Identification of unstable points in protein using analiysis prepheral of each residue

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Abstract: Engineering of proteins for stability is a challenging field since it is critical for broadening the industrial use of recombinant proteins[1]. An important factor governing the folding of any protein is the distribution of its polar and nonpolar amino acids. The nonpolar (hydrophobic) side chains in a protein tend to cluster in the interior of the molecule. In contrast, polar (hydrophile) side chains tend to arrange themselves near the outside of the molecule, where they can form hydrogen bonds with water and with other polar molecules. So it seems logical that if the polar amino acids within the protein may be a suitable candidate for non-polar mutation in an amino acid to the protein more stable. There are some polar amino acids in protein interiors, however, these are very important in defining the precise shape adopted by the protein because the pairing of opposite poles is even more significant than it is in water[2]. Therefore, it seems logical that if the residue is present within the protein, it can be a suitable candidate for mutation to non-polar amino acids to make the protein more stable. Nevertheless, some amino acids are located within the proteins, and in protein stability also plays an important role since the placement of opposite poles in the protein core is more effective than the conjugate produced by water molecules. To do this, you need to have information about the environment which surrounds the desired amino acid. In order to, a tool was developed to determine the environmental information surrounding any amino acid in the folded protein. This information includes the type of peripheral environment, neighbors, and the contribution of each of them. To evaluate the contribution of each residue to the structural stability of the protein, the surrounding hydrophobicity of each amino acid was computed. This means that each residue was considered along with its neighbors. Models were suggested for local stabilization of buried residue. Our proposed model is able to predict the hydrophobic packing and polar residue that are located individually within the hydrophobic clusters and amino acids charged with hydrogen interactions and salt bridges.

Keywords: protein engineering; Hydrophobic environments; local stabilization; hydrophobic clusters

References

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