YENEPOYA
(DEEMED TO BE UNIVERSITY)
Recognized under Sec 3(A) of the UGC Act 1956

Structural Biology

Core course for Pre-PhD: 4 credits

Yenepoya Research Centre
Yenepoya (Deemed to be University)
University Road, Deralakatte
Mangalore – 575018

Course Name: Structural Biology

1. Course Type : Core
2. Level : Ph.D. (Pre-PhD course work)
3. Credit Value: : 4 Credits
4. Total Hours : 60 (L:P:S: 10:25:25)
5. Total Marks: : 100 (IA= 40 + Final exam= 60)

6. Course Objectives

- To expose the research scholars to the important techniques and concepts associated with the emerging field of Structural Biology.
- Train the research scholars to acquire skills to design and perform experiments that are relevant for further execution of research in emerging areas of Structural Biology
- To provide exposure to advanced research topics and techniques pertaining to the principles behind Protein stability, folding and associated function and malfunction.
- Train the research scholars in Python and C driven software for protein structure calculation, interaction determination and to figure out the correlation between its dynamics with function.

7. Learning Outcome

This course will enable the students to design and analyze the detailed methodology using appropriate molecular biology, bio analytics and biophysics-driven techniques to address the biological questions from structural perspective.

8. Competencies

1. Describe different bio-analytical tools and techniques and suitable in-silico and wet lab techniques applicable in structural biology research
2. Describe NMR driven data analysis for structure calculation
3. Comprehend recombinant protein production, protein engineering and different spectroscopic/analytical techniques for undertaking complex research problems in structural biology field
4. Evaluate and apply suitable molecular biology techniques for application in structural biology research
5. Perform operations of different equipment used in analytical laboratory
6. Apply suitable in-silico and wet lab techniques to perform, analyse and interpret data
7. Apply NMR driven data analytics for structure calculation
8. Interpret the mutation and associated anomalies based on protein structure,

interaction, folding and dynamics

9. Practice of ethics, safety procedures and appropriate waste disposal protocols while conducting research.

9. Content of the Course

Module 1: Molecular techniques (10 h)

1.1 Approaches for sterile laboratory environment and its importance. Different sources of contamination and its implications.

1.2 Vector design and cloning, competent cell preparation, Transformation, Protein over expression.

1.3 Electrophoresis and blotting techniques

1.4 Assays using microbial cells: MIC and MBC

Module 2: Bio-Analytical Methods (10 h)

2.1 Different types of microscopic techniques (Optical, Fluorescence, Confocal, SEM, TEM and AFM): Mode of information obtained and its application.

2.2 Different types of Spectroscopic and their application: UV-Vis, Fluorescence, IR, CD, MS, and NMR

2.3 Different types of Separation Methods and its implication: Centrifugation-Sedimentation principle, differential centrifugation, Chromatography- types (adsorption, partition, affinity, ion exchange and size exclusion)

Module 3: Basics Principles in Biophysics (15 h)

3.1 Understanding of Structure and Bonding: Pauli Exclusion Principle, Ionization energy, electron affinity and chemical binding, Electronegativity and strong bonds, secondary bonds

3.2 Concept of the electronics structure of atoms, Molecular orbital, and Covalent bonds.

3.3 Understanding of the molecular interactions: strong or weak interactions, Stereochemistry and Chirality

3.4 Introduction to Biophysical Chemistry: Basic thermodynamics, ligand binding and co-operativity in biological systems, kinetics, diffusion, and sedimentation.

Module 4: Applied Biophysics (15 h)

4.1 Understanding of the molecular organization for proteins and peptides: sequence and primary conformation of polypeptide chain, Usual/unnatural amino acids, Predicting properties from amino acid composition, Secondary confirmation of protein and its stability, Ramchandran plot, Tertiary structure and Quaternary structure of protein, symmetry consideration, Analysis of subunits and chain arrangement of subunits,

4.2 Concept development on stability of globular protein, Protein folding and dynamics.

4.3 Exposure to cutting edge protein and peptide modification/protein engineering techniques/method and its application, different kind of ligation and labeling techniques and its utility in structural studies.

Module 5: Bio-informatics and structural data analysis (10 h)

5.1 Handling of different online resources like Swissport, PubMed and PDB for generating known information about any protein.

5.2 Learning the usage of software for NMR data processing (NMR-pipe/NMRDraw) and analysis (sparky)

5.3 Learning the usage of software for 3D structure calculation (CYANA and Xplor-NIH)

5.4 3D representation and modification of the protein/nucleic acid structure and interactions using PyMOL/MOLMOL software.

Teaching-learning methods

Modules	**Teaching-learning**		
	Lecture	Practical/Hands on	Self-study
Module 1: Molecular techniques	1.1		
	1.2		1.2
		1.3	1.3
		1.4	1.4
Module 2: Bio-Analytical Methods	2.1	2.1	2.1
	2.2	2.2	2.2
		2.3 (Team work)	2.3 (seminar)
Module 3: Basics Principles in Biophysics	3.1		3.1
	3.2		3.2 (Seminar)
		3.3 (problem set)	3.3
	3.4	3.4 (Team work)	3.4
Module 4: Applied Biophysics	4.1		4.1 (Seminar)
		4.2 (Problem set)	4.2 (Seminar)
	4.3	4.3	4.3(Seminar)

Module 5: Bio-informatics and structural data analysis		5.1(Problem+ group discussion)	5.1(seminar)
	5.2	5.2 (assignments group discussion)	5.2
	5.3	5.3 (assignments)	5.3
		5.4 (Group discussion)	5.4

10. Assessments

Formative assessments: (40 Marks)

1	Internal Exams - 40 marks each (2)	20 M
2	Seminar (2)	8 M
3	Group discussion (2 Including ethical and regulatory issues)	6 M
4	Case studies (2)	6 M

Summative Assessment: (60 Marks)

Sl. No.	Details	Q X M
Two Questions to assess the knowledge and problem solving abilities in the given context		4X10 M=40 M
1	Knowledge on application of any of the major instruments used in the In vitro and in vivo cancer research for generating data (E.g. Explain the principle and protocol for the use of Fluorescence for membrane permeability study.)	
2	Problem solving ability: Designing experimental protocol for a given research problem and interpretation of data (E.g. determination of the secondary structure and conformational state using CD data)	
3 4	Two questions to assess the analytical skills to solve a given hypothetical research problem Write the methodology for solving a given research (e.g. Generation of basic information about sequence and hydrophobicity, solubility index of any given protein /Processing of the raw data of 1D and 2D NMR and basic amino acid type determination/Basic methodology planning for determination of antimicrobial activity of a compound)	
5	Descriptive questions from module 2, 3 and 4.	4X5=20 M

*A question bank will be maintained with multiple scenarios.

Learning Resources

Reference books:

1. Atkins, P. and De Paula, J (2016). Physical chemistry for the life sciences. New York: Oxford University Press.
2. Beard, D. and Qian, H (2010). Chemical biophysics. Cambridge: Cambridge University Press.
3. Bohr, H (2009). Handbook of molecular biophysics. Weinheim: Wiley-VCH.
4. Branden, C. and Tooze, J (2012). Introduction to Protein Structure. Taylor and Francis.
5. Cantor, C. and Schimmel, P (2001). Biophysical chemistry. New York: W.H. Freeman.
6. Chang, R (2005). Physical chemistry for the biosciences. Sausalito, Calif.: University Science Books.
7. Claridge, T (2016). High-resolution NMR techniques in organic chemistry. Amsterdam: Elsevier.
8. Friebolin, H (2011). Basic one- and two-dimensional NMR spectroscopy. Weinheim: WILEY-VCH.
9. Haynie, D (2007). Biological thermodynamics. Cambridge
10. Jackson, M (2006). Molecular and Cellular Biophysics. Cambridge: Cambridge University Press.
11. Lesk, A (2016). Introduction to protein science. Oxford: Oxford University Press.
12. Logan, S (1998). Physical chemistry for the biomedical sciences. London: Taylor &Francis.
13. Narayanan, P (2010). Essentials of biophysics. Tunbridge Wells [England]: Anshan.
14. Schulz, G. and Schirmer, R (2013). Principles of Protein Structure. New York, NY: Springer.
15. Serdyuk, I., Zaccai, N. and Zaccai, G (2007). Methods in molecular biophysics. Cambridge: Cambridge University Press.
16. Voet, D. and Voet, J (2013). Principles of biochemistry. Hoboken, N.J. John Wiley & Sons.
17. Waigh, T. (2007). Applied biophysics. Chichester, England: J. Wiley & Sons.
18. Whitford, D. (2003). Protein structure & function. New York: Wiley.

Online Resources: URLs/websites

- https://www.ebi.ac.uk/Tools/msa/clustalo/
- https://spin.niddk.nih.gov/NMRPipe/doc1/
- https://www.cgl.ucsf.edu/home/sparky/
- http://www.cyana.org/wiki/index.php/CYANA_structure_calculation_with_automated_NOESY_assignment_(e-NMR_-_Extend-NMR_Workshop)
- https://nmr.cit.nih.gov/xplor-nih/
- https://pymol.org/2/
- https://www.ncbi.nlm.nih.gov/
- https://blast.ncbi.nlm.nih.gov/Blast.cgi
- https://web.expasy.org/protparam/

Student should refer leading Journals and publishers in the subject category and list is not limited to specific titles.