

This thesis leverages the CoVAMPnet neural network architecture to analyze the dynamics of apolipoprotein E (APOE), a protein involved in the development of Alzheimer's disease. CoVAMPnet offers a versatile machine learning framework for extracting meaningful features from high-dimensional molecular dynamics data and constructing Markov state models to characterize protein conformational dynamics. By applying CoVAMPnet to APOE simulations, the thesis successfully captures the protein behavior by revealing its key conformational states and structural transitions. These findings provide new insights into the dynamics of APOE and its potential role in Alzheimer's disease. The thesis also investigates the influence of a small molecule drug candidate 3SPA on APOE's conformational behavior, shedding further light on its therapeutic possibilities. Overall, this work demonstrates CoVAMPnet's effectiveness in analyzing and comparing the dynamics of larger proteins in an interpretable manner, reinforcing its potential application for complex biomolecular studies.