

## The excited state deactivation of Shikonin rationalized from its naphthoquinone parent structures

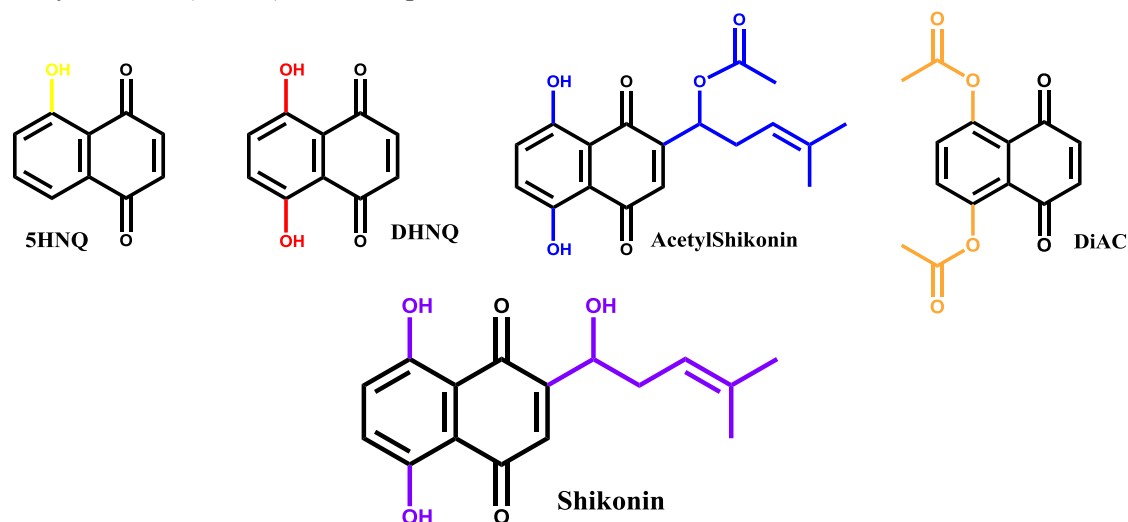
Catarina M. Pinto<sup>1\*</sup>, Estefanía Delgado-Pinar<sup>1</sup>, João Pina<sup>1</sup>, J. Sérgio Seixas de Melo<sup>1</sup>

<sup>1</sup>University of Coimbra, CQC, Department of Chemistry, 3004-535 Coimbra, Portugal

\**catarina.m.pinto@student.uc.pt*

Shikonin, a naphthoquinone dye, is a molecule of colour<sup>1</sup> with natural origin and various medicinal properties including anti-inflammatory capacity, which shows solvent dependent properties. Previous studies on this molecule have reported its photostability and theoretical predictions on the more stable conformer.<sup>2</sup> However, a complete rationalization of its excited state deactivation mechanism is still to be done.

The chemical structure of shikonin shows a core structure of a di-hydroxy-naphthoquinone with an additional non-aromatic hydroxy group. The involvement of excited state intra/ or inter molecular proton transfer is found determinant in the deactivation mechanisms of aromatic molecules.<sup>1,3</sup> In this work a comprehensive photophysical characterization has been undertaken for shikonin involving fast spectroscopic techniques (fs-UC and fs-TA)<sup>3</sup> and TD-DFT calculations aiming to clarify the excited state deactivation mechanisms of this compound. In order to fully equate the contributions of the different hydroxy groups on this mechanism, a study involving its quinone derivatives (Figure 1), 5-hydroxy-1,4-naphthoquinone (5HNQ), 5,8-dihydroxy-1,4-naphthoquinone (DHNQ), 5,8-diacetyloxy-1,4-naphthoquinone (DiAc) and acetylshikonin (AcShk), was also performed.



**Figure 1.** Chemical structures of 5-hydroxy-1,4-naphthoquinone (5HNQ), 5,8-dihydroxy-1,4-naphthoquinone (DHNQ), shikonin (Shk), acetylshikonin (AcShk) and 5,8-dioxyacetyl-1,4-naphthoquinone (DiAc).

### References

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