Effect of microhydration on DNA probe explored by Non-Adiabatic Dynamics

Lognon Elise;[A] **Monari Antonio**[A]

A) ITODYS, Université Paris Cité, 15 Rue Jean Antoine de Baïf, 75013 Paris

elise.lognon@u-paris.fr

The study of the native conformation of nucleic acids and its eventual perturbation induced by the coupling with the environment or external stimuli is fundamental to better assess the molecular mechanisms underlying their biological role.[1] Luminescent DNA probes [2] are tools of choice to evidence the presence of important structural modification of the nucleic acid structure. I will present a non-adiabatic dynamics study, performed with the surface hopping formalism,[3] on 2-thienyl-3-hydroxychromone, an environment-dependent luminescent organic DNA probe.[4] I will show that the solvent first-shell water molecules undergo a rather complex reorganization upon light excitation.[5] This also involves the triggering of a water-mediated proton transfer process which leads to the formation of the probe's tautomeric structure (Figure 1). The solvent-mediated transfer process globally diminishes the intersystem crossing efficiency, and hence the population of the triplet state manifold, as compared to the non-solvated systems. Our results also point out the non-innocent role of solvent networks in tuning complex photophysical processes, while opening competitive relaxation channels.

[1]. H. L. Lightfoot, T. Hagen, N. J. Tatum, J. Hall, FEBS Lett.2019, 593, 2083–2102.
[2]. R. W. Sinkeldam, N. J. Greco, Y. Tor, Chem. Rev.2010, 110, 2579–2619.
[3]. M. Richter, P. Marquetand, J. Gonzàlez-Vàzquez, I. Sola, L. Gonzàlez, JCTC. 2011, 7(5), 1253-1258
[4]. A. Monari, A. Burger, E. Dumont, Photochem. Photobiol. Sci.2023.
[5]. E. Lognon, A. Burger, E. Dumont, A. Monari, ChemPhotoChem. 2024, e202400078.

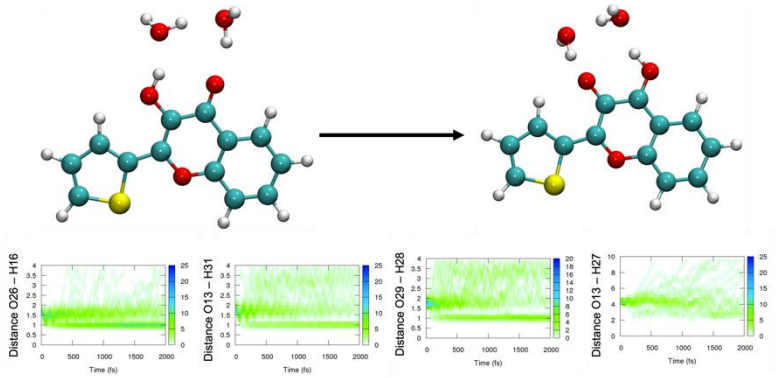

Figure 1. Tautomerization process

Keywords: Photochemistry, Non-Adiabatic dynamics, DNA probe.