Supplementary Information

Reaction pathways and free energy profiles for cholinesterase-catalyzed hydrolysis of 6-monoacetylmorphine

Yan Qiao,[1,2] Keli Han,[1,*] and Chang-Guo Zhan[2,*]

[1]*State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Science, Zhongshan Road 457, Dalian 116023, P. R. China*

[2]*Department of Pharmaceutical Sciences, College of Pharmacy, University of Kentucky, 789 South Limestone Street, Lexington, KY 40536.*

Supplementary Information Available. An additional figure for the plots of the key internuclear distances *vs* the simulation time in the MD-simulated BChE-6-MAM binding structure.

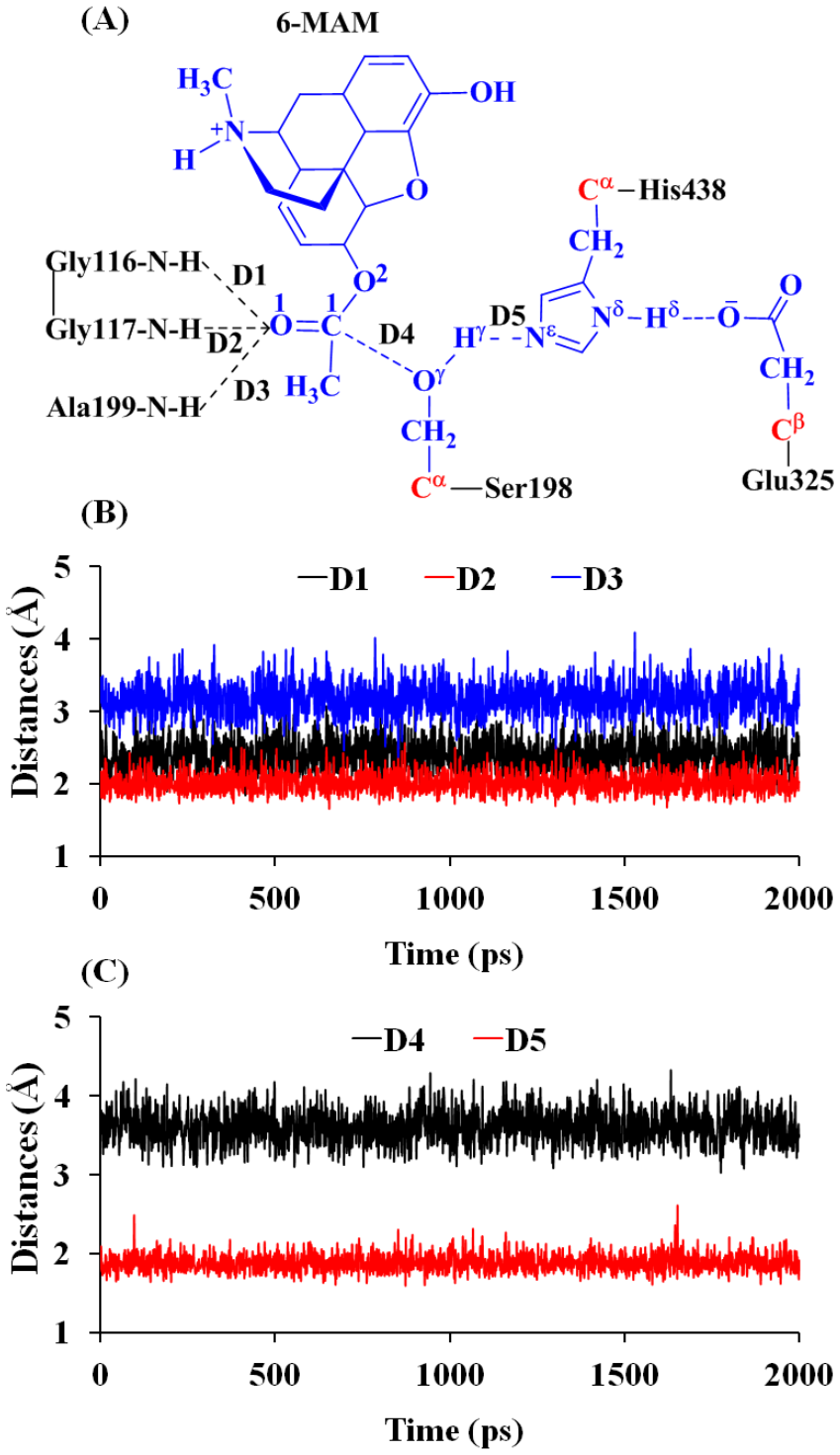

Figure S1. Key internuclear distances *vs* the simulation time in the MD-simulated BChE-6-MAM binding structure.