Unveiling the photosensitivity mechanisms of UVB filter PABA

Authors: Julia Arnanz¹, Antonio Monari², Inés Corral^{1,3} & Juan J. Nogueira^{1,3}

¹ Department of Chemistry, Universidad Autónoma de Madrid, 28049 Madrid, Spain. ² Chimie Theoretique et Modélisation – ITODYS, Université Paris Cité, 75013, Paris, France.³ Institute for Advanced Research in Chemical Sciences, 28049 Madrid, Spain.



PABA-DNA non-covalent binding

1. <u>Sampling of DNA binding sites through conventional MD</u>



2. Intercalation binding profile through Umbrella Sampling







TDM analysis^[2] allows to separate local and charge transfer (CT) states.





()→●

Local on PABA



Pure DNA CT





<u>References</u>

^[1] J. M. Allen, et al. J Photoch. Photobio. B. 1996, 32, 33–37. ^[2] F. Plasser. J. Chem. Phys. 2020, 152, 084108. ^[3] C. Chan, et al. Phys. Chem. Chem. Phys. 2020, 22, 8006–8020.

Conclusions

- PABA gets spontaneously intercalated in the DNA strand.
- PABA favours population of charge-transfer states in the DNA
- PABA deactivation routes lead to a long-lived triplet state

PABA potentially induces photodamage in the DNA



Find out more about our research!



Processes in Photoinitiated biological environments events