Role of a single arginine residue for the shift in pH optima of family 11 xylanases

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Modulation of electrostatic interaction within the catalytic cleft has been effective to change the pH optima of the family 11 xylanases. Introduction of positively charged residue (arginine) can be effective to modulate the existing electrostatic environment within the catalytic cleft. In this study we explore the factors responsible for a larger shift in pH optima towards alkaline side. Structural comparison showed the presence of a single arginine residue in the xylanases with the pH optima >6.5 at equidistance (8-9 Å) to the catalytic glutamates. A tyrosine residue is present in between the catalytic glutamates and the arginine. On the analysis of the factors for the role of the arginine into a larger shift of the pH optima up to 11, it is revealed that the pKa of the catalytic glutamates is modulated by the spatial orientation of the arginine which is intrinsic pKa and interaction energy dependent. On formulating this structural difference by using pKa System in pKa tool, it is concluded that the shift in pH optima of the enzymes towards >6.5 is very sensitive to the differences in intrinsic pKa of the tyrosine and the arginine and heavily influenced by the interaction energy between these two residues.