTER THEORY: 25 MARK

1. Organic compound Identification
  - (a) Element determination (N,S, Halogen)
  - (b) Functional groups of CHO and CHN groups
  - (c) MP/BP determination of the organic compound.

## IMSC BI 3<sup>rd</sup> YEAR 5<sup>th</sup> SEMESTER

### CORE PAPER -11

### STRUCTURAL BIOINFORMATICS

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

### Course Outcome:

It is based on structural studies and prediction of computational models for Proteins and other small biomolecules ? Structural evaluation studies for those structures which are not reported yet through experimental approaches

### UNIT – I

No. of Hours: 10 1.1. Nucleic acid structures, RNA folding, RNA loops, conformational study. 1.2. Protein-protein interactions, protein ligand interactions. DNA-binding proteins, RNA binding

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proteins. 1.3. Ramachandran plot, Structural databases:- Protein Data bank (PDB), Nucleic Acid Data Bank (NDB), Molecular modeling Data Bank (MMDB). 1.4. Protein identification and characterization:- AAComplident, TagIdent, PepIdent and Multident, PROSEARCH, PepSea, PepMAPPER, FindPept.

#### UNIT – II

Molecular modeling:-Introduction, force field, quantum chemistry, Schrödinger equation, potential energy functions. various approximations; LCAO, HF, semi-empirical calculations; single point calculations, geometry optimization methods, ZDO, MNDO, CNDO, NDDO, AM1, PM3, RM1. Molecular mechanics:-Definition, balls and springs, force fields, bond-stretching, bond-bending, dihedral motions, out of plane angle potential, non-bonded interaction, coulomb interactions, conformational search, united atoms and cut-offs.

#### UNIT – III

Antibacterial antibiotics; narrow spectrum and broad spectrum antibiotics. Recent advances in pharmaceutical Biotechnology: synthetic vaccines, DNA vaccines, edible vaccines. Policies in drug designing:- Quality assurance: ISO, WHO, certification, Good manufacturing practices, GMP, GLP, Government regulations, Chemo informatics and Pharmaco informatics. Applications of Drug Discovery and In-Silico Drug Designing, Area influencing drug discovery, pharmaco genomics and pharmaco proteomics.

#### UNIT – IV

Introduction, Structure-based drug designing approaches: - Target Identification and Validation, homology modeling and protein folding, receptor mapping, active site analysis and pharmacophore mapping, Grid maps.

### CORE PAPER -11 PRACTICAL

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. Chemical Structure development using Chems sketch / Chemdraw
  2. Various file format .mol, .mmdb, .pdb and their application
  3. Structure Visualization tool (Pymol/ Rasmol)
  4. Structure Validation Tool
  5. Active Site /Conformational Search in proteins Structure
  6. Secondary Structure prediction of Proteins
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# IMSC BI 3<sup>rd</sup> YEAR 5<sup>th</sup> SEMESTER

## CORE PAPER -12 GENOMICS & PROTEOMICS

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

### Course Outcome:

Understanding the genome and proteome involved in research ? The genomic and proteomic analysis helps out to understand the biological ways to enhance research.

### Unit-I

Introduction to Genomics, DNA sequencing methods manual & automated: Maxam & Gilbert and Sangers method. Pyrosequencing, Genome Sequencing: Shotgun & Hierarchical (clone contig) methods, Computer tools for sequencing projects: Genome sequence assembly software.

### Unit-II

Managing and Distributing Genome Data: Web based servers and softwares for genome analysis: ENSEMBL, VISTA, UCSC Genome Browser, NCBI genome. Selected Model Organisms' Genomes and Databases.

### Unit-III

Introduction to protein structure, Chemical properties of proteins. Physical interactions that determine the property of proteins. Short-range interactions, electrostatic forces, van der waal interactions, hydrogen bonds, Hydrophobic interactions. Determination of sizes (Sedimentation analysis, gel filtration, SDS-PAGE); Native PAGE, Determination of covalent structures Edman degradation.

### Unit-IV

Introduction to Proteomics, Analysis of proteomes. 2D-PAGE. Sample preparation, solubilisation, reduction, resolution. Reproducibility of 2D-PAGE. Mass spectrometry based methods for protein identification. De novo sequencing using mass spectrometric data.

### RECOMMENDED BOOKS:

1. Charles Malkoff, 2016. Exploring Genomics, Proteomics and Bioinformatics, Syrawood Publishing House.
2. A.Malcolm Campbell Discovering Genomics, Proteomics and Bioinformatics, Pearson Education India; 2 edition
3. Dunham, I., 2003. Genome Mapping and sequencing. Horizon Scientific.
4. Graur, D and W H Li, 2000. Fundamentals of molecular evolution. Sinauer Associates.

## CORE 12 PRACTICAL

Credit : 02

END SEMESTER: 25 Marks

1. Use of SNP databases at NCBI and other sites
  2. Detection of Open Reading Frames using ORF Finder
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3. Proteomics 2D PAGE database
4. Software for Protein localization.
5. Native PAGE 6. SDS-PAGE

## IMSC BI 3<sup>rd</sup> YEAR 5<sup>th</sup> SEMESTER

### DISCIPLINE SPECIFIC ELECTIVE (DSE-1)

### BIOTECHNIQUES

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

#### Course Outcome:

Understanding the use of various experimental equipment and their principles in biological evaluations. To upgrade the approaches made in evaluation of experimental calculations.

#### Unit-I

Simple microscopy, phase contrast microscopy, fluorescence and electron microscopy (TEM and SEM), pH meter, absorption and emission spectroscopy

#### Unit-II

Principle and law of absorption fluorimetry, colorimetry, spectrophotometry (visible, UV, infrared), centrifugation, cell fractionation techniques, isolation of sub-cellular organelles and particles.

#### Unit-III

Introduction to the principle of chromatography. Paper chromatography, thin layer chromatography, column chromatography: silica and gel filtration, affinity and ion exchange chromatography, gas chromatography, HPLC.

#### Unit-IV

Introduction to electrophoresis, polyacrylamide gel (native and SDS-PAGE), agarose-gel electrophoresis, immuno- electrophoresis, isoelectric focusing, Western blotting. Introduction to Biosensors and Nanotechnology and their applications.

#### RECOMMENDED BOOKS:

1. Principle and Techniques of Biochemistry and Molecular biology, 7th ed By Keith Wilson and Jhon Walker, Cambridge Press
  2. Rodney Boyer, Modern Experimental Biochemistry, Pearson Education; 3 Edition.
  3. Molecular Cloning: A Laboratory Manual (3rd Edition) Sambrook and Russell Vol. I to III,
  4. Becker, W.M., Kleinsmith, L.J., Hardin. J. and Bertoni, G. P. 2009 The World of the Cell.7th edition. Pearson Benjamin Cummings Publishing, San Francisco.
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## DSE 1 PRACTICAL

Credit : **02**END SEMESTER- **25** Marks

1. Native gel electrophoresis of proteins
2. Determination of absorption maxima of given chemicals.
3. SDS-polyacrylamide slab gel electrophoresis of proteins under reducing conditions.
4. Separation of amino acids by paper chromatography.
6. To verify the validity of Beers law and determine the molar extinction coefficient of NADH.

## IMSC BI 3<sup>rd</sup> YEAR 5<sup>th</sup> SEMESTER

### DISCIPLINE SPECIFIC ELECTIVE (DSE-2) PHARMACOGENOMICS

CREDIT- **04**END SEMESTER THEORY: **60** MARKSMID SEMESTER THEORY: **15** MARKS

#### Course Outcome:

To enhance and to understand the role of bioinformatics in Pharmaceutical research? To understand areas like drug discovery, patent filing, clinical trials on medicines.

#### UNIT-I GENERAL PHARMACOLOGY

Theories and mechanism of drug action, Pharmacokinetic principles and parameters, Factors modifying drug action- Pharmacogenetics- Chronopharmacology- Adverse effects of drugs. Drug dependence-Toxicology-Dose response relationships- Structure-activity relationships. Physiological and biochemical basis of drug action-Etiopathogenesis of diseases relevant to therapeutic use of drugs.

#### UNIT-II SYSTEMIC PHARMACOLOGY, CHEMOTHERAPY AND THERAPEUTICS

Pharmacology of drugs acting on autonomic, peripheral and central nervous systems; cardiovascular, endocrine, respiratory, renal, gastrointestinal and haemopoietic systems, treatment of diseases affecting these systems-Pharmacology of anti-microbial and anti-parasitic drugs and treatment of infective diseases- Cancer chemotherapy, immunopharmacology-Gene therapy and evidence based medicine.

#### UNIT-III BIOCHEMICAL PHARMACOLOGY

Preparing standard operative practice for Bioavailability and bioequivalence studies. Introduction to simple analytical methods-Basic principles and applications-Quantitative estimation using Colorimetry and Spectrophotometry, flame photometry, HPLC and ELISA. Toxicological Studies using chemical and biological tests-Identifying toxic drugs using chemical and biological tests (alkaloids, glycosides, steroids, barbiturates, salicylates).

#### UNIT-IV CLINICAL PHARMACOLOGY

Development of new drugs, protocol designing, phases, methodology and ethics of clinical trials, clinical pharmacokinetics and pharmacodynamic studies, post marketing surveillance, therapeutic drug monitoring, pharmacovigilance, ADR monitoring, Drug information service, drug utilization

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studies, therapeutic audit, essential drug concept and rational prescribing, GLP and GMP - Recent advances in understanding of mechanism of drug action and treatment of diseases; new drugs and new uses of old drugs.

#### RECOMMENDED BOOKS:

1. Rang H. P., Dale M. M., Ritter J. M., Flower R. J., Rang and Dale's Pharmacology, Churchill Livingstone Elsevier
2. Katzung B. G., Masters S. B., Trevor A. J., Basic and clinical pharmacology, Tata Mc GrawHill
3. Goodman and Gilman's, The Pharmacological Basis of Therapeutics
4. Ghosh MN. Fundamentals of Experimental Pharmacology. Hilton & Company, Kolkata.
5. Kulkarni SK. Handbook of experimental pharmacology. VallabhPrakashan,

### DSE 2 PRACTICAL

Credit : **02**

END SEMESTER- **25** Marks

1. Native gel electrophoresis of proteins
2. Determination of absorption maxima of given chemicals.
3. SDS-polyacrylamide slab gel electrophoresis of proteins under reducing conditions.
4. Separation of amino acids by paper chromatography.
5. To identify lipids in a given sample by TLC.
6. To verify the validity of Beers law and determine the molar extinction coefficient of NADH.

## IMSC BI 3<sup>rd</sup> YEAR 6<sup>th</sup> SEMESTER

### CORE 13

### DATA ANALYSIS & MOLECULAR MODELING

CREDIT- **04**

END SEMESTER THEORY: **60** MARKS  
MID SEMESTER THEORY: **15** MARKS

#### Course Outcome:

It enables the data analysis in biological systems. Understanding the omics study and its importance in research in today's world. Modelling of biomolecules those which are not experimentally proven. Force field and simulation calculations for predicted computational models

#### Unit-I

Sequence Databases : Nucleotide Sequence Databases, Secondary Nucleotide Sequence Databases, Protein Sequence Databases, Secondary & Specialized Protein Sequence Databases, Information Retrieval System: Entrez, Information Retrieval System: SRS. Structure Databases: Structure File Formats, Protein Structure Database Collaboration, PDB, MMDB, CATH, FSSP, DALI, SCOP.

#### Unit-II

Data Submission Tools: Nucleotide Sequence Submission Tools, Protein Submission Tools, BLASTn, tBLASTn Data Analysis Tools: Tools for Nucleotide Sequence Analysis, Tools for Protein Sequence Analysis.

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**Unit-III**

Prediction Tools: Phylogenetic Trees and Phylogenetic Analysis, Gene Prediction, Protein Structure & Function Prediction. Modelling Tools: Tools for 2D Protein Modelling, Tools for 3D Protein Modelling.

**Unit-IV**

Molecular Modeling, Quantum Mechanical and molecular orbital methods- Introduction to semi-empirical-Molecular mechanics and ab- initio techniques-Docking and Modeling substrate receptor Interactions. Software tools for modeling bio- molecules – Protein conformations- protein folding and mutational Analysis through comparative modeling

**.RECOMMENDED BOOKS**

1. Bioinformatics: Databases, Tools & Algorithms—Orpita Bosu and Simminder Kaur Thukral (Oxford Higher Education)
2. A Text Book of Bio-informatics -Singhal and Singhal (Pragati Prakashan) Molecular Modelling and drug Design (Leech)
3. Text book of Drug Design and Discovery (Edited by Povl Krosggaard–Larsen, Tommy Liljefors and Ulf Madsen) Taylor Francis Publication.
4. Molecular Modeling for Beginners: Alan Hinchliffe

**CORE 13 PRACTICAL**CREDIT : **02**END SEMESTER: **25** MARKS

1. To perform the consensus secondary structure prediction for a given protein sequence at NPS@ by selecting six different methods
2. To identify the fold for a given protein sequence using 3-D PSSM fold recognition server
3. To find the structural neighbours of a given protein (2TRX) according to SCOP, CATH, FSSP and CE. To find out if any particular structure is identified by all these classifications.
4. Protein structure prediction and validation
  - a. Primary feature computing by PROTPARAM
  - b. 3D structure by PSI-BLAST tool,
5. SWISS-MODEL and SAVS server (MODELER software)

**IMSC BI 3<sup>rd</sup> YEAR 6<sup>th</sup> SEMESTER****CORE 14****BIOMEDICAL DRUG DESIGNING**CREDIT- **04**END SEMESTER THEORY: **60** MARKSMID SEMESTER THEORY: **15** MARKS**Course Outcome:**

Practical advancement in drug delivery and discovery and its impact on human health? This study helps in understanding the human diseases and the drug reaction systems and helps out in designing more prone reactive compounds for betterment of human health and lead in drug discovery

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**Unit-I**

Introduction to Drug Design; Principles of Drug Discovery system-Strategies for Drug design and stages in drug development, Lead generation and lead optimization, Structure based Drug Design,

**Unit-II**

Docking and different methodologies of Docking, Docking Principles and types, Docking Softwares, Free Energy perturbation method. Analogue based drug Design: Structure Alignment, Molecular Descriptors, Molecular field descriptors, Methods of regression, Genetic algorithm, Validation

**Unit-III**

Introduction, Structure-based drug designing approaches: - Target Identification and Validation, homology modeling and protein folding, receptor mapping, active site analysis and pharmacophore mapping, Grid maps.

**Unit-IV**

Pharmacophore pattern- Pharmacophore identification, Pharmacokinetics-Structure based drug design-ADME properties-Quantitative Structure Activity relationships-QSAR equations, CADD. High Throughput Screening (HTS), QSAR, Database generation and Chemical libraries,

**RECOMMENDED BOOKS:**

1. Text Book of Drug Design and Discovery (Edited by Povl Krosgaard-Larsen, Tommy Liljefors and Ulf Madsen) Taylor and Francis Publication.
2. Bioinformatics basic methods and applications-S.C. Rastogi
3. Principles of Drug discovery, Badhe P
4. Drug Discovery & Clinical Research 2nd Edition 2019 by GUPTA SK, Jaypee

**PRACTICAL CORE 14****CREDIT- 02****END SEMESTER THEORY: 25 MARKS**

1. Data mining for retrieval chemical information from PUBCHEM and Ligand databases
  2. Retrieving pharmacological information from Pharma base and MSDchem database
  3. Prediction of binding affinity of ligand by protein-ligand interaction/ReLiBase database tools
  4. Ligand design and analysis by ISIS Chem Draw/ Chem Sketch, VMD and TSAR software
  5. Protein-protein interaction prediction by Hex
  6. Protein-ligand interaction prediction by Argus Lab & Autodock
  7. Paper Studies related to Drug Discovery processes.
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# IMSC BI 3<sup>rd</sup> YEAR 6<sup>th</sup> SEMESTER

## DISCIPLINE SPECIFIC ELECTIVE- 3

### BIOINFORMATICS PROGRAMMING in PERL

CREDIT- 04

END SEMESTER THEORY: 60 MARKS

MID SEMESTER THEORY: 15 MARKS

**Course Outcome:**

Scripting language helps out to develop interfaces for software, database and tool development? Helps in practical designing of web tools and servers based on the experimental data

**UNIT- I**

INTRODUCTION TO PERL Introduction to Perl - scalars, Arrays and Hashes - Perl Interpreter – Operators - Using standard Perl modules – CPAN – Array-Based Character Manipulation - simple programs. A Program to store DNA sequence, Concatenating DNA fragment, Transcription: DNA to RNA, Subroutines, scoping and subroutines, command-line arguments and arrays passing data to subroutines, modules and libraries of subroutines, fixing bugs

**UNIT -II**

CONTROL STRUCTURES IN PERL SUBROUTINES Perl debugger - Perl control structures-if, elsif, else, unless, while, do-while, until, do-until, for and foreach - Perl subroutines and Functions - simple programs. File handling - Input/Output operator - open() and close() commands –

**UNIT -III**

PERL REGULAR EXPRESSIONS AND PATTERNS Translating DNA into proteins reading DNA from files in FASTA format, reading frames, Regular expressions, restriction maps and restriction enzymes, Genbank files, Genbank libraries, separating sequence and annotation parsing, Annotations indexing, parsing PDB files, parsing BLAST files.

**Unit -IV**

Random number generators a program using randomization, a program to simulate DNA Mutation, generating random DNA, analyzing DNA, Hashes, data structures and algorithms for biology, the genetic code, Introduction to BioPERL Modules – BioSeq, BioSeqIO, BioPrimarySeq, BioSearch, BioDB

**RECOMMENDED BOOKS:**

1. Sumitabha Das, UNIX Concepts and Applications, 4th Edition, Tata McGraw-Hill, New Delhi, 2006. 2. Chan Bernard Ki Hong, Perl 5 Tutorial, First Edition, 2003.
2. James Tisdall, Beginning Perl for Bioinformatics, O'Reilly, 2001.
3. D. Curtis Jamison, Perl Programming for Biologists, John Wiley & Sons, INC., 2003.
4. Michael Moorhouse, Paul Barry, Bioinformatics Biocomputing and Perl, Wiley, 2004.

**PRACTICAL FOR BIO-PERL (DSE- 3)**

CREDIT- 02

END SEMESTER THEORY: 25 MARKS

1. PERL Variable, Commands and Operations
  2. Program for Translation of DNA Sequence to Protein sequence
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3. Retrieval of Sequence from Nucleotide databases.
4. Program for indexing sequence annotations
5. Program to Gen bank Libraries.

## **DISCIPLINE SPECIFIC ELECTIVE- 4**

### **PROJECT REPORT & SEMINAR**

CREDIT- **06**

END SEMESTER: **100** MARKS

Project Report: 60 marks, Seminar: 20 marks, Viva: 20 marks & Total: 100 Marks

#### **Course Outcome:**

Practical application and formation of small individual projects helps out student to understand the use of softwares and tools to evaluate biomolecules.

1. Bioinformatics Tools and Softwares
2. Homology Modelling
3. Computational Programming in Biology
4. Docking
5. Protein Threading
6. Phylogenetic study & Evolutionary Relationships

