Photo-induced anticancer activity and singlet oxygen production of prodigiosenes

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Supporting Information

Description of singlet oxygen quantum yield calculations (ΦΔ):

1O2 quantum yields were calculated based on literature precedents.1 9,10-Dimethylantracene was added as a 1O2 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 yields of 1O2 were calculated using Rose Bengal (RB) as a reference actinometer (ΦΔ, RB = 0.54 in CH3CN).2 ΦΔ for each photosensitizer (5, 6 and 7, ΦΔ,PS) was estimated using eq. S1 below.

ΦPS = ΦΔ RB FPS mPS mRB

Here, ΦΔ, RB is the known quantum yield of 1O2 from RB in CH3CN, m is the slope of linear portion of ∆A 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$_3$CN 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$_3$CN 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 CH3CN 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