

"PHOTOSTABLE OR PHOTODAMAGING? STRUCTURE-PHOTOPHYSICAL PROFILE RELATIONSHIPS IN DNA BUILDING BLOCKS"

Dr. Inés Corral Pérez

Departamento de Química,
Universidad Autónoma de Madrid
IADCHEM. Institute for Advanced Research in Chemistry,
Universidad Autónoma de Madrid,
28049 Cantoblanco, Madrid, Spain
ines.corral@uam.es

May 21, 2021 (Friday)

12pm (BRT time) - Google Meet

ORGANIZATION:

Prof. Dr. Antonio Carlos Borin

Instituto de Química, Universidade de São Paulo (USP), SP, Brazil

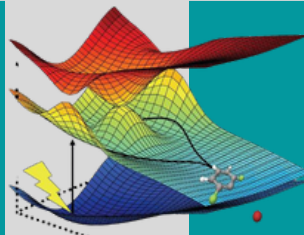
INFORMATION AND REGISTRATION:

ancborin@iq.usp.br

Registration: send a message to ancborin@iq.usp.br

with the words "Inés Corral Pérez - Virtual" on the "subject"

Deadline: May 19, 2021 (Wednesday), 06pm (BRT time)



WEBINARS
COMPUTATIONAL PHOTOCHEMISTRY



IQ - USP

ABSTRACT

Photostable or photodamaging? Structure-photophysical profile relationships in DNA building blocks

Dr. Inés Corral Pérez

Departamento de Química, Universidad Autónoma de Madrid, 28049 Cantoblanco, Madrid, Spain
IADCHEM. Institute for Advanced Research in Chemistry, Universidad Autónoma de Madrid,
28049 Cantoblanco, Madrid, Spain
ines.corral@uam.es

The current composition of the genetic alphabet is the result of the persistence of DNA and RNA monomers against multiple selection pressures operating on the early Earth, among which UV light exposure played a prominent role.[1] Despite being strong UV absorbers, native nucleobases are highly photostable systems that have developed extremely efficient mechanisms to dissipate the absorbed energy, preventing this way DNA damage.[2] Investigating the decay routes of non-canonical purine- and pyrimidine-derivatives can help elucidating the origin of the photostability of life building blocks, and at the same time identifying potential prebiotic genetic ancestors that might have composed the primordial soup.

The aim of this webinar is to provide an overview of the main photophysical properties of a selected group of nucleobase derivatives. In particular, the effect of the position and the number of carbonyl and amino substituents in the purine and pyrimidine cores' potential energy landscapes will be discussed. Furthermore, the extraordinarily efficient population of triplet states upon the replacement of carbonyl by thiocarbonyl functions in canonical purine and pyrimidine nucleobases will be rationalized in terms of the changes in the topographical features of the potential energy surfaces of these two families of heterocycles and the outcome of molecular dynamics simulations.[3]

These results will help rationalizing the relation between functionalization schemes of purine [4] and pyrimidine [5] cores and their observed photophysics, which is key to determine the electronic and structural factors that established the superiority of the five contemporary DNA and RNA nucleobases against other organic chromophores.

References:

- [1] A. C. Rios and Y. Tor, *Isr. J. Chem.*, 53 469 (2013).
- [2] A. Giussani, J. Segarra-Martí, D. Roca-Sanjuán, and M. Merchán, *Top Curr. Chem*, 355 57 (2015).
- [3] S. Arslançan, L. Martínez-Fernández, I. Corral, *Molecules*, 22 998 (2017).
- [4] C. E. Crespo-Hernández, L. Martínez-Fernández, C. Rauer, C. Reichardt, S. Mai, M. Pollum, P. Marquetand, L. González, I. Corral, *J. Am. Chem. Soc.*, 137 4368 (2015).
- [5] E. M. Arpa, M. M. Brister, S. J. Hoehn, C. E. Crespo-Hernández, I. Corral, *J. Phys. Chem. Lett.*, 11 5156 (2020).