Supporting Information

The Reaction Mechanism of Loganic Acid Methyltransferase: A Molecular Dynamics Simulation and Quantum Mechanics Study

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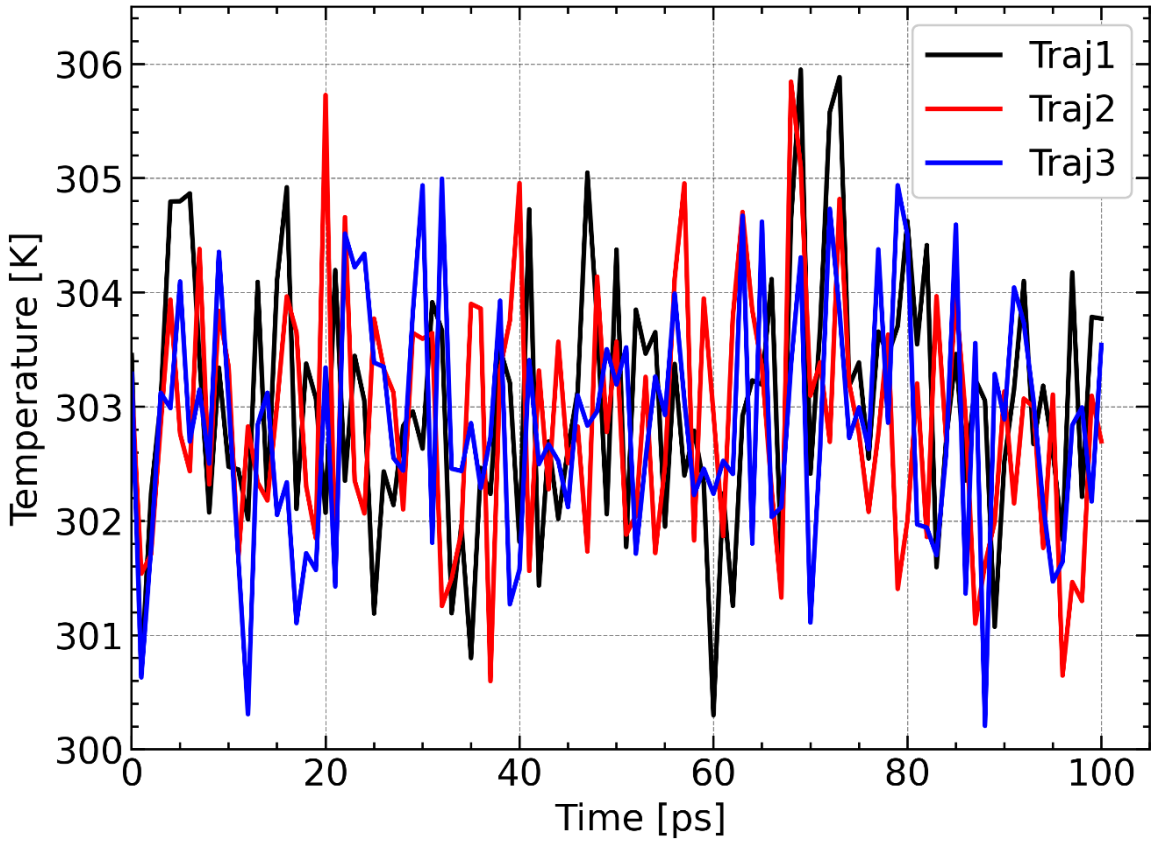

Figure S1. System temperature changes during NVT simulation for 3 different trajectories (Traj1, Traj2, Traj3).

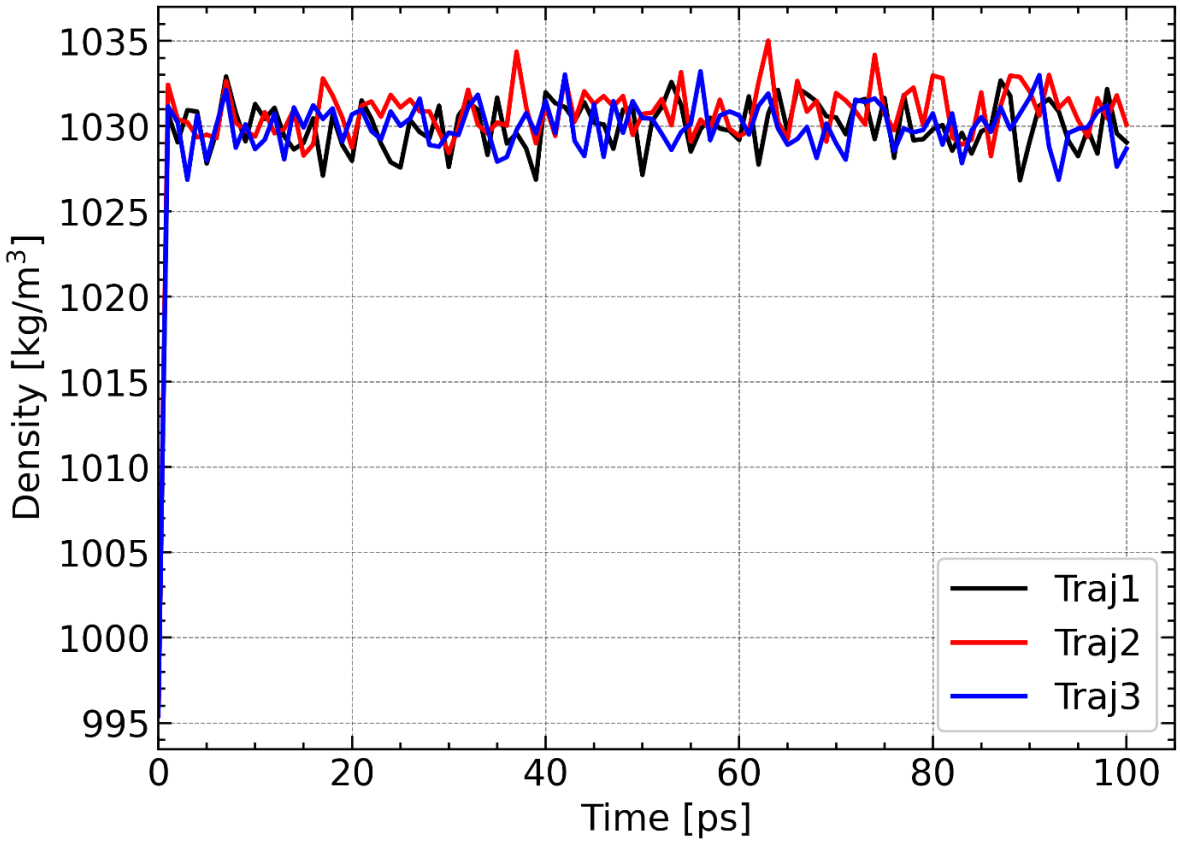

Figure S2. Changes in system density during NPT simulation for 3 different trajectories (Traj1, Traj2, Traj3).

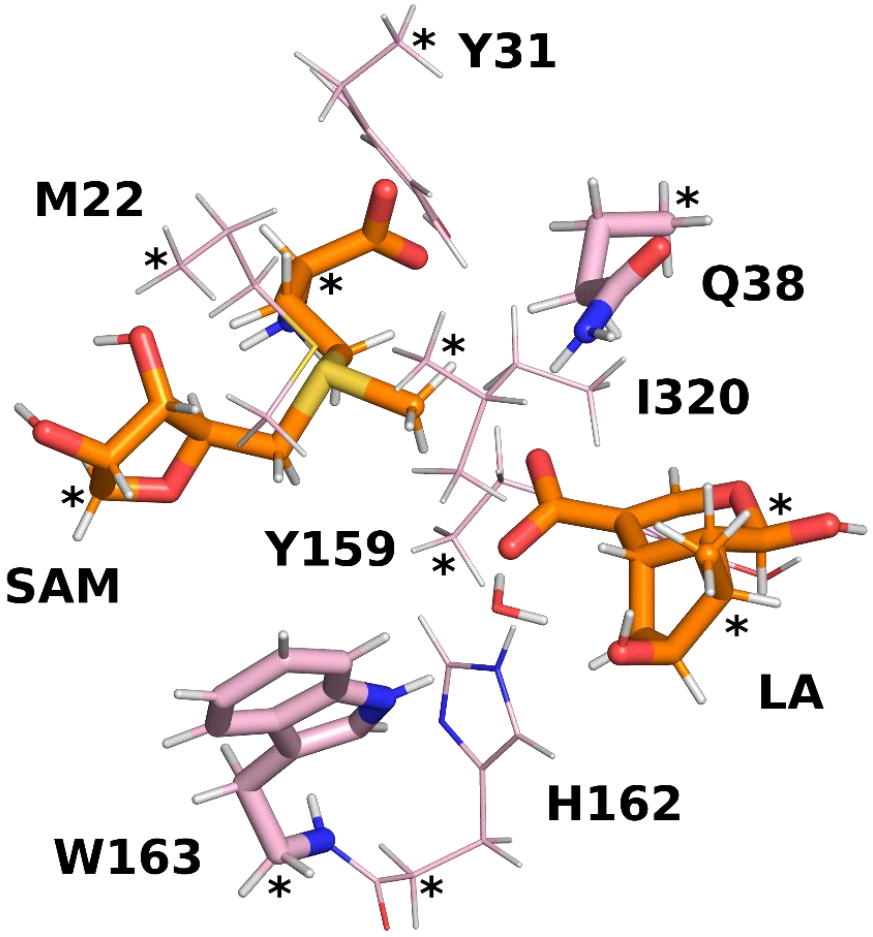

Figure S3. The structure of **Model 1** with water-mediated hydrogen bond between W163 and loganic acid. The fixed atoms are marked with an asterisk.

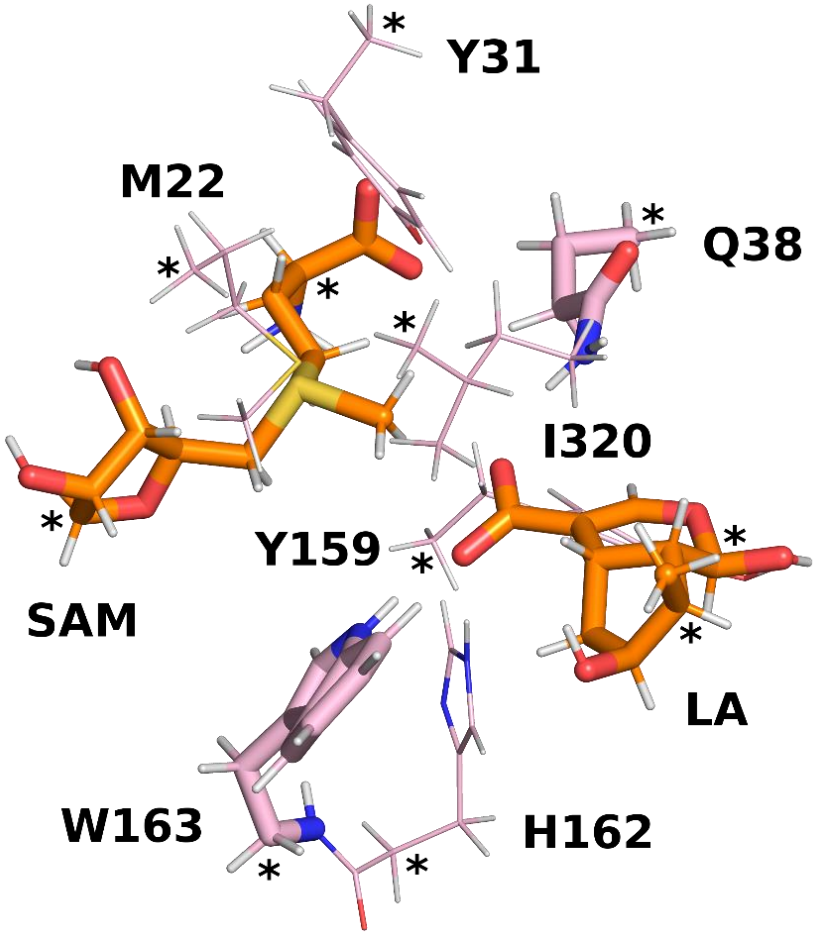

Figure S4. The structure of Model 2 with a direct hydrogen bond between W163 and loganic acid. The fixed atoms are indicated with an asterisk.

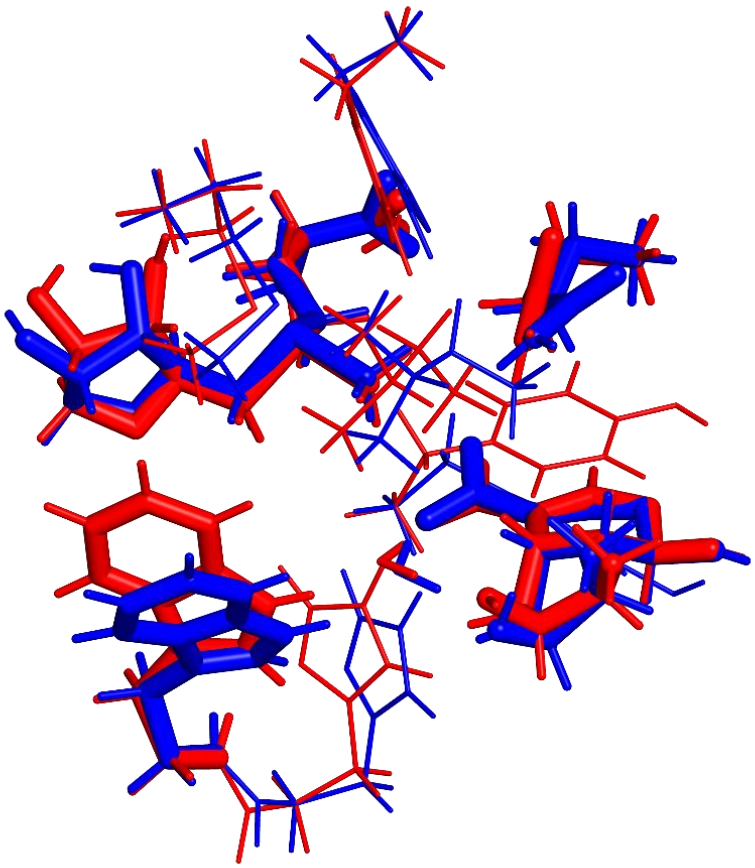

Figure S5. The initial structure from the optimization for Model 1 (in blue) superimposed on the structure of the found energy minimum (in red).

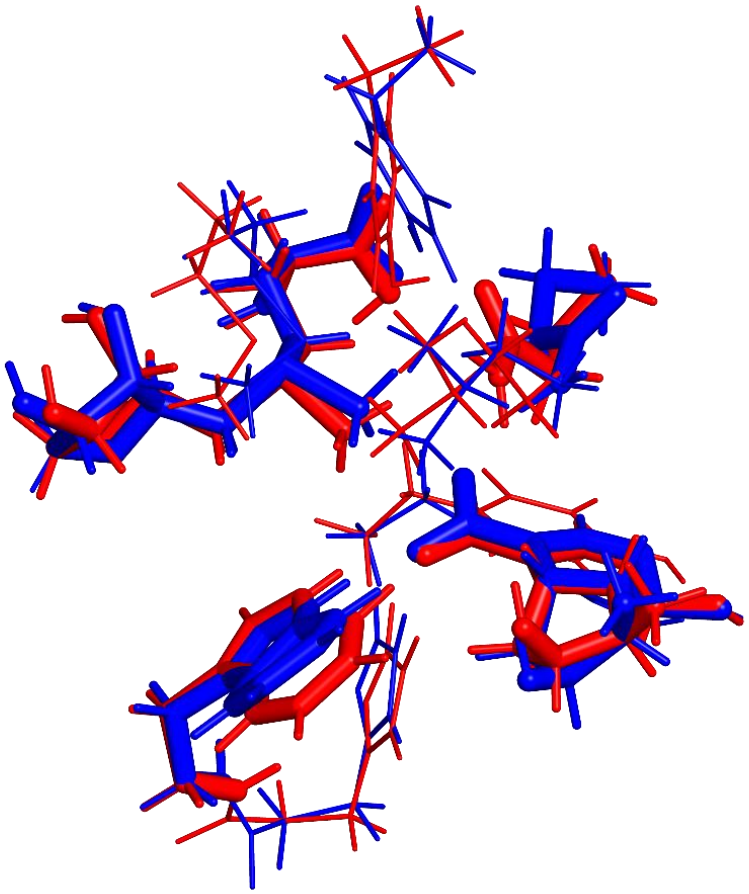

Figure S6. The initial structure from the optimization for Model 2 (in blue) superimposed on the structure of the found energy minimum (in red).

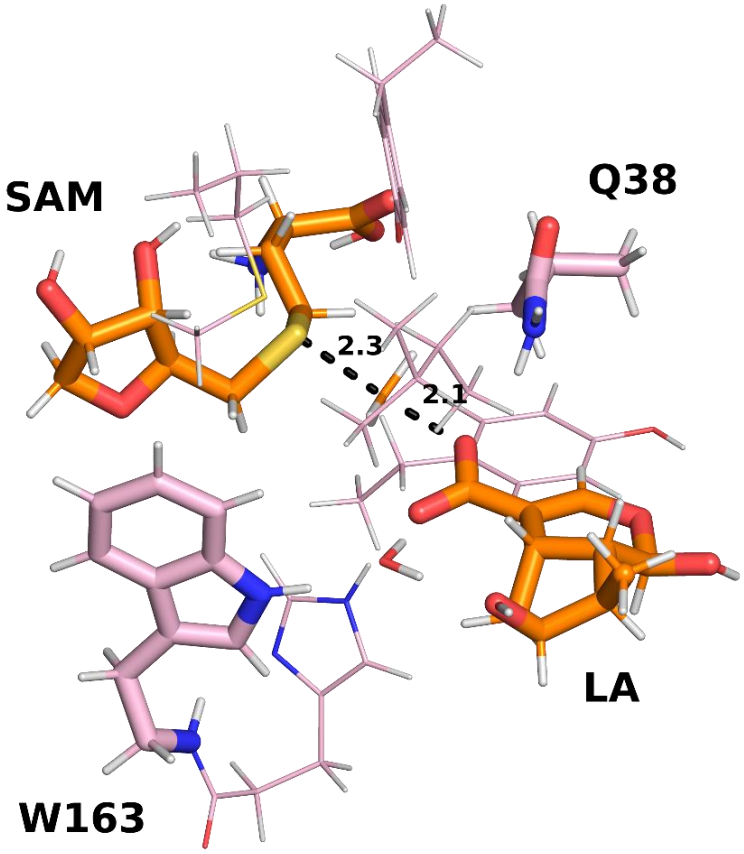

Figure S7. Optimized transition state structure for Model 1.

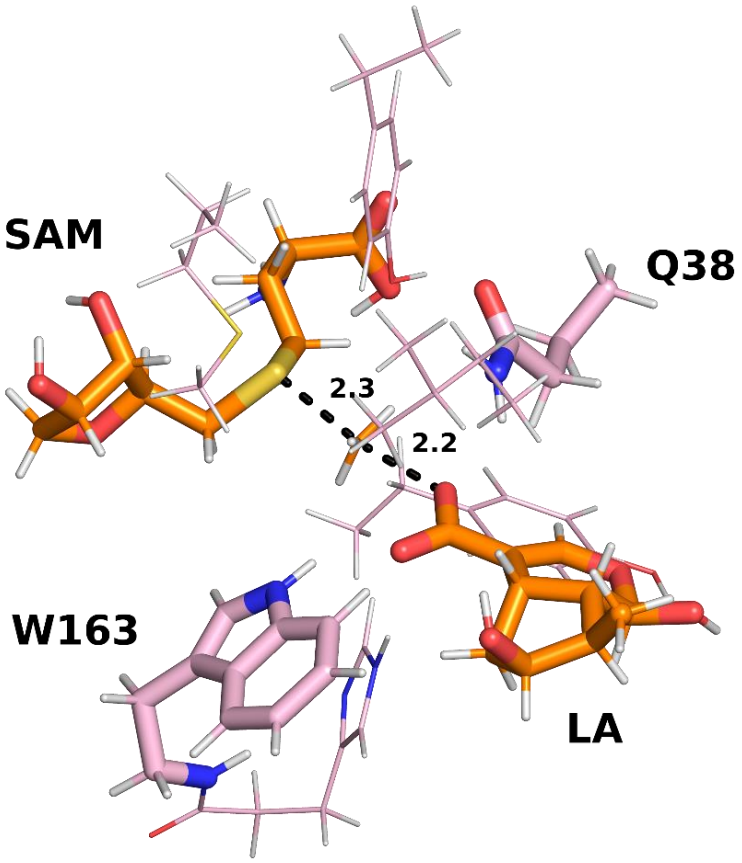

Figure S8. Optimized transition state structure for Model 2.