

Supporting Information for

Perylene bisimide with diphenylacrylonitrile on side-chain: Strong fluorescence liquid crystal with large pseudo Stokes shift based on AIE and FRET effect

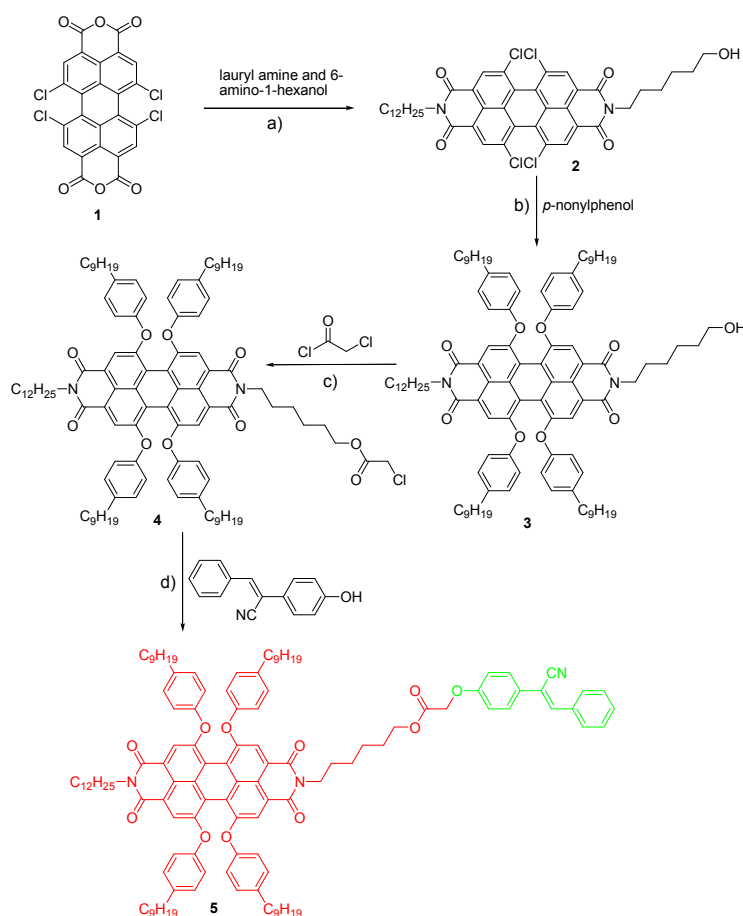
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1. The synthetic route of title compound



Scheme 1 Synthetic route of title compound: a) isopropanol, reflux, 8h, yield: 28%; b) *N*-methyl-2-pyrrolidone (NMP), K₂CO₃, 130 °C, overnight, yield: 78%; c) DCM, 35 °C, 6h, yield: 86%; d) anhydrous MeCN, K₂CO₃, reflux, overnight, yield: 75%.

2. Analytical Data

2.1. ^1H NMR and ^{13}C NMR Spectroscopy

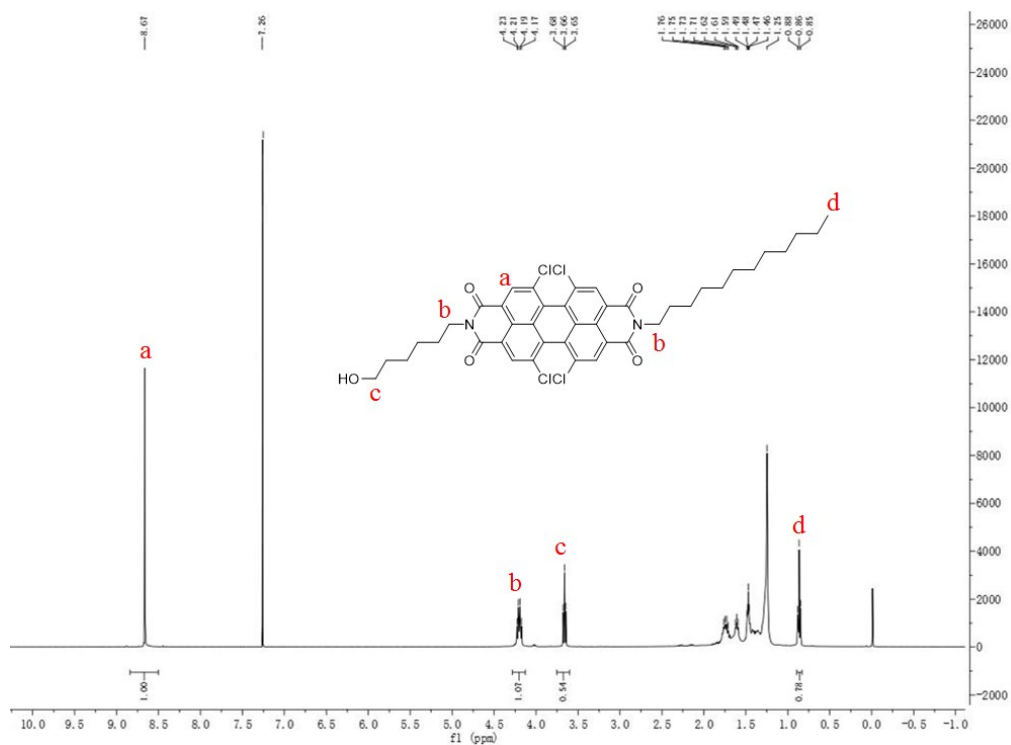


Fig.S1 ^1H NMR spectrum of PBI 2.

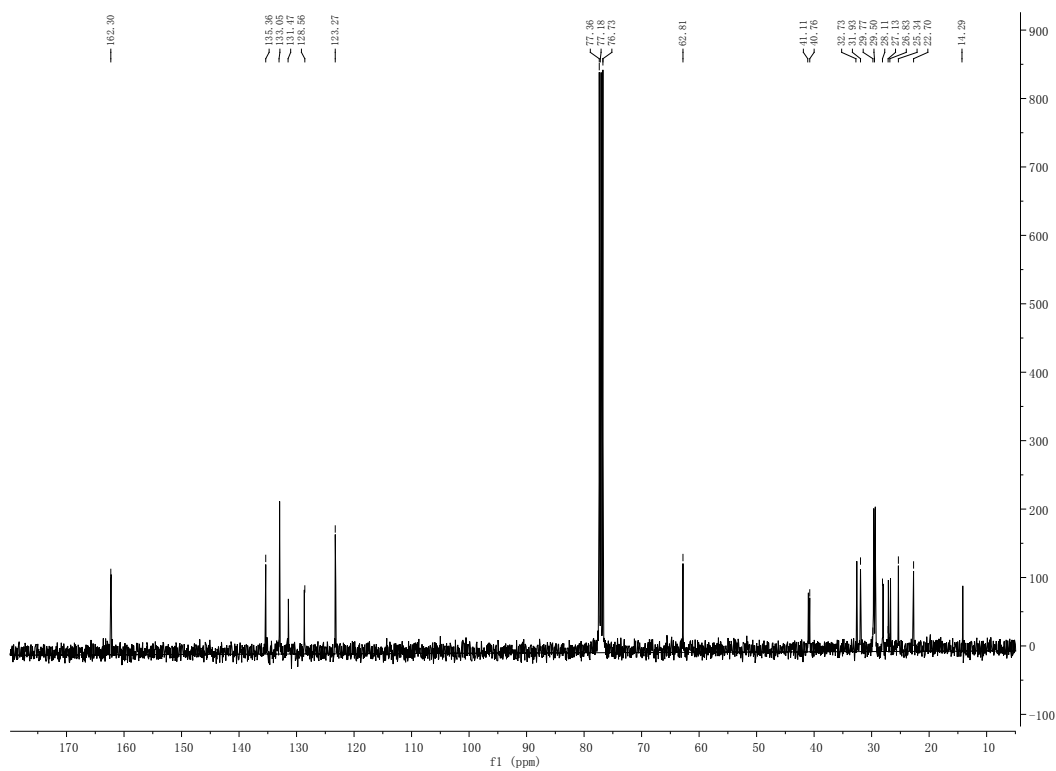


Fig.S2 ^{13}C NMR spectrum of PBI 2.

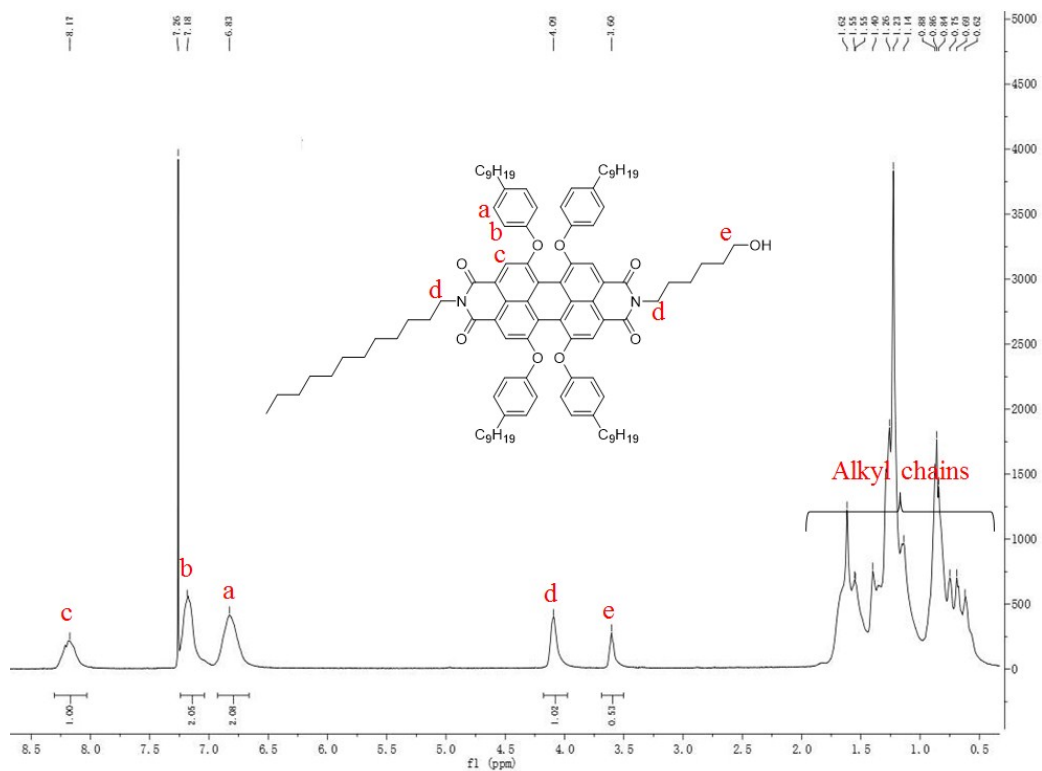


Fig.S3 ¹H NMR spectrum of PBI 3.

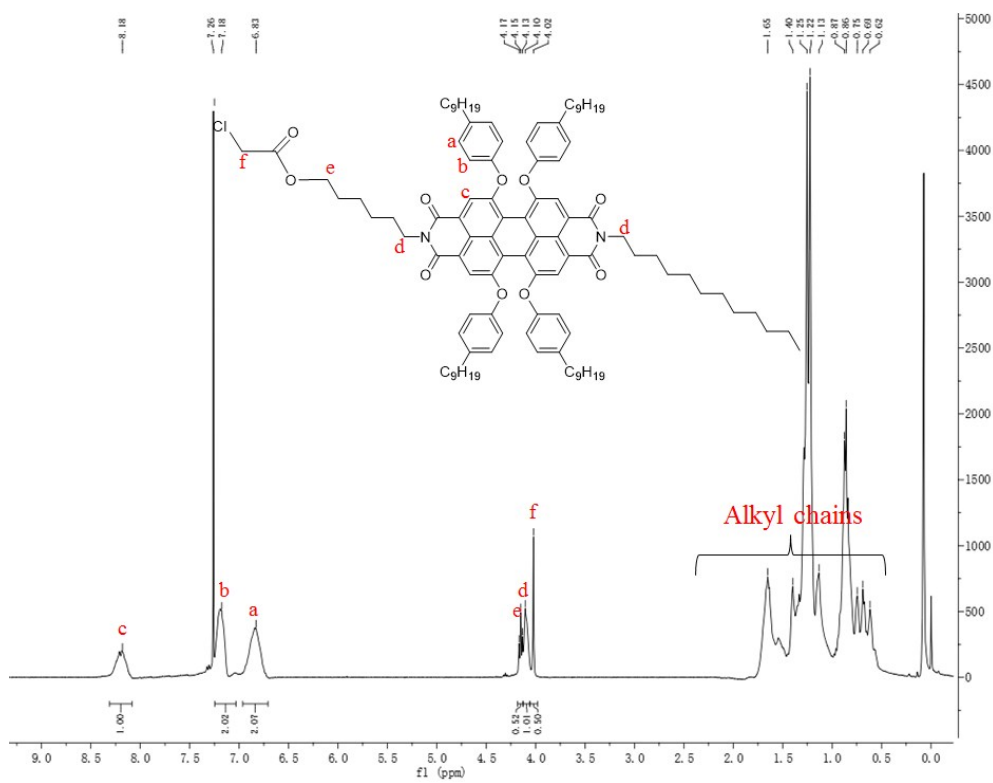


Fig.S4 ¹H NMR spectrum of PBI 4.

2.2. MALDI-TOF Mass spectrometry

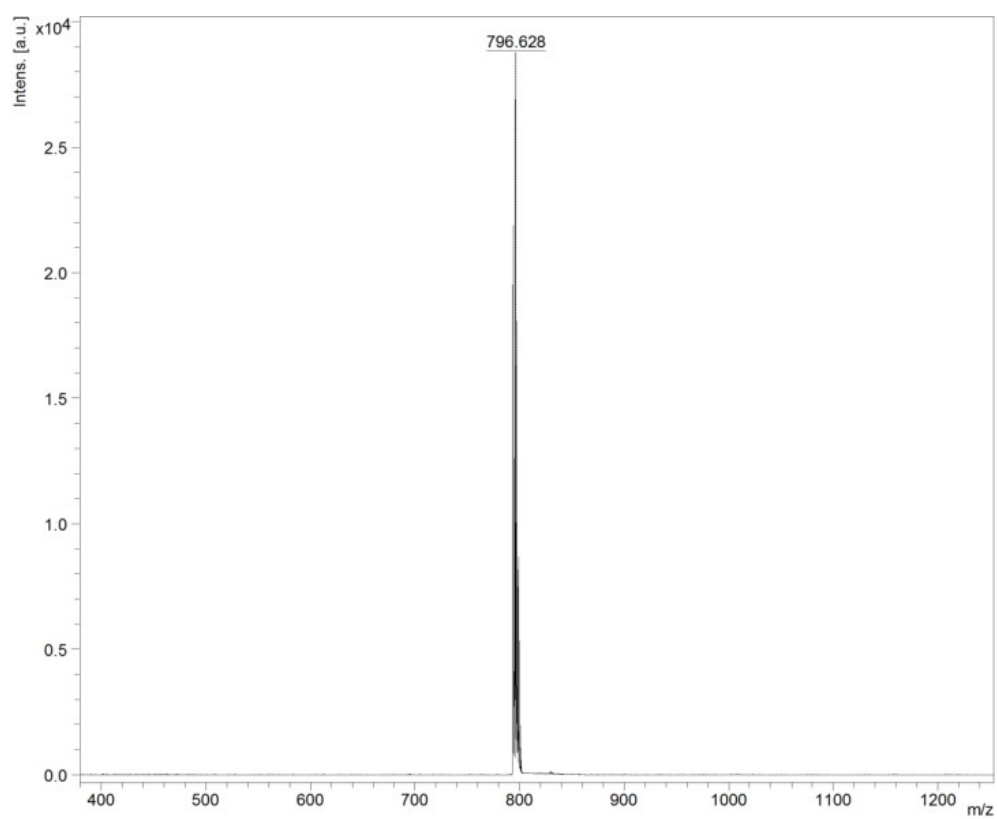


Fig. S7: MALDI-TOF mass spectrum of PBI 2.

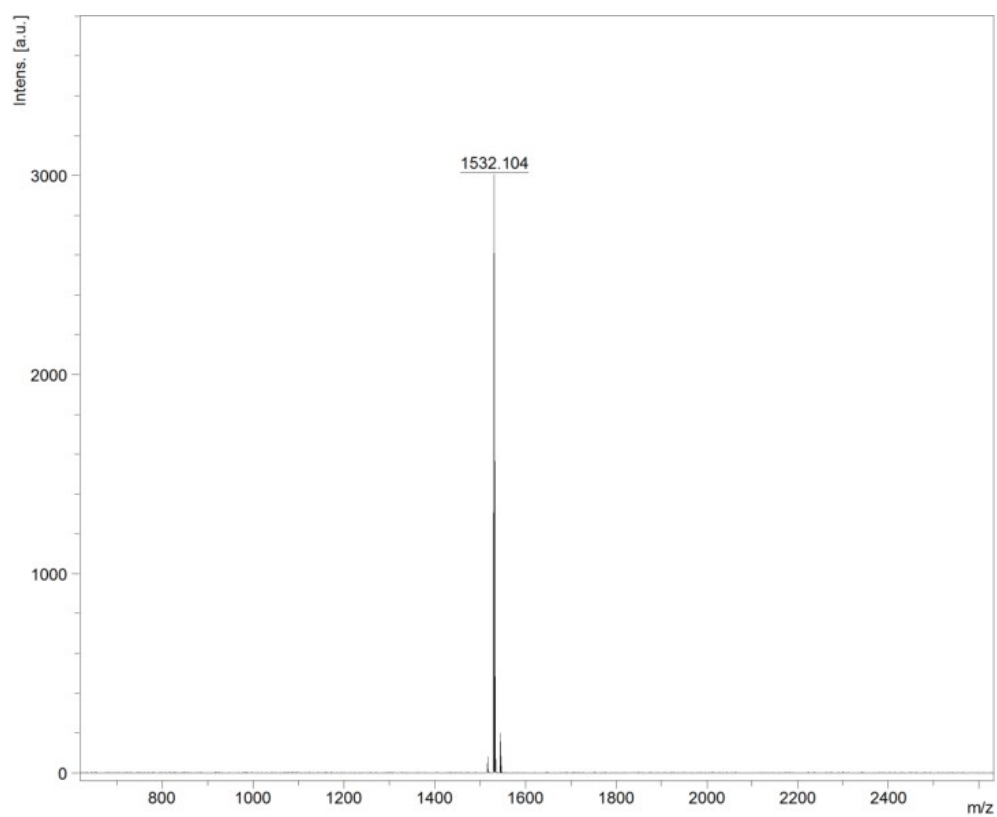


Fig. S8: MALDI-TOF mass spectrum of PBI 3.

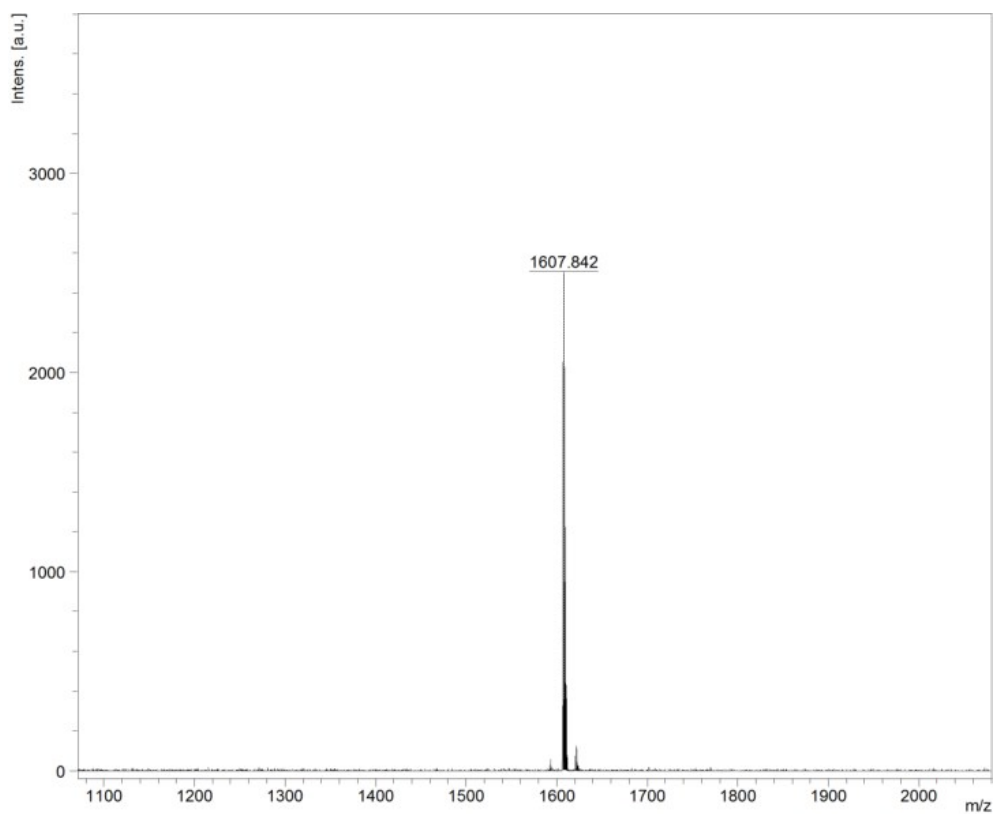


Fig. S9: MALDI-TOF mass spectrum of PBI 4.

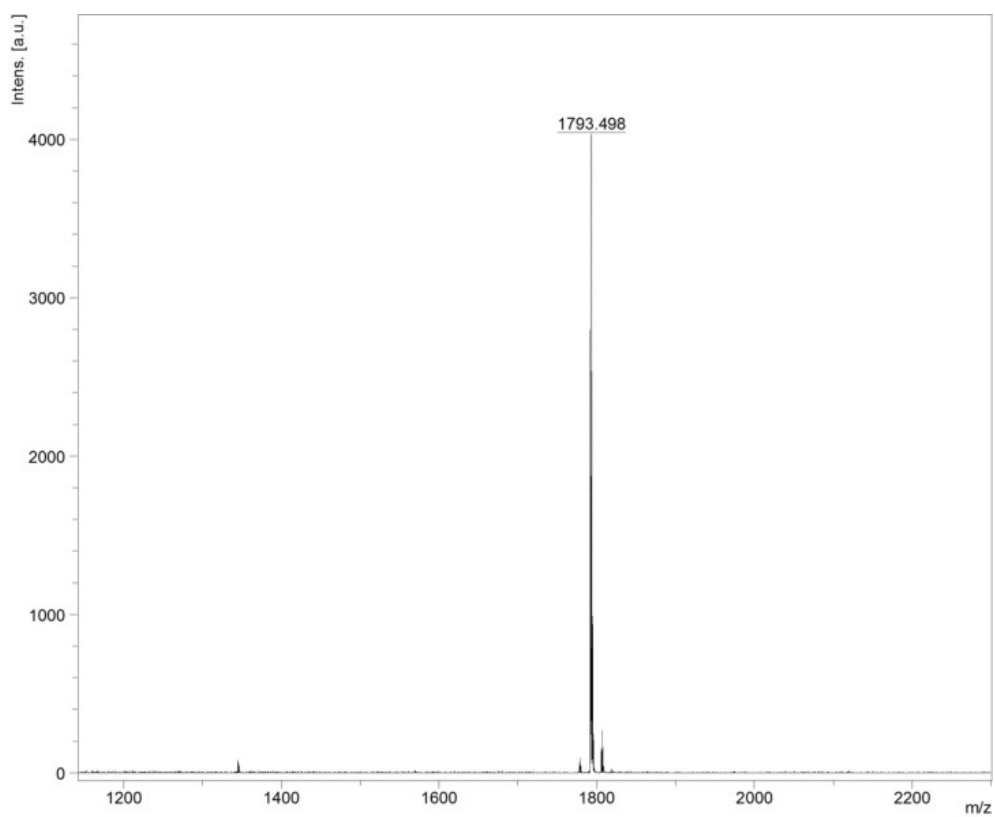


Fig. S10: MALDI-TOF mass spectrum of PBI 5.

2.3 Photophysical properties

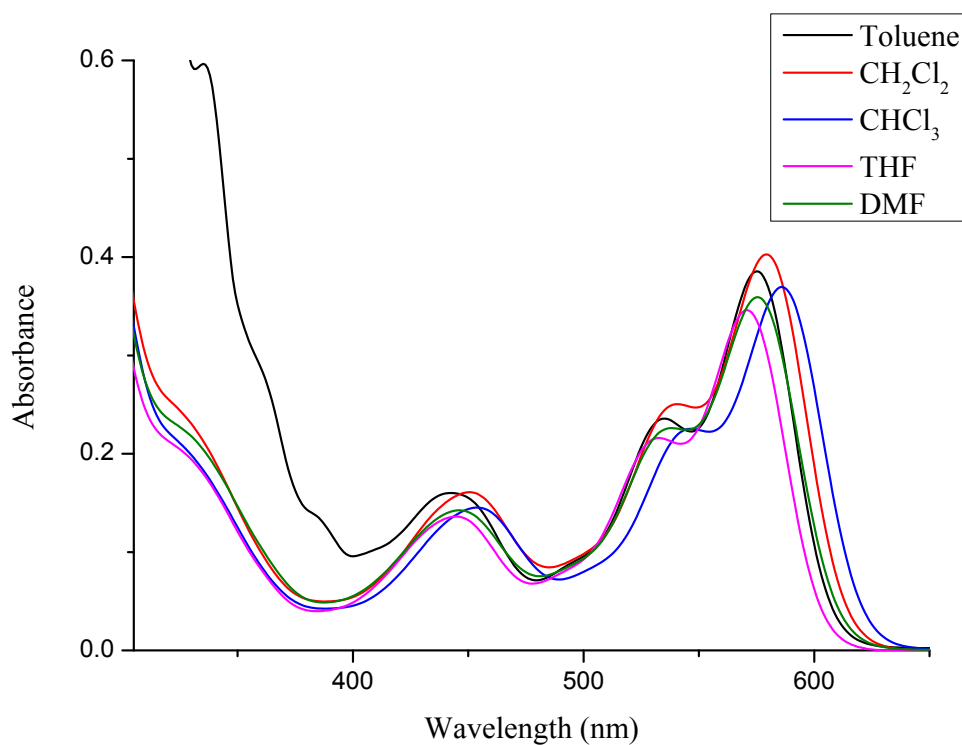


Fig. S11 The UV-Vis absorption spectra of PBI **5** in different solvents (10 μ M).

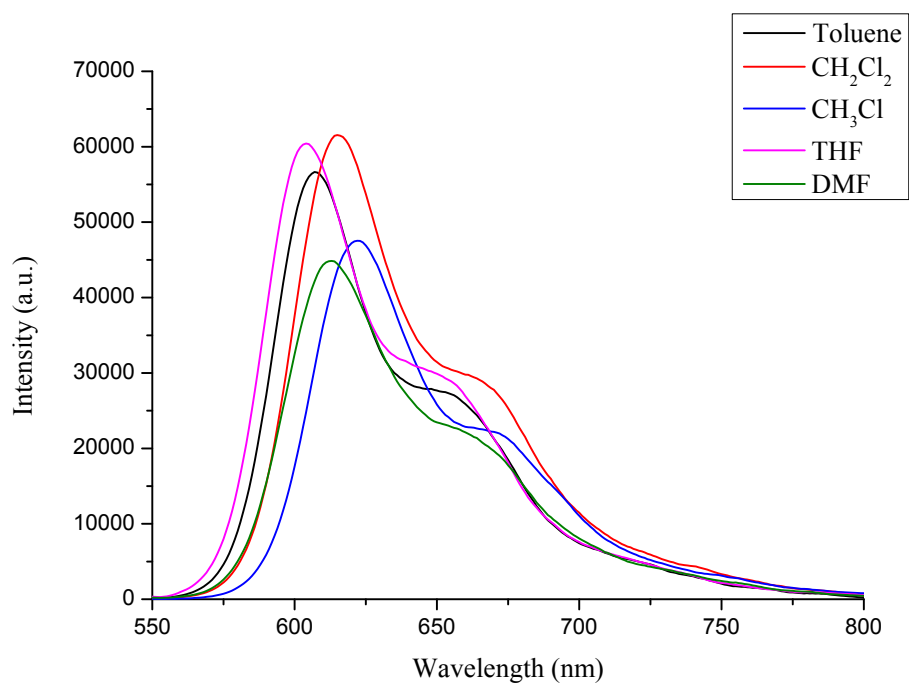


Fig. S12 Fluorescence emission spectra of PBI **5** in different solvents (10 μ M, λ_{ex} = 530 nm).

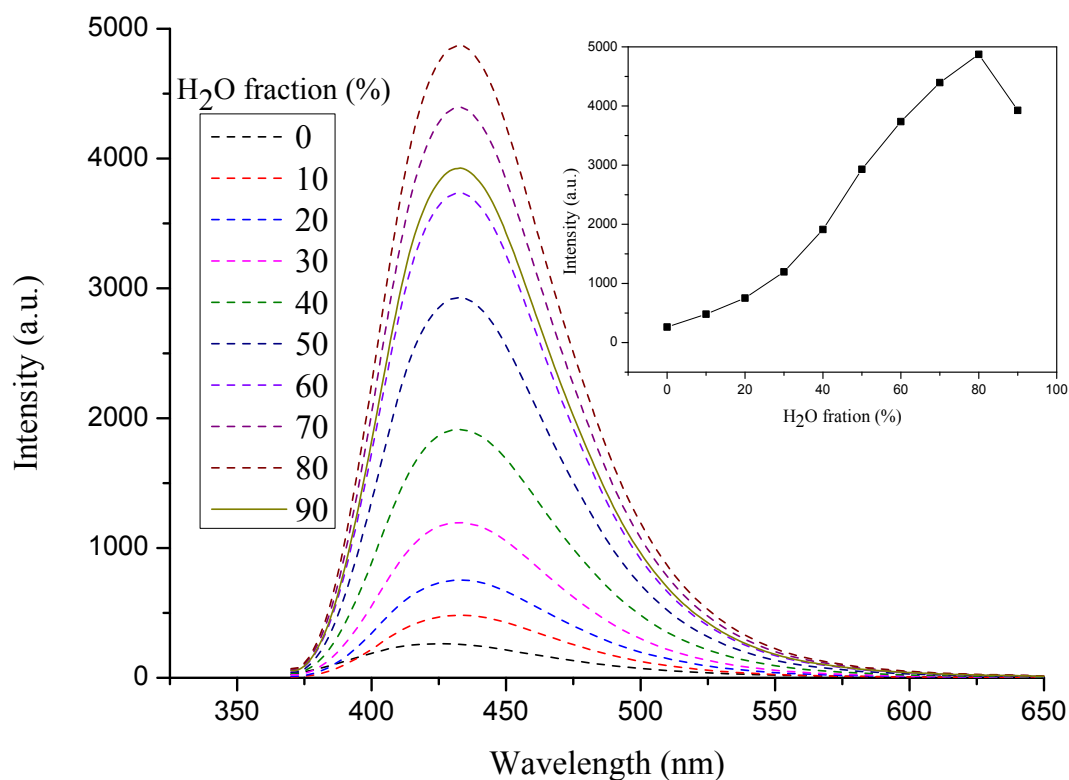


Fig. S13 Emission spectra of the hydroxyl-diphenylacrylonitrile in THF-water system ($10 \mu\text{M}$) with different water fractions (f_w), excited at $\lambda_{\text{ex}} = 330 \text{ nm}$. (The inset: Variations in intensity with f_w).

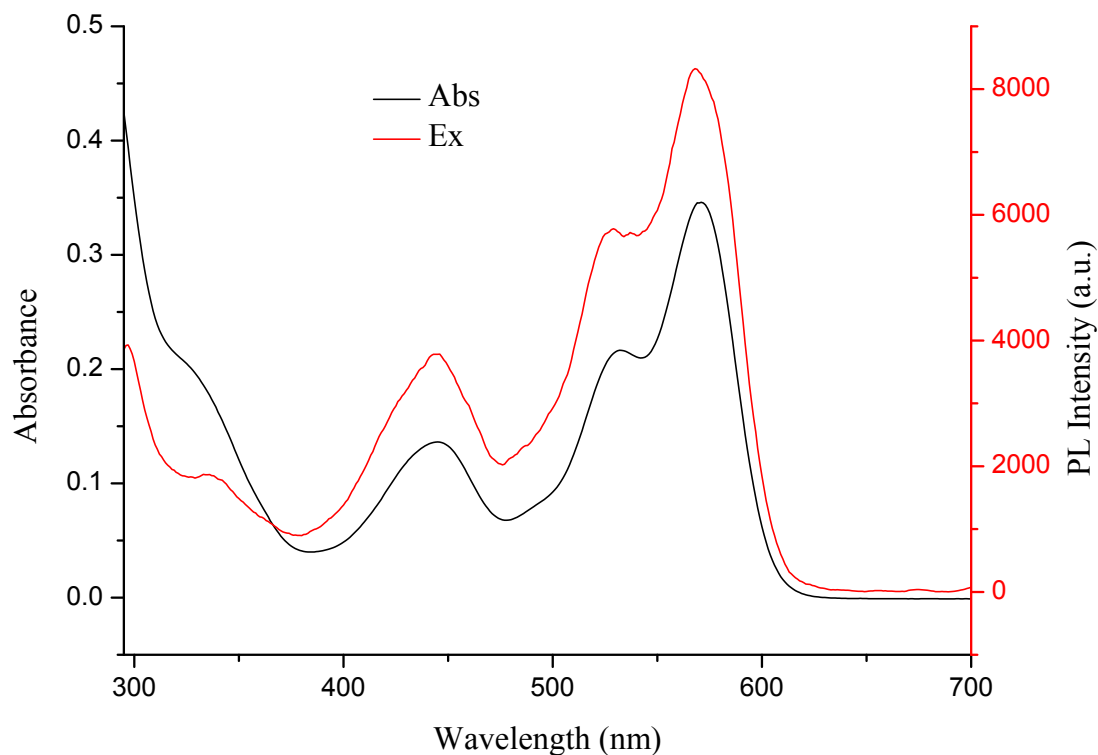


Fig. S14 The absorption and excitation spectra of PBI 5 in THF solution. ($10 \mu\text{M}$, $\lambda_{\text{em}} = 604 \text{ nm}$ was used to record the excitation spectrum).

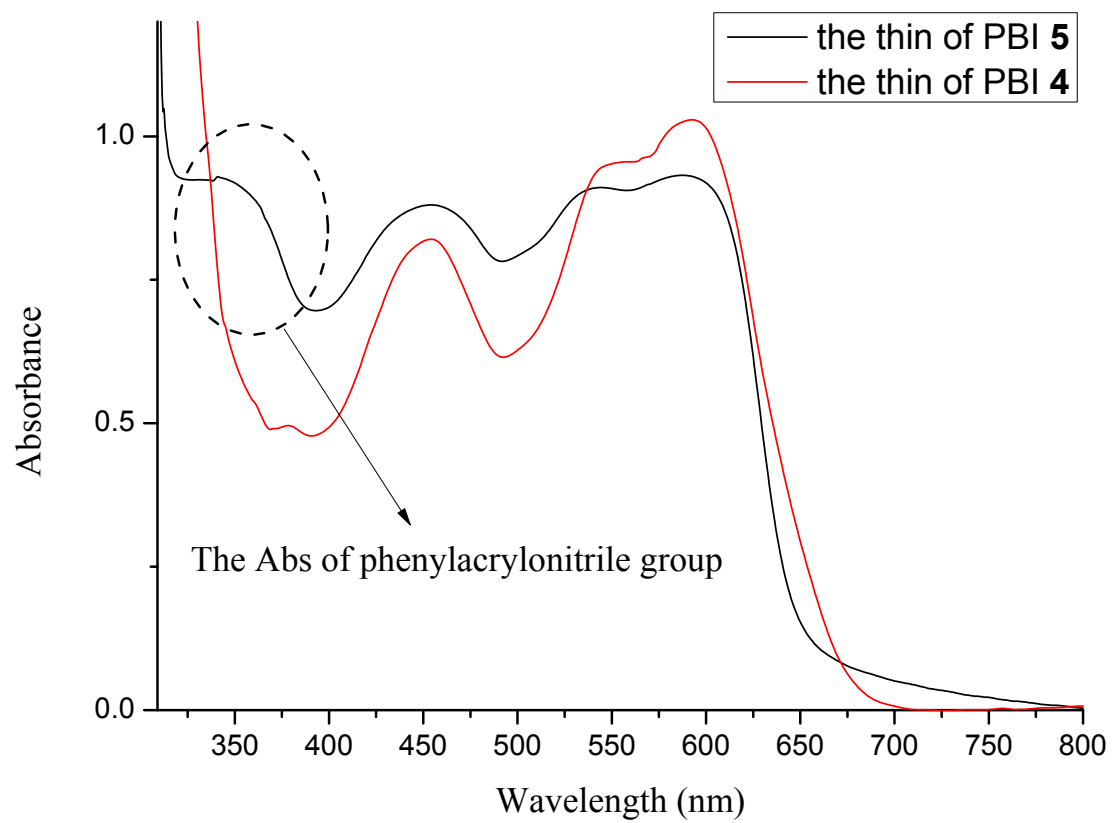


Fig. S15 The thin film absorption spectra of PBIs 4 and 5.