# **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

Course Fee: Rs. 7500/- per Semester (examination and other fee will be applicable as per university norms).

Intake capacity: 20 students

Eligibility: Bachelors / Masters Degree in life Science, pharmacy, medical, engineering, agriculture and veterinary science.

Exam Pattern: Semester Pattern (80 External / 20 Internal evaluations).

Course Structure: One year duration; Seven Theory Papers, one practical examination and one project report.

# Program Specific Outcomes

This course is expected to bring direct benefit to students of this university, strengthening ongoing university research in the area of life science's.

- **PSO1** To develop an expert manpower to help bioinformatics industry, academia and thereby society.
- **PSO2** Create an advanced research facility to carry out research in frontier areas of Bioinformatics and Computational Biology.
- **PSO3** Add the knowledge of Bioinformatics to their attained educational skills.
- **PSO4** Become a part of Mission-skill India by disseminating the knowledge of Bioinformatics to next generation.

The students will be awarded as per absolute grading system, detailed below:

Interval of Marks	Grade	Grade Points	
> or = 80 but <or =100<="" td=""><td>O (Outstanding)</td><td>10</td></or>	O (Outstanding)	10	
> or = 70 but <80	A+(Excellent)	9	
> or = 65 but <70	A(Very Good)	8	
> or = 55 but <60	B+ (Good)	7	
> or = 50 but <55	B (Above Average)	6	
> or = 45 but <50	C (Average)	5	
> or = 40 but <45	P (Pass)	4	
Less than 40	F (Fail)	0	
	Ab (Absent)	0	

Note: A student obtaining Grade F shall be considered failed and will be required to reappear in the examination.

# **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

Paper Code	Title of Paper	I.A.	U.E	Total	Credit
DBIN-01	Basics of Bioinformatics	20	80	100	04
DBIN-02	Computational Biology	20	80	100	04
DBIN-03	Bio-statistics	20	80	100	04
DBIN-04	Genomics and Proteomics	20	80	100	04
DBIN-05	Structural Biology	20	80	100	04
DBIN-06	Lab course		4	100	04
Total Marks			600		

# Semester II

DBIN-07	Molecular Modelling and Drug discovery	20	80	100	04
DBIN-08	Database management system	20	80	100	04
DBIN-09	Project report			200	08
Total Marks			400		

Total Credits 40

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### **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

## **DBIN 01: Basics of Bioinformatics**

# MM: Th 80 + IA: 20 Time: 3 Hours

### Students completing this course will be able to:

- **CO1** Access the world of Bioinformatics, different types of biological data and databases.
- **CO2** Discuss the concept of Bioinformatics and Biocomputing techniques
- **CO3** Explain and use phylogenetic analysis softwares and visualisation tools
- **CO4** Utilize the different information retrieval system and sequence search tools.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

## Unit I

Introduction to Bioinformatics: Definition and History of Bioinformatics, Internet and Bioinformatics, Introduction to Data Mining, Applications of Data Mining to Bioinformatics Problems and Applications of Bioinformatics in Biotechnology

#### Unit II

**Biocomputing:** Introduction to String Matching Algorithms, Database Search Techniques, Sequence Comparison and Alignment Techniques, Use of Biochemical Scoring Matrices, Introduction to Graph Matching Algorithms, Automated Genome Comparison and its Implication, Automated Gene Prediction, Introduction to Signaling Pathways and Pathway Regulation. Gene Arrays, Analysis of Gene Arrays

# Unit III

Bioinformatics Softwares: Clustal V, Clustal W 1.7, RasMol, Oligo, Molscript, Treeview, Alscript, Genetic Analysis Software, Phylip

Genome Information Resources – DNA sequence Databases – EMBL DDBJ, TAIR, Genbank GSDB (Genome, Sequence Database), UniGene.

#### Unit IV

Protein Information Resources: Biological Databases, Primary Sequence Databases, Composite Protein Sequence Databases - Secondary Databases, Prosite, Prints, Blocks Profiles and Identity.

Evolution of Bioinformatics: Scope, Potentials of Bioinformatics Human Genome Project.

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Reference:

- 1. Baldi, P. and Brunak, S. 1998 Bioinformatics. The MIT Press.
- 2 Lesk, A.M. 2002 Introduction to Bioinformatics. Oxford University Press.
- 4. Rastogi, S.C., Mendiratta, N. and Rastogi, P. 2004 Bioinformatics: Concepts, Skills & Applications. CBS Publishers & Distributors, New Delhi.
- 5. Mont, D.W. Bioinformatics: Sequence and Genome Analysis.
- 6. Jae K. Lee, Statistical Bioinformatics, John Wiley & Sons Inc.

9. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi (2003).

11. D. Higgins and W. Taylor (Eds), Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi (2000).

12. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley-Interscience, Hoboken, NJ (1998).

13. S. R. Swindell, R.R.Miller and G.S.A.Myers (Eds.), Internet for the Molecular Biologist, Horizon Scientific Press, Wymondham, UK, (1996).

## **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

## DBIN 02: Computational Biology

# MM: Th 80 + IA:20 Time: 3 Hours

### Students completing this course will be able to:

- CO1 Discuss the concept of Genomics and Proteomics.
- **CO2** Access and explain the tools and techniques of analyzing and visualizing structure of DNA and protein sequences.
- CO3 Discuss local and global alignment (Smith Waterman algorithms, Needleman Wunch algorithm).
- CO4 Elaborate the concept of Multiple Sequence Alignments.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

#### Unit I

Structure of DNA & Protein – Sequence analysis – pairewise sequence comparison – sequence queries against biological databases – BLAST and FASTA.

## Unit II

Multiple sequence alignments, Phylogenetic alignment – profiles and motifs – distance and similarity – evolutionary basis of sequence alignment – scores and gaps.

#### Unit III

**Protein structure visualisation**, tools structure, classification, alignment and analysis. Solvent accessibility and Interactions, Physico chemical properties, structure optimisation. Protein resource databases; Predicting Protein structure and function from sequence, Determination of structure, feature detection, secondary structure prediction, Predicting 3D structure.

### Unit IV

Genomics and Proteomics, Sequencing genomes, sequence assembly, genome on the web, annotating and analyzing genome sequences. Proteomics: biochemical pathway databases, submitting sequence to the databases.

Reference:

1. Bioinformatics : A practical guide to the analysis of genes and proteins – 2001 – AD Baxevanis & BFF Ouellette – Wiley Interscience – New York.

2. Bioinformatics : Methods and Protocols – 2000 – Stephen Misener & Stephen A. Krawetz, Humana Press, New Jersey.

3. Bioinformatics : Sequence, structure and databanks – 2000 – Des Higgins & Willie Taylor – Oxford University Press.

#### **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

#### DBIN 03: Biostatistics

# MM: Th 80 + IA:20 Time: 3 Hours

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#### Students completing this course will be able to:

- CO1 Explain the probability concept
- CO2 Discuss the Measures of Central tendency and dispersion in detail.
- **CO3** Explain the Theory of Attributes.

CO4 Apply the relevant types of tests on the provided data.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

## Unit I

Numerical Description of Data: Mean, Median, Mode, Quantiles, Standard Deviation, Variance, Coefficient of Variation; Simple Linear Regression and Correlation: Linear Regression Model, Least Squares Method, Estimating Model Parameters, Residual Sum of Squares.

#### Unit II

Probability Theory: Sample Space and Events, Axioms of Probability, Conditional Probability, Independent Events, Bayes' Formula

Random Variables: Discrete and Continuous, Expected Value, Variance; Discrete and Continuous Distributions, Chi-Square, Student's t, Snedecor's F and Z Distributions

#### Unit III

Theory of Attributes: Introduction, Dichotomy, Consistency of Data, Independence of Attributes, Association of Attributes, Rules coefficient of Association.

#### Unit IV

Estimation Theory: Unbiased Estimator; Confidence Interval: Population Mean, Population Variance; Limit Theorems: Central Limit Theorem, Strong Law of Large Number, Weak Law of Large Number.

Text Book :

1. S.C. Gupta and V.K. Kapoor, Fundamentals of Mathematical Statistics, 11<sup>th</sup> Edition, Sultan Chand & Sons, New Delhi, 2002.

2. S.P.Gupta, Statistical Methods, Sultan Chand & Sons, 1996.

3. L. Forthofer, Introduction to Biostatistics, Academic Press, 1995.

4. Robert R. Sokal and F.J. Rohlf, Introduction to Biostatistics (Biology-Statistics Series), W.H. Freeman & Company, New York, 1987.

## **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

# **DBIN 04: Genomics and Proteomics**

# MM: Th 80 + IA:20

# Time: 3 Hours

#### Students completing this course will be able to:

CO1 Explain the concept of prokaryotic and eukaryotic genomes.
CO2 Discuss about sequencing and analysis methods for genomes.
CO3 Apply learnt proteomics technique for structure predictions etc.
CO4 Perform the phylogenetic analysis using different techniques.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

## Unit I

**Diversity of Genomes:** Prokaryotic and Eukaryotic Genomes: Structure, Organization; Gene Families; Genome Analysis: Introduction, Gene prediction methods, Physical methods of sequencing, automated sequencing, genome expression and analysis.

## Unit II

Gene mapping and applications- Genetic and Physical Mapping, Integrated map; Sequence assembly and gene expression; Genome Annotation.

#### Unit III

**Phylogenetic analysis:** Evolutionary Change in Nucleotide Sequences, Rates and Patterns of Nucleotide Substitution, Models for Nucleotide Substitution and Methods for Phylogenetic analysis: Sequence Alignment, Softwares (SSearch, BLAST, FASTA, CLUSTAL), Construction of Phylogenetic Tree

## Unit IV

**Proteomics**: Definition, Transcriptomics; metabolomics. Techniques of proteomics – 2D PAGE, Multidimensional protein identification (Mud PIT) Isotopically coded affinity Tag (ICAT), Mass spectrophotometer – (MALDI –TOF) MS. Application of functional genomics in basic biology, target / marker identification, target valediction / toxicology, microbial drug resistance and drug design etc.

## References :

1. Baxevanis AD and B.F.F. Ouellette, Wiley Bioinformatics – A practical guide to the analysis of genes and proteins. (ed) – Interscience, New York, 2001.

2. Doolittle RF (1990). Molecular evolution. Computer Analysis of Protein and Nucleic acid Sequences, Methods in Enzymology, Academic Press, New York.

3. Faber K (1992) Biotransformation in Organic Chemistry, Springer Verlag.

4. Gerbardt P.Murray RG, Wood WA, Kreig NR (1994) Methods for General and Molecular Bacteriology – American Society for Microbiology Washington D.C.

## **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

## DBIN 05: Structural Biology

# MM: Th 80 + IA:20 Time: 3 Hours

#### Students completing this course will be able to:

- CO1 Account for the structure of cell membrane, proteins, DNA, RNA and other macro-biomolecules.
- **CO2** Explain basic principles of experimental methods for the determination of the structure of macromolecules.
- **CO3** Prediction of protein structures by *in-silico* methods.

**CO4** Explain the gene structure in detail

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

### Unit I

Cell Structure and Ultracell structure of Pro and Eukaryotic cells – Cell wall – cell membrane – Biomembranes – Organelles. – Diffusion – Active and Passive Transport – Osmoregulation

#### Unit II

Carbohydrates - Classification Types - Structure - Function. Lipids - Classification Types - Structure - Function.

Classification of amino Acids, Classification and three-Dimensional structure of proteins. Overview of protein structure – Primary, Secondary, Tertiary and Quartenary structures – J helix, K Pleated sheet, Ramachandran plot and bonds stabilizing protein structure.

#### Unit III

Principles of Structural Organization and Conformational Analysis. Prediction of Pprotein structure – Fold Recognition (threading), Comparative Modeling (homology), The Chou and Fasman Sheme. Basic Principles of X-ray Diffraction Studies, NMR, Mass Spectroscopy in Identifying Protein Conformation.

### Unit IV

Introduction and Physiochemical Properties of Nucleic Acids – DNA and RNA. Watson and Crick Model of DNA and the different forms of DNA. RNA structure – Principles and Prediction. Gene Structure.

Reference Books :

1. Principles of Physical Biochemistry - Van Holde, Prentice Hall.

2. Basic one & two dimensional NMR sepectroscopy, Horst Friebolin Witey VCH - 1990.

3. Lechninger Principles of Biochemistry – David L.Nelson, Michael M.cox. 3rd Edition Macmillan worth Publishers.

4. Principles of Protein structure, G.E.Shuttz and R.H.Schirmer, Springer verlag, New York.

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# **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

## DBIN 07: Molecular Modeling and Drug Discovery

# MM: Th 80 + IA:20

# Time: 3 Hours

#### Students completing this course will be able to:

- CO1 Explain the recent advances in the field of drug designing.
- **CO2** Describe the concept of QSAR, ADMET, and their applications in drug design.
- CO3 Explain the simulation and docking techniques in detail.
- **CO4** Discuss the concept of genomics and proteomics for target identification and lead design.

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

# Unit I

Recent advances in drug design methodologies, Biomolecular structure, Structure activity relationship, Pharmacokinetics, structure-based drug design.

# Unit II

Pharmacophoric pattern, ADME Properties, quantitative structure activity relationship, Use of genetic algorithms and principle component analysis in the OSAR equations.

## Unit III

Molecular modeling, quantum mechanical and molecular orbital methods, introduction to semi-empritical, molecular mechanics and ab intio techniques. Simulation techniques, potential energy surfaces, docking and modeling substrate receptor interactions.

Software tools for modeling bio-molecules. Molecular electrostatic potentials, charge analyses. Protein conformations, folding and mutation through modeling.

## Unit IV

Use of Genomics and Proteomics for understanding diseases at molecular level strategies for target identification and lead design.

Reference Books:

1. Andrew Leach, Molecular Modelling: Principles and Applications (2<sup>nd</sup> Edition), Addison Wesley Longman, Essex, England, 1996.

2. Alan Hinchliffe, Molecular Modelling for Beginners, John-Wiley, 2003.

3. N. Cohen (Ed.), Guide Book on Molecular Modeling in Drug Design, Academic Press, San Diego, 1996.

## **CENTRE FOR BIOINFORMATICS, M.D. UNIVERSITY**

# **DBIN 08: Database Management System**

# MM: Th 80 + IA:20 **Time: 3 Hours**

# Students completing this course will be able to:

- **CO1** Discuss, Design and apply different data models.
- **CO2** Explain the concept of Indexing and Hashing in databases
- CO3 Utilize the methods of data updation, curation and retrieval through structured query language (SQL)
- Access data in a database without the need of consulting the indexing system of a **CO4** database by using pointers

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question number I is compulsory covering the entire syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

#### Unit I

Data base: Introduction, Basic Technology and Data Basics, Objective of a Data base organisation, Entities & Attributes. Data Models: Introduction, Schemes & Sub Schemes, Data base Management Systems, Tree Structures, Plex Structures, Relational Databases, Normal Forms.

# Unit II

Data Base Languages: Introduction, Data Description Languages, the CODASYL Data Description Language, Query Languages, Data Dictionaries.

#### Unit III

Physical Organization: Introduction, Criteria affecting physical organization, Differences between physical & logical organization, Addressing Techniques, Index sequential organisation, Hashing.

#### Unit IV

Pointers: Chains & Ring Structures: Introduction, Physical representation of tree structures, Physical representation of plex structures, Virtual & Storage hierarchies.

Reference Books:

- 1. James Martin, Computer Database Organisation, Prentice Hall of India.
- 2. James Martin, Principles of Database Management, Prentice Hall of India

3. C.J.Date, An Introduction to Database systems, 3rd edition, Narosa Publishing House. 11