Electronic supplementary information

Near-Infrared emitting AIE multinuclear cationic Ir(III) complexes assembled nanoparticles for photodynamic therapy

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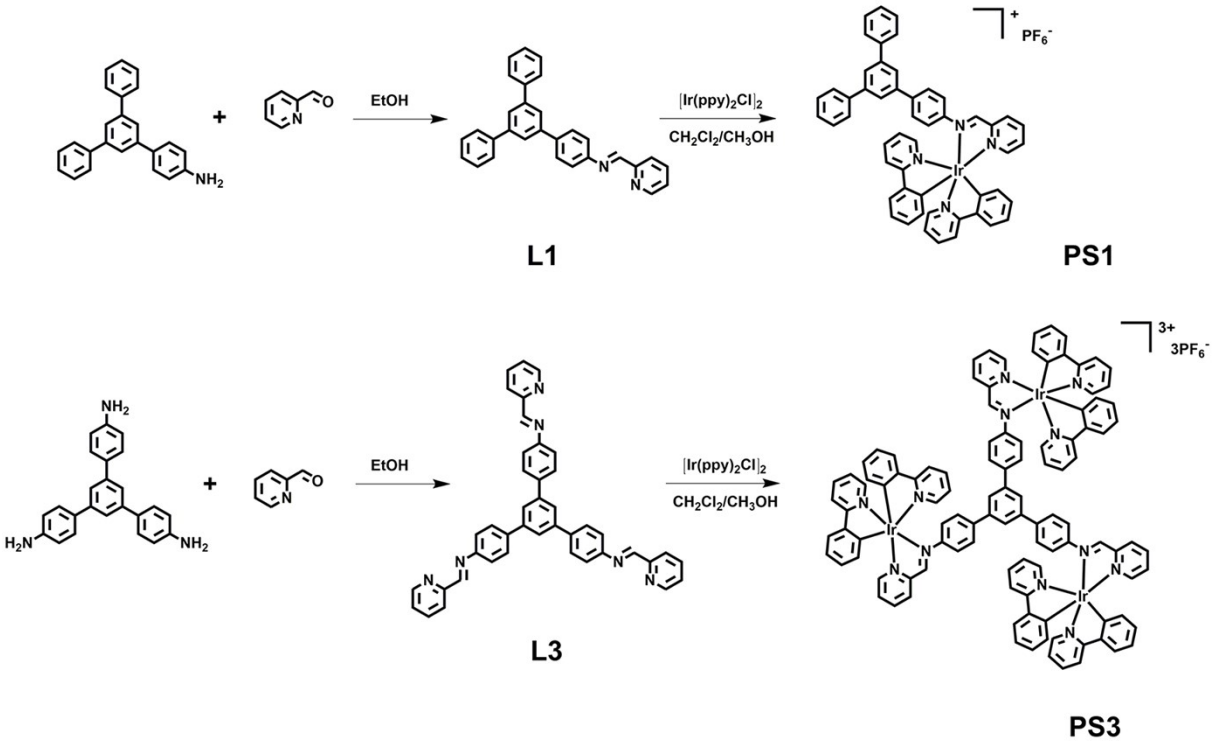
Supplementary Figures and Tables



Scheme S1 Synthetic routes of **L1**, **L3**, **PS1** and **PS3**.

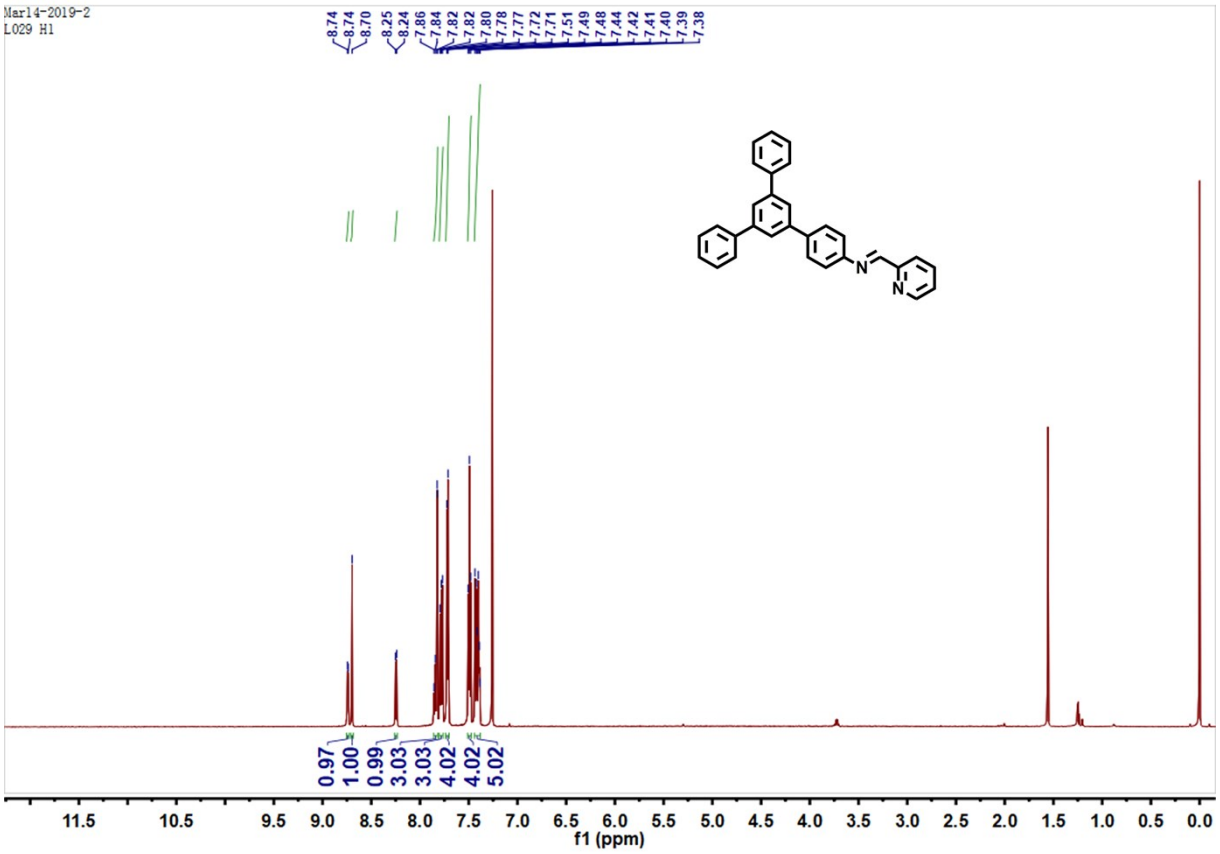


Fig. S1 ^{1}H NMR spectrum of **L1** in $CDCl_3$.

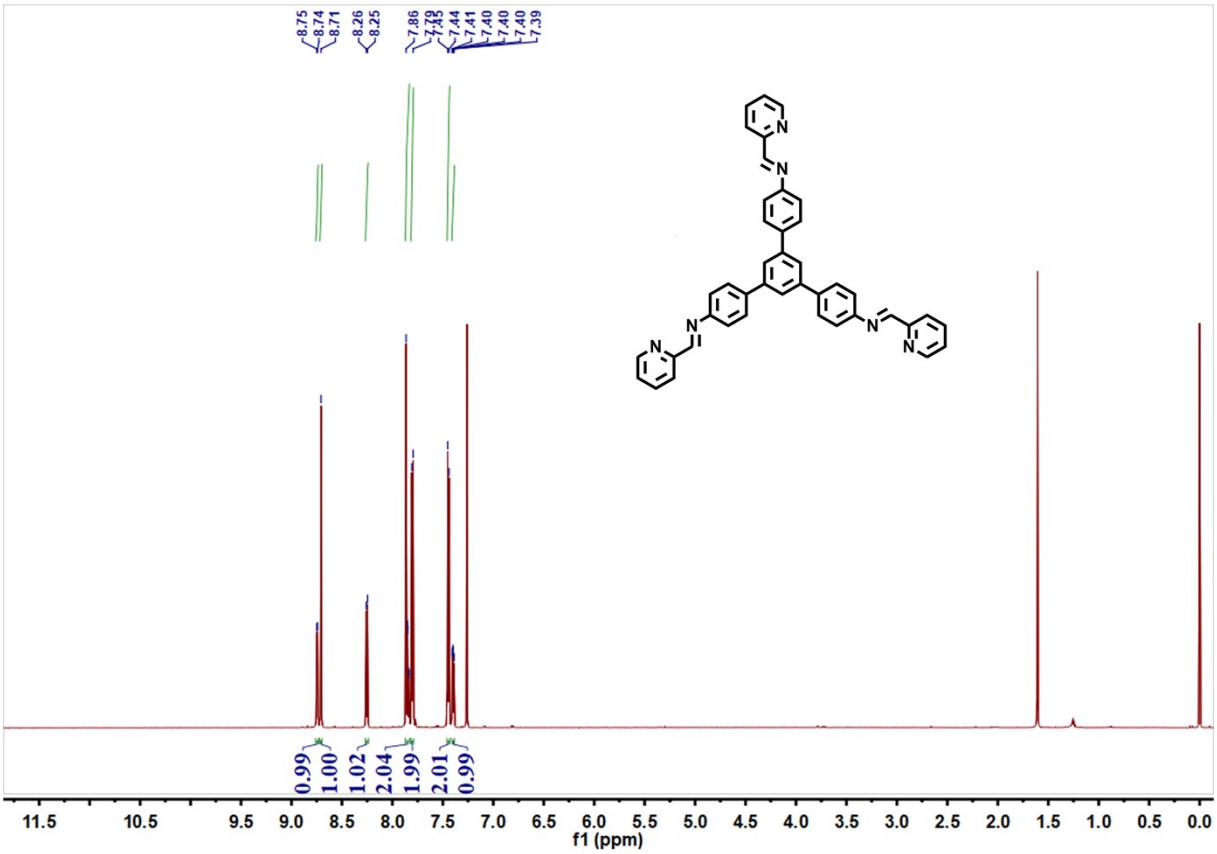


Fig. S2 ^{1}H NMR spectrum of **L3** in $CDCl_3$.

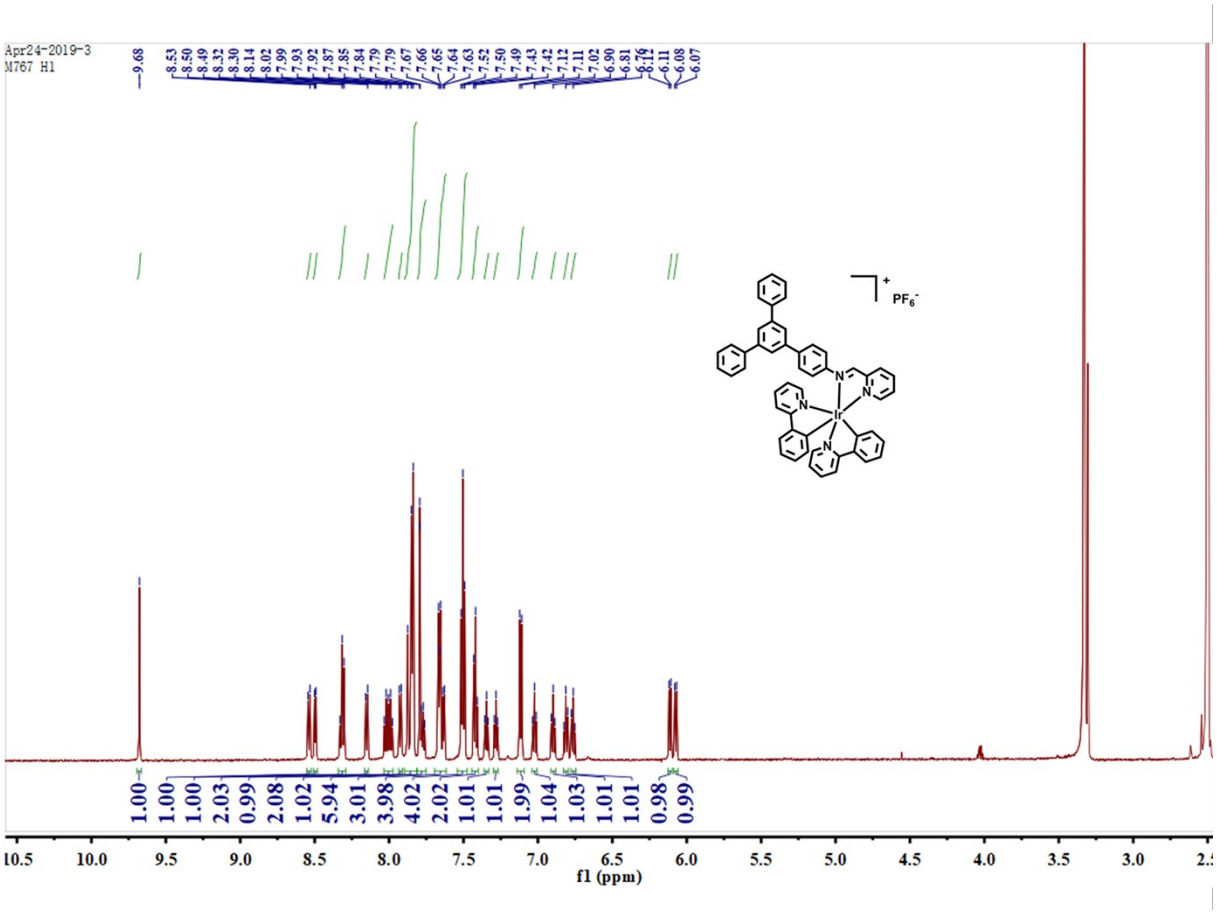


Fig. S3 ^{1}H NMR spectrum of **PS1** in DMSO-d_6.

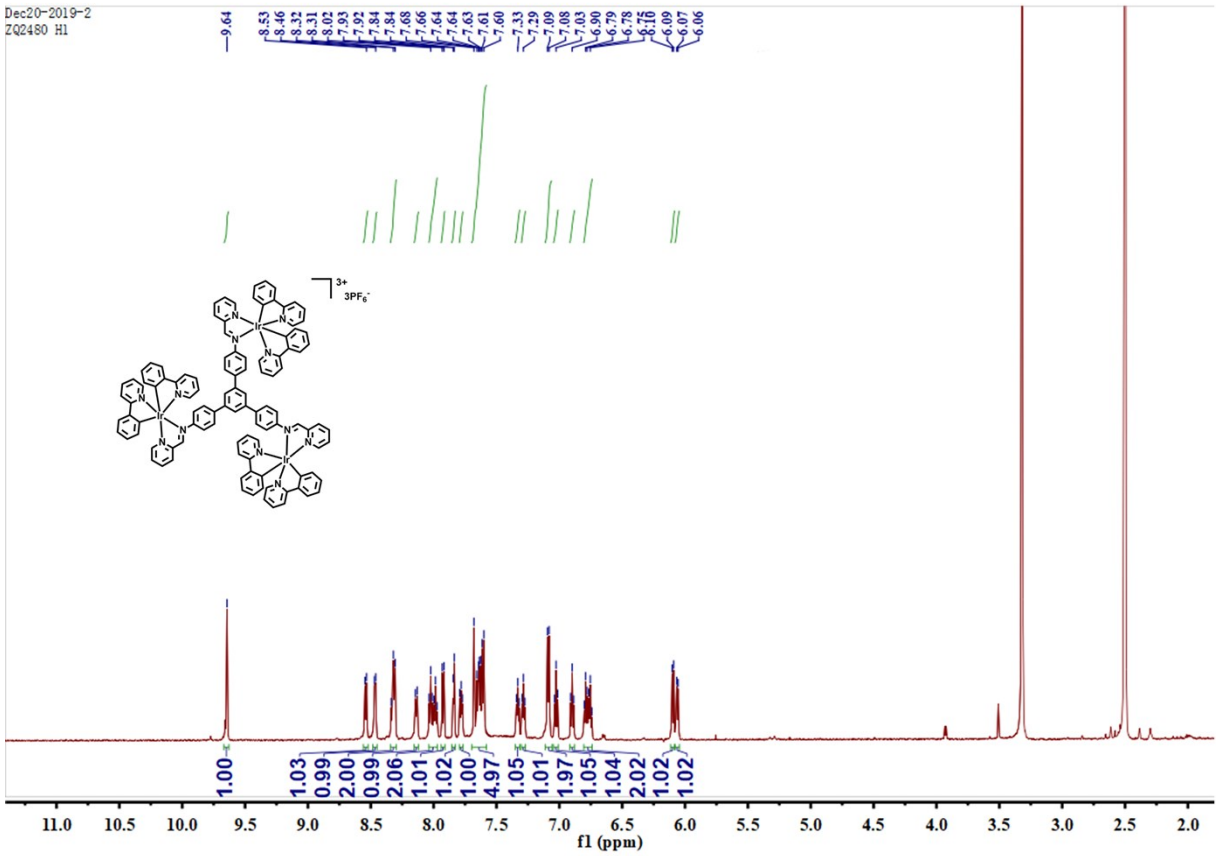


Fig. S4 ^{1}H NMR spectrum of **PS3** in DMSO-d_6.

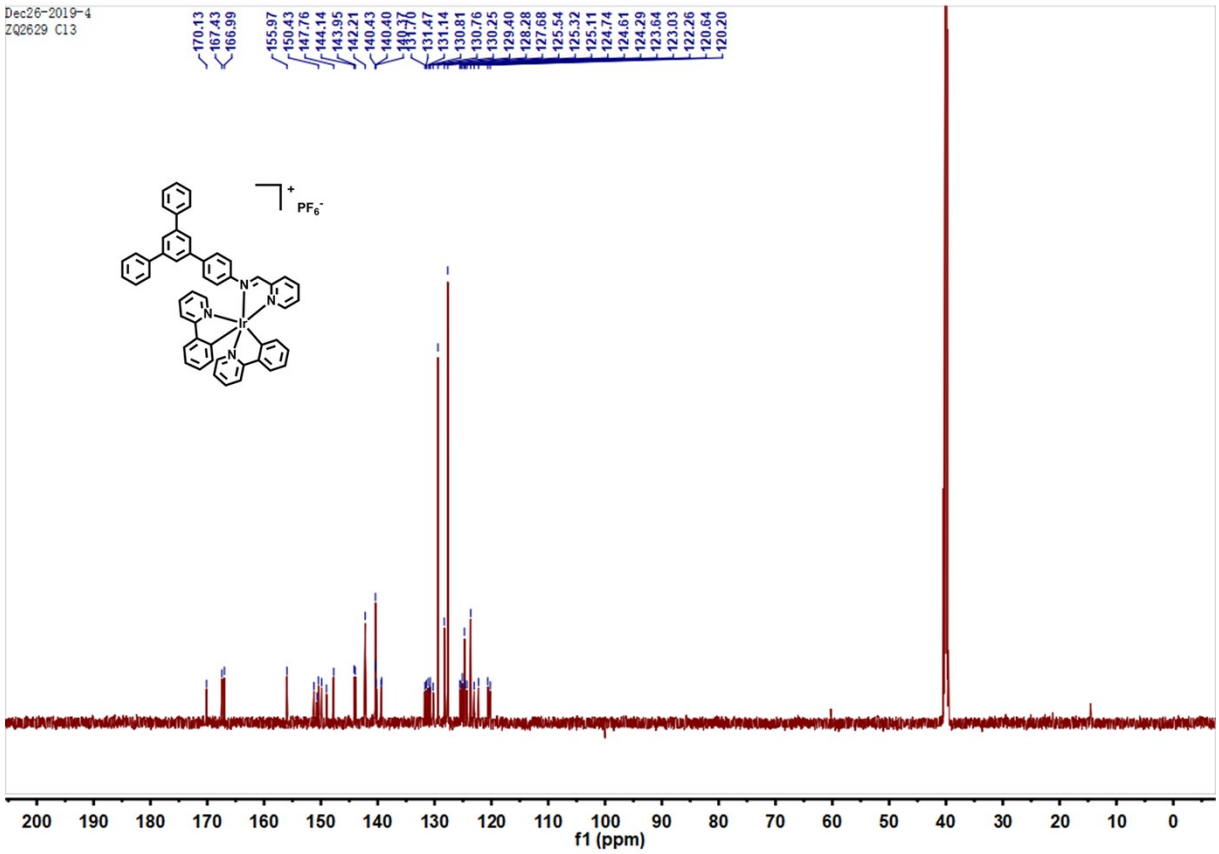


Fig. S5 ^{13}C NMR spectrum of **PS1** in DMSO-d_6.

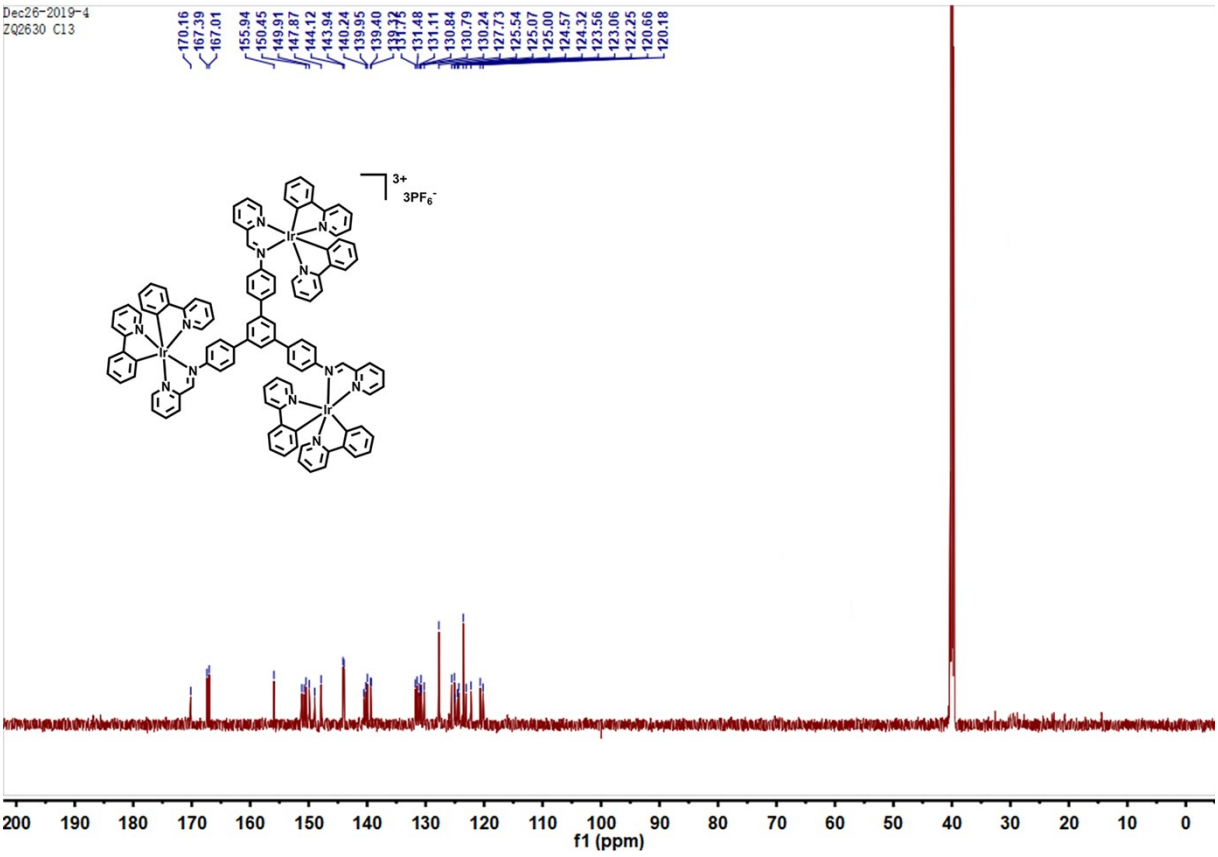


Fig. S6 ^{13}C NMR spectrum of **PS3** in DMSO-d_6.

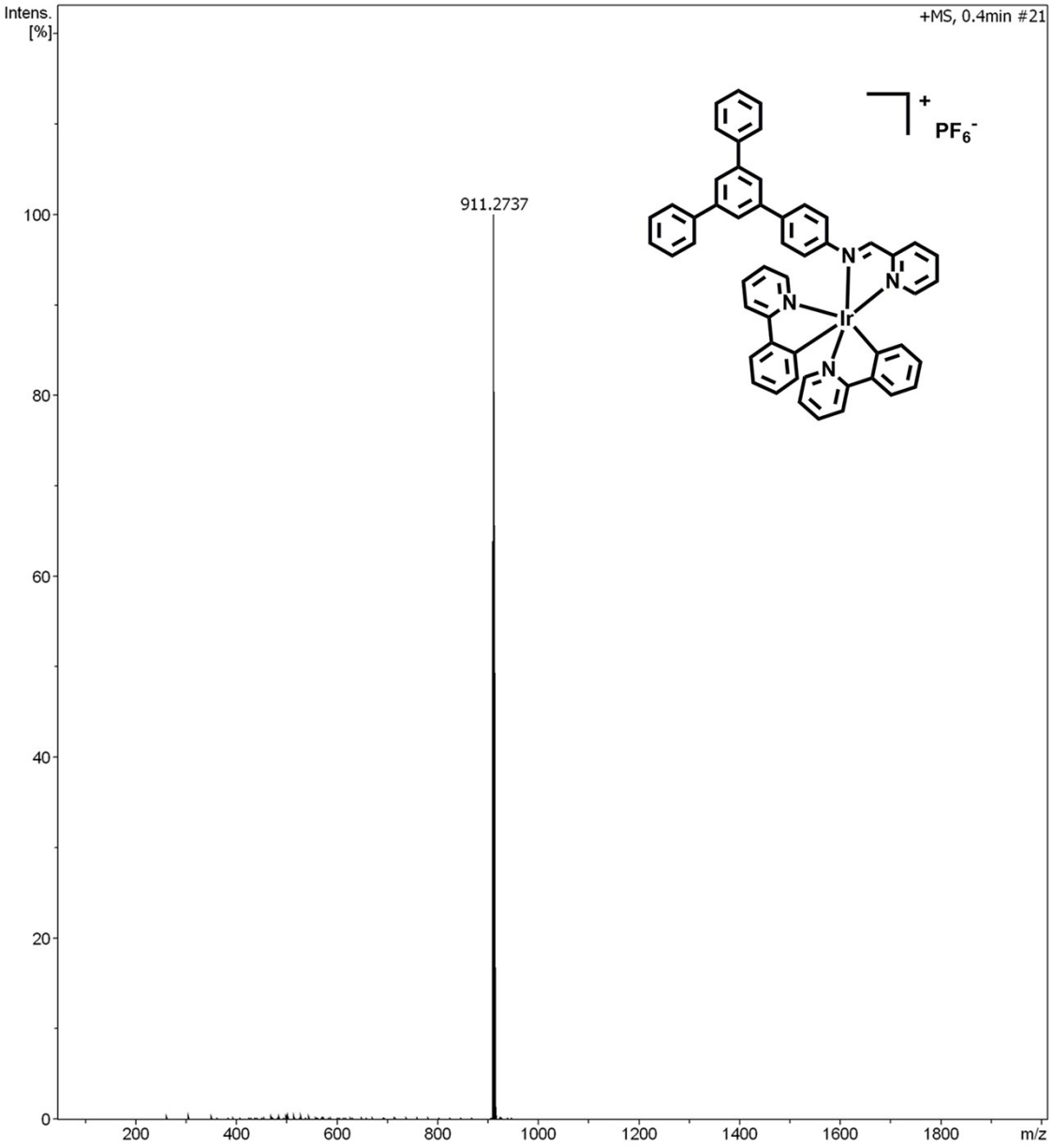


Fig. S7 ESI mass spectrum of **PS1**.

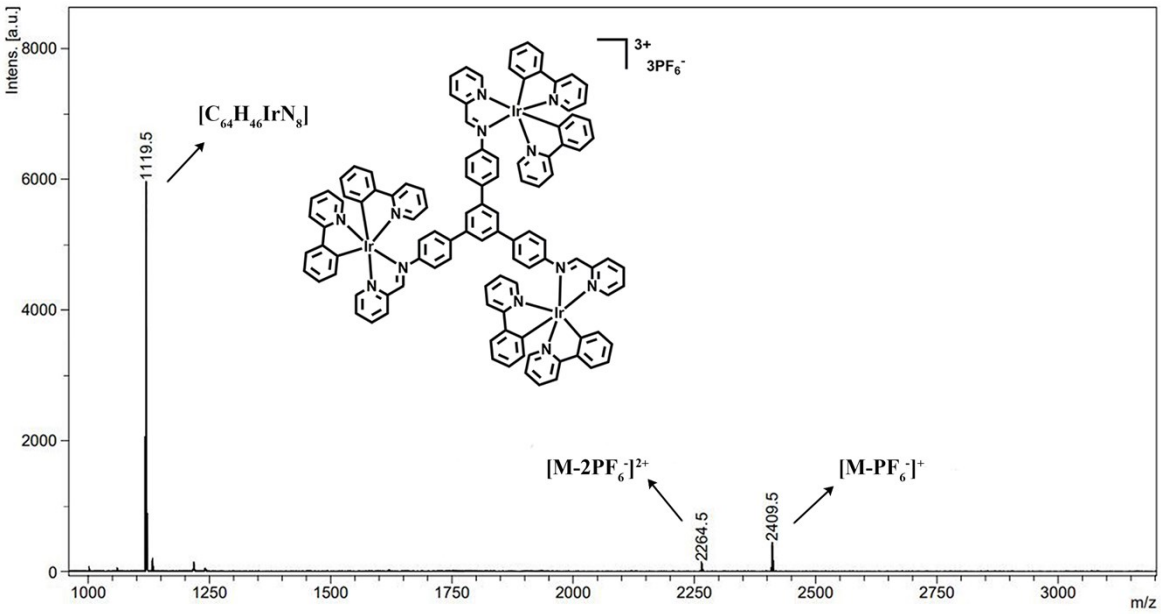


Fig. S8 MALDI-TOF mass spectrum of **PS3**.

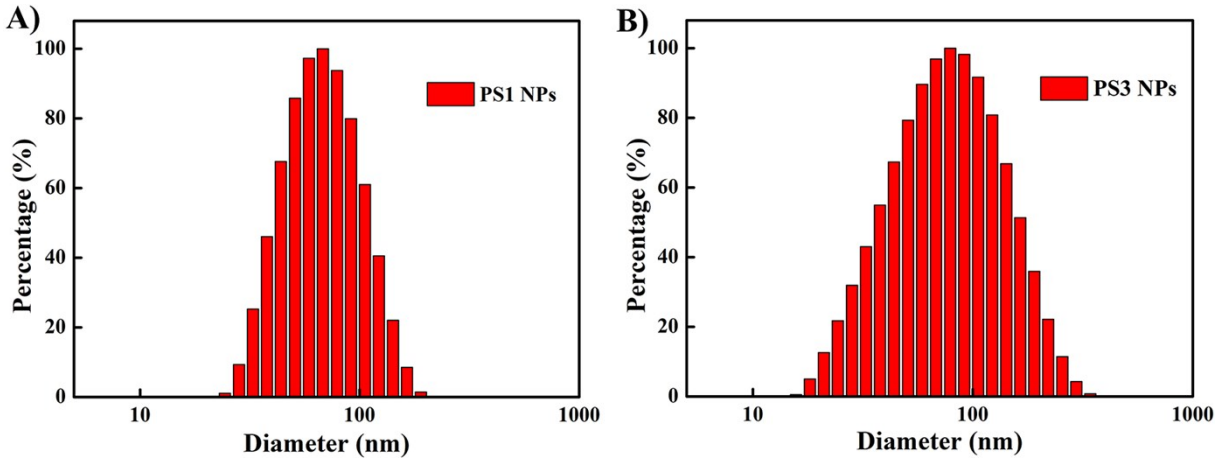


Fig. S9 DLS results of A) **PS1** NPs and B) **PS3** NPs in water at room temperature.

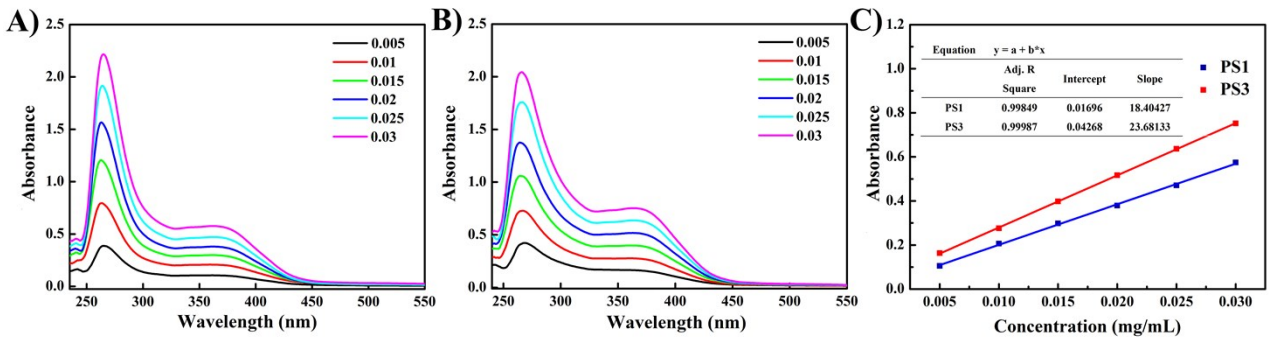


Fig. S10 UV–vis absorption spectra of A) **PS1** and B) **PS3** at different concentration in DMSO/water (v/v) =4/1. C) Standard curves of **PS1** and **PS3** in DMSO/water (v/v) =4/1.

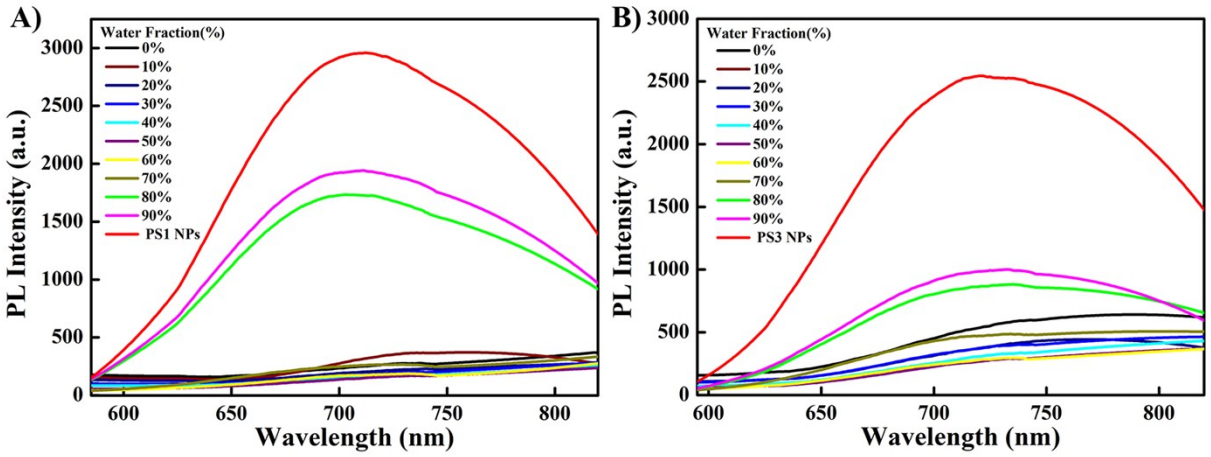


Fig. S11 A) PL spectra of **PS1** NPs in water and **PS1** in DMSO/water mixtures with different water fractions at room temperature. B) PL spectra of **PS3** NPs in water and **PS3** in DMSO/water mixtures with different water fractions at room temperature. (**PS1** or **PS3** or **PS1** NPs or **PS3** NPs) = 10^{-5} M

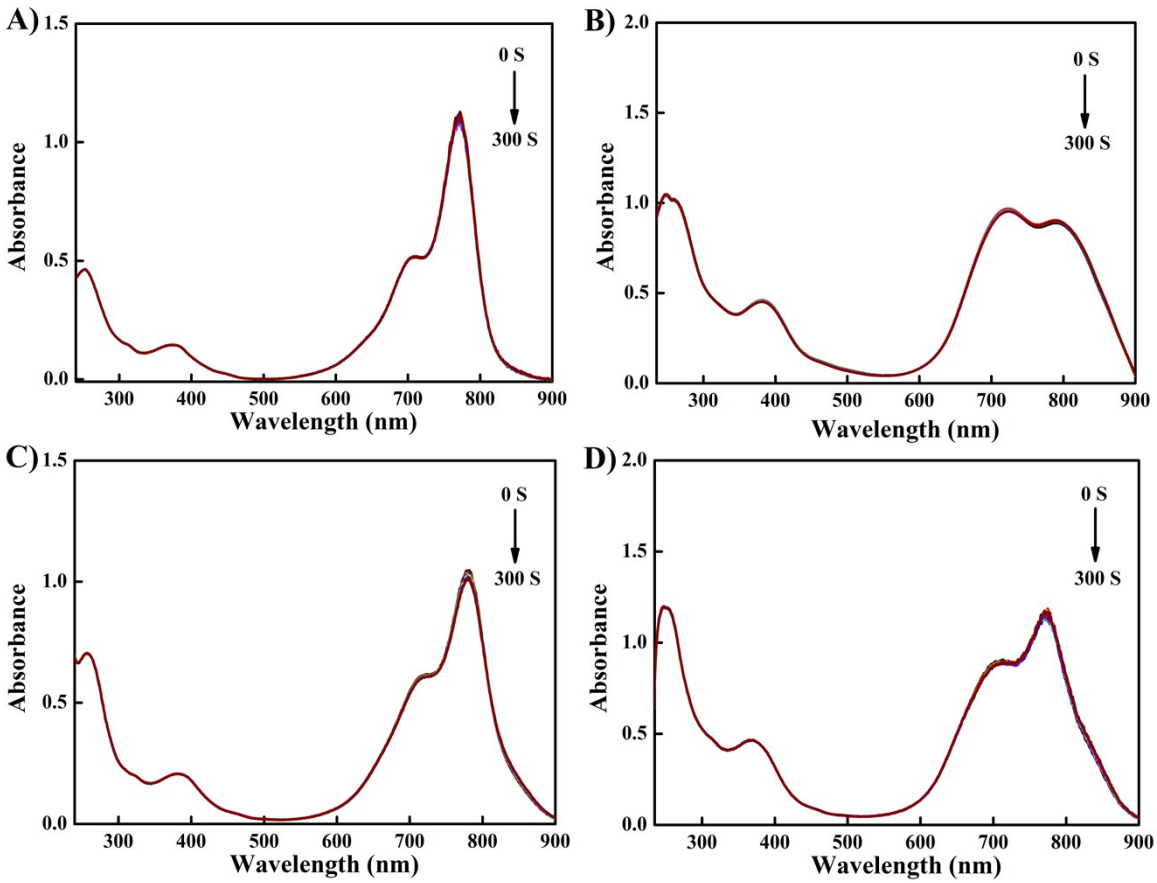


Fig. S12 UV-vis absorption spectra of ICG (6.5×10^{-6} M) in the presence of A) **PS1**, B) **PS3**, C) **PS1** NPs and D) **PS3** NPs (5×10^{-6} M) at different times under dark. The time interval of UV recording = 30 s.

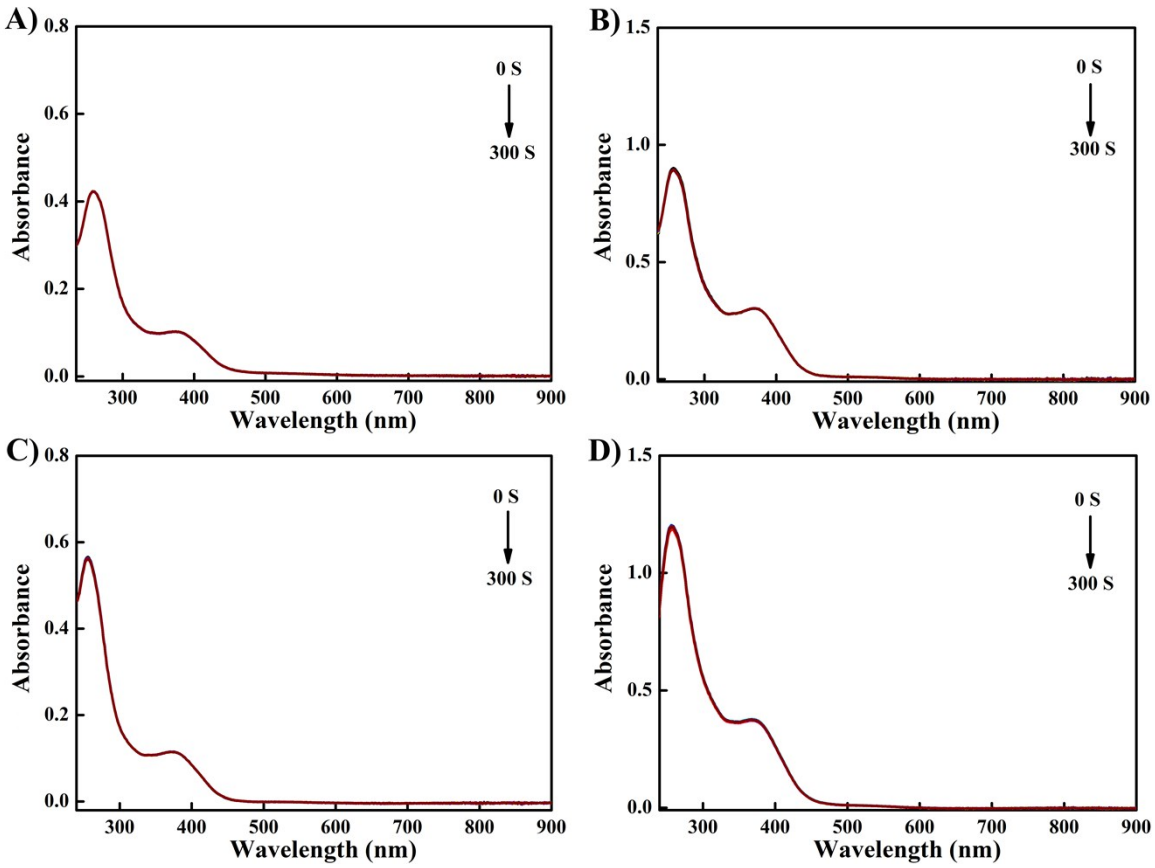


Fig. S13 UV-vis absorption spectra of A) **PS1**, B) **PS3**, C) **PS1** NPs and D) **PS3** NPs (5×10^{-6} M) at different times upon irradiation of a 450 nm LED at 20 mW cm^{-2} (0.6 J cm^{-2}). The time interval of UV recording = 30 s.

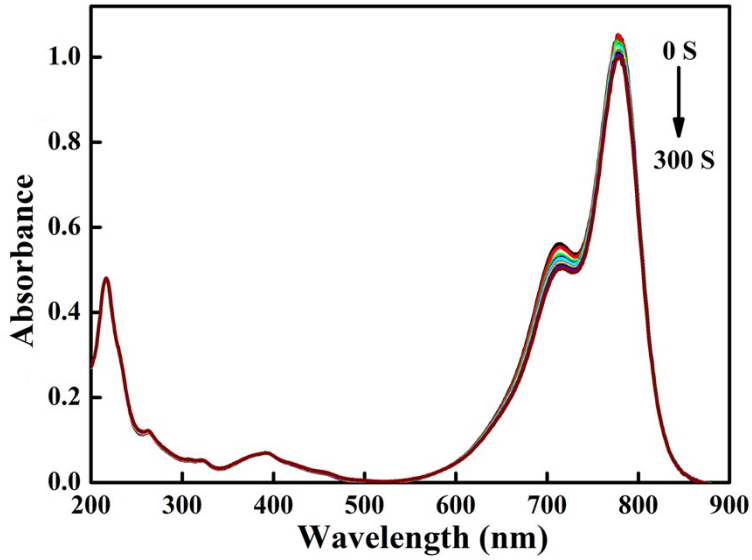


Fig. S14 UV-vis absorption spectra of ICG (6.5×10^{-6} M) at different times upon irradiation of a 450 nm LED at 20 mW cm^{-2} (0.6 J cm^{-2}). The time interval of UV recording = 30 s.

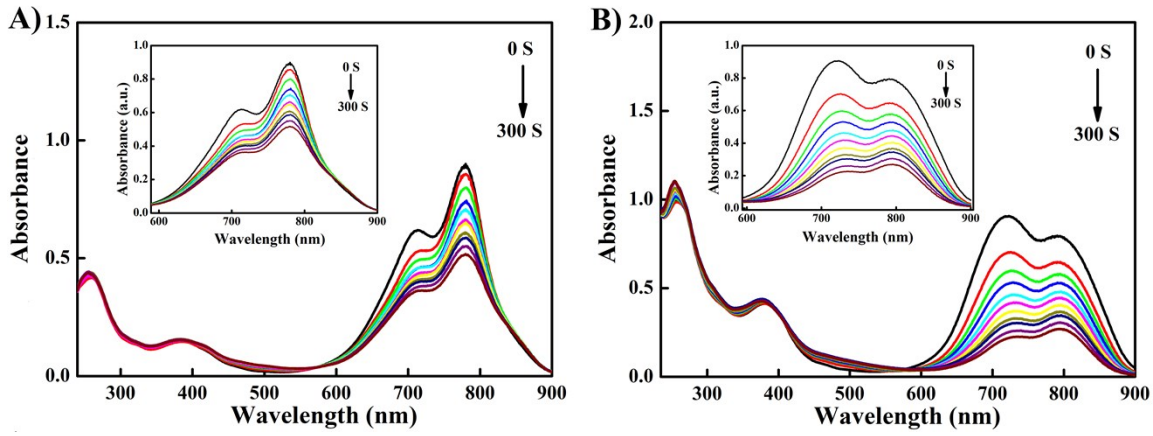


Fig. S15 UV-vis absorption spectra of ICG (6.5×10^{-6} M) in the presence of A) **PS1** and B) **PS3** (5×10^{-6} M) at different times upon irradiation of a 450 nm LED at 20 mW cm^{-2} (0.6 J cm^{-2}). The time interval of UV recording = 30 s.

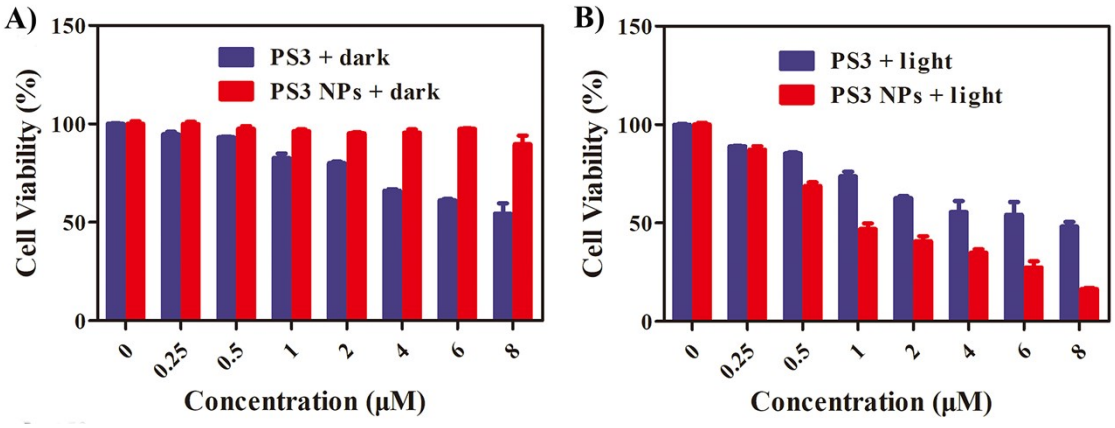


Fig. S16 The viability of HeLa cells pretreated with **PS3** and **PS3** NPs in the A) absence and B) presence of light. The cells were not washed before irradiation.

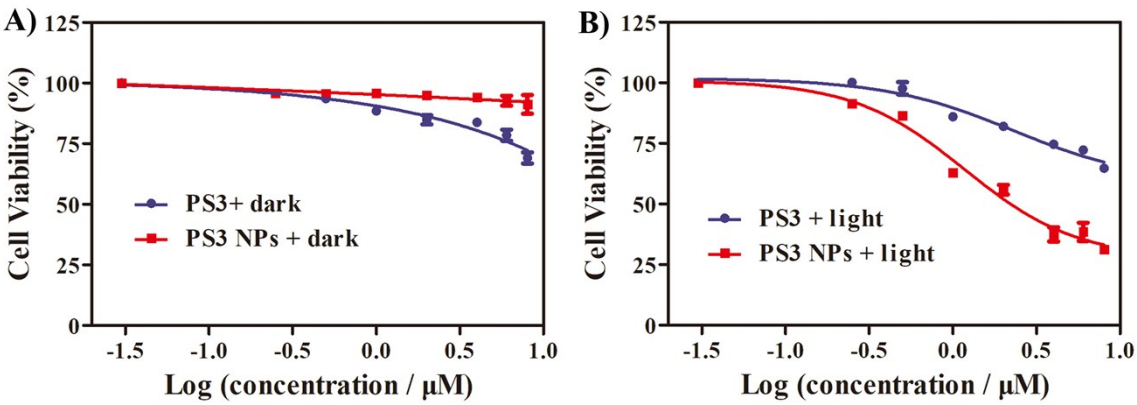


Fig. S17 The cytotoxicity dose-response curves of **PS3** and **PS3** NPs in HeLa cells A) under dark or B) light irradiation. The cells were washed before irradiation.

Table S1. The average diameter and polydispersity index (PDI) results of **PS1**/**PS3** NPs measured by DLS.

Sample	**PS1** NPs	**PS3** NPs
Average diameter (nm)	73	87
PDI	0.128	0.186

Table S2. Photophysical data of **PS1**, **PS3** and their corresponding NPs.

	λ_{abs} (nm)	λ_{em} (nm)	Φ_p (%)	T_p (ns)
PS1[a]	257; 378	710	6	53.57
PS3[a]	260; 375	730	4	24.12
PS1 NPs[b]	257; 378	710	25	60.85
PS3 NPs[b]	260; 375	730	22	32.97

[a]Measured in DMSO/water (v/v = 1/9) at 298 K (1.0×10^{-5} M, λ_{ex} = 380 nm). [b]Measured in water at 298 K (1.0×10^{-5} M, λ_{ex} = 380 nm).