Supplementary Information (SI) for Journal of Materials Chemistry B.

Supporting Information

A Dual-Targeting Photosensitizer for Simultaneous Mitochondrial and Lysosomal Disruption in Cancer and Antibacterial Photodynamic Therapy

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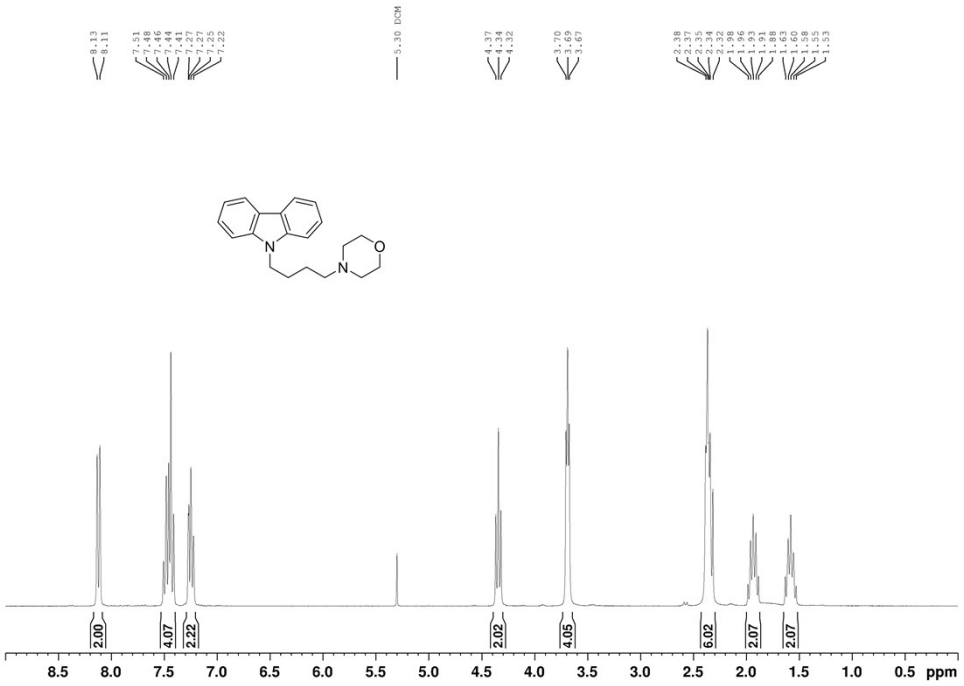

Figure S1 ^{1}H NMR spectrum of compound **1** (300 MHz, chloroform-*d*).

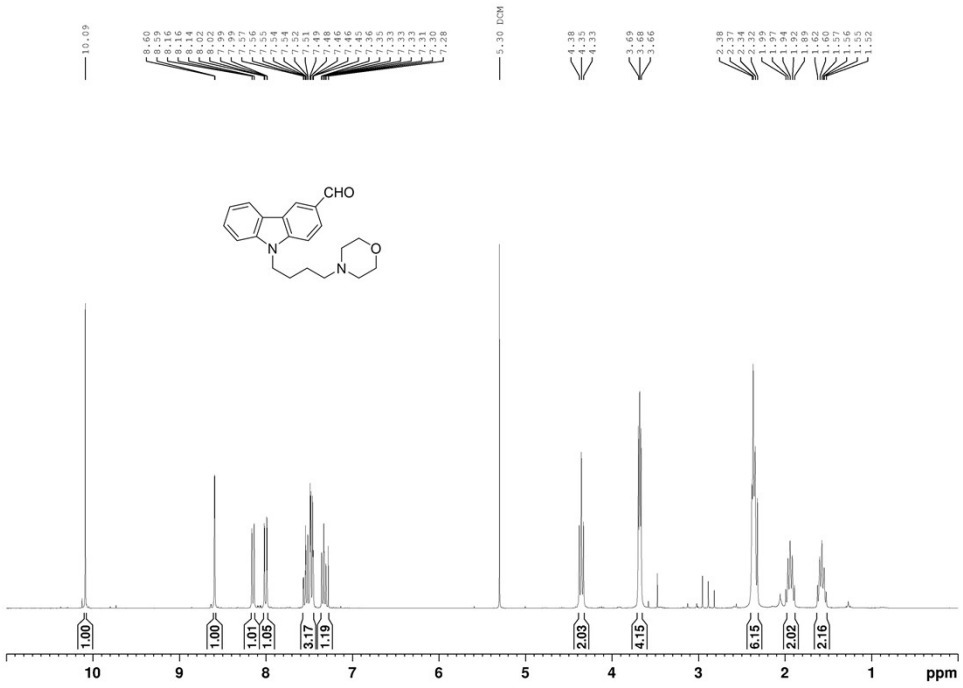

Figure S2 ^{1}H NMR spectrum of compound **2** (300 MHz, chloroform-*d*).

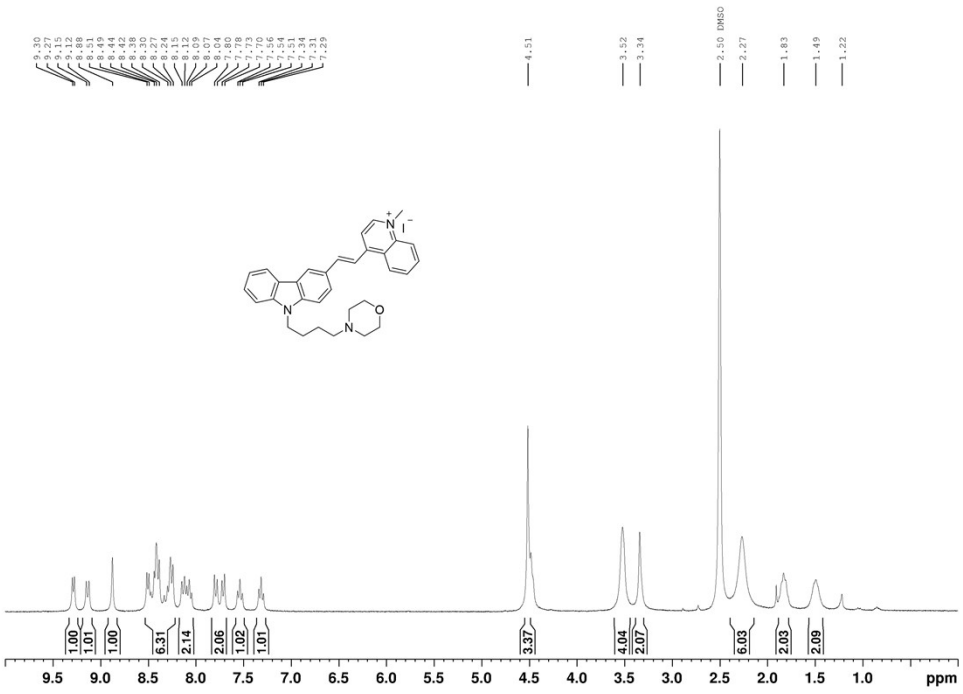

Figure S3 ^{1}H NMR spectrum of **MCQ-1** (300 MHz, DMSO- d_6).

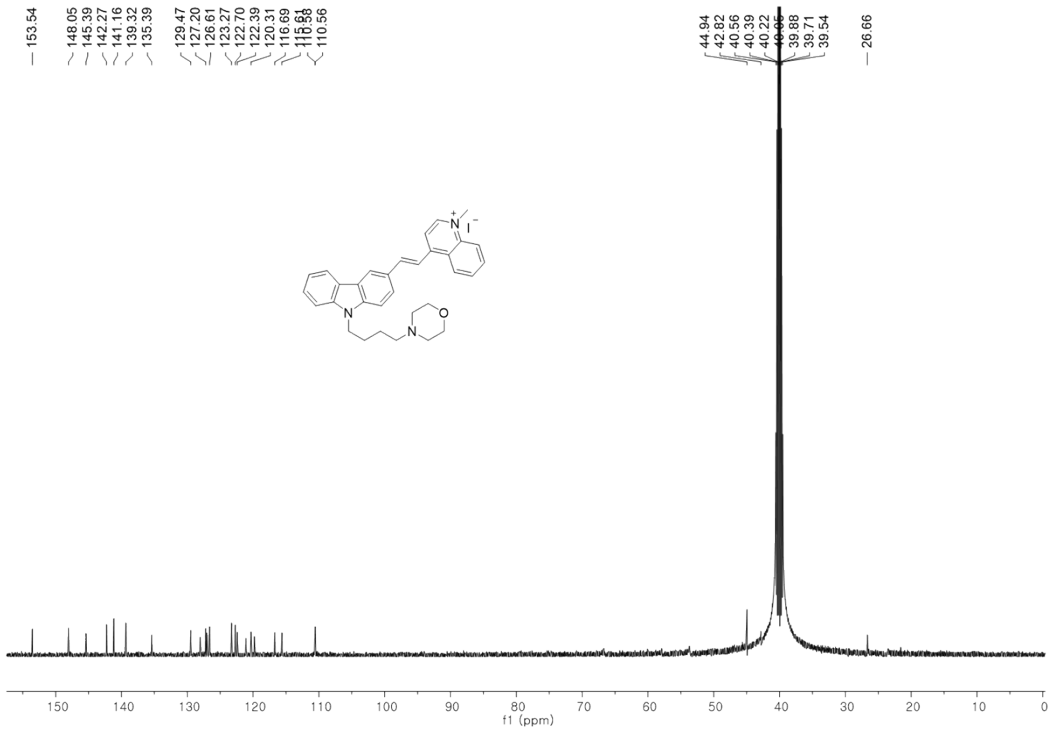

Figure S4 ^{13}C NMR spectrum of **MCQ-1** (125 MHz, DMSO- d_6).

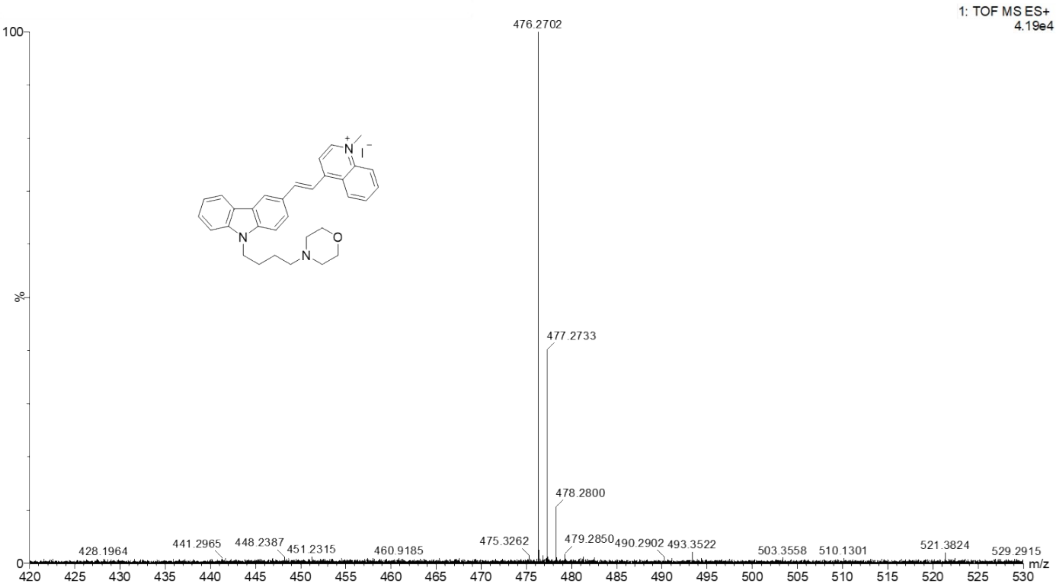

Figure S5 ESI-HRMS spectrum of **MCQ-1**.

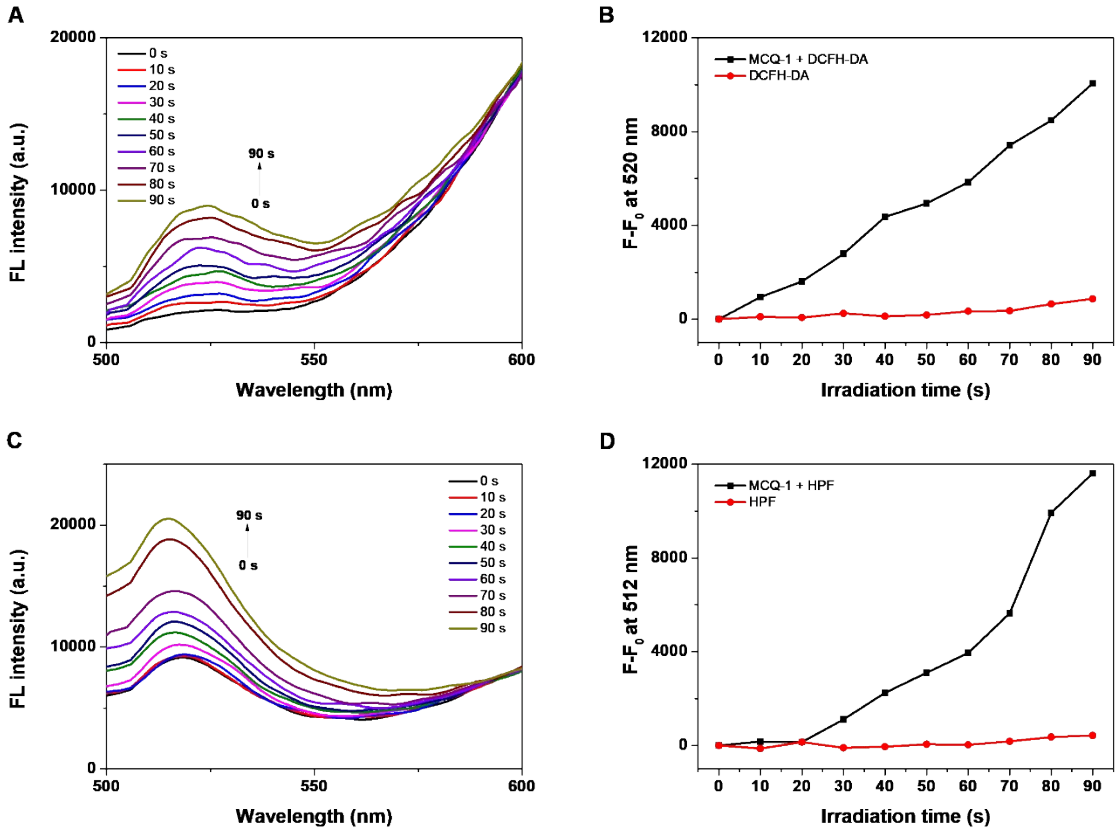

Figure S6 (A), (B) Total ROS and (C), (D) Hydroxyl radical (·OH) generation of **MCQ-1** (10 μM) in PBS under white LED irradiation (50 mW/cm^2), detected using DCFH-DA and HPF, respectively.

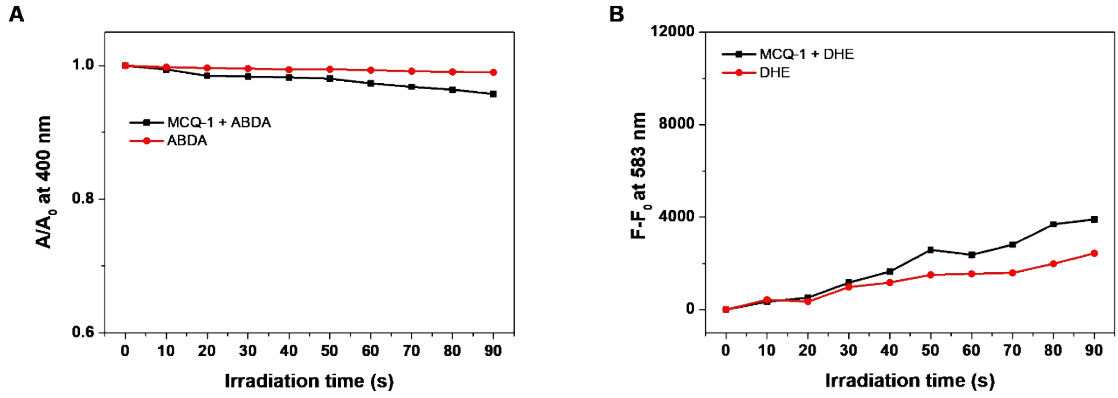

Figure S7 (A) Singlet oxygen ($^1O_2$) and (B) Superoxide radical anion ($O_2^{\bullet-}$) generation of **MCQ-1** (10 μM) in PBS under white LED irradiation (50 mW/cm^2), detected using ABDA and DHE, respectively.

Table S1. Calculated energy level and energy gap of **MCQ-1** at CAM-B3LYP/TZVP theory level.

S_n	Energy (eV)	T_n	Energy (eV)	S_1/T_n	Energy gap
S_1	3.04	T_1	1.97	S_1/T_1	1.07
S_2	3.95	T_2	2.89	S_1/T_2	0.15
S_3	4.17	T_3	3.25	S_1/T_3	-0.21
S_4	4.31	T_4	3.49	S_1/T_4	-0.45
S_5	4.50	T_5	3.63	S_1/T_5	-0.59
S_6	4.58	T_6	3.68	S_1/T_6	-0.64
S_7	4.66	T_7	3.82	S_1/T_7	-0.78
S_8	4.88	T_8	4.02	S_1/T_8	-0.98