Investigation of Protein Tertiary Structure and Intermolecular Forces of Ligand Associations through Computer Modeling

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The purpose of this project was to develop an algorithm capable of predicting protein structure. The first step was to research how other protein modeling software work like homology modeling, threading/fold recognition, and ab initio methods. Ab initio and threading/fold recognition were promising but require computational power not available in a laptop. Homology modeling was the most favorable for a learning algorithm since it uses an online database such as the PDB as a template and then computes the protein structure from there. However, the use of a learning algorithm takes away from the actual chemical bonding that makes all of the protein sequences because no one really knows how it works. With the template, the algorithm computes what the protein would look like and uses PyMOL to display the predicted protein structure. The results show striking similarities between the actual protein sequences and the learning algorithm predicted sequences. Most tertiary structures are approximately the same in shape. α-helices and β-pleated sheets appear to be roughly about the same place with about the same twists and turn respectively. Protein modeling also depends on the environment where the protein is synthesized so little red dots and “+” signs are added to simulate charges as an actual protein would. The use of an online database allows for a lighter, faster, and cheaper model of a protein.