

Singlet oxygen photogeneration by ethanolic extract of *Syzygium cumini* fruits: Theoretical elucidation through excited states computations

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The ethanolic extract of *Syzygium cumini* fruits was characterized and evaluated in the photogeneration of singlet oxygen (1O_2) under visible light radiation. This process was studied from a theoretical approach by the survey of the generated electronic excited states, after photoexcitation of the most abundant anthocyanin of the extract, i.e. delphinidin-3,5-diglucoside. It was determined that the adiabatic energy of the optimized $T_1(\pi\text{-H}^* \rightarrow \pi\text{-L}^*)$ state was 1.55 eV and that the overall energy transfer releases 0.58 eV in an exothermic process. Therefore, this state is the responsible of promoting electron transfer reactions and subsequent formation of 1O_2 through illumination. © 2018 Elsevier B.V.

Anthocyanin

Singlet oxygen

Syzygium cumini

TDDFT

Electric excitation

Energy transfer

Excited states

Fruits

Oxygen

Adiabatic energies

Electron-transfer reactions

Electronic excited state

Exothermic process

Singlet oxygen

Syzygium cumini

TDDFT

Theoretical approach

Anthocyanins