

Supporting Information

Diphenylacrylonitrile conjugated porphyrin with Near-infrared emission by AIE-FRET

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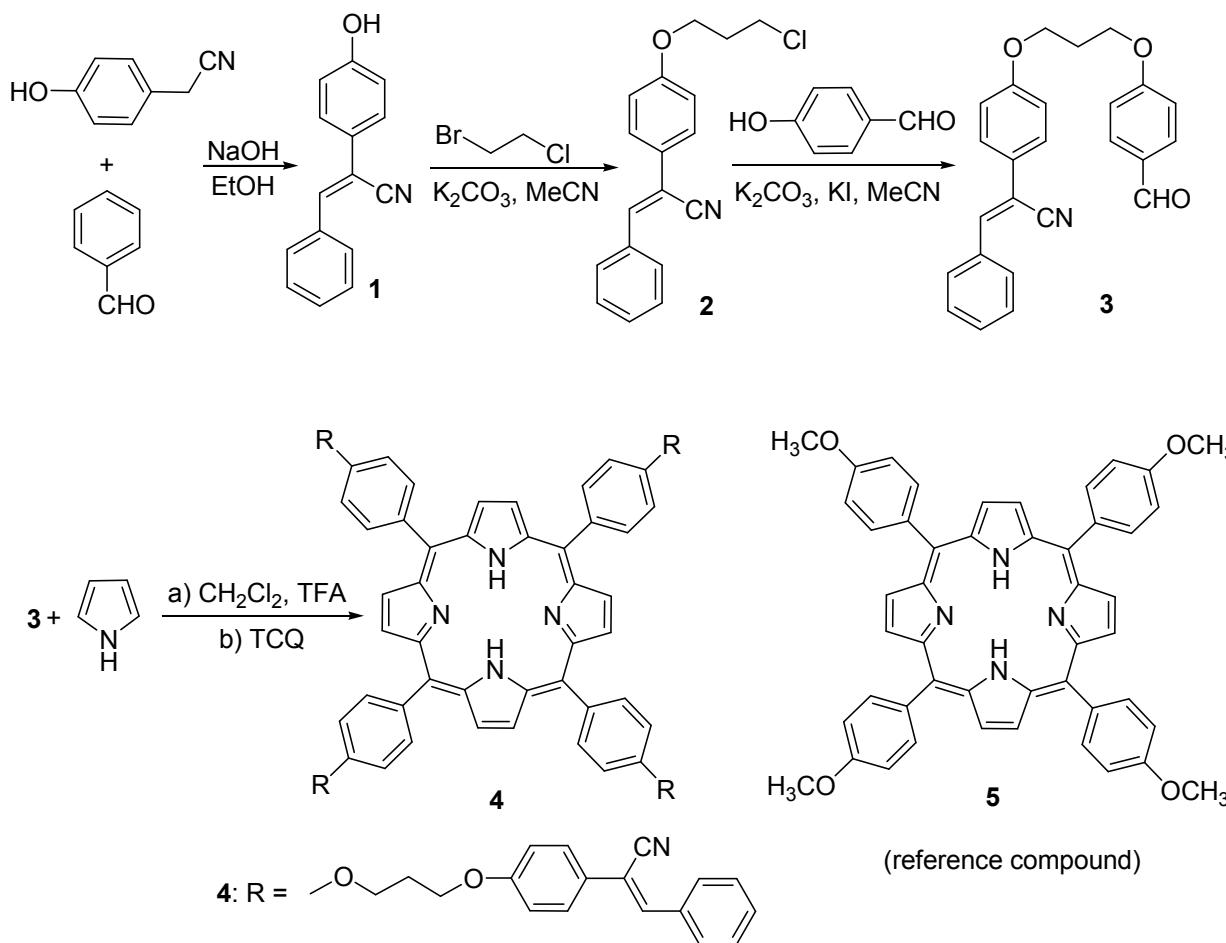
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1. General

All chemical reagents were obtained from commercial suppliers and used without further purification. The other organic solvents and inorganic reagents were purified according to standard anhydrous methods before use. TLC analysis was performed by using pre-coated glass plates. Column chromatography was carried out by using silica gel (200-300 mesh). NMR spectra were recorded in CDCl_3 on a Bruker-ARX 400 instrument at 25 °C. Chemical shifts are reported in ppm, using tetramethylsilane (TMS) as internal standard. MS spectra were obtained from Bruker mass spectrometer.

UV-Vis spectra were recorded on Varian UV-Vis spectrometer. Fluorescence spectra were measured in a conventional quartz cell (10×10×45 mm) at 25 °C on an Edinburgh Instruments FS5 spectrometer with excitation slits 1.8 nm wide and emission slits 0.9 nm wide. The fluorescence absolute Φ_F values were obtained on an Edinburgh Instruments FLS920 Fluorescence Spectrometer with a 6-inch integrating sphere. FT-IR spectra were obtained with samples in KBr matrix on a Thermo Scientific Nicolet 6700 FT-IR Spectrometer. Compounds **1**, **2** and **3** were prepared by reported method (Org. Biomol. Chem., 2017, 15, 6006-6013).



2. The synthetic process and characteristic spectra.

2.1 Synthesis of compound 4.

A mixture of compound **3** (0.38 g, 1 mmol) and pyrrole (67 mg, 1 mmol) was stirred for 60 min at room temperature in 100 mL of CH_2Cl_2 with 0.3 mL of trifluoroacetic acid (TFA), followed by oxidation with tetrachlorobenzoquinone (TCQ) (197mg, 0.8 mmol). After reaction, the solvent was removed by rotary evaporator. The crude product was further purified by silica chromatography on silica gel (eluent: CHCl_3 : ethyl acetate = 85:15), affording 40 mg of compound **4** in 9.3% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.85 (s, 8H), 8.11 (d, J = 8.0 Hz, 8H), 7.85 (d, J = 8.0 Hz, 8H), 7.67 (d, J = 8.0 Hz, 8H), 7.45-7.42 (m, 16H), 7.29 (d, J = 8.0 Hz, 8H), 7.08 (d, J = 8.0 Hz, 8H), 4.47 (t, J = 6.0 Hz, 8H), 4.38 (t, J = 6.0 Hz, 8H), 2.49 (t, J = 6.0 Hz, 8H), -2.73 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 159.9, 158.7, 140.2, 135.6, 134.8, 134.0, 132.0, 130.2, 129.1, 128.9, 127.4, 119.7, 118.2, 115.1, 112.8, 111.3, 64.8, 29.5; MALDI-TOF-MS ($\text{C}_{116}\text{H}_{90}\text{N}_8\text{O}_8$) Calcd. for m/z = 1723.692, found: 1724.386; HR-MS(ESI) Calcd. for $[\text{MH}^+] = 1724.6987$, found: 1724.6979 (MH^+), 1746.6877 (MNa^+).

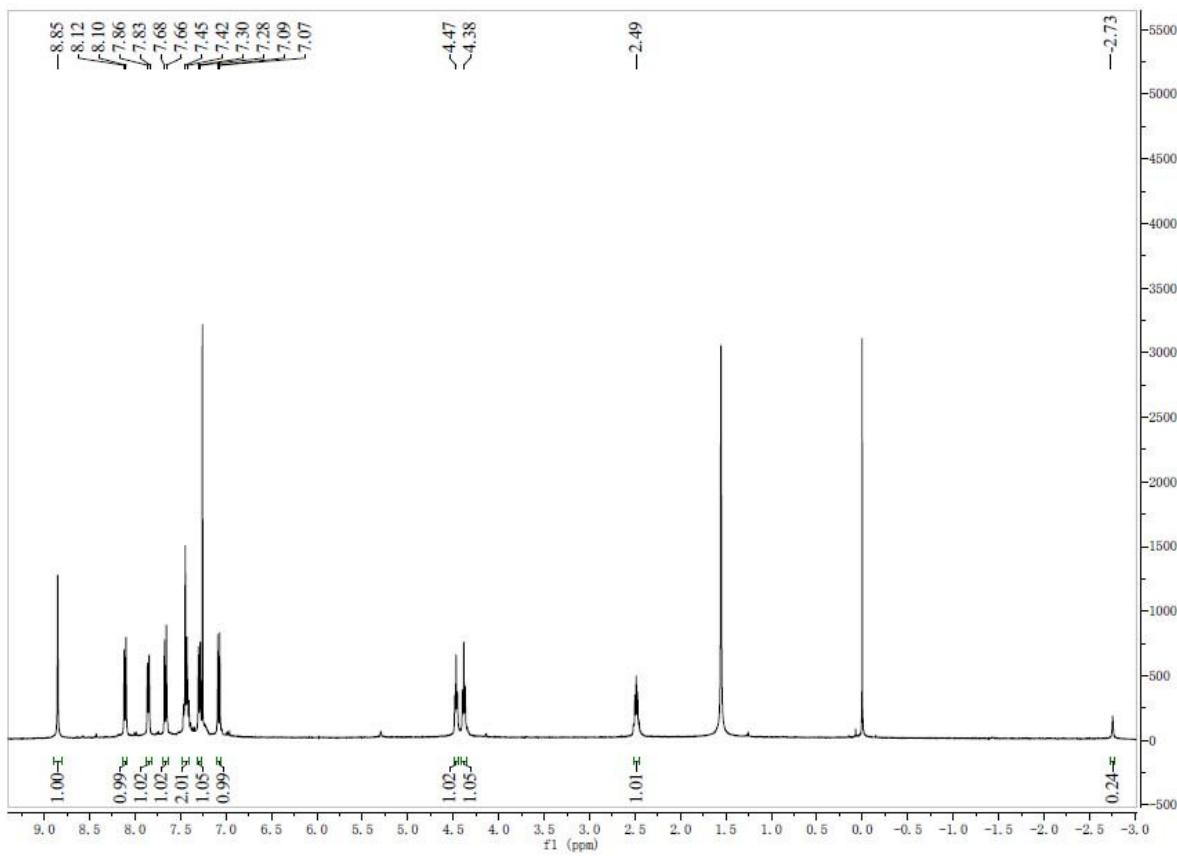


Figure S1. The ^1H NMR spectrum of compound 4

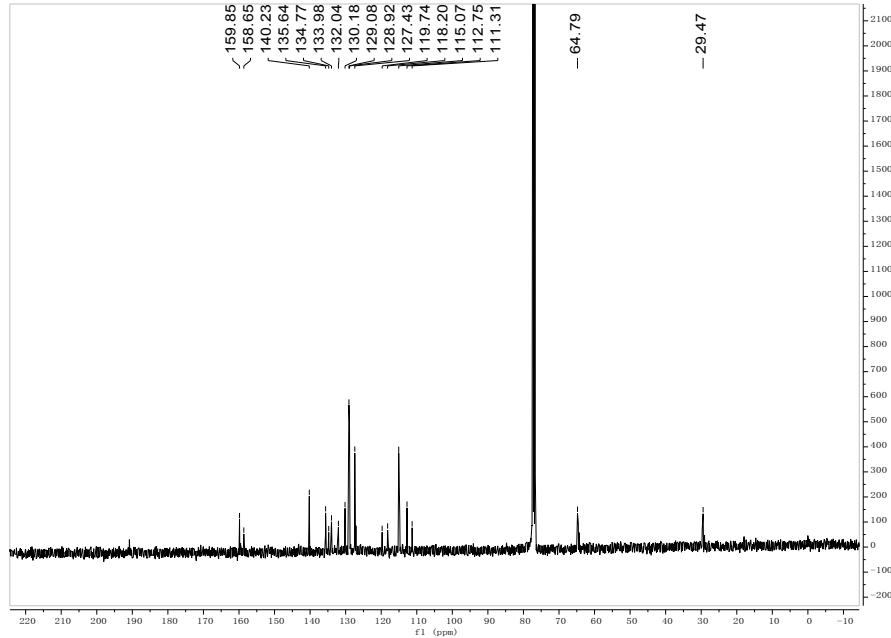


Figure S2. The ^{13}C NMR spectrum of compound 4

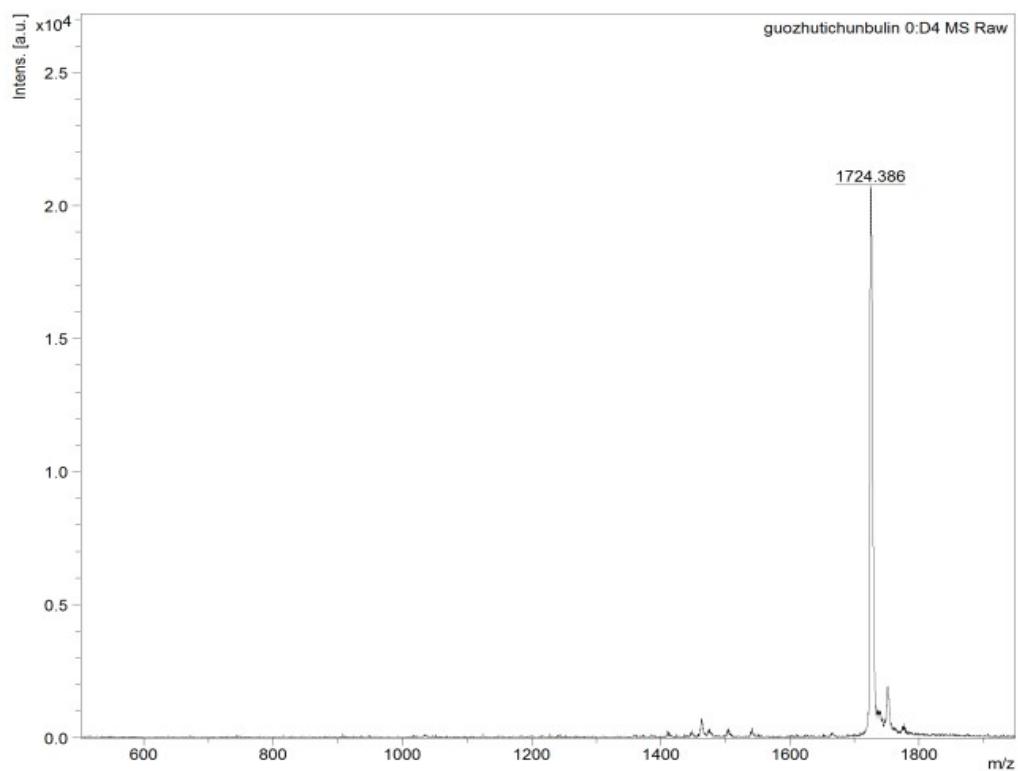


Figure S3. The MALDI-TOF-MS spectrum of compound 4

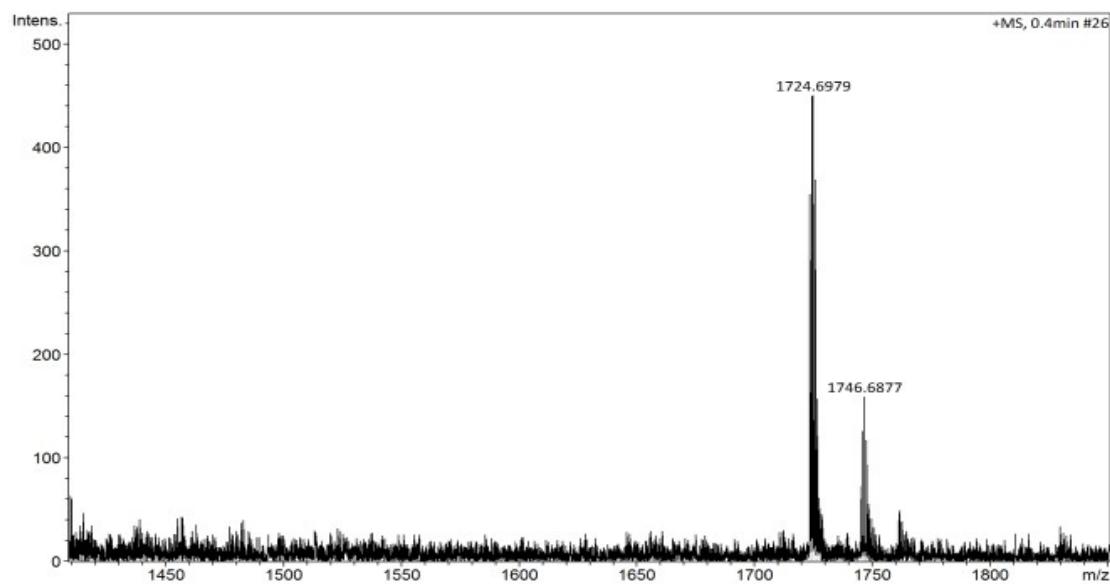


Figure S4. The The HR-MS spectrum of compound 4

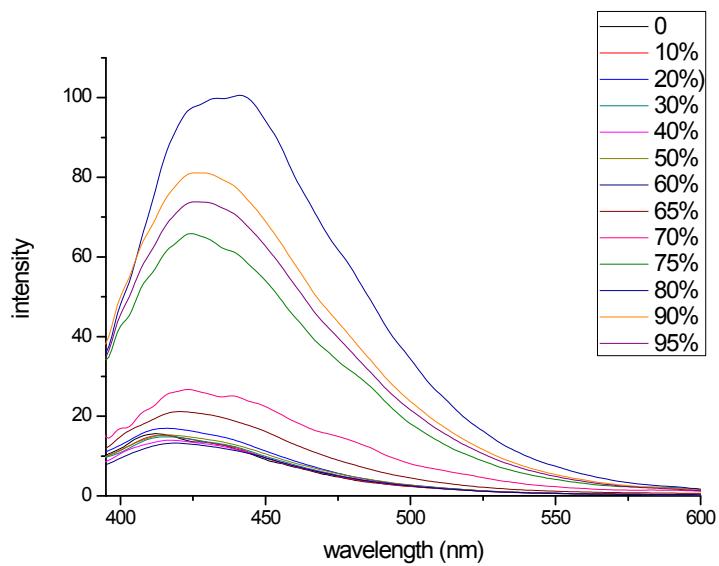


Figure S5 The fluorescence spectra of compound **3** with different fractions of H_2O in $\text{THF}/\text{H}_2\text{O}$ mixtures ($1 \times 10^{-5} \text{ M}$, $\lambda_{\text{ex}} = 330 \text{ nm}$).

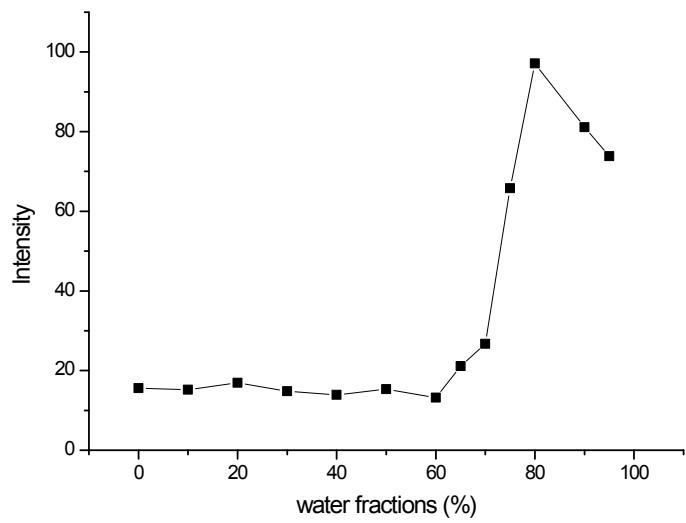


Figure S6 The line plot of fluorescence intensity change from 0-95% water fractions of sample **3**

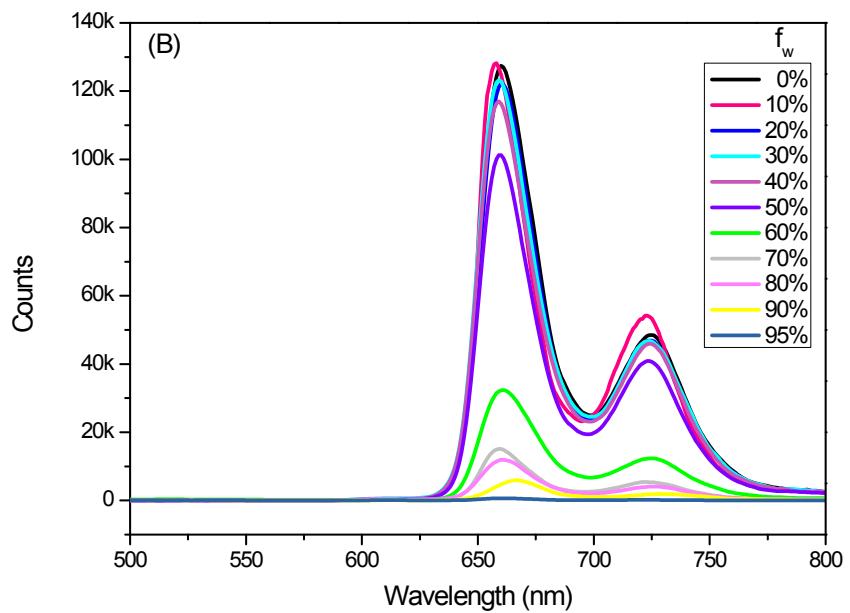


Figure S7 The fluorescence spectra of compound **5** with different fractions of H_2O in THF/ H_2O mixtures (1×10^{-5} M, $\lambda_{\text{ex}} = 420$ nm).

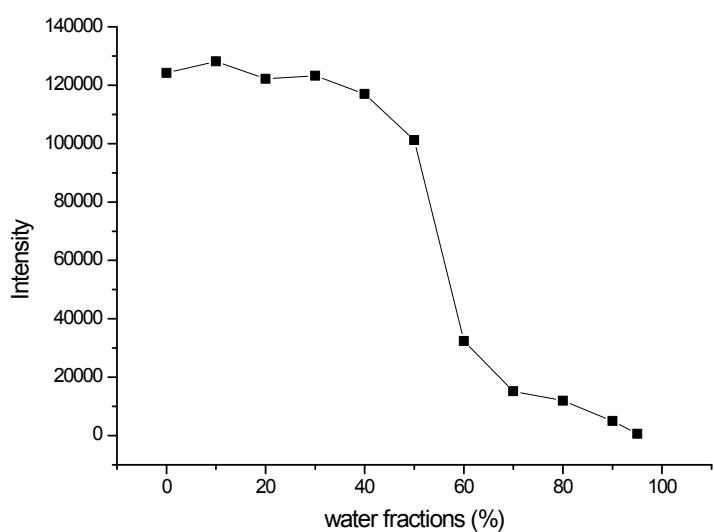


Figure S8 The line plot of fluorescence intensity change from 0-95% water fractions of sample **5**