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

Hao Su, Xiang Sheng, Yongjun Liu*

Key Laboratory of Colloid and Interface Chemistry, Ministry of Education, School of Chemistry and Chemical Engineering, Shandong University, Jinan, Shandong 250100, China

Corresponding Author: Tel.: +86 53188365576; fax: +86 53188564464. Email address: yongjunliu_1@sdu.edu.cn (Y. Liu).

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.