

Structural Biology and Bio-computing

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The Laboratory for Structural Biology and Bio-computing (Professor K. Sekar) carries out research, which is truly interdisciplinary in nature. The laboratory is involved in elucidating the three-dimensional crystal structures of protein molecules and studying the molecular mechanisms. State of the art computational and biochemical methods are used for this purpose. First, a detailed bioinformatics analyses are performed on the protein sequences to extract valuable insights about the protein molecules of interest viz. sequence evolution, variability in different regions of the sequences, similarity against already studied proteins etc. Then, the identified protein is extracted through a series of biotechnological processes, like cloning, expression and purification. The purified protein is characterized through several biochemical and biophysical techniques, like mass spectrometry, circular dichroism, protein specific assay, ITC etc. Crystallization attempts will be made to grow good diffraction quality crystals of the purified protein. When the crystals are obtained, the three-dimensional crystal structure of the protein will be solved using X-ray diffraction data. The data obtained from bioinformatics, biochemical and biophysical studies along with the structural details are analyzed to understand the molecular mechanism and function. If necessary, molecular dynamics simulations will be carried out to better understand the function and dynamics. Thus, the students are required to know some amount of mathematics and little biology. Writing computer programs (in any language) is an added advantage.