Photo-induced anticancer activity and singlet oxygen production of prodigiosenes

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Supporting Information

Description of singlet oxygen quantum yield calcuations (Φ_Δ):

$^1O_2$ quantum yields were calculated based on literature precedents.[1] 9,10-Dimethylantracene was added as a $^1O_2$ trap. The photooxidation of DMA to the corresponding endoperoxide was monitored as a function of time (over 10 min for rose bengal and over 120 min for photosensitizers **5**, **6** and **7**) and the corresponding kinetic plots are presented in Figure S3. The quantum yeilds of $^1O_2$ were calculated using Rose Bengal (RB) as a reference actinometer ($\Phi_{\Delta,\,RB} = 0.54$ in CH_3CN).[2] Φ_Δ for each photosensitizer (**5**, **6** and **7**, $\Phi_{\Delta,\,PS}$) was estimated using eq. S1 below.

$$\Phi_\Delta^{PS} = \Phi_\Delta^{RB} \frac{F^{PS}\ m^{PS}}{F^{RB}\ m^{RB}}$$

Here, $\Phi_{\Delta,\,RB}$ is the known quantum yield of $^1O_2$ from RB in CH_3CN, m is the slope of linear portion of ΔA of DMA @ 398 nm *vs.* 480 nm LED irradiation (plots and m values presented in Figure S3). F is a correction factor where $F=1-10^{-A}$ (A is the absorption of the photosensitizer at the irradiation wavelength of 480 nm).

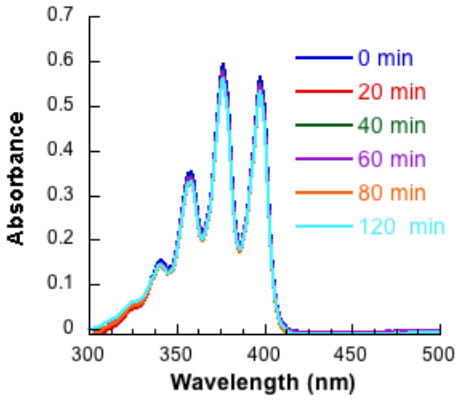

Figure S1. UV-visible spectra of 70 μM DMA collected in CH_3CN over 120 min of 480 nm LED light exposure.

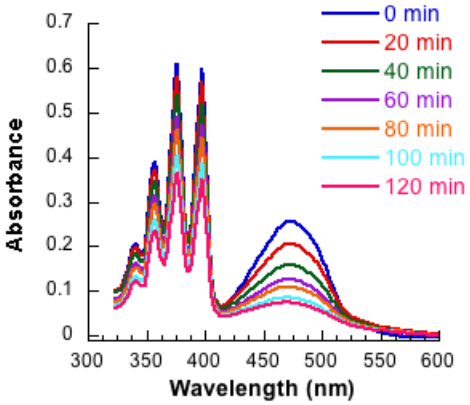

Figure S2. UV-visible spectra of 10 μM **7** and 70 μM DMA collected in CH_3CN over 120 min of 480 nm LED light exposure.

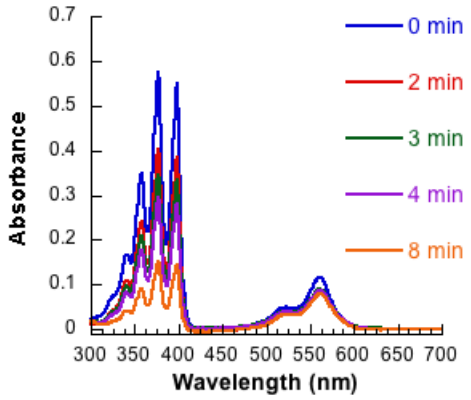

Figure S3. UV-visible spectra of 1.6 μM Rose Bengal and 70 μM DMA collected in CH_3CN over 120 min of 480 nm LED light exposure.

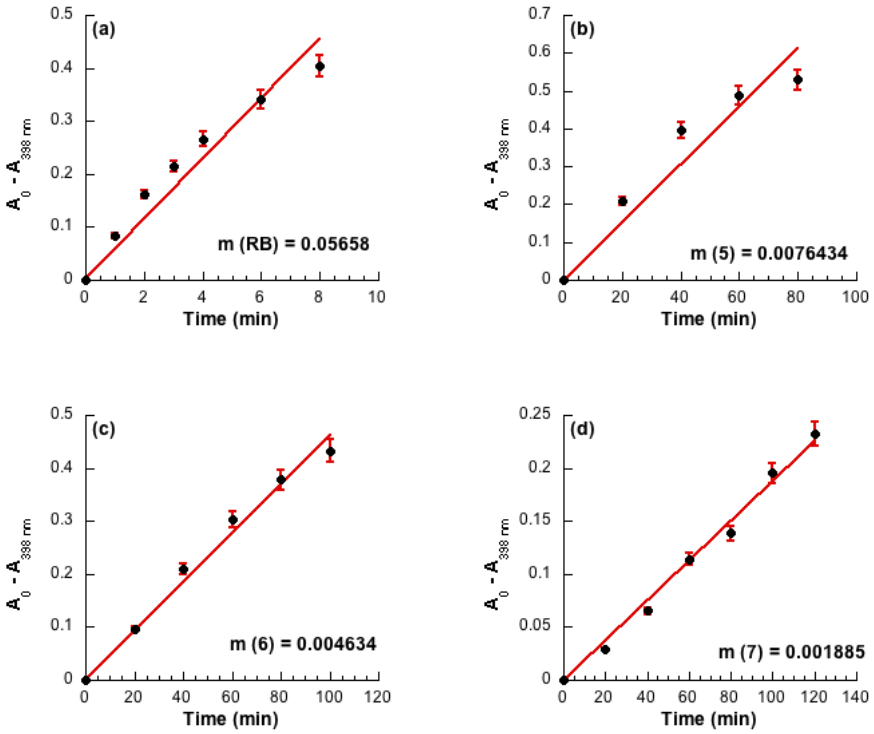

Figure S4. Plot of ΔA of DMA at 398 nm *vs.* irradiation time in the presence of (a) Rose Bengal, (b) **6** and (c) **7**.

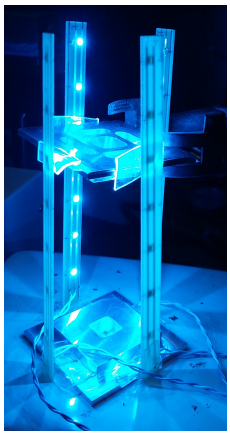

Figure S5. Image of 480 nm blue LED experimental design used as the irradiation source for the photophysical studies.

References

1. W. Li, L. Li, H. Xiao, R. Qi, Y. Huang, Z. Xie, X. Jing and H. Zhang, *RSC Adv.*, 2013, 3, 13417-13421.
2. A. M. Durantini, L. E. Greene, R. Lincoln, S. R. Martínez and G. Cosa, *J. Am. Chem. Soc.*, 2016, 138, 1215-1225.