



# BIO-INFORMATICS : ALGORITHMS AND APPLICATIONS

## PROF. MICHAEL GROMIHA

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**PRE-REQUISITES** : Basic knowledge of Biology and any computer language would be helpful

**INTENDED AUDIENCE** : Students, PhD scholars, teachers, industry

**INDUSTRIES APPLICABLE TO** : Cognizant, TCS

## COURSE OUTLINE :

Bioinformatics is an interdisciplinary field of science for analyzing and interpreting vast biological data using computational techniques. In this course, we aim to give a walkthrough of the major aspects of bioinformatics such as the development of databases, computationally derived hypothesis, algorithms, and computer-aided drug design. During the first section of the course, we will focus on DNA and protein sequence databases and analysis, secondary structures and 3D structural analysis. The second section will be devoted to applications such as prediction of protein structure, folding rates, stability upon mutation, and intermolecular interactions. Further, we will cover computer-aided drug design using docking and QSAR studies. This course is designed to nurture skills and knowledge required for aspiring students, young biologists and research scholars to develop algorithms and tools in bioinformatics.

## ABOUT INSTRUCTOR :

Prof. M Michael Gromiha received his Ph.D in Physics from Bharathidasan University, India and served as STA fellow, RIKEN Researcher, Research Scientist and Senior Scientist at Computational Biology Research Center, AIST, Japan till 2010. Currently, he is working as an Associate Professor at Indian Institute of Technology (IIT) Madras, India. He is teaching courses on bioinformatics, protein structure and function, protein interactions: computational techniques, big data analysis and handling computational biology lab. His main research interests are structural analysis, prediction, folding and stability of globular and membrane proteins, protein interactions and development of bioinformatics databases and tools. He has published over 200 research articles, 40 reviews, 5 editorials and a book on Protein Bioinformatics: From Sequence to Function by Elsevier/Academic Press. His papers received more than 9000 citations and h-index is 52. He is an Associate Editor of BMC Bioinformatics as well as Editorial Board Member of Scientific Reports, Biology Direct, Journal of Bioinformatics and Computational Biology and Current Computer Aided Drug design. He has received several awards including Oxford University Press Bioinformatics prize, Okawa Science Foundation Research Grant, Young Scientist Travel awards from ISMB, JSPS, AMBO, ICTP etc., Best paper award at ICIC2011, ICTP Associateship award, ICMR International fellowship for Senior Biomedical Scientists, INSA senior scientist award, Best paper award in Bioinformatics by Department of Biotechnology, India, Institute Research and Development Award at IIT Madras and Outstanding Performance award from Initiative for Parallel Bioinformatics (IPAB), Tokyo Institute of Technology, Japan. He is a member of the National Academy of Sciences, India.

## COURSE PLAN :

**Week 1** : Introduction, DNA sequence analysis, DNA Databases

**Week 2** : Protein structure and function, protein sequence databases, sequence alignment

**Week 3** : PAM matrix, Global and local alignment, BLAST: features and scores

**Week 4** : Multiple sequence alignment, Conservation score, phylogenetic trees

**Week 5** : Protein sequence analysis, hydrophobicity profiles, non-redundant datasets

**Week 6** : Protein secondary structures, Ramachandran plot, propensity, secondary structure prediction

**Week 7** : Protein tertiary structure, Protein Data Bank, visualization tools, structural classification

**Week 8** : Protein structural analysis, protein structure prediction

**Week 9** : Protein stability, energetic contributions, database, stabilizing residues

**Week 10** : Protein folding rates, proteins interactions, binding site residues

**Week 11** : Computer aided drug design, docking, screening, QSAR

**Week 12** : Development of algorithms, awk programming, machine learning techniques, applications using WEKA