Electronic Supplementary Material (ESI) for RSC Advances.

Concentration dependent ratiometric turn-on selective fluorescence detection of picric acid in aqueous and non-aqueous media

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Table S1: Crystal data table

Compound	**TAQP.3H_2O**
Chemical formula	C27 H27 N6 O4 P
Formula weight	530.52
Temperature	100(2)K
Crystal system	Hexagoanal
Space group	P-3
a (Å); α (°)	16.08(2); 90°
b (Å); β(°)	16.08(2); 90°
c (Å); γ (°)	6.269(8); 120°
V ($Å^3$); Z	1404(3); 2
ρ (calc.) mg m^{-3}	1.255
μ(Mo K_α) mm^{-1}	0.140
$2\theta_{max}$ (°)	56
R(int)	0.1479
Completeness to θ	95.6 %
Data / param.	2194 / 121
GOF	1.082
R1 [F>4σ(F)]	0.0863
wR2 (all data)	0.2874
max. peak/hole (e.$Å^{-3}$)	0.733/ -0.432

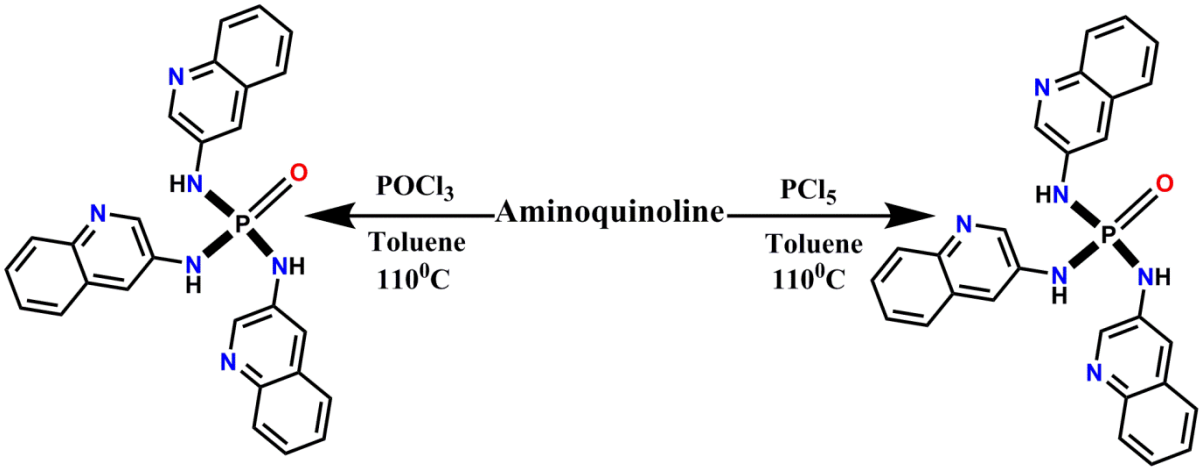
Table S2: Selected bond-lengths and angles for TAQP.3H_2O

Compound	**Bond length**		**Bond angle**	
TAQP	P(1)-O(1)	1.504(5)	O(1)-P(1)-N(1)#1	112.56(12)
	P(1)-N(1)#1	1.658(4)	O(1)-P(1)-N(1)#2	112.56(12)
	P(1)-N(1)#2	1.658(4)	N(1)#1-P(1)-N(1)#2	106.22(14)
	P(1)-N(1)	1.658(4)	O(1)-P(1)-N(1)	112.56(12)
			N(1)#1-P(1)-N(1)	106.22(14)
			N(1)#2-P(1)-N(1)	106.22(14)

Table S3: H-bonding table for TAQP.3H_2O

Compound	**D-H...A**	**d(H...A)Å**	**d(D...A)Å**	**<(DHA)°**
TAQP	N(1)-H(1)...O(1S)#3	0.88	2.876(5)	154.5
	O(1S)-H(1S)...N(13)#4	0.88(4)	2.938(5)	177(6)
	O(1S)-H(2S)...O(1)	0.88(4)	2.887(5)	167(6)
	#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -x+y+1,-x+1,z-1			
	#4 y,-x+y,-z+1			

Scheme S1:



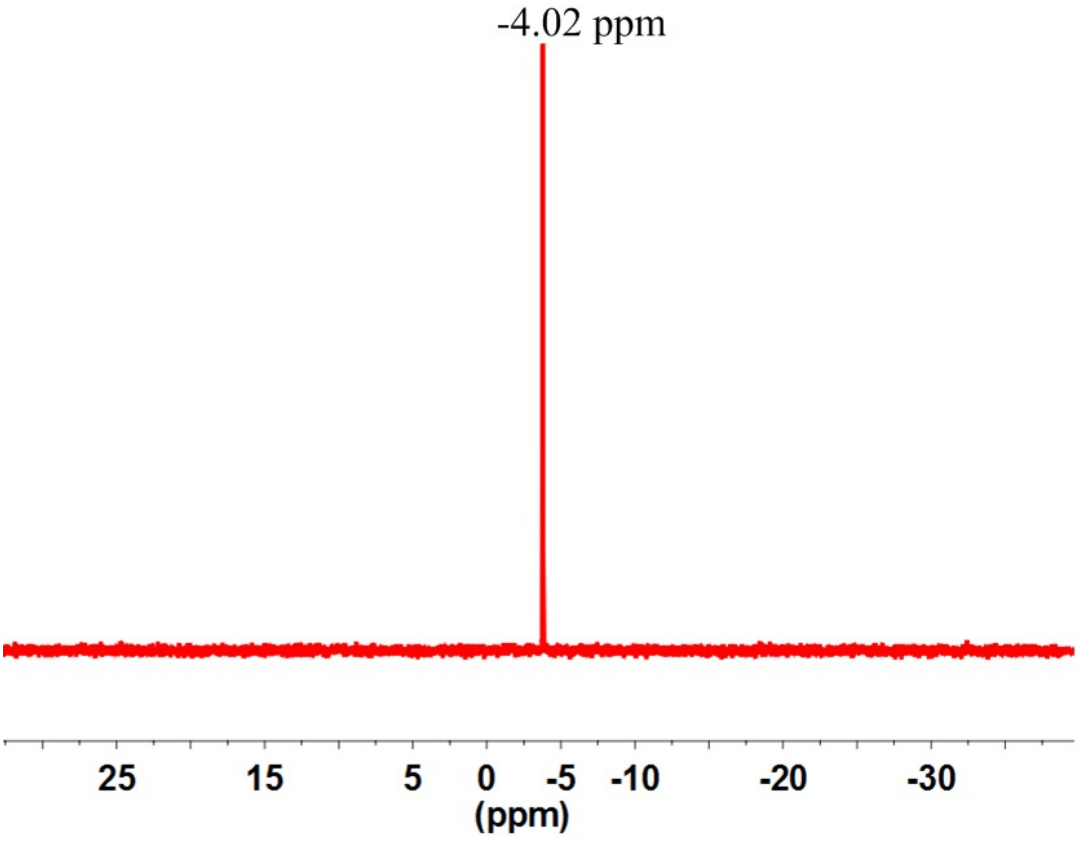


Fig. S1: ^{31}P-NMR of TAQP in DMSO-d_6

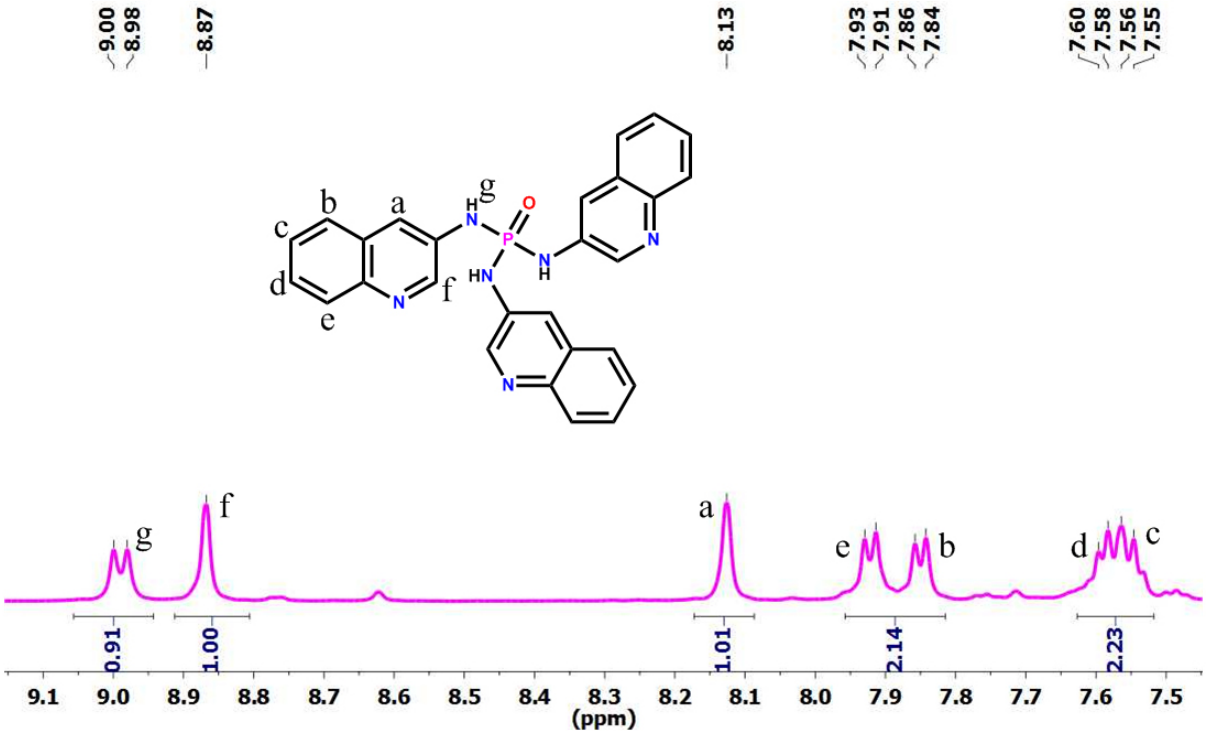


Fig. S2: ^{1}H-NMR of TAQP in DMSO-d_6

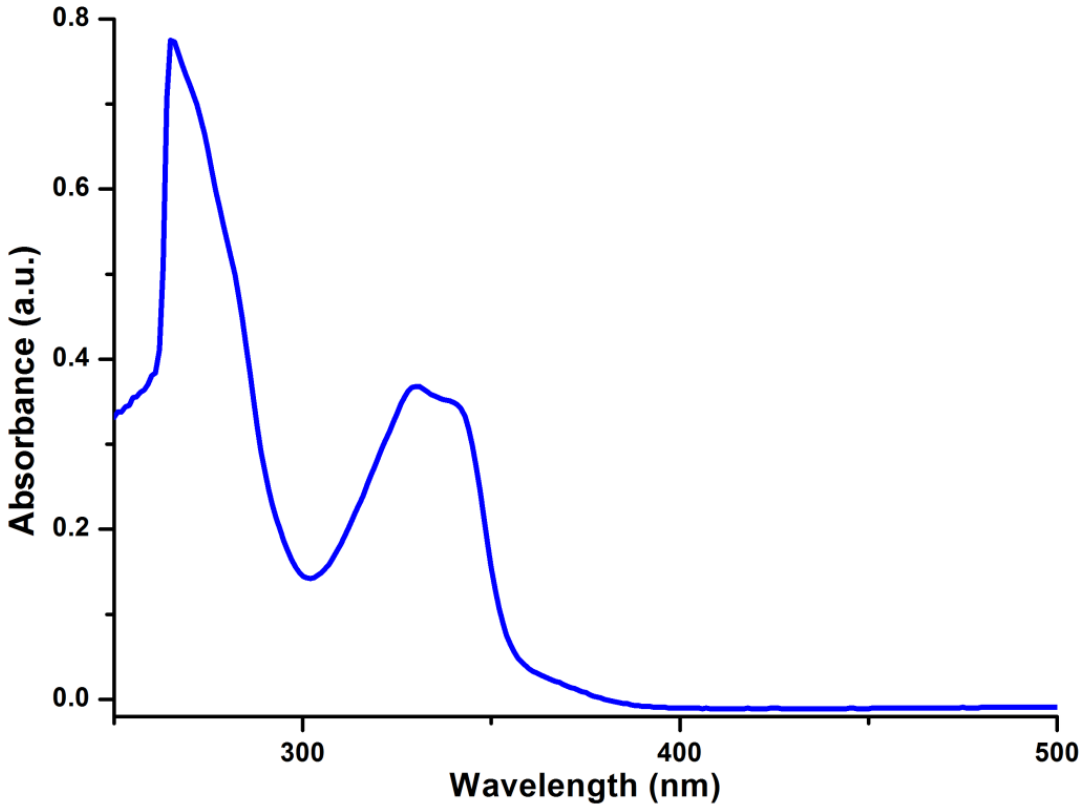


Fig. S3: Absorbance spectra of TAQP in DMF.

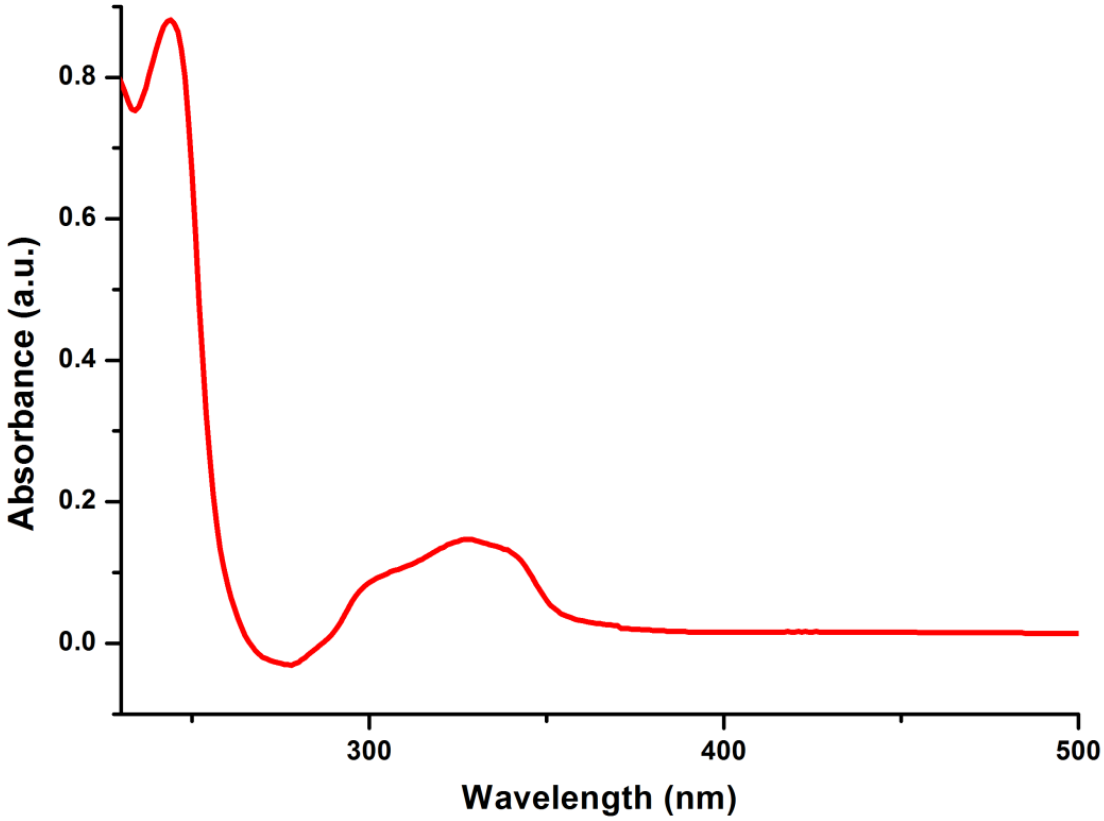


Fig. S4: Absorbance spectra of TAQP in MeOH.

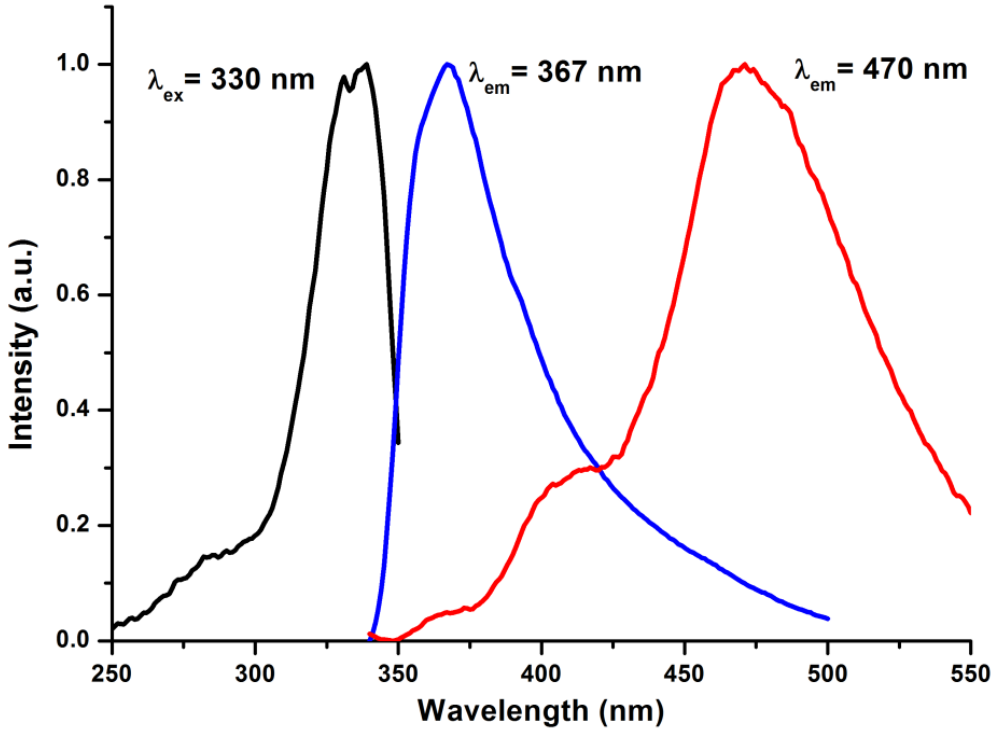


Fig. S5: Excitation and emission Spectra of TAQP in DMF: excitation spectra (black), emission at $1x10^{-3}$M concentration (blue) and emission at higher concentration $1x10^{-3}$M (red).

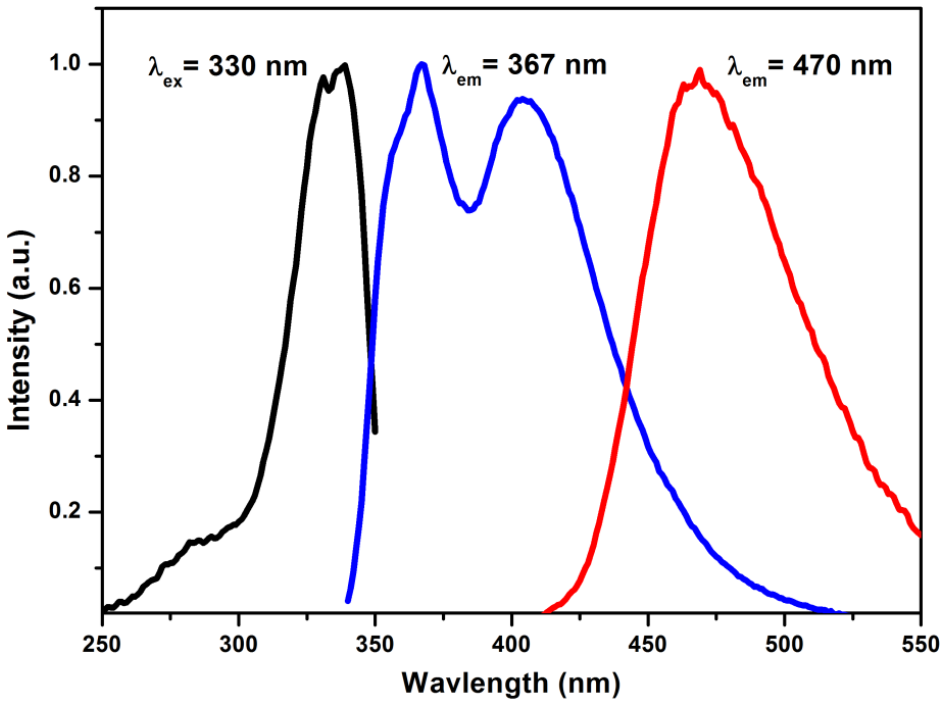


Fig. S6: Excitation and emission Spectra of TAQP in MeOH: excitation spectra (black), emission at $1x10^{-5}$M concentration (blue) and emission at higher concentration $1x10^{-3}$M (red).

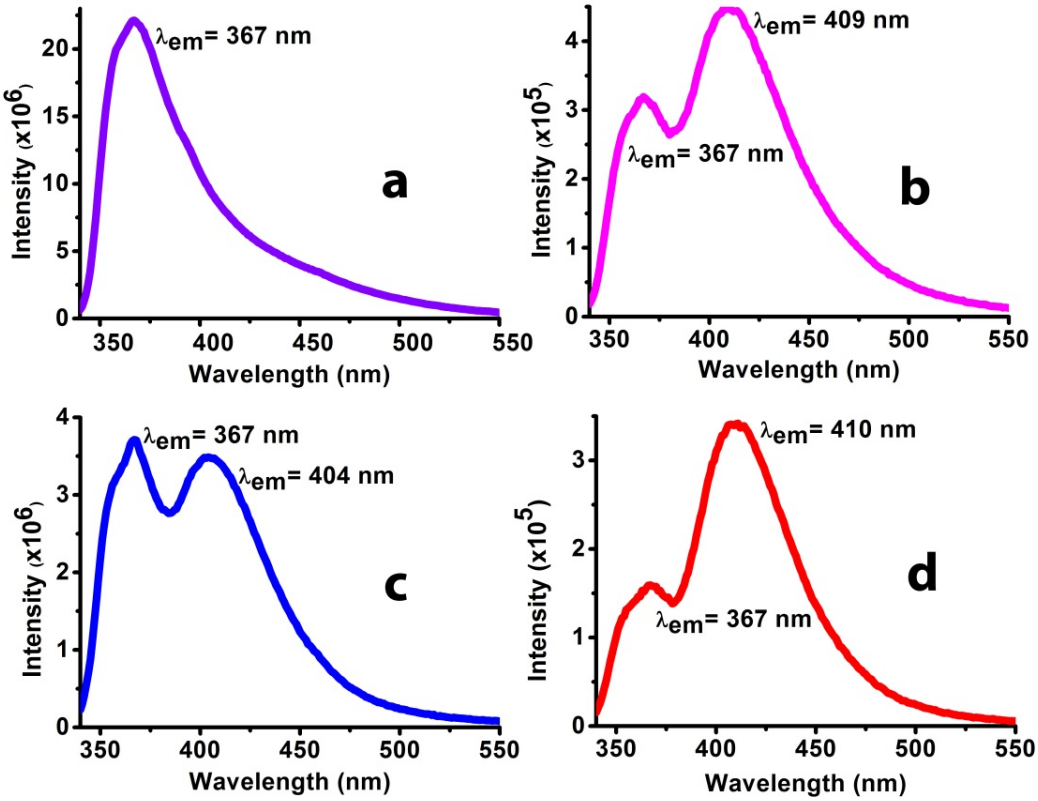


Fig. S7: Emission Spectra of TAQP in various solvents at $1x10^{-5}$M concentration: DMF (green), DMF/H_2O (pink), MeOH (blue) and MeOH/H_2O (red).

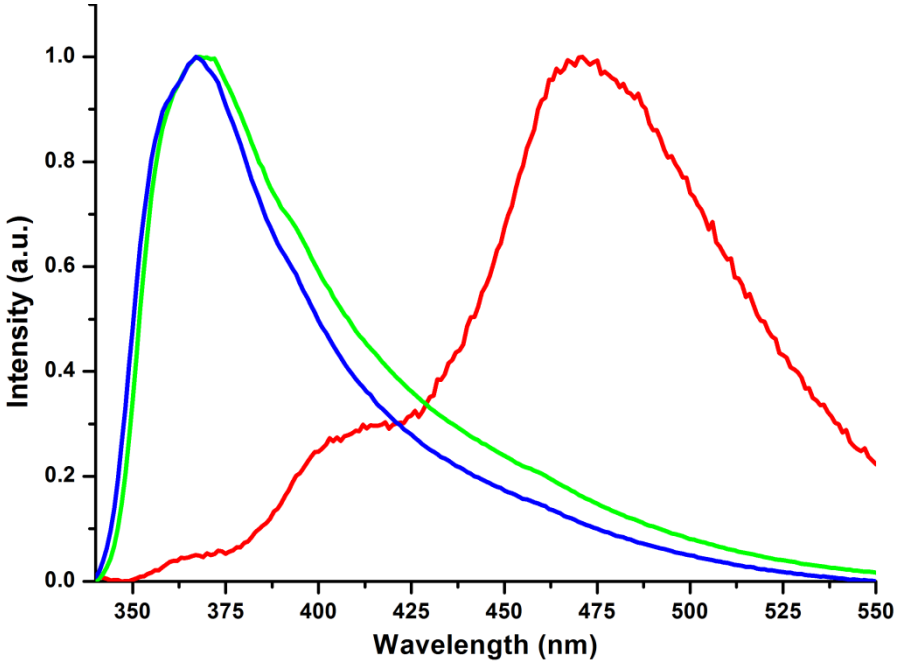


Fig. S8: Emission spectra of TAQP in DMF at different concentration: $1x10^{-3}$M (red), $1x10^{-4}$M (green), $1x10^{-5}$M (blue).

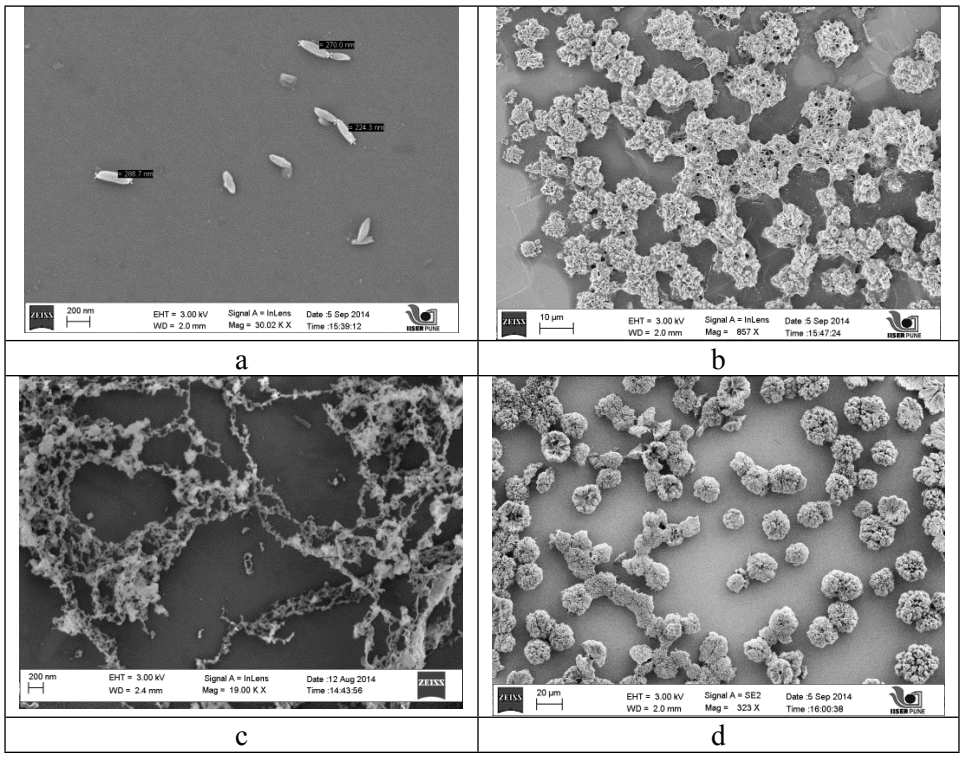


Fig. S9: FESEM images of $1x10^{-5}$M solution of TAQP in DMF (a), DMF/H_2O (b), MeOH (c) and MeOH/H_2O (d).

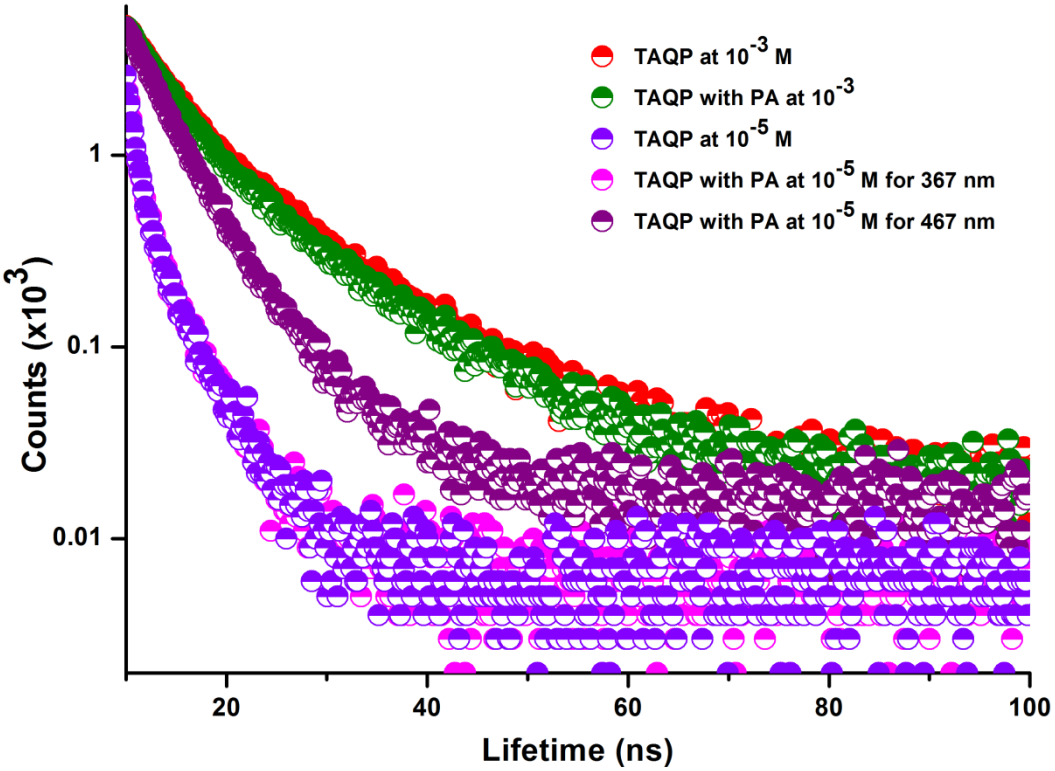


Fig. S10: Fluorescence Lifetime spectra of various samples of TAQP.

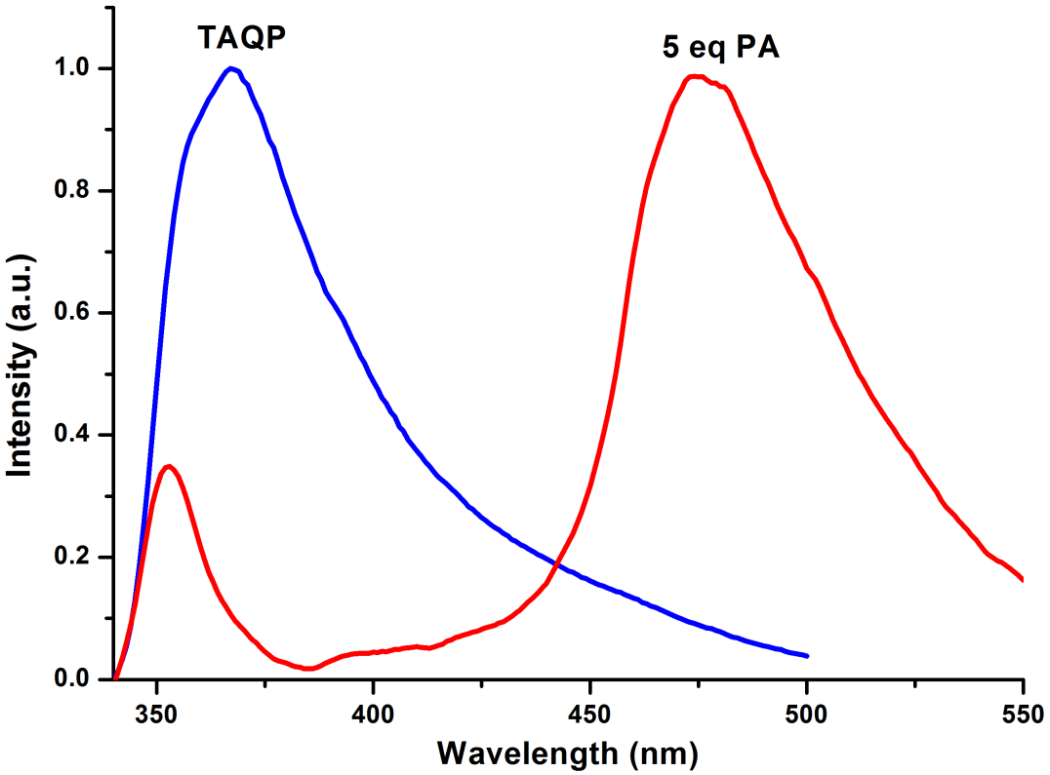


Fig. S11: Emission spectra of TAQP ($1x10^{-5}$M) before (blue) and after (red) the addition of 5 eq PA ($1x10^{-3}$M) in DMF.

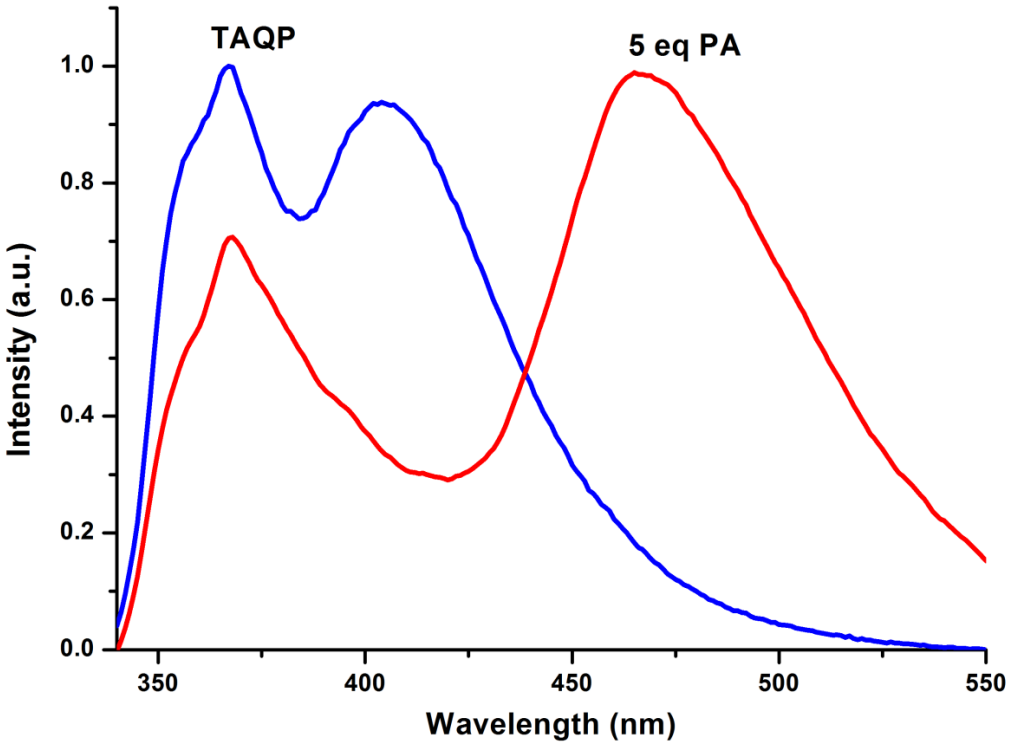


Fig. S12: Emission spectra of TAQP ($1x10^{-5}$M) before (blue) and after (red) the addition of 5 eq PA ($1x10^{-3}$M) in MeOH.

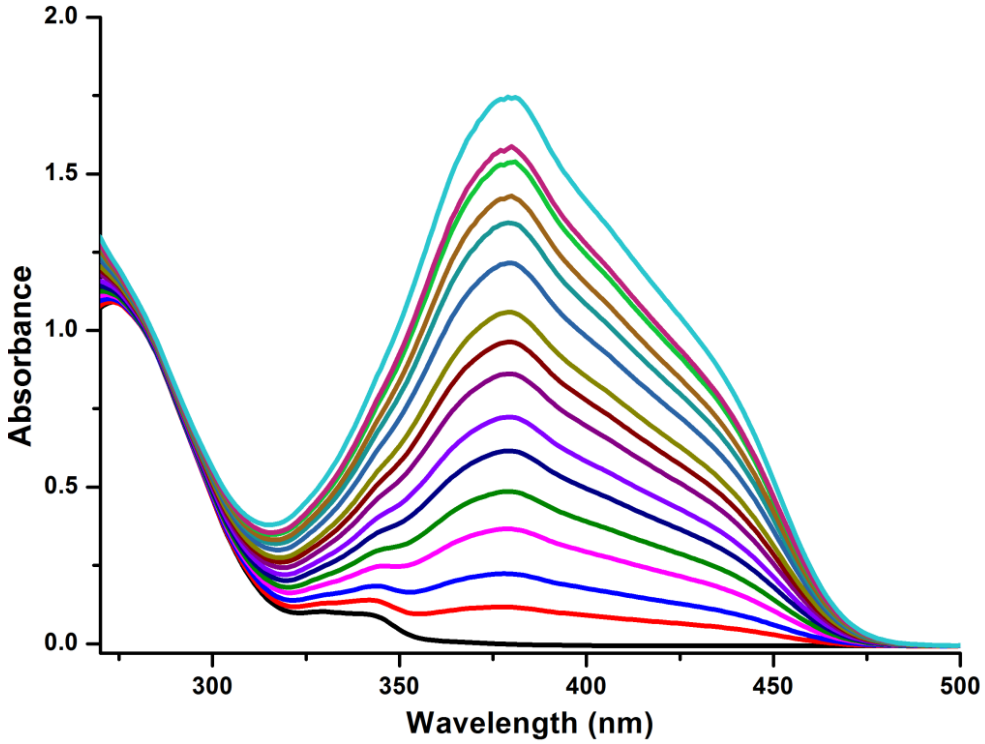


Fig. S13: Absorbance spectra of TAQP ($1x10^{-5}$M) in DMF with PA ($1x10^{-3}$M)

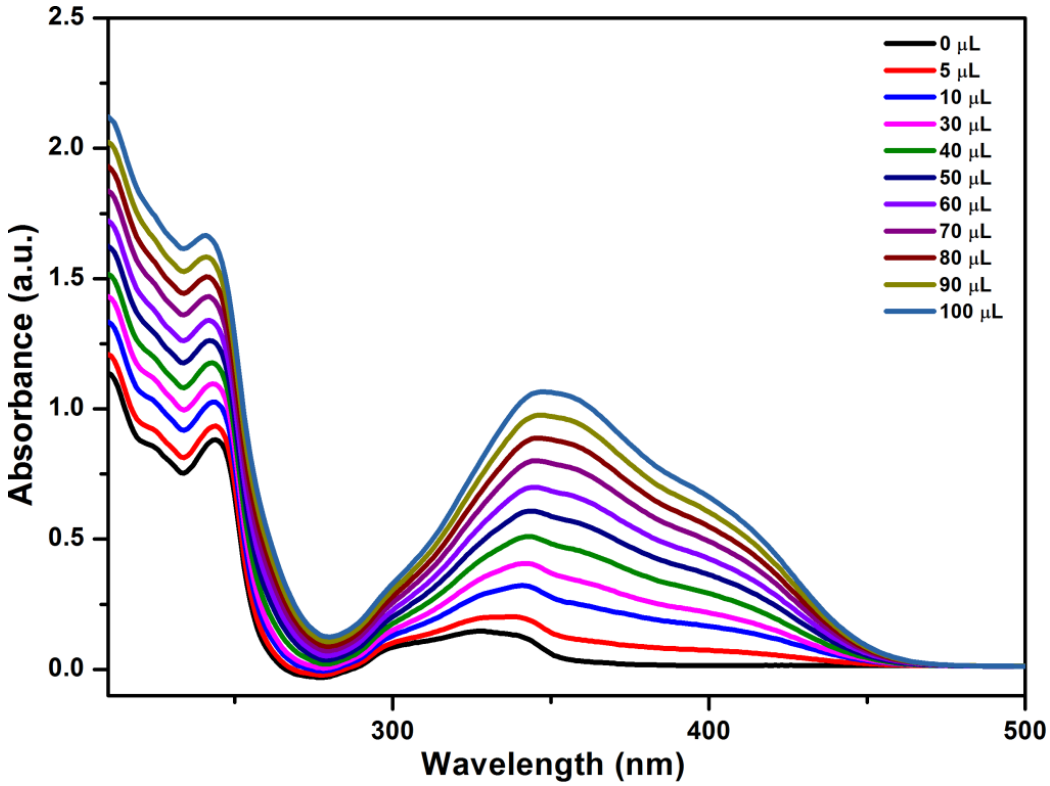


Fig. S14: Absorbance spectra of TAQP (1x10^{-5}M) in MeOH with PA (1x10^{-3}M)

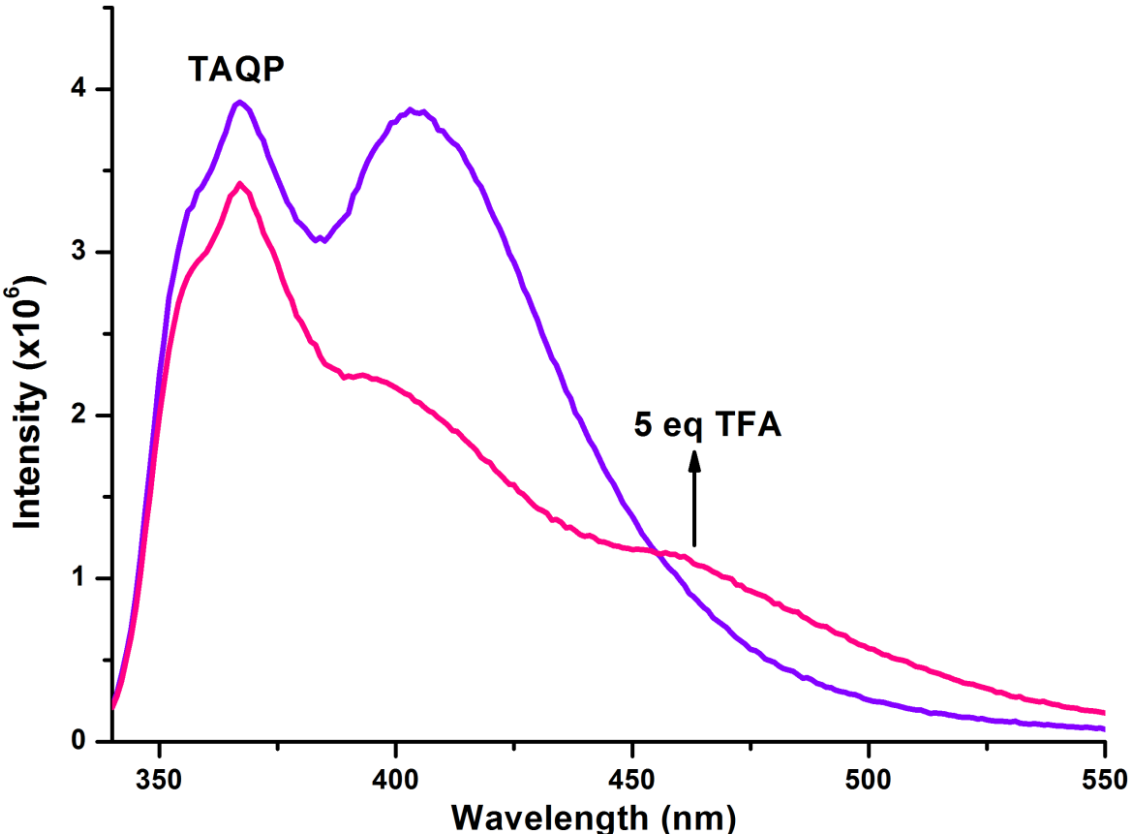


Fig. S15: Emission spectra of TAQP (1x10^{-5}M) before (purple) and after (red) the addition of TFA (1x10^{-3}M) in MeOH.

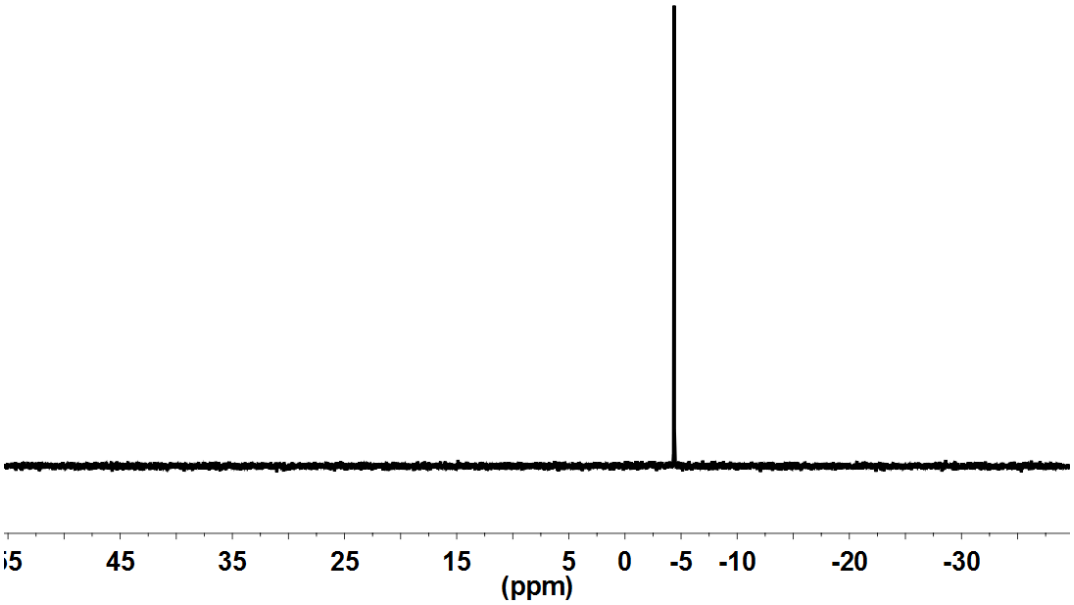


Fig. S16: ^{31}P-NMR of TAQP + 5 eq PA in DMSO-d_6.

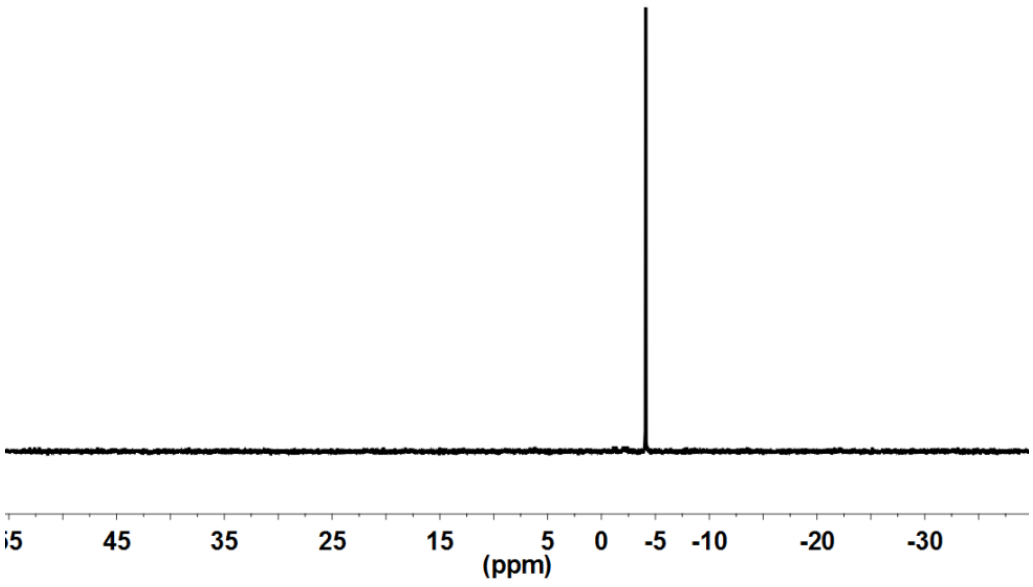


Fig. S17: ^{31}P-NMR of TAQP + 10 eq TFA in DMSO-d_6

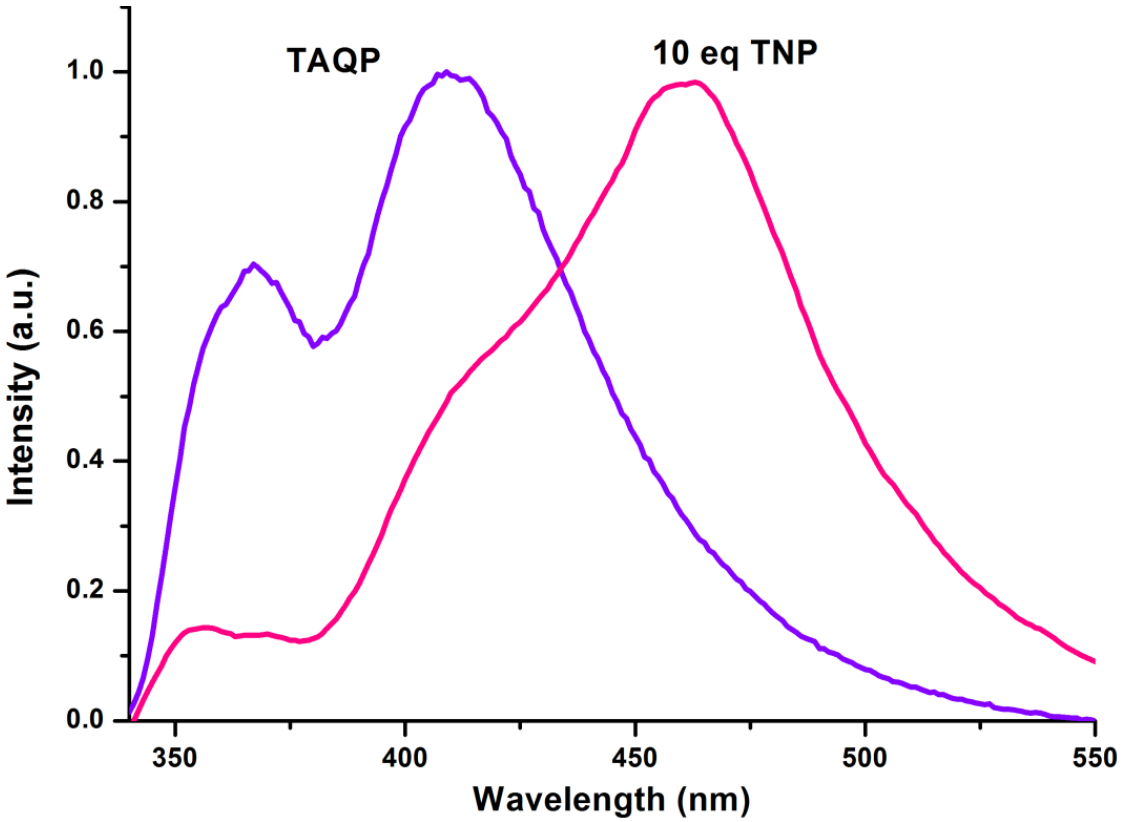


Fig. S18: Emission spectra of TAQP ($1x10^{-5}$M) before (purple) and after (red) the addition of 10 eq PA ($1x10^{-3}$M) in DMF:H_2O (6:4).

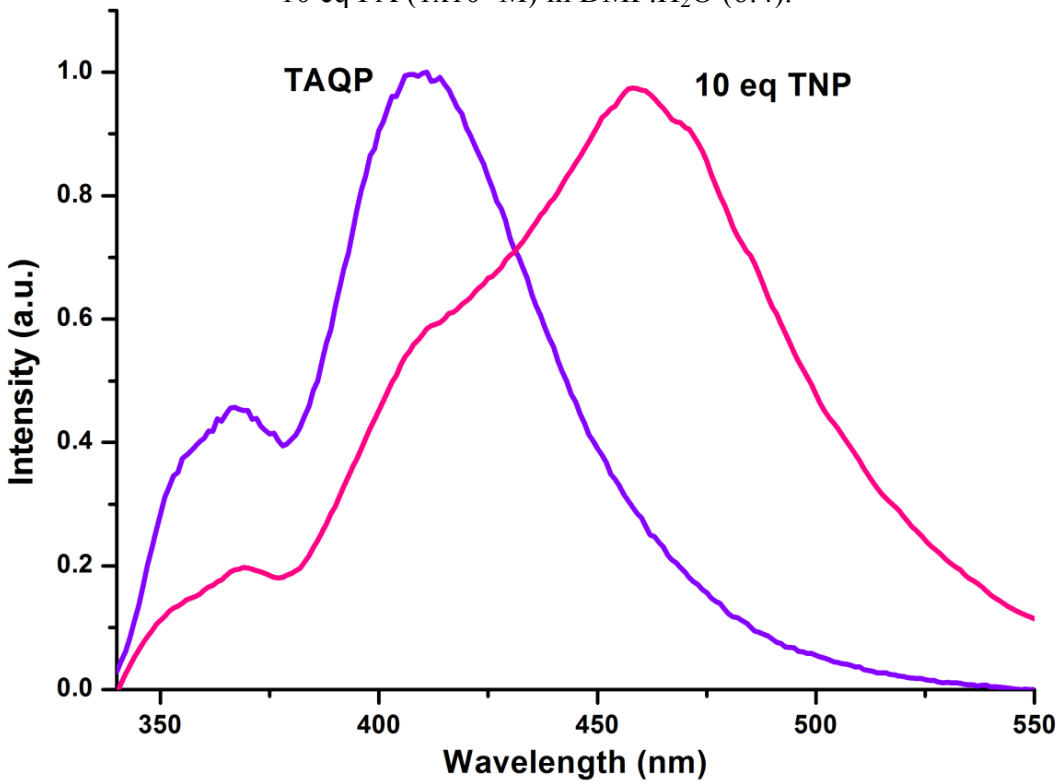


Fig. S19: Emission spectra of TAQP ($1x10^{-5}$M) before (purple) and after (red) the addition of 10 eq PA ($1x10^{-3}$M) in MeOH:H_2O (6:4).

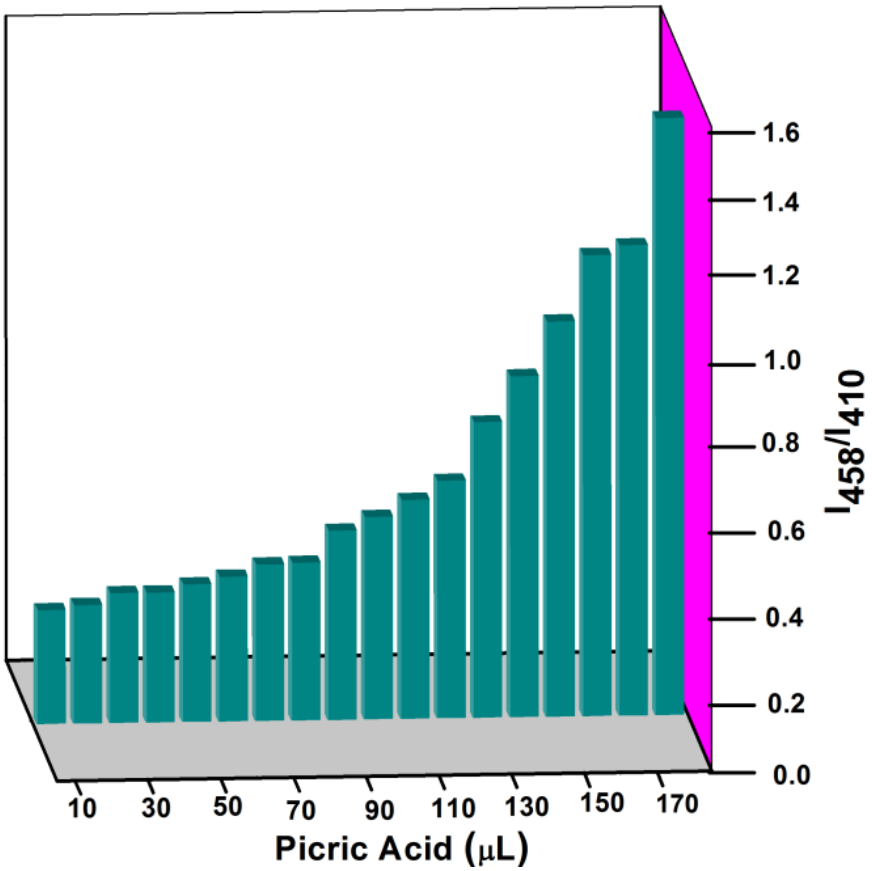


Fig. S20: Relative changes of fluorescent intensity (I_{458}/I_{410}) of TAQP ($1x10^{-5}$M) for PA in MeOH/H_2O or DMF/H_2O.

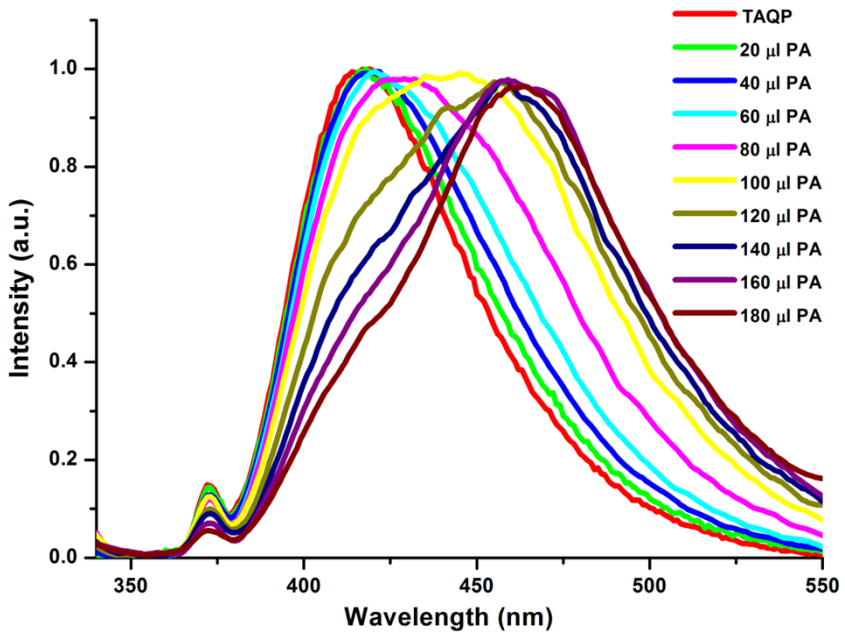


Fig. S21: Emission spectral titration of TAQP ($1x10^{-5}$M) with PA ($1x10^{-3}$M) in H_2O.

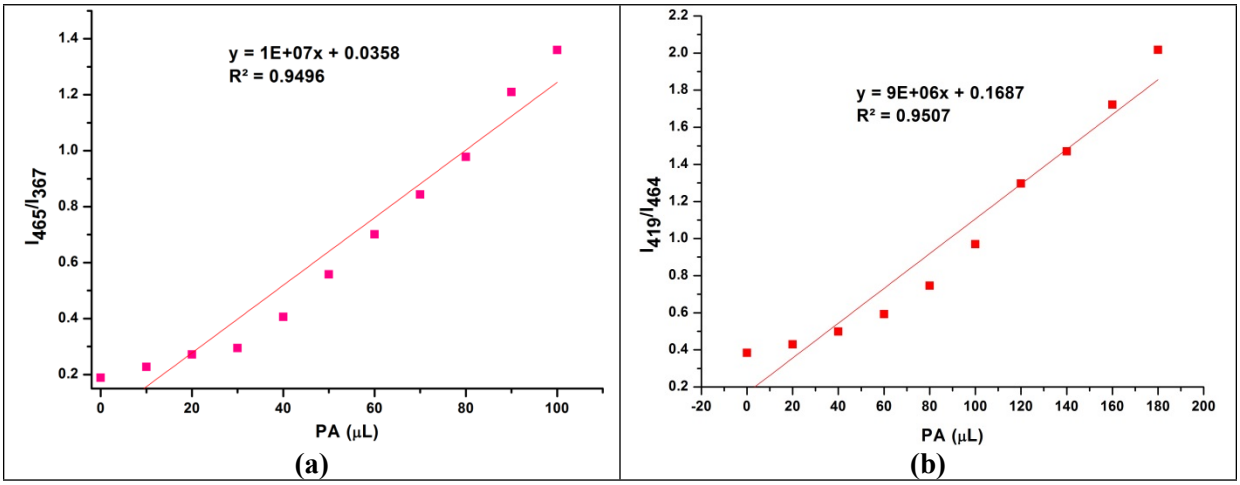


Fig. S22: Plot of luminescence ratios of TAQP (1x10^{-5}M) vs the concentration of PA in (a) DMF/H_2O mixture and (b) neat H_2O suspension. The slope of the fitted line is used for calculating the PA detection limit of TAQP.

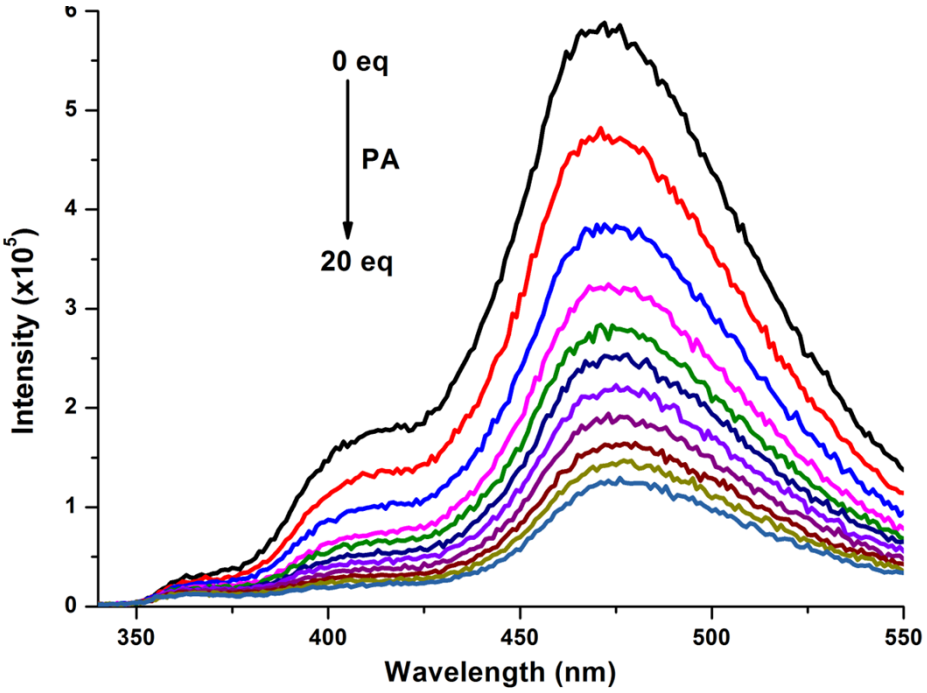


Fig. S23: Emission spectral titration of TAQP (1x10^{-3}M) with 20 equivalent of PA (1x10^{-3}M) in DMF.

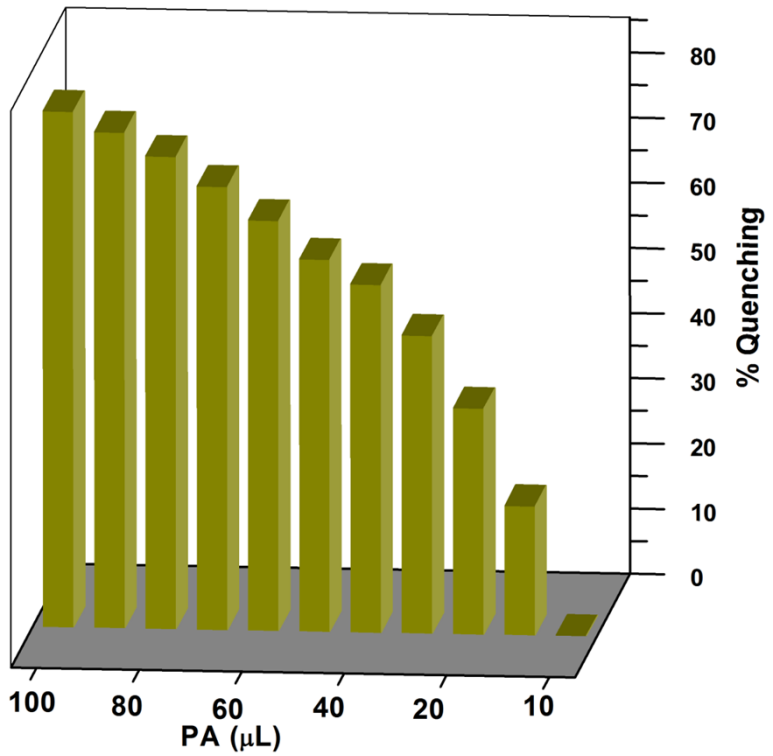


Fig. S24: Luminescence quenching plot of TAQP (1x10^{-3}M) with 20 equivalent of PA (1x10^{-3}M) in DMF

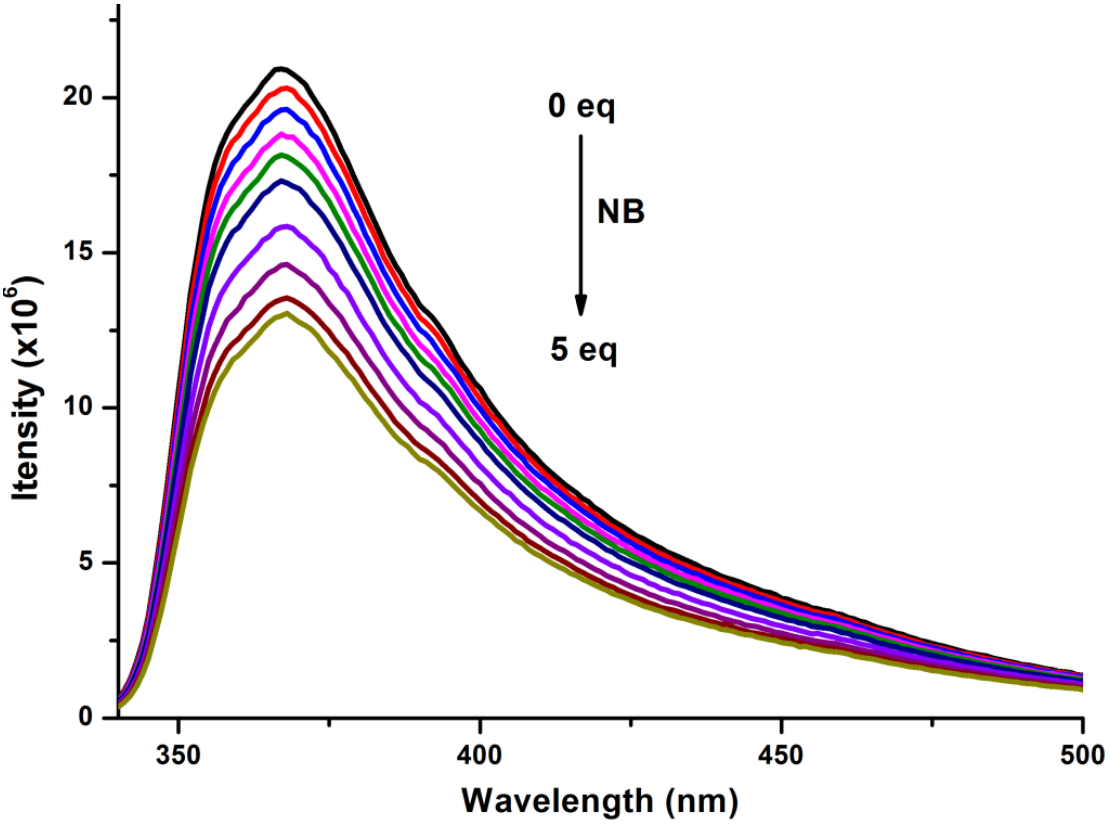


Fig. S25: Emission spectral titration of TAQP (1x10^{-5}M) with 5 equivalent of NB (1x10^{-3}M) in DMF

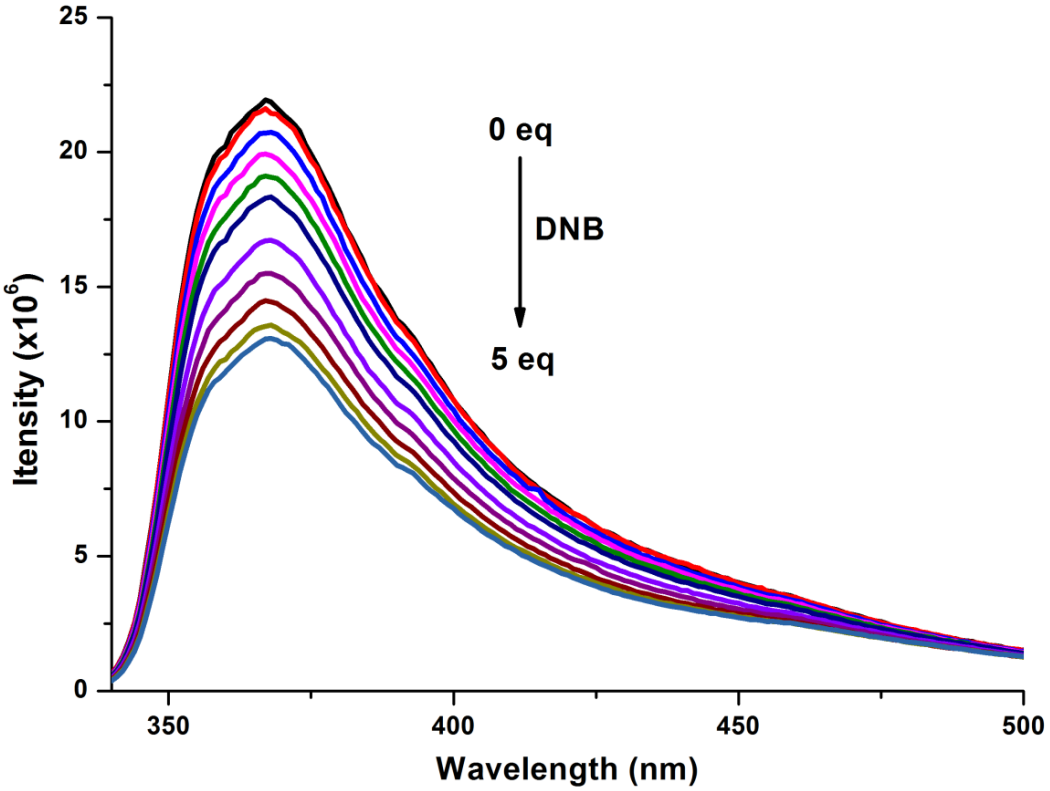


Fig. S26: Emission spectral titration of TAQP ($1x10^{-5}$M) with 5 equivalent of DNB ($1x10^{-3}$M) in DMF

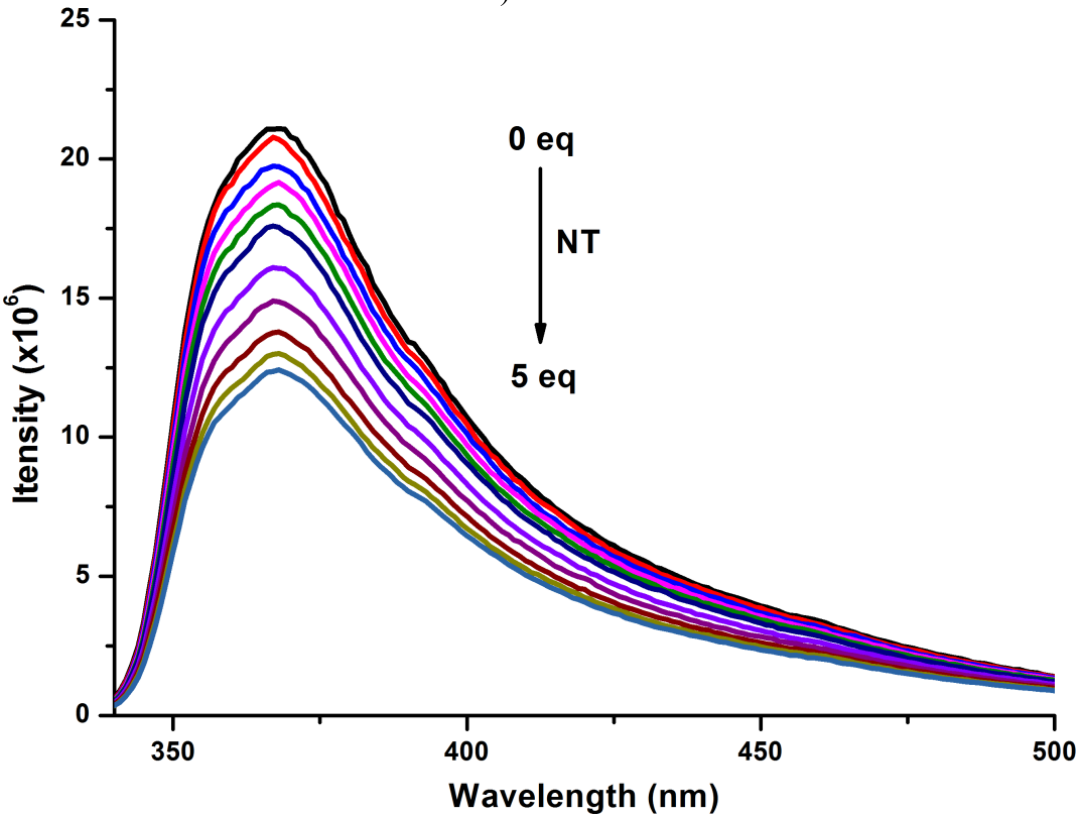


Fig. S27: Emission spectral titration of TAQP ($1x10^{-5}$M) with 5 equivalent of NT ($1x10^{-3}$M) in DMF.

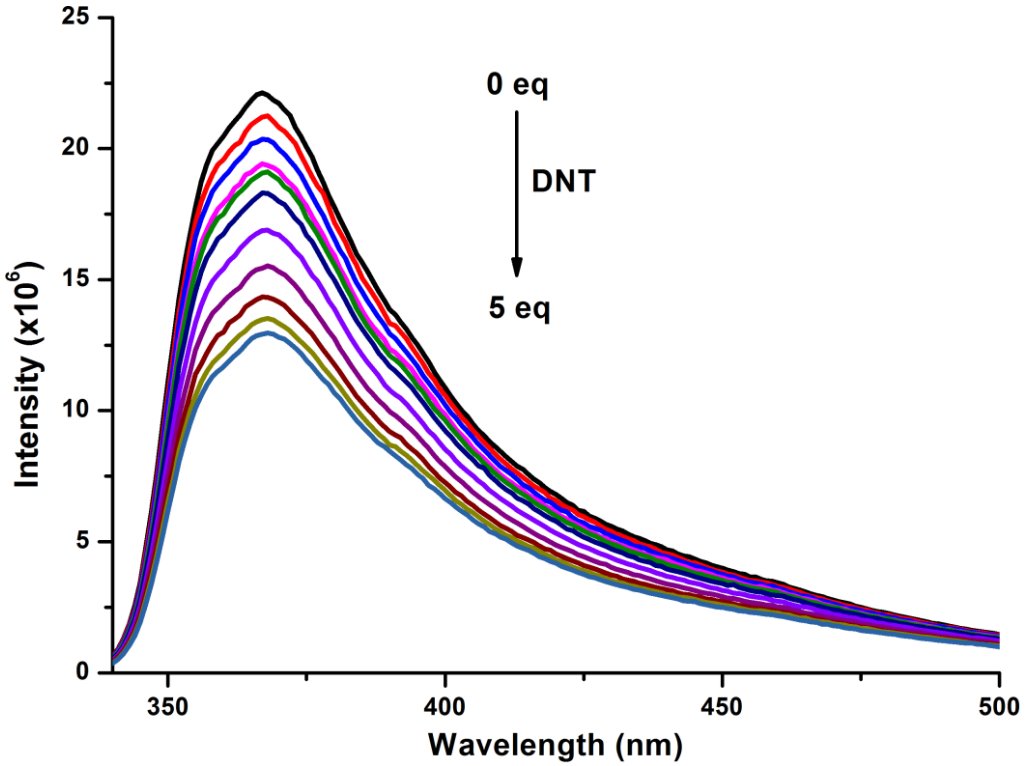


Fig. S28: Emission spectral titration of TAQP (10^{-5} M) with 5 equivalent of DNT (10^{-3} M) in DMF.

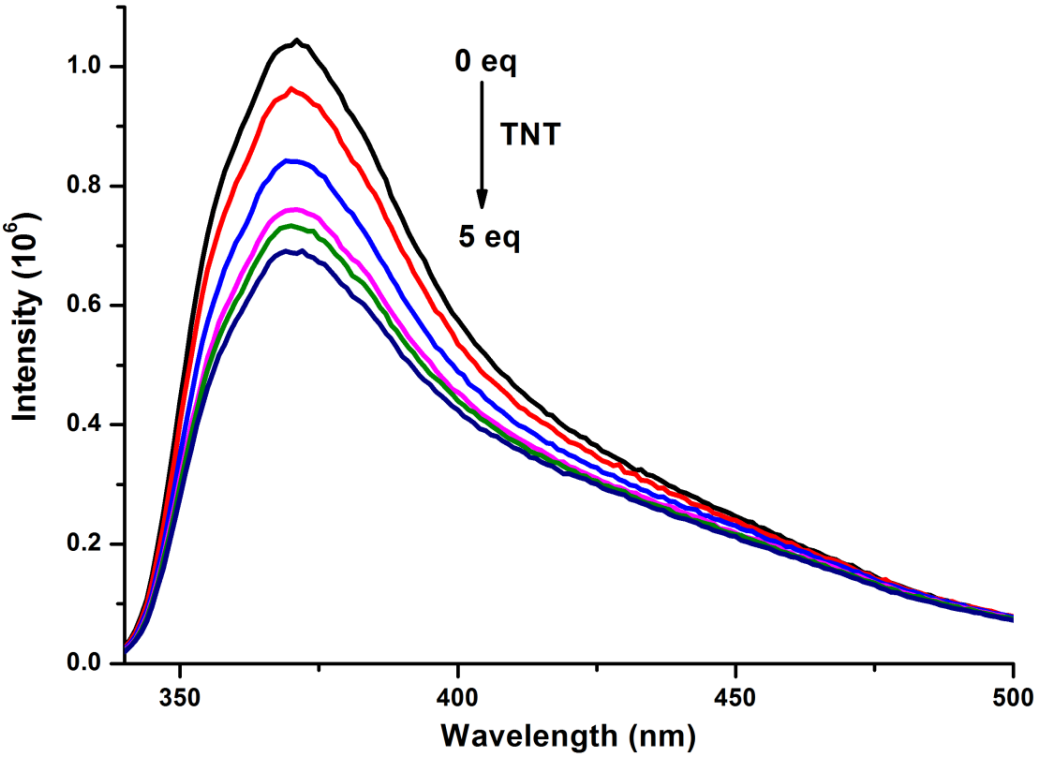


Fig. S29: Emission spectral titration of TAQP ($1x10^{-5}$M) with 5 equivalent of TNT ($1x10^{-3}$M) in DMF.

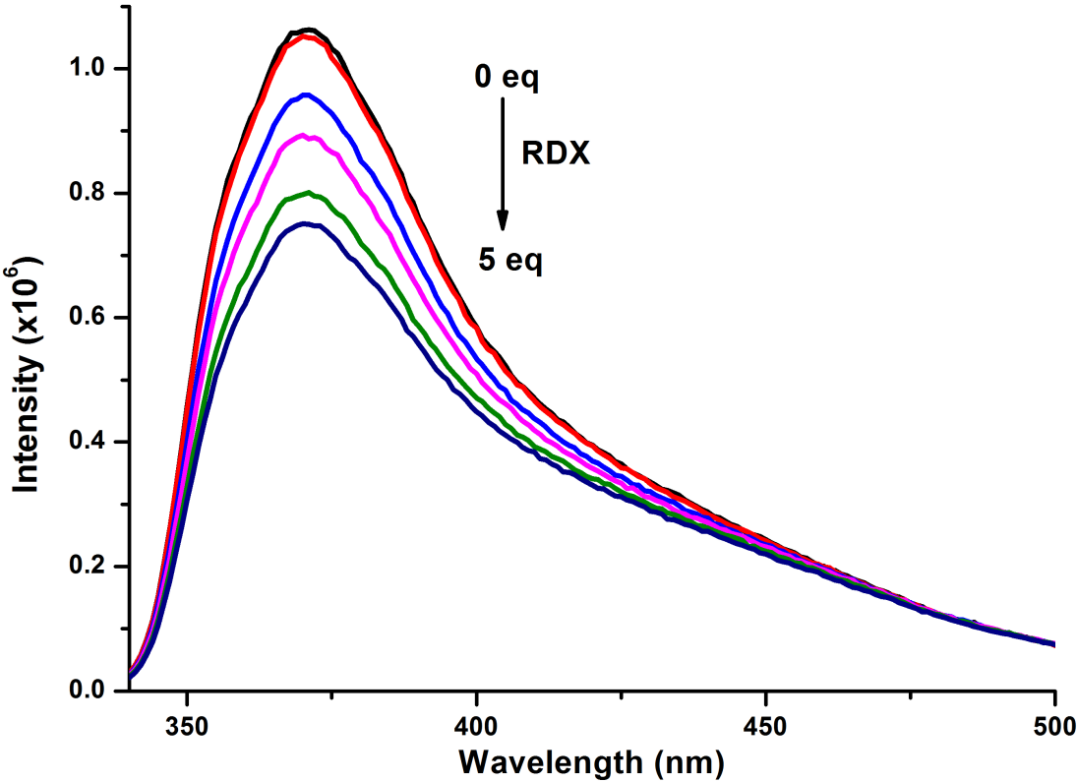


Fig. S30: Spectra of TAQP (1x10^{-5}M) with 5 equivalent of RDX (1x10^{-3}M) in DMF.

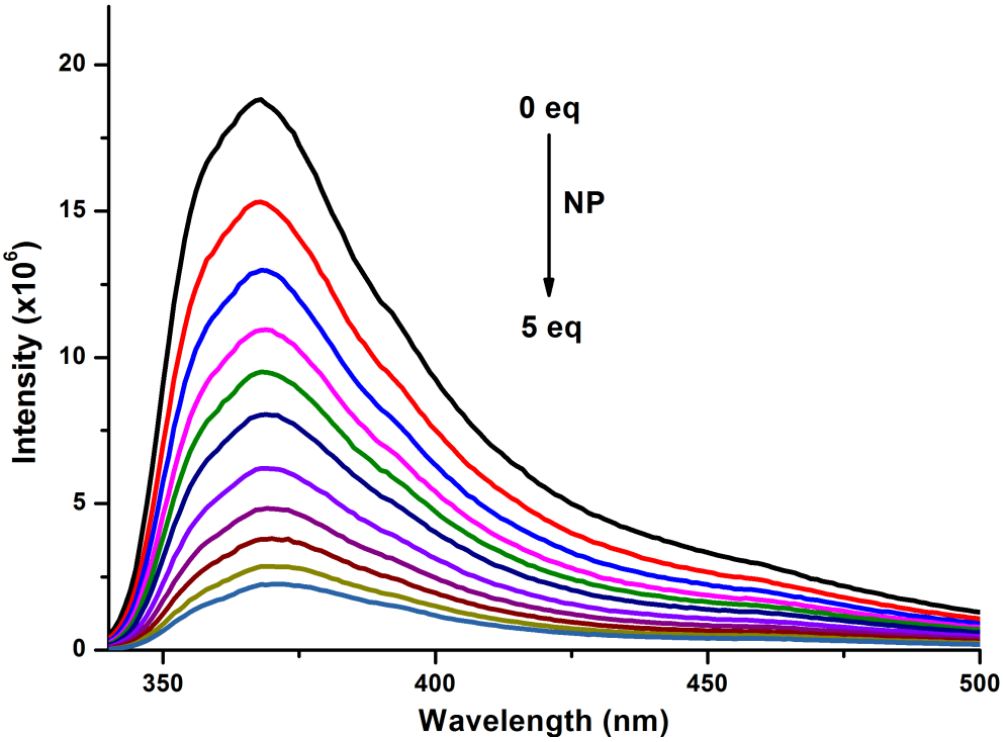


Fig. S31: Emission spectral titration of TAQP (1x10^{-5}M) with 5 equivalent of NP (1x10^{-3}M) in DMF.

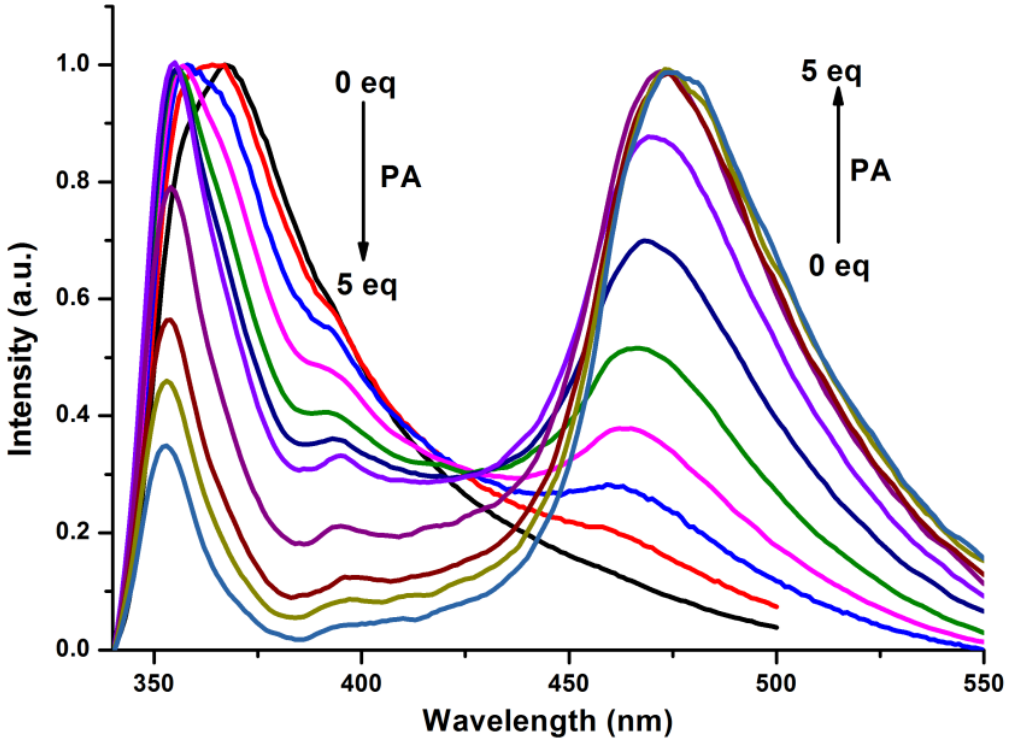


Fig. S32: Emission spectral titration of TAQP ($1x10^{-5}$M) with 5 equivalent of PA ($1x10^{-3}$M) in DMF.

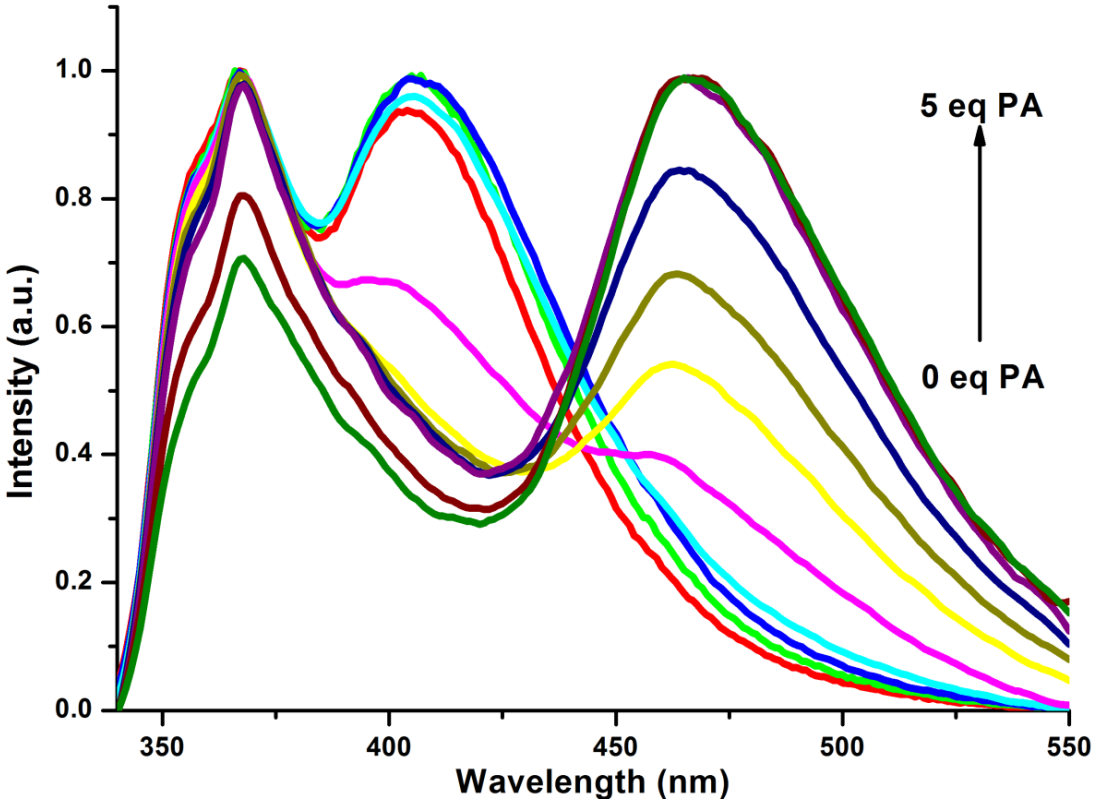


Fig. S33: Emission spectral titration of TAQP ($1x10^{-5}$M) with 5 equivalent of PA ($1x10^{-3}$M) in MeOH.

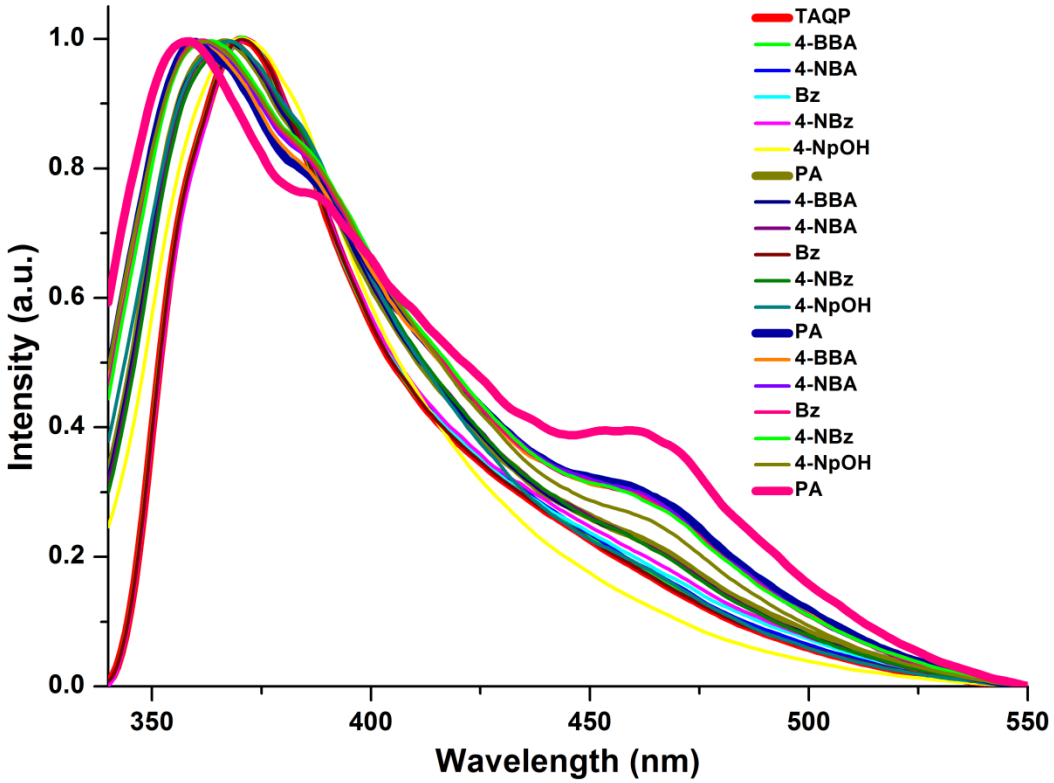


Fig. S34: Emission spectral titration of TAQP ($1x10^{-5}$M) of PA ($1x10^{-3}$M) in the presence of other interfering aromatic analytes ($1x10^{-3}$M) in DMF in incremental addition of 50µL each. These observations suggest that the formation of the peak at 465 nm is observed only in case of PA.