

Supplementary materials

Quantum Mechanics and Molecular Mechanics Study on the Reaction Mechanism of Quorum Quenching Enzyme: N-Acyl Homoserine Lactonase with C6-HSL

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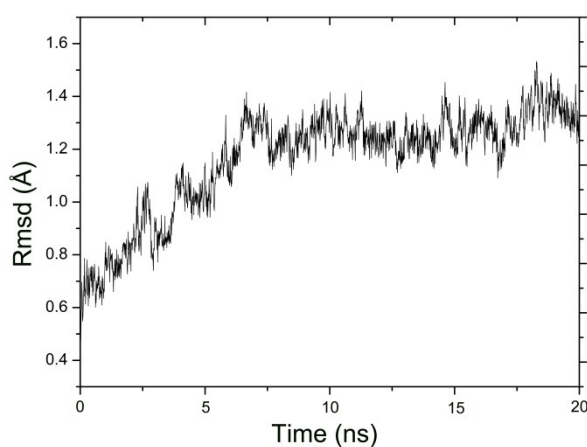


Fig. S1 The RMSD of AidH in complex with C6-HSL obtained from 20 ns MD simulation.

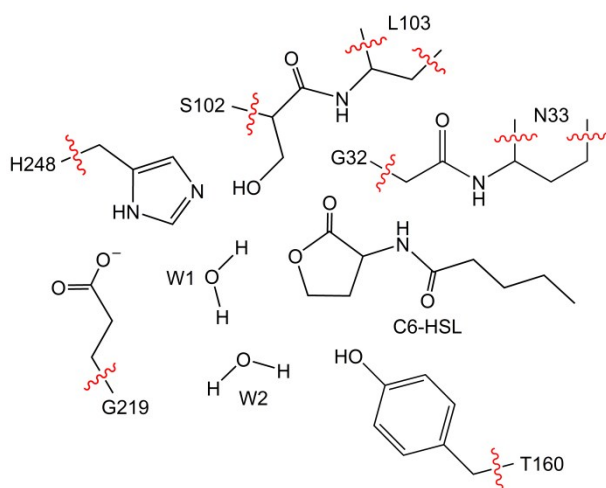


Fig. S2 QM region selected for the QM/MM calculations.

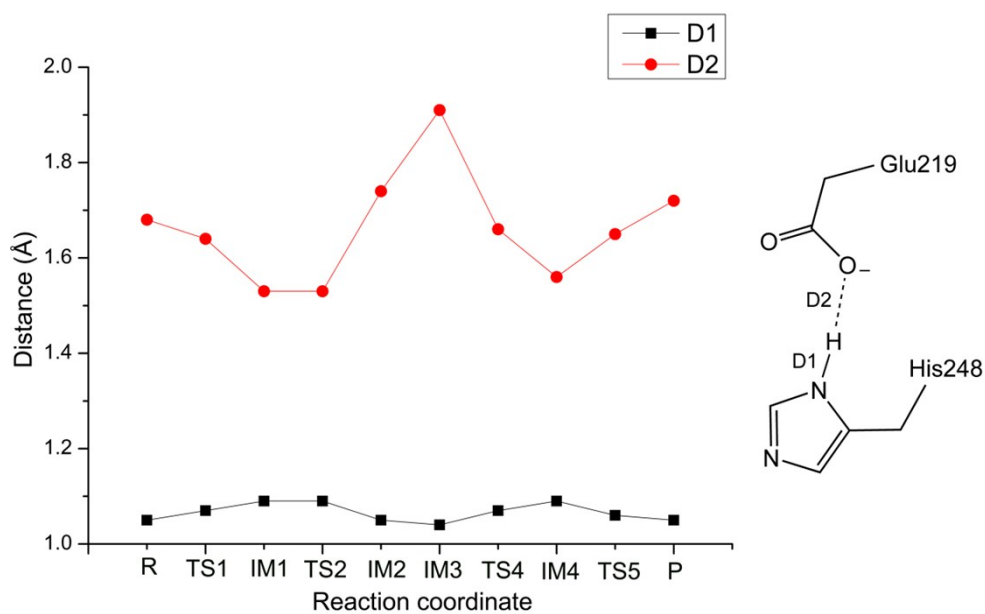


Fig. S3 Changes of two key distances along the degradation of C6-HSL.

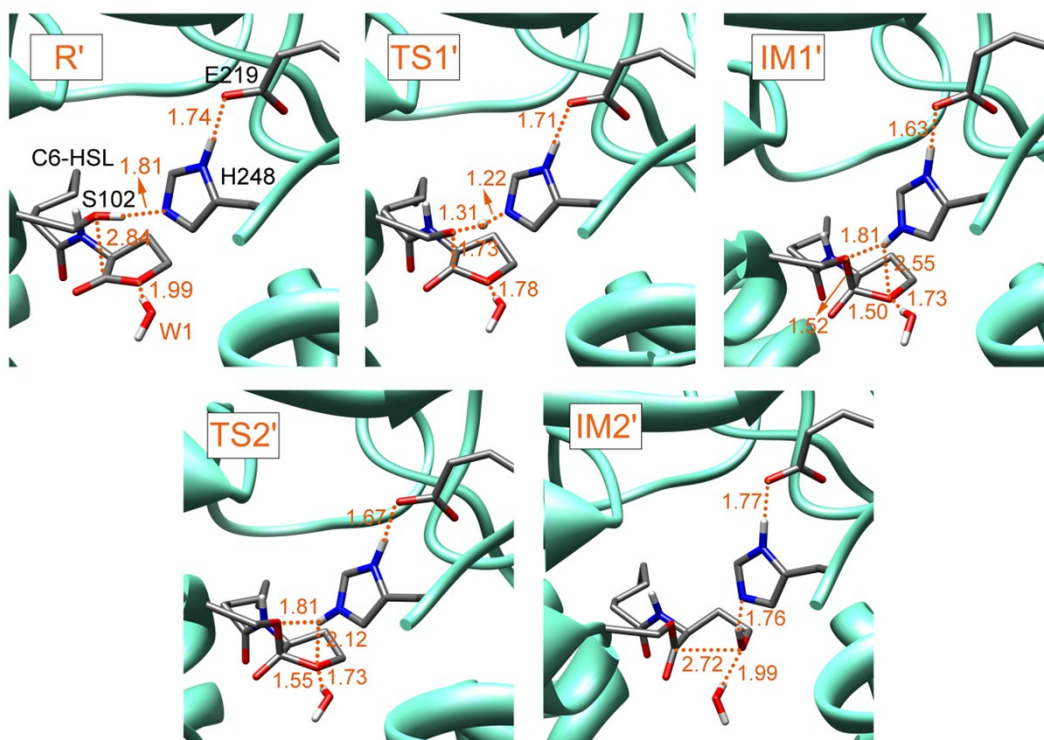


Fig. S4 Optimized structures for the first two steps of the reaction catalyzed by Y160A mutant. Distances are given in angstroms.

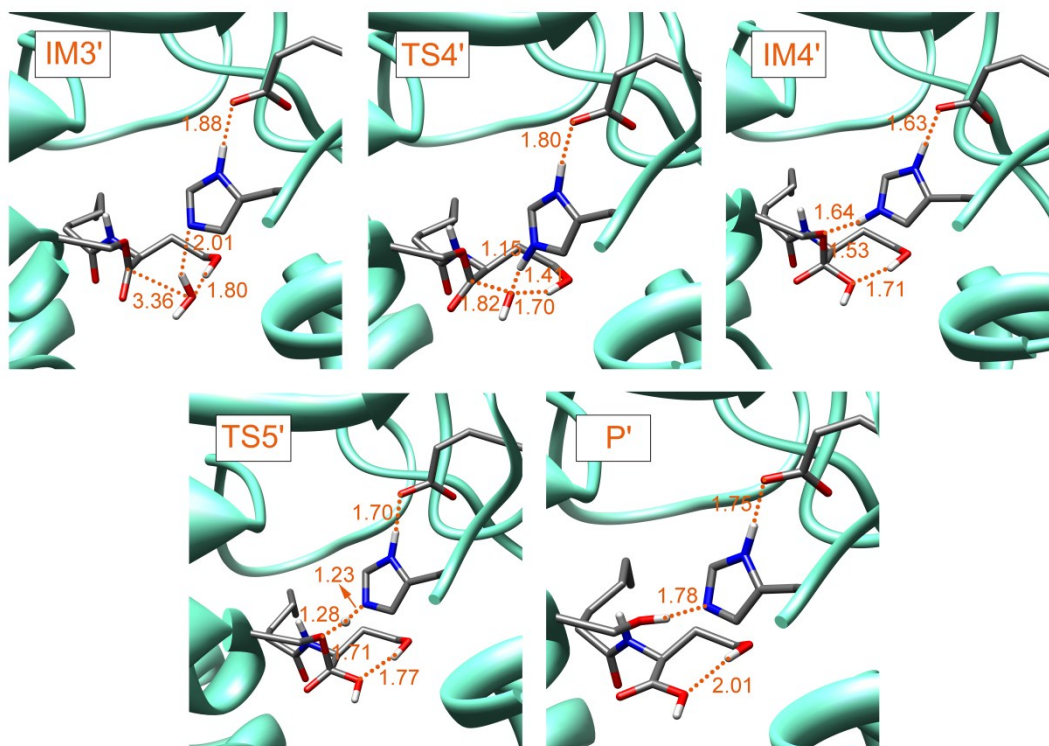


Fig. S5 Optimized structures for last two steps of the reaction catalyzed by Y160A mutant. Distances are given in angstroms.