

Femtosecond Intersystem Crossing to the Reactive Triplet State of the 2,6-Dithiopurine Skin Cancer Photosensitizer

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Electronic Supporting Information

I. Supporting Results

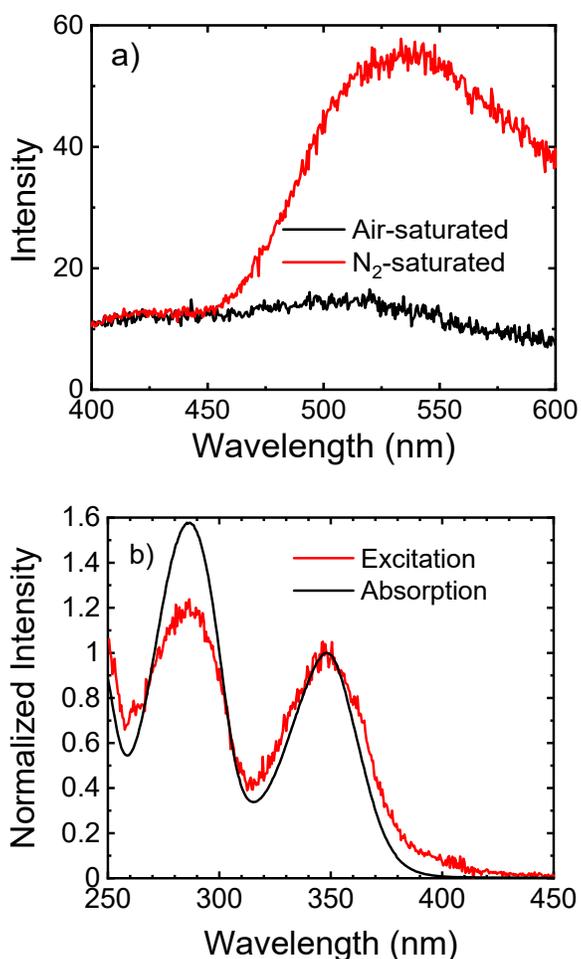


Figure S1. a) Emission spectra of deprotonated dtPur ($\lambda_{\text{exc}} = 325$ nm) in phosphate buffer pH 7.4 under air- and N₂-saturated conditions and b) excitation spectrum ($\lambda_{\text{em}} = 535$ nm) of dtPur in phosphate buffer pH 7.4.

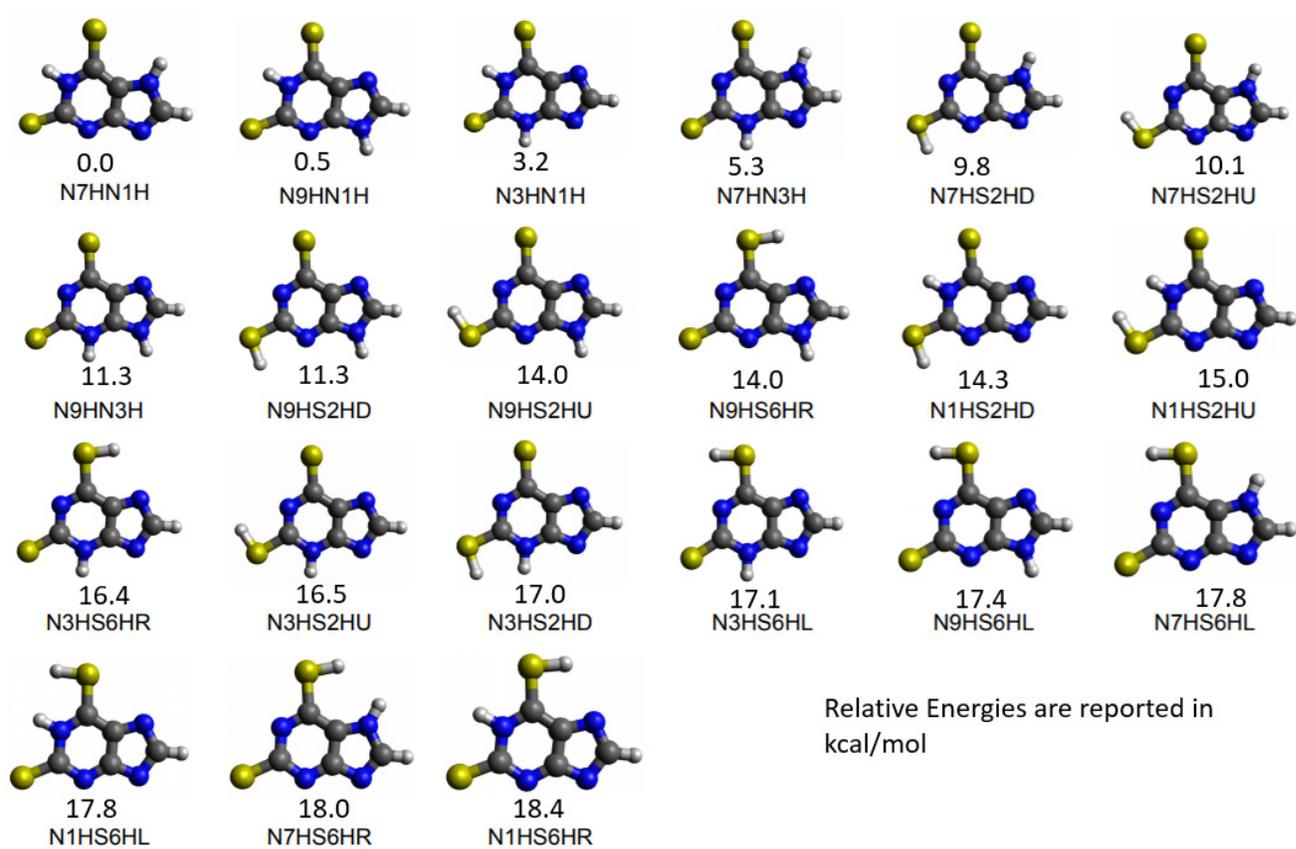


Figure S2. Ground-state optimized geometries of the 21 possible tautomers of deprotonated dtPur calculated at the B3LYP/IEFPCM/6-311+G(d,p) in water with their relative energies.

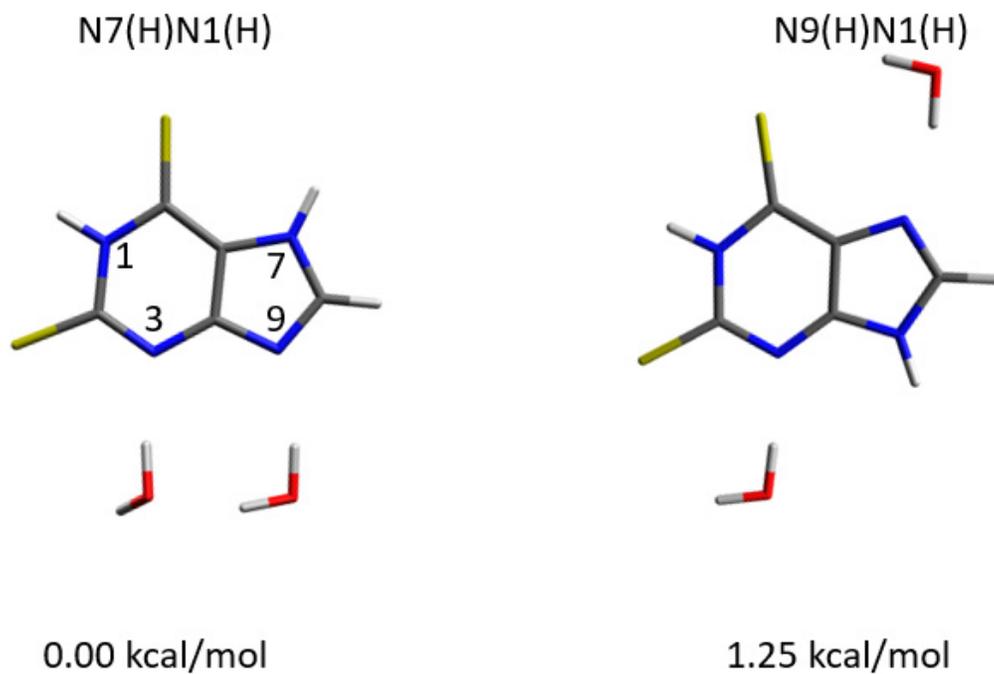


Figure S3. Ground-state optimized geometries of the N7(H)-N1(H) and N9(H)-N1(H) tautomers of deprotonated dtPur with two explicit water molecules calculated at the B3LYP/IEFPCM/6-311+G(d,p) in water with their relative energies.

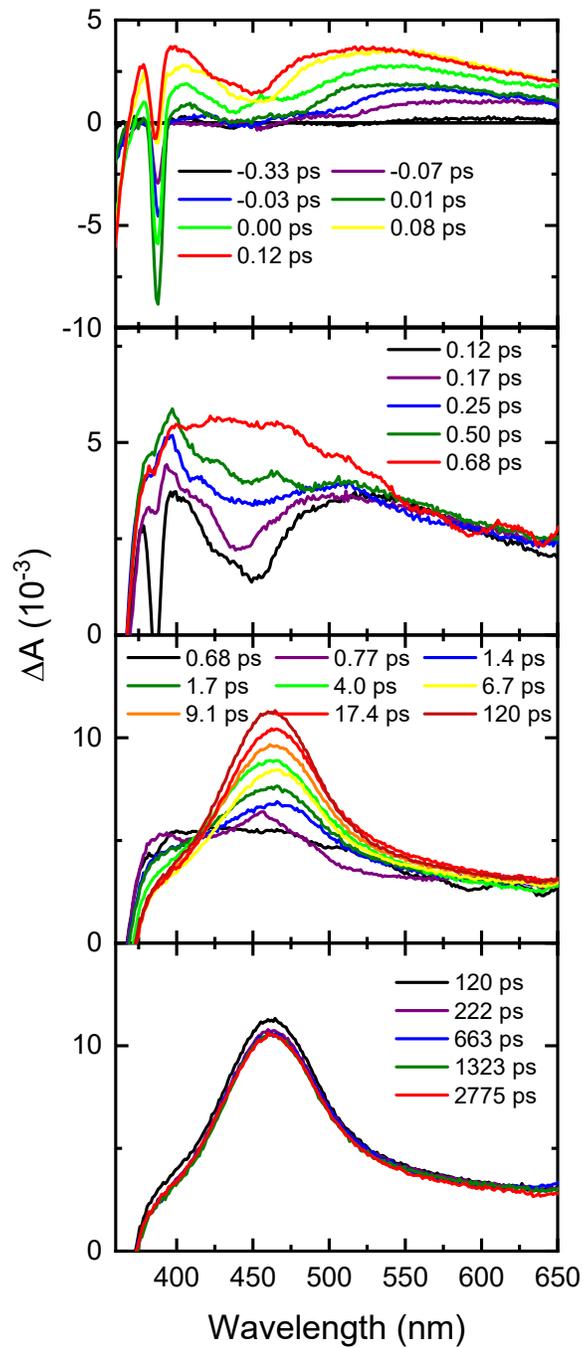


Figure S4. Transient absorption spectra of dtPur in phosphate buffer pH 7.4 upon excitation with 342 nm. The dynamics observed upon 342 nm excitation of dtPur in phosphate buffer pH 7.4 are identical to those reported in the main text where an excitation wavelength of 325 nm was used.