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Photophysics of the fluorescent guanine analog tzG

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The development of environmental sensitive fluorescent nucleoside analogues (FNA) to site-selectively characterize the structure and dynamics of nucleic acids is of high demand [1]. One of the perspective FNA is isothiazologuanosine (tzG) [2], an isomorphic and isofunctional FNA of guanosine (G). tzG can faithfully substitute G in non-canonical nucleic acid structures. tzG spectroscopic response to different environmental changes is critical to fully understand its photophysics and correctly interpret its spectroscopic signatures when it is inserted into nucleic acids.

In this work, we performed the fluorescence spectroscopy measurements of free tzG in different solvents and quantum mechanical (QM) calculations to characterize the mechanisms underlying tzG photophysics. In aprotic solvents, mainly tzG-H1 keto-amino tautomer is present and possesses short fluorescence decay ($\tau \sim 2$ ns) and low quantum yield ($\phi \sim 0.10$). In buffer, tzG-H1 and tzG-H3 keto-amino tautomers coexist in ground-state equilibrium and tzG-H1 is the main emitting species ($\phi = 0.36$, $\tau = 8.84$ ns). The two tautomers were also observed in methanol, but with a 30% decrease in ϕ and τ values for the major H1 tautomer and decreased population of tzG-H3 tautomer. QM calculations revealed the main non-radiative pathway of tzG-H1 caused by NS bond loosening, which is responsible for the solvent-sensitive ϕ and τ values. The study lays the ground for rationally using tzG as a sensitive FNA.

[1] Dziuba, D. et al., Chem. Soc. Rev. 2021, 50 (12), 7062–7107.
[2] Rovira, A. R. et al., J. Am. Chem. Soc. 2015, 137 (46), 14602–14605.

Topics

Session D. Biomedical optics and sensors technology

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