Cavity design of Bacillus circulans xylanase to increase the thermostability using computational approach

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Most proteins have small cavities inside even though they have compact globular shape. Some cavities are structurally important to the activity of proteins such as for ligand binding, enzyme catalysis, protein-protein interaction. But others have no structural role and could trigger the unfolding of protein and destabilize proteins if proteins are exposed to harsh conditions, therefore these cavities could be mutated to stabilize proteins. Previous works have enhanced the thermostability of protein by cavity-filling method. In this work, we tried to stabilize the protein by maximizing the interaction of cavity residues using computational approach. Cavities of Bacillus circulans xylanase were investigated and 12 non-catalytically important cavities were selected for mutant design. Residues of each cavity were mutated and 18 residues which have lower energy value than wildtype were suggested as stable mutants. The results of cavity redesign were validated by experiments. The details will be presented and discussed.