# Furanyl chalcone derivatives as efficient singlet oxygen quenchers. An experimental and DFT/MRCI study

Diaz-Uribe C.

Vallejo W.

Flórez J.

Trilleras J.

Gutierrez M.

Rodriguez-Serrano A.

Schott E.

Zarate X.

This study reports the antioxidant activity against singlet oxygen (1O2) of five newly synthesized furanyl chalcones (FCs) (E)-3-(5-(4-chlorophenyl)furan-2-yl)-1-arylprop-2-en-1-ones (3a-e). Their structural difference is based on the aryl substituent as follows (Ar): 3a = ?C6H4?OCH3, 3b = ?C6H3-(1,2-OCH3), 3c = ?C6H4OC6H4, 3d = ?C10H6-(OCH3) and 3e = ?C4H3O. We used a Claisen-Schmidt condensation involving a 5-(4-chlorophenyl)furan-2-carbaldehyde and the corresponding ketones under ultrasonic irradiation. Their property to 1O2 quenching was analyzed in terms of the rate constant for the process (kQ at 25 °C) determined by the Stern?Volmer model in ethanol. For the compounds 3c, 3d and 3e, the kQ values are slightly larger respect to 3a and 3b. The FCs 3c behaves as the best quencher (kQ of 8.44 (±0.09) x 107 M?1s?1). Geometry analysis and electronic structure calculations have been performed in the framework of Density Functional Theory (DFT) and DFT/Multi-Reference Configuration Interaction (DFT/MRCI) methods. According to DFT/MRCI, a physical quenching of 1O2 from the ground states of the FCs may not likely induce a spontaneous energy transfer processes but a chemical quenching mechanism may dominate the kinetics. 

DFT/MRCI

Furanyl chalcones

Singlet oxygen quenching

3 [5 (4 chlorophenyl)furan 2 yl] 1 (3,4 dimethoxyphenyl)prop 2 en 1 one

3 [5 (4 chlorophenyl)furan 2 yl] 1 (4 methoxyphenyl)prop 2 en 1 one

3 [5 (4 chlorophenyl)furan 2 yl] 1 (4 phenoxyphenyl)prop 2 en 1 one

3 [5 (4 chlorophenyl)furan 2 yl] 1 (6 methoxynaphthalen 2 yl)prop 2 en 1 one

3 [5 (4 chlorophenyl)furan 2 yl] 1 (furan 2 yl)prop 2 en 1 one

chalcone derivative

singlet oxygen

unclassified drug

analytic method

antioxidant activity

Article

Claisen rearrangement

density functional theory

drug structure

drug synthesis

energy transfer

Fourier transform infrared spectroscopy

kinetics

multireference configuration interaction

priority journal

proton nuclear magnetic resonance

rate constant

ultrasound