Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supplementary Information

Aggregation-induced emission (AIE)-Active Fluorescent Probes with Multisite-Binding Sites toward ATP Sensing and the Live Cell Imaging

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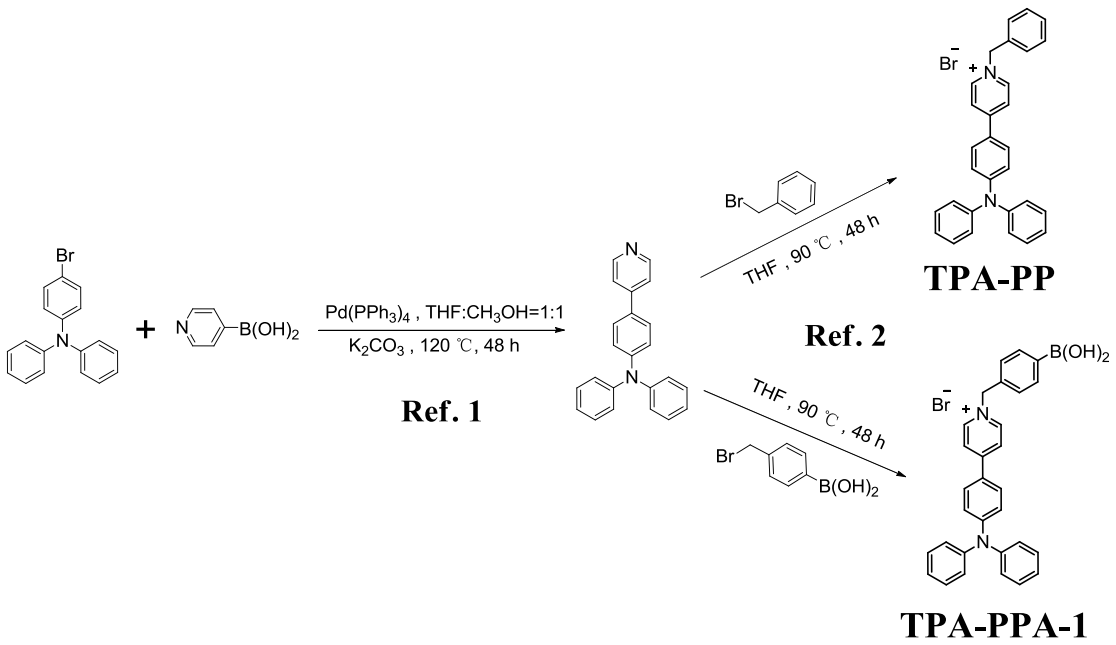
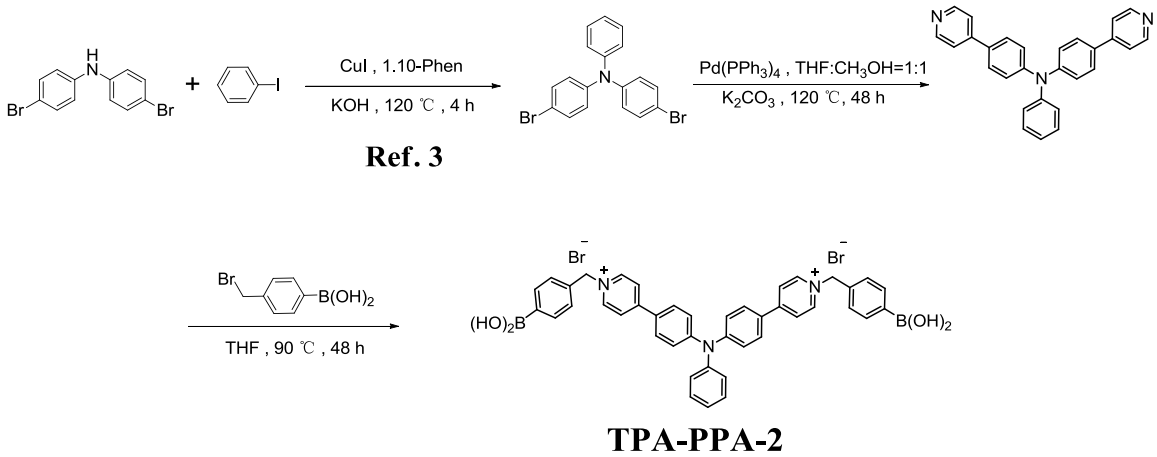
Table of Contents

Synthesis of TPA-PP and TPA-PPA-1



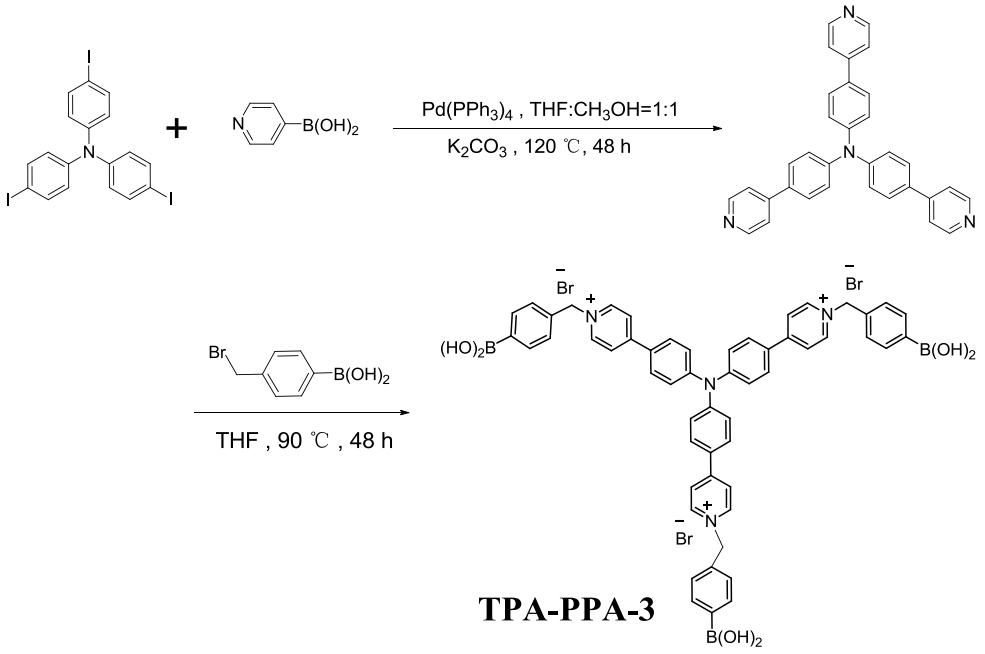
Scheme S1 The synthesis of TPA-PP and TPA-PPA-1

Synthesis of TPA-PPA-2



Scheme S2 The synthesis of TPA-PPA-2

Synthesis of TPA-PPA-3



Scheme S3 The synthesis of TPA-PPA-3

TPA-PP

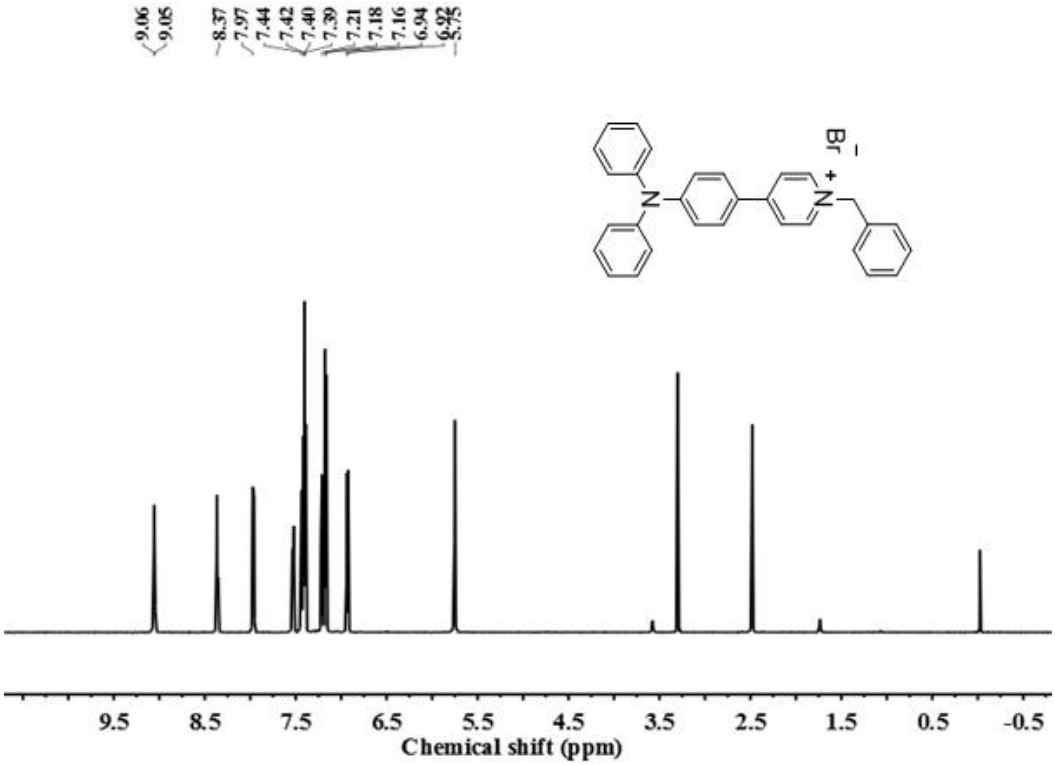


Figure S1 (a) ^{1}H NMR spectra of TPA-PP

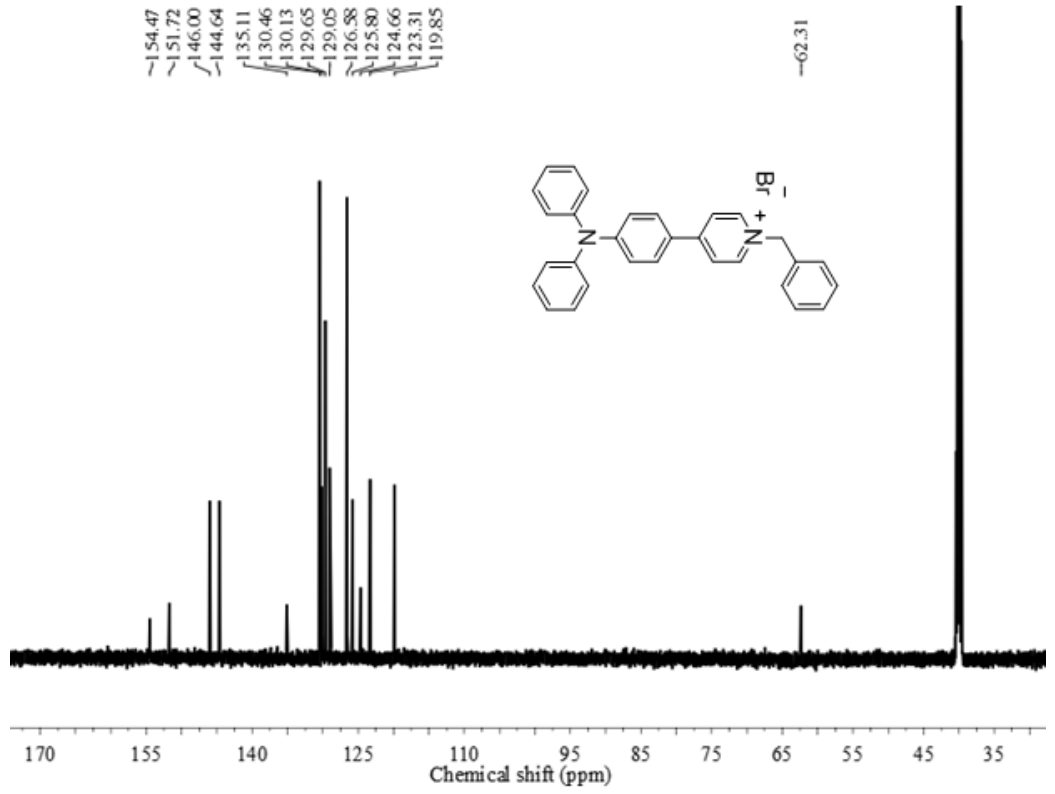


Figure S1 (b) ^{13}C NMR spectra of TPA-PP

TPA-PPA-1

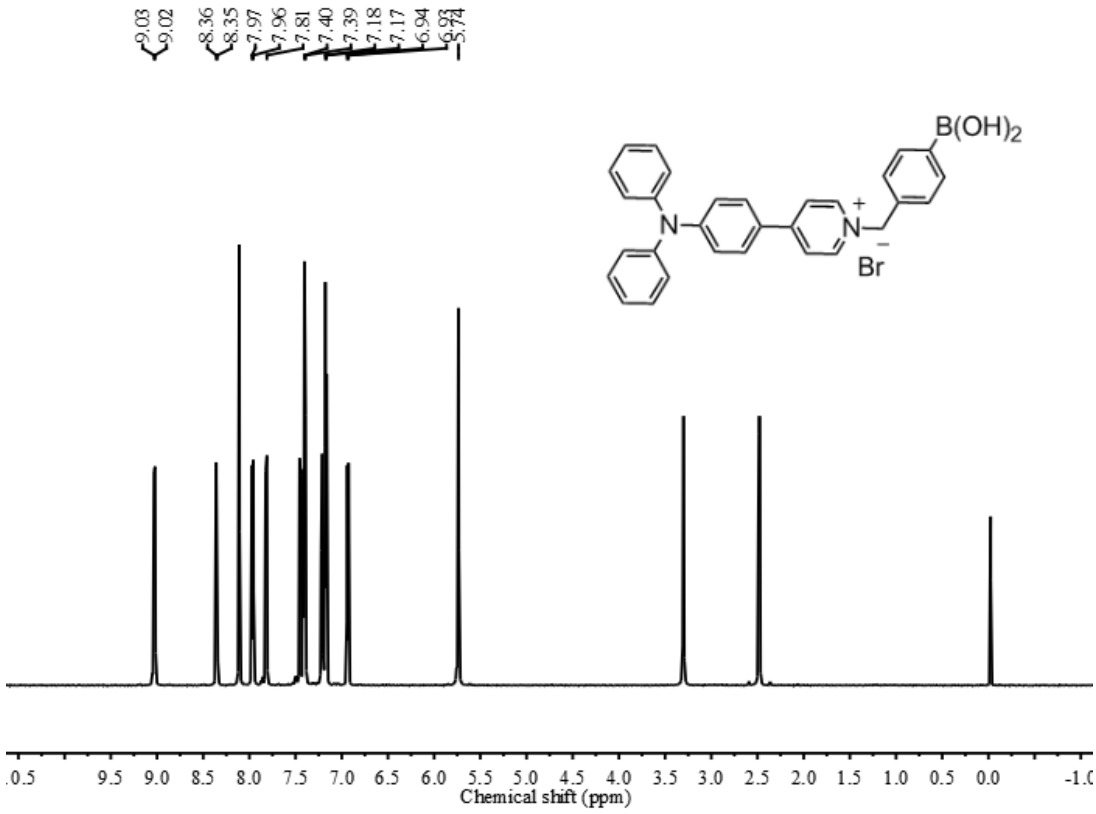


Figure S2 (a) ^{1}H NMR spectra of TPA-PPA-1

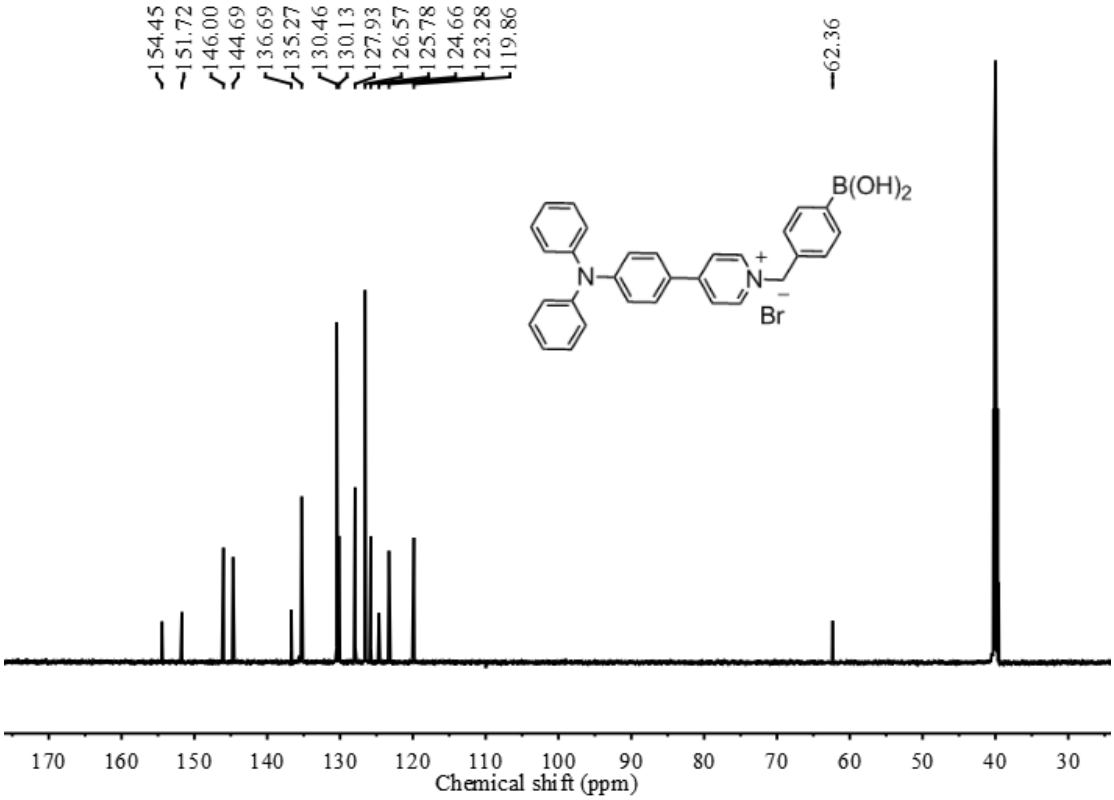


Figure S2 (b) ^{13}C NMR spectra of TPA-PPA-1

TPA-PPA-2

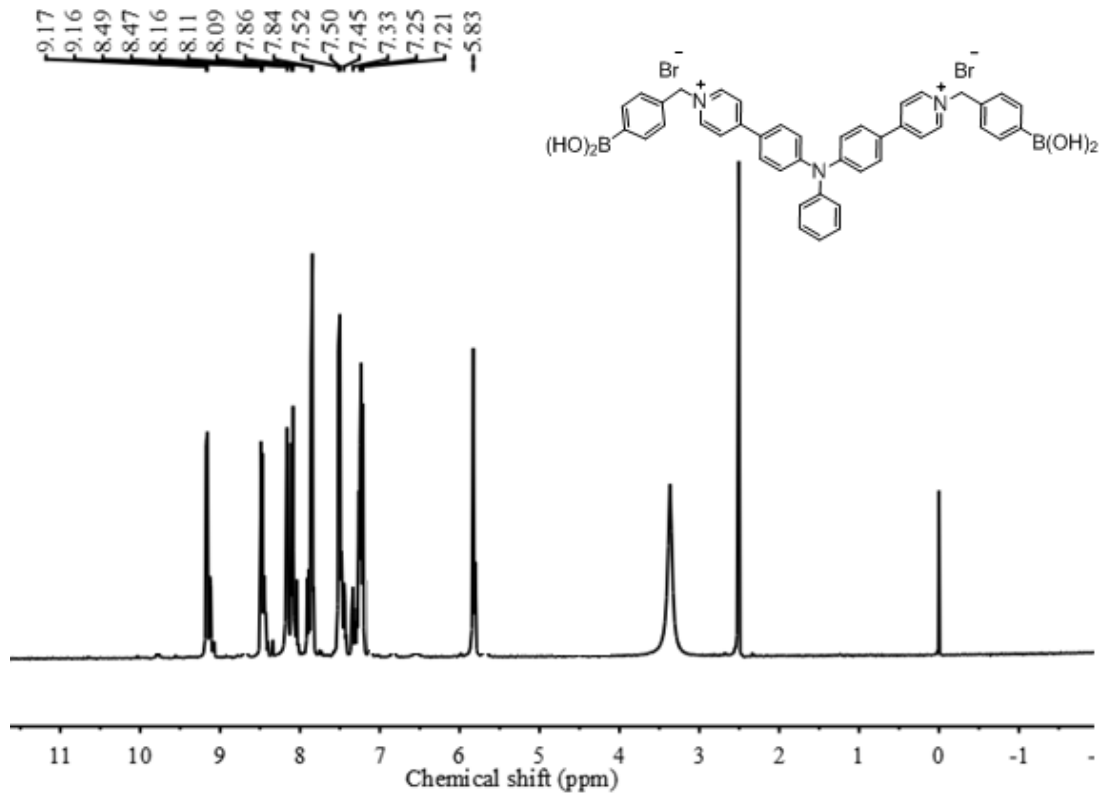


Figure S3 (a) ^{1}H NMR spectra of TPA-PPA-2

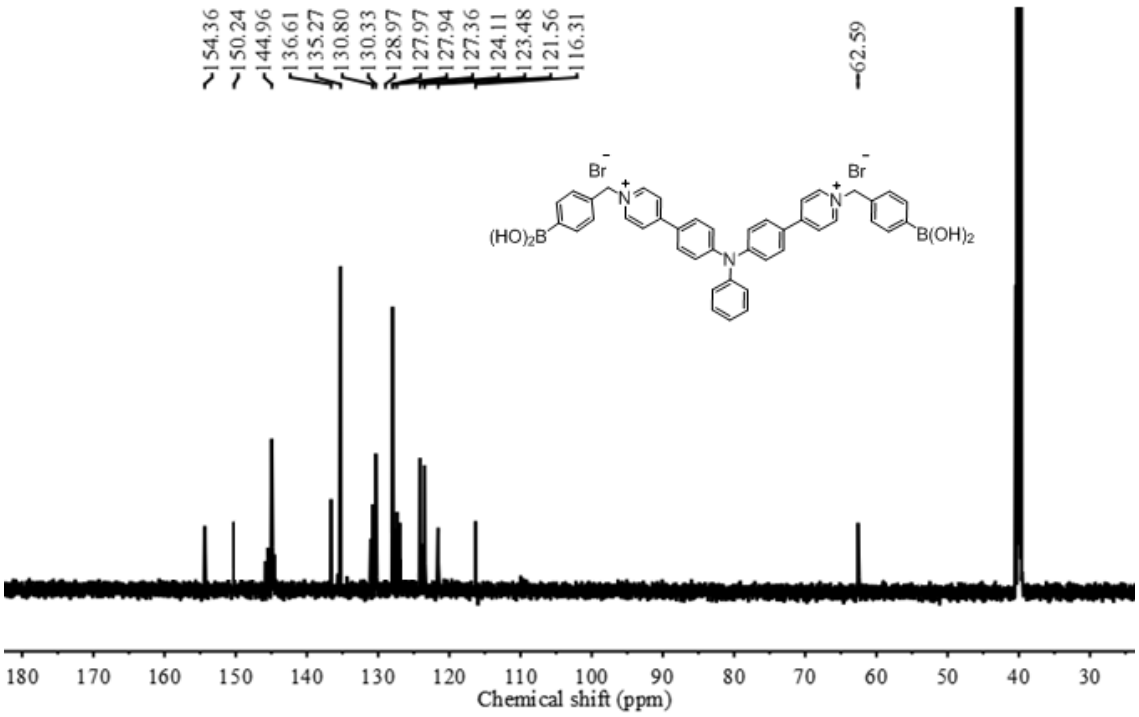


Figure S3 (b) ^{13}C NMR spectra of TPA-PPA-2

TPA-PPA-3

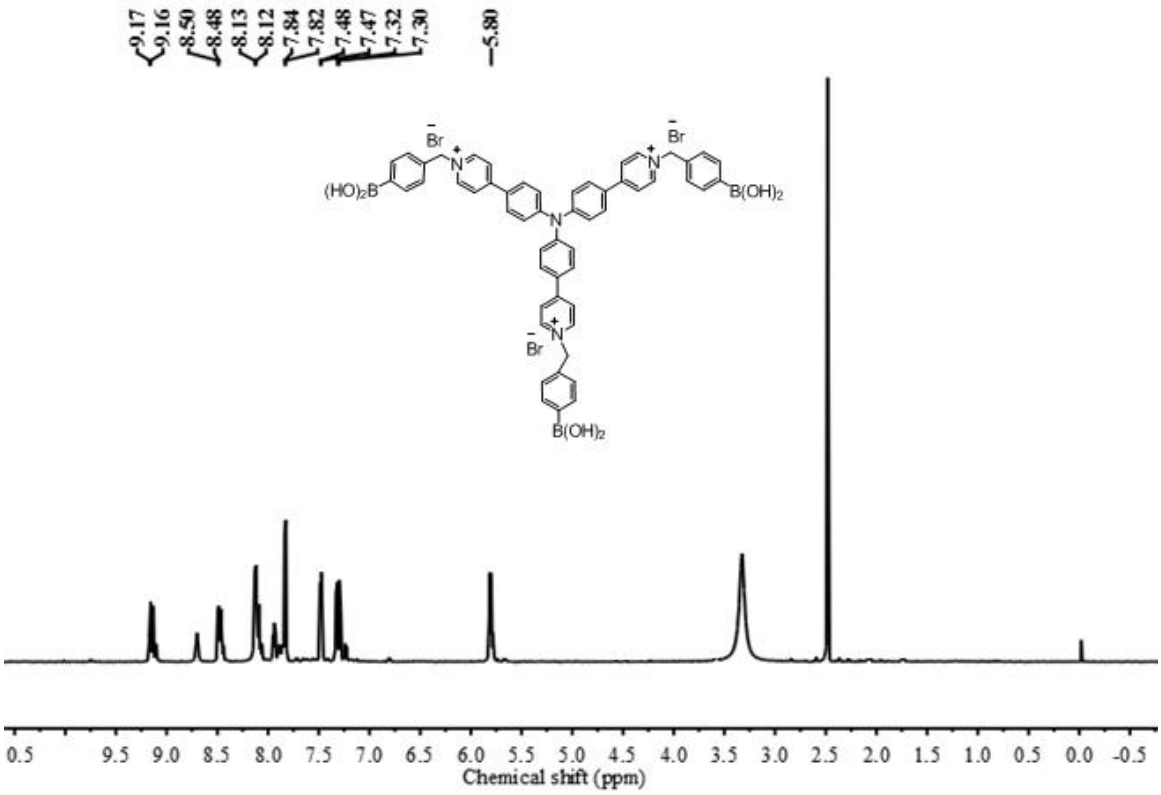


Figure S4 (a) ^{1}H NMR spectra of TPA-PPA-3

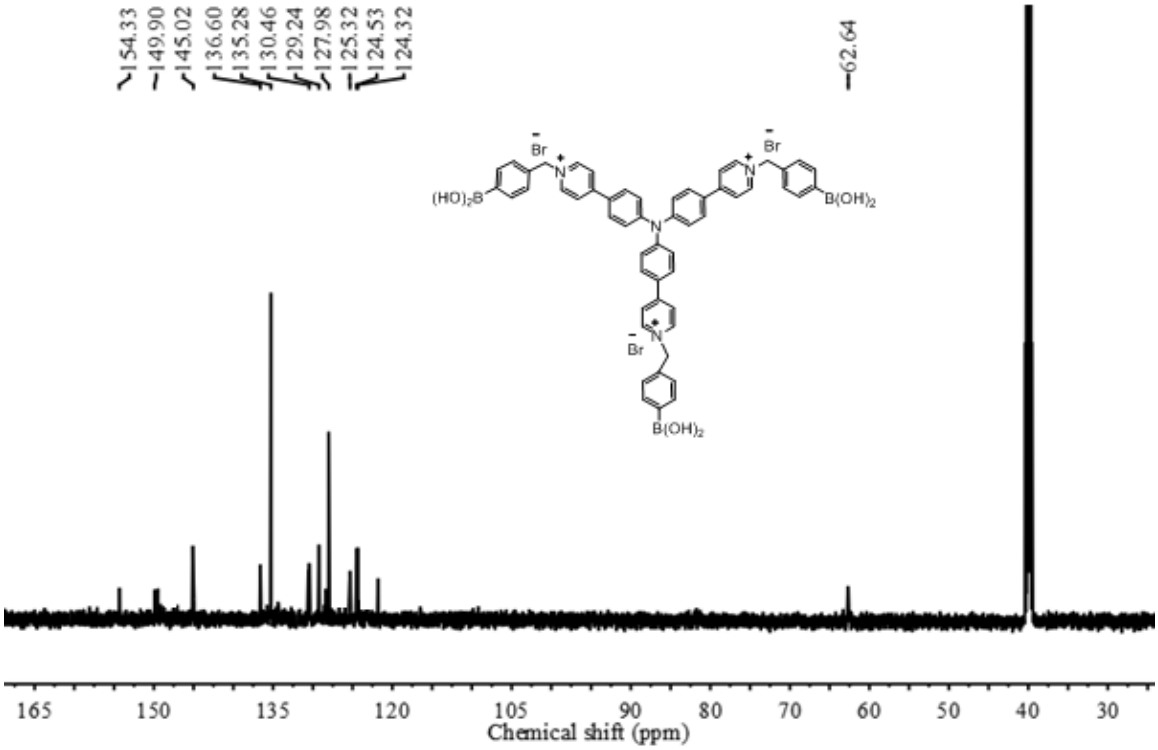


Figure S4 (b) ^{13}C NMR spectra of TPA-PPA-3

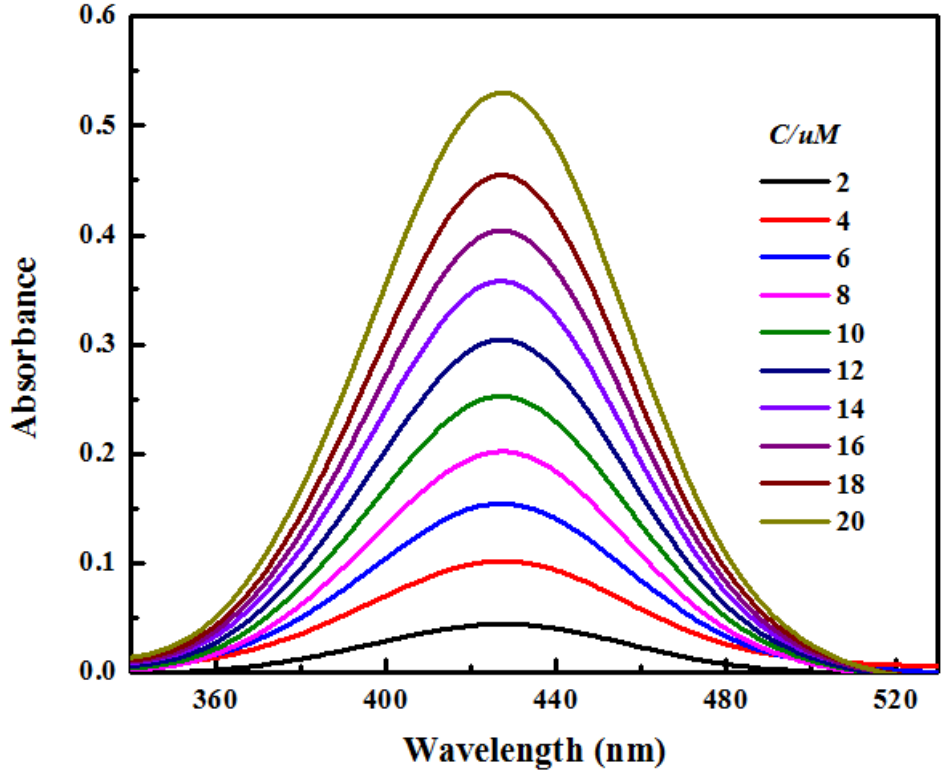


Figure S5 (a) Absorption spectra of TPA-PP at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

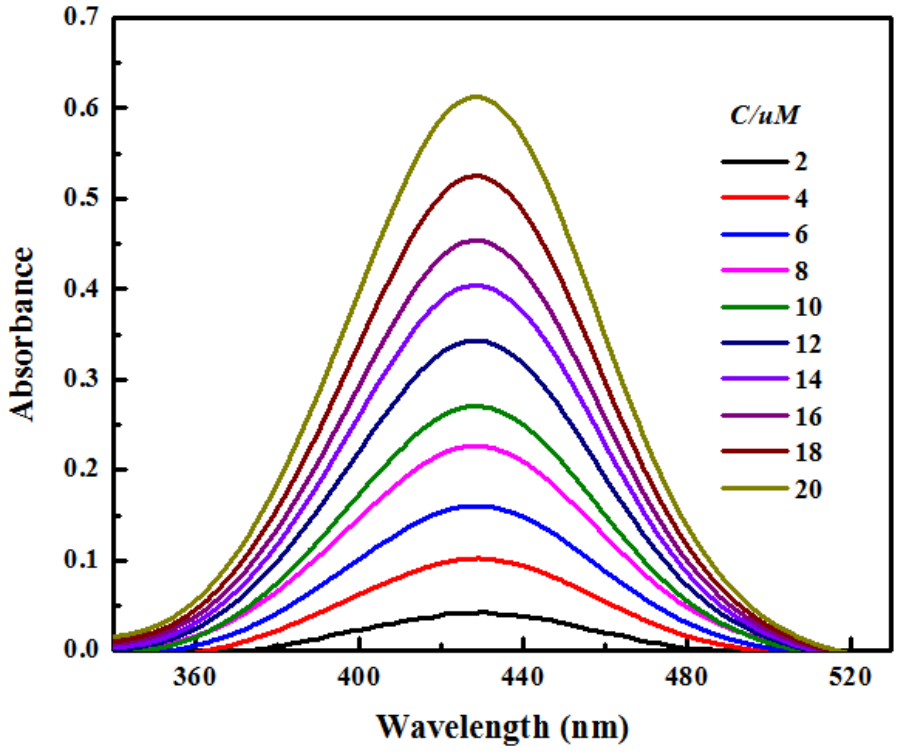


Figure S5 (b) Absorption spectra of TPA-PPA-1 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

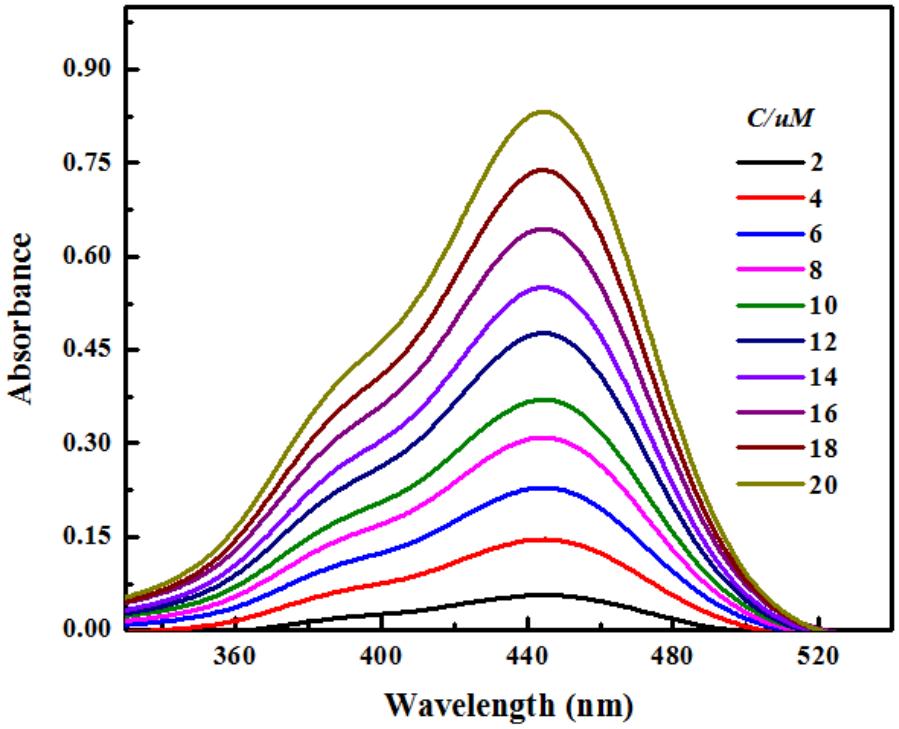


Figure S5 (c) Absorption spectra of TPA-PPA-2 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

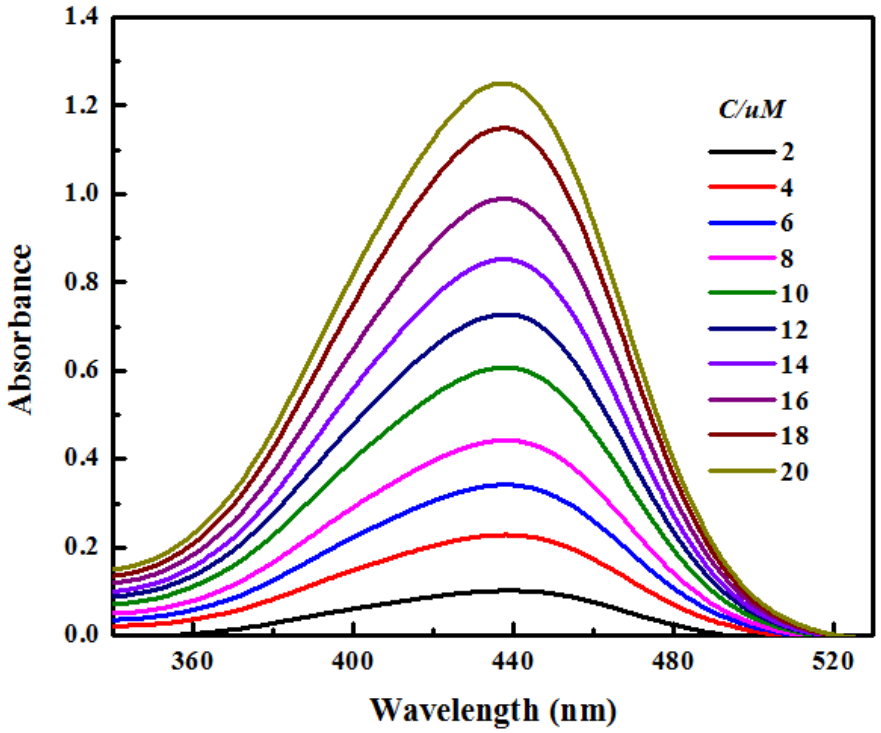


Figure S5 (d) Absorption spectra of TPA-PPA-3 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

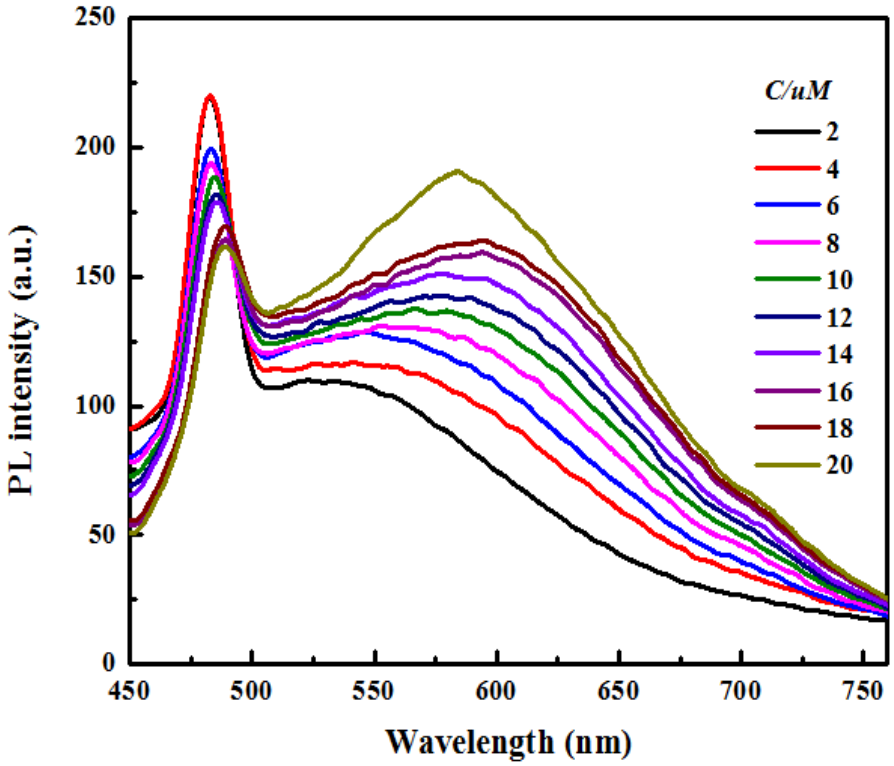


Figure S6 (a) Fluorescence spectra of TPA-PP at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

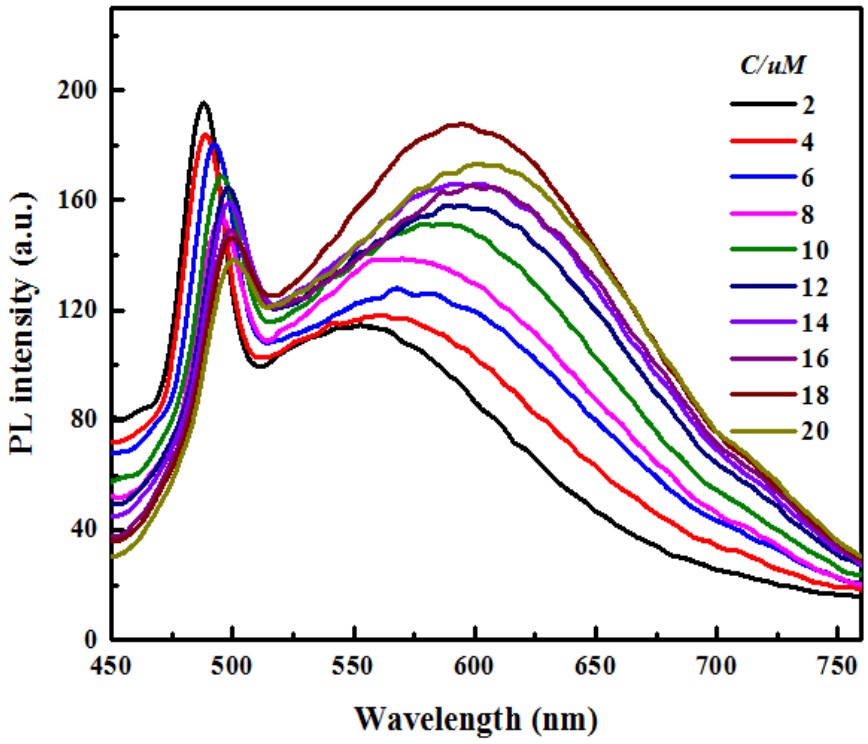


Figure S6 (b) Fluorescence spectra of TPA-PPA-1 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

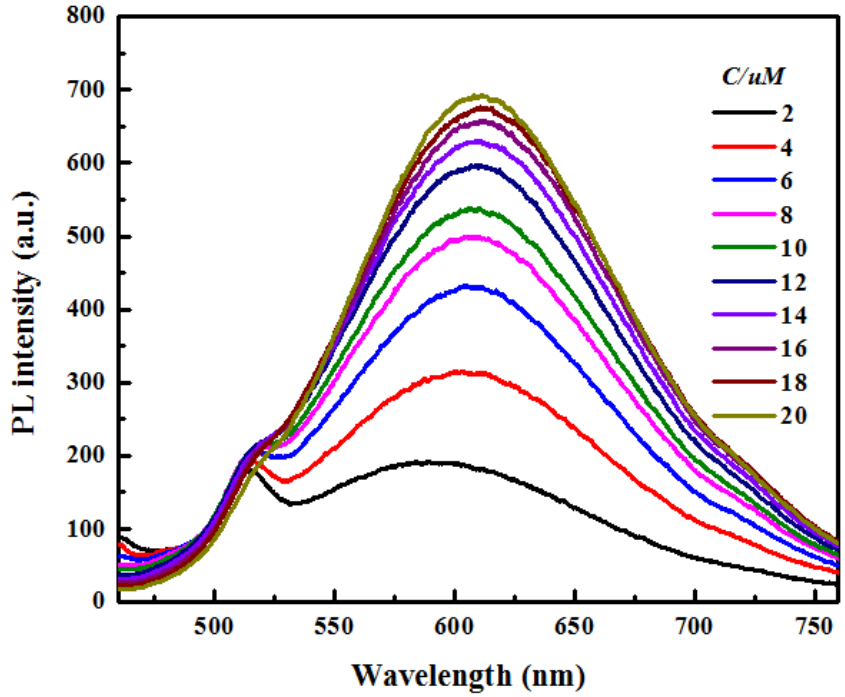


Figure S6 (c) Fluorescence spectra of TPA-PPA-2 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

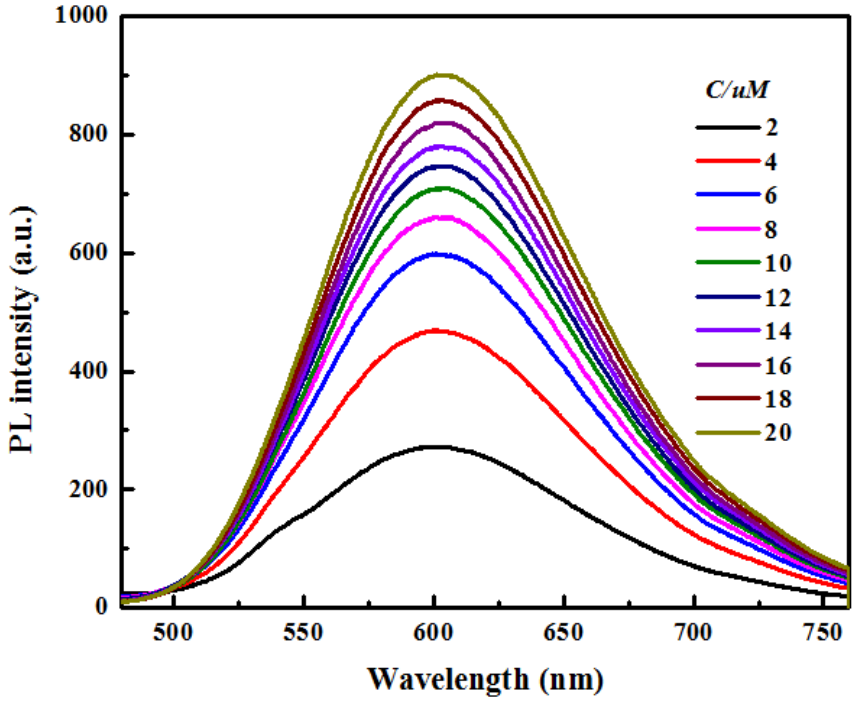


Figure S6 (d) Fluorescence spectra of TPA-PPA-3 at a range of 2-20 μM in aqueous solution containing 2 vol % DMSO.

Table S1 Fluorescence quantum yield of probes without ATP and the addition of ATP

	Without ATP			Addition of ATP		
	λ_{ex}	λ_{em}	Φ^b(%)	λ_{ex}	λ_{em}	Φ^c(%)
TPA-PP[a]	427	578	0.13	427	589	0.79
TPA-PPA-1[a]	432	591	0.16	432	594	1.72
TPA-PPA-2[a]	437	610	0.45	437	597	4.36
TPA-PPA-3[a]	451	618	0.89	451	601	26.43

[a]Conc. of TPA-PP, TPA-PPA-1, TPA-PPA-2and TPA-PPA-3：20 μM; [b]The fluorescence quantum yield without ATP; [c]The fluorescence quantum yieldwith ATP (ATP conc.: 200μM.)

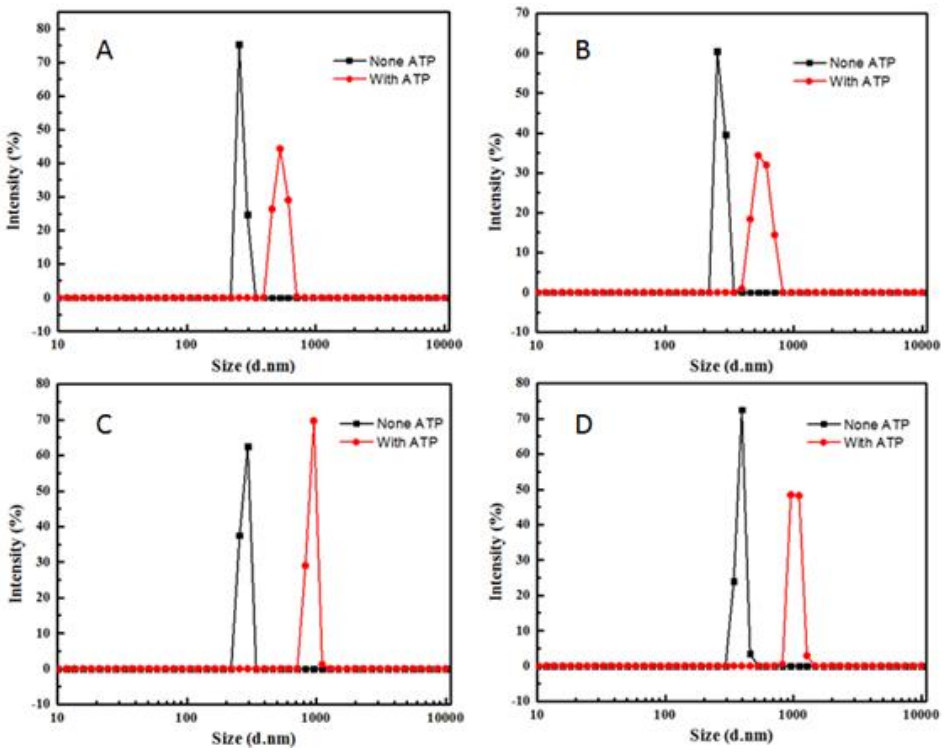


Figure S7 Particle size distributions of TPA-PP, TPA-PPA-1, TPA-PPA-2, TPA-PPA3 in aqueous solution containing 2 vol % DMSO and with the addition of ATP.

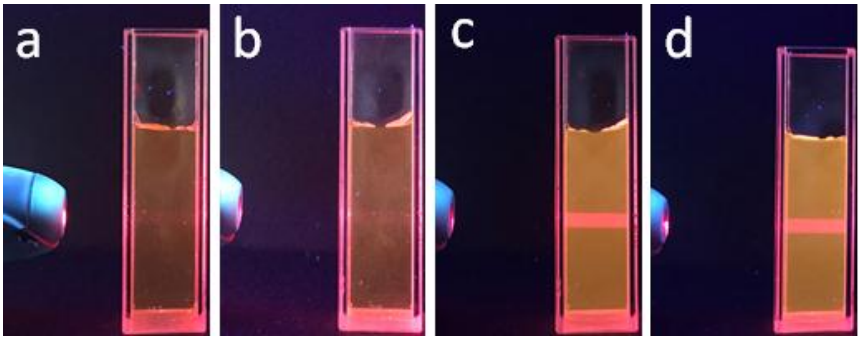


Figure S8 Tyndall effect of TPA-PPA-3 (a) in aqueous solution containing 2 vol % DMSO and (c) with the addition of ATP, (b), (d) is the corresponding photographs after two weeks.

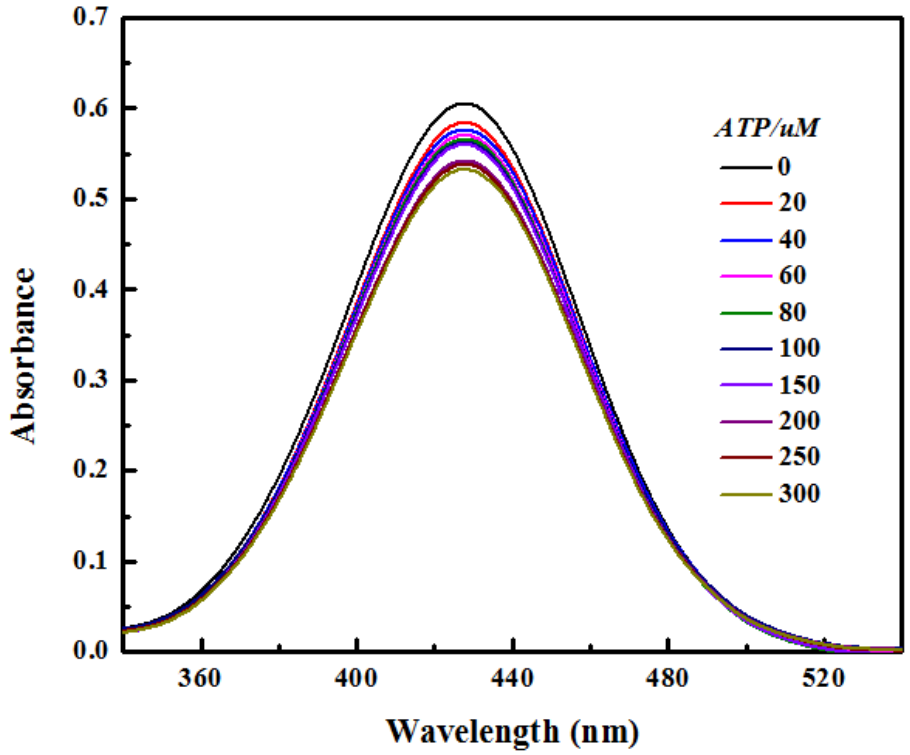


Figure S9 (a) Absorption spectra of TPA-PP upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PP concentration: 20 μM.

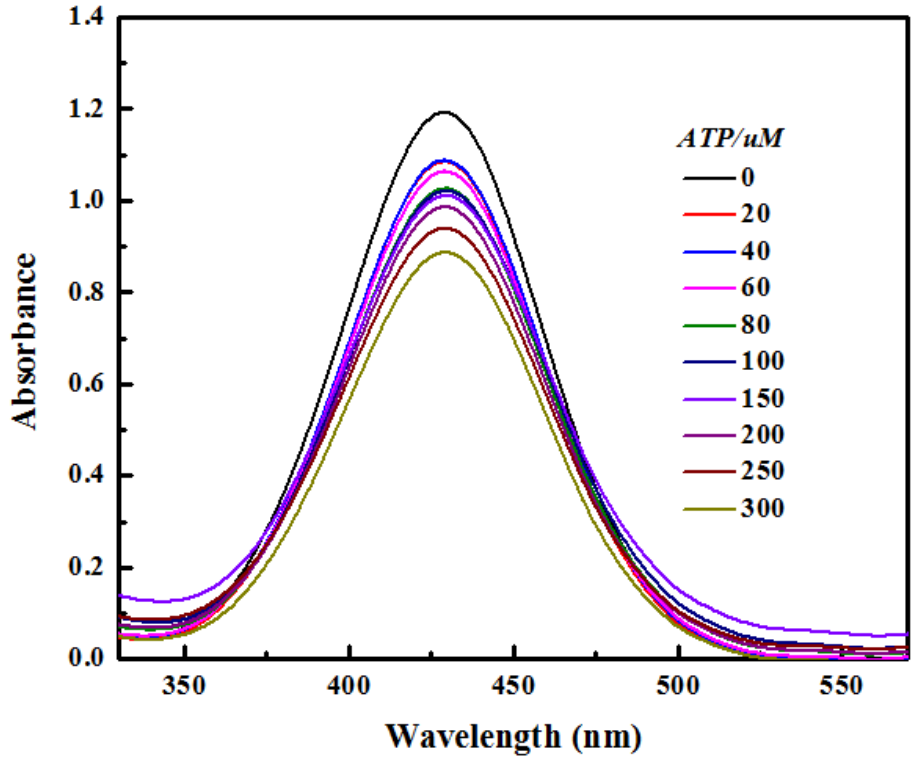


Figure S9 (b) Absorption spectra of TPA-PPA-1 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-1 concentration: 20 μM.

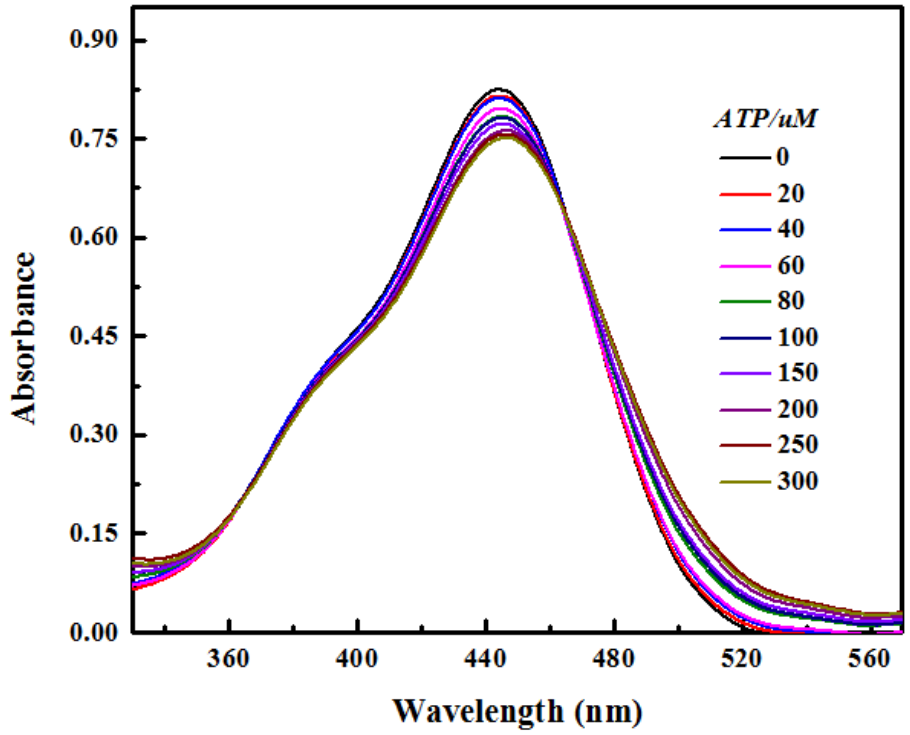


Figure S9 (c) Absorption spectra of TPA-PPA-2 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-2 concentration: 20 μM.

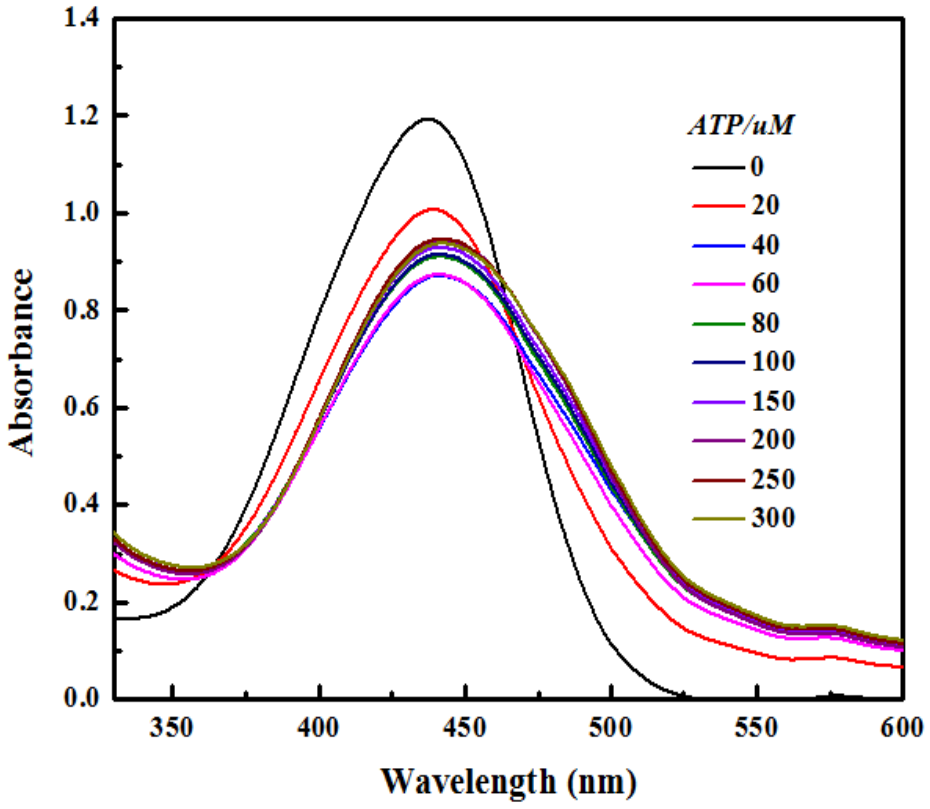


Figure S9 (d) Absorption spectra of TPA-PPA-3 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-3 concentration: 20 μM.

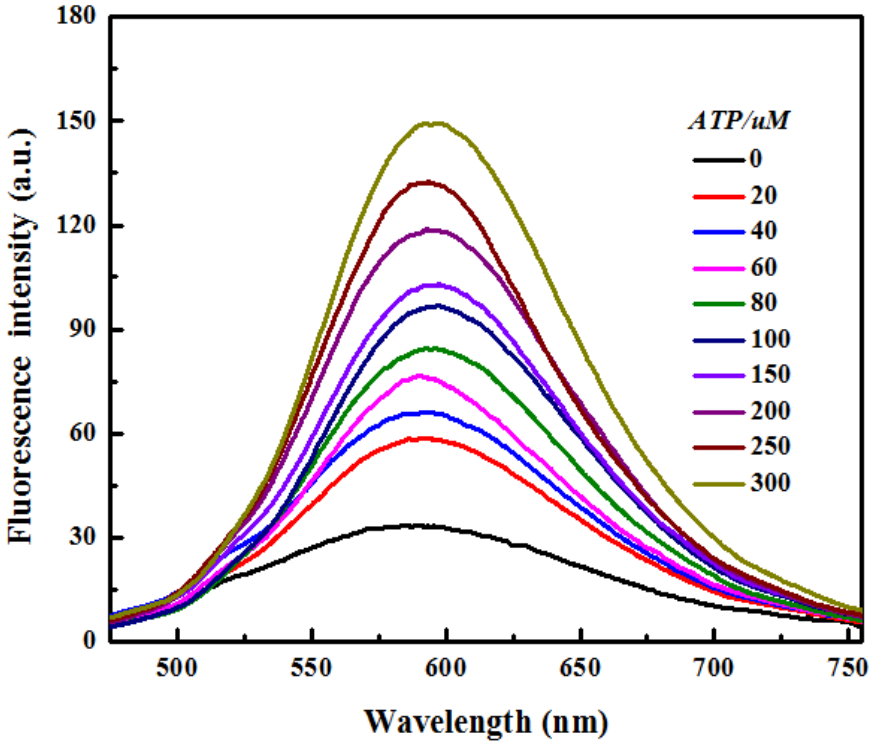


Figure S10 (a) Fluorescence spectra of TPA-PP upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PP concentration: 20 μM.

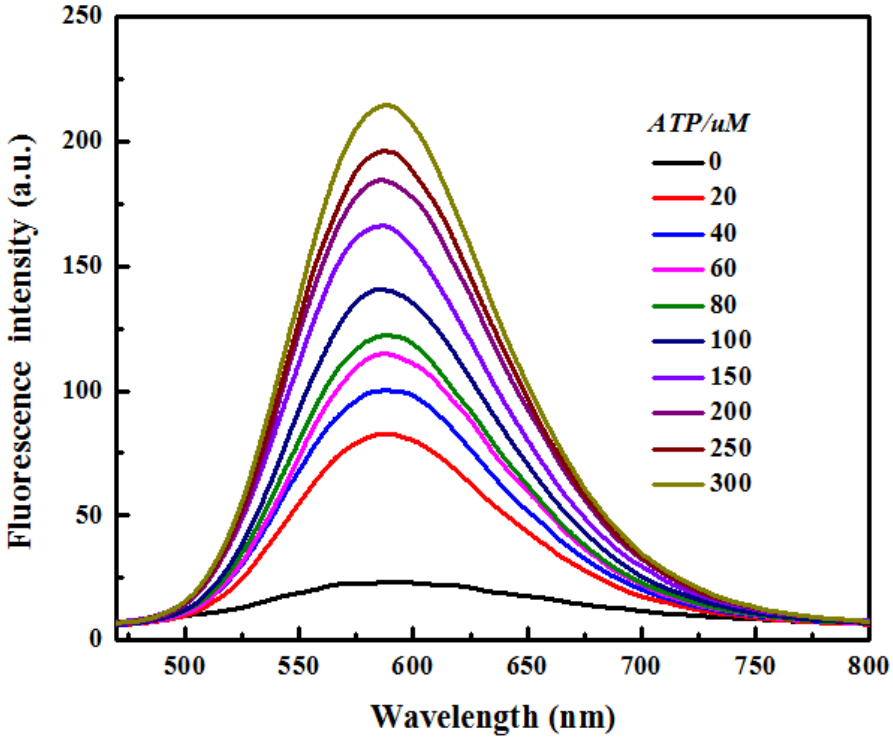


Figure S10 (b) Fluorescence spectra of TPA-PPA-1 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-1concentration: 20 μM.

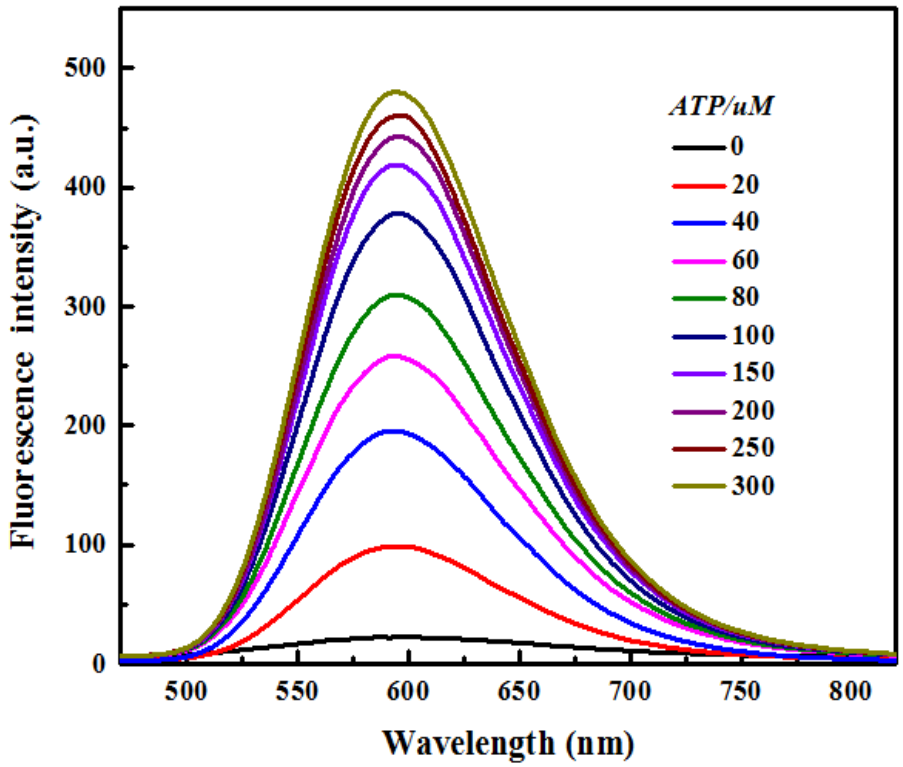


Figure S10 (c) Fluorescence spectra of TPA-PPA-2 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-2 concentration: 20 μM.

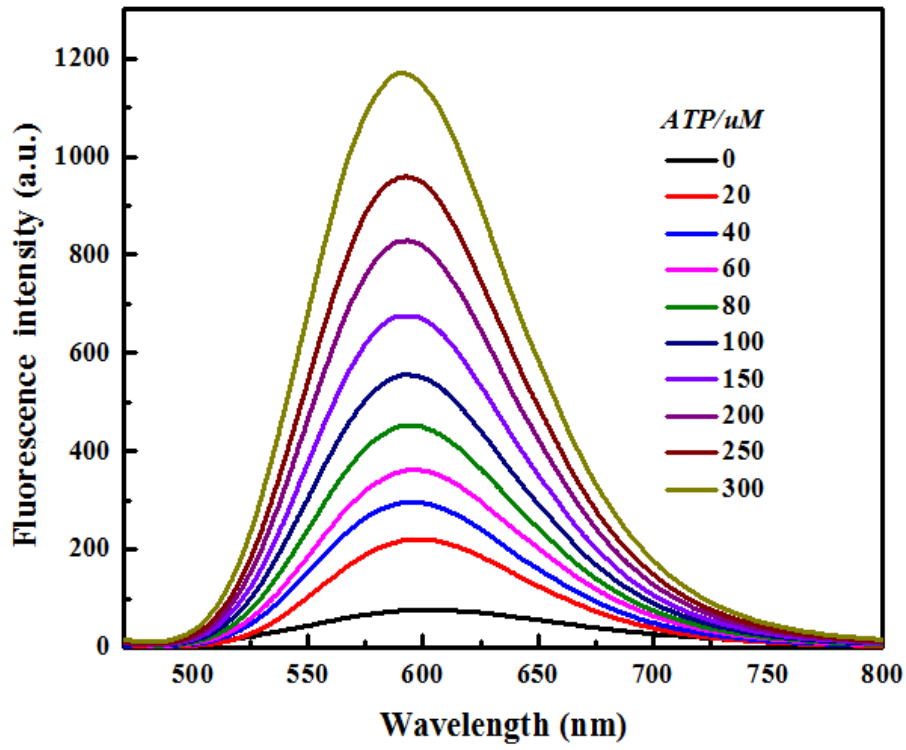


Figure S10 (d) Fluorescence spectra of TPA-PPA-3 upon the addition of ATP in aqueous solution containing 2 vol % DMSO. TPA-PPA-3 concentration: 20 μM.

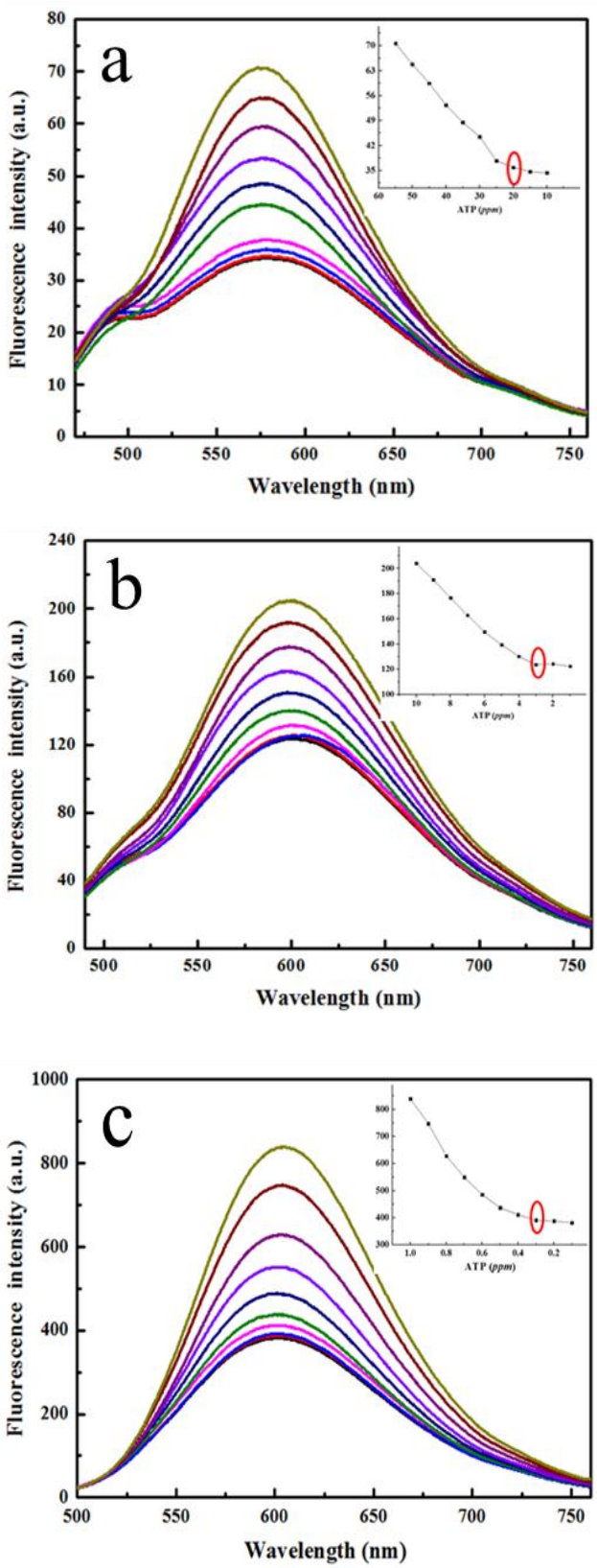


Figure S11 Fluorescence spectras of (a) TPA-PPA-1(λ_{ex} = 432 nm), (b) TPA-PPA-2 (λ_{ex} = 437 nm), (c) TPA-PPA-3(λ_{ex} = 451 nm) upon the addition of ATP in dilute solvents.

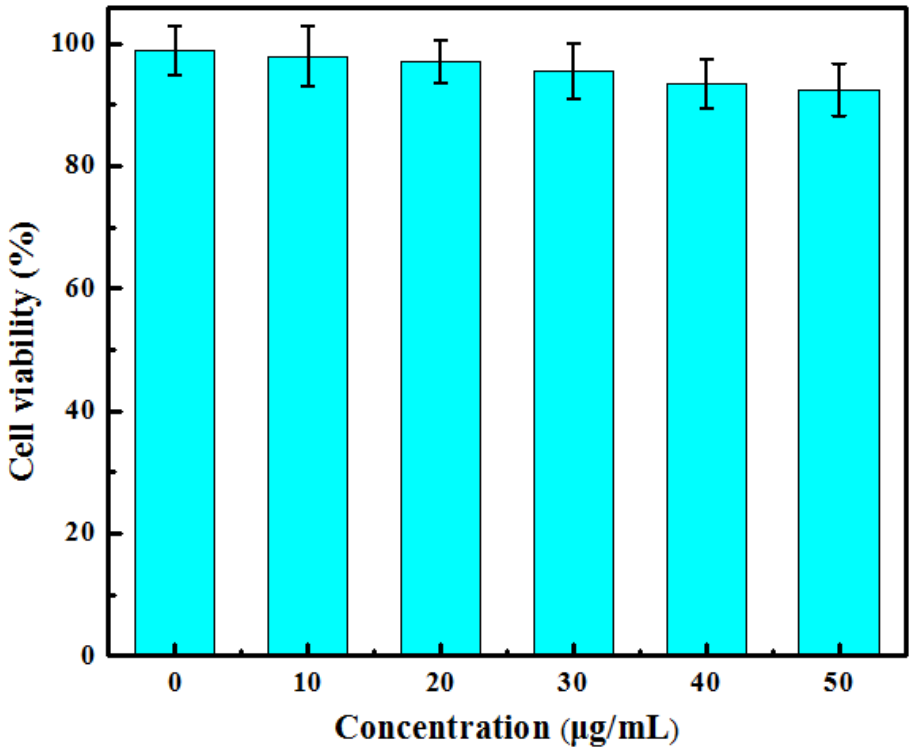


Figure S12 (a) Cell viabilities of HepG-2 cells treated with different concentrations of TPA-PP for 96 h by MTT assay

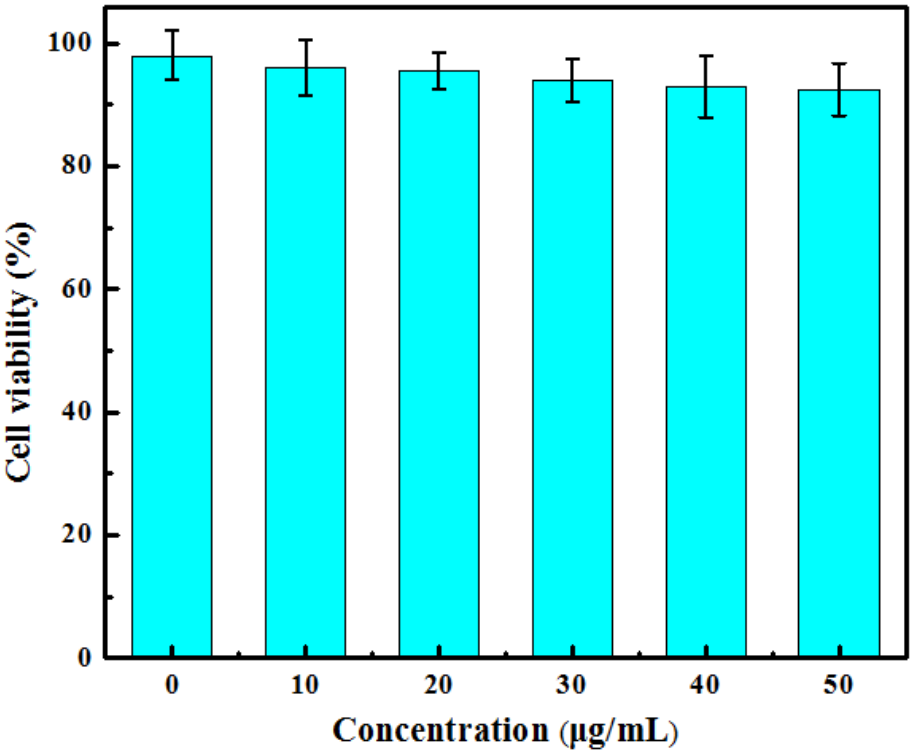


Figure S12 (b) Cell viabilities of HepG-2 cells treated with different concentrations of TPA-PPA-1 for 96 h by MTT assay

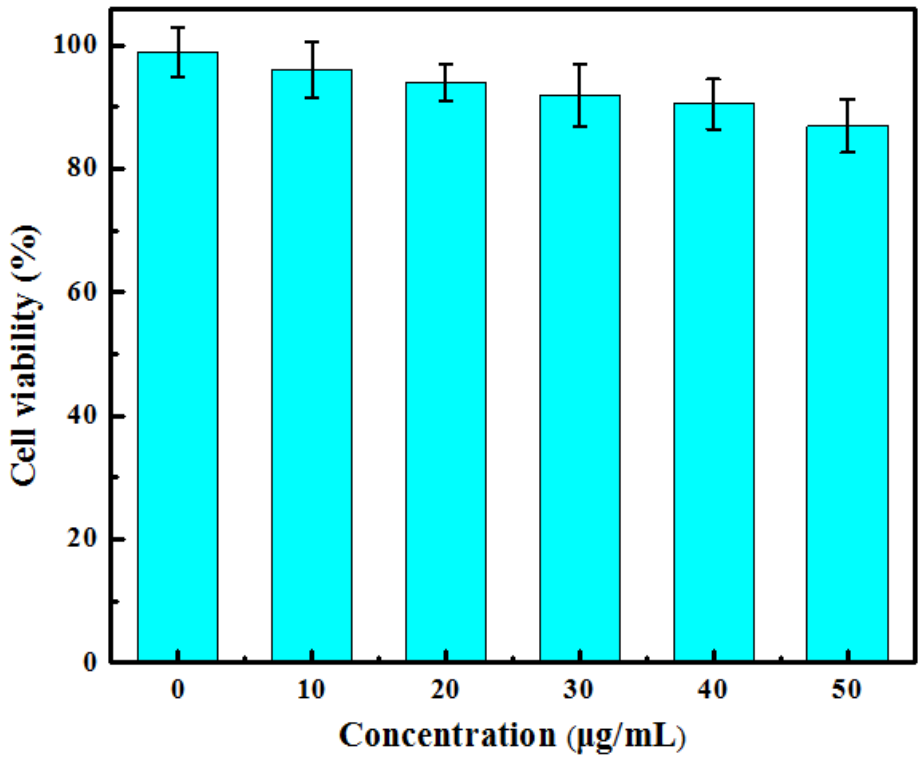


Figure S12 (c) Cell viabilities of HepG-2 cells treated with different concentrations of TPA-PPA-2 for 96 h by MTT assay

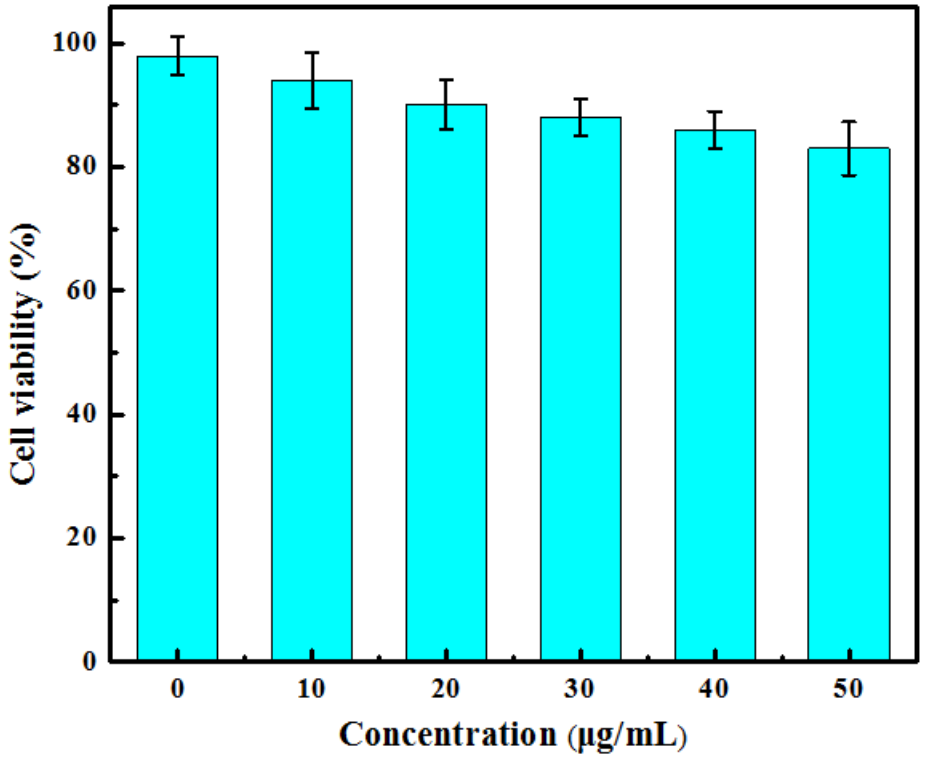


Figure S12 (d) Cell viabilities of HepG-2 cells treated with different concentrations of TPA-PPA-3 for 96 h by MTT assay

Notes and references

1 Miyaura, N.; Suzuki, A. Palladium-catalyzed cross-coupling reactions of organoboron compounds. Chem. Rev., **1995**, 95, 2457-2483.

2 Xu, Z.; Singh, N. J.; Lim, J.; Pan, J.; Kim, H. N.; Park, S.; Yoon, J. Unique sandwich stacking of pyrene-adenine-pyrene for selective and ratiometric fluorescent sensing of ATP at physiological pH. *J. Am. Chem. Soc.*, **2009**, 131, 15528-15533.

3 McIlroy, S. P.; Cló, E.; Nikolajsen, L.; Frederiksen, P. K.; Nielsen, C. B.; Mikkelsen, K. V.; Ogilby, P. R. Two-Photon Photosensitized Production of Singlet Oxygen: Sensitizers with Phenylene− Ethynylene-Based Chromophores, *J. Org. Chem.*, **2005**, 70, 1134-1146.