Biodegradation of anionic polyacrylamide mediated by laccase and amidase: docking, virtual mutation based on affinity and DFT study

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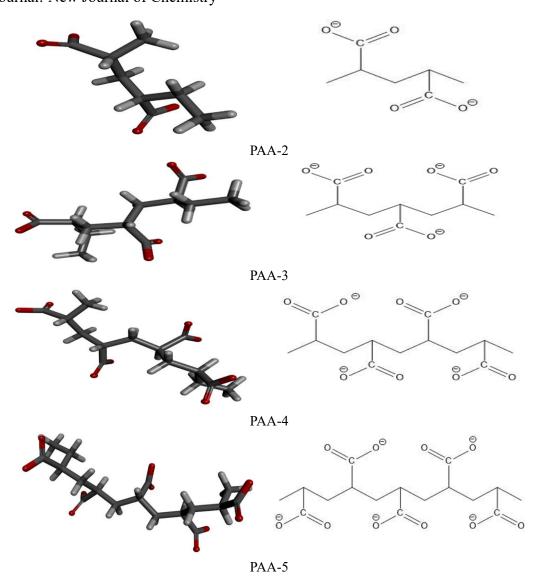


Fig.S1 Minimized stick structural models of PAA (left) (Elements: gray: carbon; white: hydrogen; red: oxygen) and chemical structures of PAA (right)

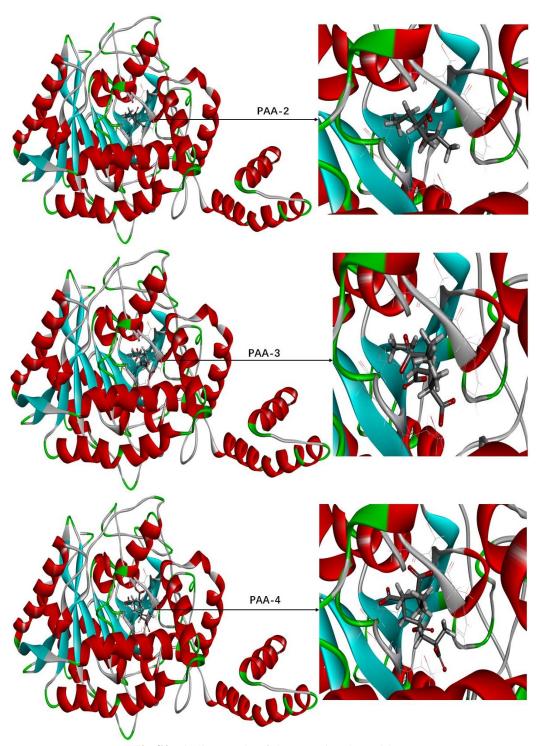
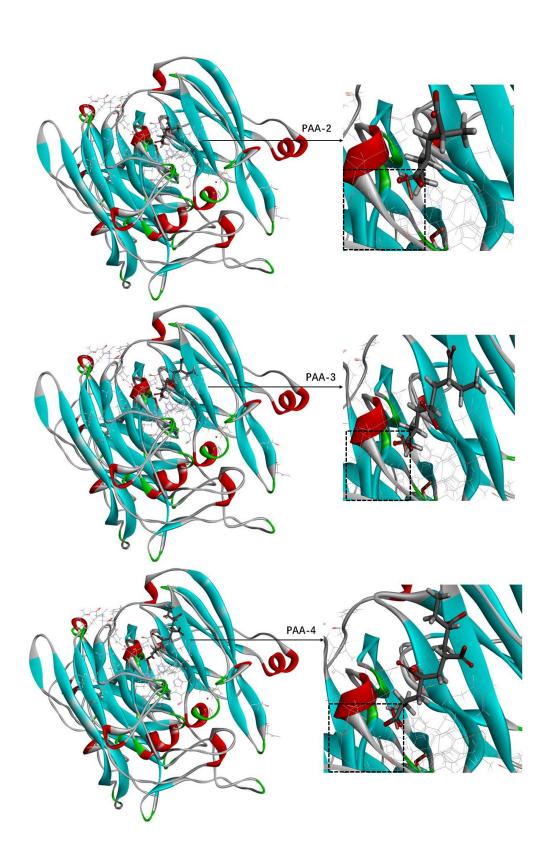


Fig.S2 Binding mode of the PAA in Rh Amidase
(The amino acids at the active site of Rh Amidase are showed as the line pattern, and the ligands are showed as stick model)



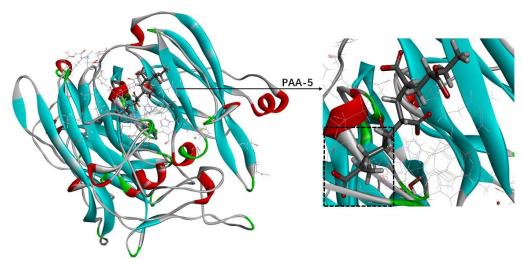


Fig.S3 Binding mode of the PAA in *B. subtilis* laccase (The amino acids at the active site of *B. subtilis* laccase are showed as the line pattern, and the ligands are showed as stick model)

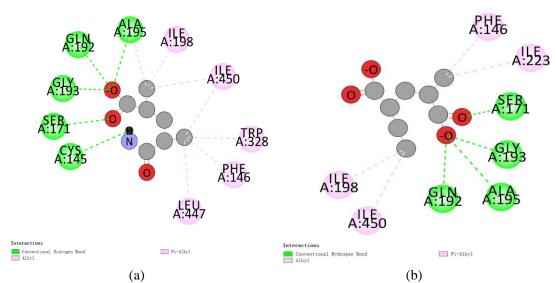


Fig.S4 2D interaction between Rh Amidase and HPAM-2(a) or PAA-2(b)

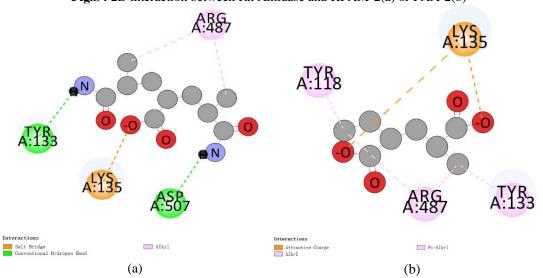


Fig.S5 2D interaction between B. subtilis laccase and HPAM-3(a) or PAA-2(b)