**Ahmedabad University**

| Course | BIO552 Computational Structural Biology | Semester | Monsoon Semester 2024 |
|---|---|---|---|
| Faculty Name(s) | Balaji Prakash | Contact | balaji.prakash@ahduni.edu.in |
| School | SAS | Credits | 3 |
| GER Category: | Not Applicable | Teaching Pedagogy Enable:NO | P/NP Course: Can not be taken as P/NP |

| Schedule | Section 1 | 11:00 am to 12:30 pm | Thu | 01-08-24 to 26-11-24 |
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| | | 11:00 am to 12:30 pm | Tue | 01-08-24 to 26-11-24 |

| Prerequisite | BCS102 Biochemistry I & BIO 107 Concepts of biology/BIO 107 Concepts of Biology/BIO107 Concepts of Biology<br>OR<br>BIO101 Introductory Biology & BIO209 Introductory Biochemistry/BIO209 Basic Biochemistry<br>OR<br>BIO101 Introductory Biology & BIO209 Introductory Biochemistry/BIO209 Basic Biochemistry |
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| Antirequisite | Not Applicable |
| Corequisite | Not Applicable |

| Course Description | Life forms exhibits extraordinary diversity in structures both at the organism level and at the molecular level. Proteins must acquire a well define three-dimensional shape to function under physiological conditions. Advancement in biophysical methods have created a repertoire of atomic level details of different biomolecules such are proteins, DNA, RNA, etc. This course aims at understanding different concepts involved in computational analysis of biomolecular structures. The students would learn about different databases related to structure biology and understand the file-formats for storing structural information. The course would provide an opportunity to learn about accessing the quality of experimentally determined structures. Students would have an opportunity to understand the challenges in structural investigation of biomolecules using conventional experimental methods and would be able to evaluate the application of computational approaches to study structural biology. Over the years tremendous advancements have been made in the field of protein structure prediction. Students would learn about different methods for structure prediction and would be able to appreciate the opportunities and challenges in this field. In addition, students would learn to model interactions between biomolecules such as protein-protein and protein-DNA interactions. The course would help students understand the significance of protein structure and thereby understand the mechanistic details of protein function. The learning from the course would enable students to pursue research in the field of structure based drug design. |
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| Course Objectives | Learn about various online resource for studying protein structures. Knowledge of experimental methods for structure determination. Learn about stereo-chemical features of proteins and visualization of structures. Evaluate methods for prediction of protein structure. Interpret concepts underlying structure comparison. Understand biomolecular interactions at structural level. |
| Learning Outcomes | To appreciate sequence-structure-function relationship. To effectively analyze protein structures and their complexes. To understand evolution at molecular level To understand how to design new functions in proteins. To learn to apply computational methods for translational research. |
| Pedagogy | Flipped classroom, lecture, group discussion, group projects. |
| Expectation From Students | To do all the assignments diligently. To read the study material suggested during the course without which it will not be possible for students to participate effectively in the class. |

| Assessment/Evaluation | <ul><li>Mid-Semester Examination:<ul><li>Written - 20%</li></ul></li><li>End Semester Examination:<ul><li>Written - 25%</li></ul></li><li>Other Components:<ul><li>Project - 25%</li><li>Assignment - 10%</li><li>Class participation (Including attendance) - 10%</li><li>Quiz - 10%</li></ul></li></ul> |
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| Attendance Policy | As per Ahmedabad University Policy. |
| Project / Assignment Details | |
| Course Material | Text Book(s)<ul><li>Structural Bioinformatics, Jenny Gu, Philip E. Bourne, 2nd Edition, Wiley, ISBN: 978-1-118-21056-7, Year: 2011,</li></ul>Reference Book<ul><li>Structural Bioinformatics: An Algorithmic Approach, Forbes J. Burkowski, 1st Edition, Chapman and Hall/CRC, ISBN: 978-1584886839, Year: 2008,</li><li>• Protein Structure and Function, Gregory Petsko and Dagmar Ringe, Oxford University Press, ISBN: 9780199556847., Year: 2008,</li></ul> |
| Additional Information | |

## Session Plan

| NO. | TOPIC TITLE | TOPIC & SUBTOPIC DETAILS | READINGS,CASES,ETC. | ACTIVITIES | IMPORTANT DATES |
|-----|-------------|--------------------------|---------------------|------------|-----------------|
|     |             |                          |                     |            |                 |