

Exploring Resveratrol Photochemistry and Photodynamic Therapy Potential

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ABSTRACT

Resveratrol is a polyphenolic compound naturally found in foods such as grapes, berries, and peanuts. Its *trans* isomer (Fig. 1a), the most stable, is known for its antioxidant activity and is commonly applied in cosmetic products. However, the incidence of UV-vis radiation can promote the isomerization of the compound to the *cis* isomer (Fig. 1b), as well as photochemical reactions [1]. Some studies have shown that specific products derived from these photochemical reactions participate in singlet oxygen generation processes, which can be used in photodynamic therapy [2].

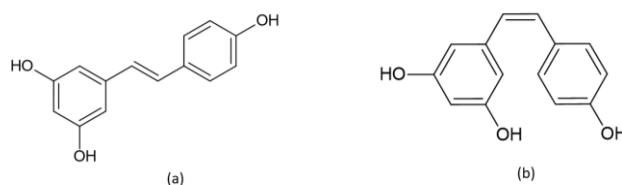


Figure 1. Molecular structures of (a) *trans*-resveratrol (b) *cis*-resveratrol

This work will present the results of DFT and TD-DFT calculations performed to investigate the photophysical properties of compounds derived from resveratrol photoexcitation. Moreover, we performed nonadiabatic dynamics simulations with surface hopping to assess the reaction pathways of *trans*-resveratrol after excitation. The thermodynamic viability of reactions involving electron and energy transfer from the resveratrol derivatives to oxygen and DNA bases was evaluated to verify the potential action of resveratrol in photodynamic therapy after excitation.

References

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- [2] Santos, D.P., Lopes, D.P.S., Moraes, R.C., Gonçalves, C.V., Rosa, L.P., Rosa, F.C.S., & Silva, R.A.A. Photoactivated resveratrol against *Staphylococcus aureus* infection in mice. *Photodiagnosis and Photodynamic Therapy*, **2019**,25, 227-236.