

# QM/MM Approach on the Structural and Stereoelectronic Factors governing Glycosylation by GTF-SI from *Streptococcus mutans*

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KEYWORDS: *GTF-SI*, *glucansucrase*, *glucans*, *QM/MM*, *mechanism*, *enzymatic catalysis*.

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## Supporting Information

1. QM/MM scan along the reaction coordinate defined as  $RC = d(C1 - O_G) - d(C1 - OD1) - d(HE2 - O_G)$ .....p.1
2. Molecular representation of the active site of the full enzyme model of GTF-SI at the Reactant structure.....p.1

Additional full enzyme model results obtained at the QM(BP68/6-31G\*)/MM(CHARMM27) level of theory.

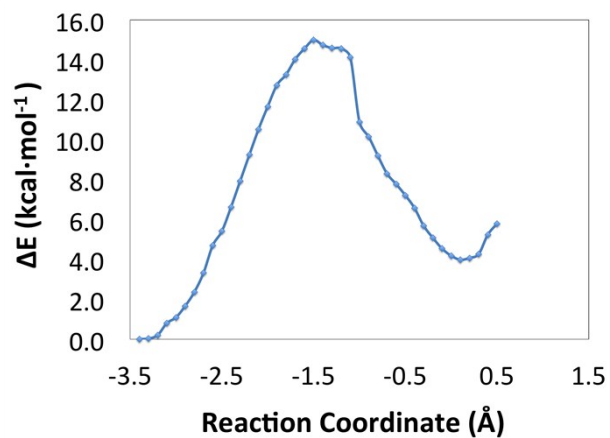


Figure S1. Energy profile for the CGE formation as a function of the asymmetric reaction coordinate (RC) at the BP86/6-31+G(d)/MM(CHARMM27) level of theory.

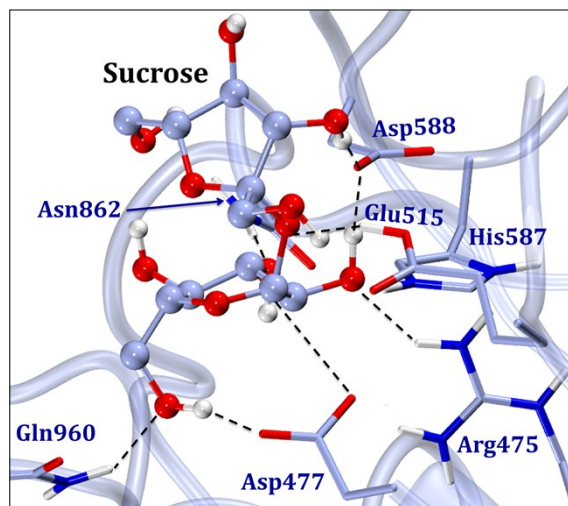


Figure S2. Snapshot of relevant interactions between sucrose and active site residues at the Reactant structure.