Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Role of conserved Arginine in GH70 family: A Computational study on the Structural Features and its Implications on the Catalytic Mechanism of GTF-SI from *Streptoccocus mutans*

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KEYWORDS: GH70, *GTF-SI, glucansucrase, glucans, QM/MM, mechanism, enzymatic catalysis.*

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Supporting Information

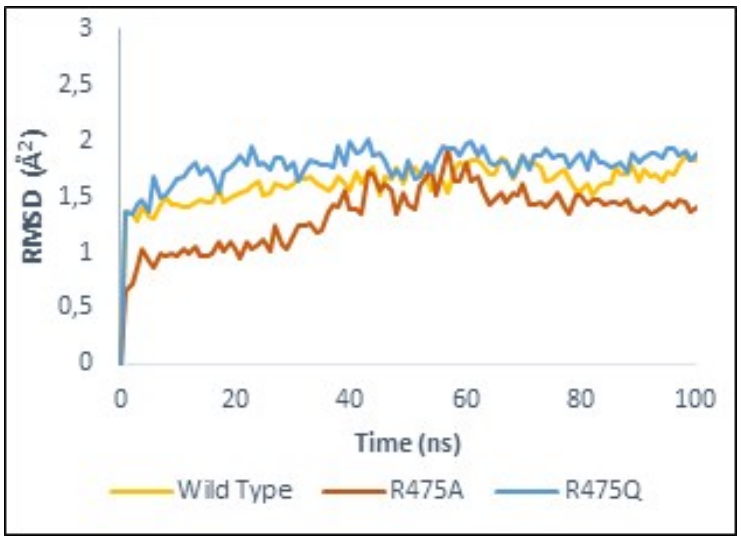

Figure S1. Root Means Square Displacements (RMSD) of the MD simulations carried out.

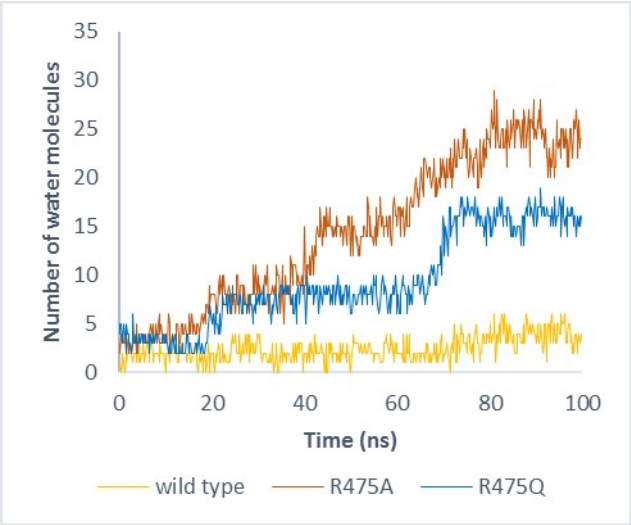

Figure S2. Average of water molecules in the active site along of MD simulations

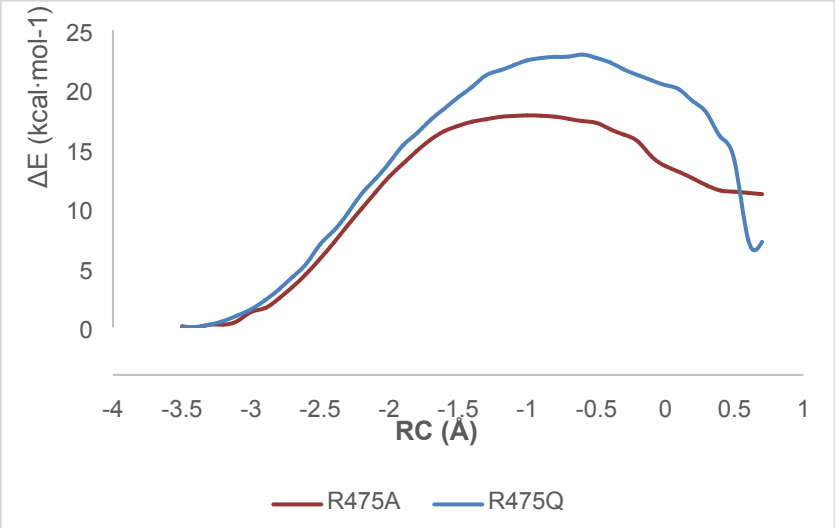

Figure S3. QM/MM scan along the reaction coordinate defined as RC = *d* (C1 – O_G)– *d*(C1– OD1) – *d* (HE2-O_G).

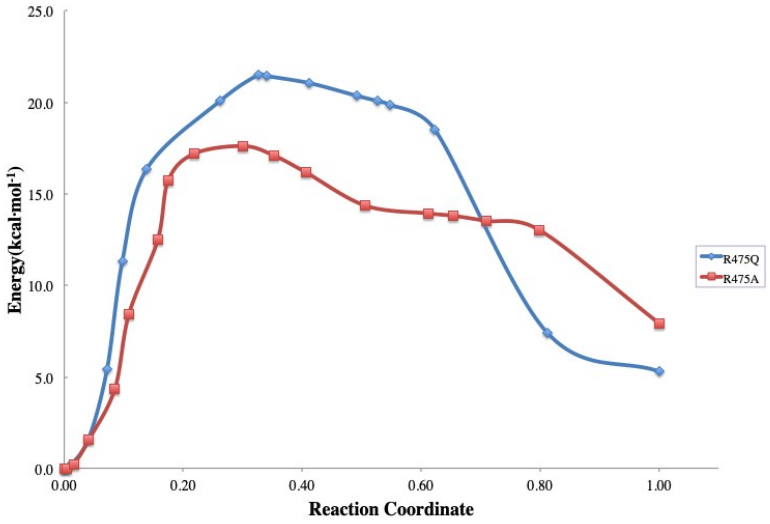

Figure S4. Minimum energy path (MEP) for the formation of CGE. The energy values are relative to the energy of the reactant and were obtained at BP86/6-31G(d) level of theory. The reaction coordinate is based on the structural difference between points along the CPR trajectory and the reactant structure. It was normalized between 0 for the reactant and 1 for the product.