Supporting Information

Investigation of the intramolecular hydrogen bonding interactions and excited state proton transfer mechanism for both Br-BTN and CN-BTN systems

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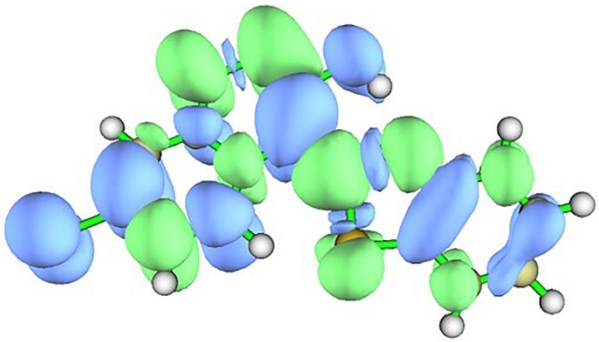
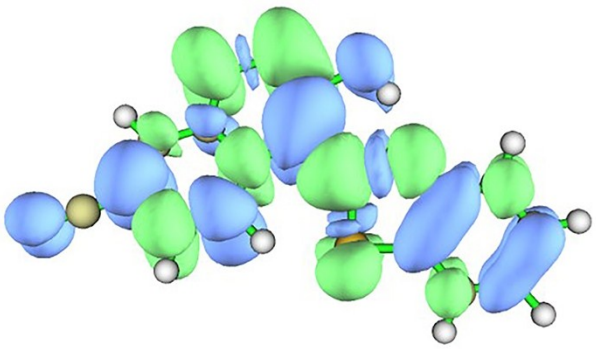


Br-BTN-enol



CN-BTN-enol

Figure S1. View of the CDD maps for both Br-BTN-enol and CN-BTN-enol systems. Herein, the regions with regions with the increasing electron density are shown in green, and those with decreasing electron density are shown in light blue.

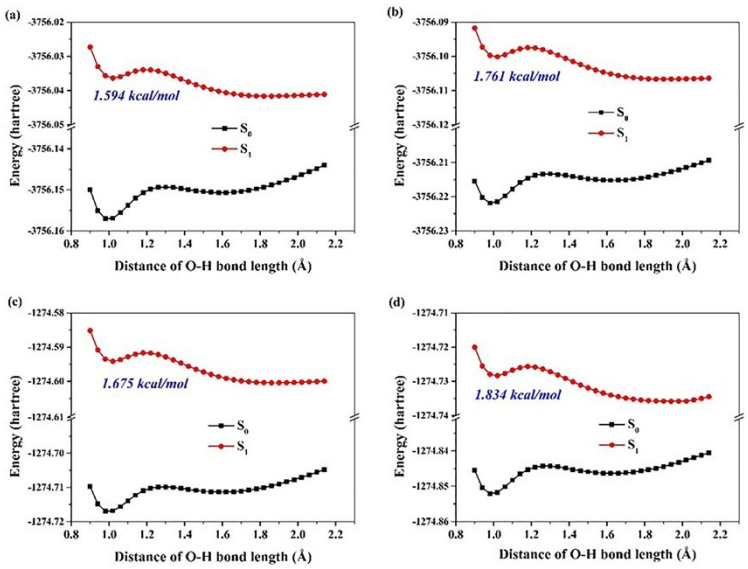


Figure S2. The constructed potential energy curves for both Br-BTN and CN-BTN systems based on fixing O-H bond length in both S_0 and S_1 states. (a) and (b) show the results of potential energy curves for Br-BTN system using Cam-B3LYP and wB97XD functionals, respectively. (c) and (d) show the results of potential energy curves for CN-BTN system using Cam-B3LYP and wB97XD functionals, respectively.

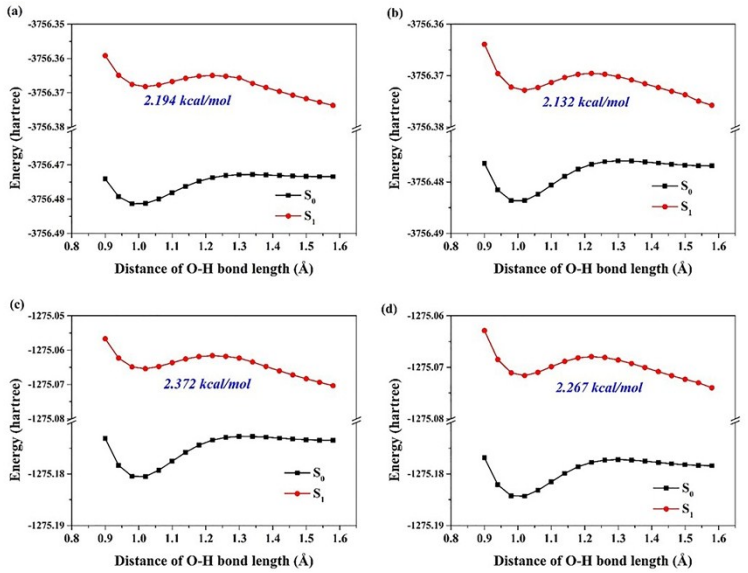


Figure S3. The constructed potential energy curves for both Br-BTN and CN-BTN systems based on fixing O-H bond length in both S_0 and S_1 states in cyclohexane and chloroform solvents. (a) and (b) show the results of potential energy curves for Br-BTN system in cyclohexane and chloroform solvents, respectively. (c) and (d) show the results of potential energy curves for CN-BTN system in cyclohexane and

chloroform solvents, respectively.

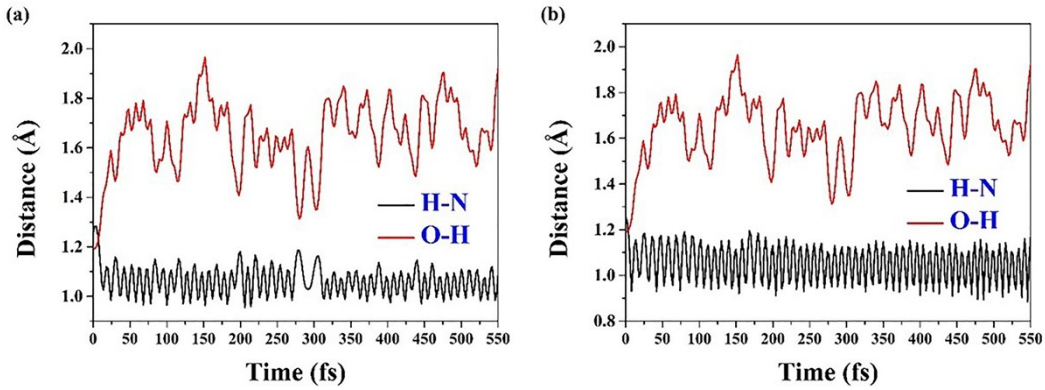


Figure S4. The time evolution of the important structural parameters (i.e., H-N and O-H bond lengths) for both Br-BTN (a) and CN-BTN (b) sampled by the excited state BOMD simulations.