This project aims to explore changes in proteins called post-translational modifications (PTMs) and understand their role in various biological processes. PTMs involve modifying specific parts of proteins (covalent modifications of amino acids side-chains or the protein's C-or N-termini), and these changes can impact various phenomena such as the regulation of enzyme activities and protein stability. There are more than 400 types of PTMs, and they play a crucial role in many biological functions. Disruptions in PTMs are linked to diseases like Alzheimer's, Parkinson's, heart failure, autoimmune diseases, and cancer.

Studying PTMs is challenging due to their transient nature and the complexity of their analysis. Advances in molecular dynamics (MD) simulations, a way to study protein structure and dynamics with the use of computational power, have shown promise. In this project, a physics-based coarse-grained molecular UNRES force field will be used to allow the study of larger systems and longer timescales compared to all-atom methods.

The project involves introducing new interaction sites representing modified protein side-chains. This requires defining these sites in a simplified (coarse-grained) representation and determining their behavior and interactions using analytical expressions. Predicting the parameters for these expressions will be treated as a machine-learning problem, making the process faster.

New interaction sites introduced into the UNRES force field, describing post-translationally modified side chains of amino acid residues, will be used to study the effect of PTMs on the binding of kinesin to microtubulin. Kinesin and microtubulins work together in a cell transportation process. The kinesin "trucks" attach to the microtubulin "roads" and move along them to transport various materials within the cell, ensuring that the right components get to the right places. Understanding how kinesin and microtubulins bind is crucial because disruptions in this process can affect the cell's internal logistics. This binding plays a vital role in maintaining the cell's health and proper functioning. This research could provide valuable insights into the role of PTMs in biological processes and diseases, contributing to the development of new treatments or interventions. Additionally, machine learning method to predict the parameters designed and tested in this project can be transferable for different cases