

Supplementary Information

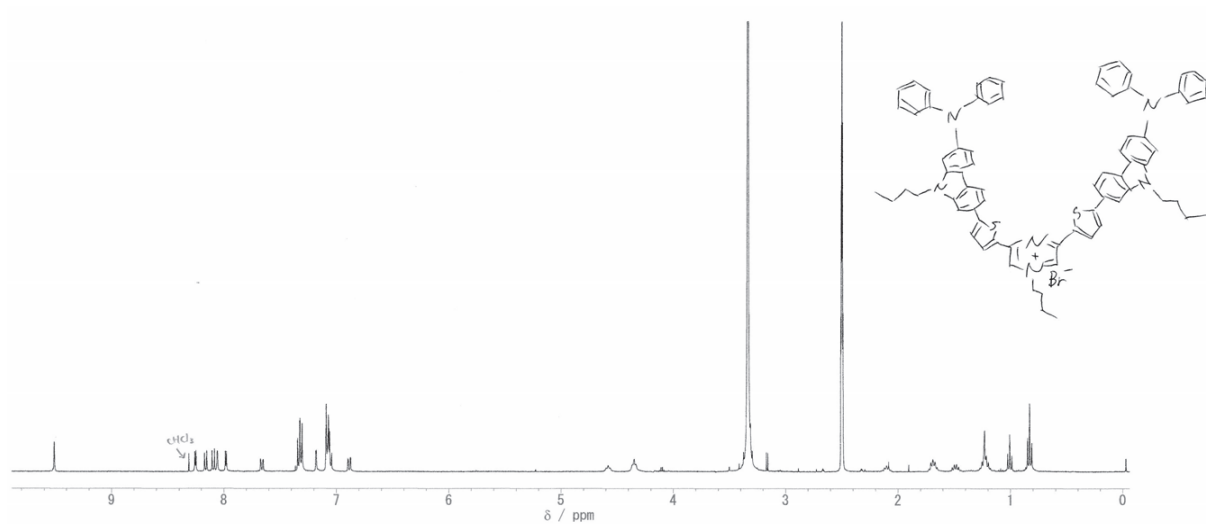
Development of D- π -A pyrazinium photosensitizer possessing singlet oxygen generation

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(a)



(b)

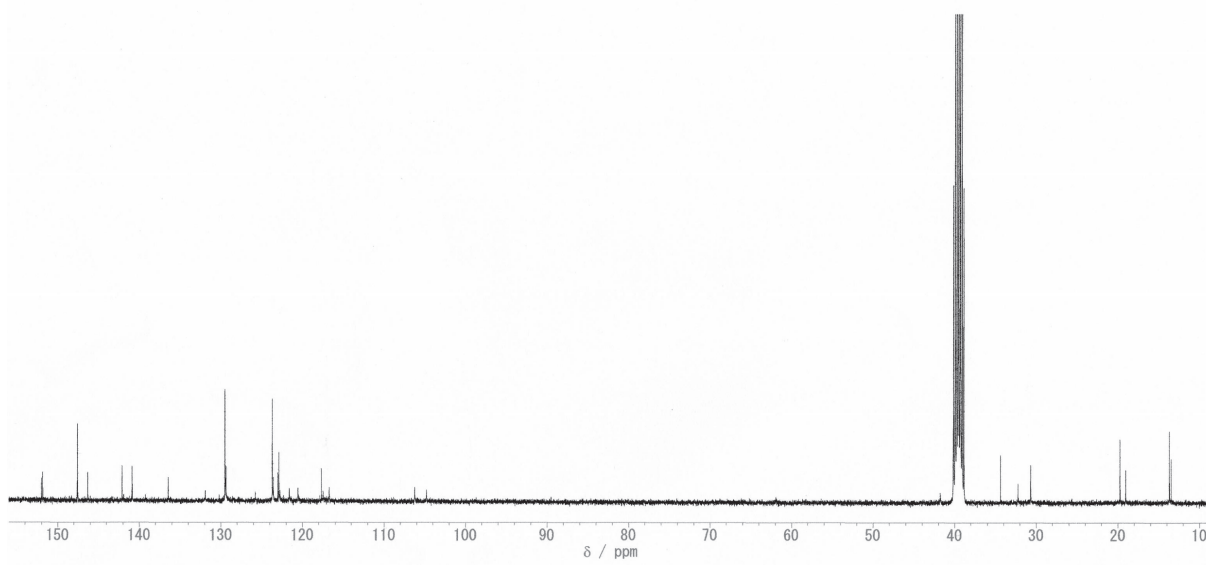
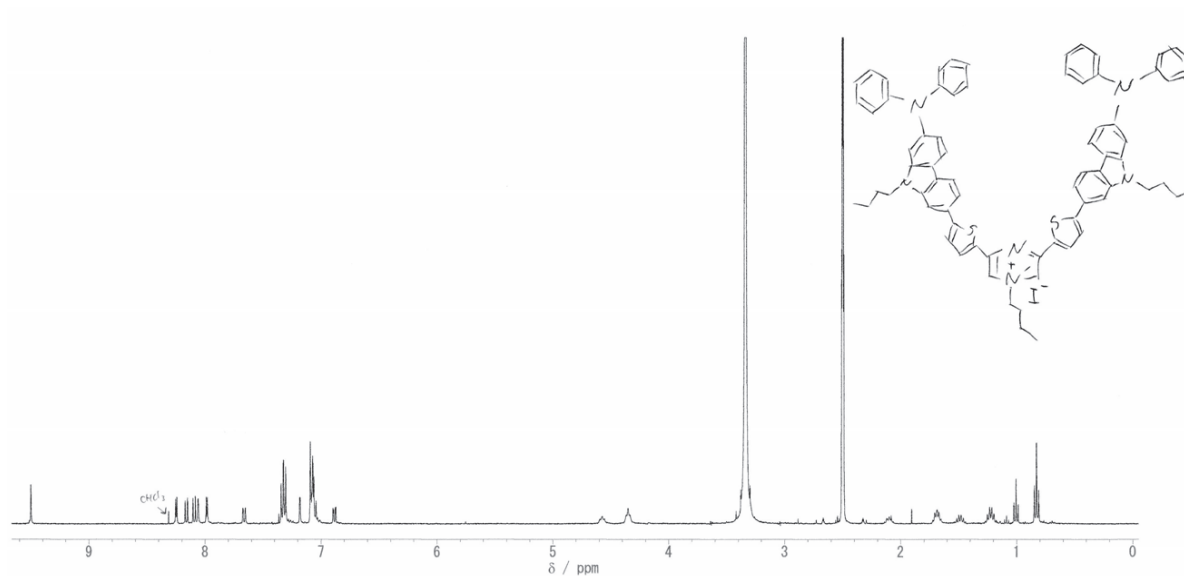


Fig. S1 (a) ¹H NMR and (b) ¹³C NMR of **OEJ-1** in DMSO-d₆.

(a)



(b)

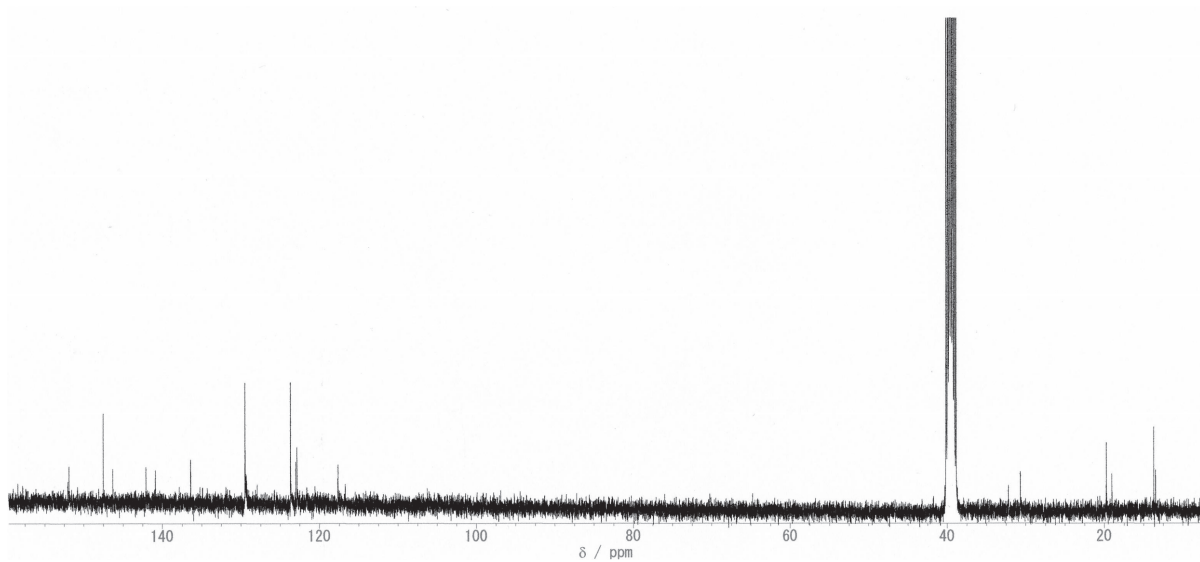


Fig. S2 (a) ¹H NMR and (b) ¹³C NMR of OEJ-2 in DMSO-d₆.

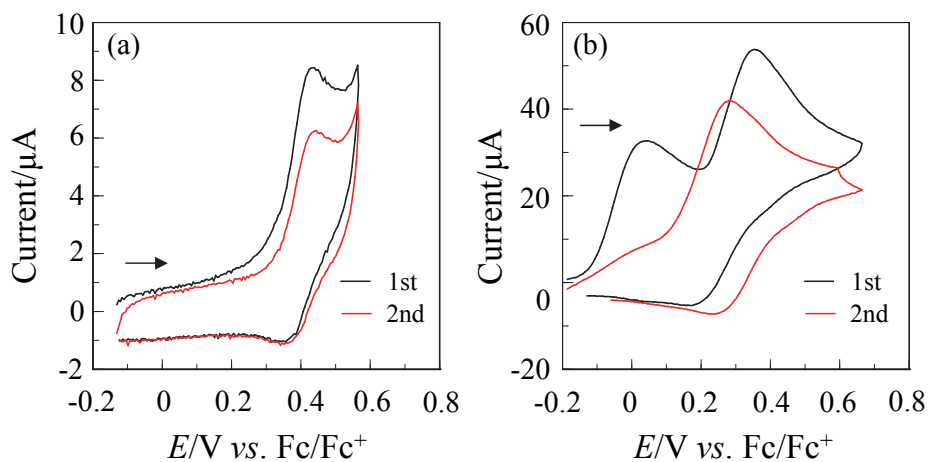
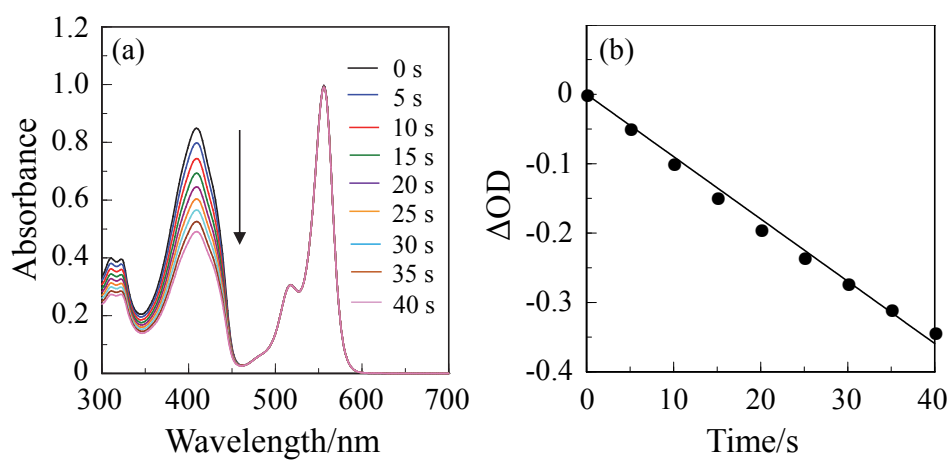


Fig. S3 Cyclic voltammograms of (a) **OEJ-1** and (b) **OEJ-2** in acetonitrile containing 0.1 M Bu_4NClO_4 at the first and the second cycles. The arrow denotes the direction of the potential scan.



Figs. S4 (a) Photoabsorption spectral change and (b) plot of ΔOD for DPBF against the photoirradiation time for the photooxidation of DPBF (4.11×10^{-5} M) using Rose Bengal (1.35×10^{-5} M) as photosensitizer under photoirradiation with 509 nm ($160 \mu\text{W cm}^{-2}$) in methanol.

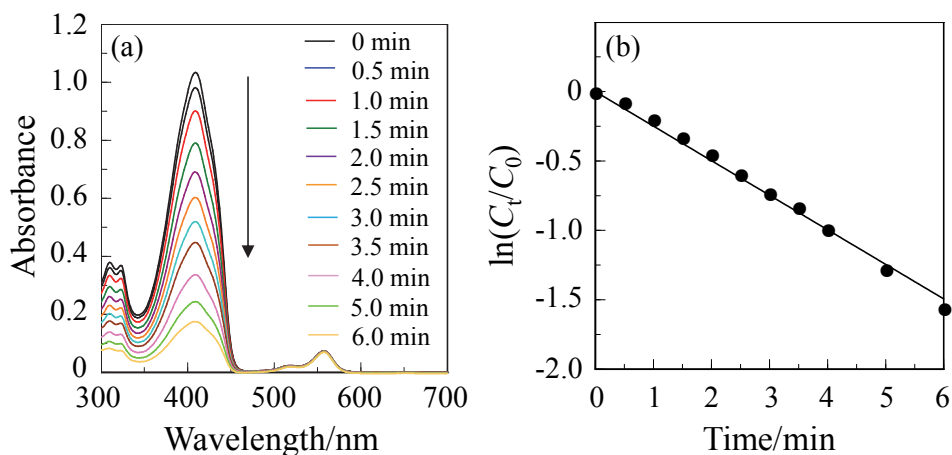


Fig. S5 (a) Photoabsorption spectral change and (b) plot of $\ln(C_t/C_0)$ for DPBF against the photoirradiation time for the photooxidation of DPBF ($C_0 = 5.0 \times 10^{-5}$ M) using Rose Bengal (1.0×10^{-6} M) as photosensitizer under photoirradiation with visible light (> 510 nm, 14 mW cm^{-2}) in methanol.

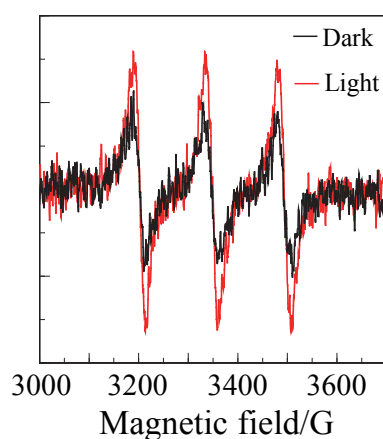


Fig. S6 The ESR spectra of 4-oxo-TEMPO which is formed by the reaction of 4-oxo-TEMP with $^1\text{O}_2$ which was generated by **OEJ-2** under irradiation with visible light (temperature 298 K, microwave power 1 mW, microwave frequency 9.439 GHz, field modulation 0.2 mT at 100 kHz, and scan time 4 min). The air-saturated THF solution containing **OEJ-2** (0.01 mM) as the photosensitizer and 4-oxo-TEMP (50 mM) as the spin-trapping agent was irradiated with visible light (> 510 nm, 14 mW cm^{-2} for 30 min) obtained by passage of xenon light through a 510 nm long path filter.

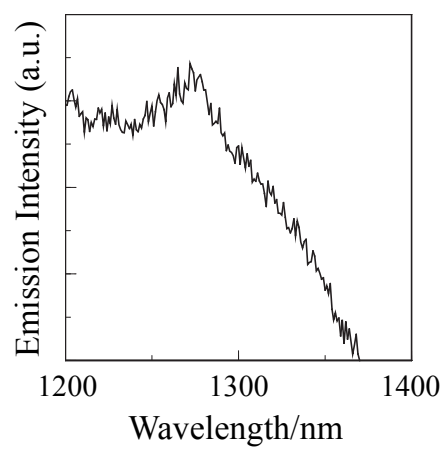


Fig. S7 Phosphorescence spectrum of $^1\text{O}_2$ produced upon the excitation of **OEJ-2** (0.07 mM) at 467 nm in THF.