

Insights into the Catalytic Mechanism of *N*-Acetylglucosaminidase Glycoside Hydrolase from *Bacillus subtilis*: A QM/MM Study

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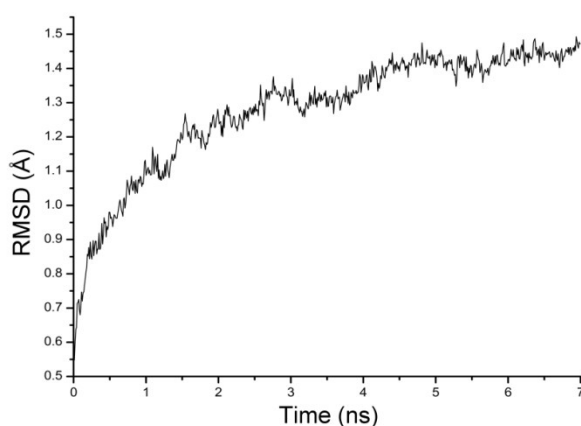


Figure S1 Time dependence of the root-mean-square deviation (RMSD) from 7ns MD simulations for substrate-enzyme complex system.

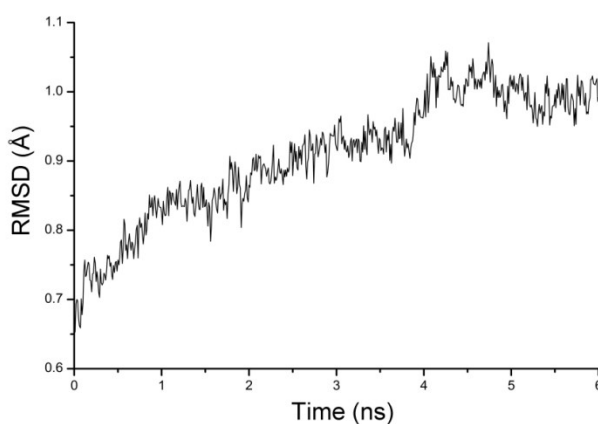


Figure S2 Time dependence of the root-mean-square deviation (RMSD) from 6ns MD simulations for Mod-A of deglycosylation step.

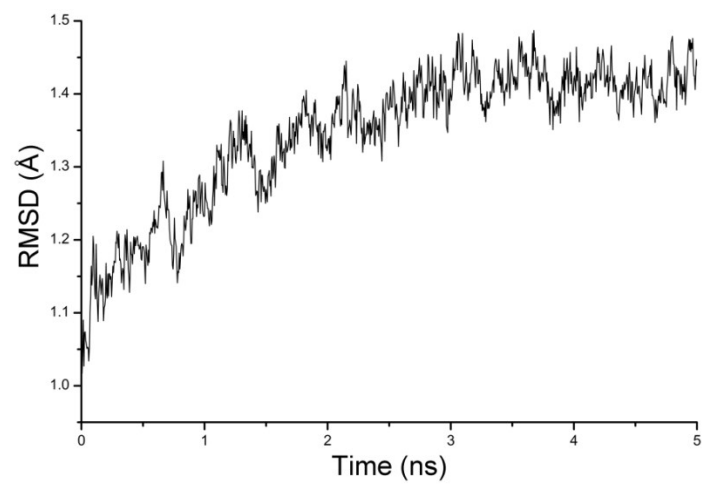


Figure S3 Time dependencies of the root-mean-square deviation (RMSD) from 5ns MD simulations for Mod-B of deglycosylation step.