

INDIAN INSTITUTE OF TECHNOLOGY TIRUPATI

भारतीय प्रौद्योगिकी संस्थान तिरुपति

Yerpedu-Venkatagiri Road, Yerpedu Post, Tirupati District, Andhra Pradesh - 517 619

1.	Title of the course	Algorithms in Computational Biology
2.	Course number	CS542L
3.	Structure of credits (L-T-P-C)	2-0-0-2
4.	New course/modification to	New
5.	To be offered by	Computer Science and Engineering
6.	Prerequisite	СоТ
7.	Course Objective(s): To explore data structures and algorithms over molecular structures, sequences, networks and pathways.	
8.	Course Content: Basic concepts in biology, 3D structural representation of proteins: crystal, nuclear magnetic resonance (NMR) and binding sites, Structural and graphical representation of ligands and pharmacophores, Molecular dynamics for protein-ligand interactions and docking, Molecular sequence and structural alignment algorithms, Protein structure prediction, Graph based representation and operations on networks of genes, proteins and pathways, Algorithms for cellular process simulation, Data visualization tools for molecular structures and graphs.	
9.	Textbook(s): 1. Philip E B and Jenny G, Structural Bioinformatics, Wiley-Blackwell, 2nd Edition, (2009). 2. David W M, Bioinformatics - Sequence and Genome Analysis, Cold Spring Harbor Laboratory Press, 2nd Edition, (2004).	
10.	Reference(s): 1. Bruce R D, Sorin I, Pavel A P and Michael S W, Algorithms in Structural Molecular Biology, MIT Press, 1st Edition, (2011). 2. Richard D, Sean E, Anders K and Graeme M, Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids, Cambridge University Press, 1st Edition, (1998). 3. Johann G and Thomas E (editors), Chemoinformatics: A Textbook, Wiley, 1st Edition, (2003).	