Annexure No.	**45 C**
SCAA Dated	**29.02.2008**

BHARATHIAR UNIVERSITY, COIMBATORE-641 046

PG DIPLOPMA IN BIOINFORMATICS

(Affiliated Colleges and University Dept.)

(with effect from 2007-2008)

Semester	Code	Subject and Paper	Exam Duration	Total marks *
I	07BIPGDT1	Paper-I : Fundamentals of Biological Systems	3	75
	07BIPGDT2	Paper-II : Computational methods for Sequence analysis.	3	75
	07BIPGDT3	Paper-III : Molecular interactions	3	75
	07BIPGDT4	Paper –IV : Systems biology	3	75
	07BIPGDP1	Practical-I : Biological Databanks and Sequence analysis *	3	100
II	07BIPGDT5	Paper-V : Programming for Bioinformatics	3	75
	07BIPGDT6	Paper-VI : Genomics	3	75
	07BIPGDT7	Paper- VII : Proteomics	3	75
	07BIPGDT8	Paper-VIII : Molecular modeling & Computer aided drug design	3	75
	07BIPGDP2	Practical-II : Computer aided Drug design*	3	100

∗ Includes 25% continuous internal assessment marks.

Practical examinations to be conducted at the end of the academic year.

07BIPGDT1 **SEM I**

FUNDEMENTALS OF BIOLOGICAL SYSTEMS

Subject description : Some basic aspects of Molecular Biology and Genetics that are relevant to the course are included in this paper.

Goals: To understand the basic structure of cell, mechanism and regulation of biological processes fundamental to genome structure and biochemistry.

Objectives: Students completing this paper should be able to understand molecular biology concept that are basic to bioinformatics.

Unit I :
Biology of cells: Cells as a unit of life, structure of prokayotic and eukaryotic cells. An overview of organells (Mitochondria, chloroplasts, ER, Golgi, ribosomes, lysosomes and peroxysomes, nucleus and nucleolus). Differences and similarities in plant and animal cells. Cellular membrane: structure, transport, channels, carriers, receptors, endocytosis, membrane potentials.

Unit II:
DNA replication; Transcription and Translation.
Cell-cell interactions and signal transductions: Intercellular junctions, signaling by hormones and neurotransmitters; receptors, G-proteins, protein kinases and second messangers.Protein traffic in cells.

Unit III:
Cell Cycle and regulation – Mitosis, Meiosis.
Mutation – Types of mutations, types of mutagenic agents and their molecular mechanism; DNA repair; Chromosomal types and structure; Mechanism by which genome undergoes changes, recombination, mutation, inversion, duplication, and transposition.

UNIT-IV
Molecules of Life: Introduction to carbohydrates-Monosacharides and their derivatives, Disacharides, Polysacharides.

Proteins –Structure of aminoacids, Different levels of organization-Primary, secondary tertiary and Quarternary structures.

Nucleic acids – Purines, pyrimidines, Nucleosides and Nucleotides, Different structural form of DNA, denaturation and renaturation of DNA

Lipids-Structure and function of Fatty acids, Triacylglycerols, sphingolipids, steroids and glycerophospholipids.

Water, small molecules-Alkaloids, glycosides, phenols, oligopeptides, Flavonoids, and terpenoids

UNIT-V

Enzymes: Units of Activity,coenzymes and metal cofactors, temperature and pH effects, Michaelis – Menten kinetics, inhibitors and activators, active site and mechanism of enzyme action, Isoenzymes, allosteric enzymes.
Metabolism of glucose: glycolysis, TCA cycle, glycogenesis, glycogenolysis and gluconeogenesis, pentophosphate shunt, ETC. Digestion of protein and protein metabolism, nitrogen balance: transamination, oxidative deamination and urea cycle. Lipid metabolism: beta oxidation. Interconnection of pathways, metabolic regulations.

REFERENCES:

1. Lehninger, A. L. 1984. **Principles of Biochemistry.** CBS publishers and distributors, New Delhi, India
2. Horton, Moran, Ochs, Rawn, Scrimgeour **Principles of Biochemistry** Prentice Hall Publishers.
3. David. E. Sadava **Cell Biology: Organelle Structure and Feunction** Jones & Bartlett publishers.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.

07BIPGDT2 **SEM I**

COMPUTATIONAL METHODS FOR SEQUENCE ANALYSIS

Subject description :This paper describes how to acquire information from biological databases, use of computational approaches to analyze this information, and interpret the results as a guide to experiments in biology.

Goals: The goal of this course is to introduce the main principles of bioinformatics. The coverage will include concepts like sequence alignments, phylogenetic trees, and structure prediction.

Objectives: Understand Genomic data acquisition and analysis, comparative and predictive analysis of DNA and protein sequence, Phylogenetic inference etc

UNIT-I

Introduction to bioinformatics, Classification of biological databases, Biological data formats, Application of bioinformatics in various fields. Introduction to single letter code of aminoacids, symbols used in nucleotides, data retrieval- Entrez and SRS.

UNIT-II

Introduction to Sequence alignment. Substitution matrices, Scoring matrices – PAM and BLOSUM. Local and Global alignment concepts, Dot plot. Dynamic programming methodology: Needleman and Wunsch algorithm. Smith–Waterman algorithm. Statistics

of alignment score. Multiple sequence alignment. Progressive alignment. Database search for similar sequences using FASTA and BLAST Programs.

UNIT-III

Evolutionary analysis: distances, Cladistic and Phenetic methods. Clustering Methods. Rooted and unrooted tree representation. Bootstrapping strategies, Use of Clustal and PHYLIP.

UNIT-IV

Gene finding methods. Gene prediction: Analysis and prediction of regulatory regions. Fragment assembly. Genome sequence assembly, Restriction Mapping, Repeat Sequence finder.

UNIT-V

Concepts of secondary structure prediction of RNA and Protein. Probabilistic models: Markov chain, Hidden Markov Models-other applications.

REFERENCES

1. **Bioinformatics – Concepts, Skills, Applications".** S.C. Rastogi, Namita Mendiratta, Parag Rastogi.
2. **Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins.** Andréa's D. Baxevanis, B.F. Francis Ouellette.
3. **Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids.** Richard Durbin et al.
4. **Computer Methods for Macromolecular Sequence Analysis**. Doolittle R.F. (Ed.) (Methods in Enzymology, VOl. 266).
5. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
6. **DNA and Protein Sequence Analysis. A Practical approach.** Bishop M.J. Rawlings C.J. (Eds.).
7. **Introduction to Bioinformatics.** Teresa. K. Atwood and David J. Parry-Smith.

07BIPGDT3 **SEM I**

MOLECULAR INTERACTIONS

Subject description : This paper deals with some of the basic features in molecular interactions.

Goals: To make the students familiar with chemical bonding and interaction between the molecules.

Objectives: Students should be able to interpret the interaction between molecules.

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; σ-bonds and π-bonds.

UNIT-II

Fundamentals of chemical bonding and non-bonding interactions:

Electrovalent bond, stability of electrovalent bond. Co- valent bond – partial ionic character of co-valent 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, 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, Metalloproteins, Pi … Pi interactions, C-H…Pi interactions.**

UNIT-V

Spectroscopy: **Principles, Theory, Instrumentation and Application of UV, IR, NMR and Circular dichroism (CD) to macro molecules.**

REFERENCES:

1. Albert cotton, F. 1971. **Chemical Application of Group Theory**. John Wiley and Sons, Inc. New York. 386 pp.
2. Spice, J. E. 1964. **Chemical Bonding and Structure**. Pergamon Press Ltd., Headington Hill Hall, Oxford. 395 pp.
3. Winter, m. j. 1996. **Chemical Bonding**. Oxford University Press, Inc., New York. 91 pp.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.

07BIPGDT4 **SEM I**

SYSTEMS BIOLOGY

Subject description : Includes the basics of analysing metabolic pathways using bioinformatics tools and also the simulation of cellular environment.

Goals: To understand the gradual maturation of genomics and proteomics into biology insilico. Convergence of genomics, proteomics, transcriptomics and metabolomics in to phenomics.

Objectives: Students should be able to understand the interaction within biological networks and simulation of cells.

UNIT – I

Introduction to Systems biology What is Systems Biology? Integrating Networks. Methods of study: Micro array – definition, types of array, Micro array analysis: Hierarchical clustering, Self-organizing maps. Applications of Micro Arrays in systems biology.

UNIT – II

Metabolomics & Metabolic Pathways

Digestion of proteins and protein metabolism, Transport metabolism, Carbohydrate metabolism – metabolism of glucose – glycolysis, TCA cycle, glycogenesis, Pentose phosphate shunt, Electron transport, Interconnection of pathways, metabolic regulation. Translating biochemical networks into linear algebra.

UNIT – III

Whole cell simulation: Principle and levels of simulation - Virtual Erythrocytes, Pathological analysis. Flux Balance Analysis

UNIT IV

Relationship analysis: Predicting ligand-binding function, Use of gene cluster, detecting protein – protein interaction.

UNIT – V

Creative Bioinformatics: Novel use for database. Use of EST database – Unigene, gene discovery, Primer design, Restriction mapping, Position specific cloning, SNP database, Target identification, Epitope identification.

REFERENCES

1. **Bioinformatics A Practical Guide to the Analysis of Genes and Proteins**. Ed. Andreas D. Baxevanis and B. F. Francis Ouellette. John Wiley & Sons, Inc., Publications (For Micro array).
2. **Nanofabrication towards Biomedical applications**. Ed. Challa S. S. R. Kumar, Joseph Hornes, Carola Leuschner. Wiley-VCH Verlag GmbH & Co.
3. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
4. Shanmughavel, P. 2006. **Trends in Bioinformatics,** Pointer Publishers, Jaipur, India.
5. **The underlying pathway structure of biochemical reaction networks.** Christopher H. Schilling *et. al*. 1998. PNAS. **95**:4193-8
6. **Towards metabolic phenomics: Analysis of Genomics Data Using Flux Balances**. Christopher H. Schilling *et. al*. 1999. *Biotechnology. Prog.* **15**: 288-295.
7. **The Minimal Gene Complement of *Mycoplasma genitalium.*** Claire M. Fraser *et. al*. 1995. *Science*, **270**: 397- 403.

8. **Molecular Classification of Cancer: Class Discovery and Class prediction by Gene Expression Monitoring.** Golub TR. *et. al*. 1999. . *Science,* **286**: 531 – 537.
9. **The *Escherichia coli* MG. 1655 *in silico* metabolic genotype: its definition, characteristics and capabilities.** Jeremy S. Edwards et. al. 2000. PNAS. **97**:5528-33.
10. **Whole cell simulation: a grand challenge of the 21st Century.** Masaru Tomita, 2001. *Trends in Biotechnology.* **19**: 205-210
11. **Cluster Analysis and Display of Genome – wide expression patterns.** Michael B.Eisen *et. al*. 1998, *Proc. Natl. Acad. Sci. USA.* **95**: 14863 – 14868.
12. **A general definition of metabolic pathways useful for systematic organization and analysis of complex metabolic networks.** Stephen Schuster *et. al*. 1999. *Nature Biotechnology*. **18**: 326-332.
13. **Of micro array and meandering data points.** Steven R. Gullans, 2000. . *Nature Genomics*. **26**: 4-5.
14. **A gene expression database for the molecular pharmacology of cancer.** Uwe Scherf *et. al*. 2000. *Nature genetics,* **24**: 236-244
15. **The transcriptional program in the response of Human Fibroblast to Serum** Viswanth R. Iyer 1999. *Science.* **283**: 83-87.

07BIPGDP1 **SEM I**

PRACTICAL – I - BIOLOGICAL DATABANKS AND SEQUENCE ANALYSIS

- Biological Databanks Sequence Databases, Structure Databases, Specialized Databases
- Data retrieval tools and methods
- Database file formats
- Molecular visualization
- Gene structure and function prediction (using GenScan, GeneMark)
- Sequence similarity searching (NCBI BLAST)
- Protein sequence analysis (ExPASy proteomics tools)
- Multiple sequence alignment (Clustal)
- Molecular phylogeny (PHYLIP)
- Analysis of protein and nucleic acids sequences,
- Sequence analysis using EMBOSS or GCG Wisconsin Package

REFERENCE:

Bioinformatics a Practical Approach by K. Mani and N. Vijayaraj, Aparna Publications, Coimbatore.

07BIPGDT5 **SEM II**

PROGRAMMING FOR BIOINFORMATICS

Subject description : This subject presents the fundamentals of programming techniques, namely sequence of execution, Selection of blocks to be executed, repetition of execution etc with the help of C programming language.

Goals: To make the students to learn problem solving, execution of programs, thinking the problems in procedure manner and apply the concepts

Objectives: On successful completion of the course the students should have:
Understood basic of approaching a problem to be computerized
Learnt the various techniques of writing codes to be executed.

UNIT-I:
Programming in C
Introduction, Data types, Operators, Expressions, Control Flow, Structures, Input and Output, Functions, Pointers and References, String Processing, File Handling

UNIT-II
Programming in C++
Basic concepts of OOPS-Introduction to C++,C vs C++-data types, variables, constants, operators and statements in c++- Functions in c++- function prototype-definition-inline functions-overloaded functions.

UNIT- III
Programming in PERL
Introduction, Basic Operators and Control Structures, Scalars, Lists, Hashes, File Manipulation, Pattern Matching and Regular Expressions, Subroutines, Text and String Processing

UNIT-IV
Python Programming
Overview, Data structures, Control Flow, Modules, Basic I/O, Exception Handling, Regular Expressions, File Manipulation, Classes, Standard library

UNIT-V
BioPERL Programming
General Bioperl classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local Database)

REFERENCES:
1. The C Programming Language, B.W.Kernighan and D.M. Ritchie 2nd Edition. Prientice Hall of India.

2. Programming Perl – Larry Wall, Tom Christiansen & John Orwant 3ed 2000- O' Reilly
3. Programming Python – Mark Lutz – 2nd Ed., O' Reilly
4. E. Balagurusamy - **"**Programming in C++ **" -** Tata Mc. Graw Hill Edition
5. Byron Gottfried, - "Programming with C**"** (Schaum's Outline Series) - Tata
6. McGrawHill Publishing Company - 1998.
7. Object oriented programming with c++ -Robert Laffore -Waite series.
8. Programming Perl - Tom Christiansen, Larry. Wall Orielly Publications

07BIPGDT6 **SEM II**

GENOMICS

Subject description : This paper deals with genome map, comparative genomics, structural genomics, functional genomics and regulation.
Goals: To make the students to familiar with genome map, comparative genomics, structural and functional genomics.
Objectives: Understand the genome architecture and to extract information like gene function, gene regulation, protein evolution and targets for drug designing

UNIT – I
Definition of Genome, Genome sequencing, Genome map: Types of Genome maps and their uses, High and low-resolution map, Map elements, Polymorphic markers, Types of maps: Cytogenetic, Linkage map, Transcript map, Physical map, Comparative map, Integrated map, STS content maps, Map repositories: NCBI – Entrez Human genome map viewer, OMIM – Online Mendelian Inheritance in Man, Linkage map resources: CEPH reference pedigree, CHLC – Cooperative human linkage center, Radiation hybrid map resources. Practical uses of genome maps: Locating genomic regions, Target identification, Arrangement of genes, SNP diagnosis, Positional specific cloning,

UNIT – II
Genome Anatomies The anatomy of the Eukaryotic Genome –The special features of metaphase chromosomes, where are the genes in the genome? Families of genes, pseudogenes – Eukaryotic organelle genomes, Repetitive DNA content of the human genome.
Transcriptomes and Proteomes
Genome Expression in outline; The RNA content of the Cell– the Transcriptome – yeast and human; The Protein content of the cell - the link between the Transcriptome and the Proteome.

UNIT – III
Annotation of the Genome: Structural annotation (Locating coding regions and other structural elements of the gene). Various approaches in gene prediction: ORF prediction, Gene prediction in prokaryotes and eukaryotes, Hidden Markov Model, Pattern discrimination, Evaluation of gene prediction methods, Prediction of promoter sequences, Functional annotation: (Prediction of gene function), Employing the similarity

in the sequence, gene family and metabolic pathway. Employing the conserved domain, Profile and motif comparison, EST Comparison. Analysis of Human Genome.

UNIT – IV

Comparative Genomics:

Purpose and Methods of comparison, Tools for genomic comparison: Applications of Comparative Genomics, Reconstruction of metabolic pathway, Predicting regulatory elements, Identifying targets, examination of domain function, analysis of conserved strings.

Genome projects and Model Organism research -Yeast; Drosophila; C. elegans; and Mouse – a comparative analysis. Comparative genomics as an aid to gene mapping and in the study of human diseases.

UNIT – V

Functional Genomics:

Gene expression analysis by cDNA micro arrays, SAGE, Strategies for generating ESTs and full length inserts; EST clustering and assembly; EST databases (DBEST, UNIGENE); Expression and regulation of entire set of genes, Sporulation Vs Vegetative condition in yeast and *Bacillus.*

REFERENCES

1. **Active Conversation of Non-coding Sequences revealed by three way species comparisons.** Inna Dubchak et al. 2000. Genome Research. 10, 1305–1306.
2. **Bioinformatics A Practical Guide to the Analysis of Genes and Proteins**. Ed. Andreas D. Baxevanis and B.F. Francis Ouellette. A. John Wiley & Sons, Inc., Publications (For mapping and comparative Genomics and COG and other database repositories).
3. **Bioinformatics Sequence and Genome Analysis**. 2001. David W. Mount. Cold Spring Harbor Laboratory Press.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
5. Shanmughavel, P. 2006. **Trends in Bioinformatics,** Pointer Publishers, Jaipur, India.
6. **Comparative genetics.** Ann Gibbons, 1998. Science. 281: 1432 – 1434.
7. **Encyclopedia or *Escherchia coli* genes and Metabolism.** Peter D. Karp et al. 1996. Eco-Cyc: Nucleic Acids Research. 10: 86-90.
8. **Structural Genomics and its importance for Gene Function Analysis.** Jeffrey et al. 2000. Nature Biotechnology. 18:283 – 287.
9. **The COG database: New developments in phylogenetic classification of Proteins from complete genomes.** Roman Tatusov et al. 2001. Nucleic Acids Research. 29:22-28.
10. **The Comprehensive Microbial Resource.** Jeremy D. Peterson et.al. 2001. Nucleic Acids Research. 29: 123 – 125.
11. **The Molecular Biology Database Collection: Updated Compilations of Biological Database Resources.** Baxevanis A.D. 2001. Nucleic Acids Research. 29 p 1-10.
12. **Genomes.** T.A. Brown, 2001. Taylor and Francis Group.

07BIPGDT7 **SEM II**

PROTEOMICS

Subject description : This paper deals with protein structure prediction and function and various tools for analysis of proteins.

Goals: Proteomics is extensively used in drug discovery, and to learn various tools for analysis of proteins.

Objectives: Taxonomy, structure-function relationship and functional aspects of the entire set cell.

UNIT – I

Protein classification: Structural elements and terminology, Helix, Sheet, Strand, Loop and coil, Active site, Architecture, Blocks, Class and Domains, Fold, Motif, PSSM, Profile. Principles of classification: Based on structural features, Phylogenetic relationship, CATH – Classification by Class, Architecture, Topology, Homology, SCOP - Structural Classification of Protein, FSSP – Fold classification based on structure – structure alignment, MMDB – Molecular Modeling Database, SARF – Spatial arrangement of backbone fragments

UNIT – II

Protein structure prediction: Use of sequence pattern, leucine zipper, coiled coil, transmembrane, signal peptide, cleavage site. Secondary structure prediction: Chou – Fasman / GOR method, Neural network, nearest neighbor method, tertiary structure prediction, threading profile, contact potential, modeling.

UNIT – III

Analytical protein and peptide separations - Complex protein and peptide mixtures, Extracting proteins from biological samples, Protein separation before digestion: 1D and 2 D Electrophoresis, Immobilized pH gradient, Sample preparation, First dimension criteria, second dimension criteria, Stabilization, Detecting protein on gel: Electro blot, Image analysis, Digital imaging, Spot detection and quantification, Gel matching. Data Analysis – Database for 2D gel.

UNIT – IV

Tools of Proteomics-

Mass Spectrometry for protein and peptide analysis:

- MALDI-TOF Analyzers
- ESI Tandem MS instrument
- Tandem Mass Analyzers
- The Triple Quadrupole Mass Analyzer
- The Ion Trap Mass Analyzer
- Q-TOF & Fourier Transform–Ion Cyclotron Resonance MS Instrument

UNIT – V

Functional Proteome Analysis: Integrated Proteome Analysis - Phage antibody as tool, Protein expression analysis, High throughput analysis for proteomics. Automation of proteomic analysis. Proteomics in plant breeding: Objectives,principles and methods, Genetic diversity analysis, Distribution of varieties, lines andcultivars, Mutant characteristics, Variability between organ and developmental stage, Identification of abiotic stress, Genetic mapping of protein markers.

REFERENCES

1. Daniel C. Leibler, (2002), **Introduction to Proteomics: Tools for New Biology**, Humana Press, Totowa, NJ.
2. Branden, Carl and Tooze John. 1999. **Introduction to Protein Structure** (2nd. Ed.),Garland Publishing, NY, USA.
3. Mount, David, W., (2001); **Bioinformatics: Sequence and Genome Analysis**, Cold Spring Harbor Lab. NY, USA
4. Pennington, S, (Editor), M. J. Dunn (Editor); (2001); **Proteomics: From Proteins Sequence to Function,** Springer Publications
5. Palzkill, Timothy; (2002); **Proteomics,** Kluwer Academic Publishers
6. Suhai, Sandor, (ed).,(2000); **Genomics and Proteomics : Functional and Computational Aspects,** Plenum Pub. Corp.
7. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.

07BIPGDT8 **SEM II**

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Subject description : This paper deals with molecular modeling, quantum mechanics, molecular mechanics pertaining to drug discovery.

Goals: Provide a broad and through background in modeling tools and docking program

Objectives: understand the theories used to build tools and their relationship and basic concepts involved in drug design.

UNIT-I

Introduction to the concepts of molecular modeling. Molecular structure and internal energy. Application of molecular graphics. Energy minimization of small molecules: Empirical representation of molecular energies. Use of force fields and the molecular mechanics method. Discussion of local and global energy minima.

UNIT-II
The techniques of molecular dynamics and Monte Carlo. Simulation for conformational analysis. *Ab initio,* dft and semi empirical methods.

UNIT-III
Macromolecular modeling. Design of ligands for known macromolecular target sites. Principles of Docking studies, Drug – receptor interactions. Classical SAR. / QSAR studies and their implications to the 3-D modeler. 2-D and 3-D database searching. Pharmacophore identification and novel drug design.

UNIT-IV
Docking-Rigid and Flexible.Finding new drug targets to treat disease, new targets for anti-cancer drugs, Drugs that rescue mutant p53's.

UNIT-V
Structure-based drug design for all classes of targets. Enzyme Inhibition strategies.

REFERENCES
1. **Molecular Modeling: Principles and Applications.** Andrew R. Leach
2. **Basic principles and applications** Hans-x
3. **Designing bioactive molecules three-dimensional techniques and applications.** Yvonne C. Martin.
4. **Exploring QSAR.** Leo, Albert, Hockma, D.H.– Hansch, Corwin.
5. **Principles of Bioinformatics,** Shanmughavel, P. 2005 , Pointer Publishers, Jaipur, India.
6. Shanmughavel, P. 2006. **Trends in Bioinformatics,** Pointer Publishers, Jaipur, India.

07BIPGDP2 **SEM II**

PRACTICAL II- COMPUTER AIDED DRUG DESIGN

- Small molecule building, using ISIS DRAW and CHEM SKETCH
- Homology Modeling using SPDBV
- Model structure refinement using SPDBV
- Model validation using What Check and Pro Check
- Docking using DOCK or AUTODOCK or AMBER