Rational design based on structural alignment for shifting pH optimum of Bacillus circulans xylanase

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Abstract

The improvement of enzyme characteristics for industrial applications remains an important work in all protein engineering endeavors. Here, a strategy to alter the pH optimum of the xylanase from *Bacillus circulans* was investigated. In this research, molecular modeling was performed to determine promising mutants before the mutations. First, the target residues for the mutation were picked out by structural alignments between *Bacillus circulans* xylanase and other xylanases having different pH optimums. The change in pK_a of a group due to the change in electrostatic potential for the mutation was calculated by using the molecular modeling software and the change in pH optimum was predicted from the change in pK_a of the catalytic residues. With the site-specific mutagenesis based on rational design, mutant xylanases having higher pH optimum were obtained while maintaining activity similar.