

## Novel approach to shift optimum pH of *Bacillus circulans* xylanase

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Electrostatic interactions are widely considered to be the primary factors upon which pH-dependence of enzyme catalysis is dependent. In search of general approach to shift pH optimum of enzymes towards alkaline side, we present a novel strategy to shift optimum pH of the enzymes. Our strategy is to introduce salt bridge interactions by introducing positively charged amino acid residues in juxtaposition of the available negatively charged residues surrounding the catalytic sites. The hypothesis was proved in *Bacillus circulans* xylanase model. The introduction of positively charged residues reduces the pKa of the negatively charged residues surrounding the catalytic sites, which raises the pKa of the catalytic glutamates, and thus increases the optimum pH of the enzyme. Mutation sites were kept at farther distance ( $>10 \text{ \AA}$ ) from the catalytic site to preserve the activity of the enzyme. Computational approach was applied to predict the shift in optimum pH in mutant models using Delphi, and mutation experiments were performed to verify the hypothesis and prediction. The details will be presented and discussed.