Course	**Discipline Specific Elective**
Semester	V
Paper Number	MBTDS5012T & MBTDS5012P
Paper Title	BIOINFORMATICS AND STRUCTURAL ENZYMOLOGY
No. of Credits	6
Theory/Composite	Composite
No. of periods assigned	4 Theory + 4 Practical
Course description/objective	1. Students will be introduced to the principles of Bioinformatics. 2. Students will be provided with an essence of the different tools and aspectsof Bioinformatics. 3. Students will learn about structure-function relationship in functioning of enzymes, enzyme regulation and enzyme immobilization technique for commercial application of enzymes. 4. An overview of protein information sources, protein tertiary structure prediction, biological databases, searching of databases and information retrieval would be provided. 5. Students would be introduced to data generating techniques and bioinformatics problems. 6. Students would be familiarized with techniques in bioinformatics by means of project/ computer based practicals.
Syllabus	**Theory** **Module A: Bioinformatics-I and Structural Enzymology (40 marks)** **UNIT I:** History of Bioinformatics. The notion of Homology.Sequence Information Sources, EMBL, GENBANK, Entrez, Unigene, Annotated databases; Sequence format; Types of Biological Databases & Information Retrieval. Global & Local alignment: Overview of Needleman–Wunsch & Smith–Waterman methods. Mutation/Substitution Matrices: PAM250 & BLOSUM62, Pairwise Sequence Alignments and Multiple Sequence Alignment, Phylogenetic Analysis. **UNIT II:** Protein Information Sources, PDB, SWISSPROT, TREMBL; Protein Structural Classification and Visualization. Protein Tertiary Structure Prediction - Homology Modeling, Threading and Fold Recognition, Overview of MD Simulations and applications. **UNIT III:** Searching Databases: Sequence Retrieval System (SRS), Entrez, Sequence Similarity Searches-BLAST, FASTA, Exposure to the methods of Data Submission. Characteristics of Protein-protein, Protein-DNA and Protein-RNA interaction surfaces.Solvent-Accessible Surface area of Protein: SASA, interactive tool for the exploration of macromolecular interfaces: PISA; **UNIT IV**: Enzyme classification; Zymogens and their activation (Proteases and Prothrombin). Structures and mechanisms of Serine protease (Chymotrypsin), Restriction endonuclease, Metalloenzyme carbonic anhydrase, aldolase and alcohol dehydrogenase. Enzyme regulation: Transition-state analog, product inhibition, feedback control, covalent modification. Allosteric enzymes with special reference to aspartate transcarbomylase. Cooperativity, Comparison with Hemoglobin, Multifunctional enzyme-e.g. Fatty Acid synthase,

	site directed mutagenesis and enzyme engineering, Immobilized enzyme reactors. Application of immobilized and soluble enzyme in health and industry. **No. of Classes:** 3 Classes per week **Module B: Bioinformatics-II (10 marks)** **UNIT V: Introduction of Data Generating Techniques and Bioinformatics problem posed by them:** Restriction Digestion, Blots, PCR and Primer designing; Microarrays; Next-generation sequencing; Genome Annotation: Pattern and repeat finding; Gene identification tools. **No. of Classes:** 1 Class per week **Practical** Bioinformatics project: 1. Retrieval of information of a protein of interest, 2. Sequence similarity searches, Sequence analysis, Homology modeling of protein, 3. Structure analysis using PyMol, Interactomics 4. Gene analysis and primer designing.
Readings	1. Biochemistry – Stryer. 2. Structural Bioinformatics and Genome Analysis – D.W. Mount. 3. Principles of Gene Manipulation & genomics-Primrose &Twyman. 4. Relevant scientific literature.
Evaluation	Theory: Continuous Internal Assessment: 10 marks End-Semester Theory Examination: 50 marks Practical: Continuous Internal Assessment: 32 marks End-Semester Examination: 8 marks
Paper Structure for End Sem Theory	Module A (40 marks) Bioinformatics-I (20 marks) One Compulsory question of 6 marks comprising objective problems Any two from three questions each carrying 7 marks. No part question will be of more than 4 marks. Structural Enzymology (20 marks) Any two from three questions each carrying 10 marks. No part question will be of more than 5 marks. Module B (10 Marks) 1 Compulsory question of 5 marks. Any two out of three questions (2 x 2.5= 5 marks)