Supplementary Information

Methoxypolyethylene Glycol Substituted Zinc Phthalocyanines for Multiple Tumor-Selective Fluorescence Imaging and Photodynamic Therapy

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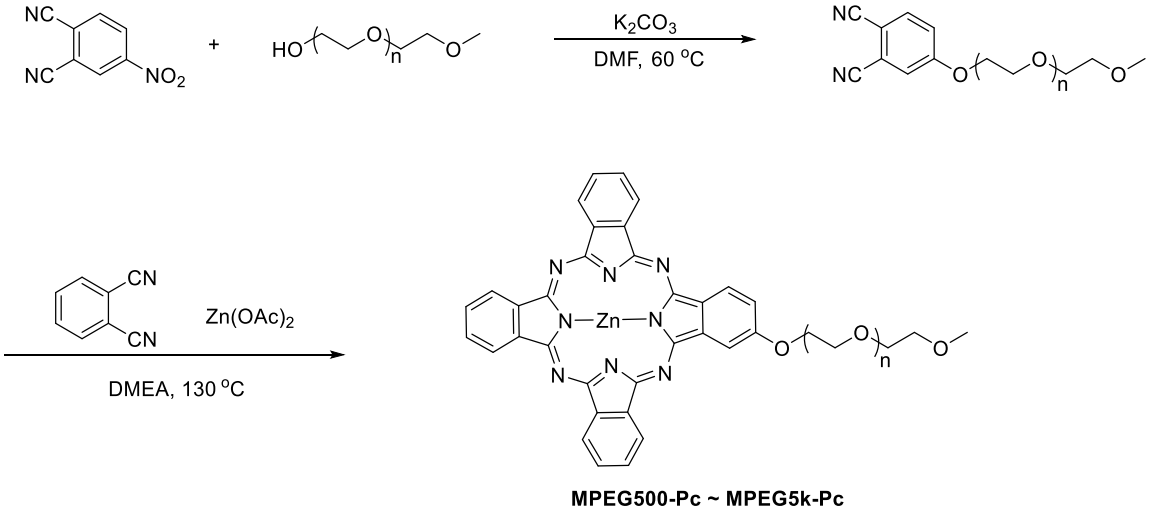

MPEG500-Pc ~ MPEG5k-Pc

Figure S1. Synthesis procedure of **MPEG500-Pc ~ MPEG5k-Pc**

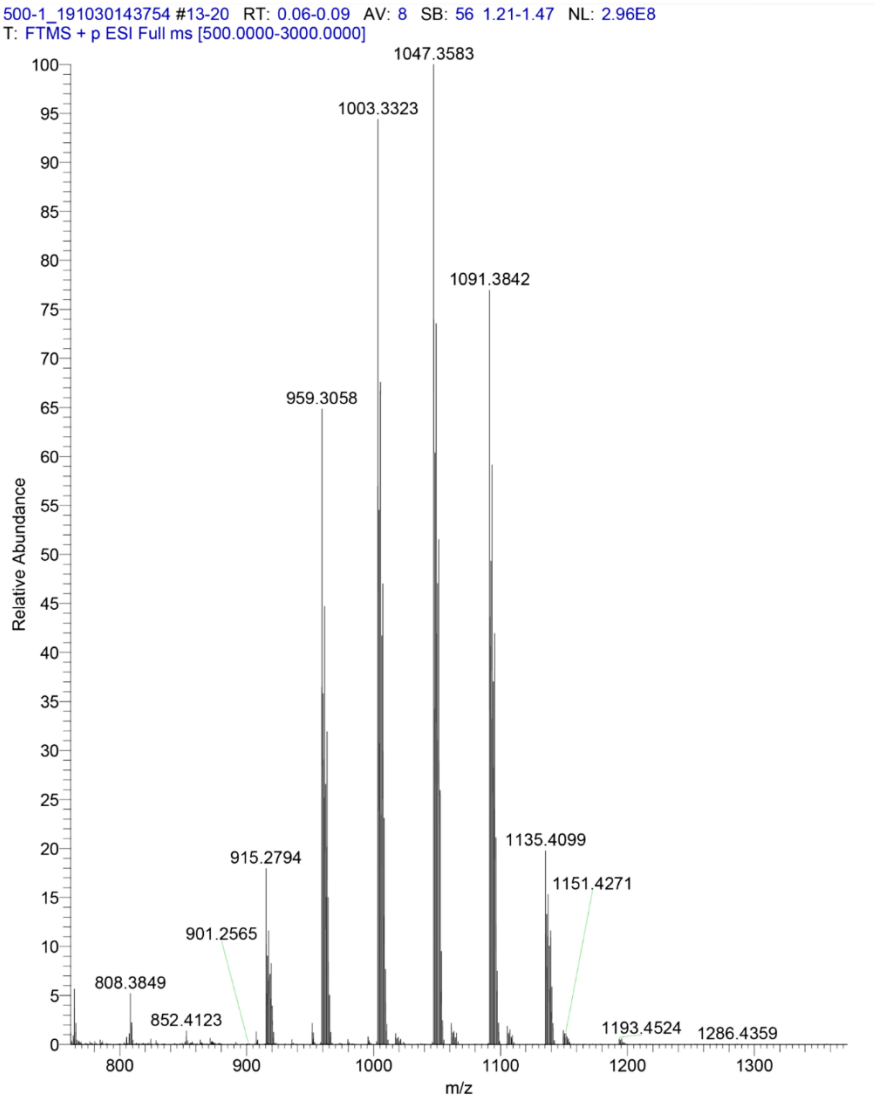

Figure S2. HR-MS (ESI) spectra of **MPEG500-Pc**

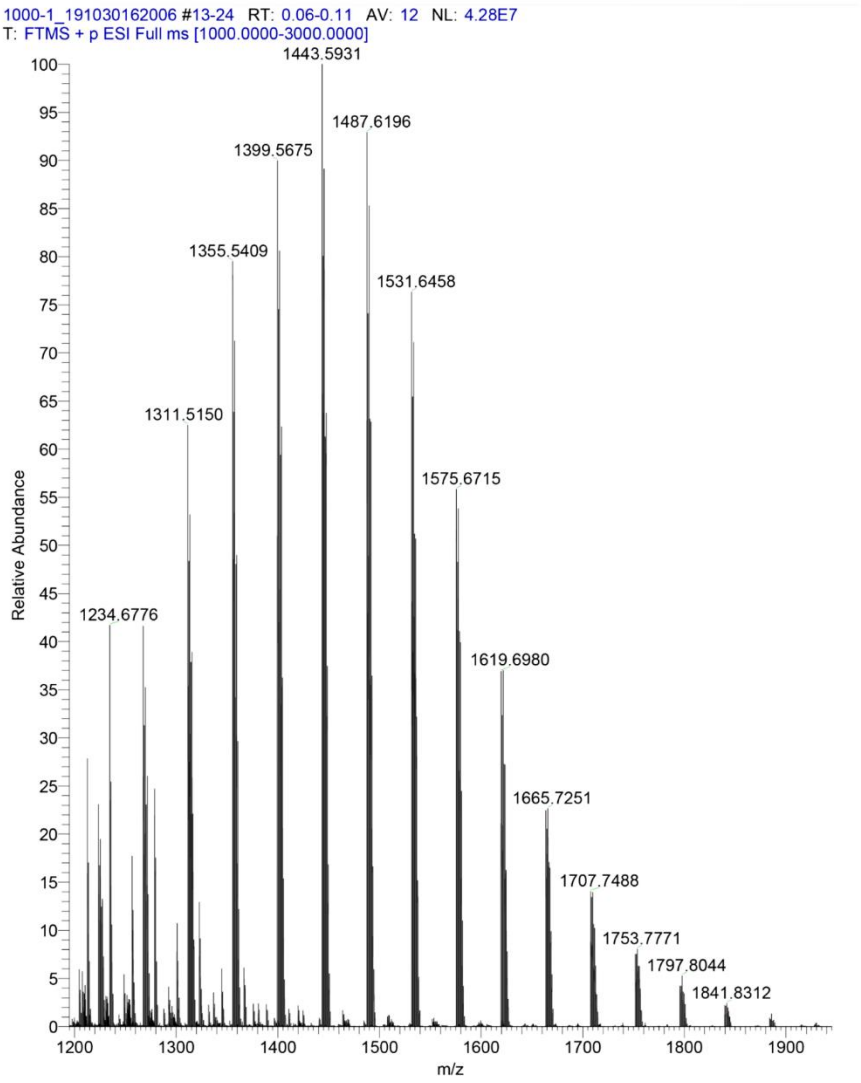

Figure S3 HR-MS(ESI) of **MPEG1k-Pc**

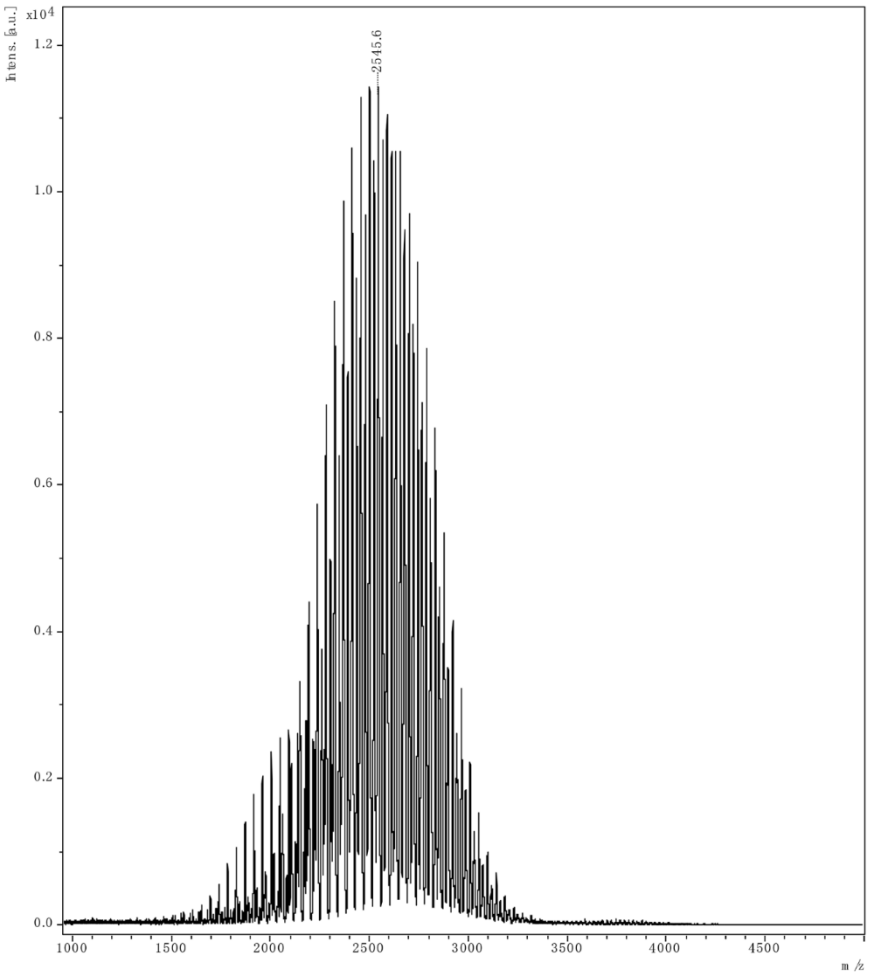

Figure S4 MALDI-TOF-MS of **MPEG2k-Pc**

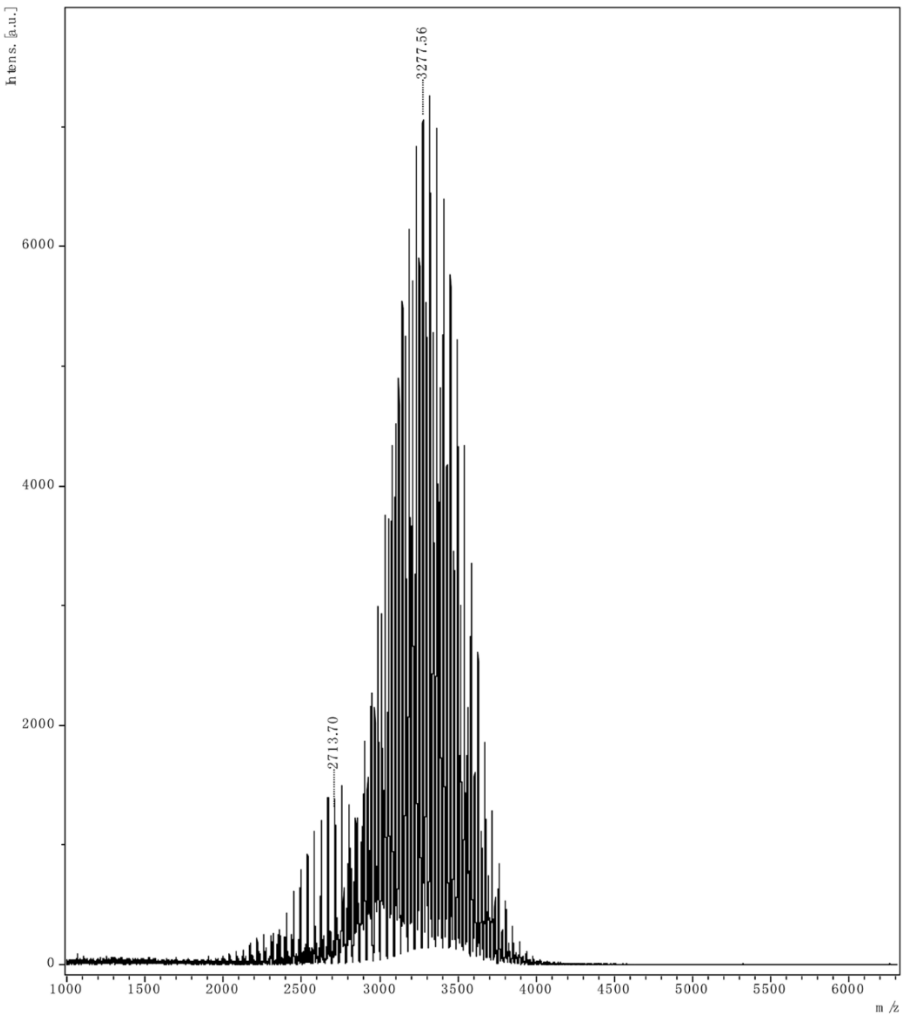

Figure S5 MALDI-TOF-MS of **MPEG3k-Pc**

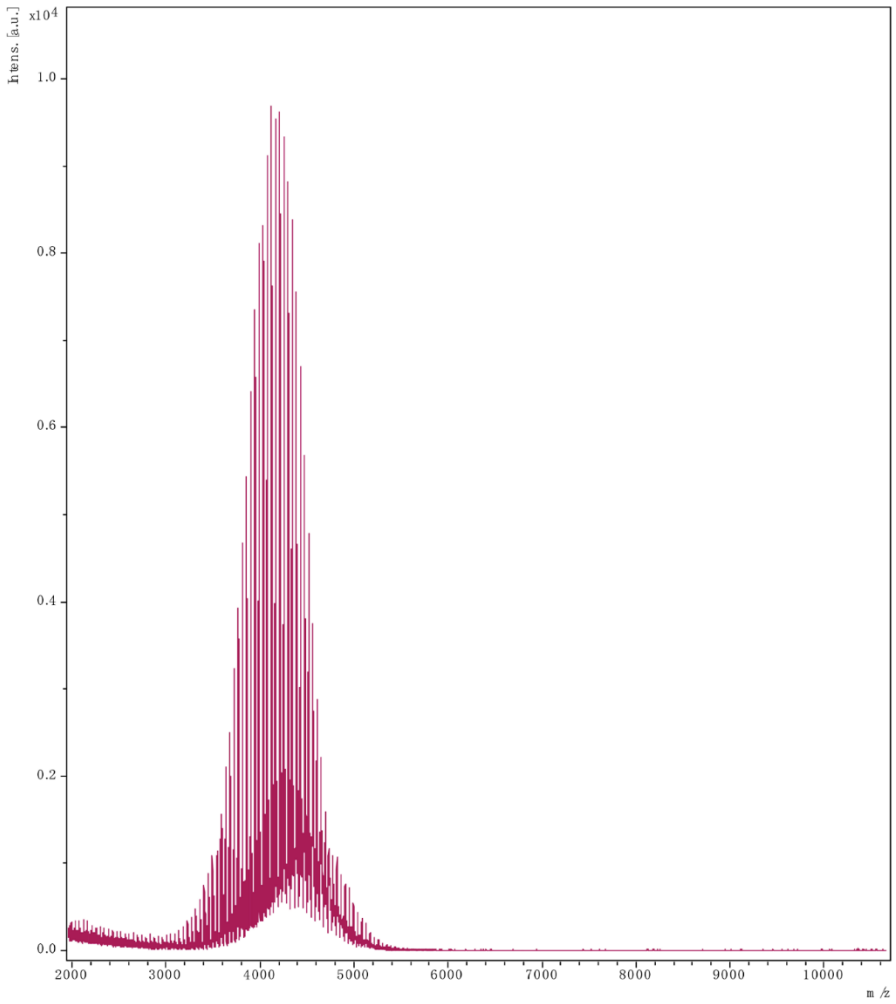

Figure S6 MALDI-TOF-MS of **MPEG4k-Pc**

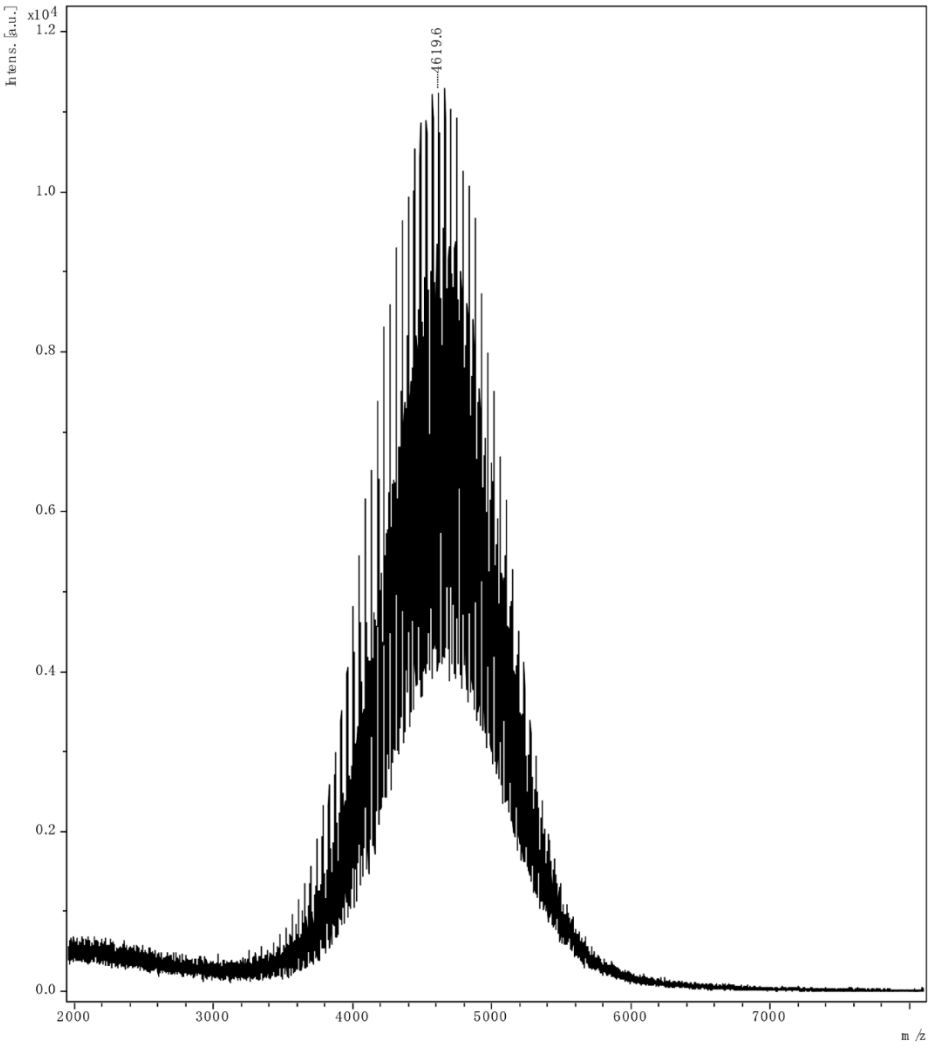

Figure S7 MALDI-TOF-MS of **MPEG5k-Pc**

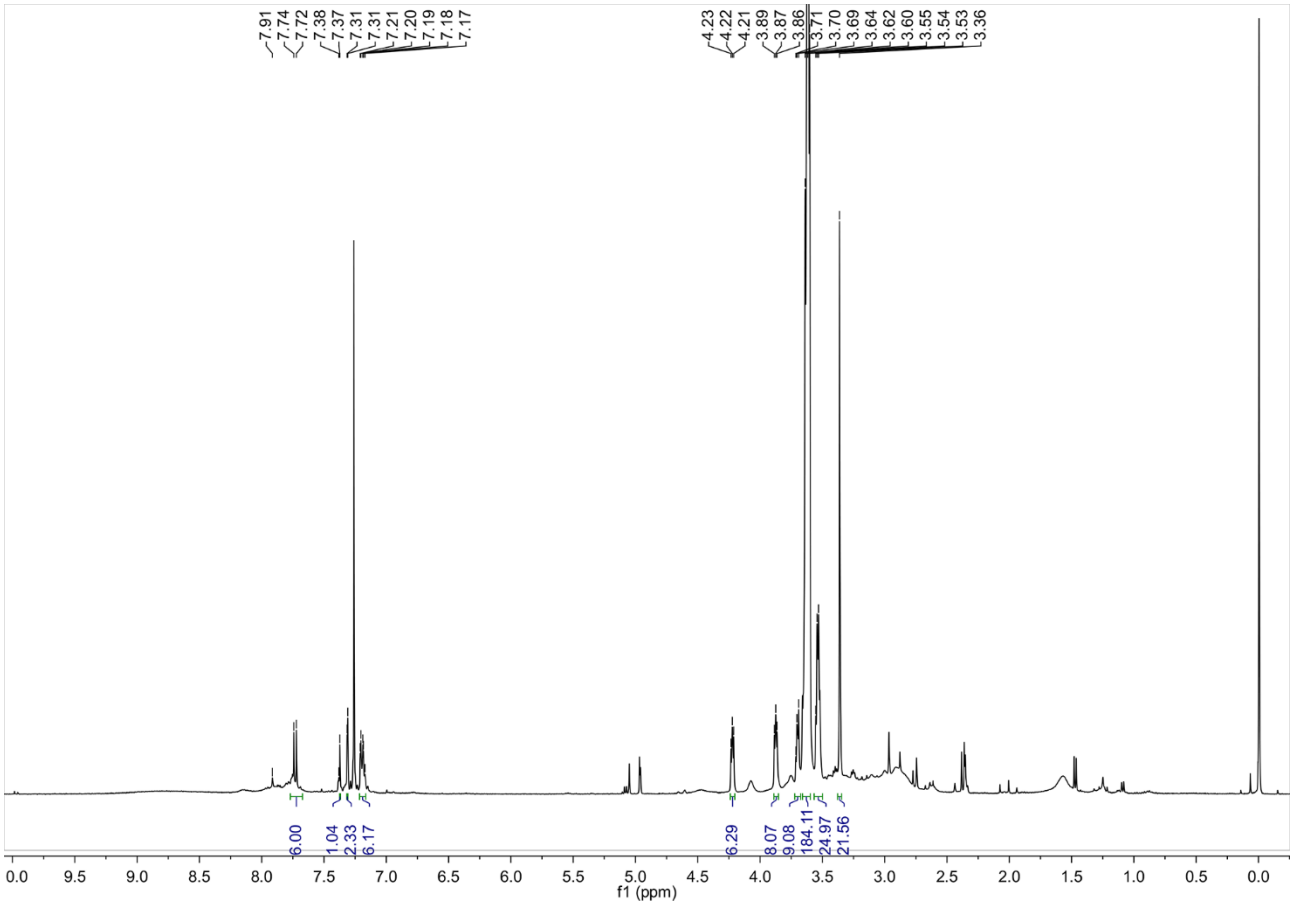

Figure S8 ^{1}H NMR spectrum of **MPEG500-Pc** (400 MHz, $CDCl_3$)

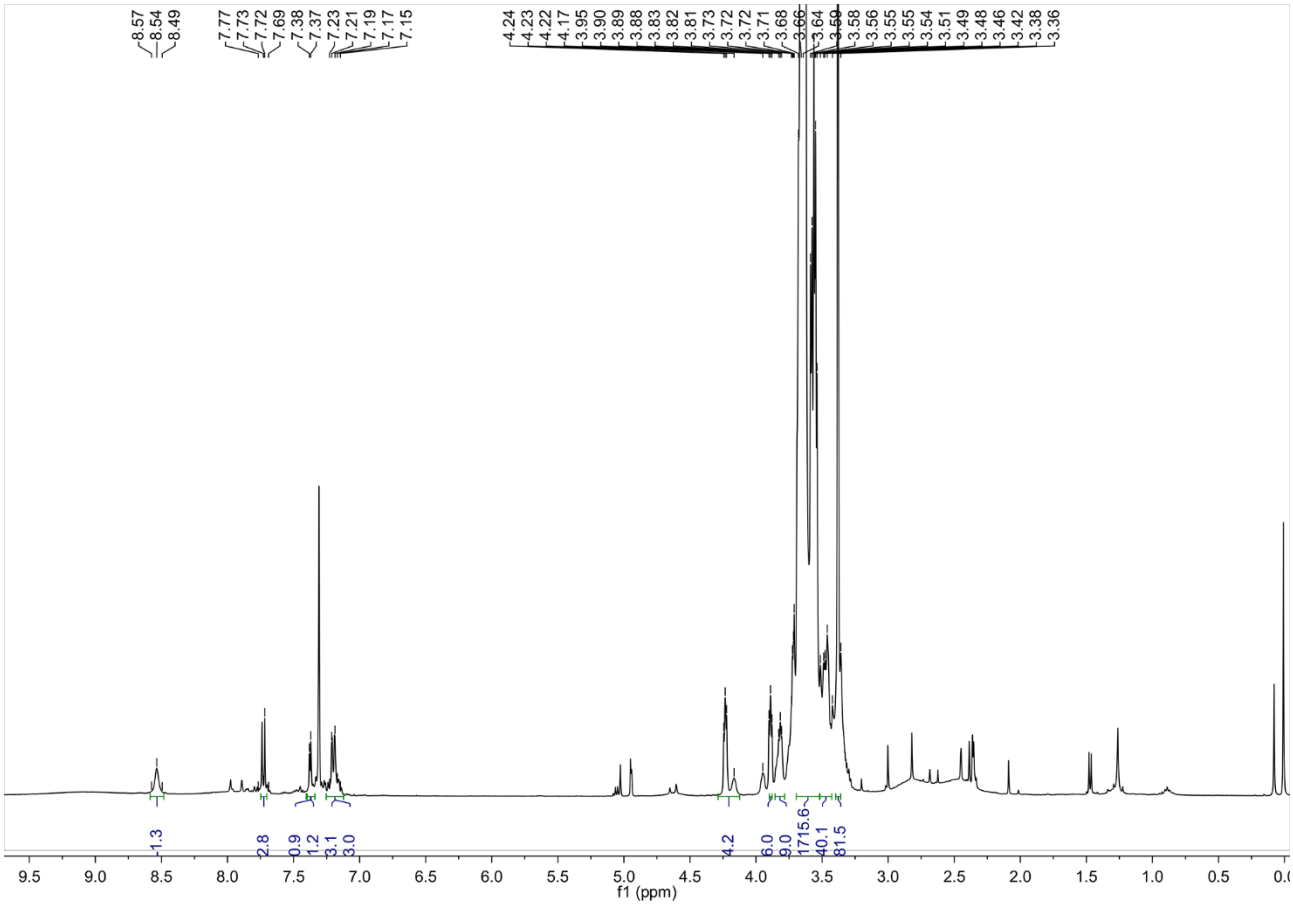

Figure S9 ^{1}H NMR spectrum of **MPEG1k-Pc** (400 MHz, $CDCl_3$)

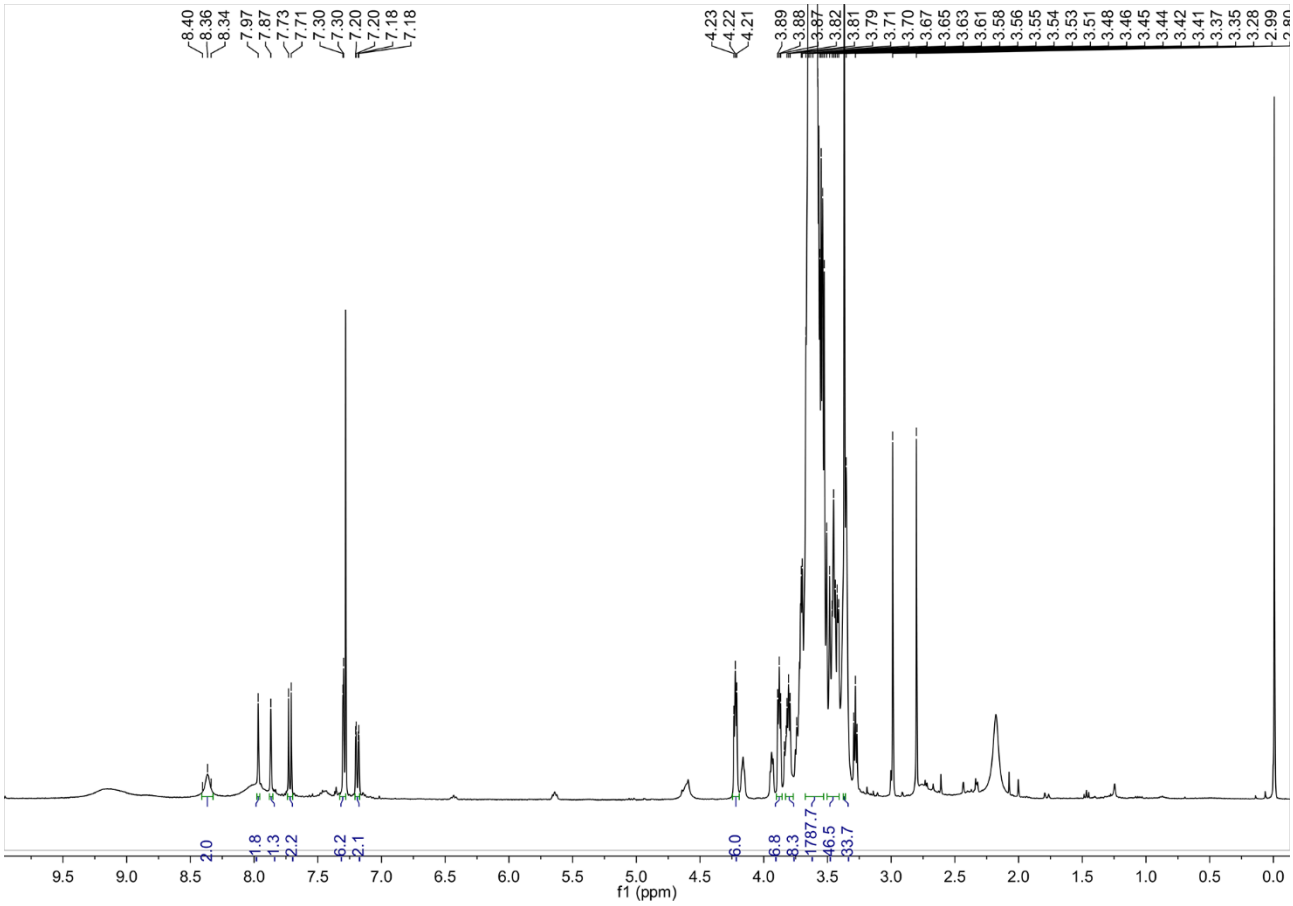

Figure S10 ^{1}H NMR spectrum of **MPEG2k-Pc** (400 MHz, $CDCl_3$)

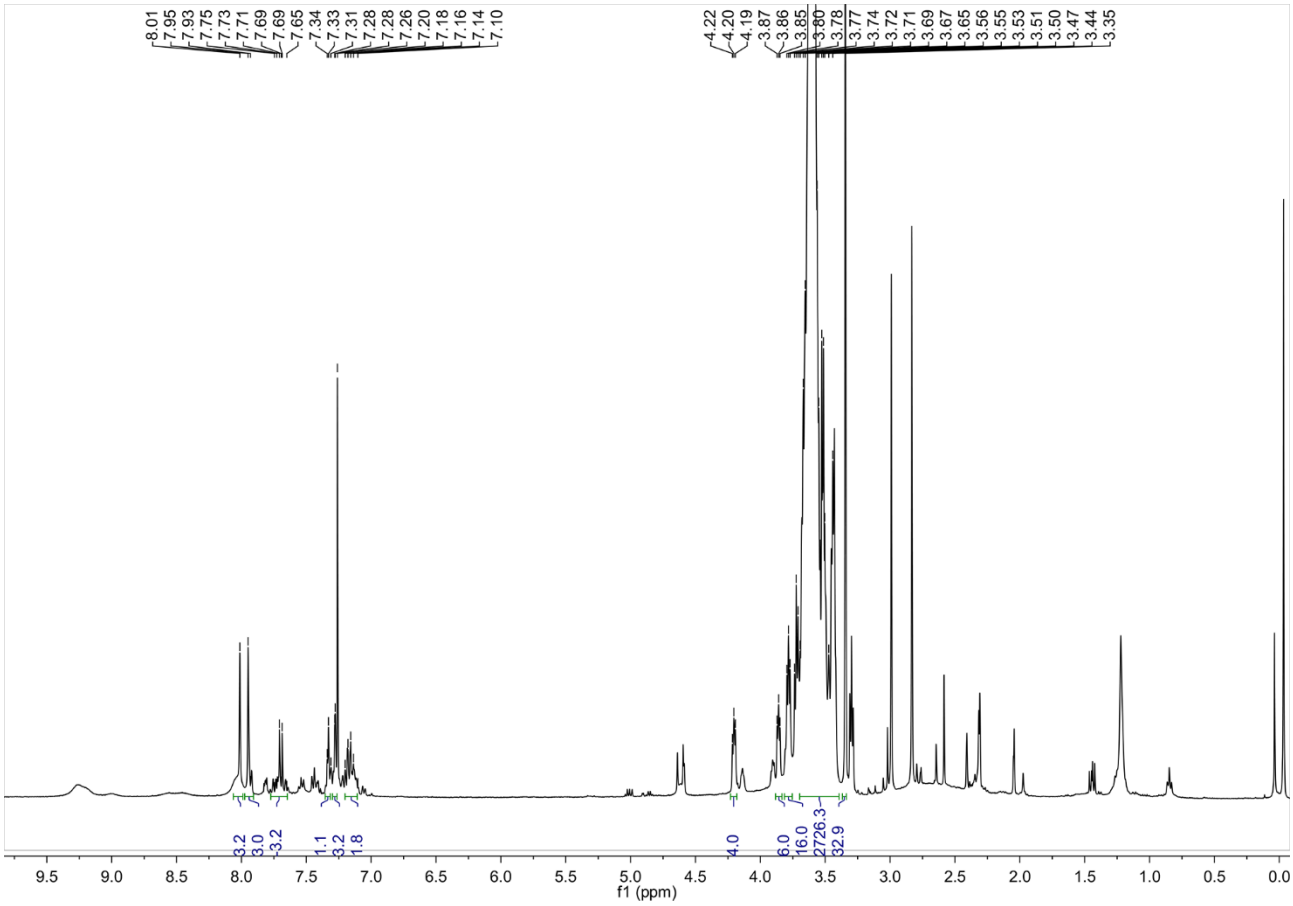

Figure S11 ^{1}H NMR spectrum of **MPEG3k-Pc** (400 MHz, $CDCl_3$)

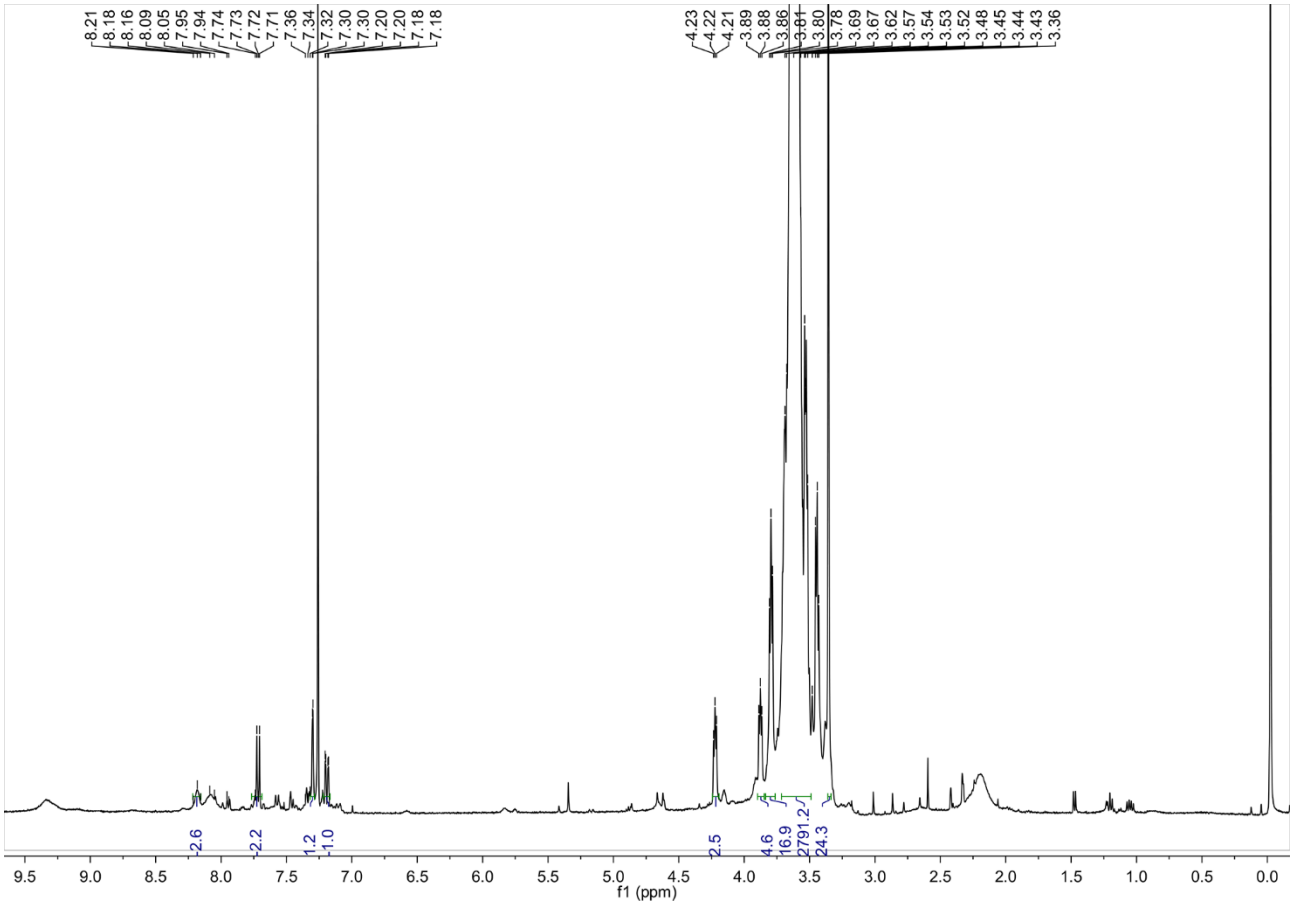

Figure S12 ^{1}H NMR spectrum of **MPEG4k-Pc** (400 MHz, $CDCl_3$)

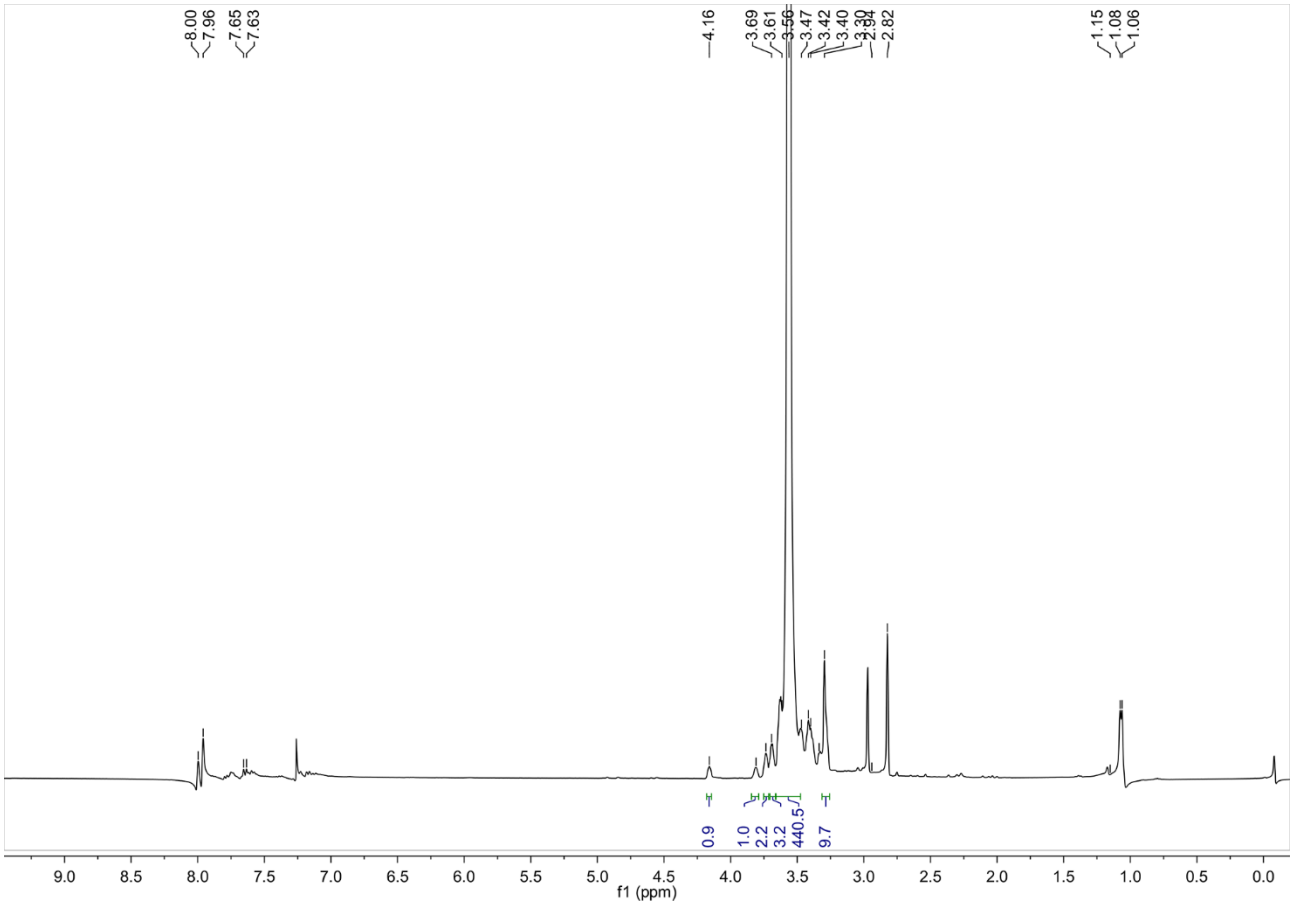

Figure S13 ^{1}H NMR spectrum of **MPEG5k-Pc** (400 MHz, $CDCl_3$)

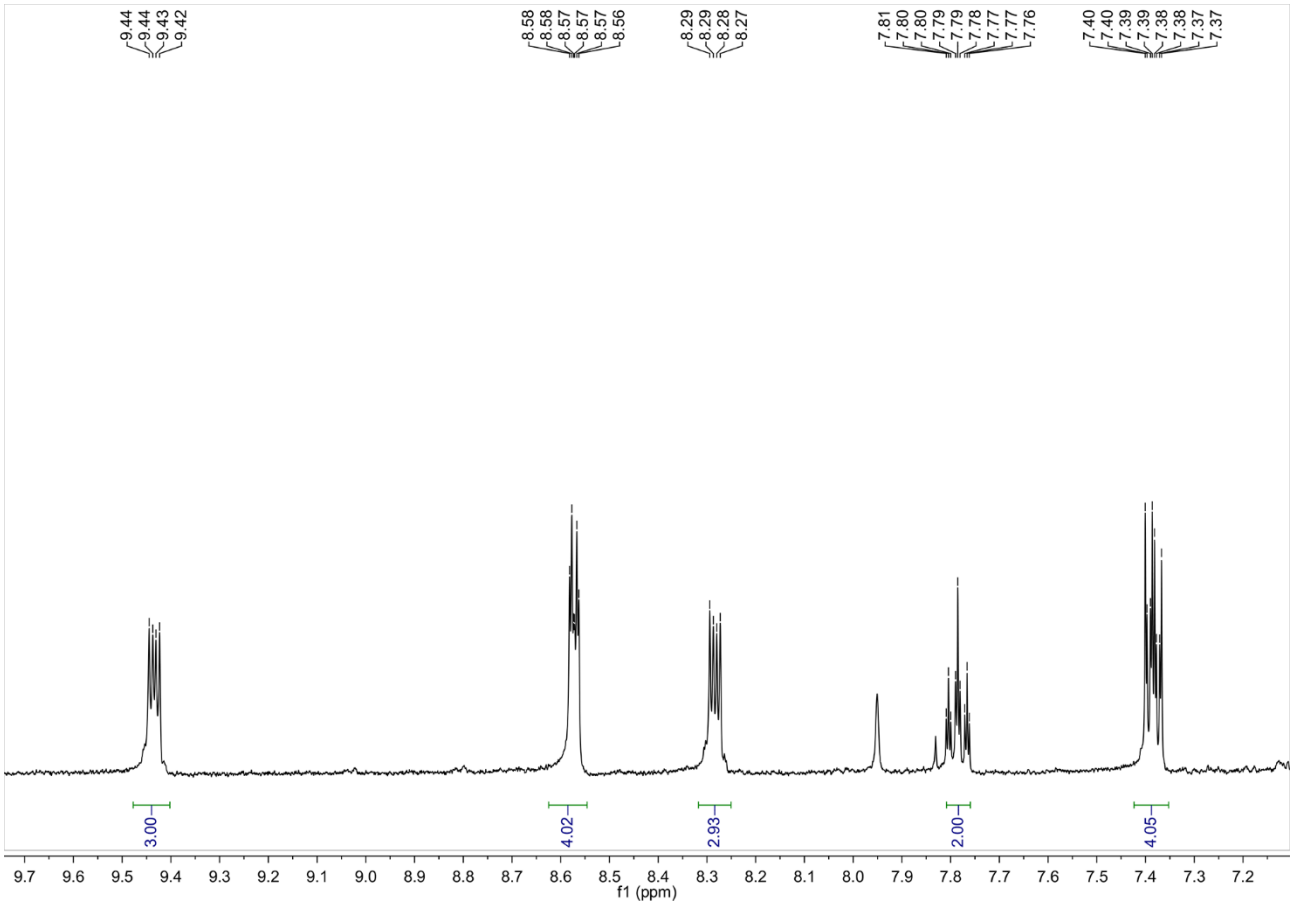

Figure S14 ^{1}H NMR spectrum of **ZnPc** (400 MHz, $CDCl_3$)

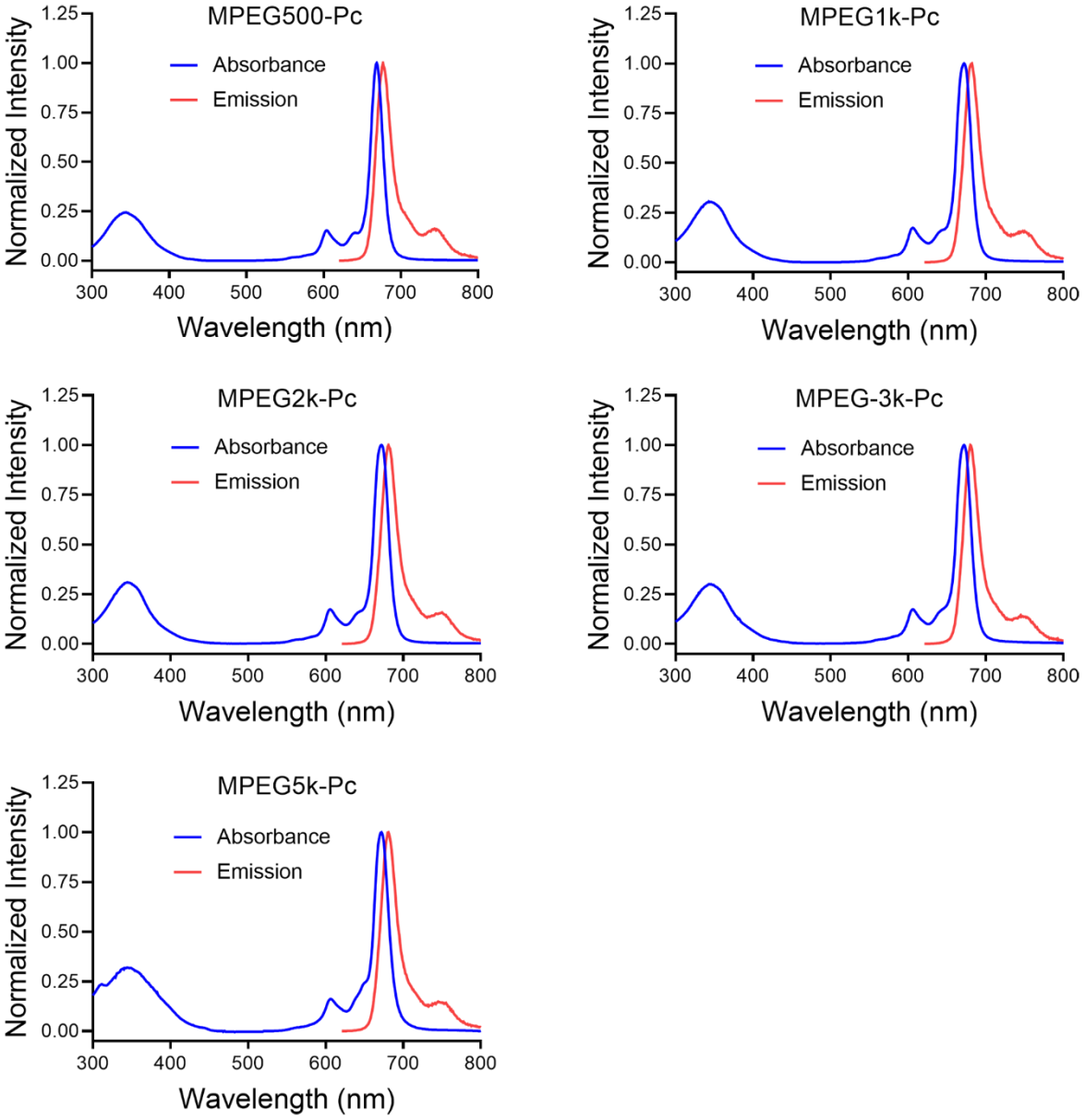

Figure S15. The UV-Vis absorbance spectra (blue) and Fluorescence emission spectra (red, excited at 610 nm) of **MPEG500-Pc**, **MPEG1k-Pc**, **MPEG2k-Pc**, **MPEG3k-Pc** and **MPEG5k-Pc** in DMF.

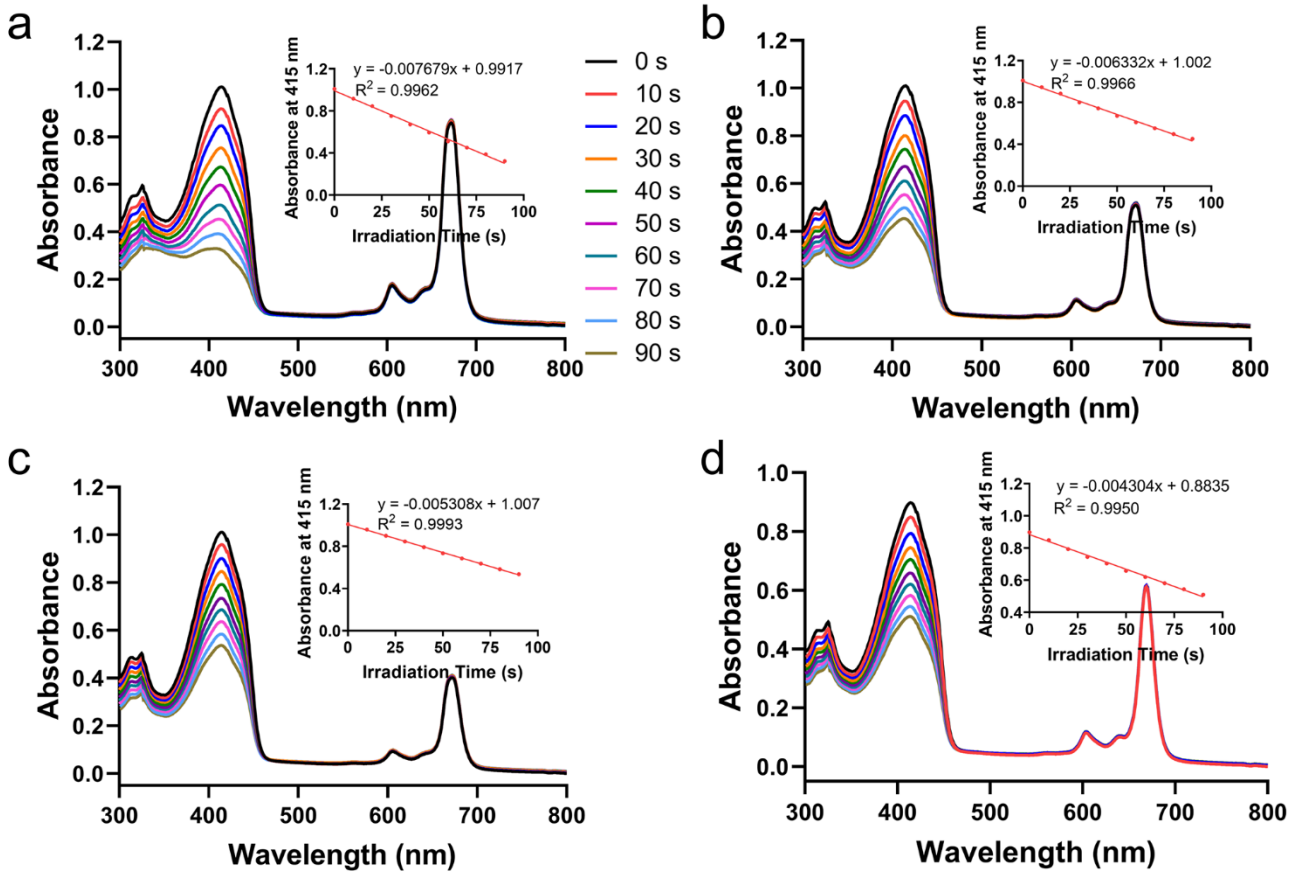

Figure S16. Photo-degradation curves of DPBF in the presence of MPEG500-Pc (a), MPEG2k-Pc (b), MPEG3k-Pc (c) and ZnPc (d) under 670 nm laser irradiation and linear fitting (inset) of DPBF absorbances versus irradiation time.

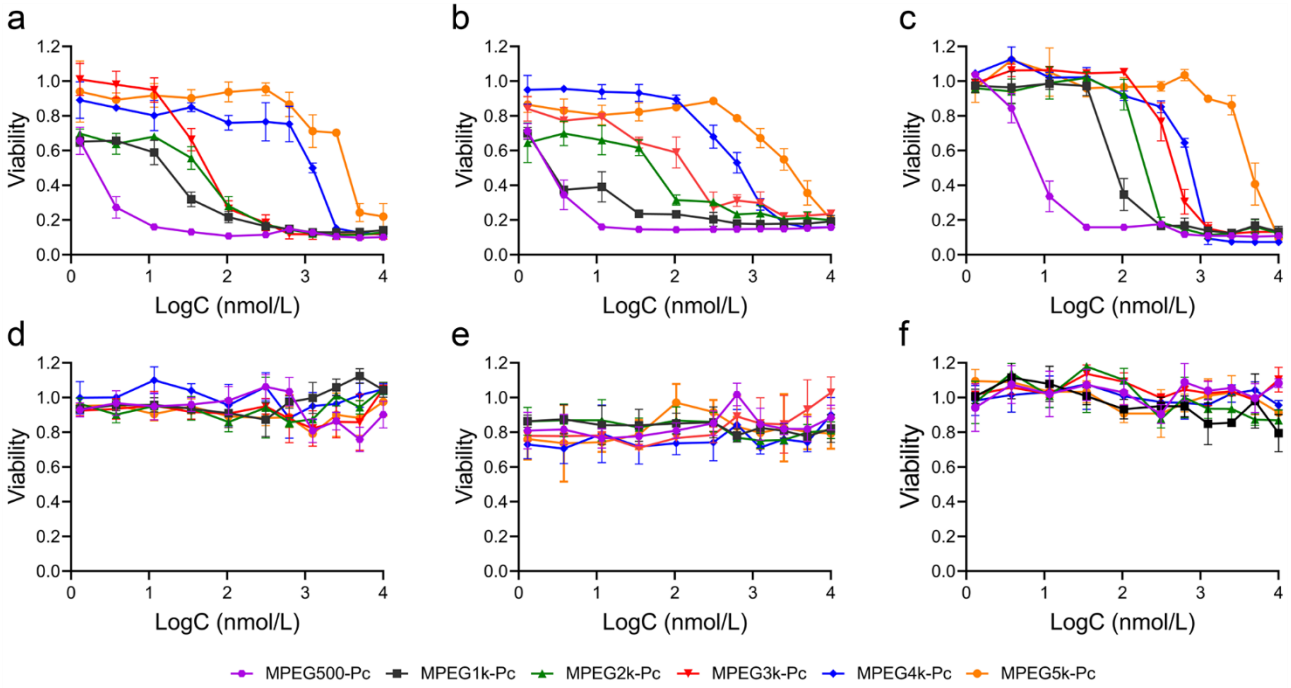

Figure S17. *In vitro* phototoxicity (a~c) and dark toxicity (d~f) of MPEG-Pcs, on NCI-H520 cells (a,

d), LO2 cells (b, e) and FaDu cells (c, f) for 48 h in the absence of irradiation (mean ± s.d., n = 3).

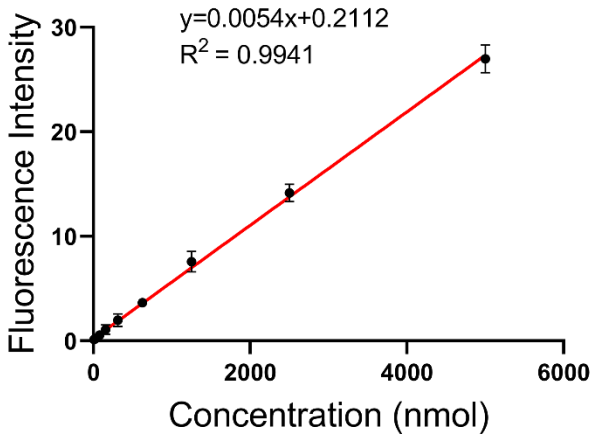

Figure S18 Standard curve of concentration versus fluorescence intensity. The concentration of MPEG4k-Pc (in 0.25% Triton X-100) was determined using the equation y=0.0054x+0.2112 with an R^2 value of 0.9941, where y is fluorescence intensity and x is concentration.

We also calculated the uptake percentage of MPEG4k-Pc according to the standard curve using the curve fitting equation (Figure S18) at 5 μM after incubation for 4 h, with uptake percentage about 1%, 10^6 ~10^7 molecules per cell.

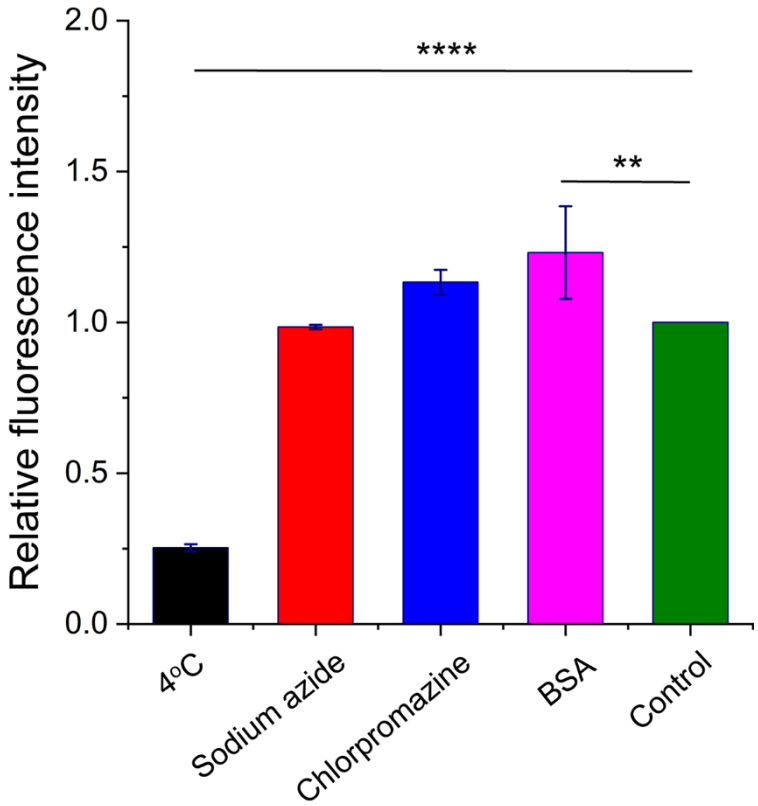

Figure S19 Effect of inhibitors of endocytosis and BSA on uptake of MPEG4k-Pc by MCF-7 cells. (**$P < 0.01$, ****$P < 0.001$)

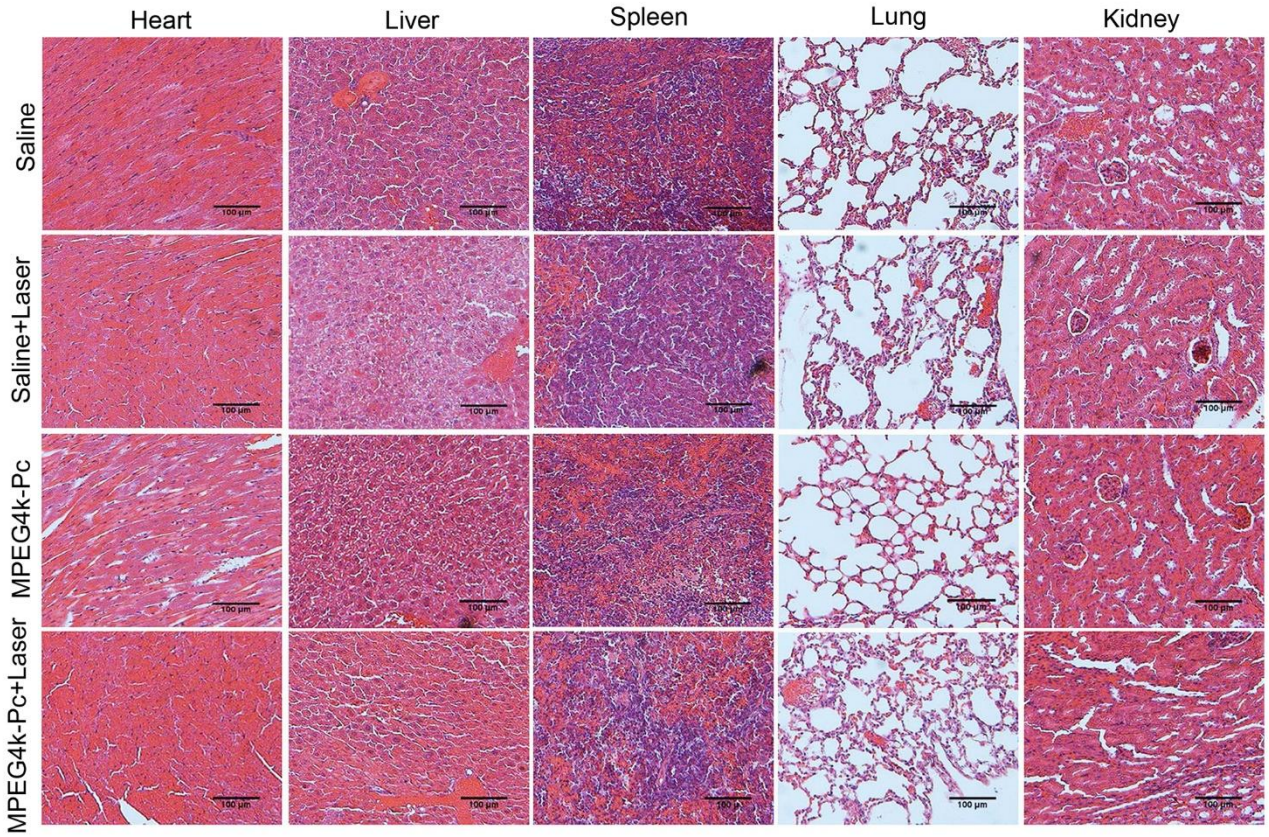

Figure S20. Histological analysis of the tumors, heart, liver, spleen, lung, and kidney of control, no illumination and illumination groups, respectively.

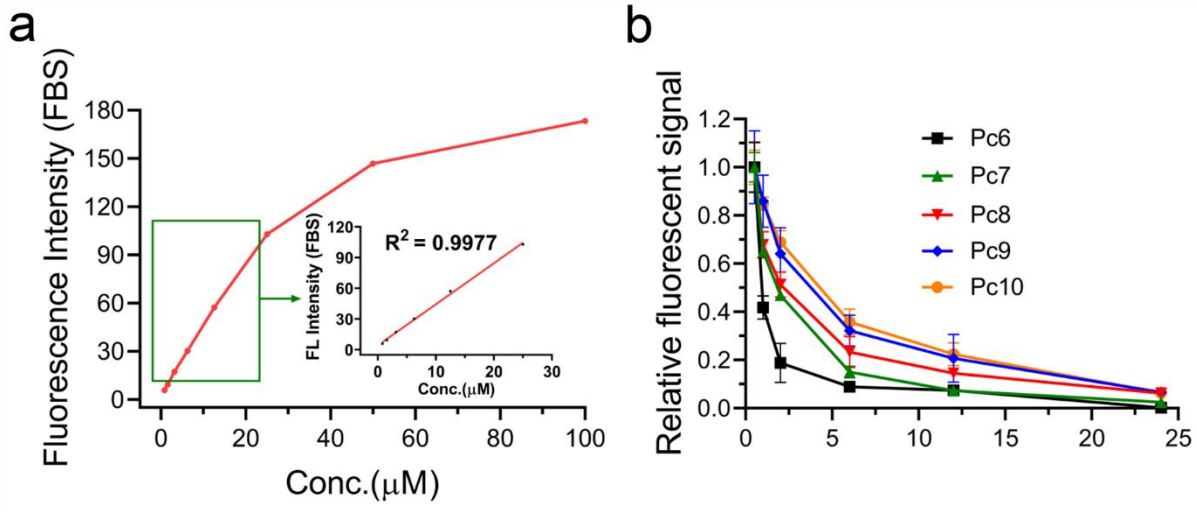

Figure S21. Pharmacokinetic study of MPEG1k-Pc ~ MPEG5k-Pc: (a) Relationship between concentration and fluorescence intensity of MPEG4k-Pc in FBS. (b) Plasma concentration of MPEG1k-Pc~MPEG5k-Pc marked by relative fluorescence intensity changed with time after i.v. injection of 40 nM/20g, 2×10−4 M, respectively (mean ± s.d., n = 3).

Table S1. In vitro phototoxicity of the MPEGylated ZnPc

Compd.	IC50 (nM)			
	FaDu	MCF-7	NCI-H520	L02
MPEG500-Pc	9.66	7.33	1.47	2.11
MPEG1k-Pc	78.05	85.75	5.76	3.47
MPEG2k-Pc	218.68	69.14	11.29	34.50
MPEG3k-Pc	456.13	157.93	31.52	113.89
MPEG4k-Pc	706.67	1135.67	1221.67	696.33
MPEG5k-Pc	4285.67	5063.00	2960.33	2533.67