Supporting Information

Optical property and singlet oxygen generation of phthalocyanine derivative with strong two-photon-absorbing chromophores in the periphery

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Instrumentation and reagents

¹H NMR and ¹³C NMR spectra were recorded on Varian Mercury VX300 FT-NMR spectrometer in CDCl₃ (Varian, USA) operating at 298 K. Elemental analysis was performed by Vario EL III (German). Mass spectra were recorded on Finnigan Trance Mass spectrometer. MALDI-TOF was operated on Voyager-DE-STR. UV-vis spectra were obtained using a Schimadzu 160A spectrometer. Fluorescence spectra were recorded on a Hitachi F-4500 fluorescence spectrophotometer. Two-photon absorption were determined by Z-scan measurement in DMF (1×10^{-3} M) at 830, 850 and 870 nm with Ti: Sapphire laser (Mira 900, Coherent; 2.5 ps, 76 MHz, $I_0 = 0.03$ GW/ cm²). Singlet oxygen experiment was performed by exposing the solution of sample to a halogen lamp (300 W). Between with them, there is a filter (FS2-GG420), which used to filter off the light that wavelength shorter than 420 nm.

DPBF and DBU were purchased from Acros and used without further purification. 4-hydroxyphthalonitrile and 4, 6-Bis-[2-(4-diethylamino-phenyl)-vinyl]-pyrimidin-2-ol were synthesized as in the literatures. All other beginning chemicals are commercially available and were used as received unless stated otherwise. The solvent was dried as normal procedure and the solution of samples were prepared freshly and wrapped in silver paper before measurement.

Optical Spectrum

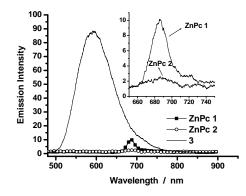


Fig. S1 Emission spectra of the three compounds ($\lambda_{ex} = 460 \text{ nm}$)

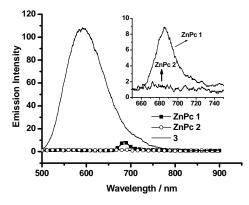


Fig. S2 Emission spectra of the three compounds ($\lambda_{ex} = 480 \text{ nm}$)

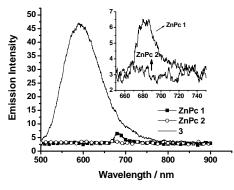


Fig. S3 Emission spectra of the three compounds ($\lambda_{ex} = 470$ nm, the concentration of ZnPc is 4×10^{-7}

M)

Note: The inset in Fig. S1, S2 and S3 are the argument of the emission of ZnPc 1 and 2 between 650 and 750 nm.

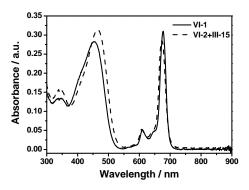


Fig. S4 The absorption of ZnPc 1 (1 μ M) and the mixture of ZnPc 2 (1 μ M) with Compound 3 (4 μ M).

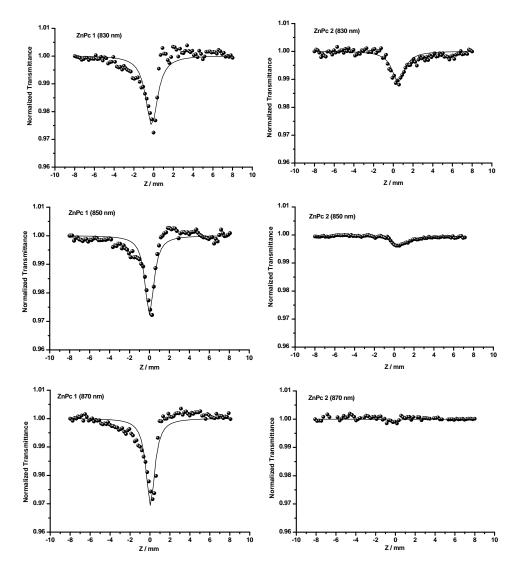


Fig. S5 Z-scan curves of the ZnPc 1 and 2 in DMF at 830, 850 and 870 nm.