5th SEMESTER

DISCIPLINE SPECIFIC ELECTIVE – DSE

BI516D   **BIO-INFORMATICS – STRUCTURAL BIO-INFORMATICS**

CREDITS: THEORY = 4, PRACTICAL = 2

UNIT –I

Principles of protein structure: Primary, Secondary, Tertiary structure, Quaternary structure, Protein secondary structure; Introduction: Hydrogen bond, Defining a secondary structure element.

UNIT-II

Methods for predicting secondary structure (GOR and J-Pred): Experimental methods for protein structure determination: Nuclear magnetic resonance (NMR), Protein tertiary structure modeling.

UNIT-III

Protein tertiary structure modeling: Basic concepts, Protein folding and dynamic simulation, Modeling protein side-chains, Comparative modeling, modeling approaches.

UNIT-IV

Introduction to RNA Secondary structure prediction, Methods for RNA Secondary structure prediction, Limitation of RNA Secondary structure prediction.

PRACTICALS

1. Protein structure prediction tools- PROCHECK, SOPMA.
2. Working on tools- Pfam, AACompIdent.
3. Working on tools: Translate, reverse translate,
4. RNA structure prediction software.

REFERENCES

- Basic Bioinformatics - S. Ignacimuthu
- Introduction to Bioinformatics: A Theoretical and Practical Approach
  Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Cheminformatics
- Structural Bioinformatics (Methods of Biochemical Analysis, V. 44) - by Philip E. Bourne (Editor), Helge Weissig (Editor), 2000.
- Understanding DNA - by Chris Calladine, Horace Drew, Ben Luisi, and Andrew Travers