Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supplementary Information

Quinoxaline Based D-A-D Molecules: High Contrast Reversible Solid-state Mechano- and Thermo-Responsive Fluorescent Materials

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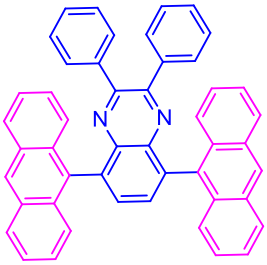


AnQ

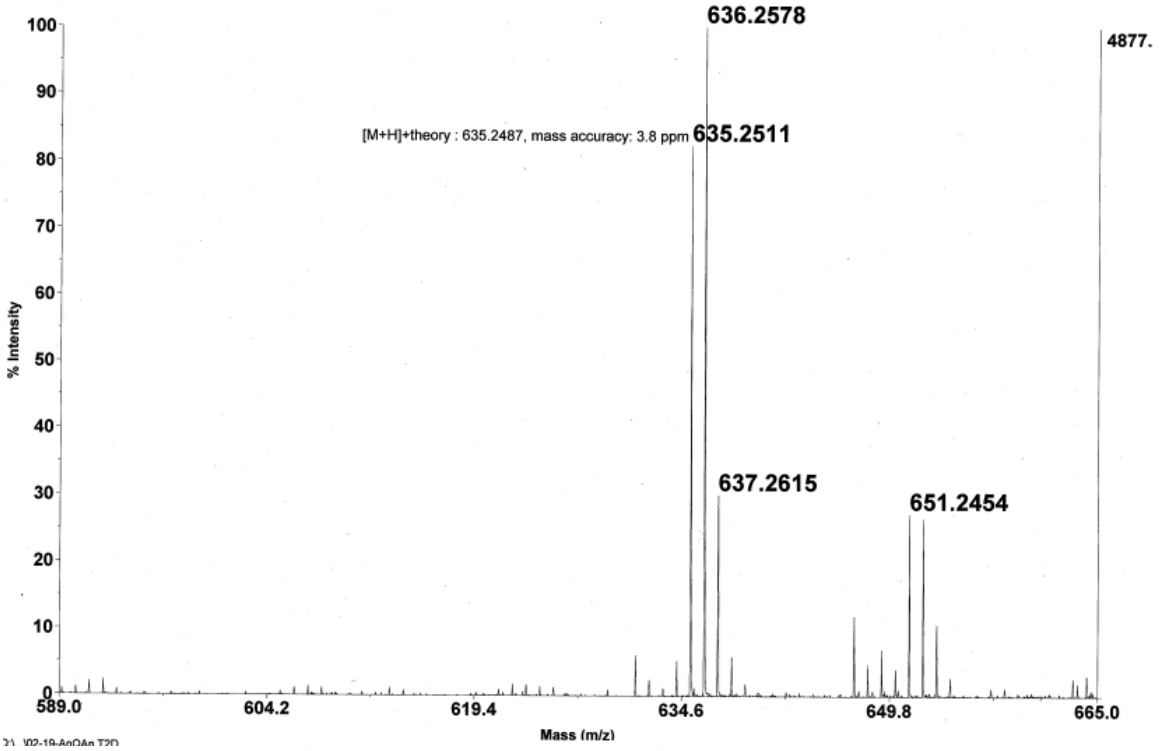


Figure S1. HR-MS mass spectrum of **AnQ**.

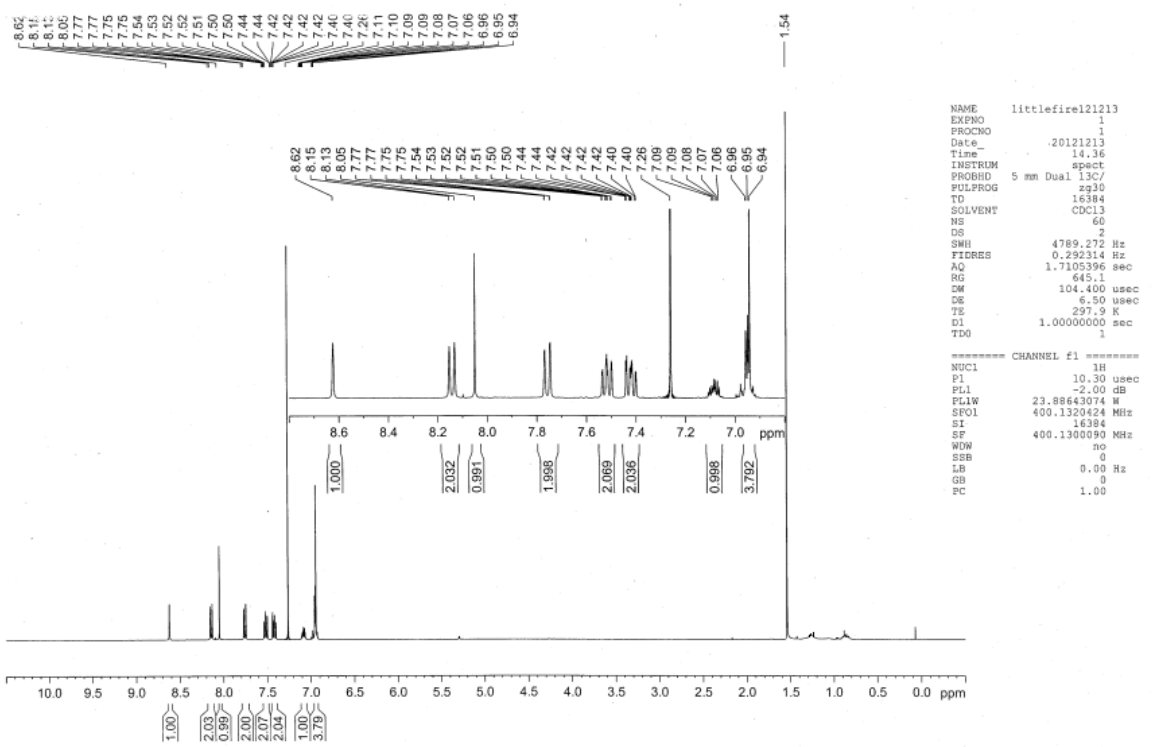


Figure S2. ^{1}H NMR spectrum of **AnQ** in $CDCl_3$.

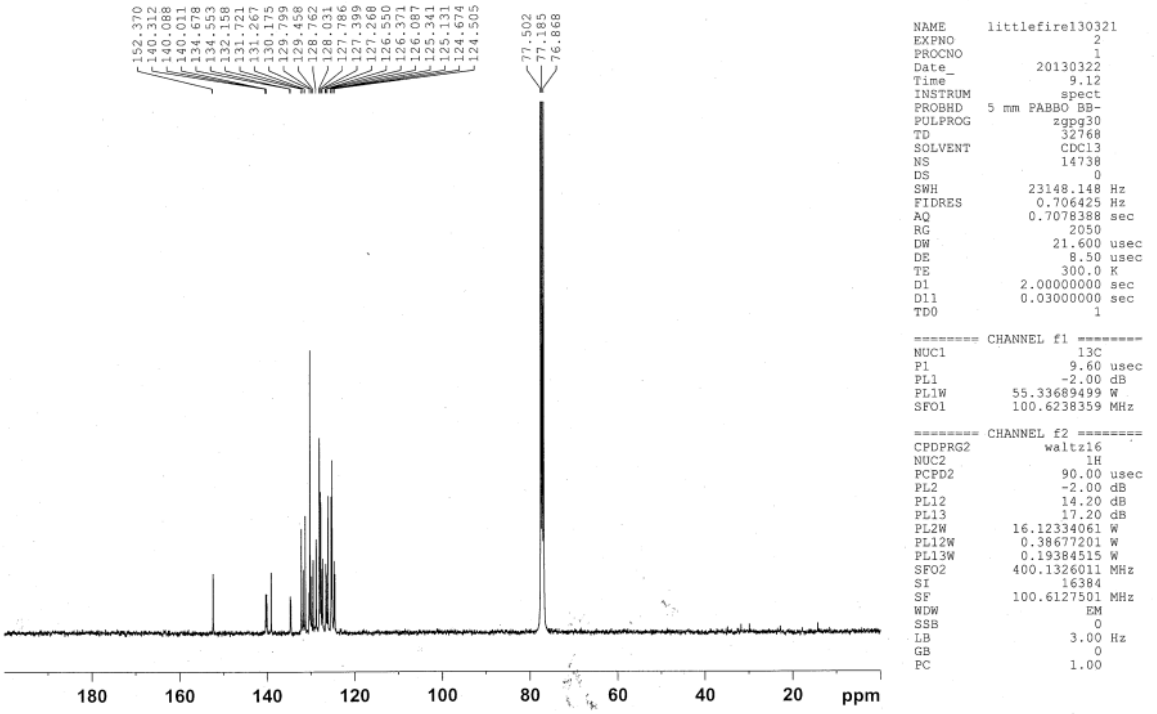
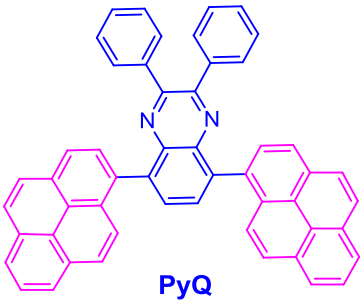


Figure S3. ^{13}C NMR spectrum of **AnQ** in $CDCl_3$.



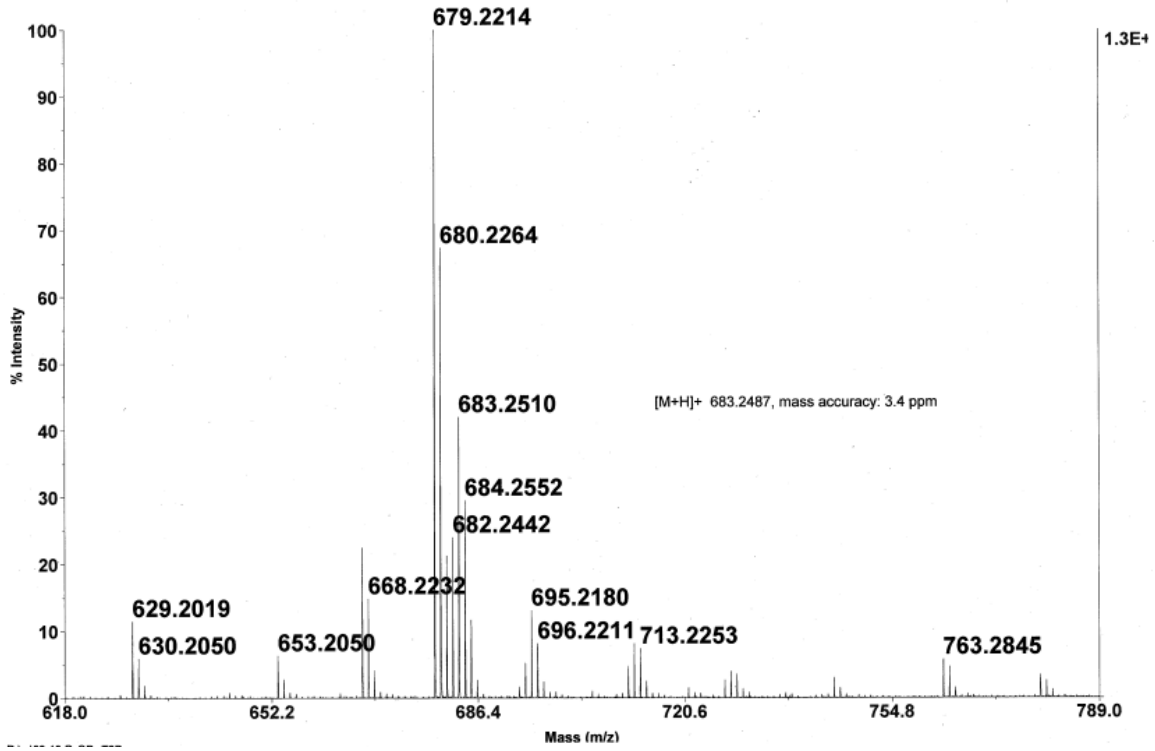


Figure S4. HR-MS mass spectrum of **PyQ**.

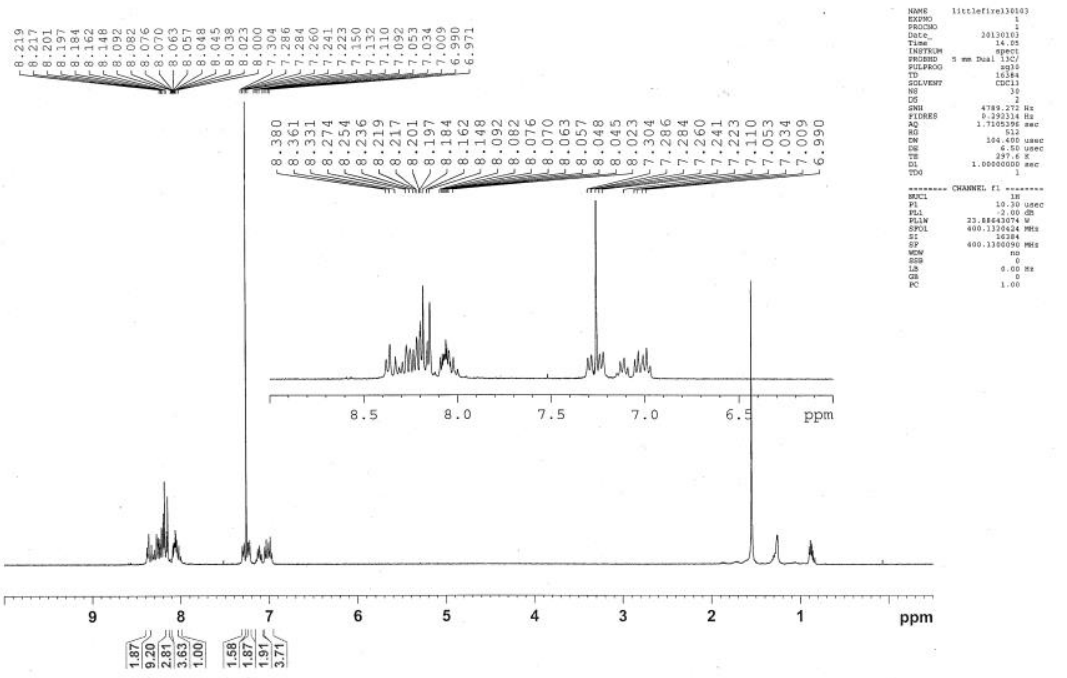


Figure S5. ^{1}H NMR spectrum of **PyQ** in $CDCl_3$.

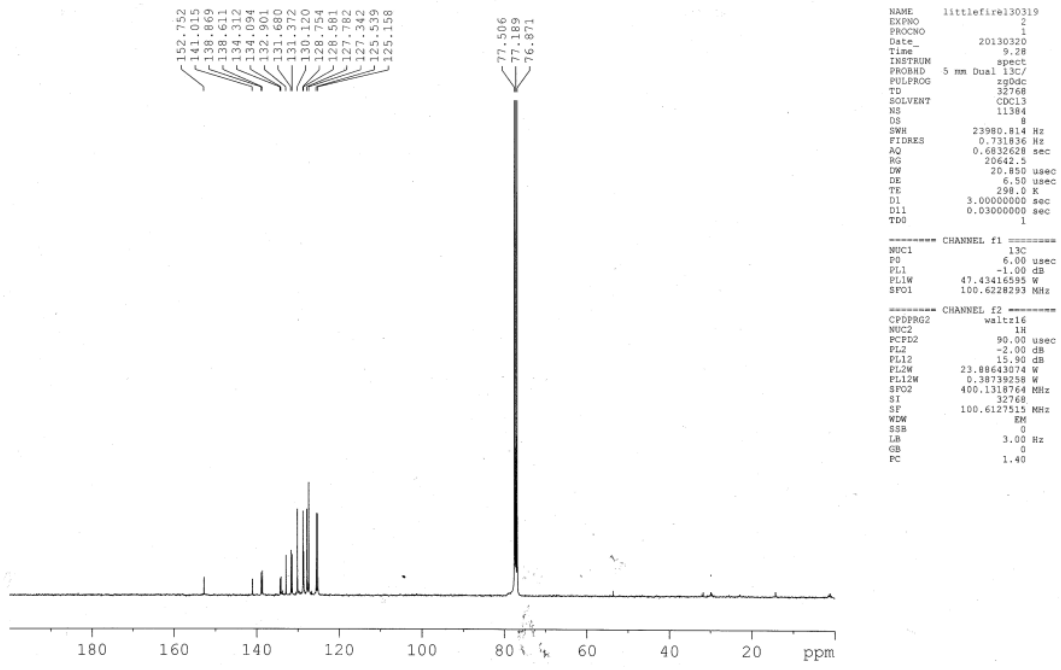


Figure S6. ^{13}C NMR spectrum of **PyQ** in $CDCl_3$.

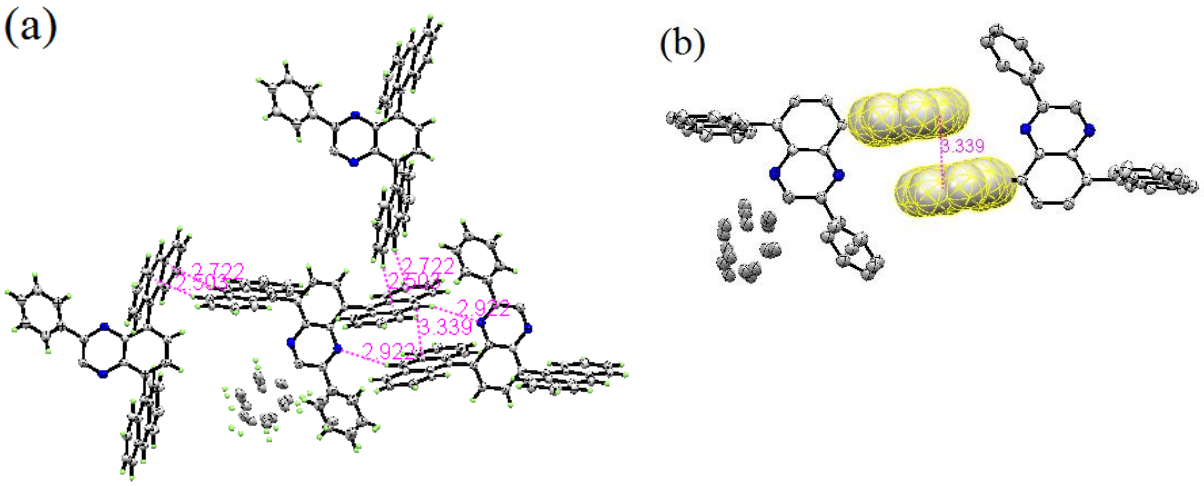


Figure S7. (a) Molecular stacking structures of **AnQ** depicting C–H···N and C–H···π interactions; (b) Representation of π-π interactions between AnQ dimer.

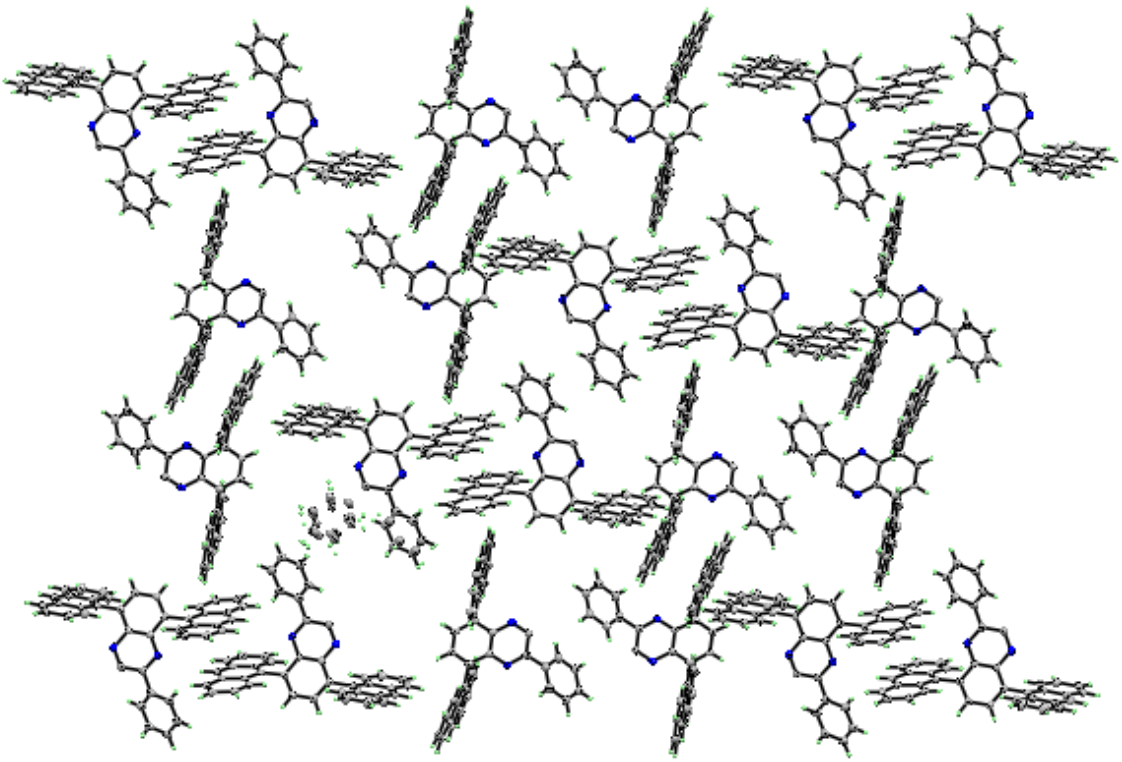


Figure S8. Higher order molecular stacking structures of **AnQ**.

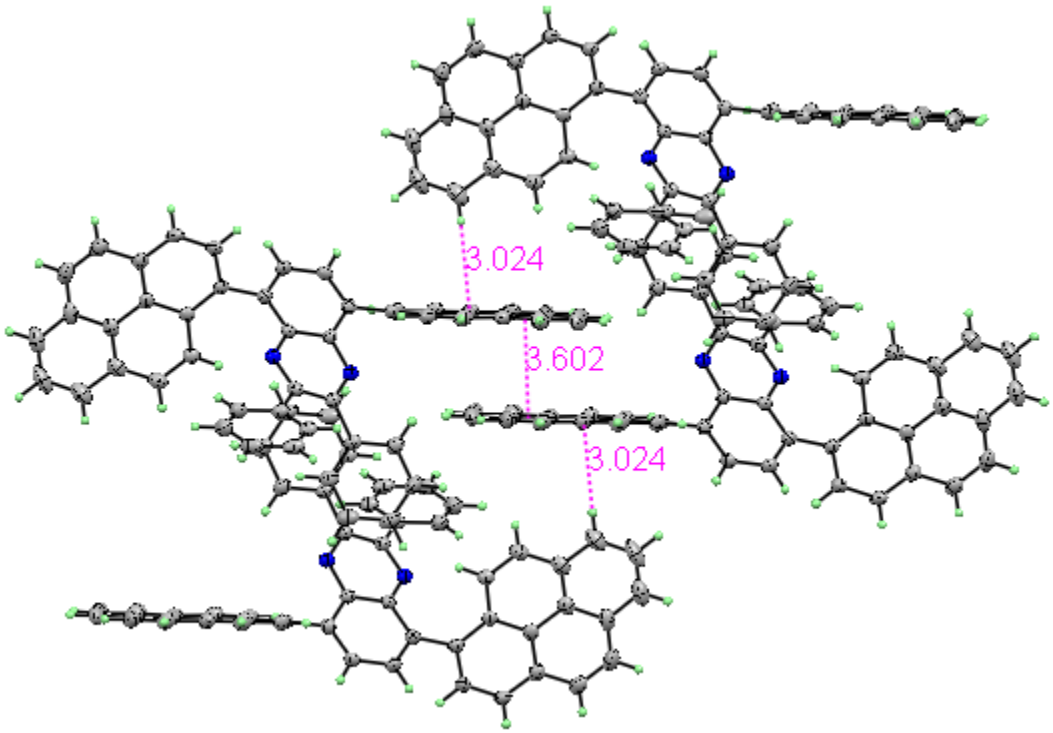


Figure S9. Molecular stacking structures of **PyQ** depicting π–π and C–H···π interactions.

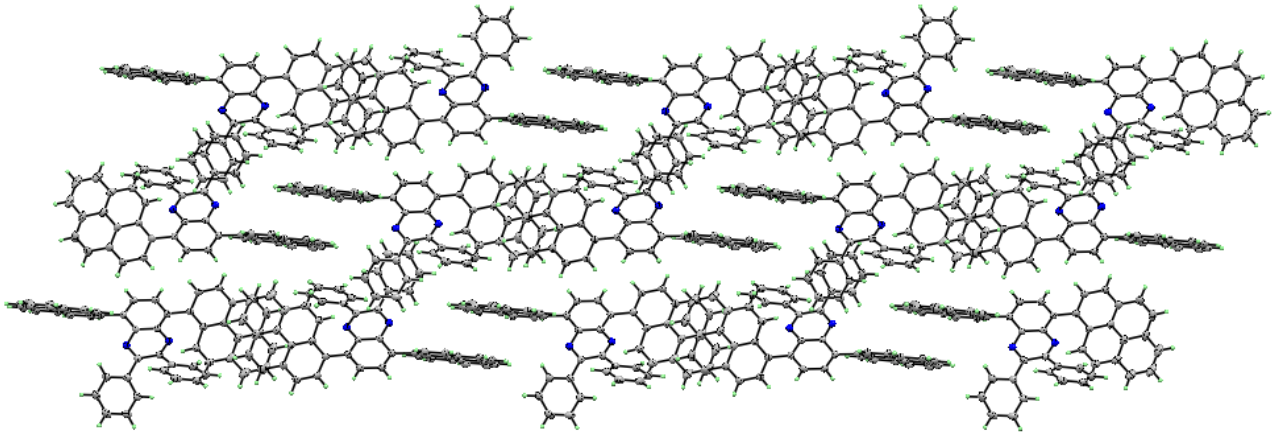


Figure S10. Higher order molecular stacking structures of **PyQ**.

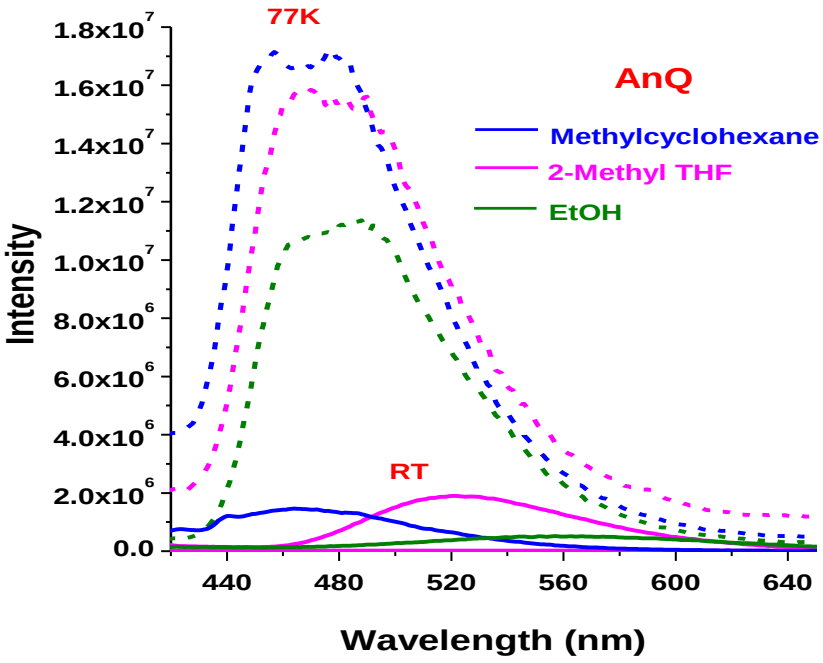


Figure S11. PL spectra of **AnQ** in various solvents at 77 K (⋯) and RT (—) (1×10^{-6} M).

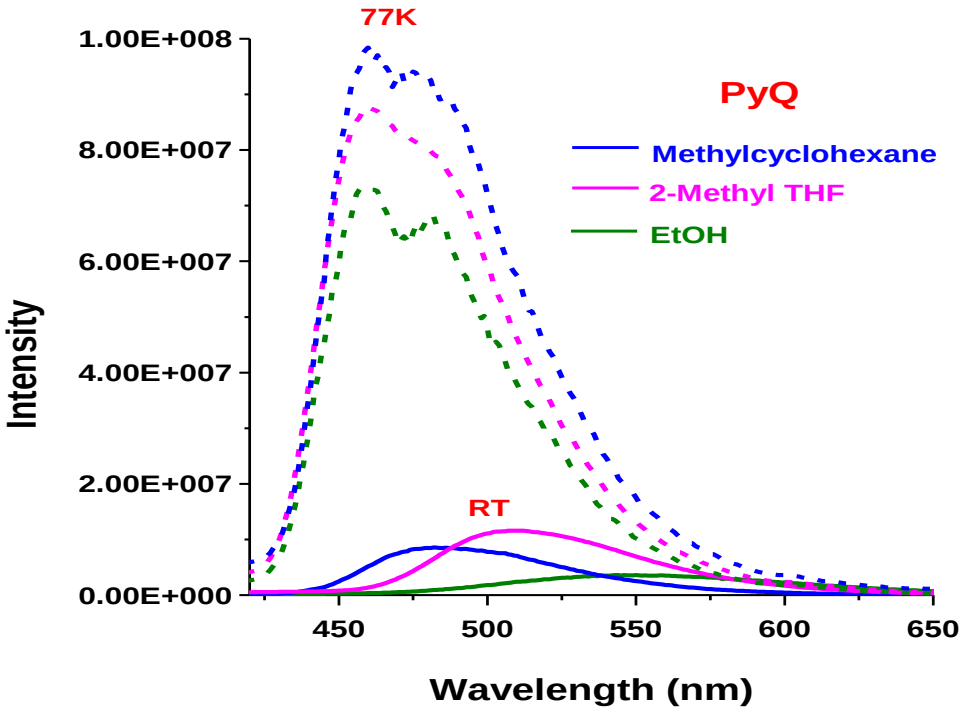


Figure S12. PL spectra of **PyQ** in various solvents at 77 K (⋯) and RT (—) (1×10^{-6} M).

Table S1. Emission data of **AnQ** and **PyQ** at room temperature and 77 K

	Methylcyclohexane		2-MeTHF		EtOH	
	RT	77 K	RT	77 K	RT	77 K
AnQ	469	457	523	468	563	467
PyQ	483	460	512	460	557	460

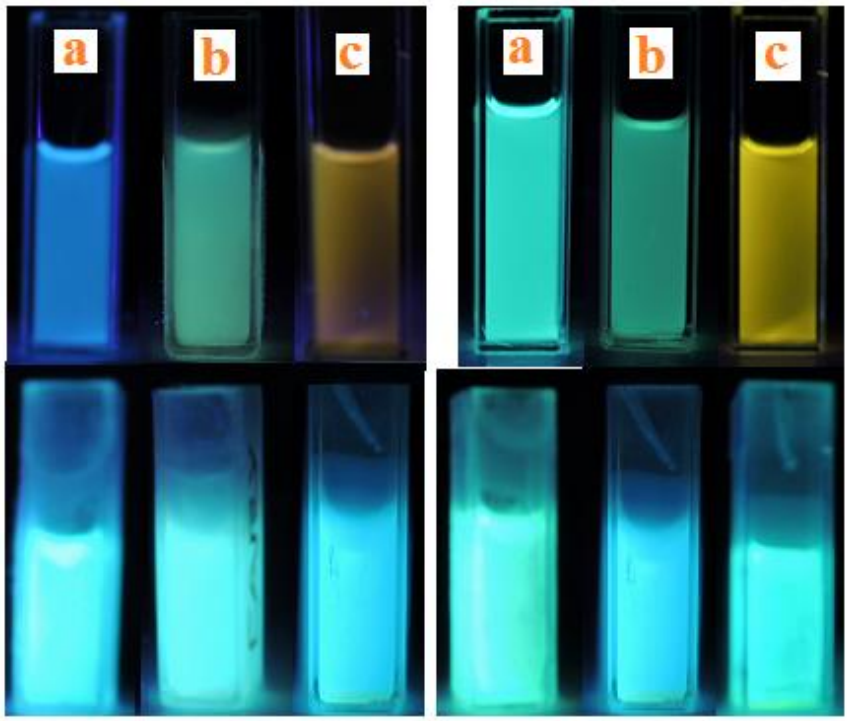


Figure S13. Photograph of **AnQ** (left) and **PyQ** (right) in three different solvent at r.t. (above) and 77 K (below) taken under UV-lamp (365 nm) (**a**: methylcyclohexane; **b**: 2-methyl THF; **c**: EtOH).

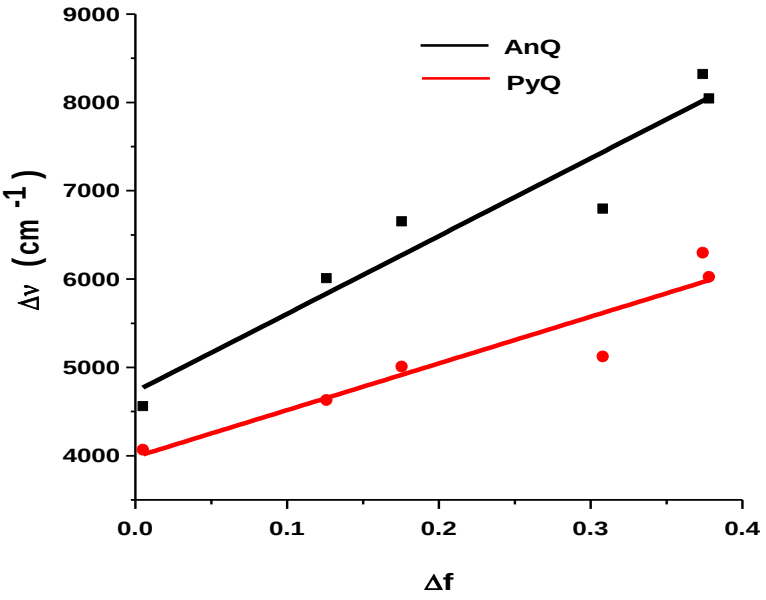


Figure S14. Plot of Stokes shift (Δν) of **AnQ** and **PyQ** verses *Δf* of their solutions.

Figure S15. Photograph of **AnQ** in different solvents taken under UV-lamp (365 nm).

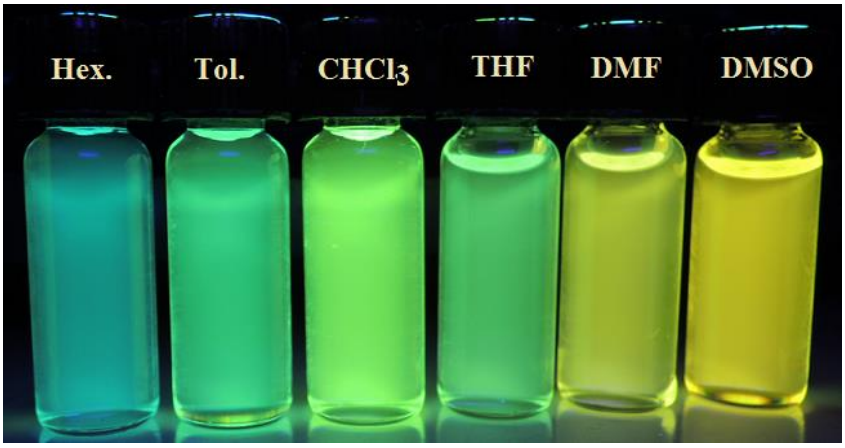


Figure S16. Photograph of **PyQ** in different solvents taken under UV-lamp (365 nm).

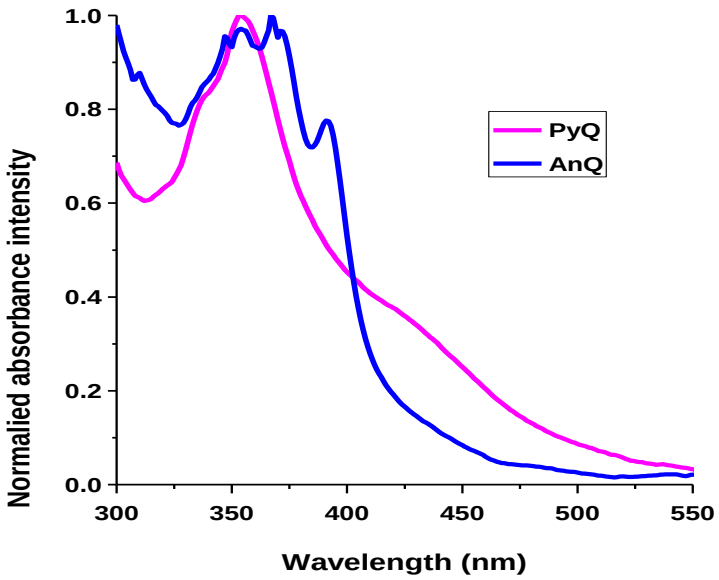


Figure S17. Absorption spectra of **AnQ** and **PyQ** in the solid state.

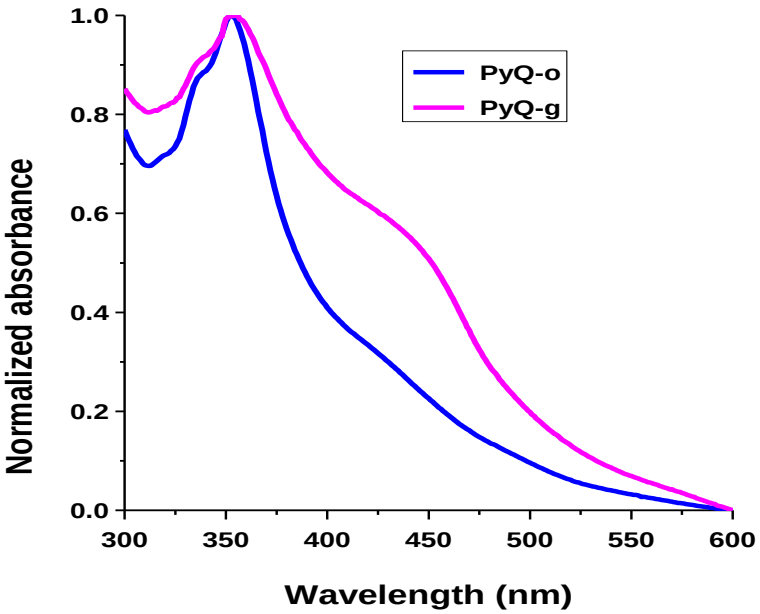


Figure S18. Absorption spectra of **PyQ-p** and **PyQ-g** in the solid state.

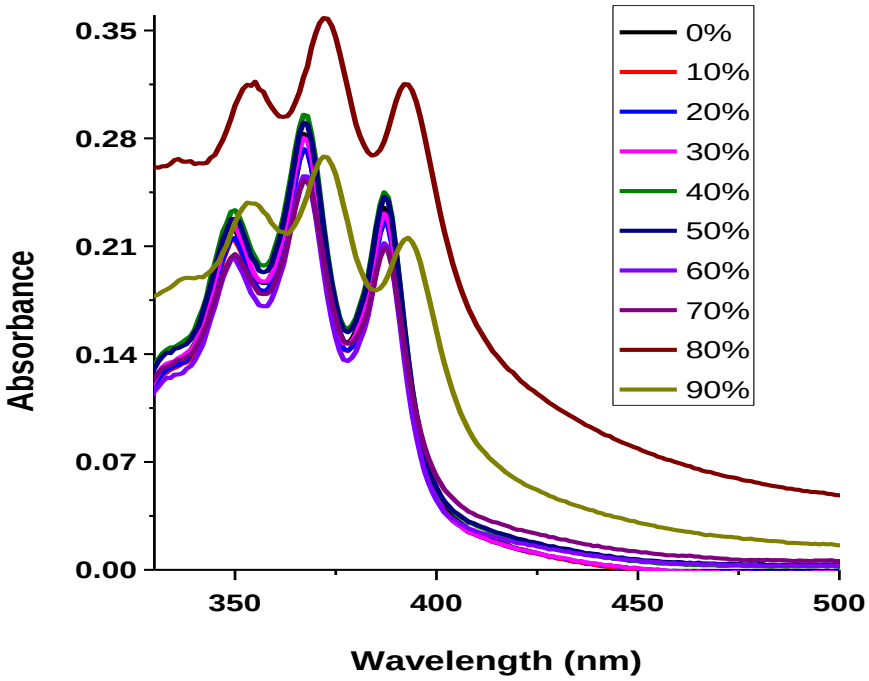


Figure S19. Absorption spectra of **AnQ** in various THF/water mixtures respectively.

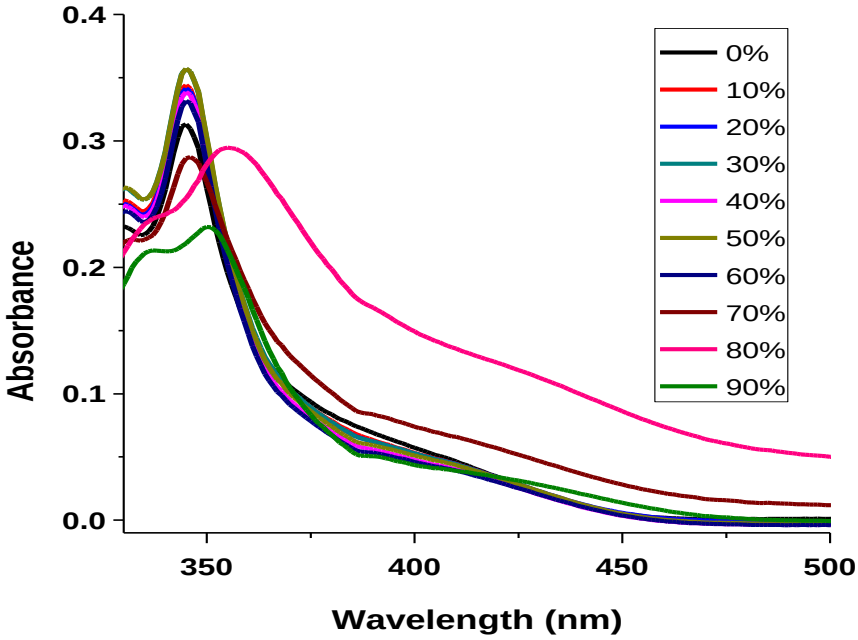


Figure S20. Absorption spectra of **PyQ** in various THF/water mixtures respectively.

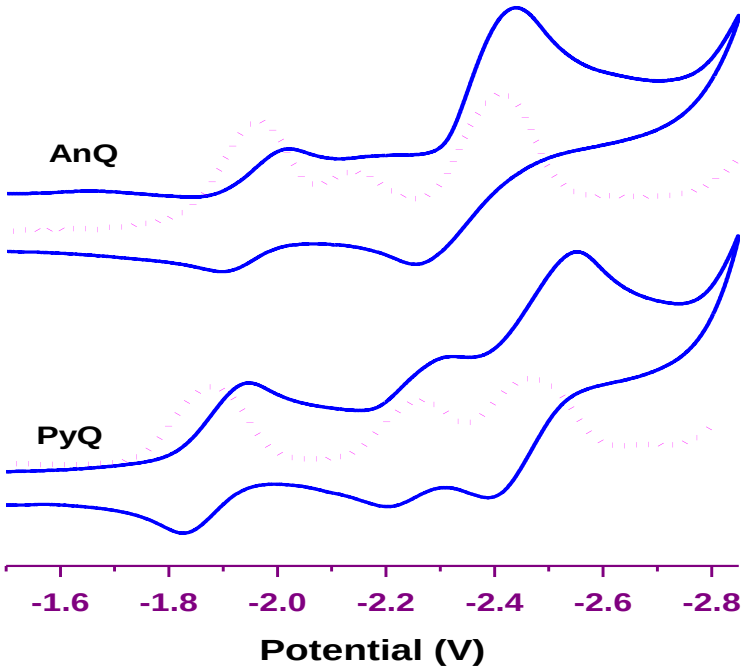


Figure S21. Comparison of reduction waves of cyclic voltammograms of **AnQ** and **PyQ** recorded in CH_2Cl_2 containing 0.1 M TBAP as supporting electrolyte recorded at 50 mV s^{-1} scan speed.

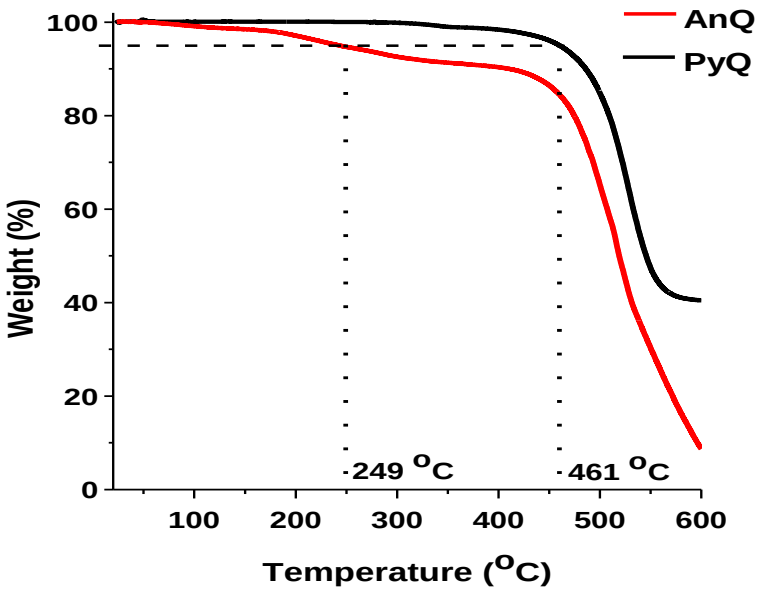


Figure S22. TGA thermograms of **AnQ** and **PyQ** recorded under nitrogen at a heating rate of 10 °C min^{-1}.

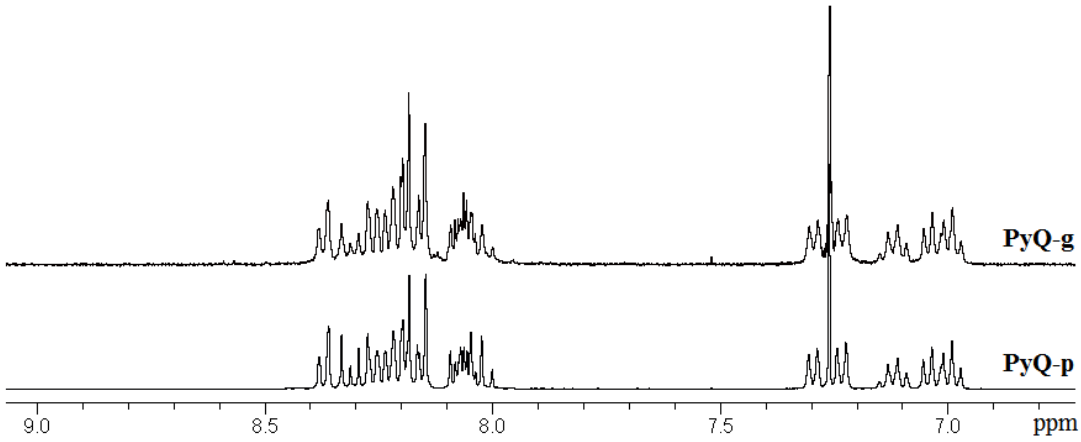


Figure S23. ^{1}H NMR spectra of **PyQ-p** and **PyQ-g** in the selected region recorded in $CDCl_3$.

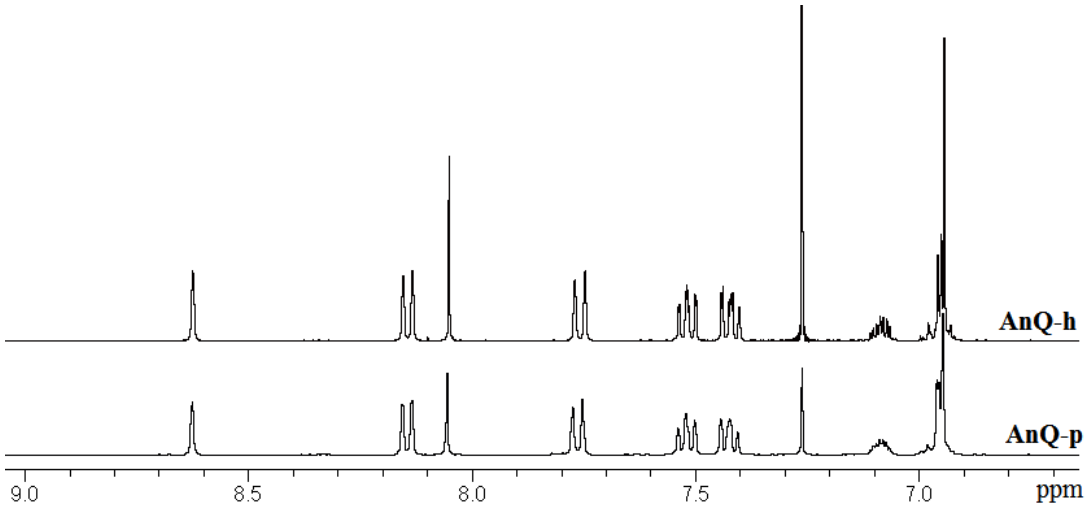


Figure S24. ^{1}H NMR spectra of **AnQ-p** and **AnQ-h** in the selected region recorded in $CDCl_3$.

Table S2. Crystallographic data and structure refinements of **AnQ** and **PyQ**.

	AnQ	**PyQ**
formula	$C_{48}H_{30}N_2$	$C_{52}H_{30}N_2$
Formula wt	634.74	682.78
T, K	373(10)	373(10)
crystal system	monoclinic	monoclinic
space group	P 2_1/n	C 2/c
a, Å	8.1522(2)	25.1073(11)
b, Å	26.7993(7)	11.3157(5)
c, Å	16.6605(4)	12.0314(5)
α,deg	90	90
β,deg	95.2500(10)	96.390(2)
γ,deg	90	90
V,Å^3	3624.60(16)	3397.0(3)
Z	4	4
density, mg/m3	1.163	1.335
μ/mm^{-1}	0.067	0.077
θ range, deg	2.46 to 27.21	2.55 to 27.18
no. of reflections measured	31159	14035
R(int)	0.0367	0.0372
Goodness-of-fit on F^2	1.141	1.043
R1 [I > 2σ(I)]	0.0683	0.0487
wR2 [I > 2σ(I)]	0.1814	0.1075
R1 (all data)	0.1076	0.0841
wR2 (all data)	0.1977	0.1237