Computational Study of the Relative Stability of Tautomers of Modified RNA Nucleobases in Aqueous Media

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This study analyzes the energetics and stability of the tautomers of modified emissive RNA nucleobases synthesized by Shin et al. [1], which is useful for biological imaging. Optimized geometries and relative stabilities are computed for the stable compounds and their tautomers in gas phase and water using density functional theory B3LYP/6-31++G(2df, 2p). We also present the thermodynamics properties for each tautomer structures. The theoretical results show that there are tautomeric forms of modified RNA bases that should be present in water. These tautomers cause unexpected peaks in the experimental spectra of the modified RNA bases [2].

References

[1] Shin, D.; Sinkeldam, R.W.; Tor, Y. Emissive RNA Alphabet. *Journal of the American Chemical Society* **2011**, *133*, 14912-14915.
[2] Gedik, M.; Brown, A. Computational Study of the Excited State Properties of Modified RNA Nucleobases. *Journal of Photochemistry and Photobiology A: Chemistry* **2013**, *259*, 25-32.

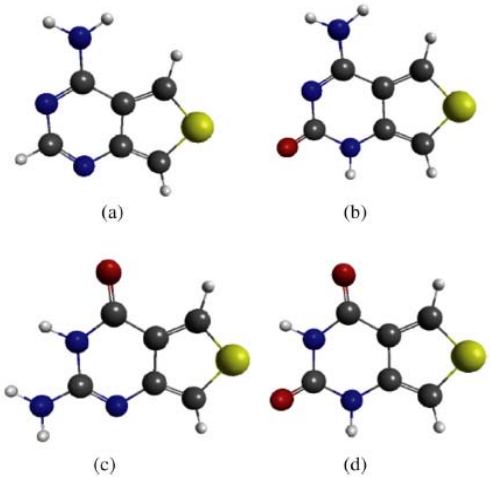

Figure 1. Structures of the modified RNA nucleobases in water. Atomic representations: S = yellow, N = blue, O = red, C = gray, H = white.
(a) thAdenine,
(b) thCytosine,
(c) thGuanine,
(d) thUracil.
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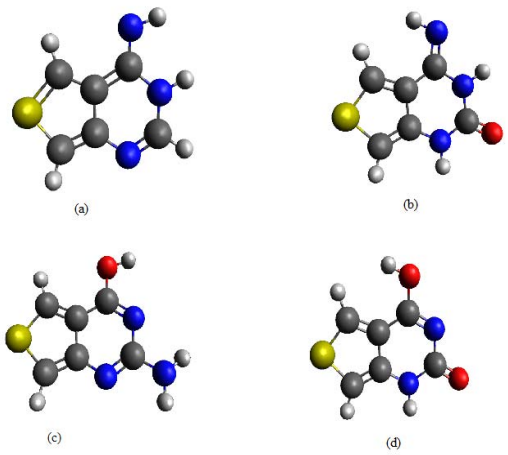

Figure 2. Examples of tautomers of modified RNA nucleobases in water. Atomic representations: S = yellow, N = blue, O = red, C = gray,
H = white.
(a) Imino tautomer of thAdenine
(b) Imino tautomer of thCytosine
(c) Enol tautomer of thGuanine
(d) Enol tautomer of thUracil.