

Supporting information

Theoretical study of the mechanism of proton transfer in the esterase EstB from *Burkholderia gladioli*

Liang Chen^{1,2#}, Xiangqian Kong^{1#}, Zhongjie Liang¹, Fei Ye¹, Kunqian Yu¹, Weiyi Dai², Daocheng Wu^{2*}, Cheng Luo^{1,3*}, and Hualiang Jiang¹

¹Drug Discovery and Design Center, State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China

²The Key Laboratory of Biomedical Information Engineering of the Ministry of Education, School of Life Science and Technology, Xi'an Jiaotong University, Xi'an 710049, China

³Center for Systems Biology, Soochow University, Jiangsu 215006, China

[#]These authors contributed equally to this work

^{*}Correspondence: Daocheng Wu and Cheng Luo

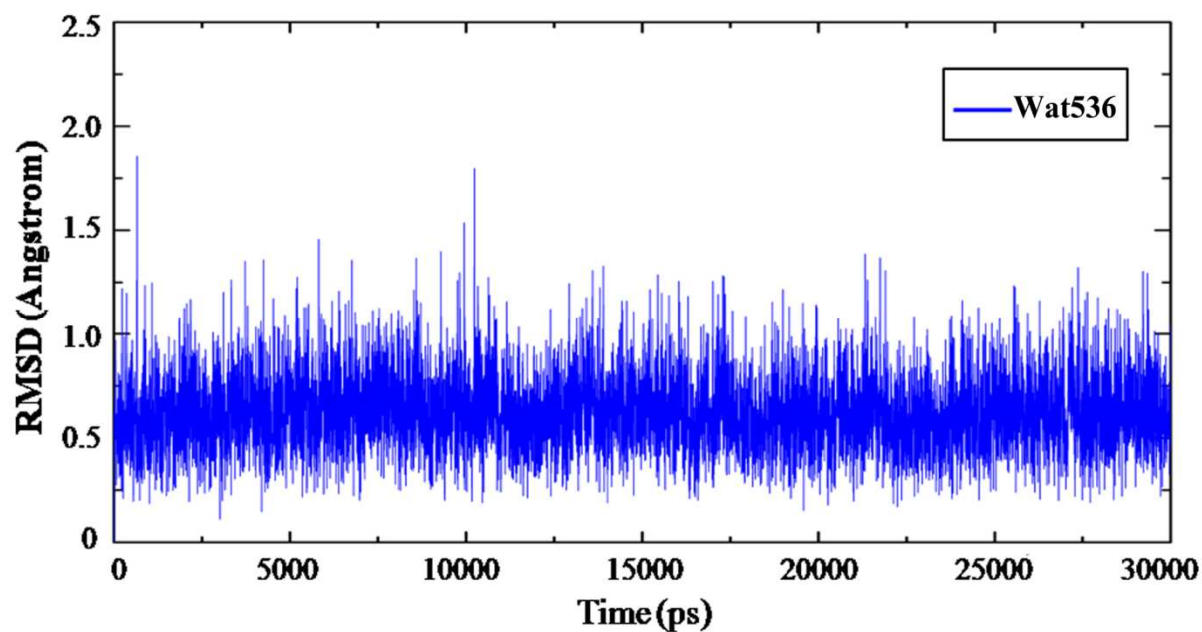


Figure S1. Time dependencies of the weighted root-mean-square deviations for Wat536 from their initial positions during the 30-ns simulation.

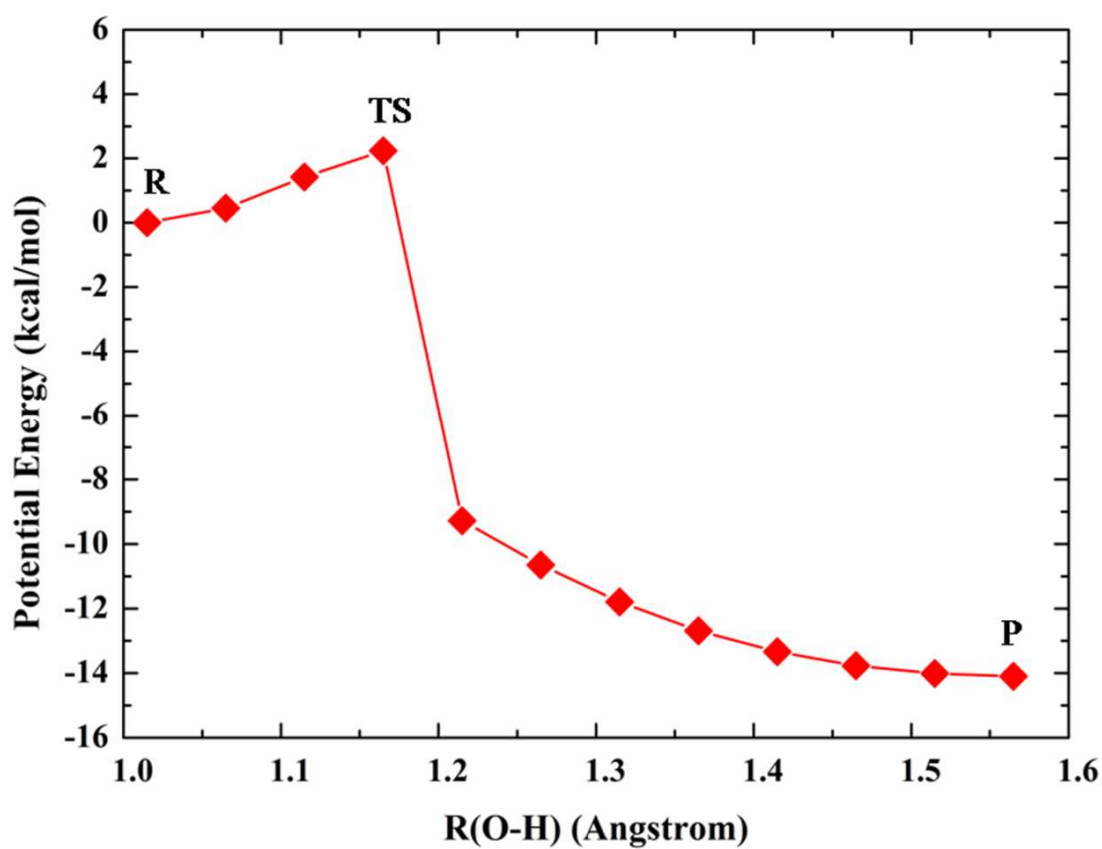


Figure S2. Potential energy curve for the PT reaction in EstB determined at the

ONIOM (B3LYP/6-31G*:AMBER) level. (R) is the reactant; (TS) is the transition state; (P) is the immediate product. All of the stationary points of potential energy along the PT pathway are marked with filled squares.

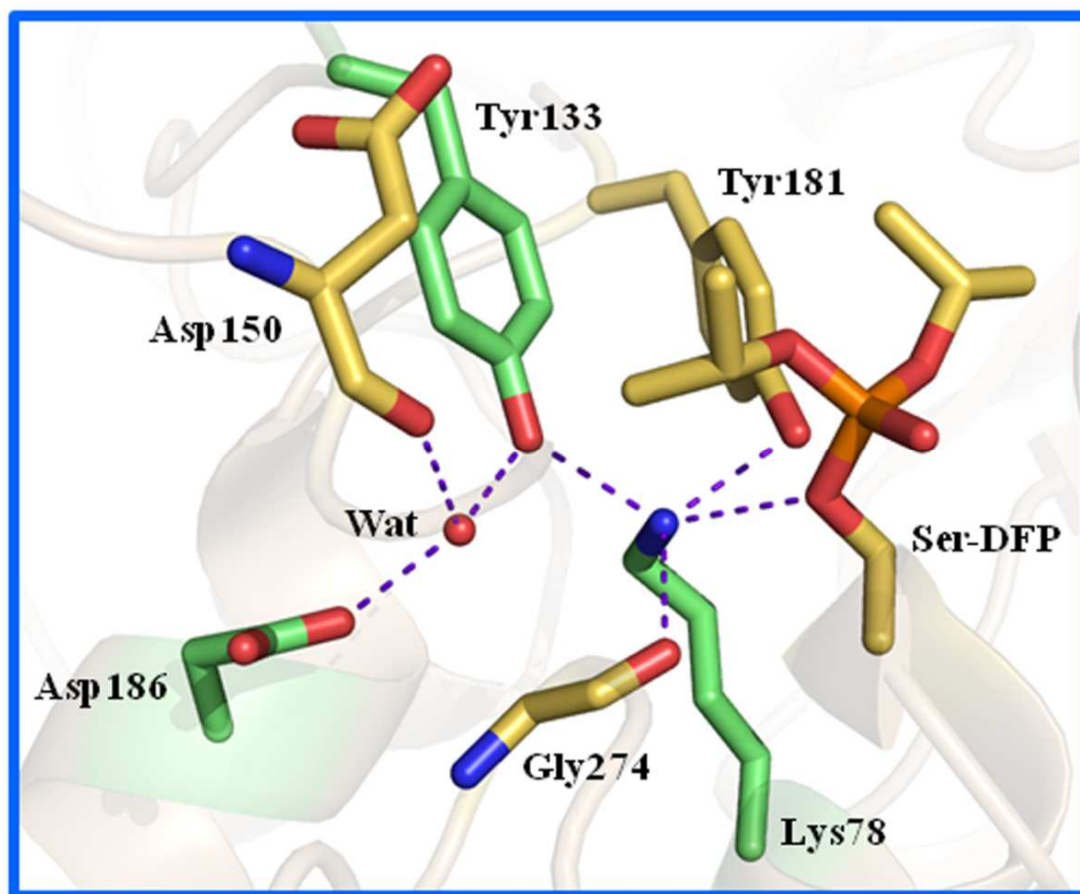


Figure S3. Stereoview of the hydrogen bonding network surrounding the water molecule in the EstB-DFP complex. (PDB code: 1CI9, chain B).

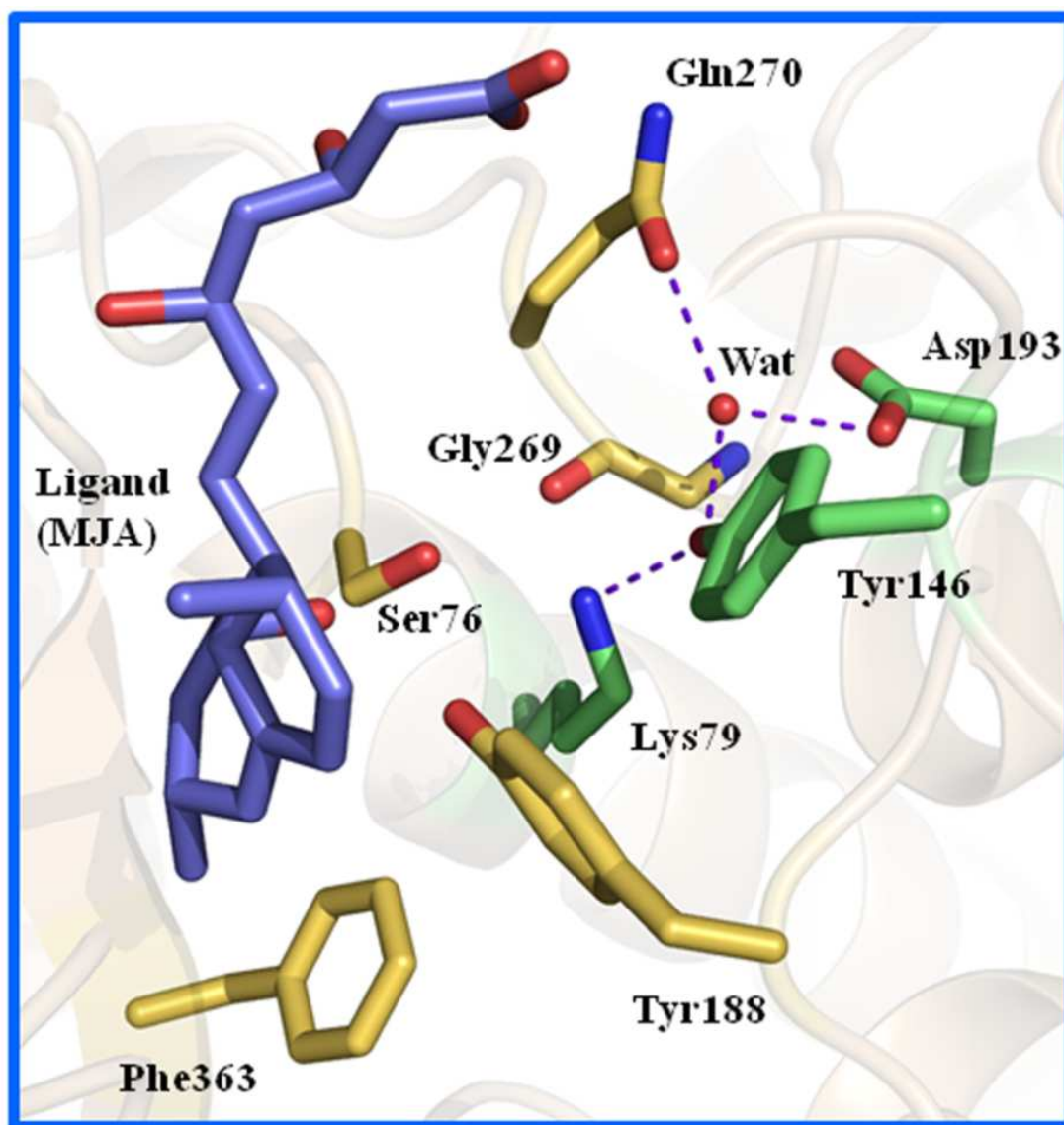


Figure S4. Active site residues and the water molecule in the LovD-MJA complex (PDB code: 3HLD).