Electronic Supplementary Information

Altering Synthetic Fragments to Tune the AIE Properties and Self-assemble Grid-like Structures of TPE-based Oxacalixarenes

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1. ^{1}H NMR and ^{13}C NMR spectra of 1a and 1b

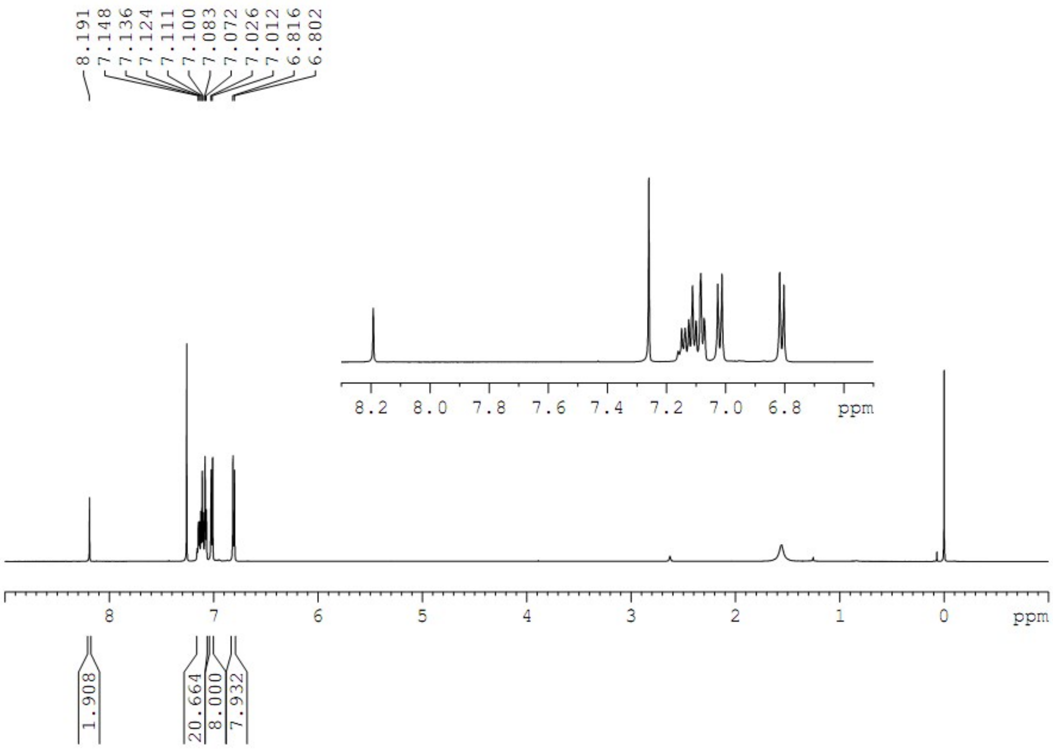

Fig. S1 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **1a.**

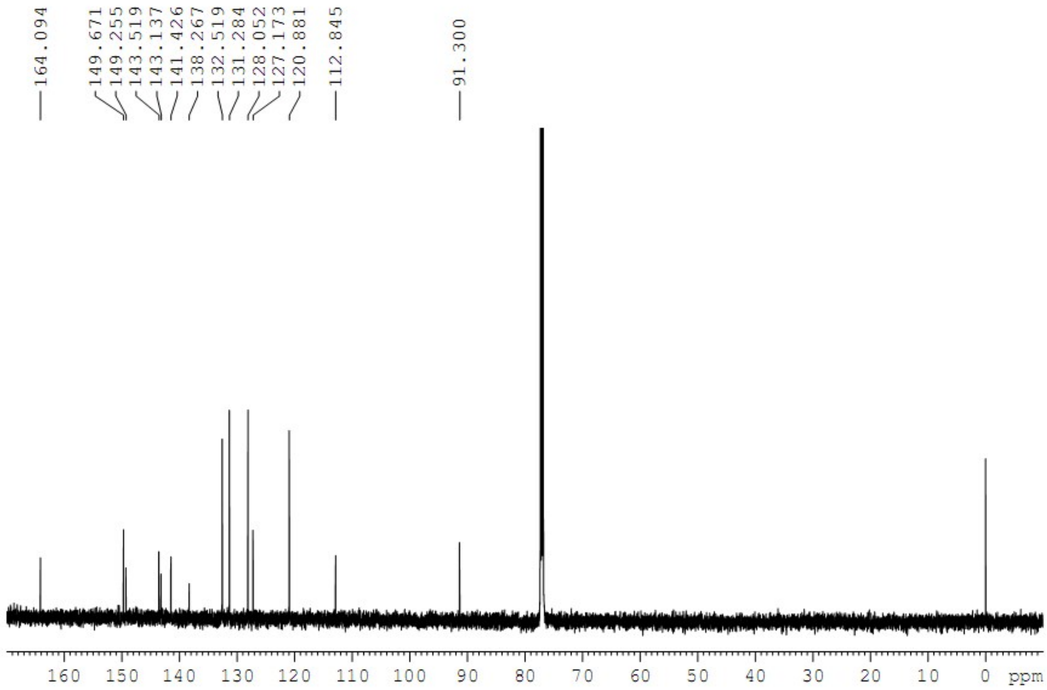

Fig. S2 ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of **1a.**

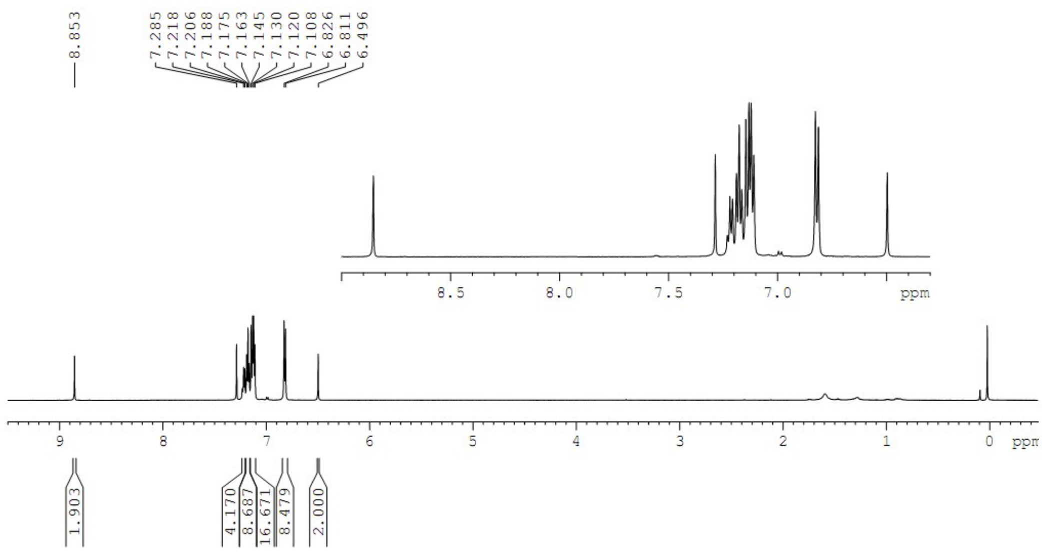

Fig. S3 ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **1b.**

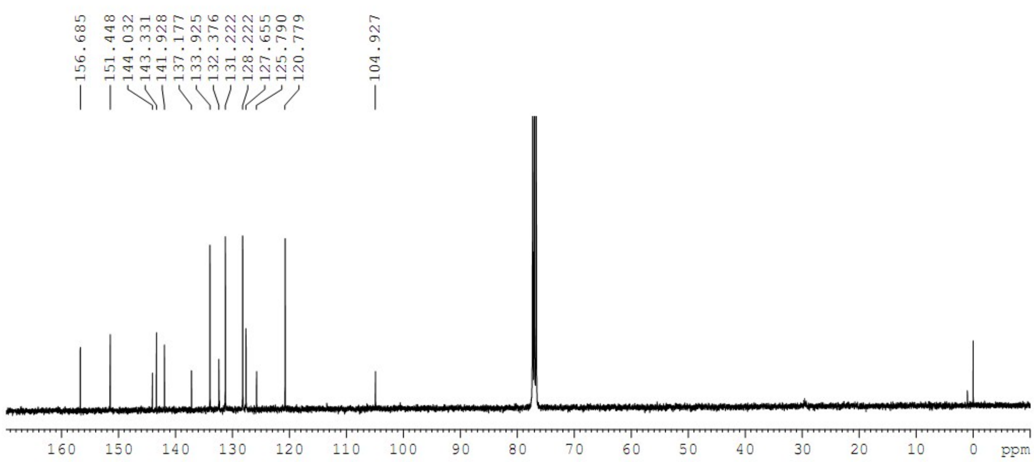

Fig. S4 ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of **1b.**

2. IR spectra of 1a and 1b

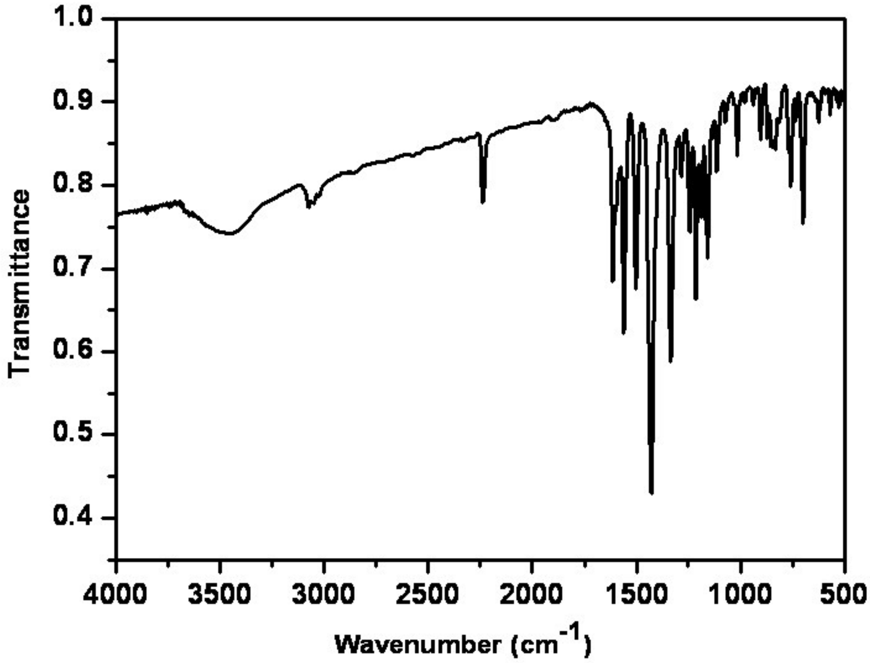

Fig. S5 IR spectrum of **1a**.

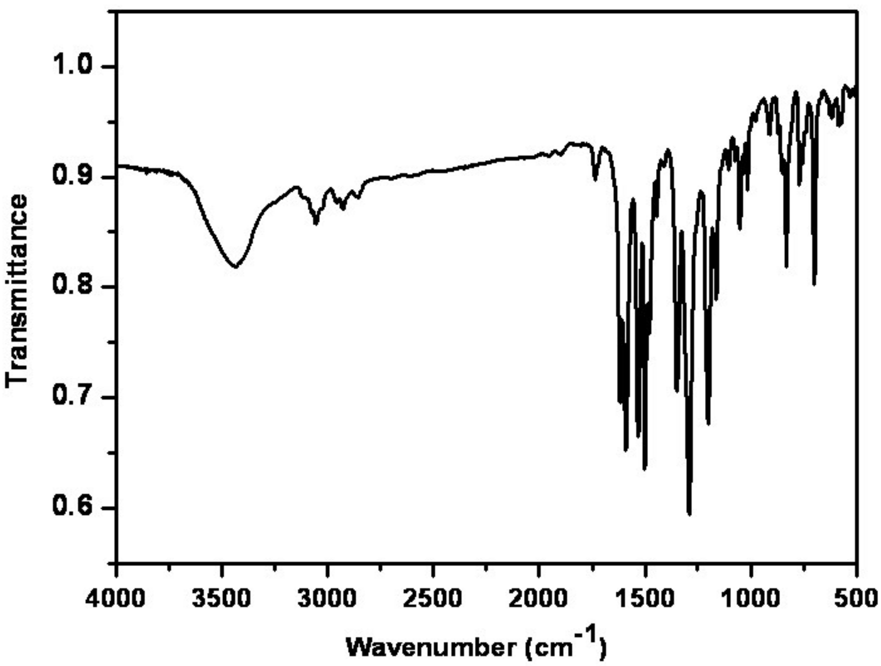

Fig. S6 IR spectrum of **1b**.

3. Crystal structure of 1a.

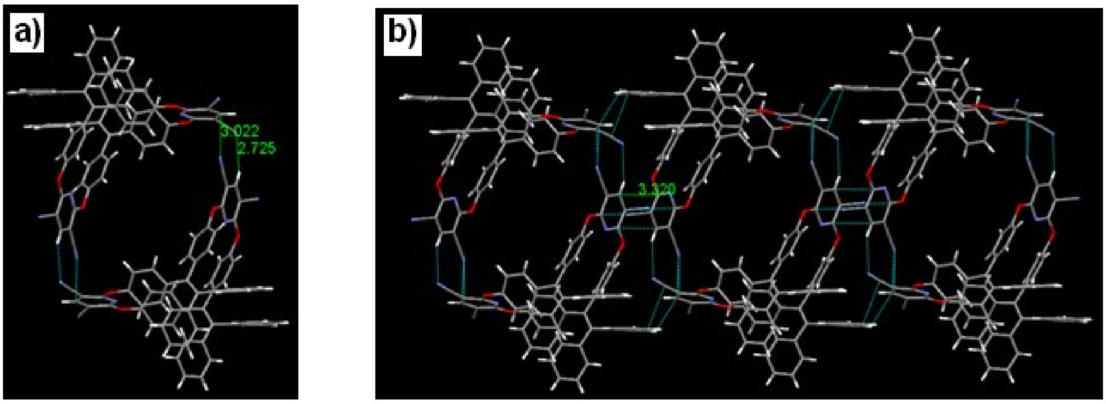

Fig.S7 The dimmer structures (a), and one-dimensional linear grid structure (c) of oxacalixarene **1a.**

4. Crystal structure of 1b.

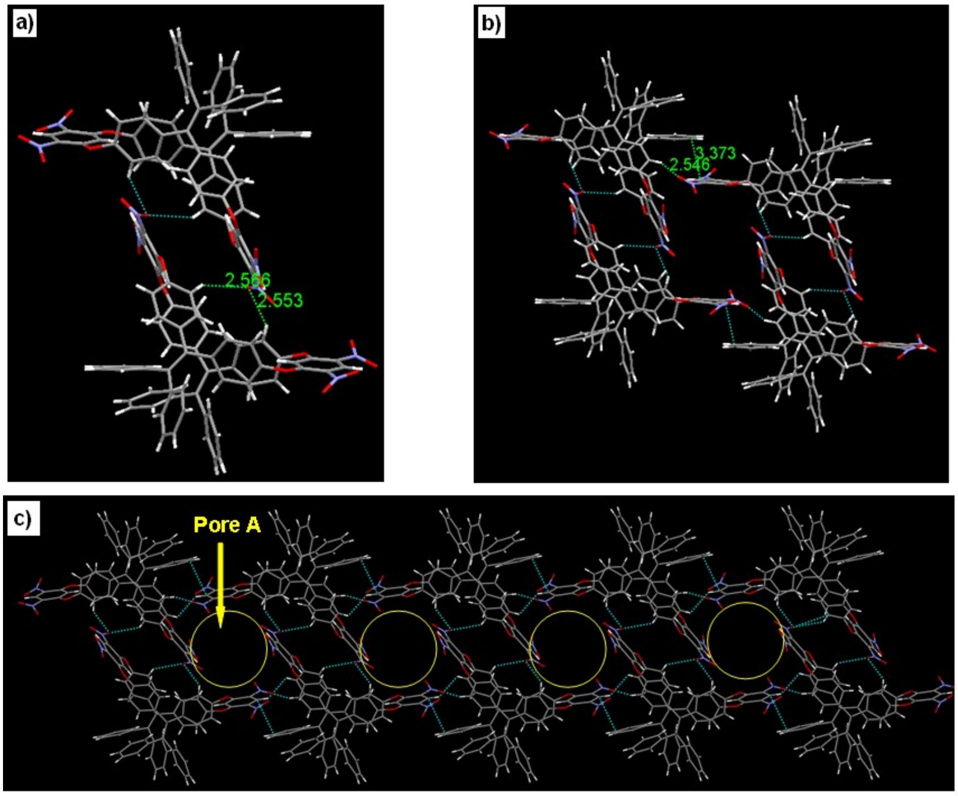

Fig. S8 The dimmer structures (a), the grid-like pore A (b) and one-dimensional linear grid structure (c) of oxacalixarene **1b.**

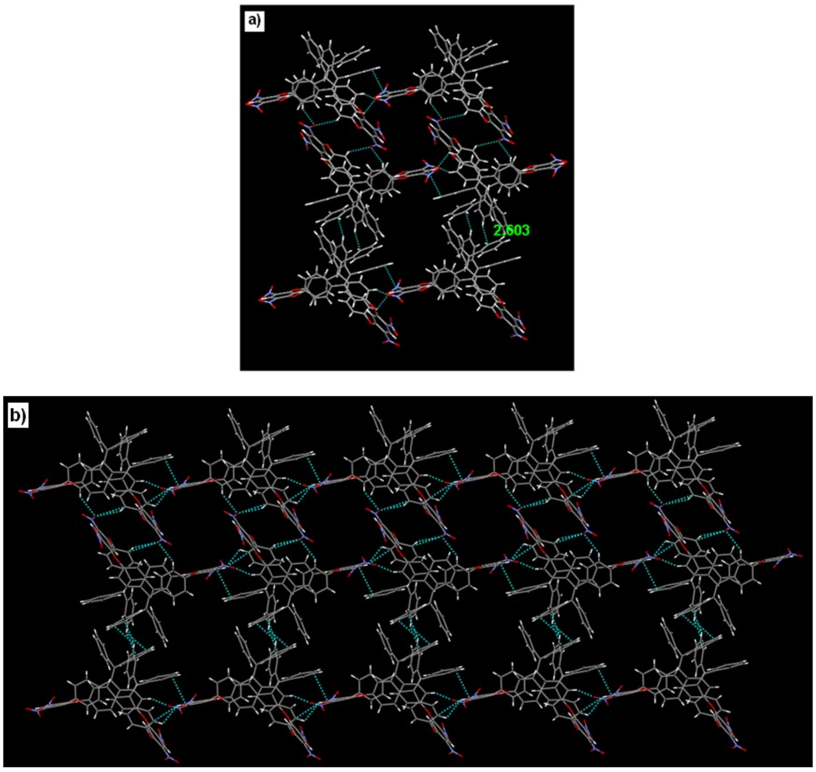

Fig. S9 The grid-like pore B (a) and two-dimensional grid structure (b) of oxacalixarene **1b.**

5. The Self-assemblies of 1a in water/THF

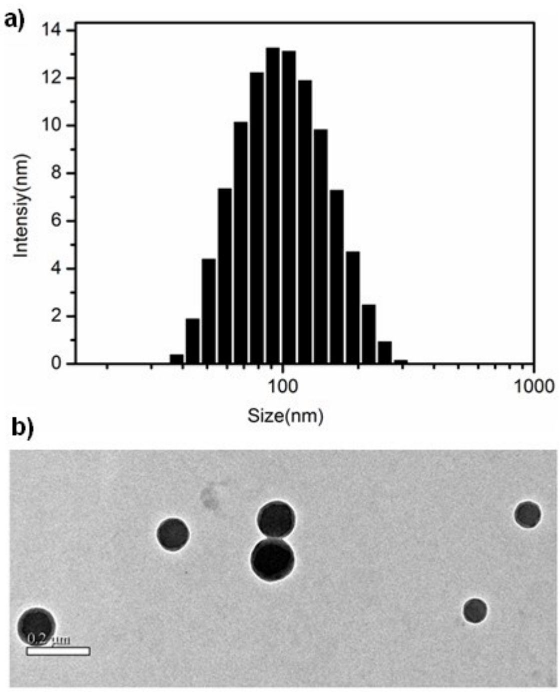

Fig.S10 The hydrodynamic size (a) and TEM image (b) of **1a** in water/THF (95/5) with concentration of 0.1 mg/mL.

6. The fluorescent titration experiments of 1a for different quenchers.

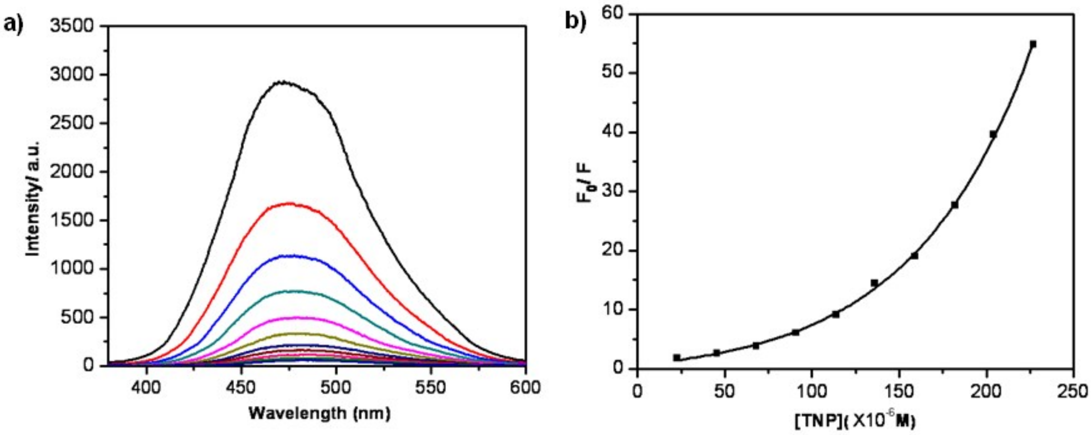

Fig. S11 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of TNP at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with TNP.

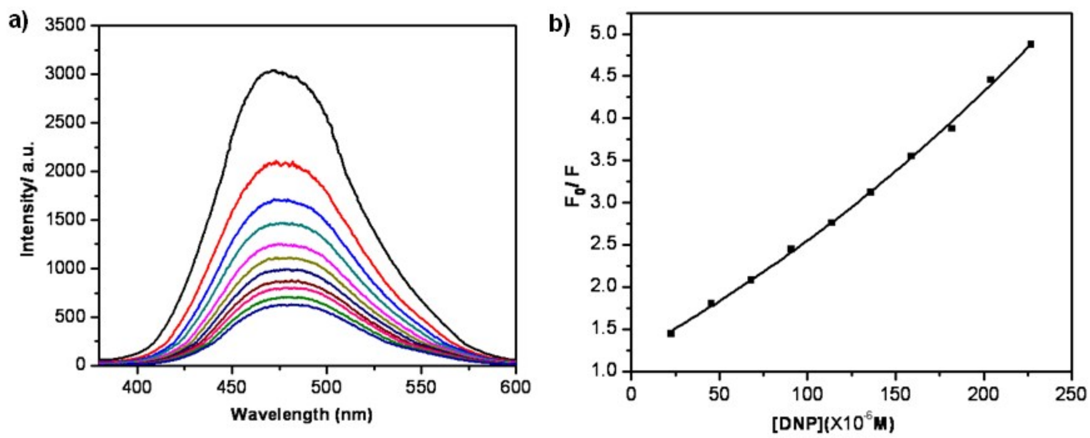

Fig.S12 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of DNP at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with DNP.

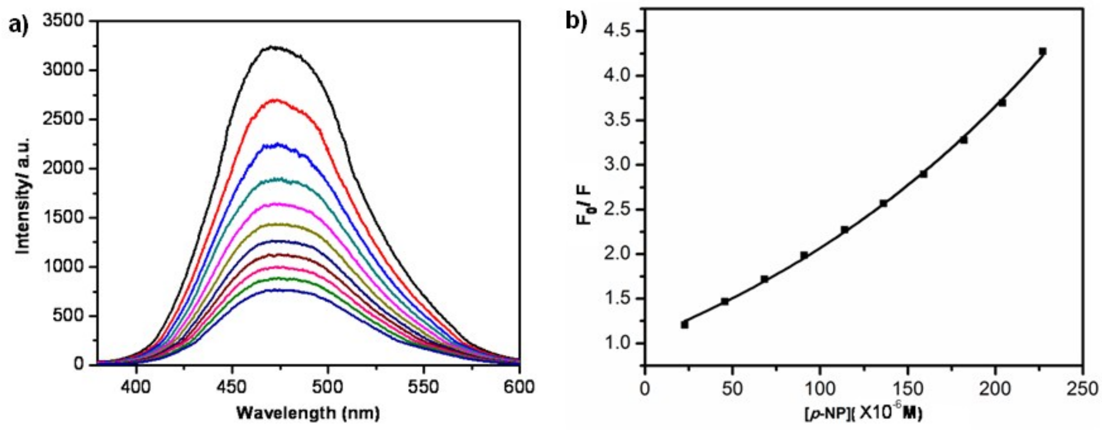

Fig. S13 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of *p*-NP at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with *p*-NP.

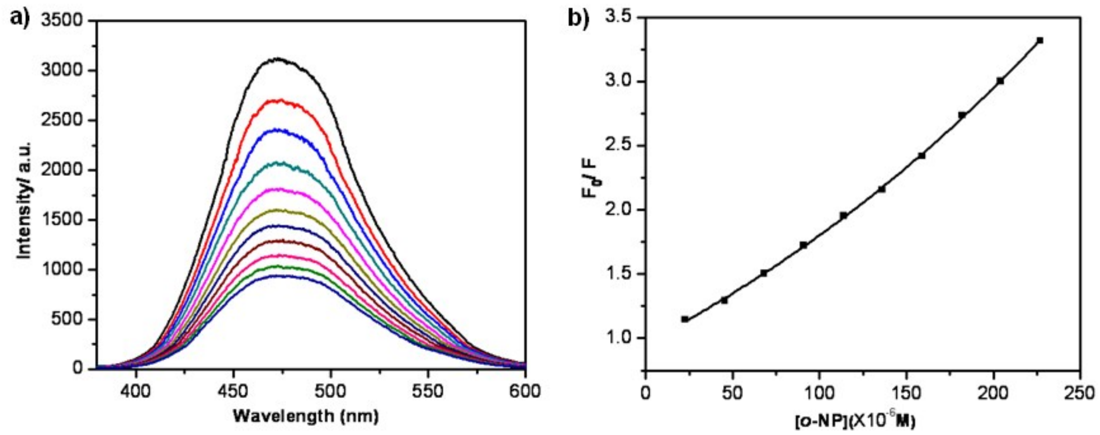

Fig. S14 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of *o*-NP at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with *o*-NP.

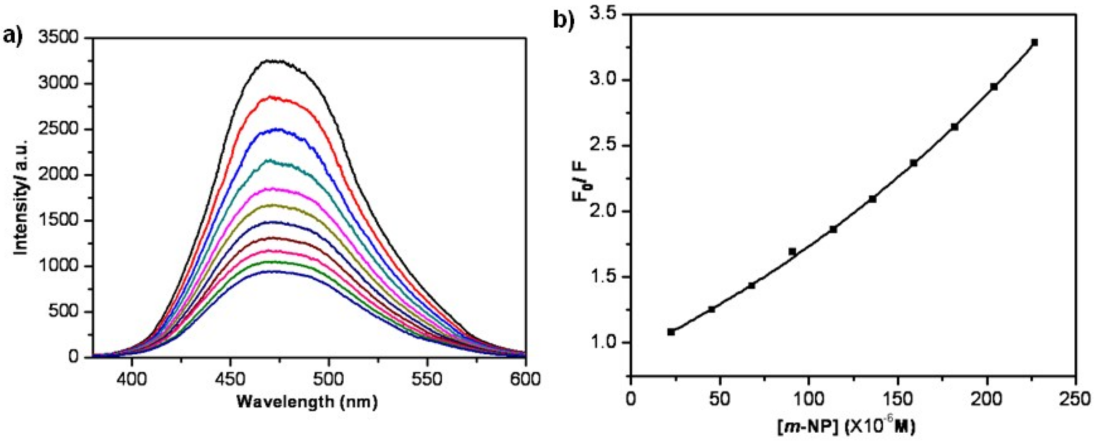

Fig. S15 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of *m*-NP at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with *m*-NP.

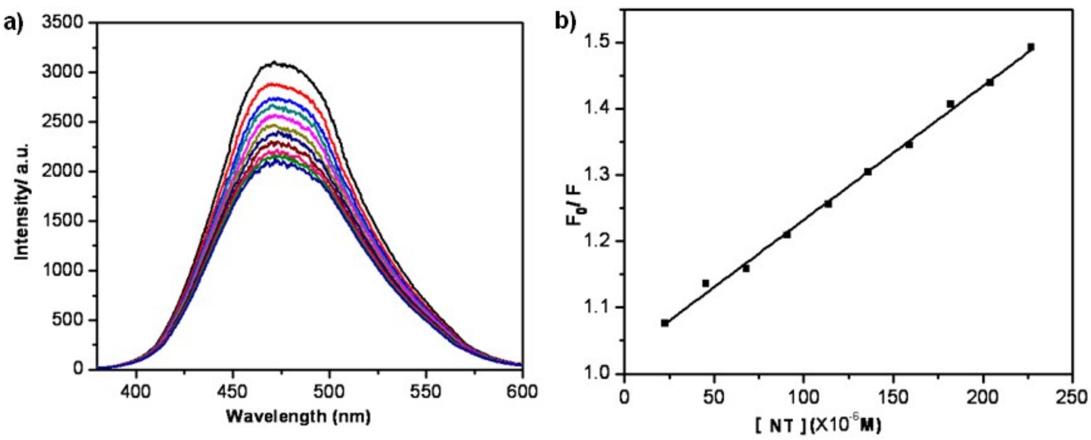

Fig. S16 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of NT at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with NT.

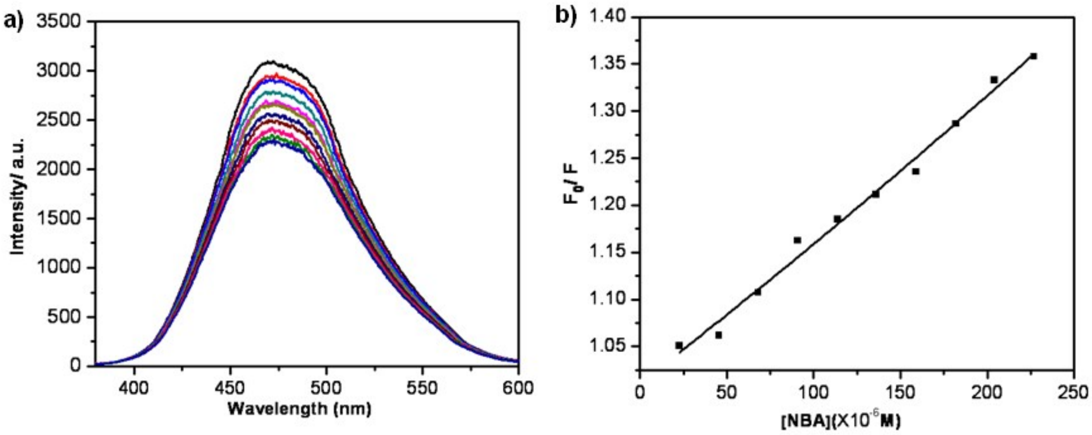

Fig. S17 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5 × 10^{-6} M) in presence of NBA at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with NBA.

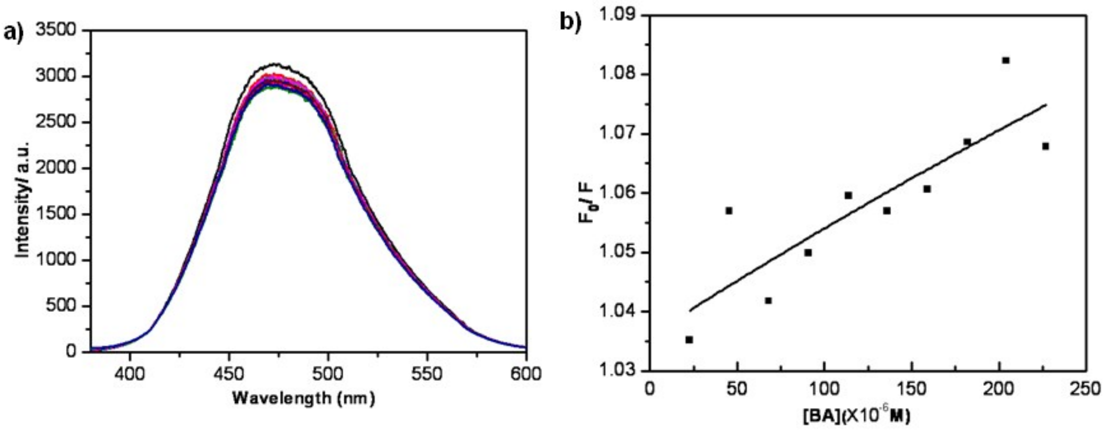

Fig S18 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5 × 10^{-6} M) in presence of BA at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with BA.

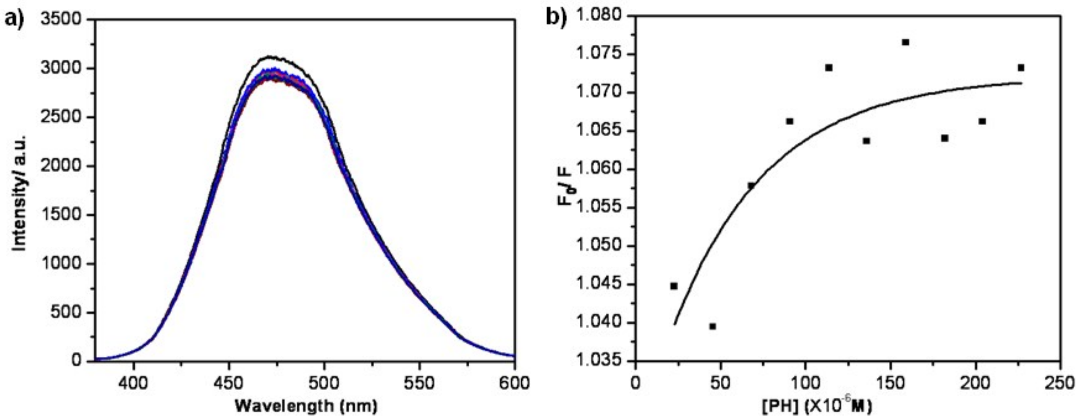

Fig. S19 (a) Emission spectra (λ_{ex} = 350 nm) of **1a** (4.5×10^{-6} M) in presence of PH at various concentration (0, 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 equiv.). (b) The nonlinear curve-fitting for the quenching constant of **1a** with PH.

Table S1. Summary of fluorescence quenching constants of **1a**.

Quencher	TNP	DNP	*p*-NP	*o*-NP	*m*-NP	NT	NBA	BA	PH
K (M^{-1})	1.7×10^{4}	5.8×10^{3}	6.0×10^{3}	5.2×10^{3}	5.4×10^{3}	1.6×10^{3}	1.3×10^{3}	1.6×10^{2}	1.3×10^{2}

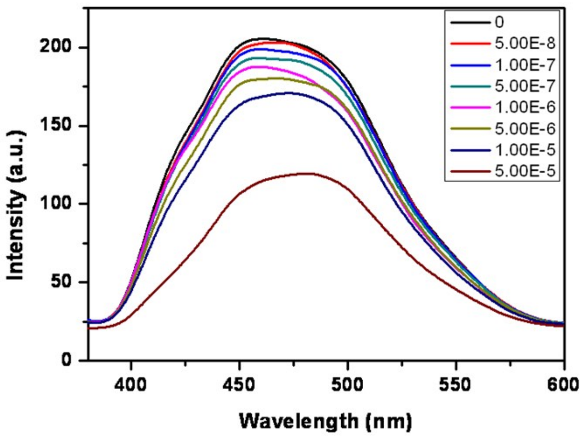

Fig. S20 Changes in the fluorescence spectra of 1a (5.0×10^{-7} M) with different concentrations of TNP.