Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Understanding the Different Activities of Highly Promiscuous MbtI by Computational Methods

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Supporting Information

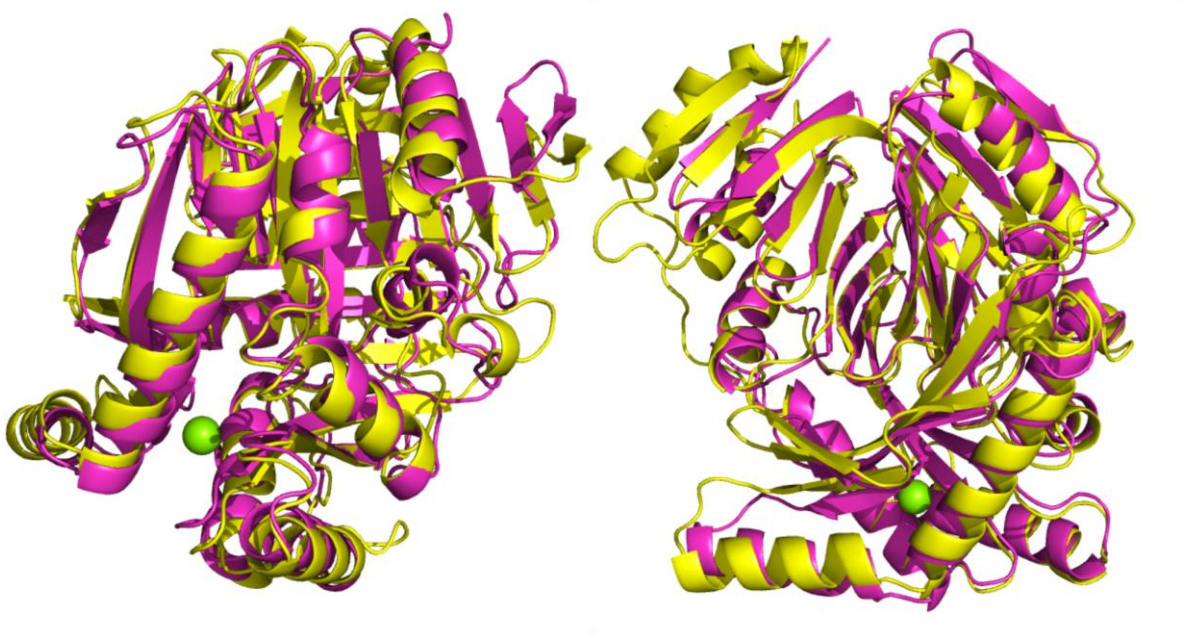

Figure S1. X-Ray Structures Irp9 (2FN1, in purple), MbtI (2G5F, in yellow). The Magnesium atom is in green.

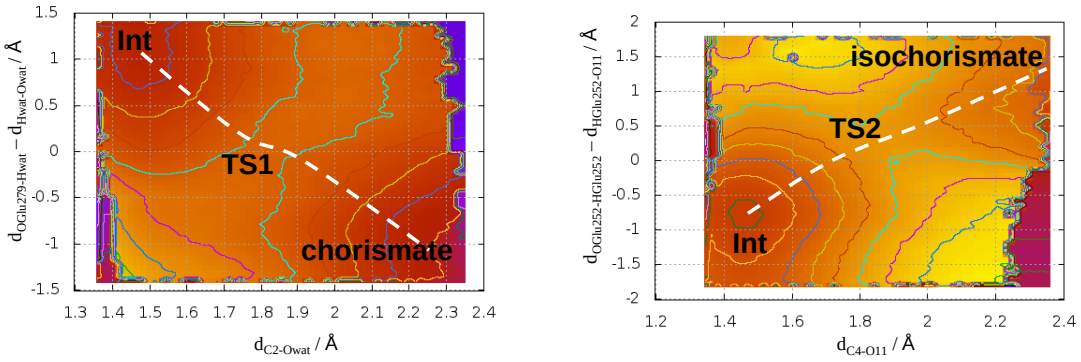

Figure S2. 2D-PMFs performed at 300 K and corrected at M06-2X level, to study the IS activity of MbtI. Isoenergetic lines are drawn every 5 kcal·mol^{-1}, dark red regions correspond to the minima, while yellow colour represent higher energies on the surface.

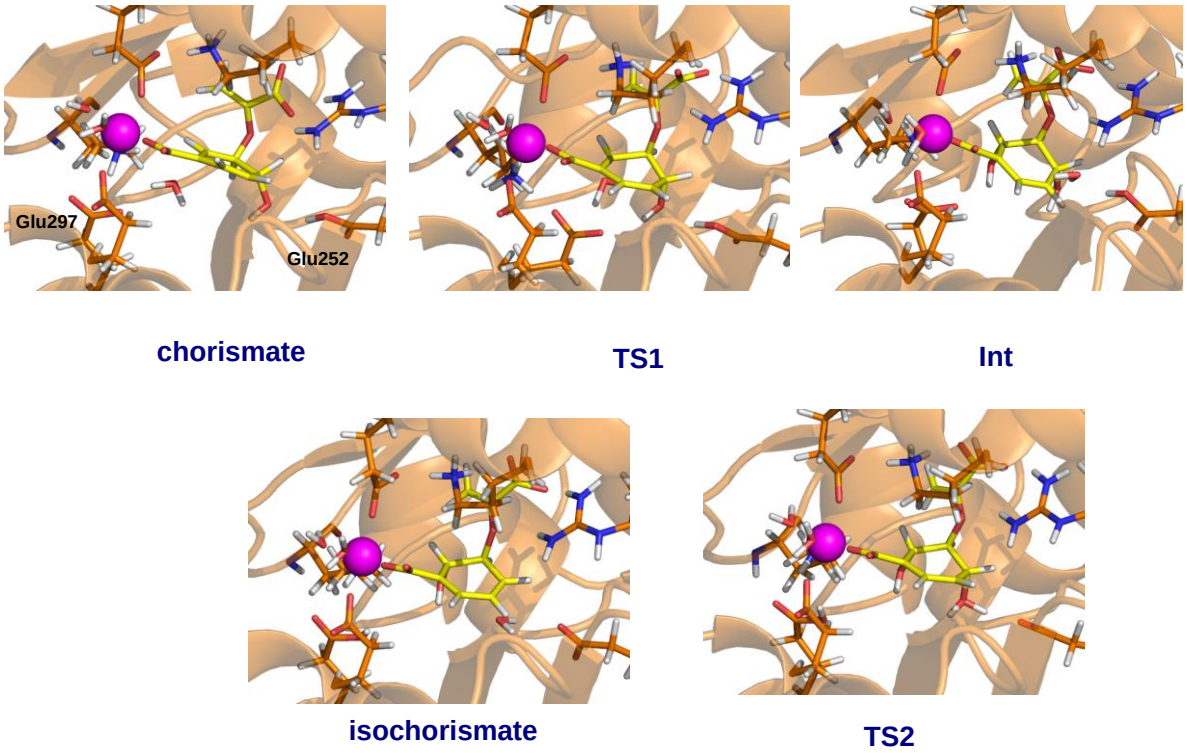

Figure S3. Representative structures of the substrate in the reactant (chorismate), intermediate, products (isochorismate) and transition states located in the active site of the MbtI

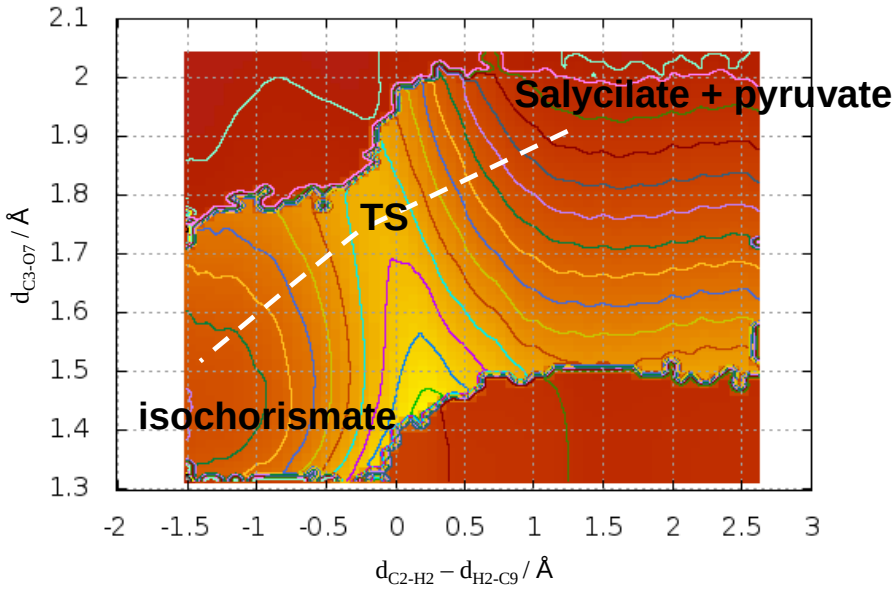

Figure S4. 2D-PMF with M06-2X corrections performed at 300 K to study the IPL activity of MbtI. Isoenergetic lines are drawn every 5 kcal·mol^{-1}, dark red regions correspond to the minima, while yellow colour represent higher energies on the surface.

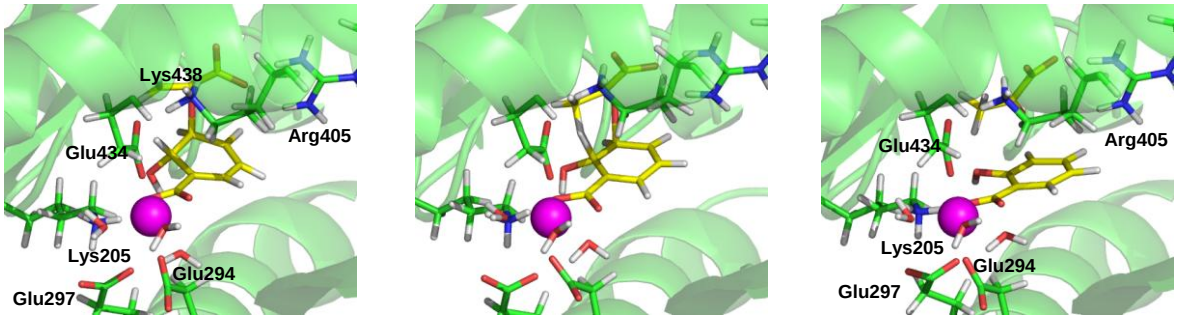

Figure S5. Representative structures of the substrate in the reactant (isochorismate), TS and products (salicylate and pyruvate)

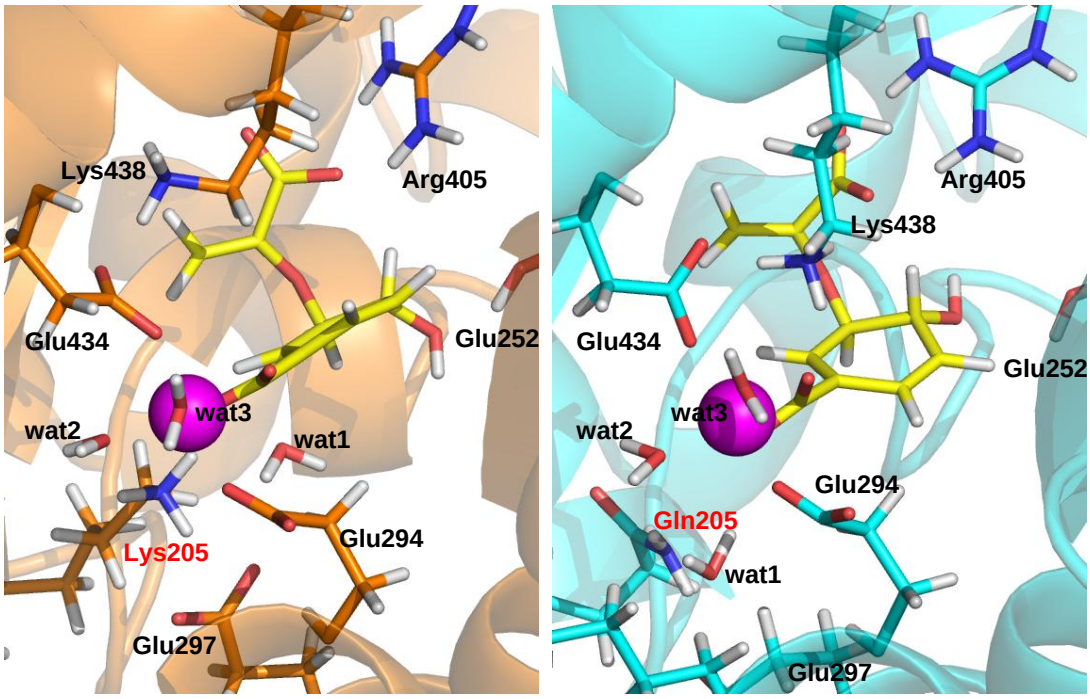

Figure S6. Representative snapshots of the K205Q mutated enzyme (right) compared to the wild-type (left). Chorismate is represented in yellow sticks. The magnesium atom is in purple.

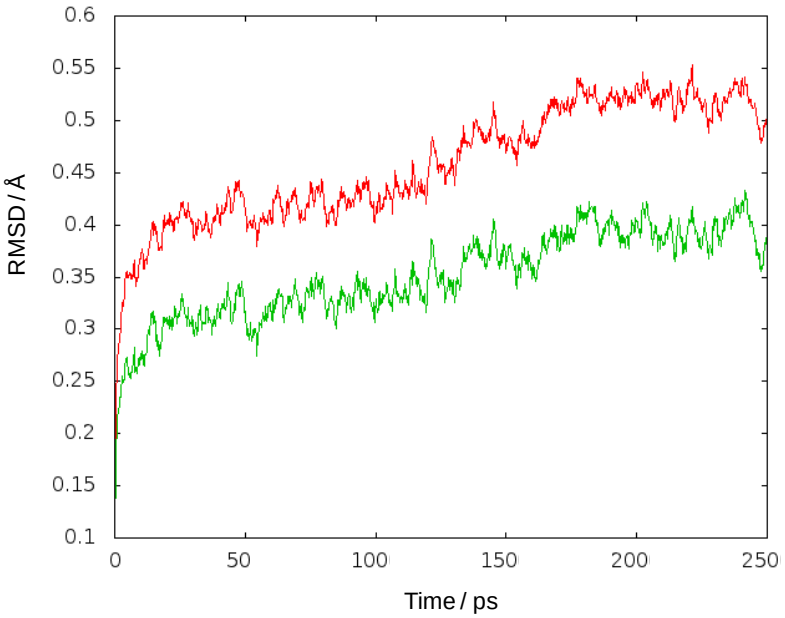

Figure S7. Time dependent root mean square deviation (RMSD) of the position of the atoms obtained along 250 ps of QM/MM MD simulations starting from the optimized structure of MbtI with chorismate molecule and Mg2+ cation in active site. Red line corresponds to the RMSD measured on atoms of the backbone of the protein while red line corresponds to RMSD calculations including sidechain of residues without hydrogen atoms.