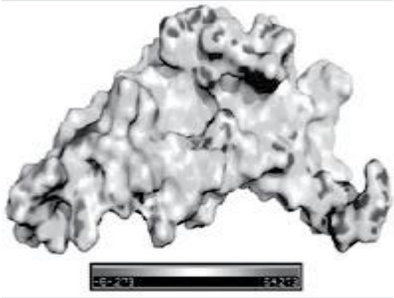
16BI401 STRUCTURAL BIOINFORMATICS



Source:
Dr. D. Vijaya Ramu
BT, VU Dirisala et al., (2013) Molecular
Biotechnology 55: 277-287.

Hours Per Week :

L	T	P	C
3	1	-	4

Total Hours :

L	T	P
45	15	-

WA/RA	SSH/HSH	CS	SA	S	BS
5	45	-	8	2	5

Course Description and Objectives:

This course offers insights into biophysical concepts of macromolecules and the conformational analysis and forces that determine the protein and nucleic acid structure. The objective of this course is to provide knowledge on structures, size and shape of macromolecules using various tools such as X-ray crystallography and NMR.

Course Outcomes:

The student will be able to:

- utilize the tools to perform structural analysis of macromolecules.
- understand the basic principles of various methods of spectroscopy and its applications.
- comprehend the concepts behind X-ray diffraction and X-ray crystallography.

SKILLS:

- ✓ *Analyze open reading frames (ORF).*
- ✓ *Perform restriction mapping insilico.*
- ✓ *Perform codon optimization.*
- ✓ *Analyze protein sequences by BLAST.*

ACTIVITIES:

- *Determine the structure of protein.*
- *Identify domains in the gene sequences.*

UNIT - 1 **L-9, T-3**

INTRODUCTION TO LEVELS OF STRUCTURES IN BIOLOGICAL MACROMOLECULES : Basic strategies in biophysics; Principles and concepts used in biophysical analysis of life processes; Biomolecules and their interactions; Size and shape of macromolecules.

UNIT - 2 **L-9, T-3**

CONFORMATIONAL ANALYSIS: Forces that determine protein and nucleic acid structure - basic problems, polypeptide chain geometries, potential energy calculations, observed values for rotation angles, hydrogen bonding, hydrophobic interactions, ionic interactions and disulphide bonds.

UNIT - 3 **L-9, T- 3**

STRUCTURAL ANALYSIS OF MACROMOLECULES: Prediction of protein structure and nucleic acids; General characteristics of nucleic acid - geometries, glycosidic bond rotational isomers and those puckering backbone rotational isomers and ribose puckering forces stabilising ordered forms, base pairing and base stacking tertiary structure of nucleic acids.

UNIT - 4 **L-9, T-3**

SPECTROSCOPY AND METHODS OF VISUALIZATION: Absorption spectroscopy; Linear and circular dichroism; Emission spectroscopy; Nuclear magnetic resonance spectroscopy; Methods of direct visualisation; Macromolecules as hydrodynamic particles; Macromolecular diffusion; Ultracentrifugation; Viscometry.

UNIT - 5 **L-9, T-3**

X-RAY DIFFRACTION: X-Ray crystallography; X-Ray diffraction; Determination of molecular structures; Generation of guttation coordinates.

TEXT BOOK:

1. R.Cantor and P.R. Schimmel , "Biophysical Chemistry", Vol. I and II, W.H. Freeman and Co., 1985.

REFERENCE BOOKS:

1. M. Daniel , "Basic Biophysics for Biologists", Agro Botanical Publishers,1998.
2. K.E. van Holde, W. C. Johnson and P. S. Ho, "Principle of Physical Biochemistry", Prentice Hall, New York, 1998.