## Unveiling the photosensitivity mechanisms of UVB filter PABA

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*Para*-aminobenzoic acid is a formerly used UVB filter that was found to react with the DNA when exposed to sunlight.[1] Molecular Dynamics (MD) and Umbrella Sampling simulations show that the neutral species of PABA binds favourably DNA by intercalation between two nucleobase pairs, while the binding of the anionic species is not feasible from the thermodynamic and kinetic points of view. Simulation of the joint PABA-DNA absorption spectrum by Quantum Mechanics/Molecular Mechanics (QM/MM) calculations on top of a MD ensemble of geometries, followed by transition density analysis, suggests that charge transfer states could play a role in the deactivation of the system and lead to the formation of radical species that might trigger DNA lesions.[2] Moreover, the identification of relevant deactivation routes of excited PABA in vacuum revealed the favourable population of a long-lived triplet state, which can participate in photosensitising mechanisms, such as energy transfer processes to thymine or to molecular oxygen.[3]

[1] J. Photoch. Photobio. A: Chemistry, 83, 223-228 (1994). DOI: 10. 1016/1010-6030(94)03827-9.

[2] Chem. Sci., 8, 5682-5691 (2017). DOI: 10.1039/C7SC01600J.

[3] J. Photoch. Photobio. A: Chemistry, 7, 100042, (2021) DOI: 10.1016/j.jpap.2021.100042.

**Authors:** Prof. MONARI, Antonio (ITODYS-CTM. Université Paris Cité); Prof. CORRAL PÉREZ, Inés (Department of Chemistry. Universidad Autónoma de Madrid); Prof. NOGUEIRA, Juan J. (Department of Chemistry. Universidad Autónoma de Madrid); ARNANZ SEBASTIÁN, Julia (Department of Chemistry. Universidad Autónoma de Madrid)

Presenter: ARNANZ SEBASTIÁN, Julia (Department of Chemistry. Universidad Autónoma de Madrid)

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