

Supporting Information

Unravelling the intramolecular cyclization mechanism of oxidized tryptophan in aqueous solution as a function of pH

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Figure S1. Page 2

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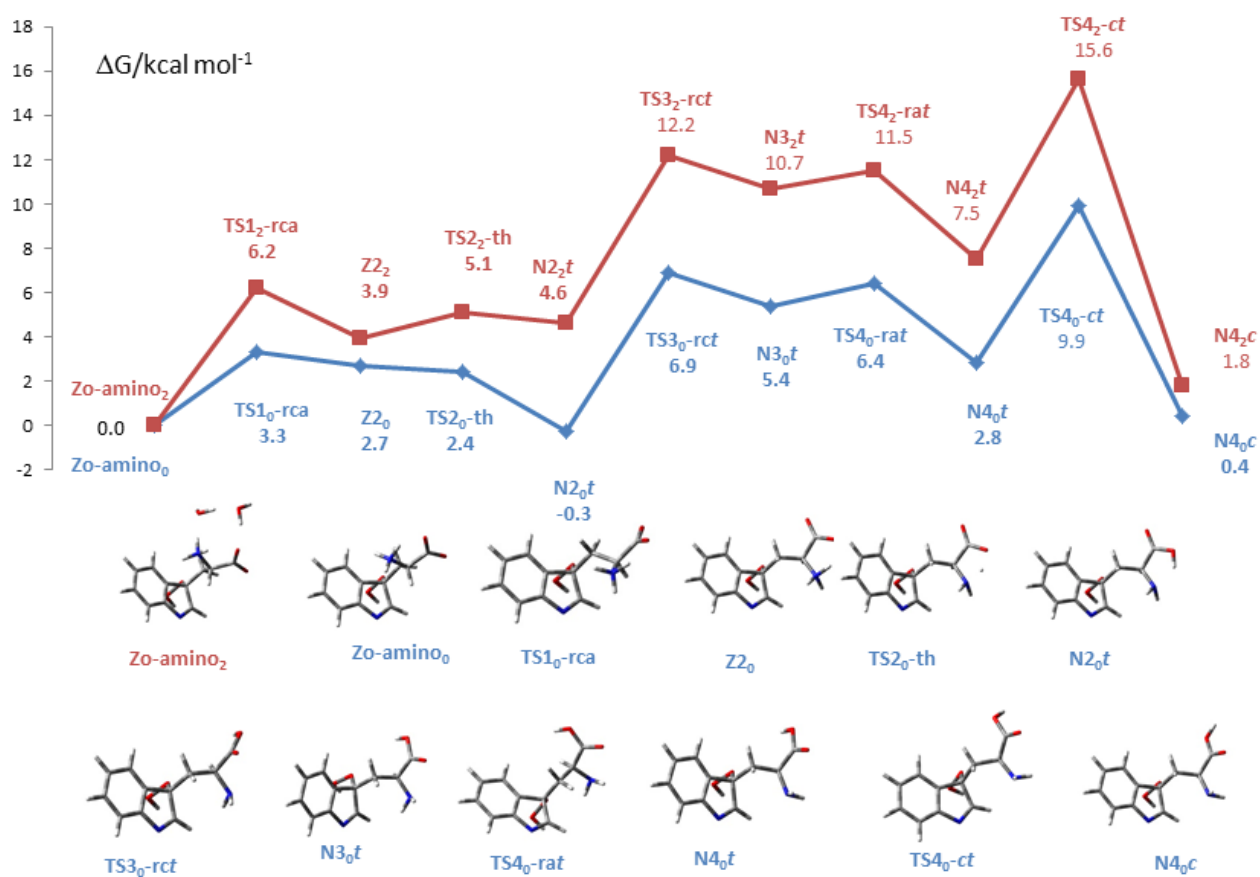


Figure S1. Gibbs energy profiles for the initial proton transfer from the ammonium to the carboxylate group, and conformational rearrangements to arrive at the neutral Trp-OOH conformer ready to undergo cyclization along the C-route considering zero and two explicit water molecules.

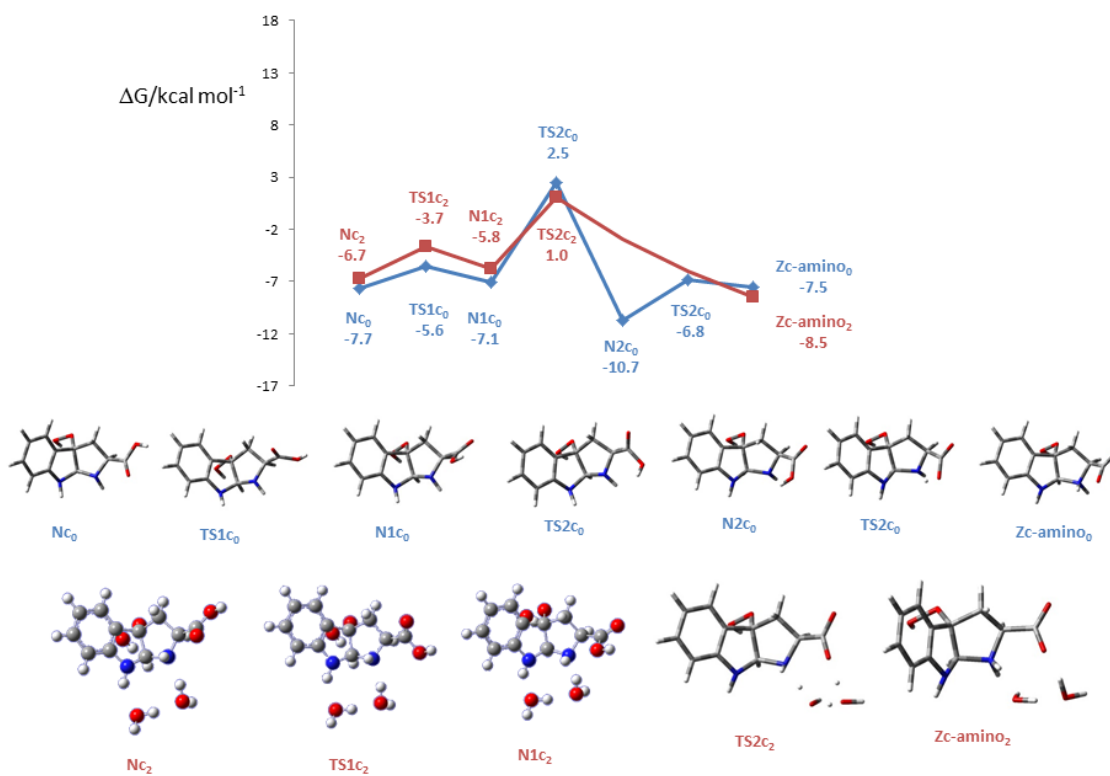


Figure S2. Gibbs energy profiles for the routes from **N2** to **Zc-amino** considering zero and two explicit water molecules