

## Electronic Supplementary Information (ESI)

### **Phenothiazin-N-yl-capped 1,4-diketo-3,6-diphenylpyrrolo[3,4-c]pyrrole exhibiting strong two-photon absorption and aggregation-enhanced one- and two-photon excitation red fluorescence**

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## 1. NMR spectra of DPPC4

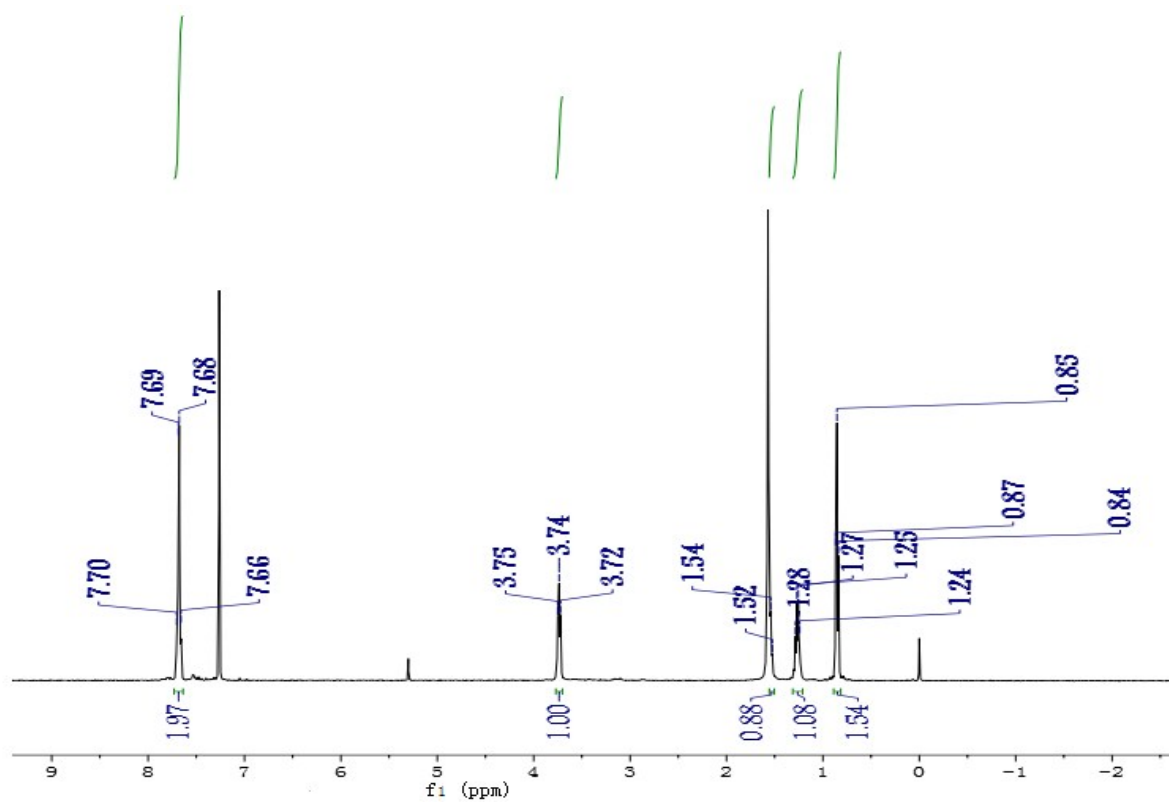
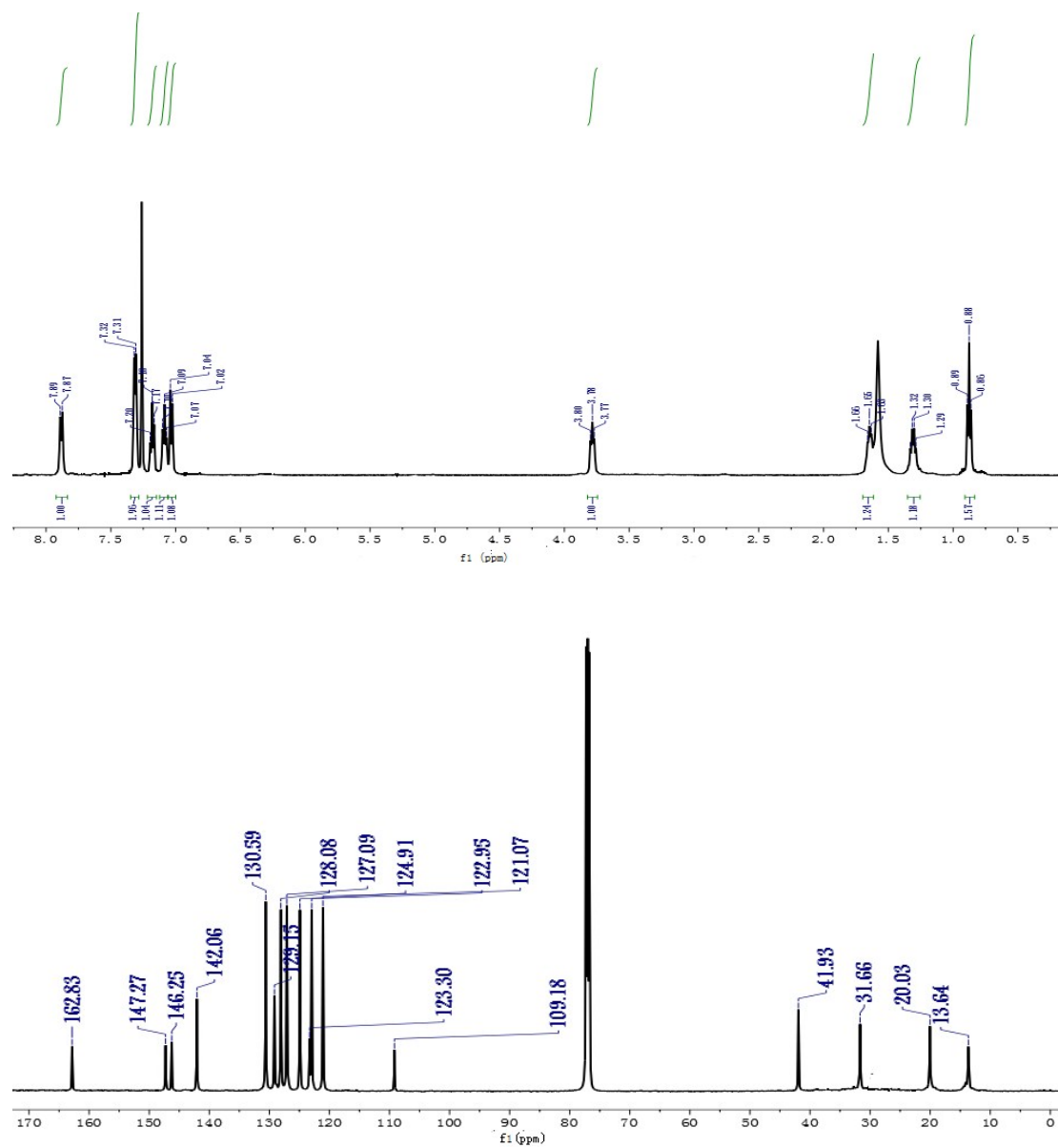
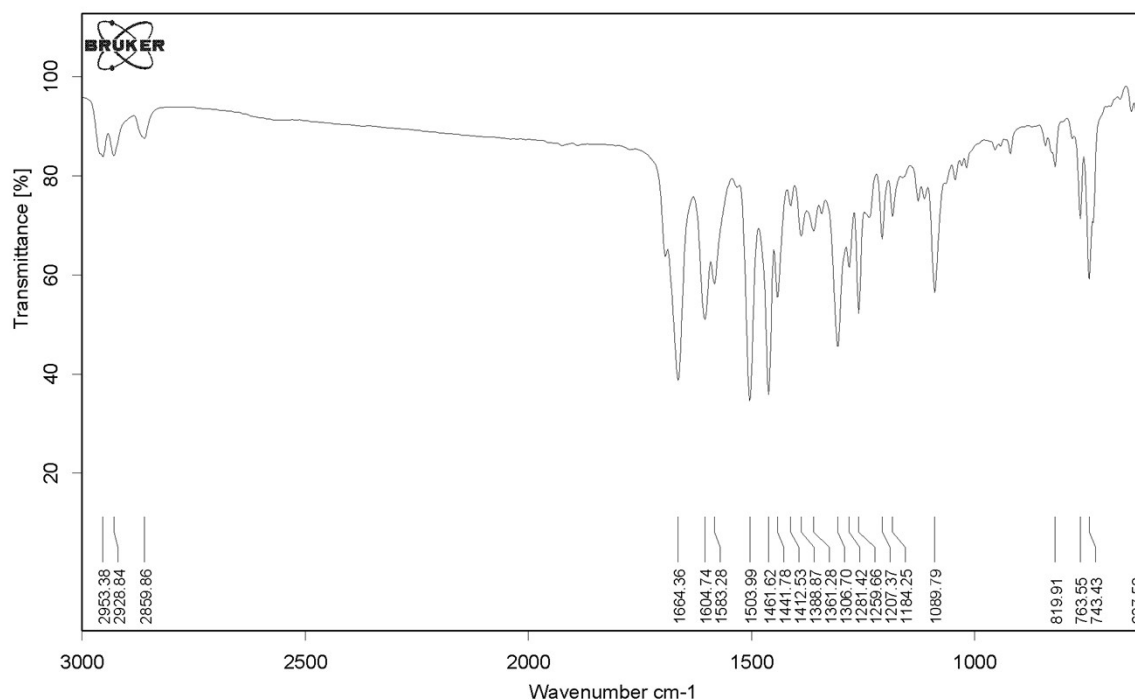


Fig. S1  $^1\text{H}$  NMR spectra of DPPC4.

## 2. NMR and IR spectra of PDPP

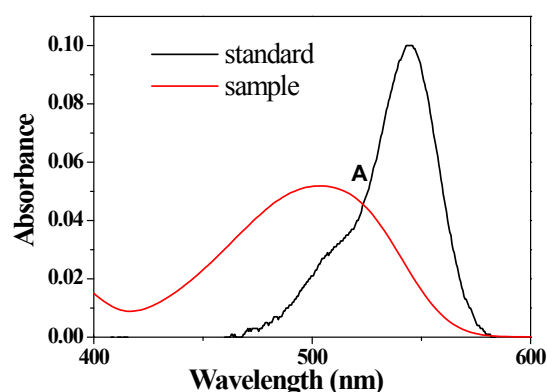




**Fig. S2** <sup>1</sup>H and <sup>13</sup>C NMR and IR spectra of PDPP.

## 2. Determination of Quantum Yields

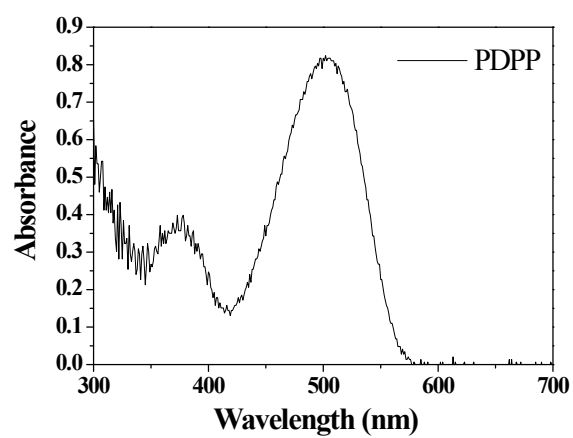
The solution fluorescence quantum yield ( $\Phi$ ) was determined by a dilute solution method using Rhodamine B in methanol as the standard(r). The same procedure is used for measuring the absorbance of the standard and samples (The maximum absorbance of standard is  $0.1 \pm 0.02$ ). Both of the UV absorption curves will have an intersection (A) (Fig. S2). If the absorbance of Intersection point (A) lies between 0.05 and 0.03 (When absorbance is above 0.05, self-absorption may occur), the wavelength at the intersection will be used later for excitation. The emission spectra of the standard and samples are recorded.  $\Phi_s$  was calculated according to the following equation:  $\Phi_s = \Phi_r [A_s/A_r][F_r/F_s][n_s/n_r]^2$ , where  $\Phi_r$  and  $\Phi_s$  are the respective fluorescence quantum yields of standard and samples,  $A_r$  and  $A_s$  are the respective absorbances of standard and the measured samples at the excitation wavelength,  $F_r$  and  $F_s$  are the area under the corrected emission curve of standards and the samples, and  $n_r$  and  $n_s$  are the respective refractive indices of the corresponding solvents of the solutions.



**Fig. S3** Absorption spectra of the reference (Rhodamine B in methanol) and sample ( PDPP in THF ).

### 3. Determination of the molar extinction coefficients

The molar extinction coefficients measurement was carried out on a Hitachi U-4100. The absorption spectra were taken using a 1.0 cm pathlength quartz-cell. Absorption spectra were recorded for samples(  $1.0 \times 10^{-5}$  M ) and the molar extinction coefficients were calculated from the absorbance values in the standard solutions, using the Beer - Lambert law  $Abs_{\lambda} = \epsilon c L$ , where Abs is the absorbance at each wavelength,  $\epsilon$  ( $M^{-1}cm^{-1}$ ) is the molar extinction coefficient,  $c$  (mol/L) is the concentration of the samples in the solution and  $L$  (cm) is the optical pathlength. First, we prepare the concentration for  $1.0 \times 10^{-3}$  M THF solution of PDPP, and then 1ml THF solution of PDPP ( $1.0 \times 10^{-3}$  M) was added into 9 mL THF, the concentration for  $1.0 \times 10^{-5}$  M THF solution of PDPP was prepared.



**Fig. S4** Absorption spectra of the PDPP in THF at  $1.0 \times 10^{-5}$  M.