1. Virtual Box and Ubuntu to simulate the folding of proteins
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3. Abstract

Studying biomolecule functions at a molecular level can be facilitated through this method. It can be applied to examine the structures of organisms from any source. Progress in comprehending this technique can result in medical breakthroughs, offering new avenues to help patients Using software like Virtual Box we are able to download a program called Ubuntu. By using Ubuntu we are able to program it to create 3D images of proteins folding or knotting. Protein knots are rare and intriguing topological features where the polypeptide chain of a protein forms a closed loop that passes through itself. These knots can influence protein stability, function, and dynamics, and their study provides valuable insights into the folding and unfolding processes of proteins. The knots that are formed allow for stability and can enable active sites. By programming the Chrymotryspsin Inhibitor 2 (CI2), we are able to visualize the folding because it has only three conformation states, (1) the folding states, (2) unfolded states, and (3) the transition states. The transition states are a bit more complicated than the folded and unfolded states. Using CI2 in Ubuntu allows us to visually understand the functions of the biomolecules at the molecular level. Since CI2 only has three main states, it makes it easy to see the different stages as the temperature changes. The knot forms on CI2 during the folded and unfolded stages. In order to view these changes, we relied on visualization software (VMD) to aid the actual trajectory of CI2 when it flipped between the sages. Due to technical difficulties (files were lost during a software reboot) and other unfortunate circumstances, we were not able to interpret the data.