

A theoretical study on the catalytic mechanism of oxalyl-CoA decarboxylase, an enzyme for treating urolithiasis

Xiang Sheng^a, Yongjun Liu^{*a,b}, Rui Zhang^c

^aSchool of Chemistry and Chemical Engineering, Shandong University, Jinan, Shandong 250100, China

^bNorthwest Institute of Plateau Biology, Chinese Academy of Sciences, Xining, Qinghai 810001, China

^cSchool of Agriculture, Ludong University, Yantai, Shandong 264025, China

Fig. S1 The energy profile of proton transfer process from 4'-NH₂ to the hydroxyl anion using IM2 as the starting structure.

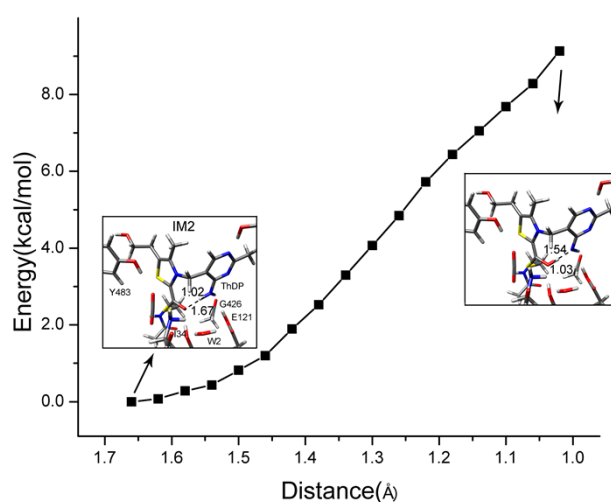


Fig. S2 The energy profile of proton transfer process from 4'-NH₂ to the hydroxyl anion using IM3 as the starting structure.

