Predicting protein structure and drug docking sites through computational methods

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Proteins are complex molecules, composed of one or more polypeptide chains, that play critical roles within the body. Understanding the interactions between proteins and ligands, such as small molecules is central to understanding the biological function and identifying candidate drugs. The purpose of this project was to create a computational workflow for accurately predicting protein structures and predicting potential molecular drug docking sites. A reliable computational approach would allow for a more efficient way for drug design and discovery in an easier and faster way. A combination of computational tools were used to retrieve an established protein/ligand structure, visualize the protein and its ligand, and run simulations to predict docking of the ligand with a test protein. AlphaFold was used to predict the protein structure based on its amino acid sequence that was fetched in Chimera. Chimera was used to save the literature structure protein as a dimer and monomer, and ligand site. It was used again to visualize the accuracy of AlphaFold's predicted protein and the reference protein by aligning the structures. Autodock Tools were used to prepare the protein for docking and then used in Autodock Vina at an exhaustiveness of 100. Autodock Vina was used to perform simulations on the accuracy of where the program would place the ligand (where the drug would dock). The docking sites of the predicted ligand were not a complete match. Therefore, further investigation should be done to determine if this methodology can be used as an accurate and effective simulation for drug docking.