



STRUCTURAL BIOLOGY

PROF. SAUGATA HAZRA

Department of Biotechnology
IIT Roorkee

TYPE OF COURSE : Rerun | Core | UG/PG**COURSE DURATION** : 12 Weeks (24 Jan' 22 - 15 Apr' 22)**EXAM DATE** : 23 Apr 2022

PRE-REQUISITES : This is an introductory course so anyone should follow it, basic knowledge of biology might be helpful

INTENDED AUDIENCE : Biotechnology/Pharmaceuticals/Bioinformatics /Chemistry and related programs
Also it would be a nice introductory course to, research scientists in biotechnology, pharma industry, veterinarians and clinicians/medical people involved in basic research.

INDUSTRIES APPLICABLE TO : Pharmaceutical, Biotechnology, Biochemical Engineering

COURSE OUTLINE :

Post NGS (Next Generation Sequencing) era has completely changed the way of understanding research, especially in the field of biomedical science. Today the complete genome sequencing of an organism is done in a few days providing the researchers with thousands of genes hence thousands of protein sequences. But to proceed further we need to understand the three-dimensional architecture of the protein molecules. The current course would take an initiative to educate the students in gathering knowledge about the structural units forming biological macromolecules, their architectural hierarchies, the basics of the structural biology techniques, their pros and cons, how to read and visualize 3D structure files, etc.

ABOUT INSTRUCTOR :

Prof. Saugata Hazra is a Professor in the Department of Biotechnology at the Indian Institute of Technology, Roorkee. An alumnus of IIT Kharagpur, Prof. Hazra has obtained his Ph.D. degree from the University of Illinois; Chicago (2004- 2010) in Structural Biology and Structure based Drug Designing and post-doc from St. Jude Children Research Center, Memphis, USA (2010-2011) and Albert Einstein College of Medicine, NY, USA, in the major area of Structural Biology. He joined IIT Roorkee in 2014. Current research in his group centers on catalytic divergence of enzymes involved in antimicrobial drug resistance and structure based enzyme engineering towards waste valorization. Prof. Hazra is teaching UG/PG courses like Macromolecular Crystallography, Bioinformatics, Computational Biology, and Biochemistry since his joining in IITR. He has published in several peer reviewed journals and recipient of awards like James graduate fellowship, DST-Young Scientist Award and Frontiers of Engineering from Royal Academy of Engineering etc. throughout his career.

COURSE PLAN :

Week 1: Introduction: What is post NGS era, why structural biology become so important, How to read biological macromolecules, Sequence to structure to function relationship, Protein as our target study molecule

Week 2: Protein Architecture: amino acids structure and function, Primary, secondary, tertiary and quaternary structure of protein; Motifs and domains of protein structures; Conformational analysis, Protein folding

Week 3: Bonds and energies in macromolecules- Covalent, Ionic, coordinate, hydrophobic and Vander walls interactions

Week 4: Enzymes: introduction to enzymes, how enzyme develop magic pockets, enzyme-ligand interaction, Structure-function relationship

Week 5: Structural Biology Techniques: Basics of macromolecular crystallography, Nuclear Magnetic Resonance (NMR) and Cryo-Electron microscopy, advantages and disadvantages of all the processes: comparative discussion

Week 6: Macromolecular Crystallography: Crystallization and Data Collection Crystallization, method of protein crystallization, thermodynamics and kinetics of protein crystallization, structural genomics project

Week 7: Macromolecular Crystallography: Data Analysis X-ray diffraction and Bragg equation, scattering factor, Structure factor expression, Phase problem and methods for phase determination, structure determination of macromolecules by crystallography technique

Week 8: Reading and Understanding 3D structure files: Introduction to PDB data, RCSB, reading PDB files, related calculations

Week 9: 3D structure Visualization: Visualization of macromolecules using Pymol and Coot

Week 10: Introduction to Molecular Dynamics Simulation: Need of simulation in studying biology, Building realistic atomistic model, Size and Times scale of macromolecular movements...

Week 11: Applicative measures01: Case studies: Structure based drug designing

Week 12: Applicative measures02: Case studies: Protein Engineering