

Supplemental Materials: Molecular Mechanisms of Succinimide Formation from Aspartic Acid Residues Catalyzed by Two Water Molecules in the Aqueous Phase

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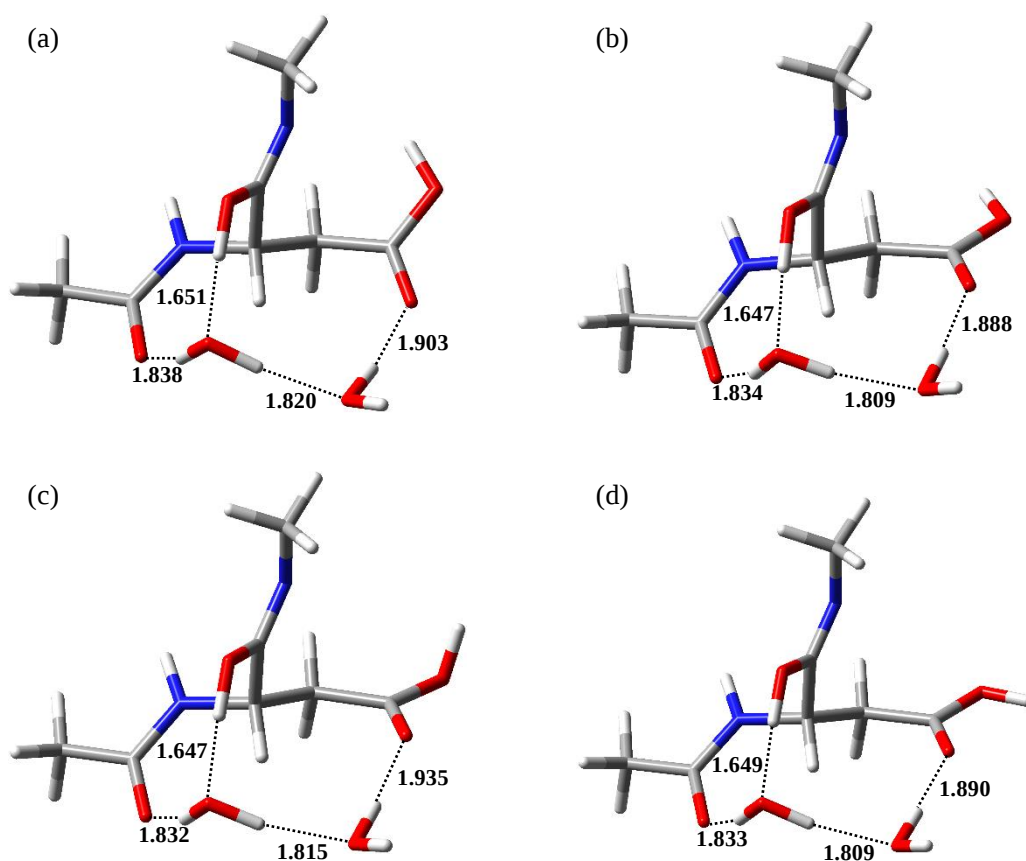


Figure S1. Optimized geometries of (a) TS3 ($\varphi = -113^\circ$, $\psi = -96^\circ$, $\chi_1 = -176^\circ$), (b) IM2 ($\varphi = -114^\circ$, $\psi = -97^\circ$, $\chi_1 = -172^\circ$), (c) TS4 ($\varphi = -114^\circ$, $\psi = -98^\circ$, $\chi_1 = -171^\circ$), and (d) IM3 ($\varphi = -113^\circ$, $\psi = -97^\circ$, $\chi_1 = -172^\circ$). Selected interatomic distances are presented in Å. Carbon, hydrogen, nitrogen, and oxygen atoms are illustrated in gray, white, blue, and red, respectively.

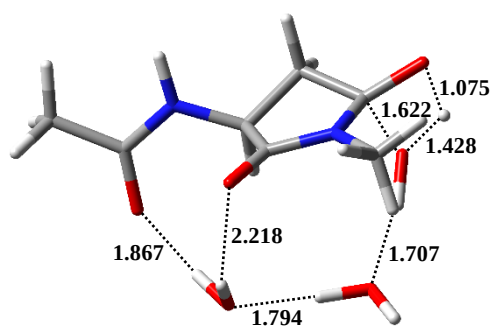


Figure S2. Optimized geometries of TS of the direct pathway for the formation of the Suc residue from TH1 ($\varphi = -97^\circ$, $\psi = -149^\circ$, $\chi_1 = 158^\circ$). Selected interatomic distances are presented in Å. Carbon, hydrogen, nitrogen, and oxygen atoms are illustrated in gray, white, blue, and red, respectively.