Supporting information

Room-Temperature Orange-Red Phosphorescence by Way of Intermolecular Charge-Transfer in Single-Component Phenoxazine-Quinoline Conjugates, and Chemical Sensing

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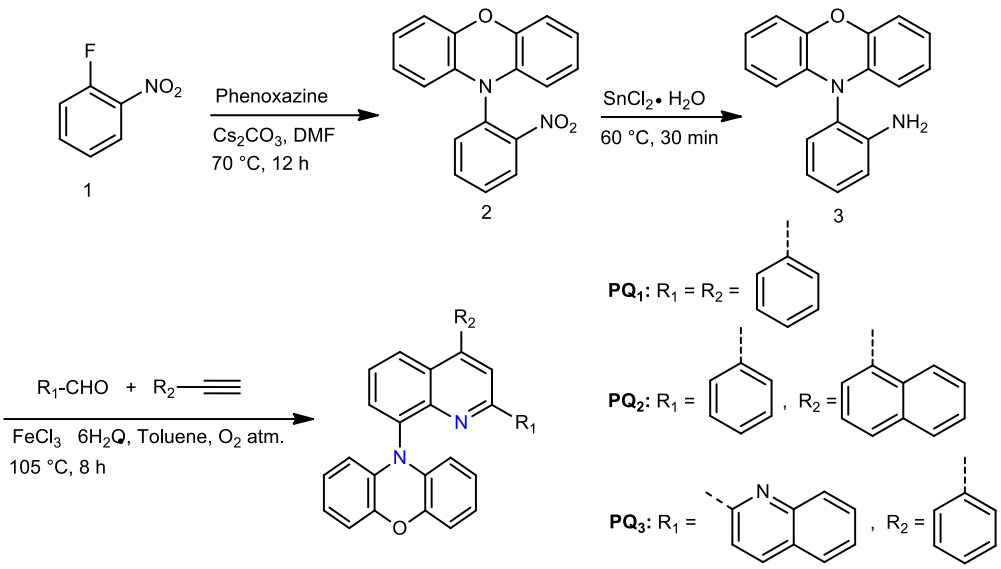
Experimental details

General. All the reagents and deuterated solvents were obtained from commercial sources and used without any further purification, unless otherwise mentioned. Dimethyl formamide (DMF) was dried and distilled over calcium hydride. Cesium carbonate (Cs_2CO_3) was activated by flame dry method. ^{1}H and ^{13}C NMR spectra were recorded in Bruker AVHDN 400 with working frequencies of 400.245 MHz for ^{1}H and 100.6419 MHz for ^{13}C nuclei, respectively, using $CDCl_3$ and CD_2Cl_2 as solvent. Chemical shifts were quoted in ppm relative to tetramethylsilane, using residual solvent peak as a reference standard. High Resolution Mass Spectroscopy (HRMS) were carried out using an Agilent 6540 accurate–mass Q-TOF LC/MS (Agilent Technologies, U.S.A.). Spectroscopic grade solvents were used for all spectroscopic measurement. Steady state and temperature dependent UV-vis(visible) absorption were measured by Agilent Technologies Cary 8454 UV/vis instrument in a conventional quartz cell cuvettes. Steady-state emission, phosphorsescence and lifetimes were measured using HORIBA Fluorolog-3 spectrofluorometer (Model: FL3-2-IHR). All the measurement techniques were discussed earlier[1].

Synthesis of Donor-Acceptor molecular system, PQ1, PQ2 and PQ3



Scheme 1. Synthesis of **PQ1-PQ3**

10-(2-nitrophenyl)-10H-phenoxazine (**2**). Cs_2CO_3 (3.46 g; 10.63 mmol) was taken in a 250 mL two-neck round bottom flask and it was heated under schlenk line for 1 h. After cooling to RT, 10H-phenoxazine (1.3 g; 7.09 mmol) and dry DMF (20 mL) were added to it. Then, 1-fluoro-2-nitrobenzene (1.0 g, 7.09 mmol) was added to this mixture and allowed to stir at 70 °C for 12 h. The reaction mixture was monitored by TLC. After consumption of starting materials, the reaction mixture was poured into ice water. The yellow precipitate appeared which was filtered out and recrystallized using ethyl acetate/hexane to obtain **2** (3.74 g; 88 %) as red powder. ^{1}H NMR ($CDCl_3$): δ 8.16 (d, 1H, *J* = 8 Hz), 7.85 (t, 1H, *J* = 8 Hz), 7.67 (t, 1H, *J* = 8Hz), 7.33-7.28 (m, 1H), 6.73-6.58 (m, 7H) ppm. ^{13}C NMR ($CDCl_3$): δ 135.44, 134.35, 132.84, 129.99, 126.41, 123.33, 122.21, 120.94, 115.88, 112.89 ppm.

2-(10H-phenoxazin-10-yl)aniline (**3**). To a stirred solution of **2** (2.0 g, 6.94 mmol) in 5N HCl, $SnCl_2$•$2H_2O$ (3.13 g, 13.88 mmol) were added and stirred at 60 °C for 30 min. After completion

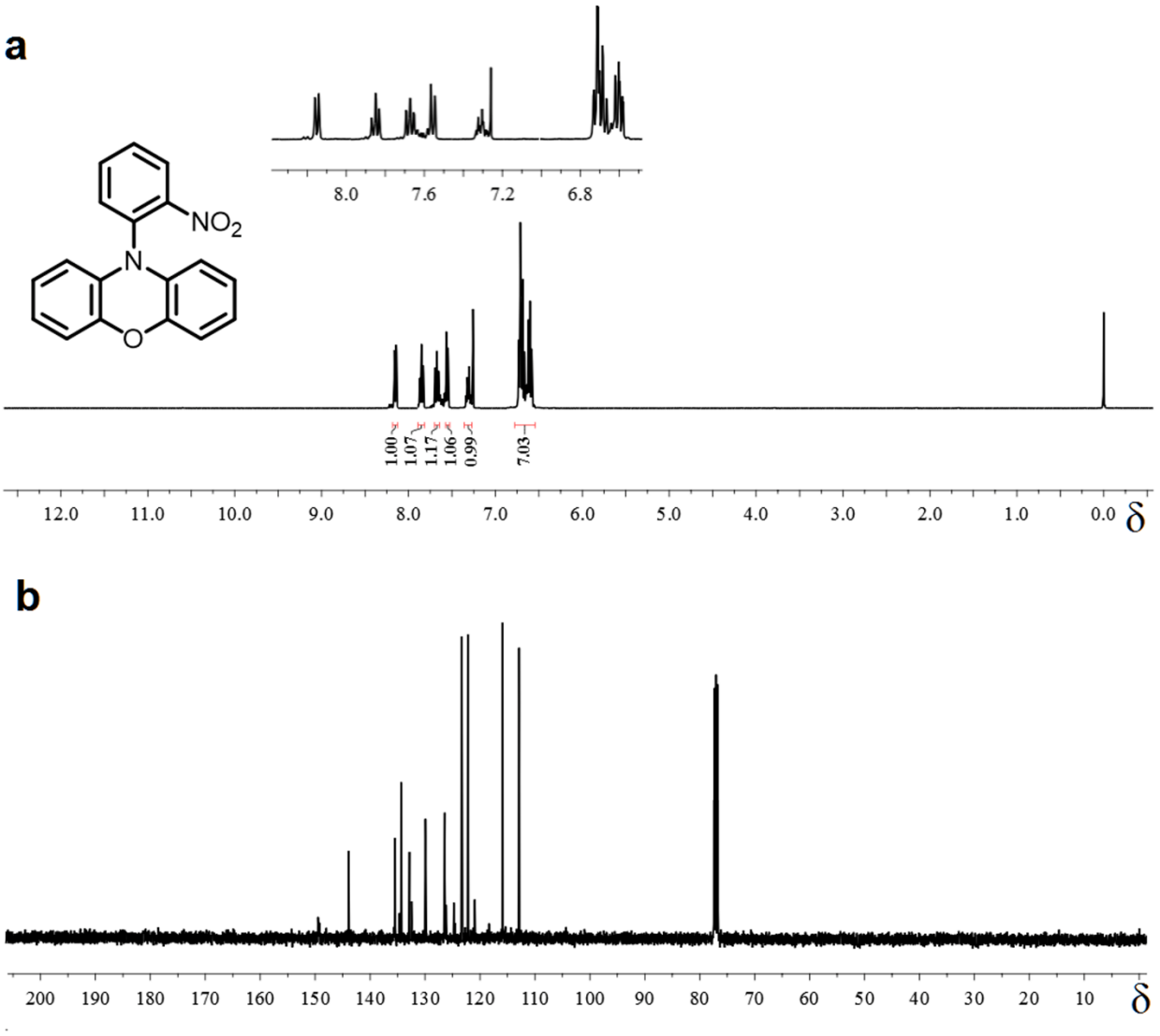
of the reaction, 5M NaOH solution was added to neutralize the excess acid. The aqueous phase was extracted with ethyl acetate (3 × 10 mL). This organic layer was dried with anhydrous Na_2SO_4 and evaporated to dryness which afforded a pale yellow solid (1.82 g, 88 %). ^{1}H NMR ($CDCl_3$): δ 7.12 (d, 2H, *J* = 8 Hz), 6.88 (d, 2H, *J* = 8 Hz), 6.69-6.58 (m, 6H), 6.01-5.98 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$): δ 146.43, 144.04, 134.99, 131.52, 129.19, 123.18, 120.90, 116.99, 115.20, 113.25 ppm. HRMS (ESI): m/z calcd for $C_{18}H_{14}N_2O$: 274.1106, found [M-H$^+$]: $C_{18}H_{15}N_2O^+$, 275.1182 (calcd 275.1179).

General synthesis procedure of PQ1, PQ2 and PQ3. A multicomponent condensation reaction[1] among **3** (1.0 g, 3.87 mmol), aromatic aldehyde (1 equiv.) and aromatic acetylene (1 equiv.) were undertaken in a 50 mL round bottom flask in presence of $FeCl_3$•$6H_2O$ (104.6 mg, 0.387 mmol) at oxygenated condition. The mixture was heated at 105 °C for 8 h. After completion of the reaction, mixture was taken in ethyl acetate and washed with brine solution. This organic layer was dried with anhydrous Na_2SO_4 and evaporated to dryness. The crude product was purified by column chromatography (SiO_2: ethyl acetate:hexanes, 95:5 v/v) to afford desired product.

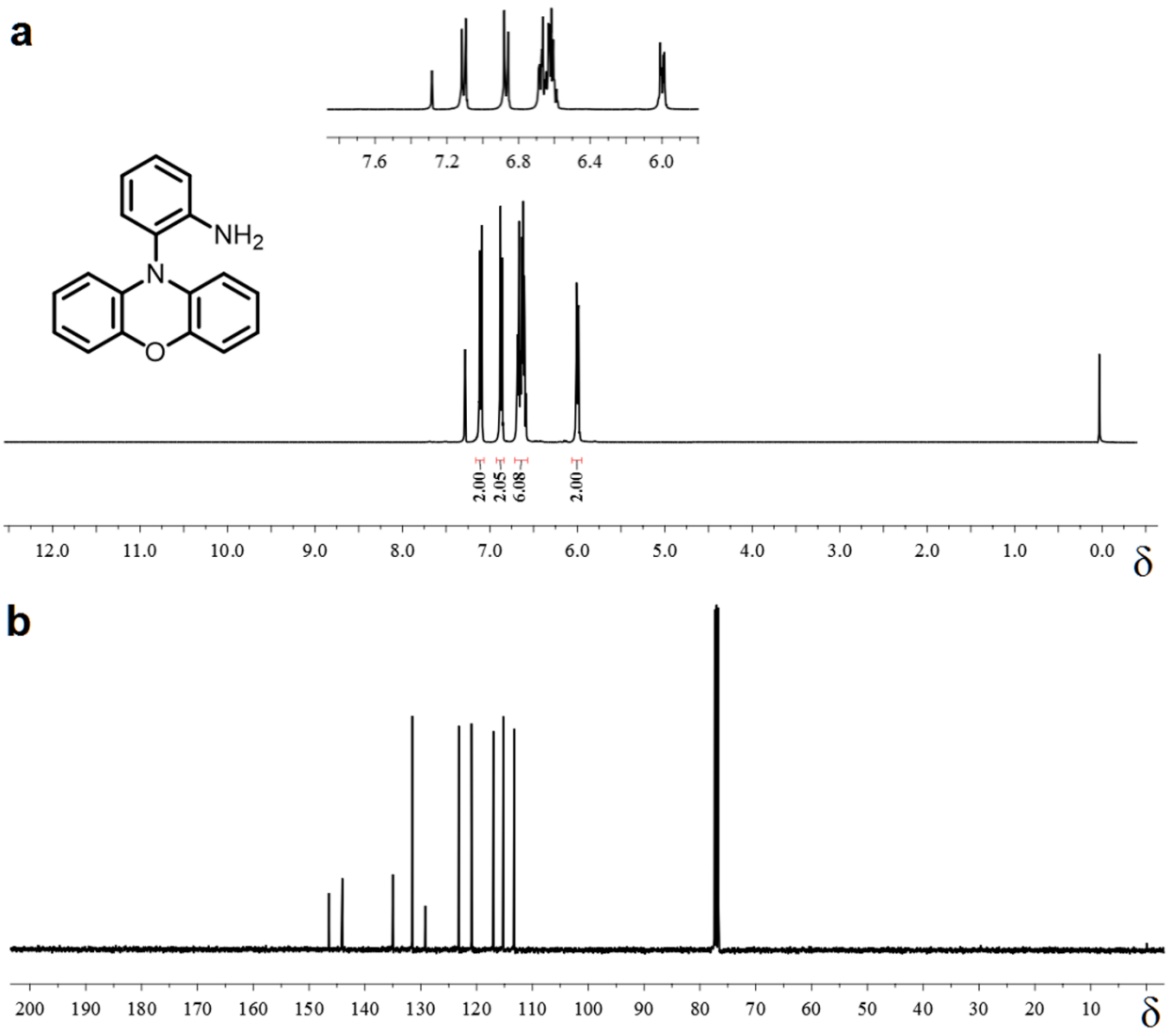
10-(2,4-diphenylquinolin-8-yl)-10H-phenoxazine (**PQ1**): ^{1}H NMR ($CDCl_3$): δ 8.00 (t, 3H, *J* = 8 Hz), 7.86 (s, 1H), 7.83 (d, 1H, *J* = 8 Hz), 7.61-7.54 (m, 6H), 6.77 (d, 2H, *J* = 8 Hz), 6.61 (t, 2H, *J* = 8 Hz), 6.48 (t, 2H, *J* = 8 Hz), 5.87 (d, 2H, *J* = 8 Hz) ppm. ^{13}C NMR ($CDCl_3$): δ 156.34, 149.84, 145.20, 143.90, 139.32, 138.40, 136.70, 135.11, 133.62, 133.03, 129.89, 129.05, 128.69. 127.89, 127.55. 126.80. 126.49, 122.96, 120.93, 119.34, 115.23, 113.97 ppm. HRMS (ESI): m/z calcd for $C_{33}H_{22}N_2O$: 462.1732, found [M-H$^+$]: $C_{33}H_{23}N_2O^+$, 463.1807 (calcd 463.1805).

10-(4-(naphthalen-1-yl)-2-phenylquinolin-8-yl)-10H-phenoxazine (**PQ2**): ^{1}H NMR ($CDCl_3$): δ 8.05 (m, 4H), 7.09 (s, 1H), 7.82 (d, 1H, *J* = 8 Hz), 7.66 (t, 1H, *J* = 8 Hz), 7.58-7.35 (m, 9H), 6.79 (d, 2H, *J* = 8 Hz), 6.64 (t, 2H, *J* = 8 Hz), 6.54 (br, 2H), 5.96 (br, 2H) ppm. ^{13}C NMR ($CDCl_3$): δ 156.24, 148.49, 145.24, 144.19, 138.81, 135.25, 133.59, 133.20, 131.96, 129.63, 129.47, 128.97, 128.68, 128.44, 127.59, 127.24, 126.68, 126.53, 126.30, 125.99, 125.35, 123.02, 121.00, 120.50, 115.29, 114.02 ppm. HRMS (ESI): m/z calcd for $C_{37}H_{24}N_2O$: 512.1889, found [M-H$^+$]: $C_{37}H_{25}N_2O^+$, 513.1962 (calcd 513.1961).

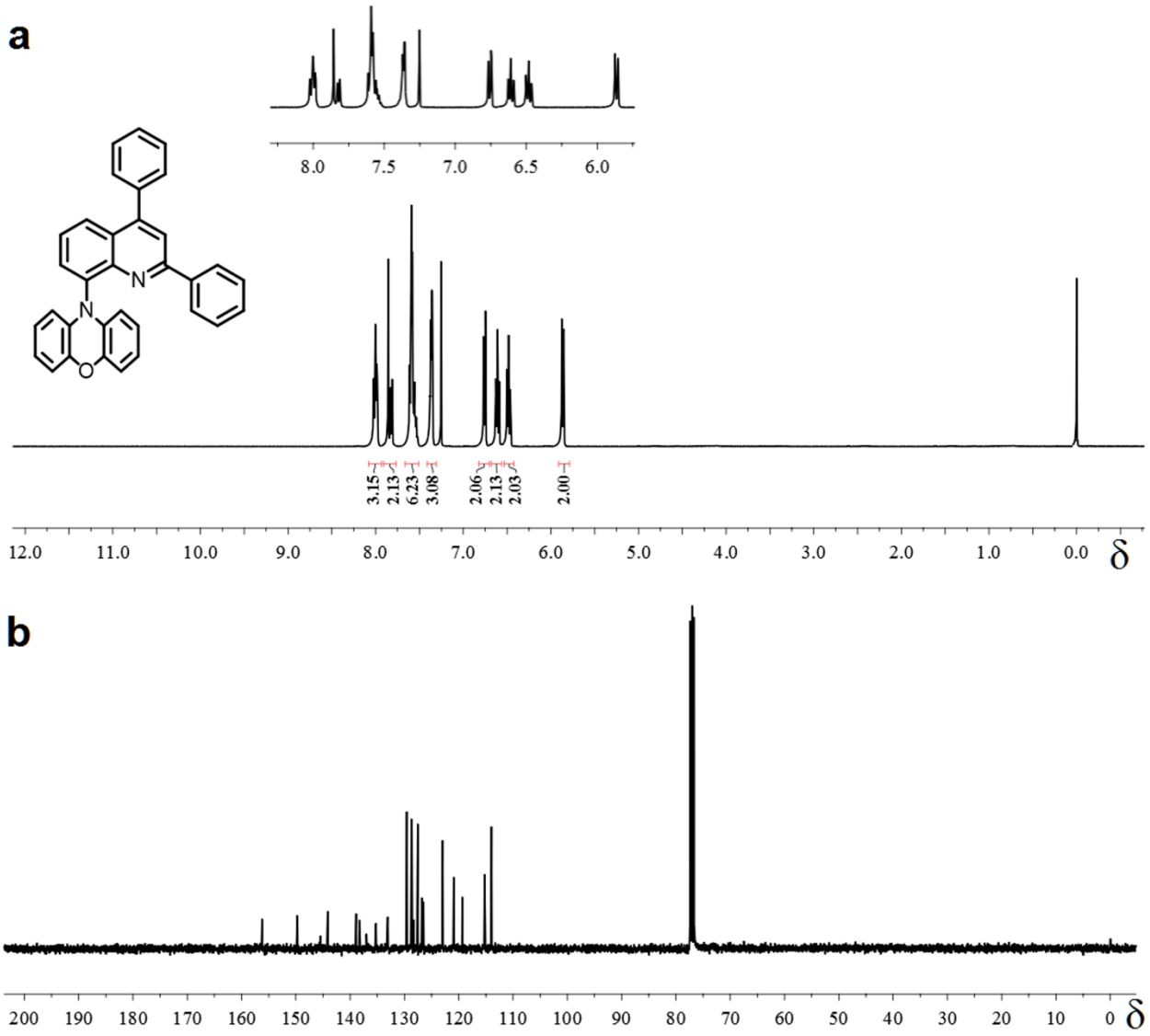
10-(4-phenyl-[2,2'-biquinolin]-8-yl)-10H-phenoxazine (**PQ3**): ^{1}H NMR ($CDCl_3$): δ 8.82 (s, 1H), 8.49 (d, 1H, *J* = 8 Hz), 8.16-8.08 (m, 3H), 7.87 (d, 1H, *J* = 8 Hz), 7.80 (d, 1H, *J* = 8 Hz), 7.70-7.50 (m, 8H), 6.81 (d, 2H, *J* = 8 Hz), 6.62 (t, 2H, *J* = 8 Hz), 6.49 (t, 2H, *J* = 8 Hz), 5.92 (d, 2H, *J* = 8 Hz) ppm. ^{13}C NMR ($CDCl_3$): δ 145.23, 144.20, 138.35, 136.71, 135.31, 133.02, 132.90, 131.16, 129.76, 128.63, 127.57, 127.01, 123.25, 123.06, 121.58, 121.05, 120.09, 119.93, 116.78, 115.51, 115.26, 114.15, 113.09 ppm. HRMS (ESI): m/z calcd for $C_{36}H_{23}N_3O$: 513.1841, found [M-H$^+$]: $C_{36}H_{24}N_3O^+$, 514.1916 (calcd 514.1914).



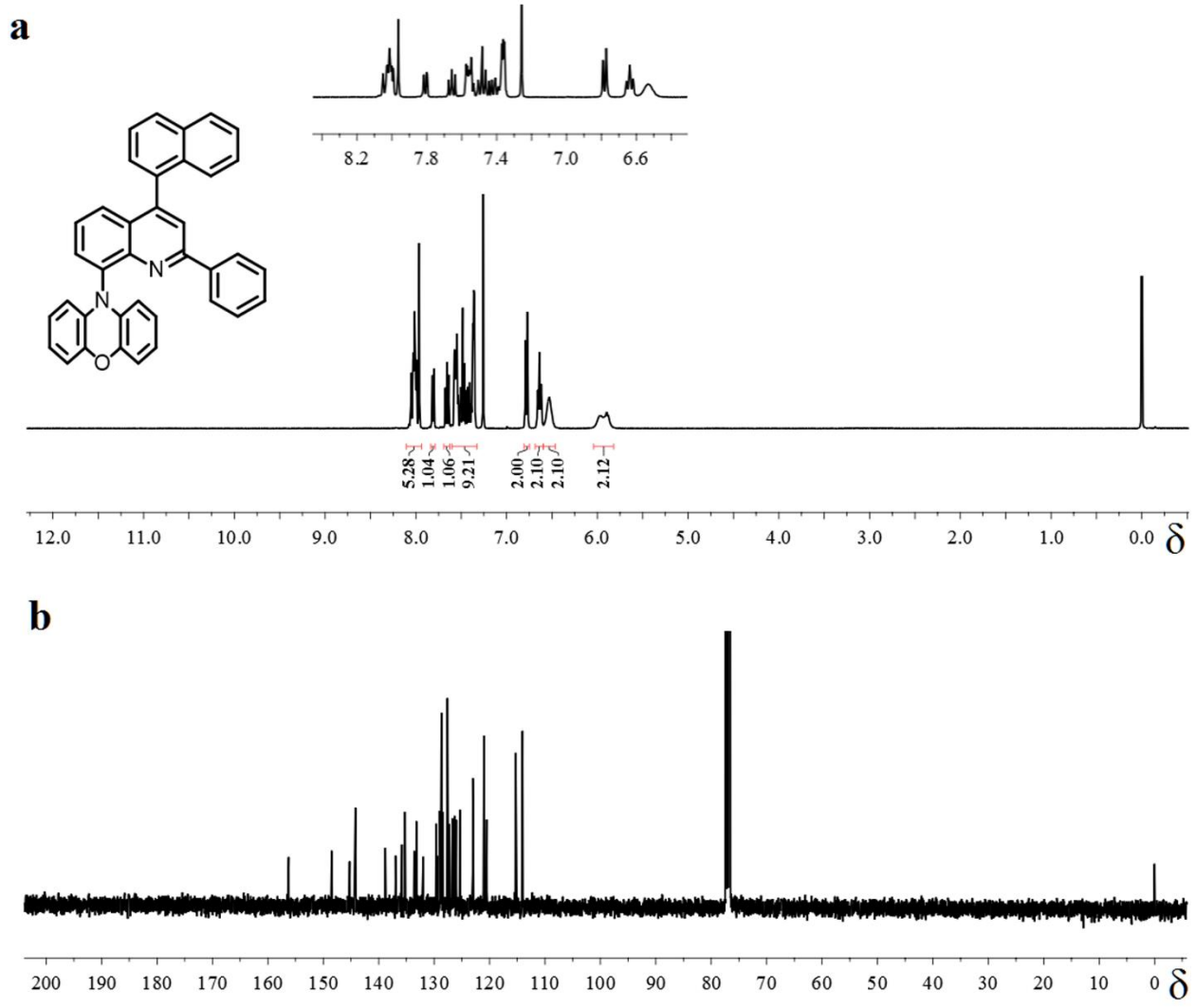
Supporting Figure S1. (a) ^{1}H and (b) ^{13}C NMR spectra of **10-(2-nitrophenyl)-10H-phenoxazine (2).**



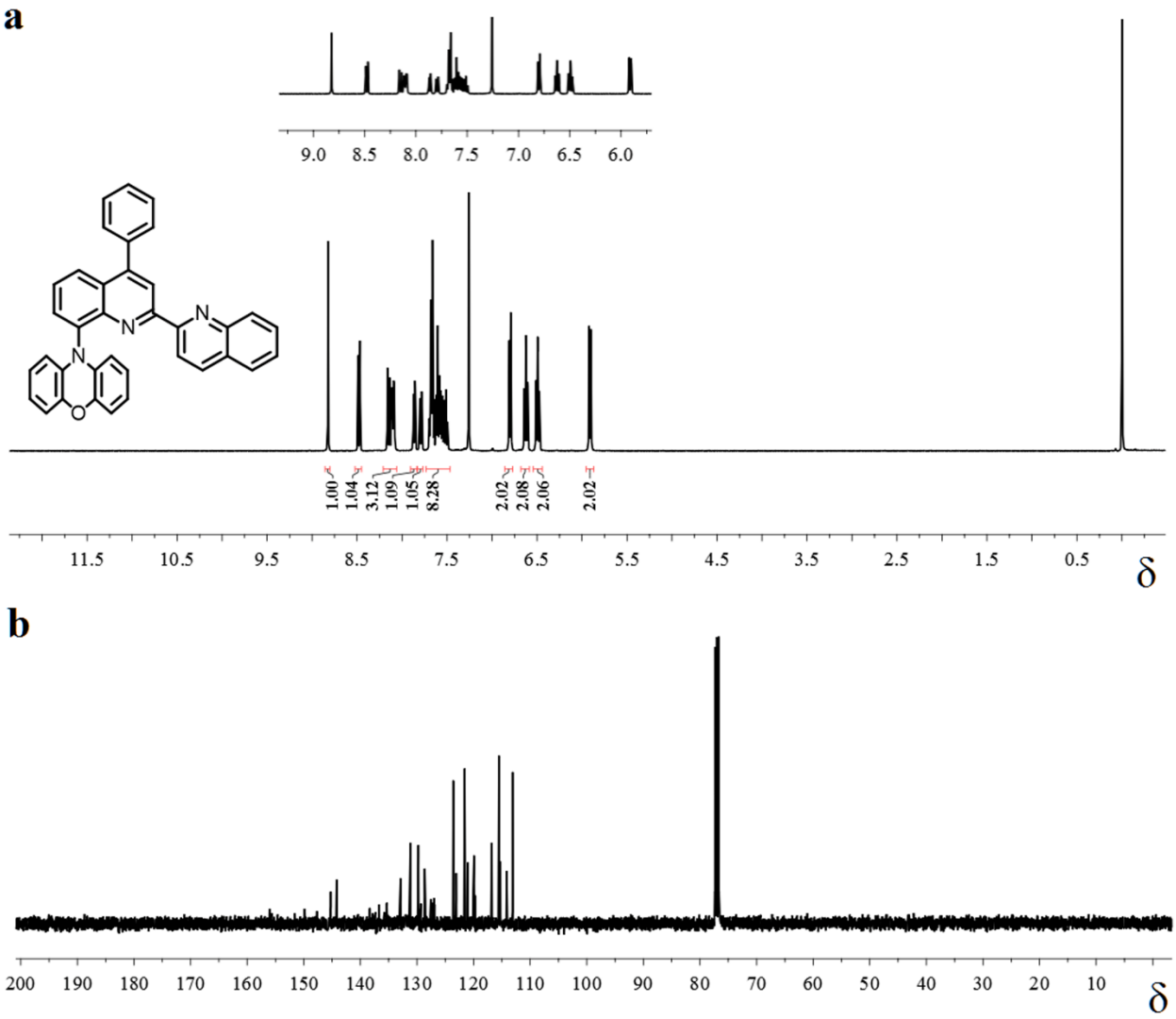
Supporting Figure S2. (a) ^{1}H and (b) ^{13}C NMR spectra of **2-(10H-phenoxazin-10-yl)aniline** (**3**).



Supporting Figure S3. (a) ^{1}H and (b) ^{13}C NMR spectra of **PQ1**.



Supporting Figure S4. (a) ^{1}H and (b) ^{13}C NMR spectra of **PQ2**.



Supporting Figure S5. (a) ^{1}H and (b) ^{13}C NMR spectra of **PQ3**.

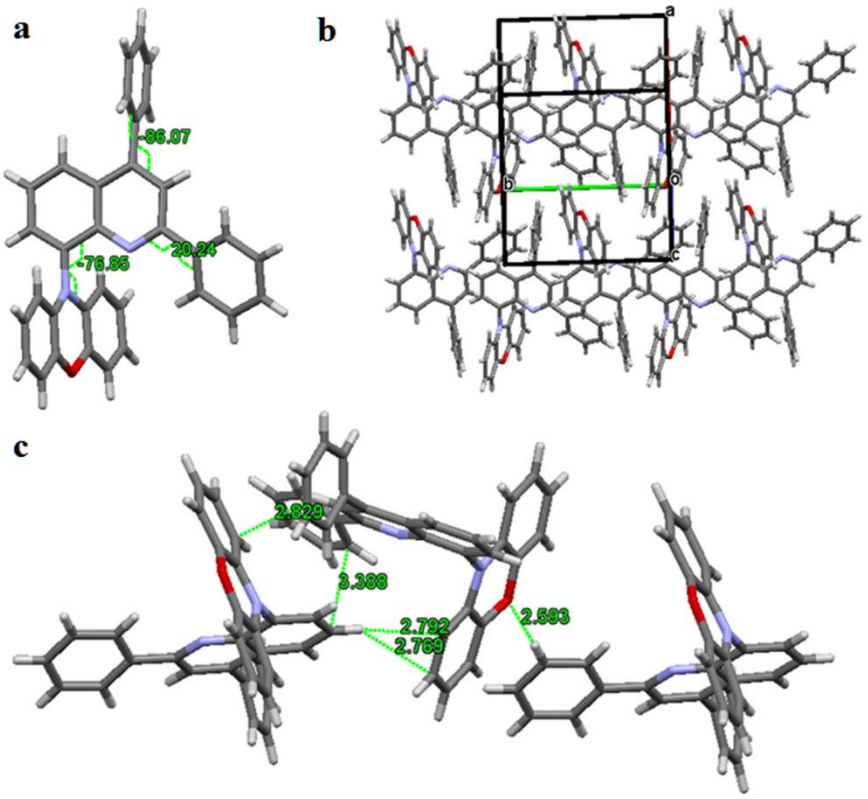
Single crystal X-ray diffraction (SCXRD)

Preparation of the PQ1 crystal. **PQ1** (20 mg, 0.04 mmol) was dissolved in 1.0 mL of toluene and resulting solution was diffused with hexane (1.0 mL). The mixture was allowed to evaporate to yield cubic-shaped yellow crystals suitable for X-ray diffraction.

Preparation of PQ2 crystal. **PQ2** (20 mg, 0.037 mmol) was dissolved in 1.0 mL of ethyl acetate and resulting solution was diffused with hexane (1.0 mL). The mixture was allowed to evaporate to yield cubic-shaped yellow crystals suitable for X-ray diffraction.

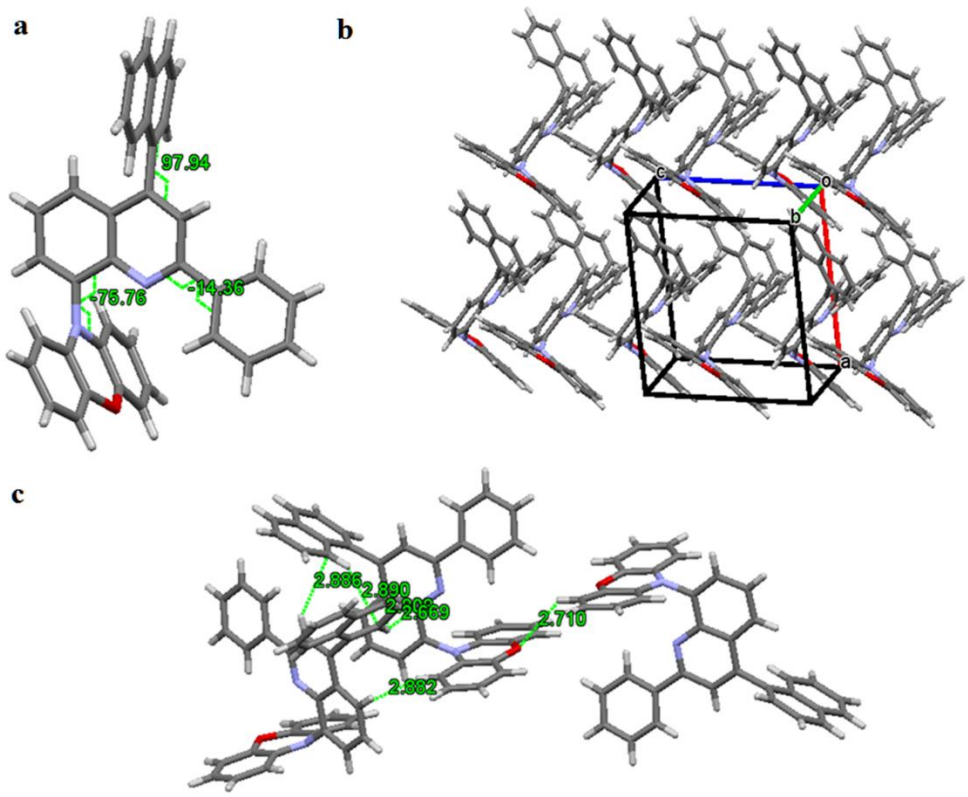
Preparation of PQ3 crystal. **PQ3** (20 mg, 0.037 mmol) was dissolved in 1.0 mL of toluene and resulting solution was diffused with hexane (1.0 mL). The mixture was allowed to evaporate to yield cubic-shaped yellow crystals suitable for X-ray diffraction.

X-ray analysis of PQ1 at RT. The X-ray analysis of **PQ1** shows that the phenoxazine and phenyl rings attached to C8, C2, and C4 atoms of quinolinyl moiety are deviated from planarity by their corresponding torsion angles which were found to be -76.85(0)°, 20.24(0)° and 86.07(0)° when viewed along the atoms of C11–N2–C8–C9, C24–C23–C2–N1 and C18–C17–C4–C3, respectively (Fig. S6 and Table S1). Furthermore, the Figs. S6b, S6c show three intermolecular C–H•••π interaction between the H6 atom of quinolinyl moiety to the adjacent phenoxazine ring (C6–H6•••C13, 2.769 Å, C6–H6•••C12, 2.792 Å), and C12 atom of phenoxazine ring with H3 atom of adjacent quinolinyl moiet (C3–H3•••C12, 2.829 Å). In addition, intermolecular hydrogen bond between O1 of phenoxazine and H25 atom of other molecule (O1•••H25, 2.593 Å) and a co-facial π•••π interaction from the two neighboring molecules were also seen (C24•••C6: 3.388 Å) in the crystal.



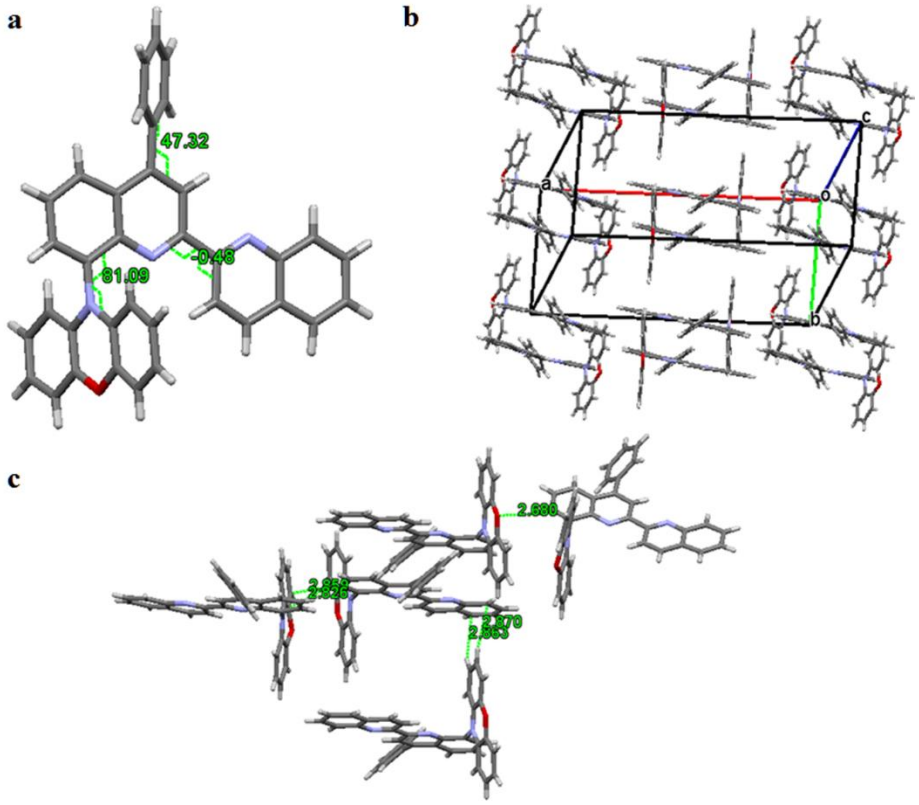
Supporting Figure S6. (a) Dihedral angles, (b) crystal packing and (c) intermolecular interactions in **PQ1**.

X-ray analysis of PQ2 at RT. The X-ray analysis of **PQ2** shows that the phenoxazine and phenyl rings attached to C8, C2, and napthyl ring attached at C4 atoms of quinolinyl moiety are deviated from planarity by their corresponding torsion angles which were found to be -75.76(0)°, -14.36(0)° and 97.94(0)° when viewed along the atoms of C11–N2–C8–C9, C24–C23–C2–N1 and C18–C17–C4–C3, respectively (Fig. S7 and Table S1). Moreover, figs S7b, S7c shows five strong intermolecular C–H•••π interactions (C3–H3•••C32, 2.886 Å, C32–H32•••C18, 2.890 Å, C18–H18•••C10, 2.809 Å, C18–H18•••C19, 2.669 Å, C12A–H12A•••C5, 2.882 Å) and one intermolecular H-bonding interaction between phenoxazine oxygen to hydrogen atom of the next molecule (O1•••H15, 2.710 Å).



Supporting Figure S7. (a) Dihedral angles, (b) crystal packing and (c) intermolecular interactions in **PQ2**.

X-ray analysis of PQ3 at RT. The X-ray analysis of PQ3 shows the substituent attached at C2, C4 and C8 of the quinolone moiety are deviated from the planarity by -0.48 (1)°, 47.32 (0)° and 81.09 (3)° when viewed along C24–C23–C2–N1, C18–C17–C4–C3 and C11–N2–C8–C9, respectively (figure S8, table S1). Additionally, there are four intermolecular C–H•••π interactions (C13–H13•••C26, 2.863 Å, C14–H14•••C29, 2.870 Å, C7–H7•••C15B, 2.859 Å, C7–H7•••C16B, 2.826 Å) and one intermolecular hydrogen bonding between O1 and H7B (2.680 Å) (fig S8.).



Supporting Figure S8. (a) Dihedral angles, (b) crystal packing and (c) intermolecular interactions in **PQ3**.

Table S1. Dihedral angles in the crystals

	C24–C23–C2–N1	C18–C17–C4–C3	C11–N2–C8–C9
PQ1	20.24(0)°	86.07(0)°	-76.85(0)°
PQ2	-14.36(0)°	97.94(0)°	-75.76(0)°
PQ3	-0.48 (1)°	47.32 (0)°	81.09 (3)°

Table S2. Crystal data for **PQ1**-**PQ3**

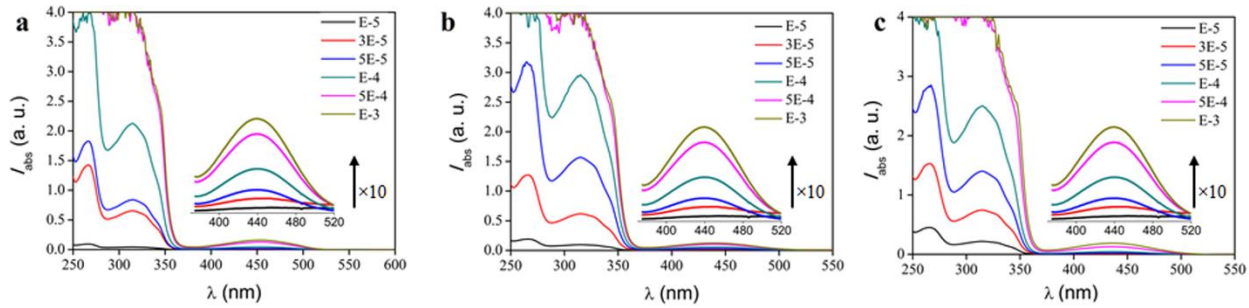
	PQ1	**PQ2**	**PQ3**
CCDC	1848419	1848420	1848421
Empirical formula	C33 H22 N2 O	C37 H24 N2 O	C36 H23 N3 O

Formula weight	462.53	512.58	513.57
Temperature	294(2)	298(2)	297(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space Group	P 21/n	P 21/c	P 21/c
Unit cell dimensions	a = 11.8020(4) Å b =11.3673(5) Å c = 17.9736(8) Å α = 90° β = 93.9950(10)° γ = 90°	a = 10.5680(8) Å b =26.2012(17) Å c = 9.6104(8) Å α = 90° β = 99.121(3)° γ = 90°	a = 25.5532(12) Å b = 12.6598(6) Å c = 17.1127(6) Å α = 90° β = 106.0600(10)° γ = 90°
Volume	2405.42(17) Å^3	2627.4(3) Å^3	5319.9(4)
Z	4	4	8
Density(calculated)	1.277 Mg/m^3	1.296 Mg/m^3	1.283 Mg/m^3
Absorption coefficient	0.077 mm^{-1}	0.078 mm^{-1}	0.078 mm^{-1}
F(000)	1056	1072	2144
Crystal size	0.32 × 0.28 × 0.22 mm^3	0.38 × 0.21 × 0.11 mm^3	0.34 × 0.26 × 0.23 mm^3
Theta range for data collection	2.272 to 26.410°	1.952 to 25.035°	2.03 to 26.438°
Index ranges	-13 <= h <=14, -14 <= k <=13, -22 <=l <=22	-12 <= h <= 12, -31 <=k <=31, -11 <= l <=11	-31 <= h <=31, -15 <= k <=15, -21 <= l <=20
Reflections collected	40593	43355	87317
Independent reflection	4934	4697	6499
Completeness to θ	100 %	100 %	99.7 %
Absorption correction	Multi-Scan	Multi-Scan	Multi-Scan
Max. and min. transmission	0.976 and 0.983	0.968 and 0.986	0.976 and 0.982
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	4913/0/326	4641/0/362	10918/0/720
Goodness-of-fit on F2	1.015	1.071	1.159

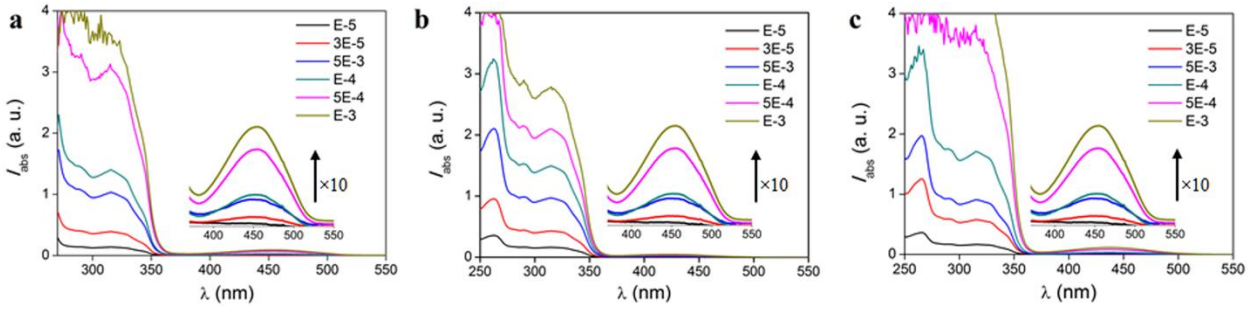
Final R indices [I>2σ(I)]	R = 0.0578 wR2 = 0.1410	R = 0.0521 wR2 = 0.1334	R = 0.0989 wR2 = 0.1586
R indices(all data)	R = 0.1382 wR2 = 0.1848	R = 0.0804 wR2 = 0.1586	R = 0.1647 wR2 = 0.1820
Largest diff. peak and hole	0.205 and -0.175 e.Å^{-3}	0.432 and -0.168 e.Å^{-3}	0.246 and -0.276 e.Å^{-3}

UV-vis analysis of PQ1-PQ3 in solutions

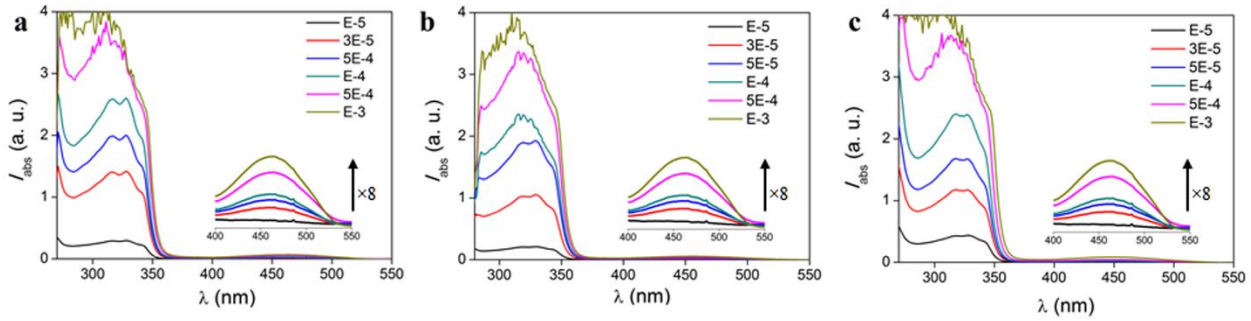
Concentration dependent absorption spectra of PQ1-PQ3 in various solvent



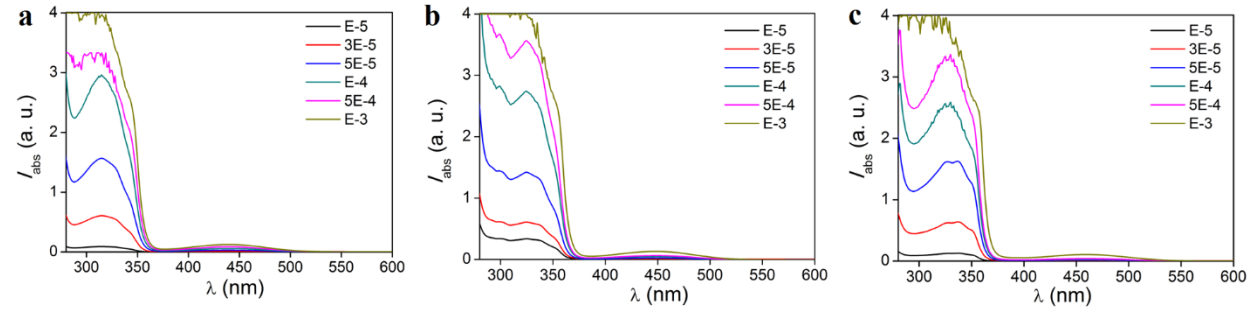
Supporting Figure S9. Concentration dependent absorption spectra of **PQ1** in (a) cyclohexane, (b) 1,4-dioxane and (c) THF.



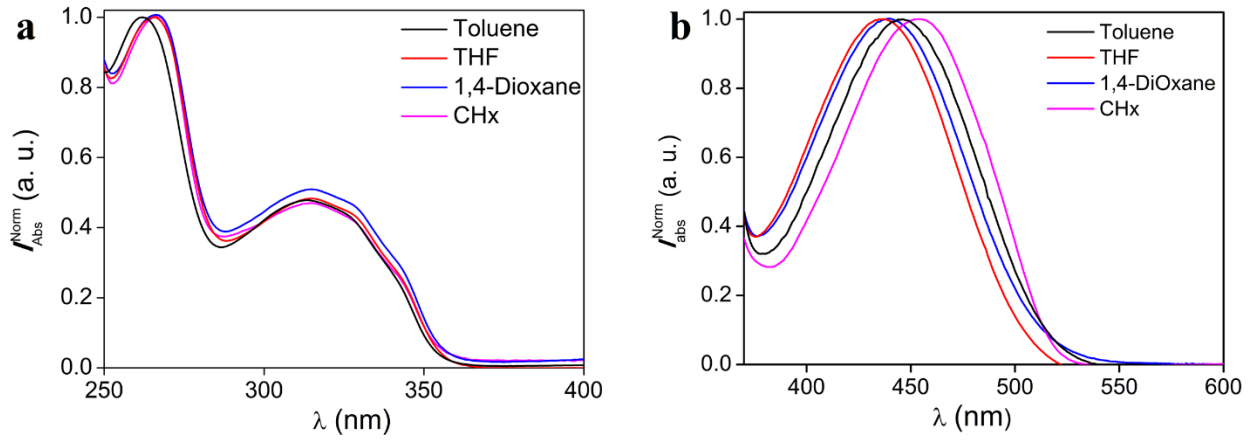
Supporting Figure S10. Concentration dependent absorption spectra of **PQ2** in (a) cyclohexane, (b) 1,4-dioxane and (c) THF.



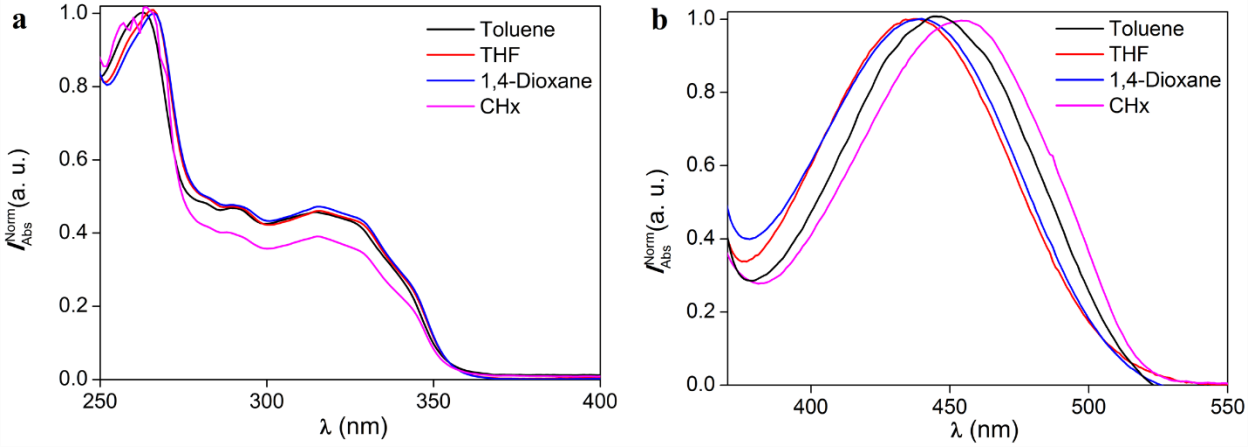
Supporting Figure S11. Concentration dependent absorption spectra of **PQ3** in (a) cyclohexane, (b) 1,4-dioxane and (c) THF.



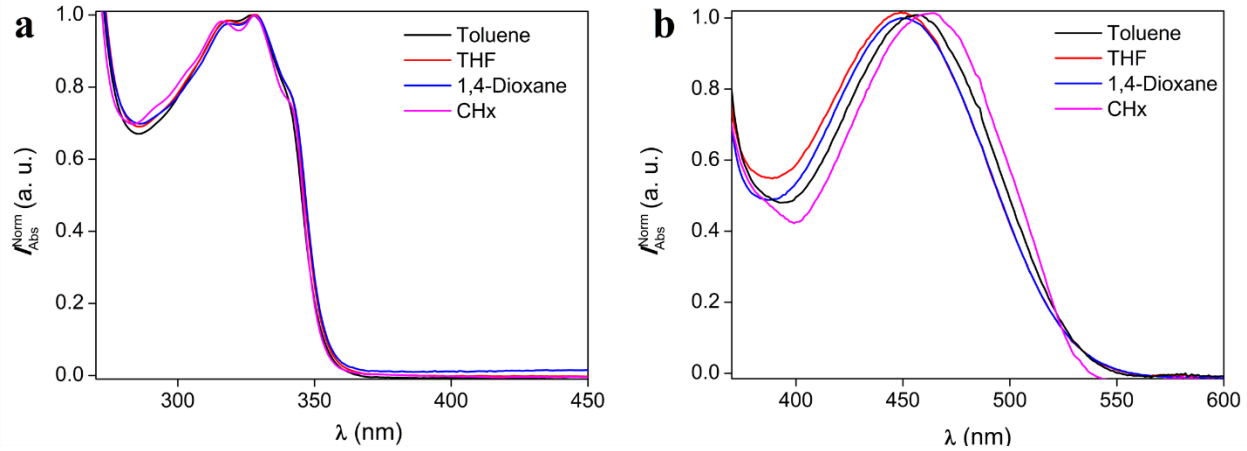
Supporting Figure S12. Concentration dependent absorption spectra in chloroform of (a) **PQ1**, (b) **PQ2** and (c) **PQ3**.



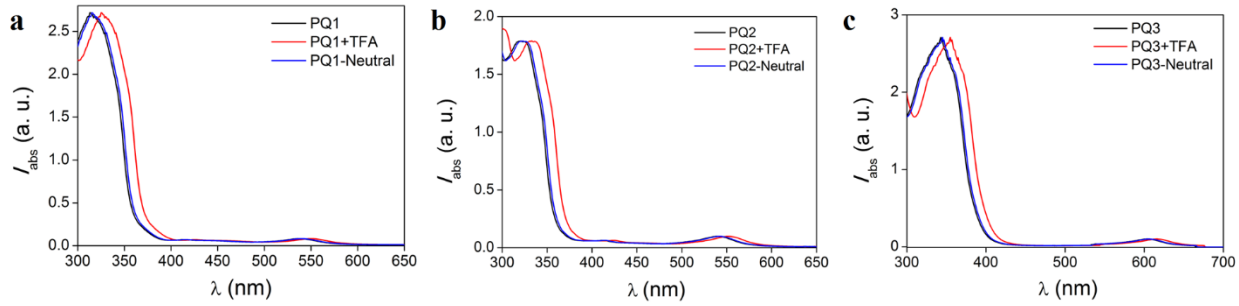
Supporting Figure S13. Solvent dependent absorbance spectra of **PQ1** at (a) 10^{-5} M and (b) 10^{-3} M concentration.



Supporting Figure S14. Solvent dependent absorbance spectra of **PQ2** at (a) 10^{-5} M and (b) 10^{-3} M concentration.

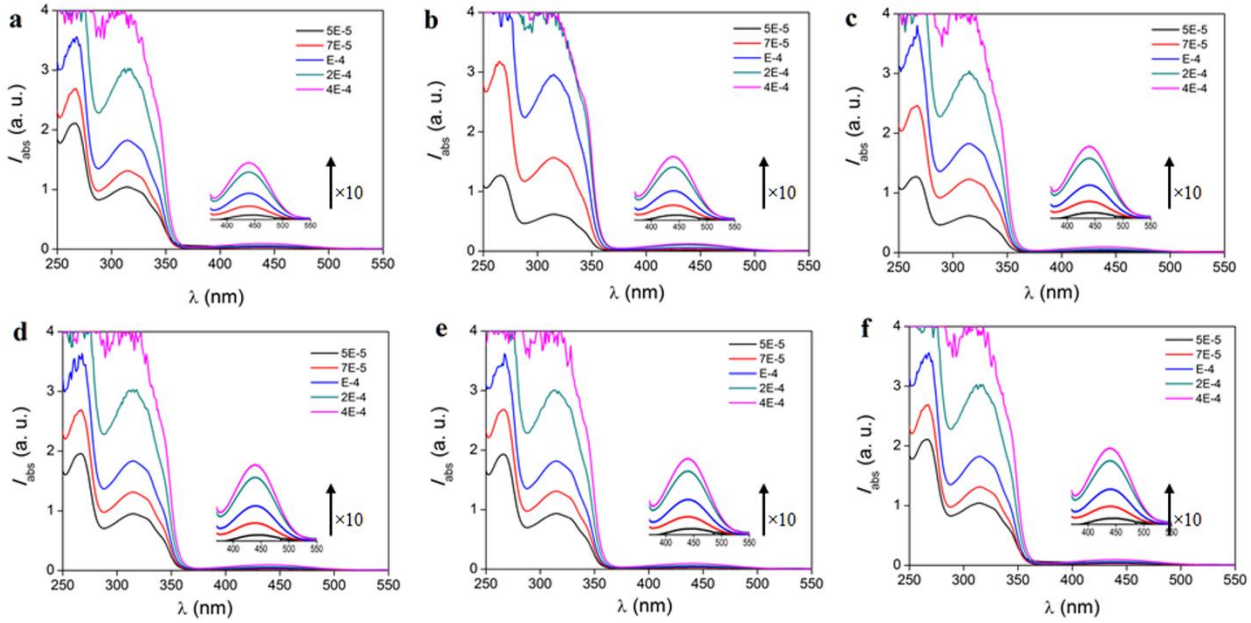


Supporting Figure S15. Solvent dependent absorbance spectra of **PQ3** at (a) 10^{-5} M and (b) 10^{-3} M concentration.

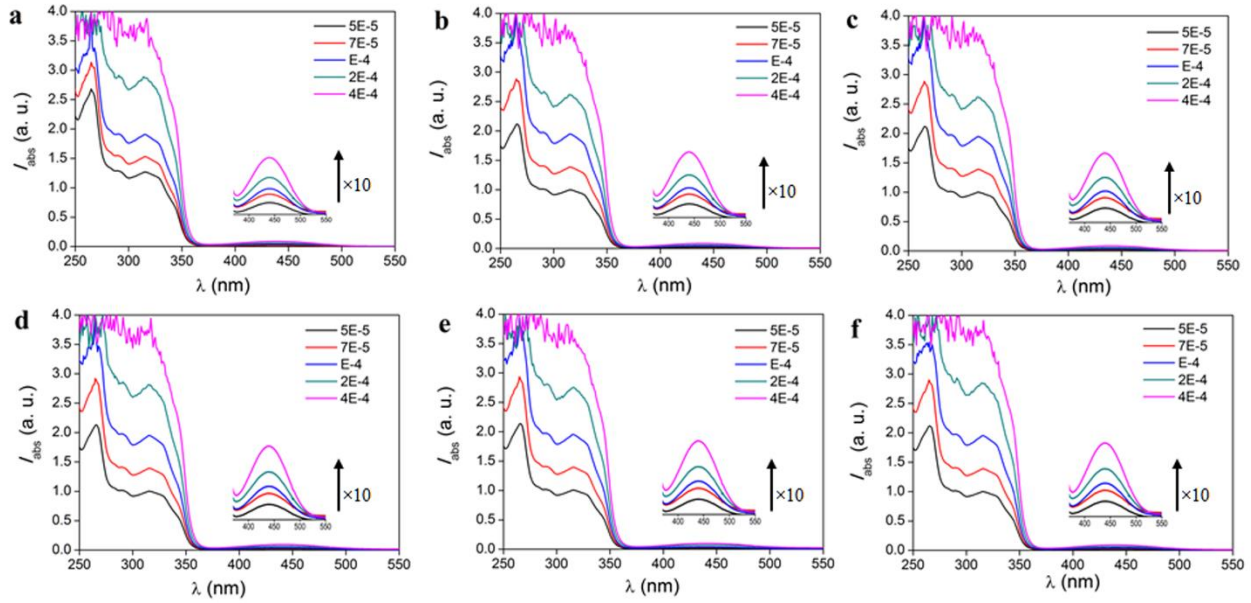


Supporting Figure S16. Absorption spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in DCM with added acid and base.

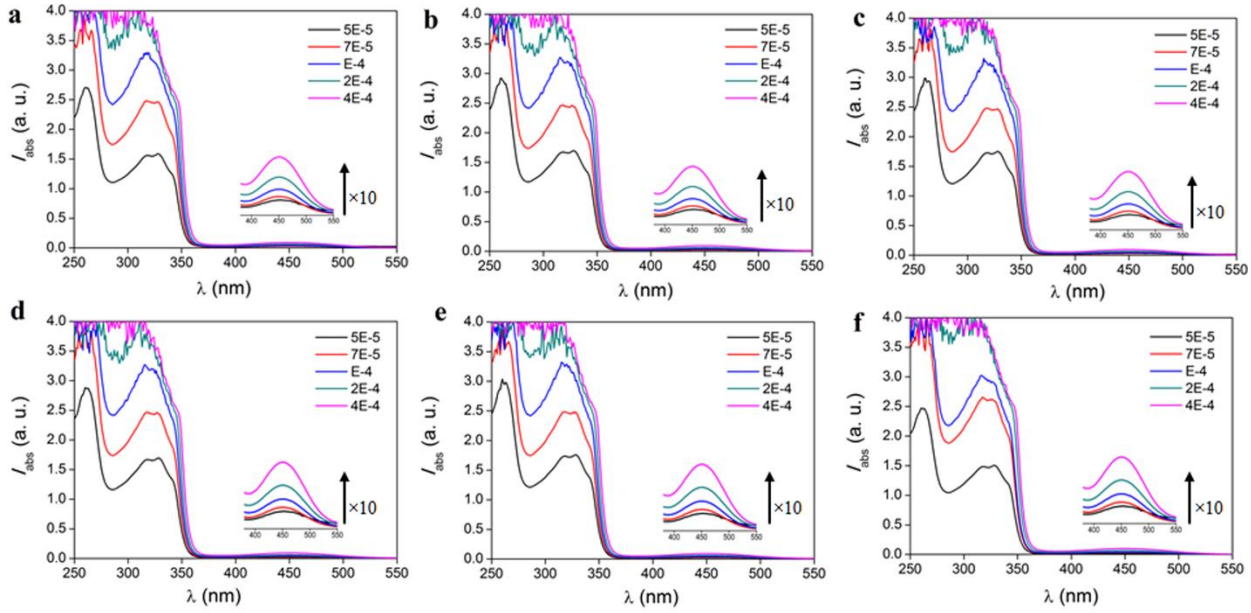
Temperature dependent absorption of PQ1-PQ3 in toluene



Supporting Figure S17. Concentration dependent absorption spectra of **PQ1** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K in toluene.

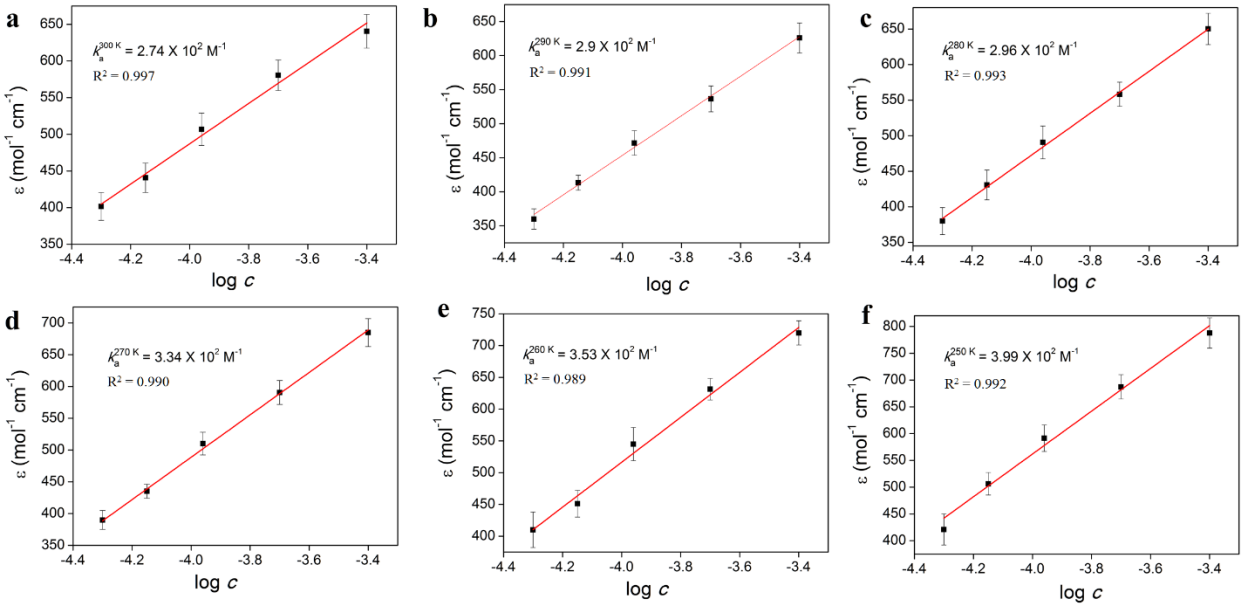


Supporting Figure S18. Concentration dependent absorption spectra of **PQ2** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K in toluene.

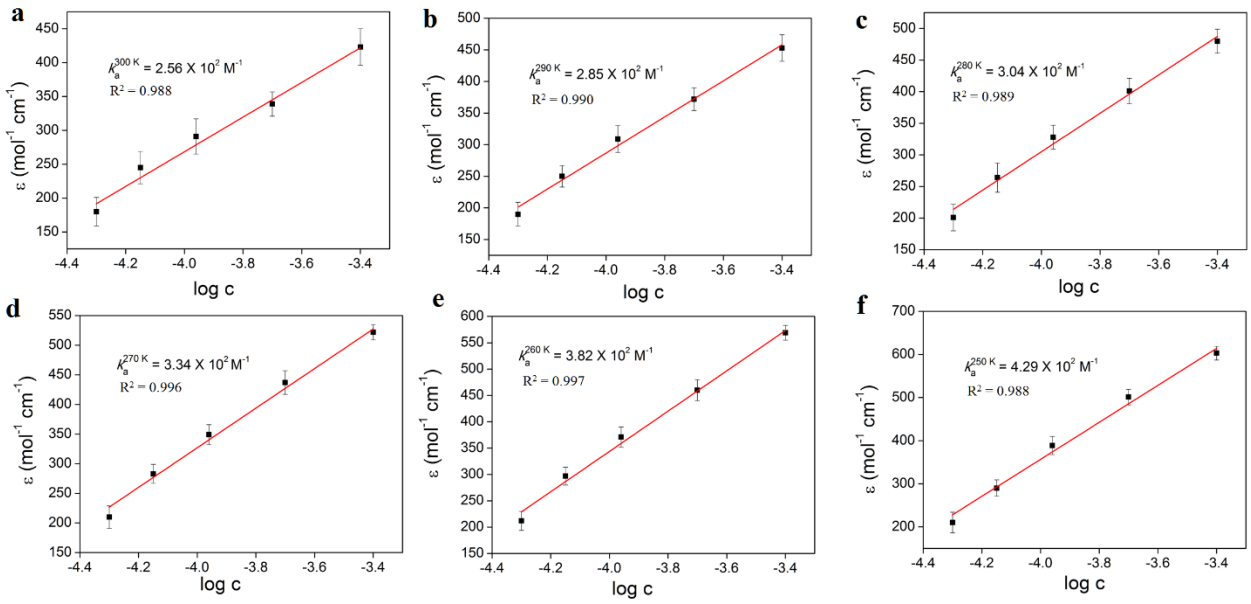


Supporting Figure S19. Concentration dependent absorption spectra of **PQ3** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K in toluene.

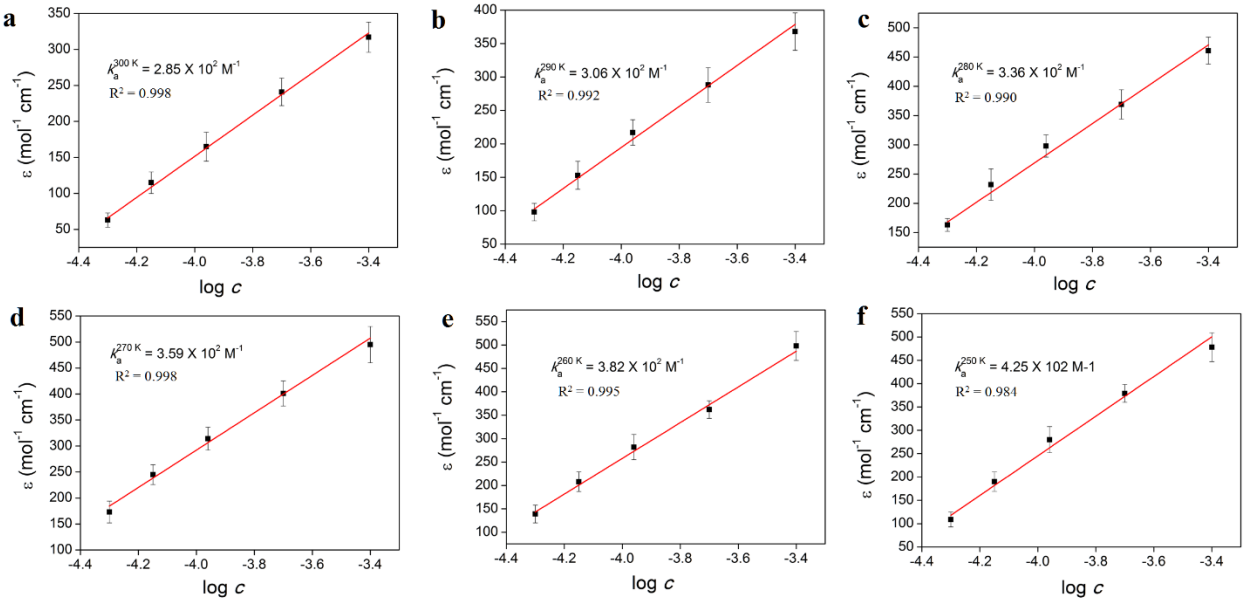
Temperature dependent association constant (k_a) of PQ1-PQ3 in toluene



Supporting Figure S20. Temperature dependent association constant (k_a) of **PQ1** in toluene **PQ3** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K.

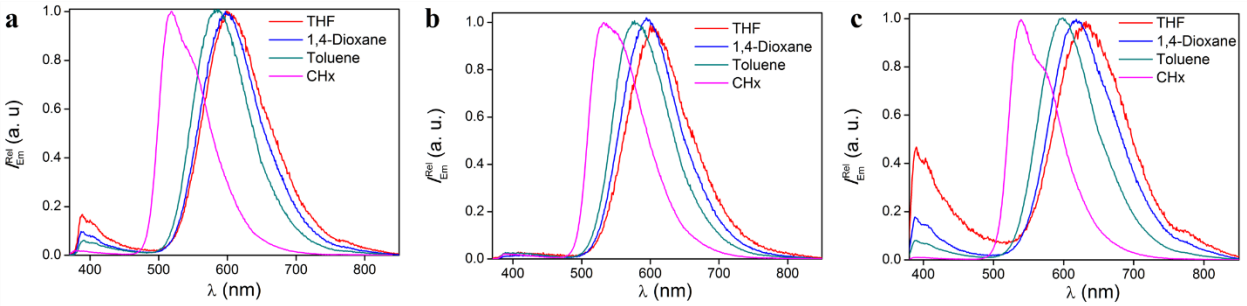


Supporting Figure S21. Temperature dependent association constant (k_a) of **PQ2** in toluene **PQ3** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K.

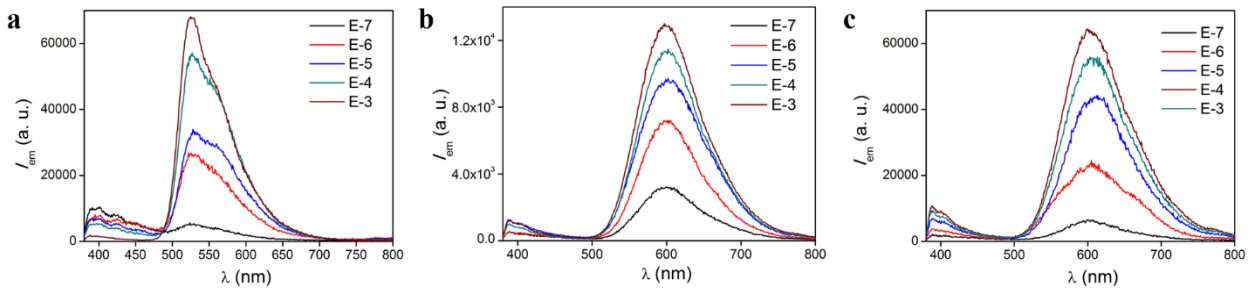


Supporting Figure S22. Temperature dependent association constant (k_a) of **PQ3** in toluene **PQ3** at (a) 300 K, (b) 290 K, (c) 280 K, (d) 270 K, (e) 260 K and (f) 250 K.

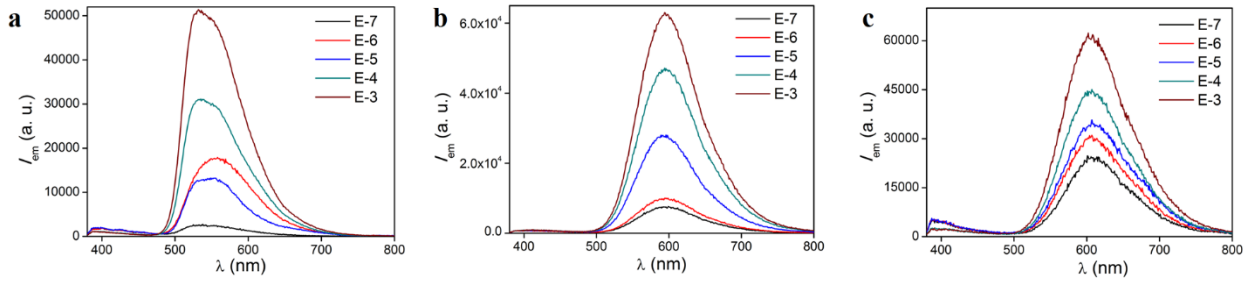
Solvent dependent emission spectra of PQ1-PQ3



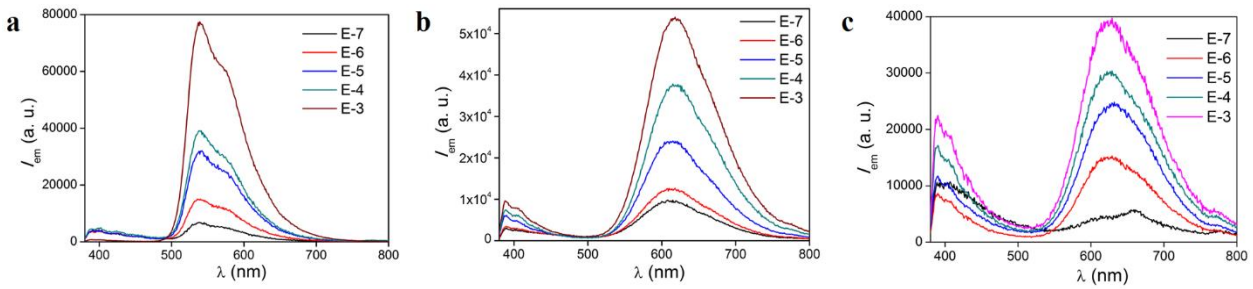
Supporting Figure S23. Solvent dependent emission spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** (O_2 free condition).



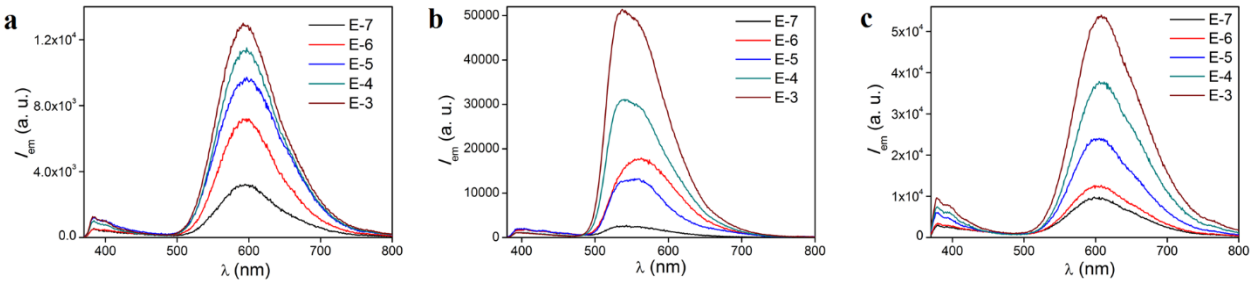
Supporting Figure S24. Concentration dependent emission spectra of **PQ1** in (a) CH, (b) DOX and (c) THF.



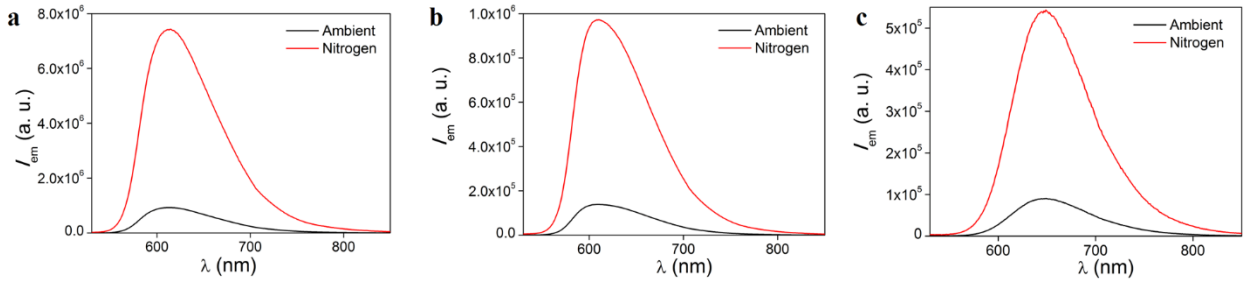
Supporting Figure S25. Concentration dependent emission spectra of **PQ2** in (a) CH, (b) DOX and (c) THF.



Supporting Figure S26. Concentration dependent emission spectra of **PQ3** in (a) CH, (b) DOX and (c) THF.



Supporting Figure S27. Concentration dependent emission spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in $CHCl_3$.

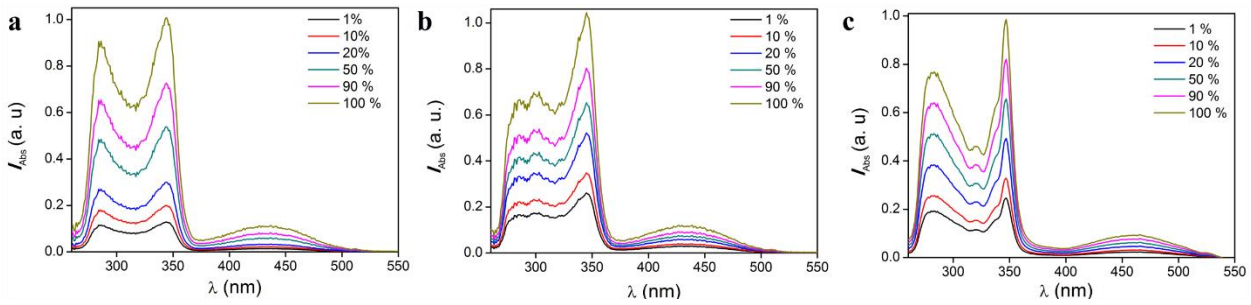


Supporting Figure S28. Emission spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in DCM at ambient and nitrogen atmosphere.

Table S3. Solvent dependent lifetimes of **PQ1**, **PQ2** and **PQ3**.

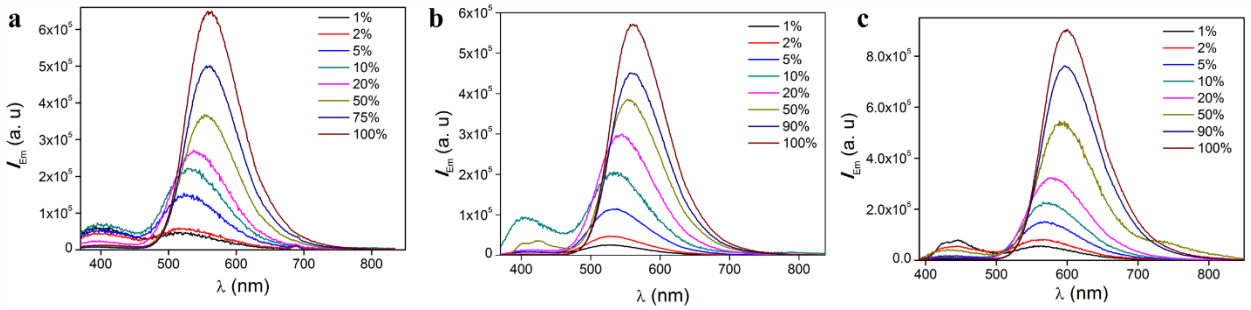
	CH		DOX		$CHCl_3$		THF	
	τ_{PF} (ns)	τ_P (μs)	τ_{PF} (ns)	τ_P (μs)	τ_{PF} (ns)	τ_P (μs)	τ_{PF} (ns)	τ_P (μs)
PQ1	3.1	18.1	3.7	23.1	3.1	22.1	1.8	34.2
PQ2	4.2	12.7	5.1	14.7	6.2	18.3	2.1	7.6
PQ3	1.7	41.4	2.4	42.9	2.2	47.1	1.1	57.1

Concentration dependent (w/w) absorption spectra of PQ1-PQ3 in PMMA matrix

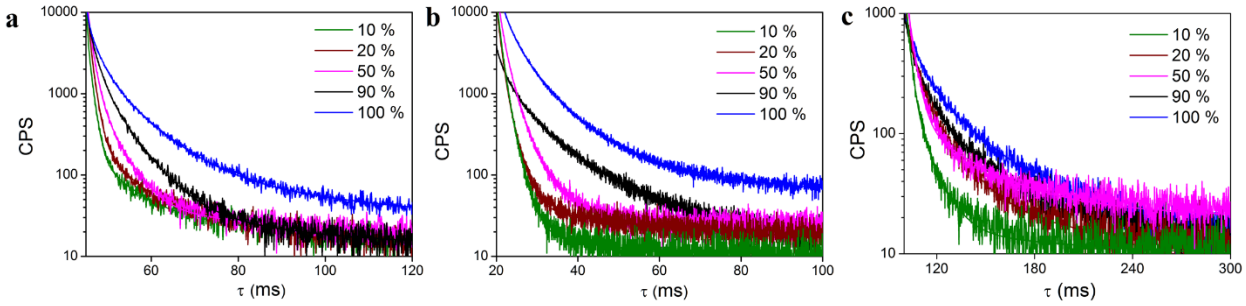


Supporting Figure S29. Concentration dependent absorption spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in PMMA supported matrix.

Concentration dependent (w/w) emission spectra of PQ1-PQ3 in PMMA matrix



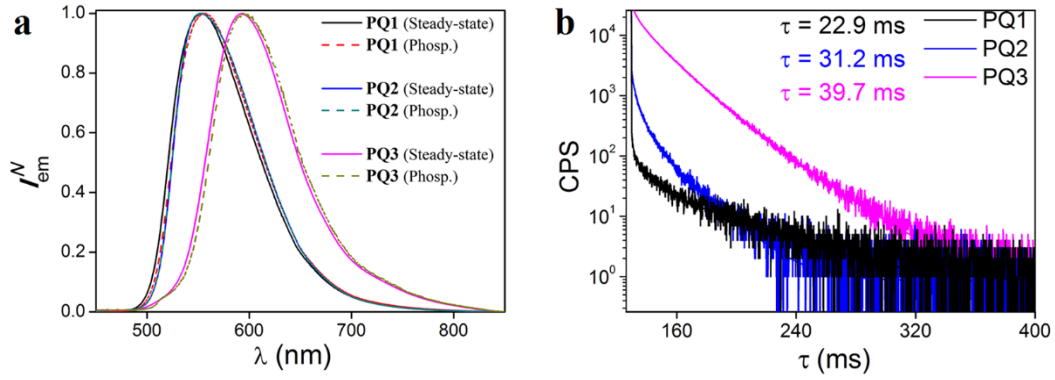
Supporting Figure S30. Concentration dependent emission spectra of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in PMMA supported matrix.



Supporting Figure S31. Concentration dependent phosphorescence decay kinetics of (a) **PQ1**, (b) **PQ2** and (c) **PQ3** in PMMA supported matrix.

Table S4. Lifetime values of **PQ1-PQ3** in thin films

%	10	20	50	90	100
PQ1	3.23	7.59	12.1	13.12	14.6
PQ2	7.92	15.77	21.92	22.53	25.7
PQ3	10.37	20.49	30.72	31.22	32.8



Supporting Figure S32. (a) Stead state emission and phosphorescence of **PQ1**, **PQ2**, and **PQ3** in crystals. (b) Lifetimes of the conjugates.

Computational Analysis

Table S5. Enthalpy change for **PQ1**

		Thermal Correction	Single point energy	Corrected enthalpy (H)	Change in enthalpy (ΔH)
BLYP-D	Monomer	0.443630	-1454.667920	-1454.22429	-0.011808 Hartree
	Dimer	0.892377	-2909.352765	-2908.460388	-7.409 kcal/mol
B3LYP-D3	Monomer	0.484959	-1455.048759	-1454.5638	-0.19498 Hartree
	Dimer	0.920827	-2910.067925	-2909.147098	-12.235 kcal/mol
M06-2X	Monomer	0.463853	-1454.459179	-1453.995326	-0.027809 Hartree
	Dimer	0.928546	-2908.947007	-2908.018461	-17.45 kcal/mol
M06-L	Monomer	0.458931	-1454.874556	-1454.415625	-0.016814 Hartree
	Dimer	0.919632	-2909.767696	-2908.848064	-10.55 kcal/mol

Change in enthalpy (ΔH) = $H_{Dimer} - 2H_{Monomer}$

Table S6. Enthalpy change for **PQ2**

		Thermal Correction	Single point energy	Corrected enthalpy (H)	Change in enthalpy (ΔH)
BLYP-D	Monomer	0.488982	-1607.998869	-1607.509887	-0.014452 Hartree
	Dimer	0.983923	-3216.018149	-3215.034226	-9.068 kcal/mol
B3LYP-D3	Monomer	0.505083	-1608.643179	-1608.138096	-0.010001 Hartree
	Dimer	1.015575	-3217.301768	-3216.286193	-6.275 kcal/mol
M06-2X	Monomer	0.510834	-1608.008064	-1607.49723	-0.007728 Hartree
	Dimer	1.023343	-3216.025531	-3215.002188	-4.849 kcal/mol
M06-L	Monomer	0.505698	-1608.452740	-1607.947042	-0.016486 Hartree
	Dimer	1.013498	-3216.924068	-3215.91057	-10.345 kcal/mol

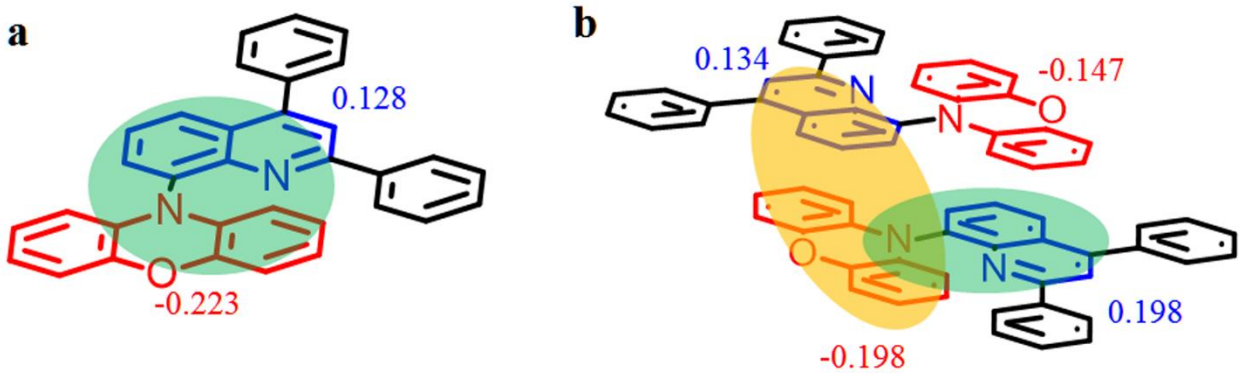
Change in enthalpy (ΔH) = $H_{Dimer} - 2H_{Monomer}$

Table S7. Enthalpy change for **PQ3**

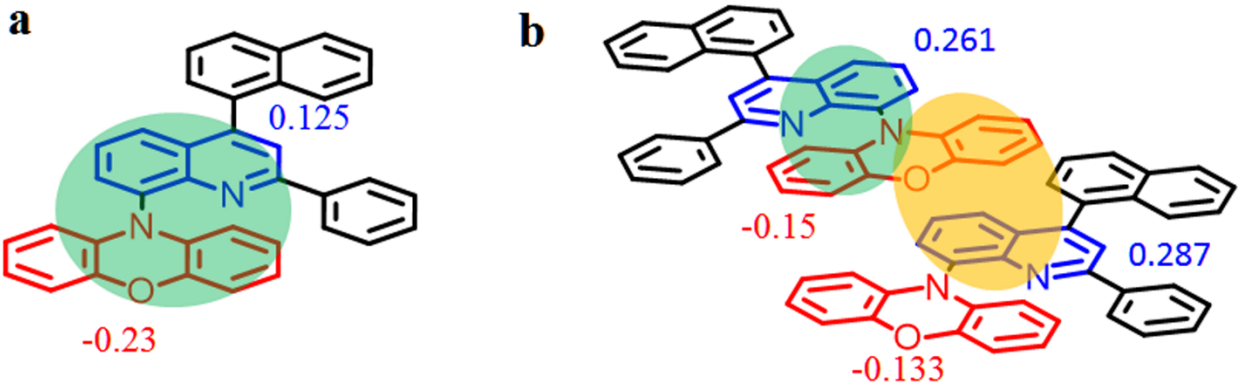
		Thermal Correction	Single point energy	Corrected enthalpy (H)	Change in enthalpy (ΔH)
BLYP-D	Monomer	0.507488	-1624.299809	-1623.792321	-0.015157 Hartree
	Dimer	1.021786	-3248.620985	-3247.599199	-9.511 kcal/mol
B3LYP-D3	Monomer	0.522417	-1624.702298	-1624.179881	-0.01964 Hartree
	Dimer	1.050994	-3249.439342	-3248.379402	-12.324 kcal/mol
M06-2X	Monomer	0.527775	-1624.059424	-1623.531649	-0.023132 Hartree
	Dimer	1.059210	-3248.145640	-3247.08643	-14.515 kcal/mol
M06-L	Monomer	0.523096	-1624.518764	-1623.995668	-0.013825 Hartree
	Dimer	1.048633	-3249.053794	-3248.005161	-8.675 kcal/mol

Change in enthalpy (ΔH) = $H_{Dimer} - 2H_{Monomer}$

Natural population analysis (NPA) of PQ1 and PQ2

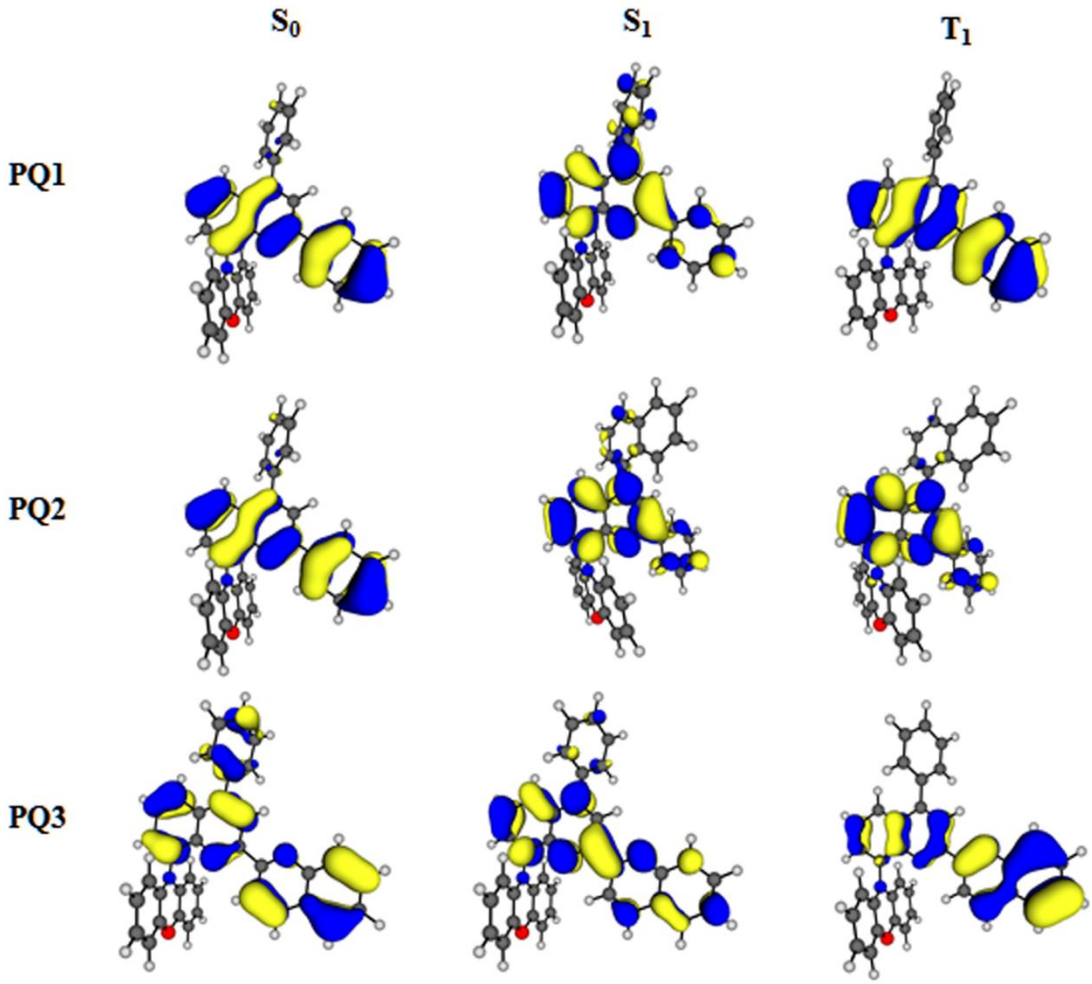


Supporting Figure S33. Natural population analysis (NPA) of **PQ1** (a) monomer and (b) dimer.

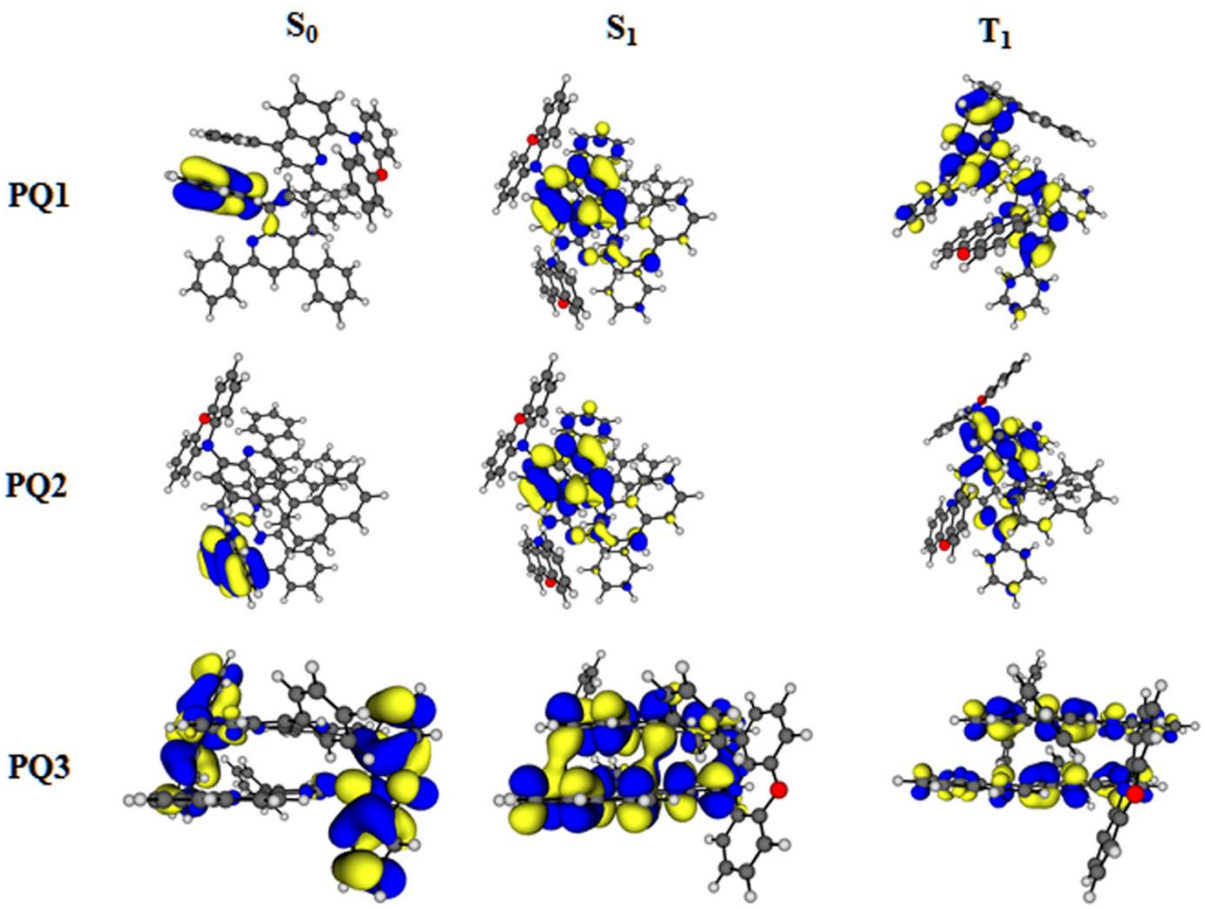


Supporting Figure S34. Natural population analysis (NPA) of **PQ2** (a) monomer and (b) dimer.

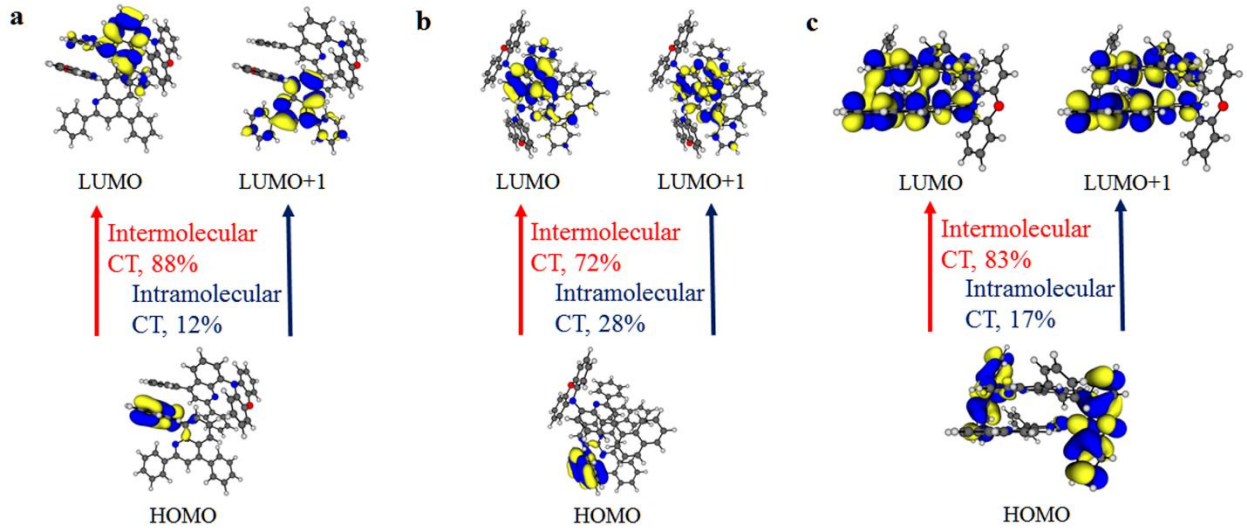
Calculated Isosurface of PQ1-PQ3 monomer and dimers



Supporting Figure S35. Calculated isosurface of **PQ1-PQ3** monomers at M06-2X/6-31G(d) level of theory.



Supporting Figure S36. Calculated isosurface of **PQ1-PQ3** dimers at M06-2X/6-31G(d) level of theory.



Supporting Figure S37. Degree of charge transfer in the dimers of **PQ1-PQ3**

Supporting Table S8. Calculated orbital energy of **PQ1**

		B3LYP-D3 (eV)	**M06-2X (eV)**
S_0	Monomer	-4.481	-5.92
	Dimer	-4.52	-5.78
S_1	Monomer	-1.85	-1.02
	Dimer	-1.92	-2.07
T_1	Monomer	-2.30	-2.80
	Dimer	-2.03	-2.12
ΔE_{ST}	Monomer	0.69	0.521
	Dimer	0.11	0.05

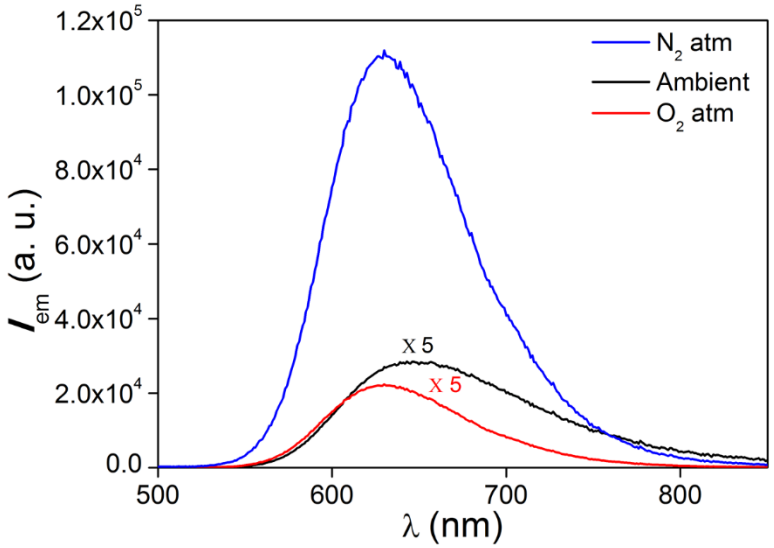
Supporting Table S9. Calculated orbital energy of **PQ2**

		B3LYP-D3 (eV)	**M06-2X (eV)**
S_0	Monomer	-4.49	-5.91
	Dimer	-4.75	-6.08
S_1	Monomer	-1.83	-1.03
	Dimer	-1.88	-2.02
T_1	Monomer	-2.25	-2.81
	Dimer	-2.01	-2.16
ΔE_{ST}	Monomer	0.42	1.78
	Dimer	0.13	0.14

Supporting Table S10. Calculated orbital energy of **PQ3**

		B3LYP-D3 (eV)	**M06-2X (eV)**
S_0	Monomer	-4.52	-5.98
	Dimer	-4.58	-5.89
S_1	Monomer	-2.01	-2.19
	Dimer	-2.15	-2.93
T_1	Monomer	-2.38	-2.88
	Dimer	-2.19	-3.02
	Monomer	0.37	0.69

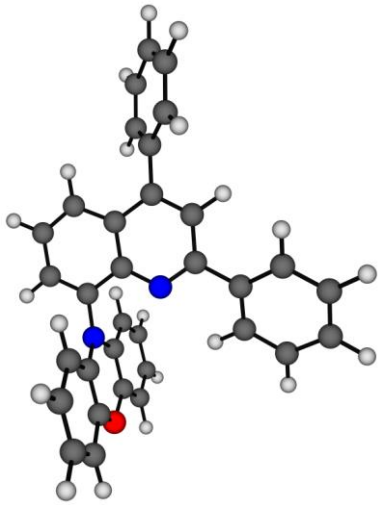
ΔE_{ST}	Dimer	0.04	0.09



Supporting Figure S38. Emission spectra of **PQ3** in PBS:DMSO (9:1 v/v) mixture at various conditions.

Coordinate

PQ1



7	1.916625000	-1.471472000	0.076432000
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6	2.513556000	-1.175083000	-1.166374000
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6	-4.291756000	-0.419201000	0.002667000
6	1.867282000	-1.386311000	-2.388890000
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6	0.174889000	-3.155569000	0.240005000
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6	-2.176478000	-2.576827000	0.255405000
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6	1.997770000	-1.178788000	2.525456000
1	0.985118000	-1.555333000	2.614833000
6	-1.185322000	-3.531431000	0.314780000
1	-1.445353000	-4.580181000	0.424877000
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6	3.829125000	-0.676015000	-1.193267000
6	0.835230000	3.089446000	-0.507373000
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6	2.509920000	-1.107413000	-3.598884000
1	1.981564000	-1.283952000	-4.531461000
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	6	-6.237286000	-1.464539000	-1.016462000
	1	-6.658831000	-2.112623000	-1.780140000
	6	4.466448000	-0.392451000	-2.392950000
	1	5.481030000	-0.008040000	-2.354243000
PQ1$_2$	7	-2.768154000	-0.745003000	-0.695337000
	7	-4.979545000	-0.755625000	0.922001000
	8	-5.107123000	1.980847000	0.151322000
	6	-3.008996000	-1.891338000	-0.018942000
	6	-2.166660000	-3.044320000	-0.096174000
	6	-4.488034000	0.269751000	1.765674000
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	6	-0.827334000	-1.774901000	-1.649660000
	1	0.064025000	-1.676159000	-2.252545000
	6	-5.670620000	-0.351417000	-0.247045000
	6	-1.496009000	0.609712000	-2.201132000
	6	0.028585000	-3.997991000	-1.001199000
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	6	-4.492847000	-3.081495000	1.503909000
	1	-5.386377000	-3.090330000	2.120139000
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	6	-6.975747000	-0.873629000	-2.224195000
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	6	0.561738000	-4.571712000	0.164370000
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	6	-2.092473000	2.947208000	-2.482234000
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	6	-0.298084000	2.007138000	-3.790626000
	1	0.479135000	2.111945000	-4.542230000
	6	-6.412858000	1.419007000	-1.735205000
	1	-6.426109000	2.478674000	-1.968870000
	6	-7.034297000	0.477343000	-2.558546000
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	6	0.546165000	-4.391545000	-2.244048000
	1	0.143893000	-3.949787000	-3.150617000
	6	-1.089974000	3.101822000	-3.443838000
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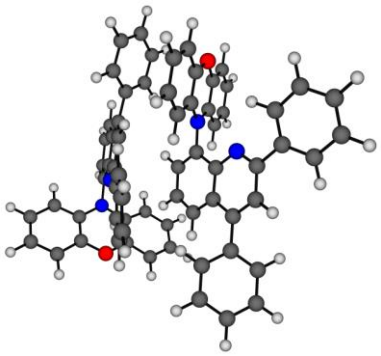

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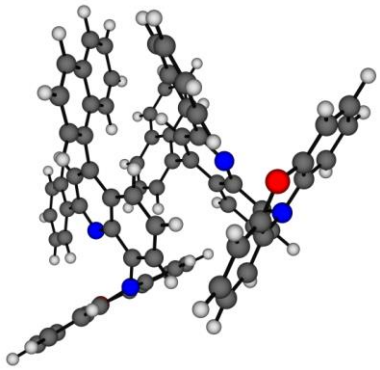

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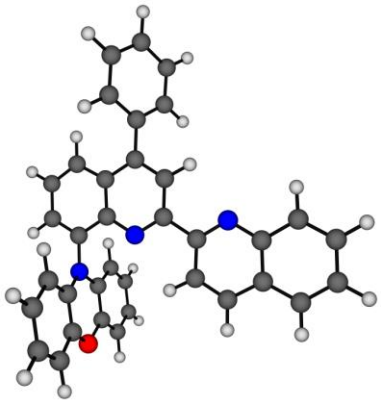	6	-2.316213000	-0.250662000	-0.020360000
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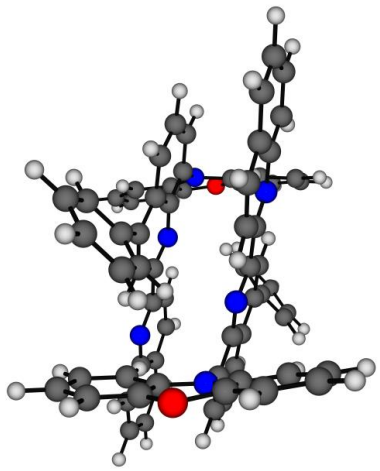

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(1) Bhattacharjee, I.; Acharya, N.; Bhatia, H.; Ray, D. Dual Emission through Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence, and Their Thermal Enhancement Via Solid-State Structural Change in a Carbazole-Quinoline Conjugate. *J. Phys. Chem. Lett.* **2018**, *9*, 2733-2738.