

Supporting Information

Dual Fluorescence of Tetraphenylethylene-Substituted Pyrenes with Aggregation-Induced Emission Characteristics for White-Light Emission

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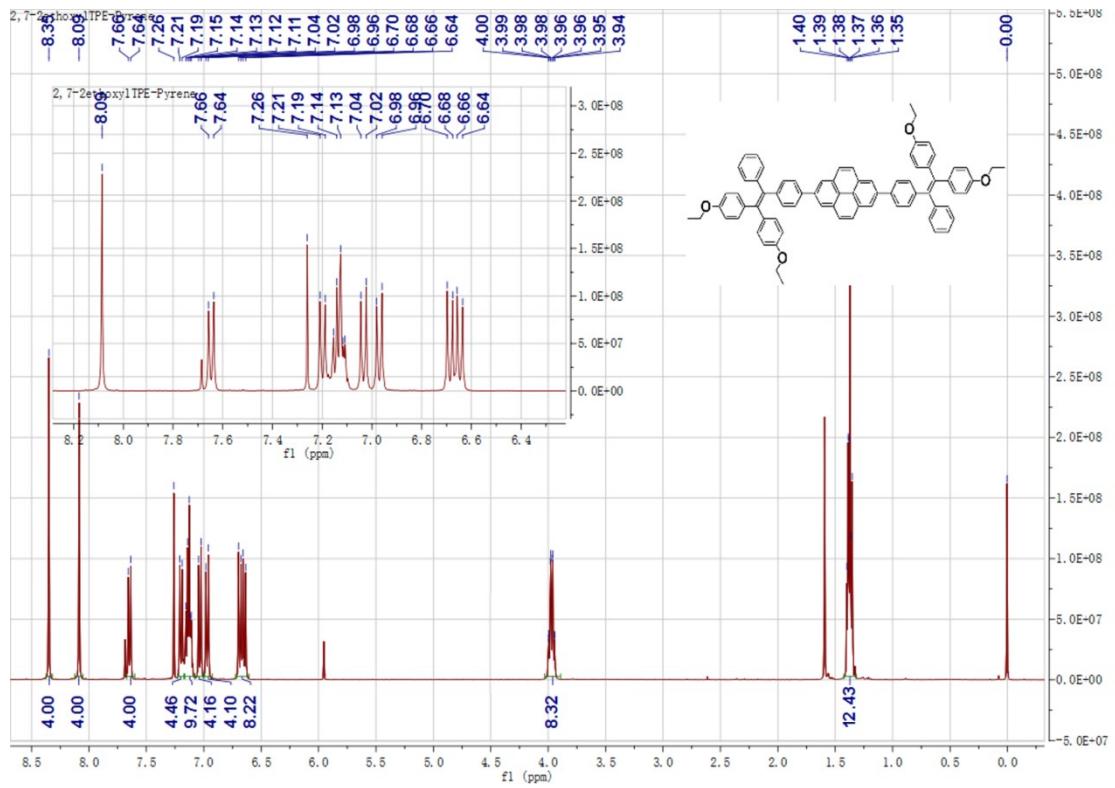


Fig. S1. ^1H NMR spectrum of **2a** in CDCl_3 .

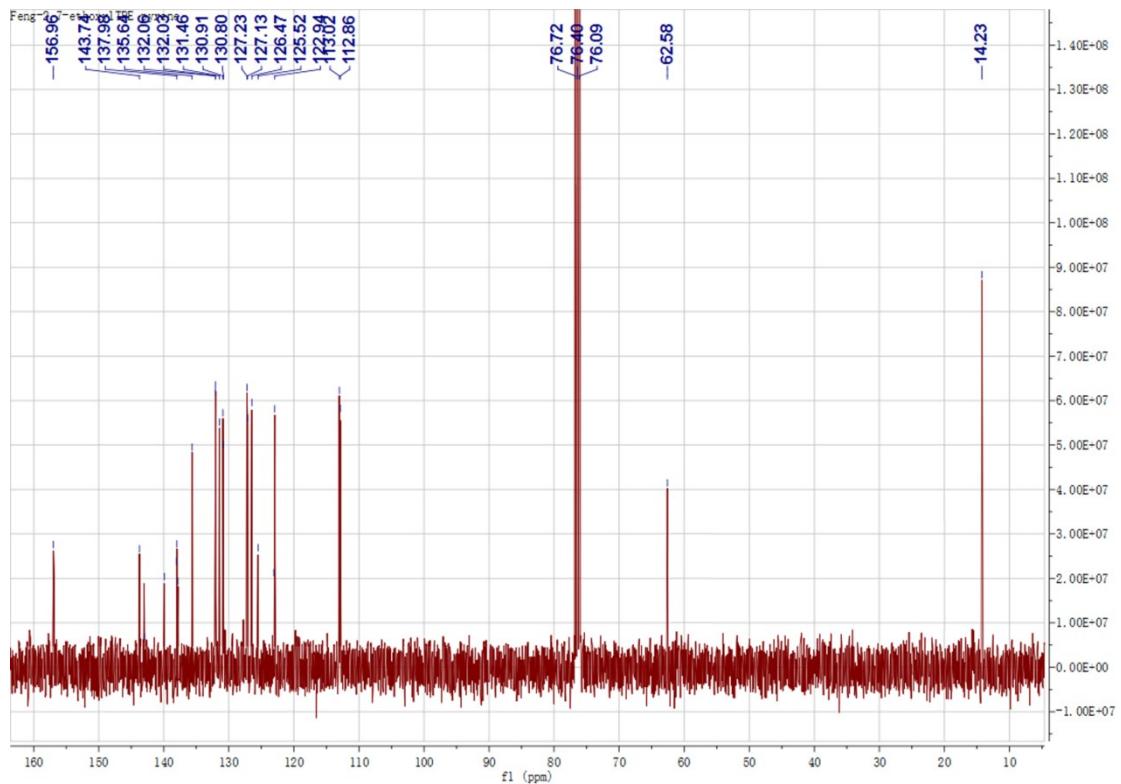


Fig. S2. ^{13}C NMR spectrum of **2a** in CDCl_3 .

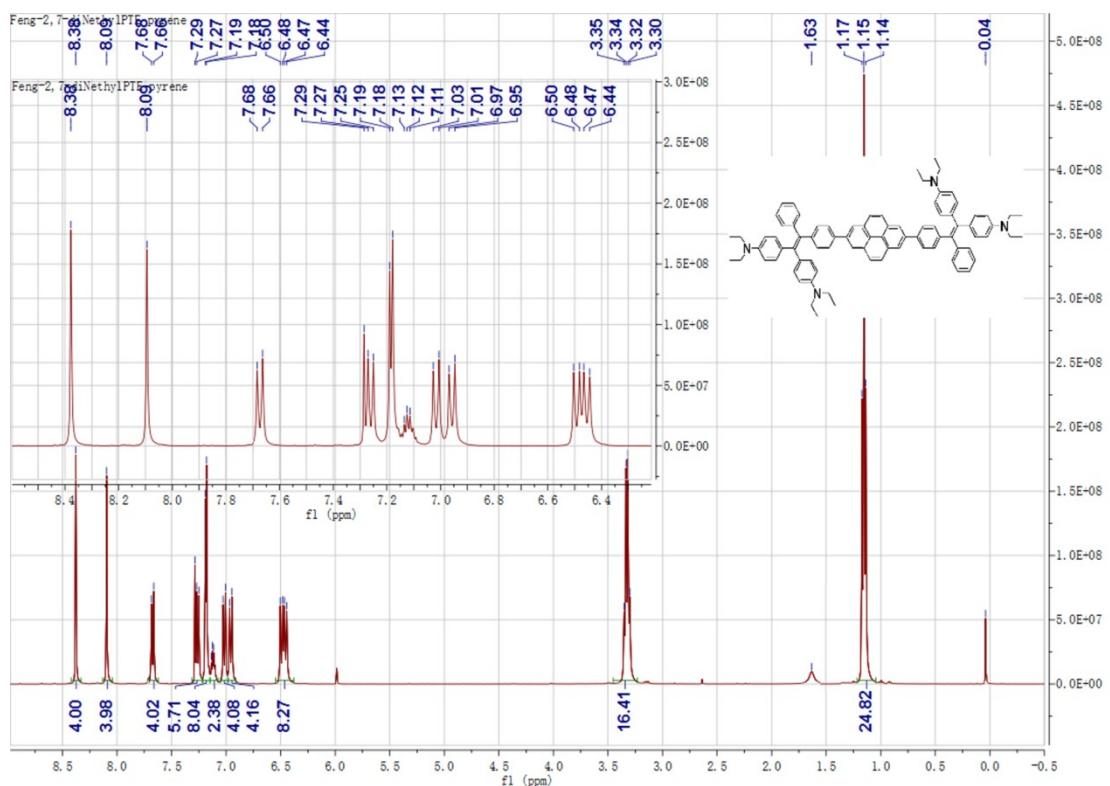


Fig. S3. ¹H NMR spectrum of **2b** in CDCl_3 .

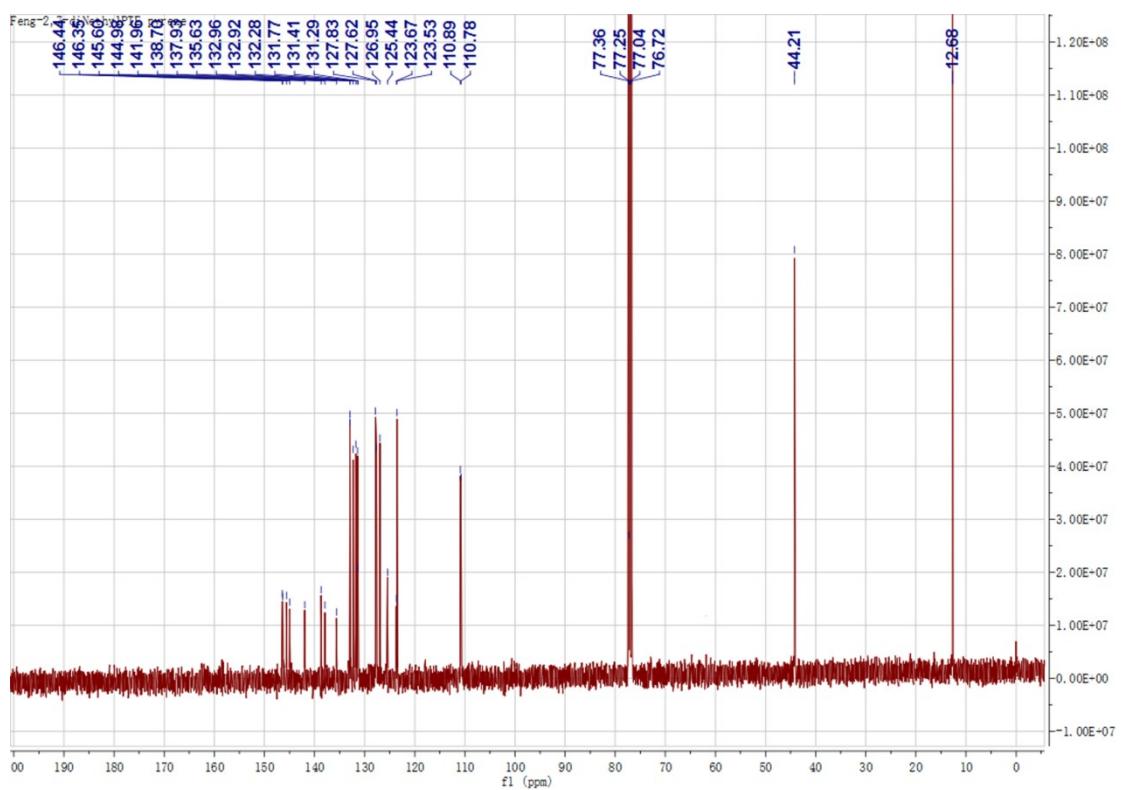


Fig. S4. ¹³C NMR spectrum of **2b** in CDCl_3 .

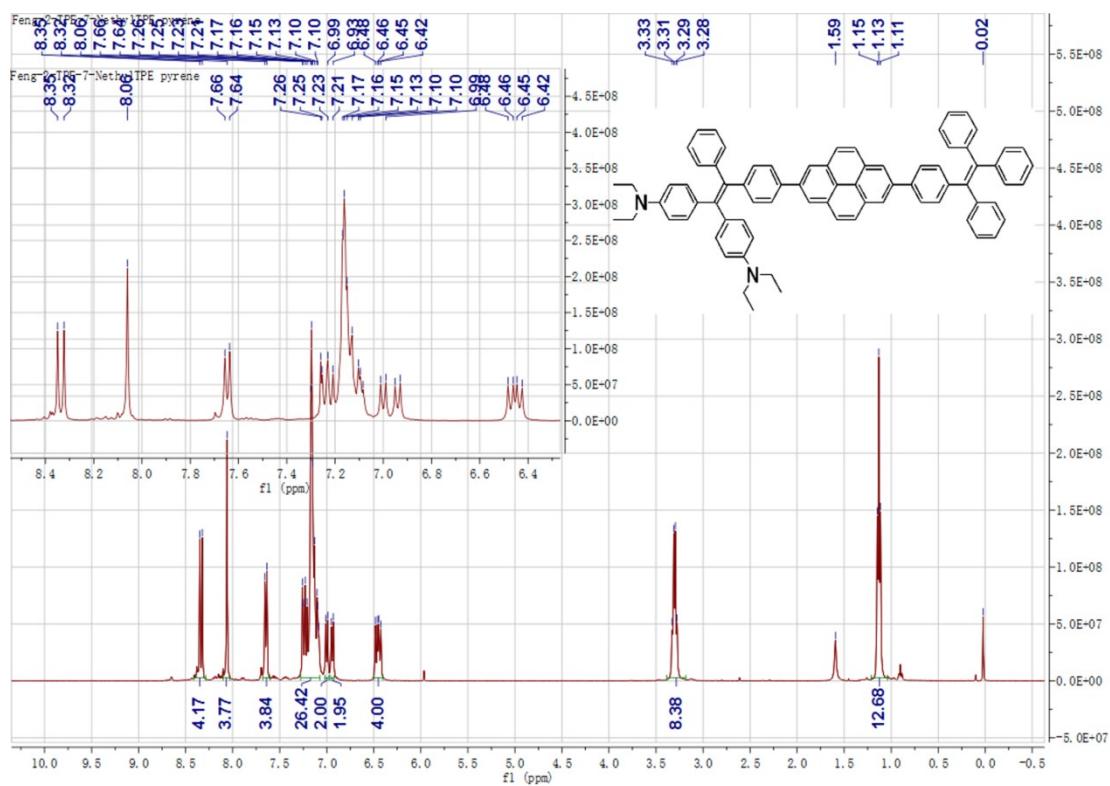


Fig. S5. ¹H NMR spectrum of **2c** in CDCl_3 .

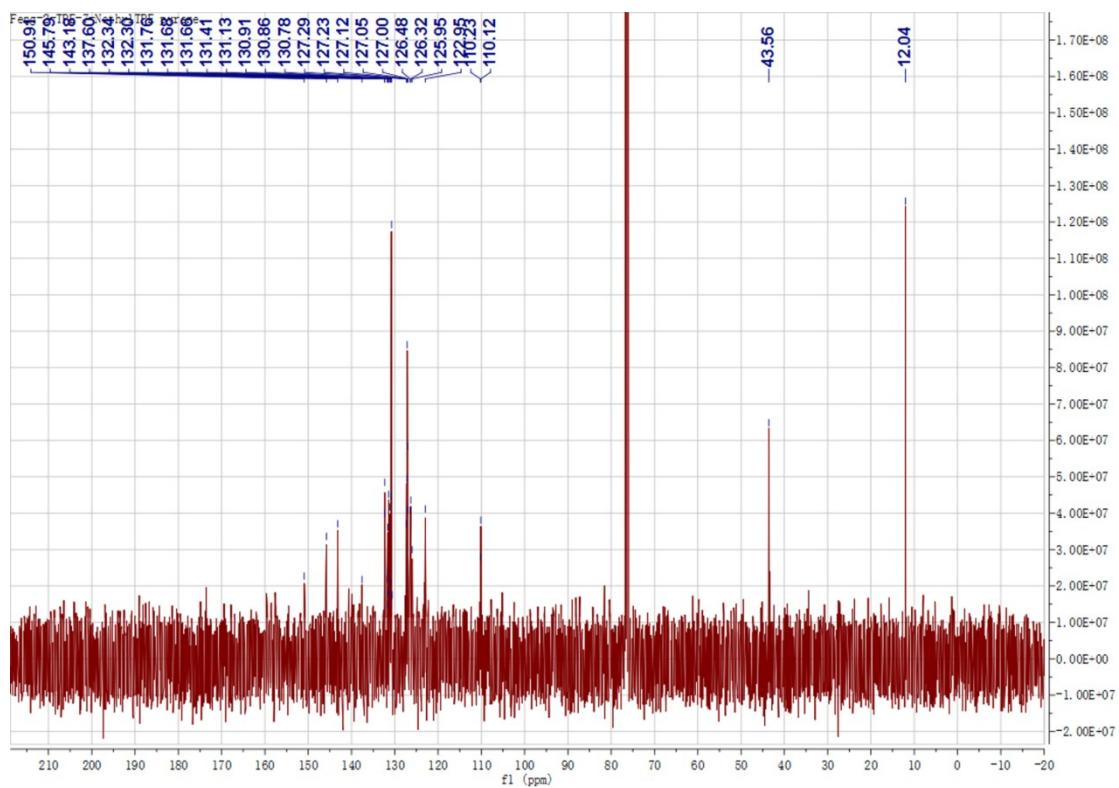


Fig. S6. ¹³C NMR spectrum of **2c** in CDCl_3 .

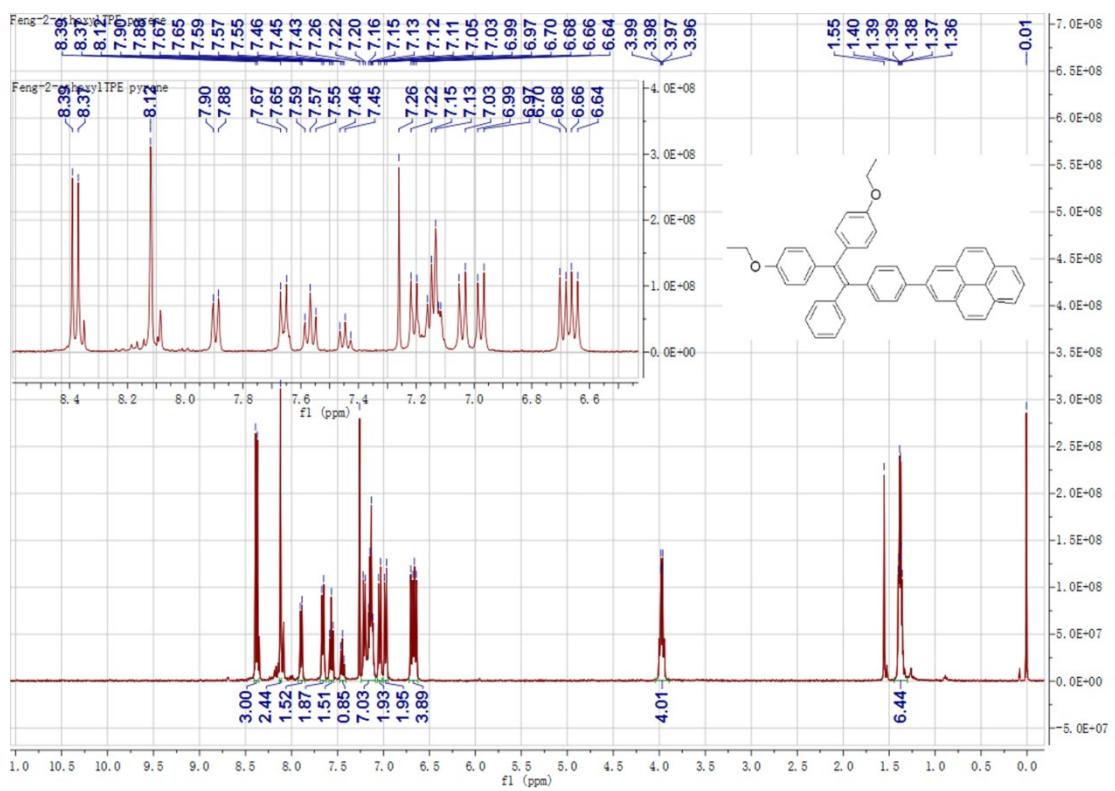


Fig. S7. ^1H NMR spectrum of **3** in CDCl_3 .

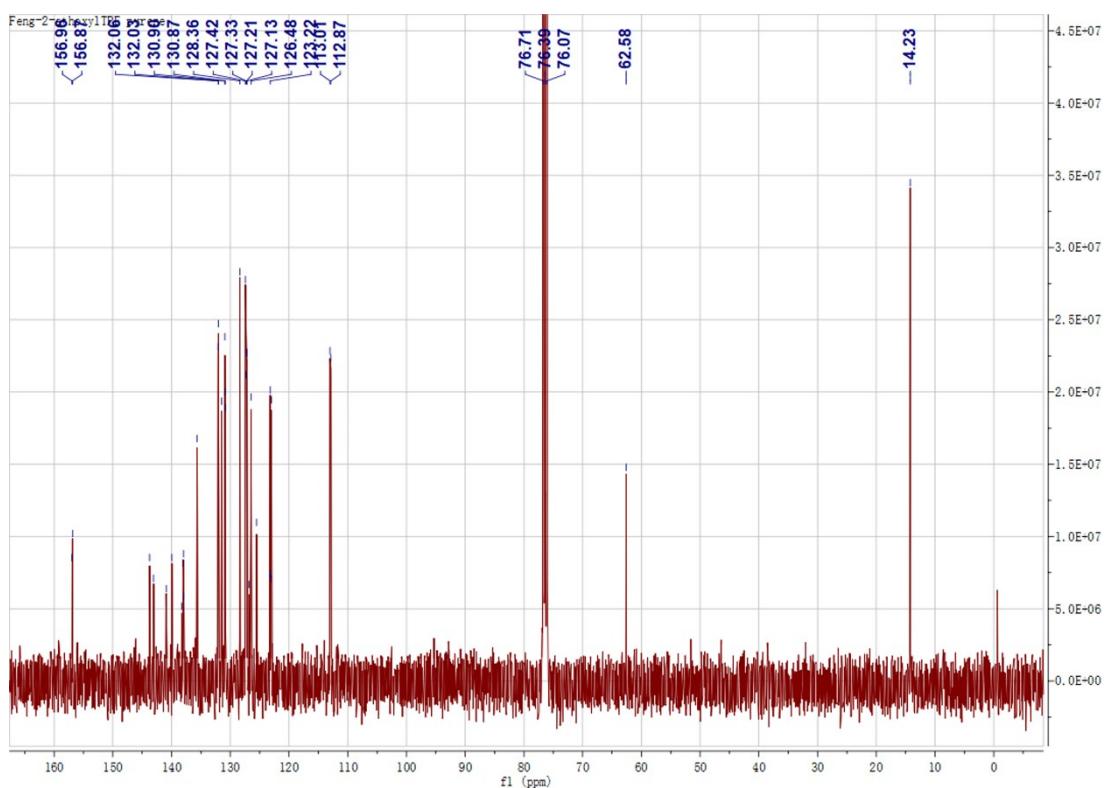


Fig. S8. ^{13}C NMR spectrum of **3** in CDCl_3 .

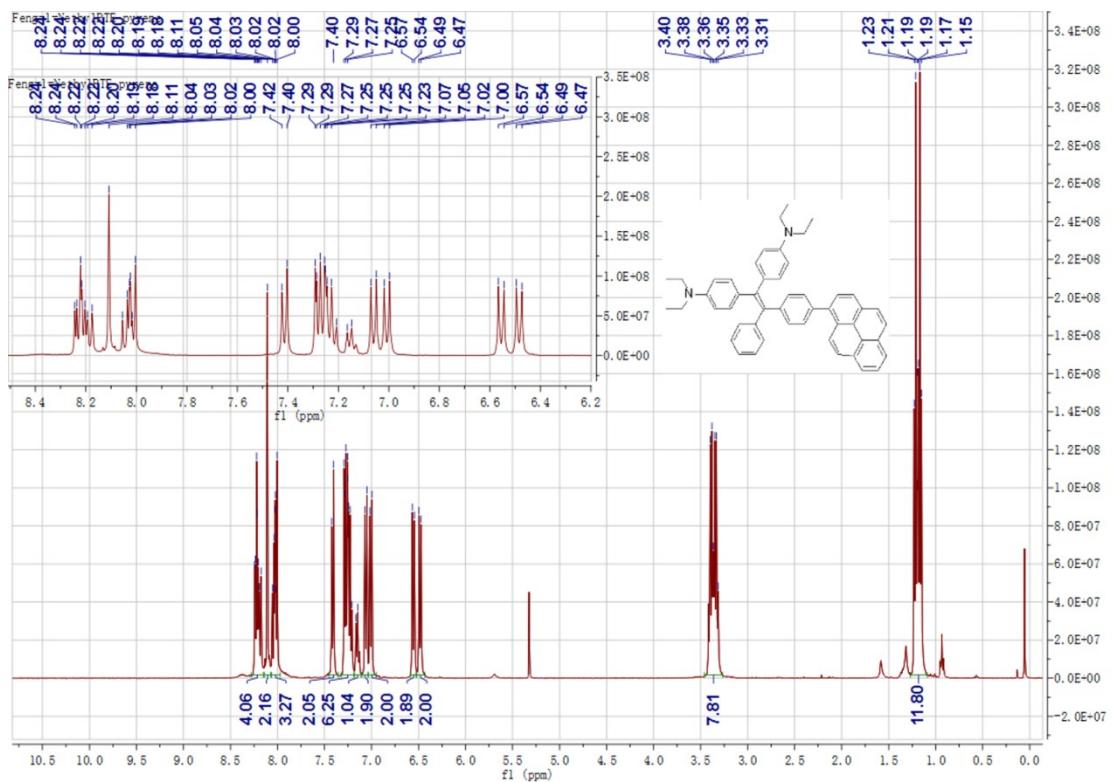


Fig. S9. ¹H NMR spectrum of **4** in CDCl_3 .

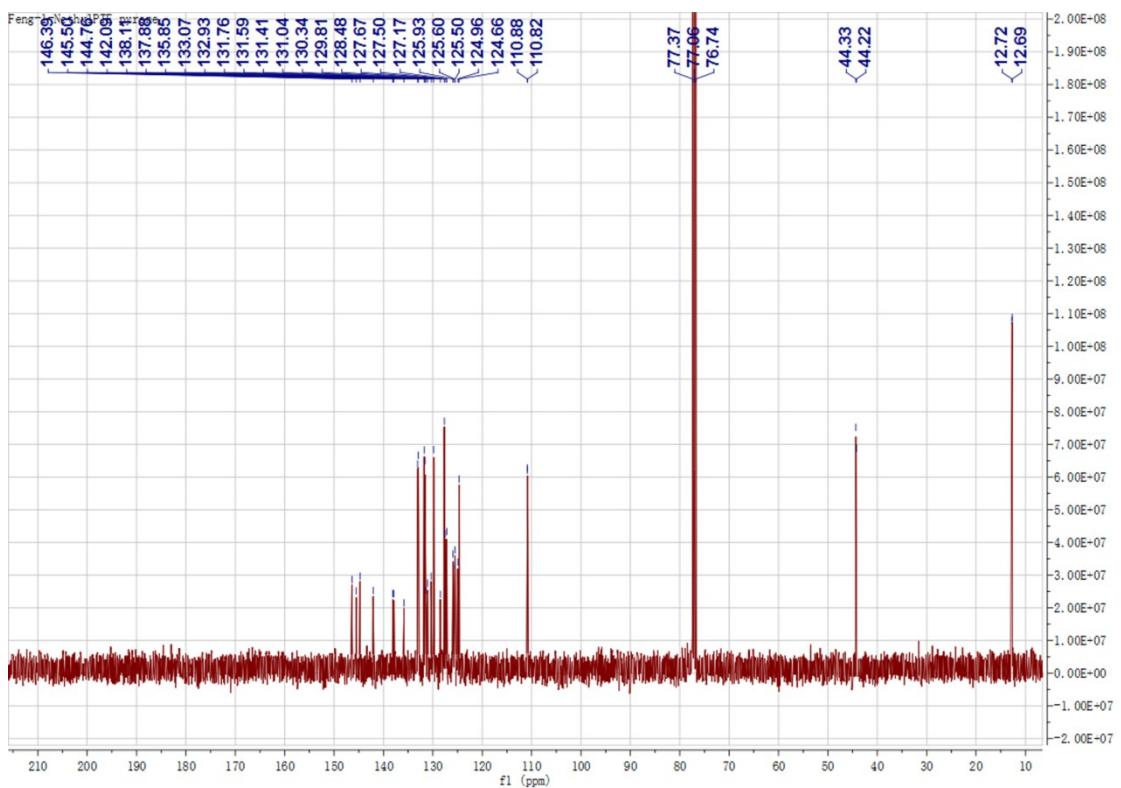


Fig. S10. ¹³C NMR spectrum of **4** in CDCl_3 .

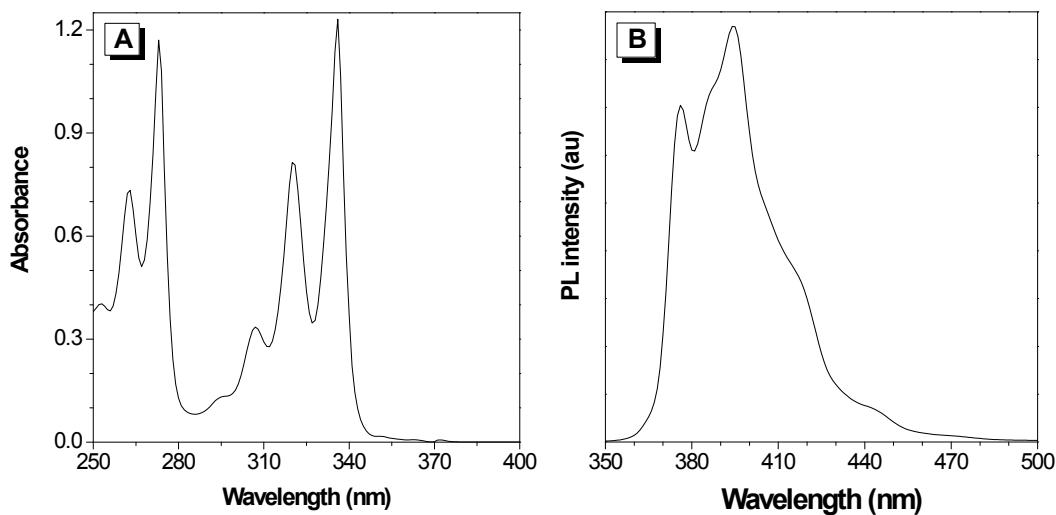


Fig. S11. (A) UV/Vis and (B) PL spectra of pyrene in THF (10 μM).

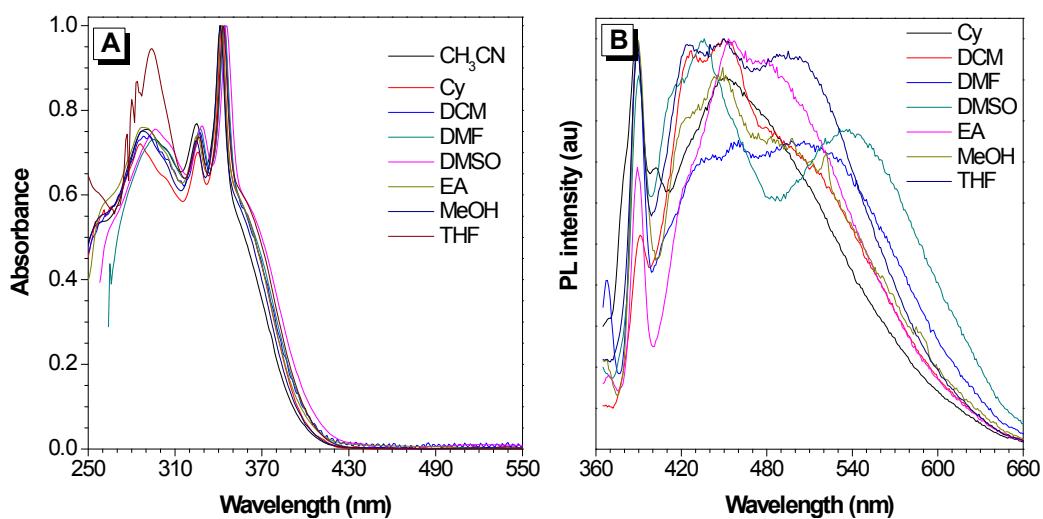


Fig. S12. (A) UV/Vis and (B) PL spectra of **2a** in different solvents (10 μM). $\lambda_{\text{ex}} = 347$ nm.

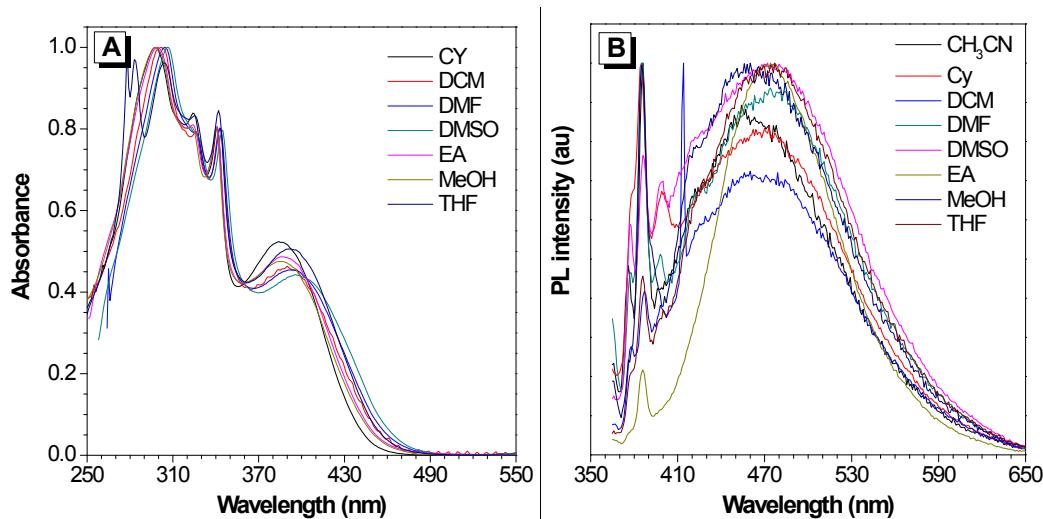


Fig. S13. (A) UV/Vis and (B) PL spectra of **2b** in different solvents (10 μM). $\lambda_{\text{ex}} = 351$ nm.

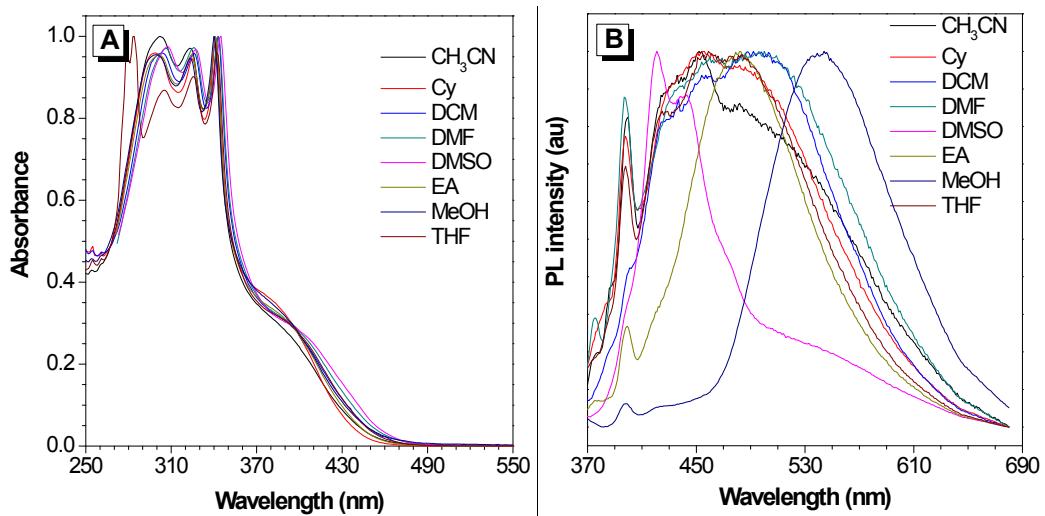


Fig. S14. (A) UV/Vis and (B) PL spectra of **2c** in different solvents (10 μ M). $\lambda_{\text{ex}} = 348$ nm.

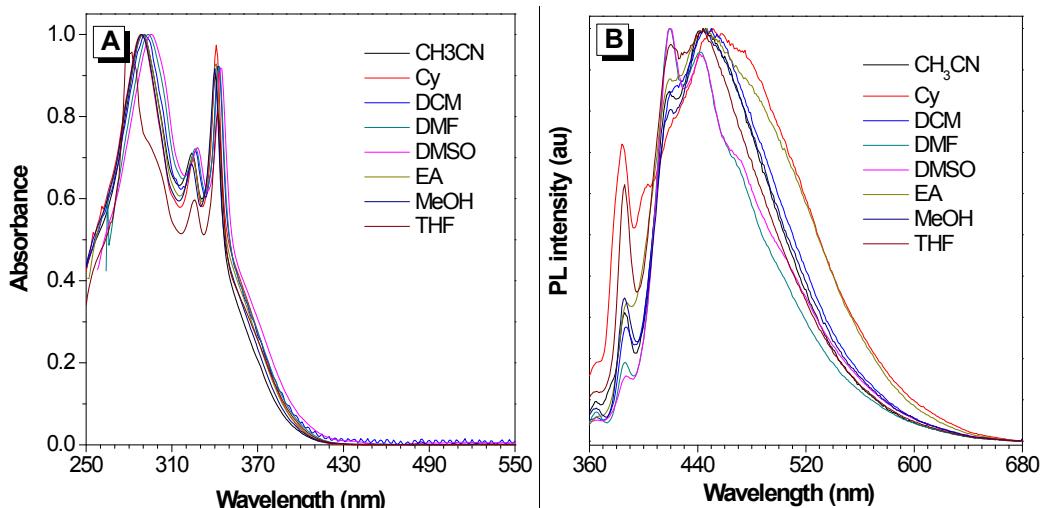


Fig. S15. (A) UV/Vis and (B) PL spectra of **3** in different solvents (10 μ M). $\lambda_{\text{ex}} = 347$ nm.

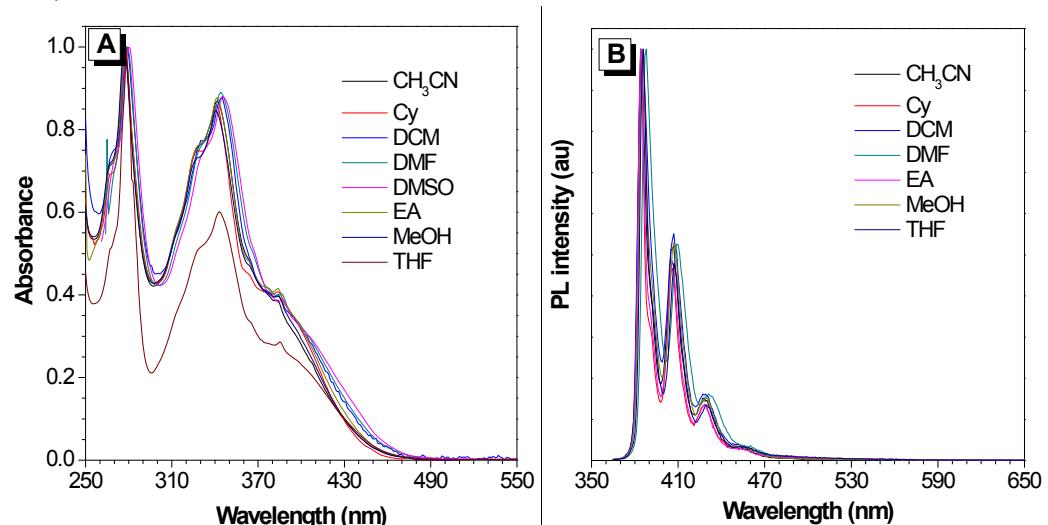


Figure S16. (A) UV/Vis and (B) PL spectra of **4** in different solvents (10 μ M). $\lambda_{\text{ex}} = 350$ nm.

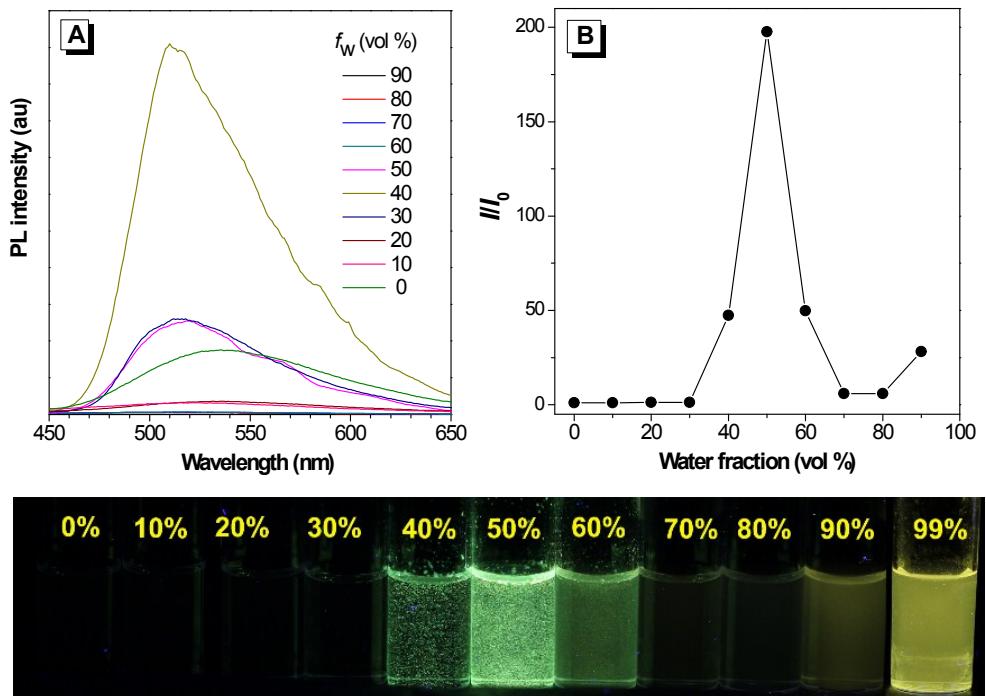


Fig. S17. (A) PL spectra of **2b** in THF/water mixtures with different water fractions (f_w). (B) Plot of relative PL intensity (I/I_0) versus the composition of THF/water mixtures of **2b**, where I_0 is the PL intensity in pure THF solution. Below: photographs in THF/water mixtures taken under UV illumination. Excitation wavelength: 365 nm.

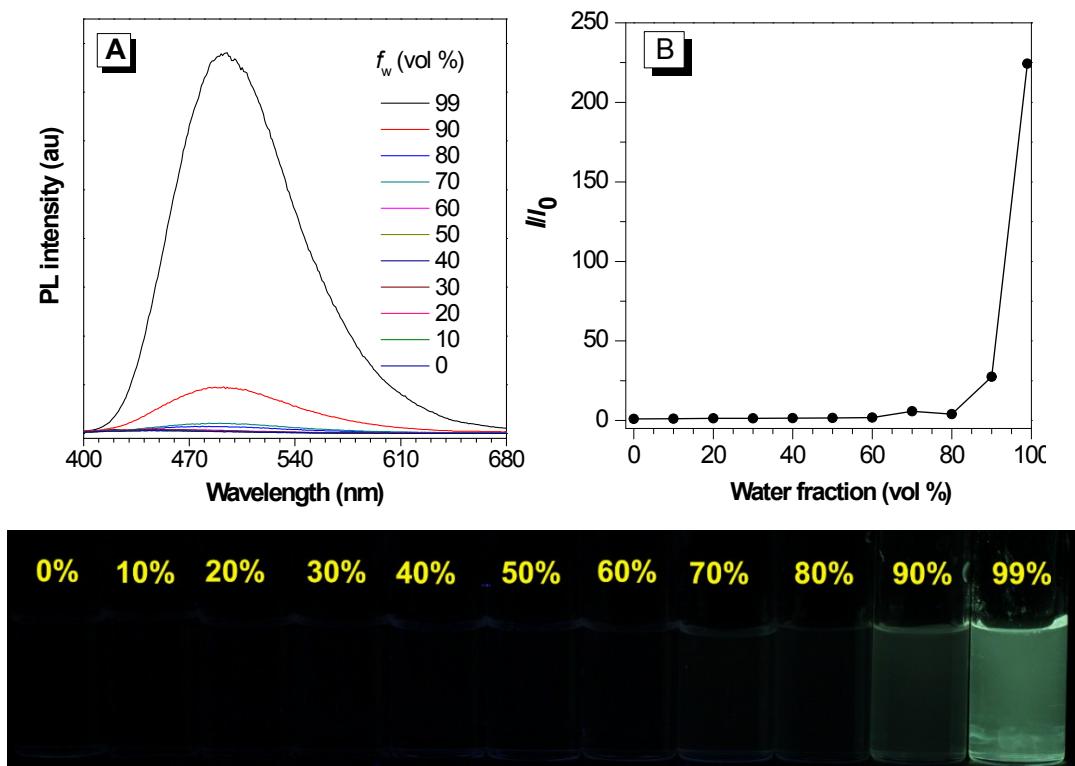


Fig. S18. (A) PL spectra of **3** in THF/water mixtures with different water fractions (f_w). (B) Plot of relative PL intensity (I/I_0) versus the composition of THF/water mixture of **3**.

3, where I_0 is the PL intensity in pure THF solution. Below: photographs in THF/water mixtures taken under UV illumination. Excitation wavelength: 365 nm.

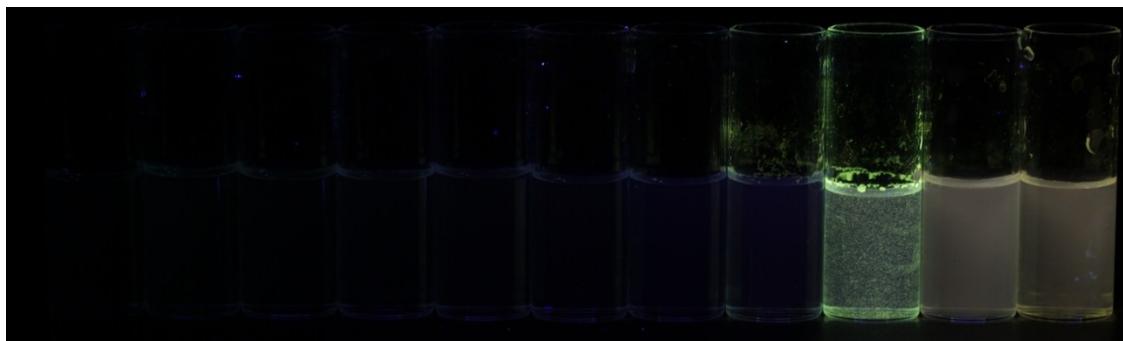


Fig. S19. Photographs of compound **2c** in THF/water mixtures taken under UV illumination. Excitation wavelength: 365 nm.

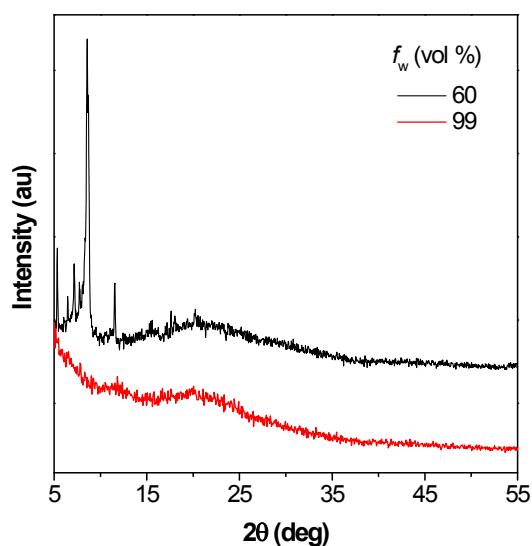


Figure S20. XRD diffractogram of **2a**.

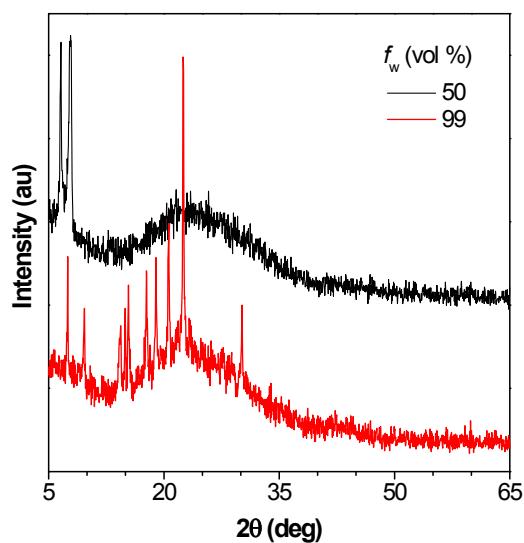


Fig. S21. XRG diffractogram of **2b**.

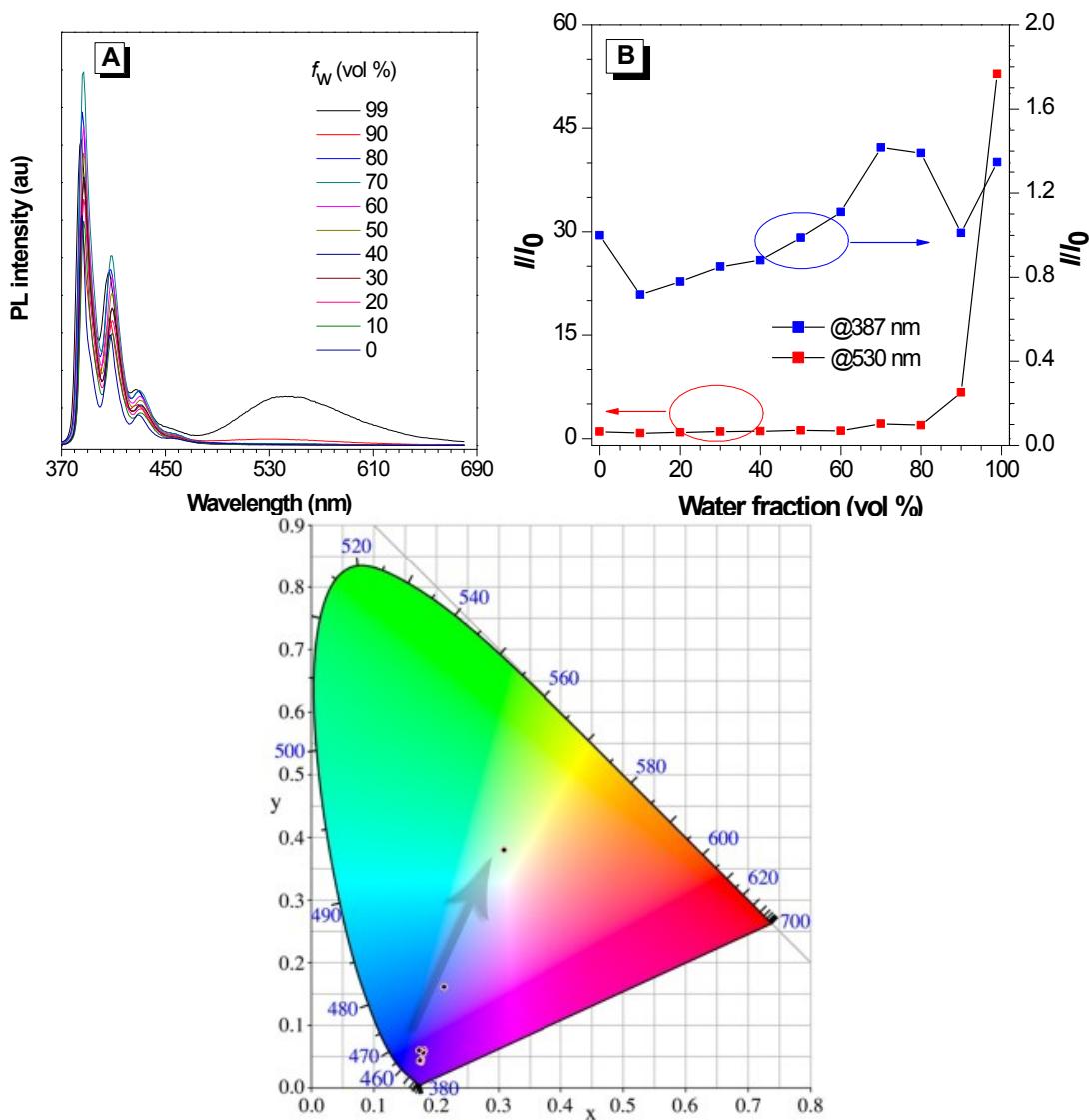


Table S1. Optical properties of **2-4** in various solvents at room temp^a

Cpd	$\lambda_{\text{abs}}/\lambda_{\text{em}}$ (nm)							
	CH ₃ CN	cyclohexane	CH ₂ Cl ₂	DMF	DMSO	EA	MeOH	THF
2a	291, 341/454	286, 342/456	292, 344/456	295, 344/457	297, 345 /456	288, 342 /456	288, 341/456	294, 343/462
2b	--	298, 341/ 47	302, 343/449	304, 345/447, 508	306, 344 /421, 531	299, 341 /453	298, 340/451	304, 325, 394/500
2c	302, 324/452	299, 325/456	304, 325/492	306, 325/500	308, 328 /421, 443	301, 324 /482	299, 323/544	304, 342, 390/435
3	290, 324/446	288, 323/451	291, 327/450	293, 327/419, 442	296, 328 /419, 442	290, 324 /447	289, 324/441	279, 342/441
4	278, 341/384, 407, 428	278, 341/384, 406, 428	278, 345/385, 407, 429	279, 344/388, 409, 431		277, 341 /384, 406, 429	277, 341/385, 407, 430	278, 341, 400/386, 407, 429

^a All measurements were performed under degassed conditions at a concentration of 10 μ M. Abbreviation: λ_{abs} = absorption maximum, λ_{em} = emission maximum, DMF = dimethylformamide, DMSO = dimethylsulfoxide, EA = ethyl acetate.

Table S2. The quantum yield of **2-4** in THF and mixture solvents of THF/H₂O at room temp

compound	Φ_F (%) in THF	Φ_F (%) In THF/H ₂ O	Φ_F (%) in solid state
2a	0.8	--	46.7
2b	0.6	6.7 (90%)	3.8
2c	0.6	12.0 (90%)	6.8
3	0.5	42.1 (90%)	19.8
4	0.8	22.1 (80%) / 28.8 (90%)	9.7

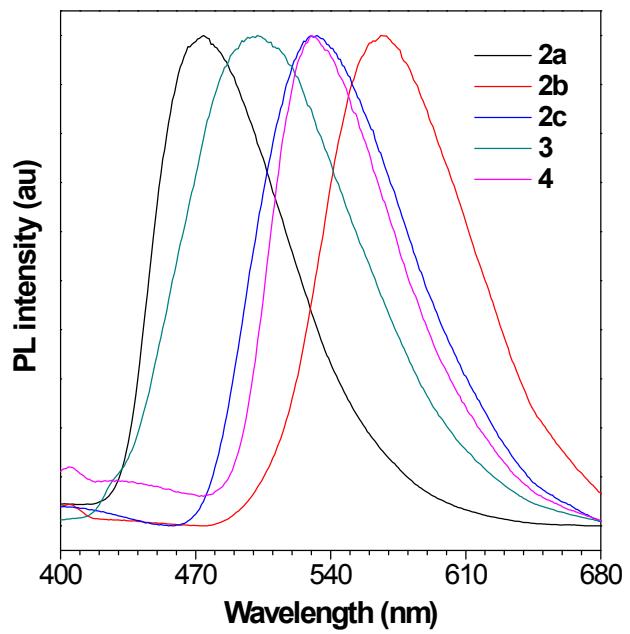


Figure S23. PL spectra of **2–4** in the solid state.

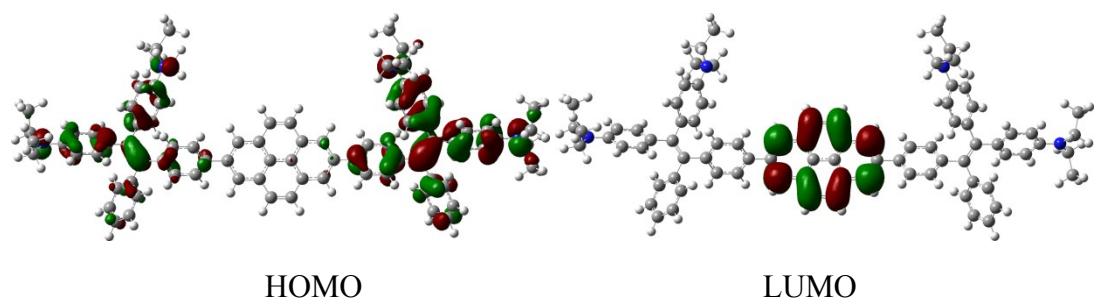


Figure S24. Computed molecular orbital plots of **2b** calculated by B3LYP/6–31G*.