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

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Fig. S1 The energy profile of proton transfer process from 4’-NH\textsubscript{2} to the hydroxyl anion using IM2 as the starting structure.
Fig. S2 The energy profile of proton transfer process from 4’-NH$_2$ to the hydroxyl anion using IM3 as the starting structure.