Post Graduate Diploma in Bioinformatics (P.G.D.B.I)

SEM	Course Code	Course	Course Title	Hrs / Week	Credit	CIA Mark	SE Mark	Total Marks
I	20PDBI1C1	Core I	Fundamental of Bioinformatics	6	4	25	75	100
	20 PDBI1C2	Core II	Statistics for Bioinformatics	6	4	25	75	100
	20PDBI1C3	Core III	Basic Structural Biology	6	4	25	75	100
	20PDBI1C4	Core IV	Computer Programming	6	4	25	75	100
	20PDBI1C5P	Core V	C Programming and Web Publishing – Practical	6	4	25	75	100
TOTAL				**30**	**20**	**125**	**375**	**500**
II	20PDBI2C1	Core VI	Database Management Systems	6	4	25	75	100
	20PDBI2C2	Core VII	Genomics and Proteomics	6	4	25	75	100
	20PDBI2C3	Core VIII	Computational Biology	6	4	25	75	100
	20PDBI2C4	Core IX	Molecular Modelling and Drug Design	6	4	25	75	100
	20PDBI2C5P	Core X	Bioinformatics - Practical	6	4	25	75	100
TOTAL				**30**	**20**	**125**	**375**	**500**
GRAND TOTAL				**60**	**40**	**250**	**750**	**1000**

Post Graduate Diploma in Bioinformatics (P.G.D.B.I)
<u>Programme Specific Outcome</u>
At the end of the programme, students will be able to:
- Explain the fundamental principles of Bioinformatics and statistical applications in bio informatics.
- Outline the process of generation, manipulation and representation of molecules for drug modeling.
- Describe the basic structure of biological molecules, process of acquiring the structures and the interaction between the molecules.
- Develop and apply basic computer programming to build biological algorithms and models to study their relationships.
- Deduce the interrelationship between genomics and Proteomics, techniques involved in analyzing proteomics and its applications.

SEMESTER I: CORE - I
FUNDAMENTAL OF BIOINFORMATICS

Subject Code: 20PDBI1C1   **Max. Marks 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks: 75**

Unit I: **18 Hours**
Bioinformatics – an Overview, Definition – Scope and History of Bioinformatics Networks – Internet in Bioinformatics, #EMBnet – Commercial Databases and Software's, # Intranet and Internet Packages. Role of Bioinformatics.

Unit II   **18 Hours**
Languages – Basics of C Programming, Array, Structure and Function. Perl – Basics, String handling. HTML – Basics, Text handling, Image handling, Links and Tables. #XML – Basics, data binding and record sets#.

Unit III   **18 Hours**
Introduction to Biological database – Protein Information Resources – Biological Databases, Primary Sequence Databases, Protein Sequence Databases, and Nucleotide Sequence Database-#Secondary Databases, Metabolic pathway databases#.

Unit IV   **18Hours**
Genome Information Resources – DNA sequence Databases – EMBL DDBJ, Genbank GSDB (Genome, Sequence Database), #UniGene-Comprehensive microbial Resource,#Sequence alignment – local and global alignment.

Unit V   **18 Hours**
Evolution of Bioinformatics – Scope – Potentials of Bioinformatics, Human Genome Project – Application of Bioinformatics #Bioinformatics in India – Future of Bioinformatics#. Cheminformatics – Ayurinformatics.

#-----------#Self-study portion

Text Books:
   T.B 1. Attwood T.K and D.J. Parry-Smith, Introduction to Bioinformatics, PearsonEducation Ltd., New Delhi (2004).

   T.B 2 .Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, NewDelhi (2003).

Unit I: Chapter I Section 1, 8-11. T.B - 1
Unit II: Chapter II Section 6- 9. T.B - 2
Unit III: Chapter I Section 1.2, 1.1, 3.2. T.B -3
Unit IV: Chapter VIII Section 180-191 T.B -3
Unit V: Chapter V Section 1-23. T.B - 2

Books for References:

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

2. Andrea Cabibbo, Richard Grant and Manuela Helmer-Citterich (Eds.), The Internet for Cell and Molecular Biologists (2nd Edn.), Horizon scientific Press, Norwich, UK (2004).

Web reference:
https://www.epictraining.ca/course/15958/biological databases/-distance
https://bioinformatics.mit.edu/

COURSE OUTCOMES:

CO 1: Identify the scope of Computational Biology and Bioinformatics.

CO2. Ability to design programs with interactive Input and Output program c.

CO3.The Study of understanding biological information. Retrieval methods for DNA sequence.

CO4. Gain the knowledge Major Biological Databases and Information.

CO5. Determine the analyzed molecular biology, clinical medicine and other disciplines.

Mapping with programme outcomesand programme specific outcomes

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓	✓	✓		✓	✓	✓
CO2	✓	✓	✓		✓	✓		✓	✓	✓
CO3	✓	✓	✓	✓	✓	✓		✓	✓	✓
CO4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO5	✓	✓	✓	✓	✓	✓		✓	✓	✓

Number of matches (✓)   -   44
Mapping Score   -   88 %
If number of matches (✓) ≥35 (ie.) 70% and above -   -   High

Prepared by: **Checked by:**
1. Mr.K.Gobalan   -   1. Dr. A. Khaleel Ahamed.
                                                       2. Dr. J. Sebastin Raj

<div align="center">

SEMESTER I: CORE II
STATISTICS FOR BIOINFORMATICS

</div>

Subject Code: 20PDBI1C2	**Max Marks: 100**
Hours / Week: 6	**Internal Marks: 25**
Credit: 4	**External Marks: 75**

Unit I   **18 Hours**

Measures of central Tendency – Arithmetic Mean – Median – Mode – Quartiles –Range – #Quartile deviation – Mean deviation#. Quartiles– Calculation of Quartiles – Standard Deviation.

Unit II   **18 Hours**

Probability – Frequency Theory of Probability – Limitations – View of Probability – Addition Theorem – Multiplication Theorem - #Baye's Theorem and related problems#.

Unit III   **18 Hours**

Theoretical Distributions – Binomial, Poisson and Normal – Importance of Normal Curve # fitting of the Distributions and its properties - Z-score, P-value and E-value#.

Unit IV   **18 Hours**

Theory of Attributes – Introduction – Dichotomy – Consistency of Data – Independence of Attributes – Association of Attributes – #Rules coefficient of Association#.

Unit V   **18Hours**

Sampling Distributors – Large and small sample tests – Theories of probability, Student's t^2 test, X^2 test, F-test – and chi square test for goodness of fit #. Normal test and their applications#.

#----------# Self-study portion

Text Books:

T.B 1: Gupta S.C and V.K. Kapoor, Fundamentals of Mathematical Statistics, 11th Edition, Sultan Chand & Sons, New Delhi, 2002.
T.B 2: Pillai R.S.N and V. Bagavathi and S. Chand Statistics (1984).

Unit I: Chapters 9 Sections 121 - 129. **T.B-1**
Unit II: Chapters 18Sections 686-695. **T.B-1**
Unit III: Chapters 19 Sections 735 - 748 **T.B-1**
Unit IV: Chapters 5 Sections 35-42.**T.B-2**
Unit V: Chapters 1 Sections 222-224. **T.B-2**

Books for Reference:
1. Gupta, S.P., Statistical Methods, Sultan Chand & Sons, 1996.
2. Forthofer, L., Introduction to Biostatistics, Academic Press, 1995.
3. Robert R. Sokal and F.J. Rohlf, Introduction to Biostatistics (Biology- Statistics Series), W.H. Freeman & Company, New York, 1987.

Web References:

1. https://nptel.ac.in/courses/statistics 102103012/s

COURSE OUTCOMES:

CO1: Determine the category of measures of central tendency, dispersion and correlation for analysis of data.
CO2: Improve the new concepts of probability and random variables.
CO3: Identify the application some standard distributions and their properties.
CO4: Gain the knowledge about frequency theory of probability and its related problems.
CO5: Intellectual about the rule's coefficient of association.

Mapping with Programme Outcomes and Programme Specific Outcomes:

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓			✓		✓		
CO2	✓		✓	✓	✓	✓		✓	✓	✓
CO3	✓		✓	✓		✓		✓	✓	
CO4	✓		✓	✓	✓	✓		✓	✓	✓
CO5	✓	✓	✓	✓		✓	✓	✓	✓	

Number of matches (✓)   -   34
Mapping Score   -   68 %
If number of matches (✓) ≥30 (ie.) 60% and above   - Moderate

Prepared by:
1. Mr.Gobalan

Checked by:
1. Dr. A. Khaleel Ahamed.
2. Dr. T. Nargis Begum

Semester I: CORE III
BASIC STRUCTURAL BIOLOGY

Subject Code:20PDBI1C3   **Max Marks: 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks :75**

Unit I   **18 Hours**

Cell Structure and Ultra cell structure of Prokaryotic and Eukaryotic cells – Cell wall – cell membrane – Biomembranes – Organelles. – Diffusion – #Active and Passive Transport#.

Unit II   **18 Hours**

Carbohydrates – Classification Types – Structure – Function. Lipids –Classification Types – Structure – Function.

Unit III   **18 Hours**

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#.

Unit IV   **18 Hours**

Classification of amino Acids. Classification and three-Dimensional structure of proteins. Overview of protein structure – Primary, Secondary, Tertiary and Quaternary structures.#Ramachandran plot and bonds stabilizing protein structure#.

Unit V   **18 Hours**

Principles of Structural Organization and Conformational Analysis. Prediction of protein structure - Modeling homology, Chou and Fasman method. Basic Principles of X-ray Diffraction Studies, #NMR#, Mass Spectroscopy in Identifying Protein Conformation#.

#........# Self-study portion

Text Books:

1. Van Holde, Principles of Physical Biochemistry –Prentice Hall. 2006

2. Horst FriebolinWitey, Basic One & Two dimensional NMR sepectroscopy–VCH – 1990.

Books for References:
1. Lechninger, David L. Nelson, Michael M. Cox., Principles of Biochemistry –3rd Edition Macmillan worth Publishers, 2000.
2. G.E.Shultz and R.H.Schirmer,Principles of Protein structure, Springer –Verlag, New York. 2002.

Web References:

https://nptel.ac.in/courses/102103012/

Course Outcomes:
CO1 Acquire the basic and fundamental concepts of cell biology.
CO2 Explain the knowledge in basic energy sources.
CO3 Apply the principle, Physiochemical properties, structure of nucleic acids.
CO4 Appraise the basic science of Protein structure including mechanisms.
CO5 Formulate the key experimental processes required to evaluate protein structure, functions and to apply them to solve biochemical problems.

Mapping withProgramme outcome and Programme Specific Outcome

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓				✓		✓
CO2	✓		✓	✓	✓			✓		✓
CO3	✓		✓	✓				✓		✓
CO4	✓		✓	✓	✓			✓		✓
CO5	✓	✓	✓	✓	✓			✓	✓	✓

Number of matches (✓)   -   34
Mapping Score   -   68 %
If number of matches (✓) ≥30 (ie.) 60% and above   - Moderate

Prepared by: **Checked by:**
1. Dr. T. Nargis Begum   -   1. Dr. J. Sebastin Raj
                                                         2Dr.A. Khaleel Ahamed

Subject Code: 20PDBI1C4   **Max Marks: 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks: 75**

Unit I   **18 Hours**
Block diagram of computer (input and output devices) generation – advantages and limitations of computers – Basics of operating systems DOS, Windows NT and XP, UNIX – #Application software's#.

Unit II   **18 Hours**
Introduction to internet, service on internet – internet tools, HTML, text formatting – Adding images – Tables – Frames to web pages. Web services – WWW, URL, DNS – Servers, WEB servers, Browsers, IP Addressing, Communication Technology – Networking: LAN, #WAN and MAN, wireless communication#.

Unit III   **18 Hours**
Identifiers and keywords – Constants, Variables and data types – #Operations and Expression – Data input and output#.

Unit IV   **18 Hours**
Control structure – If and Switch statement – While, Do – While and for statements – Goto statement, #Arrays - 1 D array -2 D array#.

Unit V   **18 Hours**
Web Publishing Internet – WWW – Designing web site – Basics of creating a web page with HTML – Linking – Text formatting – #Adding Images and background to HTML pages – Tables– Image maps#.Function – User defined functions – Defining and assessing functions – Passing arguments - Functions prototypes – character strings – string functions – recursion – storage classes – structure – union.

-----------#Self-study portion

Text Books:

T.B 1: Balagurusamy E., Object Oriented Programming with C++" — TMH-2000.
T.B.2: Monica D'Souza & Jude D'Souza "Web Publishing" — TMH– 2001.

Unit I: Chapters III Sections 1-37.T.B-1

Unit II: Chapters II Sections49-210.T.B-1

Unit III: Chapters IV Sections 65-175.T.B-1

Unit IV: Chapters VI Sections 2-59. T.B-2

Unit V: Chapters VII Sections 11-109. T.B-2

Books for Reference:
1. Robert Lafore., Object Oriented Programming in C++ - Galgotia.2000.
2. YeshwantKanetkar., let us C++ -– BPB. 2001
3. Steve Wright., Instant HTML Programmer's Reference — WROX Press Ltd.2011.

Web reference:
1. https://ocw.mit.edu/courses/computer program /7-06- -spring-2007.
2. https://ocw.mit.edu/courses/biology/7-06-computer application-spring-2010/

COURSE OUTCOMES:
CO 1: Develop the foundation for higher studies in the field of Computer Application.
CO 2: Ability to design programs with Interactive Input and Output
CO 3: Gain ability to develop responsive web applications
CO 4: Explore different web extensions and web services standards.
CO 5: Acquire knowledge and skills for creation of web site considering both client and server-side programming.

Mapping with programme outcomes and programme specific outcomes:

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓		✓		✓	✓	✓
CO3	✓	✓	✓	✓		✓		✓	✓	✓
CO4	✓	✓	✓	✓		✓		✓	✓	✓
CO5	✓	✓	✓	✓		✓		✓	✓	✓

No. of matches   40
Mapping Score   80%
If number of matches ≥35 (i.e.) 70% and above   High

Prepared by: **Checked by:**
1. Mr. K.Gobalan   1. Dr.A.Khaleel Ahamed.
                                           2. Dr. T. Nargis Begum

C PROGRAMMING AND WEB PUBLISHING - PRACTICAL

Subject Code:20PDBI 1C5P	**Max Marks: 100**
Hours / Week: 6	**Internal Marks: 25**
Credit: 4	**External Marks : 75**

1. Factorial of a given number.
2. Sorting and merging two arrays of numbers.
3. Sorting names in alphabetical order.
4. Reversing a given string.
5. Checking for palindrome.
6. String Manipulation – String copy, String length, String concatenation, String comparisonand String reverse.
7. Mean, median, mode and standard deviation calculations.
8. Storing and retrieving amino acid sequences using structure data types.
9. Swapping two values using pointers.
10. File Processing – Creation and simple processing.
11. Computing amino acid composition of a given protein sequence.
12. Enumerate RNA Secondary Structure.

*Web Publishing***:**
1. Create a web page for your University / College using HTML. The opening page shouldprovide hyperlinks to other pages (add animation and sound effects appropriately).
2. Creating a web page to get protein sequence data and compute and display amino acid composition.
3. Creating a web page to get nucleic acid sequence data and compute and display base composition.

Text Books:

1:E. Balagurusamy. Object Oriented Programming C++. Third Edition 2006.
2:A. Jitender. Introduction to HTML."Web Publishing" – Monica D'Souza & Jude D'Souza – TMH– 2001. Third Edition 2008.

Books for References:

1. Gary J. Bronson (A First Book of ANSI C Third Edition 2001).
2. Jitender Kumar Chakra, Programming with C and C++. (Second Edition 2006).
3. Yes want Kantar. let us C++ – BPB. (2000)
4. Steve Wright., Instant HTML Programmer's Reference — WROX Press Ltd. 2011.

Web reference:
1. https://www.youtube.com/watch?v=c program/k1pp

2. https://www.youtube.com/watch?v=html /k1O9jBHgsxs

COURSE OUTCOMES:
CO1: Describe the C programming concepts like Structures, Pointers and Command line
 arguments and data structures
CO2: Identify the application of some basic programs in C and Web based   application.

CO3: Acquire the knowledge Practice the use of conditional and looping statements.

CO4: Illustrate the structure; implement arrays, functions and pointers.

CO5**:** Improve the new skills to handle strings and files.

Mapping with programme outcomes and programme specific outcomes:

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓	✓	✓	✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓		✓		✓	✓	✓
CO3	✓	✓	✓	✓		✓		✓	✓	✓
CO4	✓	✓	✓	✓		✓		✓	✓	✓
CO5	✓	✓	✓	✓		✓		✓	✓	✓

No. of matches   40
Mapping Score   80%
If number of matches ≥35 (i.e.) 70% and above   High

Prepared by:
1. Mr.K.Gobalan

Checked by:
1. Dr.A.KhaleelAhamed
2. Dr. Y. Arsia Tarnam

Semester II: CORE VI
DATABASE MANAGEMENT SYSTEMS

Subject Code:20PDBI 2C1   **Max Marks: 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks :75**

Unit I   **18 Hours**
Data base: Introduction – Basic Technology and Data Basics – #Objective of a Data base organization – Entities & Attributes #.

Unit II   **18 Hours**
Data Models: Introduction – Schemes & Sub Schemes – Data base Management Systems – File Database – Tree Structures. #Relational Databases – Normal Forms #.

Unit III   **18 Hours**
Data Base Languages: Introduction – Data Description Languages – the CODASYL Data Description Language – #Query Languages – Data Dictionaries #.

Unit IV   **18 Hours**
Physical Organization: Introduction – Criteria affecting physical organization –Differences between physical & logical organization – #Addressing Techniques –Index sequential organization – Hashing #.

Unit V   **18 Hours**
Database security: Data Classification– Database access Control – Types of Privileges – Cryptography- Statistical Databases- Distributed Databases- Processing. #Object Oriented Databases-XML Databases#.

#................# Self-study portion

Text Book:

T.B. 1. James Martin, Computer Database Organization, Prentice Hall of India, 2016

Books for Reference:

1. James Martin, Principles of Database Management, Prentice Hall of India, 2012

2. C.J. Date, An Introduction to Database systems, 3rd edition, Narosa Publishing House, 2004

Web References:

https://nptel.ac.in/courses/106105175/

Course outcomes

CO1 Acquire the basics, concepts, objectives of Database.

CO2 Describe the fundamental elements of data models and database management systems.

CO3 Apply and use data manipulation language to query update and manage a data base.

CO4 Analyze the physical and logic database designs and addressing techniques: indexing methods and Hashing.

CO5 Construct a simple database system with the understanding of essential DBMS concepts such as Database security.

Mapping withProgramme outcome and Programme Specific Outcome

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✓		✓	✓		✓			✓	
CO2			✓	✓		✓	✓		✓	
CO3	✓	✓	✓	✓		✓			✓	✓
CO4	✓		✓	✓		✓			✓	✓
CO5		✓	✓	✓	✓	✓			✓	✓

If number of matches () $\geq$ 30 (ie.) 60% and above –Moderate

Prepared by: **Checked by:**

1. Dr. T. Nargis Begum   -   1. Dr. J. Sebastin Raj

2. Dr. A. Khaleel Ahamed

*****

SEMSTER II: CORE VII
GENOMICS AND PROTEOMICS

Subject Code:20PDBI 2C2   **Max Marks: 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks: 75**

Unit I   **18**
Hours

The genetic material – Identification of genetic material, genetic code, concept of gene – operon concept – lac and trp operons, [#]promoters and repressors.

Unit II   **18**
Hours

Different types of genome maps and their uses, genetic and physical mapping techniques – Genomics – definitions – pharmacogenomics – taxicogenomics – [#]prokaryotic and eukaryotic genome – genome relationships – human genomics.

Unit III   **18**
Hours

Genomics Whole genome analysis – Physical methods of sequencing – automated sequencing – genome expression and analysis – serial analysis. [#]code micro assay and microchips.

Unit IV   **18**
Hours

Proteomics Definition – Transcriptomics; Proteomics, 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 toxicology, microbial drug,tumour immunology, vaccine discovery, drug design.

Unit V   **18**
Hours

Proteome and technology – Primary attributes for protein identification – protein super families. A brief account of genetic engineering –Vectors used in genetic engineering-Genomic DNA library-Cloning and modification methods-#Site Directed mutagenesis-Commercial applications.

#.............# Self-study portion

Text Books:

T.B. 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.

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

Books for References:

1. K. Faber. Biotransformation in Organic Chemistry, Springer Verlag. 1992.
2. P.Gerbardt, R. G.Murray, W. A.Wood, N. R.Kreig. Methods for General and Molecular Bacteriology – American Society for Microbiology Washington D.C., 1994.

Web Reference:

1.https://courses.lumenlearning.com/boundless-biology/chapter/genomics-and-proteomics/

2. https://www.ncbi.nlm.nih.gov/books/NBK19861/

Course Outcomes:
On completion of this course, the student will be able to:

CO1. Infer the basic concepts of genomics, transcriptomics and proteomics.
CO2. List and discuss the use of genomics and proteomics in human health.
CO3. Suggest and outline solution to theoretical and experimental problems in Genomics and Proteomics fields.
CO4. Helpful to those students who want to work in core facilities and commercial biological and medical laboratories as well as in their postgraduate studies.
CO5. Deals with a rapidly evolving scientific area that introduces students into genomes, proteomes
and databases that store various data about genes, proteins, genomes and proteomes.

Mapping with Programme Outcomes and Programme Specific Outcomes.

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✔		✔	✔		✔				✔
CO2	✔		✔	✔	✔	✔	✔		✔	✔
CO3	✔	✔		✔	✔	✔	✔		✔	✔
CO4	✔	✔	✔	✔	✔	✔				✔
CO5	✔		✔	✔	✔	✔	✔		✔	✔

No of matches   36
Mapping Score   72%
If number of matches ≥ 35 (ie) 70% and above   High

Prepared by: **Checked by:**

1.H.F.Seyed Mafiya Haniff   1.Dr.A.Nishanthini

                                                        2.   Dr.A.Khaleel
Ahamed

SEMSTER II: CORE VIII
COMPUTATIONAL BIOLOGY

Subject Code:17PDBI2C3   **Max Marks: 100**
Hours / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks :75**

Unit I   **18**
Hours

Structure of DNA & Protein – Sequence analysis – pairwise sequence comparison – sequence

queries against biological databases – BLAST and FASTA – #multifunctional tools for analysis#.

Unit II   **18**

Hours

Multiple sequence alignments, Phylogenetic alignment – profiles and motifs – distance and

similarity – #evolutionary basis of sequence alignment – scores and gaps#.

Unit III 18

Hours

Protein structure visualization – tools structure – classification, alignment and analysis. Solvent accessibility and Interactions – Physico-chemical properties, structure optimization. #Protein resource databases#.

Unit IV 18

Hours

Predicting Protein structure and function from sequence – Determination of structure – feature detection – secondary structure prediction – Predicting 3 D structure. #Protein modeling#.

Unit V 18

Hours

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#.

#---------------# **Self-study portion**

Text Books:

T.B-1 A.D.Baxevanis, B.F.F. Ouellette Bioinformatics: A practical guide to the analysis of genes and proteins– Wiley Interscience – New York, 2001.

T.B-2 StephenMisener& Stephen A. Krawetz, Bioinformatics: Methods and Protocols HumanaPress, New Jersey, 2000.

    Unit I Chapters III Sections 3-21.**T.B-1**

    Unit II Chapters III Sections 20.3-4.21.**T.B-1**

    Unit III Chapters III Sections 22-55.**T.B-1**

    Unit IV Chapters V Sections 5.1-5.6.**T.B-2**

    Unit V Chapters VII Sections 151-166.**T.B-2**

Books for Reference:

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

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

CO 1. Describe different types of biological database and sequence submission tools.
CO 2. Summarize the basics of sequence alignment and various approaches in phylogenetic analysis.
CO 3. Assess the structure, properties and interactions of protein and its databases.
CO 4. Explain the structure and various approaches in 3D structure prediction.
CO 5. Classify and explain the tools and algorithms used for genome sequencing assembly.

Mapping with Programme Outcomes and Programme Specific Outcomes

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✔	✔		✔		✔	✔		✔	
CO2	✔			✔	✔	✔			✔	✔
CO3	✔	✔	✔	✔	✔	✔	✔	✔	✔	✔
CO4	✔		✔	✔	✔	✔		✔	✔	✔
CO5	✔	✔		✔		✔	✔		✔	

Number of matches (✓)   -   36
Mapping Score   -   72 %

If number of matches (✓) ≥35 (ie.) 70% and above -   High

Prepared by: **Checked by:**

1.Dr. Y. ArsiaTarnam   1. Dr. J. Sebastinraj
                                                    2. Dr. A. Khaleel Ahmed

SEMSTER II: CORE IX
MOLECULAR MODELING AND DRUG DESIGN

Unit I   18 Hours

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

Unit II   18 Hours

Molecular basis of drug action, Pharmacophoric pattern, ADME Properties, quantitative structure activity relationship, #Use of genetic algorithms and principle component analysis in the QSAR equations#.

Unit III   18 Hours

Molecular modeling, quantum mechanical and molecular orbital methods, introduction to semi-empirical, molecular mechanics and abintio techniques.Simulation techniques, potential energy surfaces, docking and modeling substrate – receptor interactions#.

Unit IV   18 Hours

Historic development of drug discovery, Modern drug discovery Software tools for modeling bio-molecules. #Molecular electrostatic potentials, charge analyses. Protein conformations, folding and mutation through modeling#.

Unit V   18 Hours

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

#.................# **Self-study portion**

Text Books:

T.B-1 Andrew Leach, Molecular Modelling: Principles and Applications, 2nd Edition, Addison
Wesley Longman, Essex, England, 1996.

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

Unit I Chapters XI Sections 12.1.**T.B-1**
Unit II Chapters X Sections 10.1-10.9.**T.B-2**
Unit III Chapters VIII Sections 8.1-8.9.**T.B-2**
Unit IV Chapters VII Sections 7.1-79.**T.B.1**
Unit V Chapters I Sections 1.1-1.10.**T.B-1**

Books for Reference:

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

Course Outcomes:

On the completion of the course students will be able to:

CO 1. Discuss various techniques and concepts used in structure-based drug design.
CO 2. Describe the algorithms used in drug analysis.
CO 3. Analyze the principles involved in molecular modeling and drug design.
CO 4. Demonstrate the various tools employed in drug discovery and its applications.
CO 5. Systematize about genomics and proteomics in disease analysis at molecular level.

Mapping with Programme Outcomes and Programme Specific Outcomes

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✔	✔		✔	✔	✔	✔		✔	✔
CO2	✔	✔			✔	✔	✔			✔
CO3	✔			✔	✔	✔			✔	✔
CO4	✔		✔	✔	✔	✔		✔	✔	✔
CO5	✔		✔	✔		✔		✔	✔	

Number of matches (✓)   -   34
Mapping Score   -   68 %
If number of matches (✓) ≥30 (ie.) 60% and above   - Moderate

Prepared by: **Checked by:**

1. Dr. Y. ArsiaTarnam   1. Dr. J. Sebastinraj
                                                             2. Dr. A. Khaleel Ahmed

SEMESTER II: CORE X
BIOINFORMATICS – PRACTICAL

Subject Code:17PDBI2C5P   **Max Marks: 100**
Hrs / Week: 6   **Internal Marks: 25**
Credit: 4   **External Marks :75**

1. Multiple alignments- using CLUSTAL W

2. Phylogenetic Analysis using NJ plot.

3. BLAST, FASTA programs for sequence database search.

4. Small molecule building using che1nDraw or chem. Sketch.

5. Evaluation of protein structure by Swiss PDB viewer and by other molecular visualization tools.

6. Calculation of phi – psi angles - Ramachandran plot.

7. Homology modeling of a given protein sequence.

8. Small molecule building using chemSketch.

9. Metabolic pathway prediction

10. Docking Using Patch Dock.

Text Books:

T.B-1 D. Andreas, B.F. Baxevanis, Francis Ouellette, Bioinformatics- A Practical Guide to the Analysis of Genes and Proteins, Wiley-Interscience, 3rd edition, 2006.

T.B-2 A. Baxevanis and B.F. Ouellette, Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley-Inter science, Hoboken, NJ, 1998.

Books for References:

1. S.C. Rastogi, Namita Mendiratta Parag Rastogi. Bioinformatics Concepts, Skills & Applications, CBS Publishers & Distributors, First edition, 2003.

2. K. Teresa, Attwood and J. David, Parry Smith, Introduction to Bioinformatics, Pearson Education, 1999.

Course Outcomes:

On the completion of the course students will be able to:

CO 1. Describe about sequencing alignment and similar search tool
CO 2. Provide hands on training on various tools and techniques employed in biological sequence analysis.
CO 3. Explain about protein structural analysis using Bioinformatics tools.
CO 4. Expose to several DNA and protein databases.
CO 5. Practice methods and tools used for phylogenetic analysis.

Mapping with Programme Outcomes and Programme Specific Outcomes:

	PO1	PO2	PO3	PO4	PO5	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	✔	✔		✓	✔	✔	✔		✔	✔
CO2	✔	✔			✔	✔	✔			✔
CO3	✔			✔	✔	✔			✔	✔
CO4	✔		✔	✔	✔	✔		✔	✔	✔
CO5	✔	✔		✔		✔	✔		✔	

Number of matches (✓)   -   34
Mapping Score   -   68 %
If number of matches (✓) ≥30 (ie.) 60% and above   -   Moderate

Prepared by: **Checked by:**

1. Dr. Y. ArsiaTarnam   1. Dr. J. Sebastinraj
                                                     2. Dr. A. Khaleel Ahmed

******