

CHEMISTRY  
COLLEGE OF ARTS AND SCIENCES

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE students

FOR APPLICATION YEAR: 2023

PROJECT TITLE: Machine learning for the function and dynamics of protein complexes

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**Project Description**

Research in the Dima group focuses on understanding the role of various structural and cellular factors in the mechanical response of biological molecules ranging from small RNA molecules and multi-domain proteins to large fibrillar assemblies that play crucial roles in fundamental processes such as the maintenance of the cell shape, cell mobility, cell-cell adhesion, axonal growth, and cellular division.

A project for a UPRISE student is "Machine learning for the function and dynamics of protein complexes". Microtubules, large multi-filament polymeric complexes which are the main component of the cell cytoskeleton, play fundamental roles in cellular processes ranging from cellular transport to mitosis. These roles are all intimately connected with microtubules' ability to depolymerize under controlled cellular conditions. This control is exerted by a large array of microtubule associated proteins (300 or so species), which form transitory complexes with microtubules over different timescales. Recent experimental results strongly suggest that many of these protein co-factors are molecular machines that work by converting chemical energy into mechanical work, which is then applied to the microtubule polymer lattice. However, little is known about the details of the process, especially for molecular machines composed of multiple monomers, such as microtubule severing proteins. The goal of this project is to determine the relationship between the steps in the functional cycle of such molecular machines and the structural changes taking place inside the machines and of their substrates, which are important during processes such as cell division, neuronal growth, and cell-cell adhesion.

The UPRISE student will gain experience with (1) machine learning (data science) methods in chemistry, (2) simulation software designed to follow protein dynamics, (3) data analysis that couples results of simulations with experimentally derived data, (4) learning how to search databases of protein sequences and structures, and (5) learning how to read scientific papers.