DEPARTMENT OF CHEMISTRY
COLLEGE OF ARTS AND SCIENCES

APPLICATION DEADLINE: 03/01/2024

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

Ruxandra Dima
College of Arts and Sciences
304 Crosley Tower
Cincinnati OH 45221
dimari@ucmail.uc.edu
Phone: 513 556 3961
Fax: 513 556 9239

Maria Kelly
College of Arts and Sciences
1308 Crosley Tower
Cincinnati OH 45221
kelly3mi@mail.uc.edu
Phone: 513 556 9687

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 processes such as the maintenance of the cell shape, cell mobility, cell-cell adhesion, and cellular division.
A project for a UPRISE student is “Data science and 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 maintain their structural integrity and to depolymerize only under controlled cellular conditions. Cellular factors that enable the control of microtubules dynamics are the large array of microtubule associated proteins, which form transitory complexes with microtubules over different timescales. Recent experimental results strongly suggest that many of these protein co-factors work in groups and their interactions are intimately connected with changes in the microtubule lattice. However, little is known about the details of such processes. The goal of this project is to determine the relationship between the steps in the development of interactions between microtubule associated proteins and

the structural changes taking place inside the microtubules, which are important during processes such as 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. Prof. Dima will be the mentor for the UPRISE student. However, because of Prof. Dima's travel for sabbatical leave during the Spring 2024 semester, students will meet with Maria Kelly, the senior graduate student in the Dima group, during the application process. Maria's contact information is kelly3mi@mail.uc.edu or by phone at 513 556 9687. Her office is in 1308 Crosley Tower.