Electronic Supplementary Material (ESI) for RSC Advances.

A QM/MM Study of the Catalytic Mechanism of Succinic Semialdehyde Dehydrogenase from *Synechococcus* sp.PCC 7002 and *Salmonella typhimurium*

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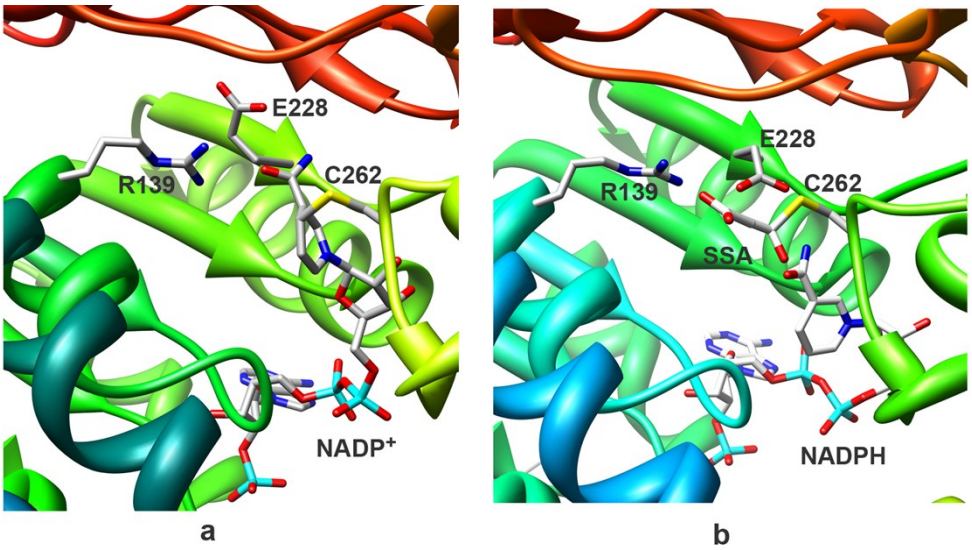

Figure S1 Multiple conformations of the nicotinamide portion of the NAD(P)$^+$ and the catalytic glutamate residue. (a) When the nicotinamide ring of the NAD(P)$^+$ enters the active site, the side chain of the catalytic glutamate residue rotates away from the active site. (b) When NAD(P)$^+$ is reduced to NAD(P)H, the nicotinamide moves away from the active site, allowing the catalytic glutamate residue to rotate back in.

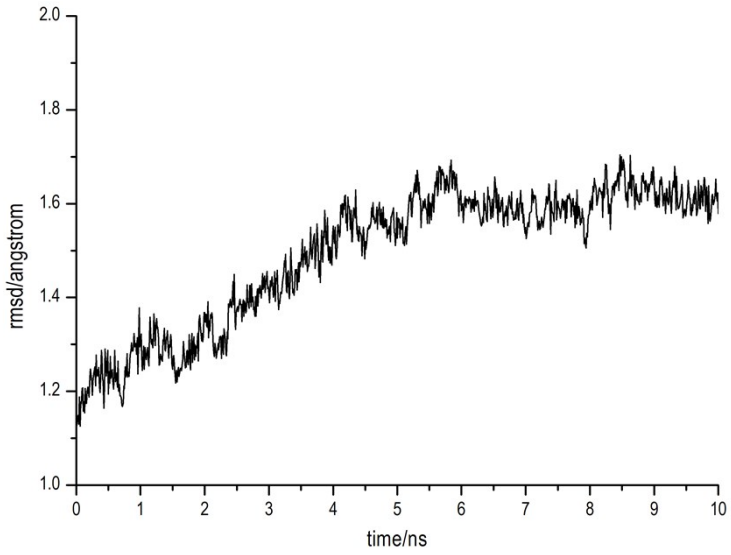

Figure S2 Time dependence of RMSD (Å) from 10ns MD simulation for the initial model chosen from the crystal structure of *Sy*SSADH in complex with NADP$^+$ (PDB code: 4ITA).

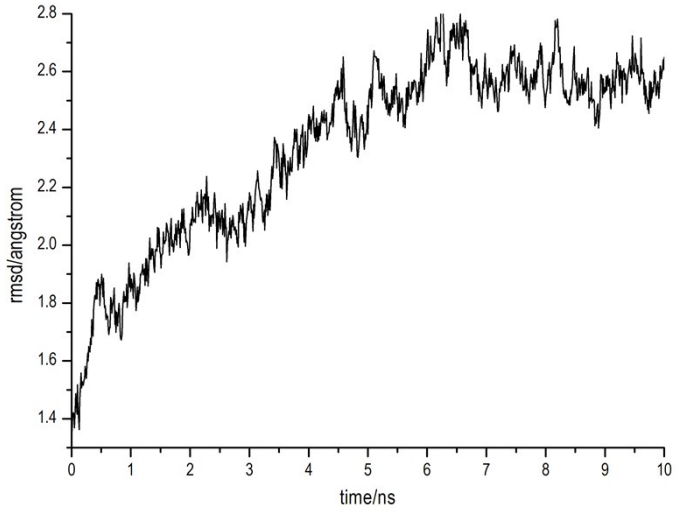

Figure S3 Time dependence of RMSD (Å) from 10ns MD simulation for the initial model chosen from the crystal structure of *St*SSADH in complex with NAD^+ (PDB code: 3EFV).

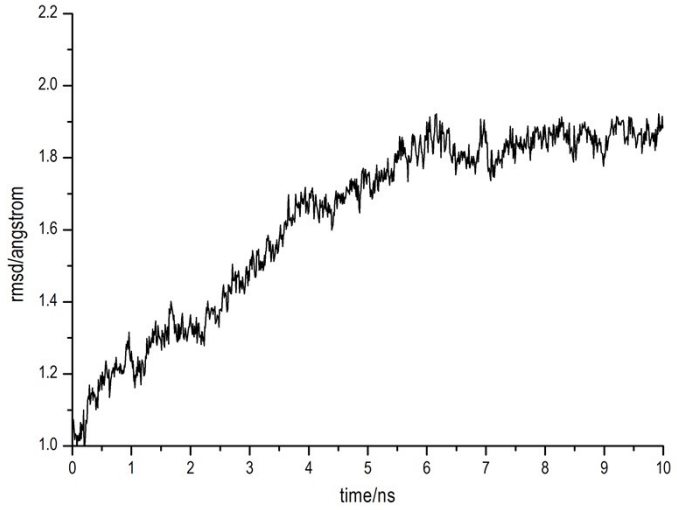

Figure S4 Time dependence of RMSD (Å) from 10ns MD simulation for the initial model chosen from the crystal structure of *Sy*SSADH in complex with NADPH and SSA (PDB code: 4ITB).

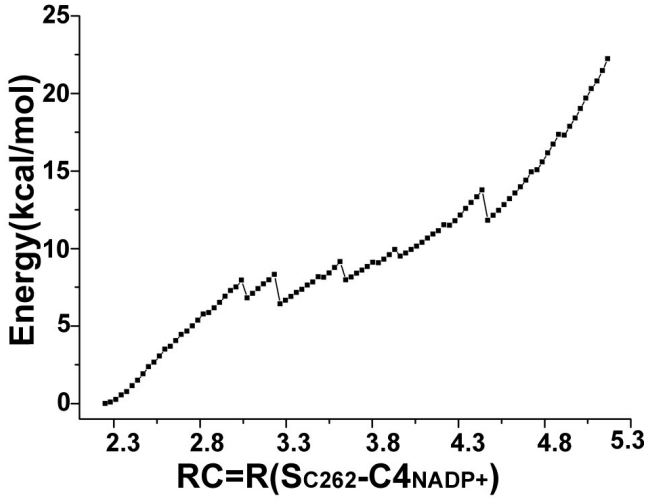

Figure S5 The calculated energy profile along the reaction coordinate defined by RC=R(S_{C262}-$C4_{NADP+}$) for the cleavage of the covalent linkage.

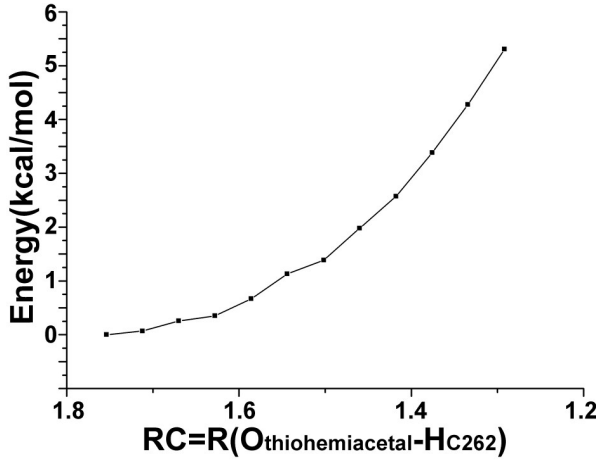

Figure S6 The calculated energy profile along the reaction coordinate defined by RC=R($O_{thiohemiacetal}$-H_{C262}) for the proton transfer from the main chain amide of C262 to the oxygen atom of the intermediate.

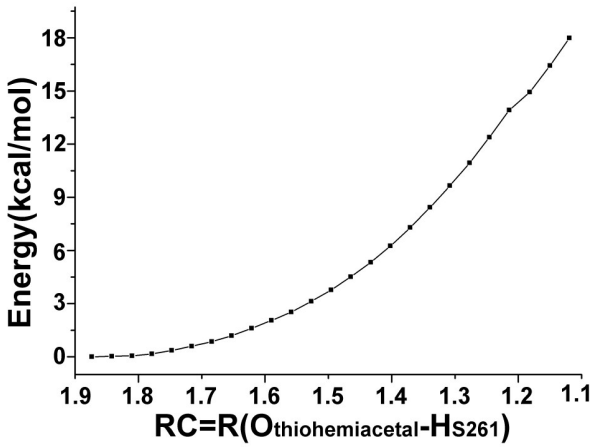

Figure S7 The calculated energy profile along the reaction coordinate defined by RC=R($O_{thiohemiacetal}$-H_{S261}) for the proton transfer from the side chain hydroxyl of S261 to the oxygen atom of the intermediate.

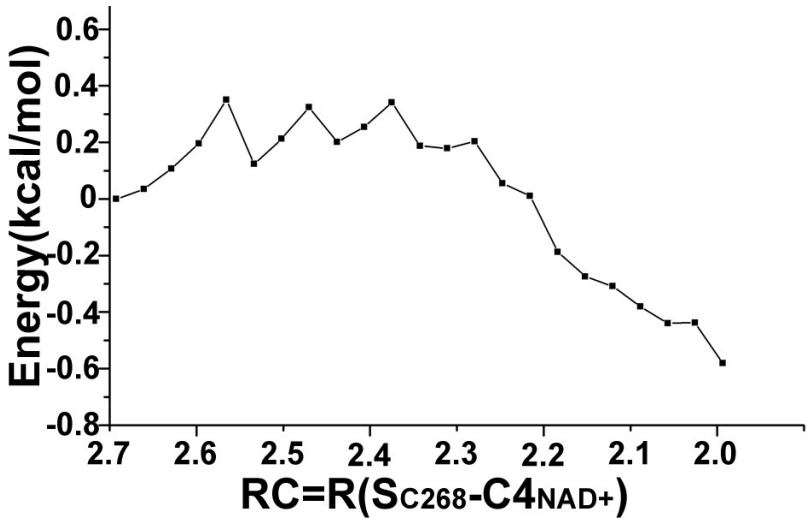

Figure S8 The calculated energy profile along the reaction coordinate defined by RC=R(S_{C262}-$C4_{NAD+}$) for the formation of a cysteine-NAD adduct.