Novel (E)-1-(pyrrole-2-yl)-3-(aryl)-2-(propen-1-one) derivatives as efficient singlet oxygen quenchers: Kinetics and quantum chemical calculations

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Chalcones constitute an important group of natural and synthetic products that have been screened due to their wide range of pharmacological applications. Herein, we studied the antioxidant activity of five newly synthetized (E)-1-(pyrrole-2-yl)-3-(aryl)-2-(propen-1-one) (PAPs) derivatives against singlet oxygen (1O<inf>2</inf>). The differences among the compounds are related to aryl substitution in the p-position where: 3a = C<inf>6</inf>H<inf>5</inf>, 3b = 4-H<inf>3</inf>COC<inf>6</inf>H<inf>4</inf>, 3c = 4-FC<inf>6</inf>H<inf>4</inf>, 3d = 4-ClC<inf>6</inf>H<inf>4</inf>, 3e = 4-BrC<inf>6</inf>H<inf>4</inf>. The PAPs were synthesized using a Claisen-Schmidt condensation reaction between 2-acetylpyrrole and aromatic aldehydes under ultrasonic irradiation (yields between 79-86%) and were characterized by IR, mass spectrometry, NMR and quantum chemical calculations. The total singlet oxygen quenching rate constants (k<inf>Q</inf>) of the PAPs were measured spectrophotometrically in ethanol at 25°C and determined by using the Stern-Volmer model. As the character of the EWGs is increased from 3a to 3e, the k<inf>Q</inf> diminishes smoothly. The best quencher is found to be the 3a compound (where the aryl group is unsubstituted) with a k<inf>Q</inf> = 5.71 (±0.21) × 107 M-1 s-1, which is similar to those for other antioxidants e.g. flavonoids. These results suggest these compounds are efficient quenchers of singlet oxygen and their potential applicability in biological systems. © 2015

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