

Supporting Information

A novel heteroacene 2-(perfluorophenyl)-1*H*-imidazo[4,5-*b*]phenazine for selective sensing of picric acid

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Figure S5 Change in PL intensity of compound **PFIPZ** (10 μM) upon titration with picric acid

Materials

The chemical reagents 2,3-phenazinediamine, pentafluorobenzaldehyde and picric acid were purchased from Aldrich Company and used as received. All other chemicals were used as received without further purification.

Methods

FT-IR spectrum was measured as KBr pellets on Perkin Elmer spectrum GX. ^1H and ^{19}F NMR spectra were recorded on Bruker 300-MHz spectrometers. MALDI-TOF mass spectrometric measurements were finished on Shimadzu Biotech AXIMA-TOF²™. The UV-vis and fluorescence spectra were carried out on Shimadzu UV-2501 and RF-5301 spectrophotometer, respectively. Cyclic voltammetry measurements were conducted on a CHI 604E electrochemical analyser with glassy carbon (diameter: 1.6 mm; area: 0.02 cm²) as a working electrode, and platinum wires as a counter electrode and a reference electrode, respectively. Fc⁺/Fc was used as an internal standard. Potentials were recorded versus Fc⁺/Fc in a solution of anhydrous acetonitrile with 0.1 M tetrabutylammoniumhexafluorophosphate (TBAPF₆) as a supporting electrolyte at a scan rate of 100 mV s⁻¹, by empirical formulas, $E_{\text{LUMO/HOMO}} = -[4.8 - E_{\text{Fc}} + E_{\text{re/ox}}^{\text{onset}}]$ eV, where $E_{\text{Fc}} = 0.22$ eV (measured in our setup). The fluorescent quantum yield (QY) in the solution was determined using fluorescein ($\phi = 0.79$ in 0.1 M NaOH) as standard using the equation:

$$\phi_s = \frac{F_s}{F_r} \frac{n_s^2}{n_r^2} \frac{A_r}{A_s} \phi_r \quad (1)$$

In this equation, subscripts s and r represent the sample and reference, respectively. F is the integral area of the fluorescence spectra, n is the refractive index of the solution, A is the absorbance, ϕ is the fluorescence quantum yield.

Synthesis of 2-(perfluorophenyl)-1*H*-imidazo[4,5-*b*]phenazine (PFIPZ)

In a round bottom flask, 2,3-diaminophenazine (210 mg, 1 mmol) and pentafluorobenzaldehyde (216 mg, 1.1 mmol) was dissolved in nitrobenzene (20 mL) under N₂. The mixture was heated to reflux for 12 hours and cooled down to room

temperature. Then, nitrobenzene was distilled under vacuum. The solid residue was purified by flash column chromatography (silica gel) with ethyl acetate: hexane = 1:2, and compound **PFIPZ** (79 mg, 0.2 mmol) was obtained as orange color powder in yield of 20%.

^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 13.51 (s, 1H), 8.53 (s, 2H), 8.25 (dd, $J = 6.7, 3.4$ Hz, 2H), 7.92 (dd, $J = 6.8, 3.3$ Hz, 2H). ^{19}F NMR (282 MHz, $\text{DMSO-}d_6$) δ -138.73 (qd, $J = 10.1, 4.9$ Hz, 2F), -149.41 – -149.83 (m, 1F), -161.01 – -161.41 (m, 2F).

HR-MS, Calcd for $\text{C}_{19}\text{H}_7\text{F}_5\text{N}_4$, 386.3; Found, 386.7.

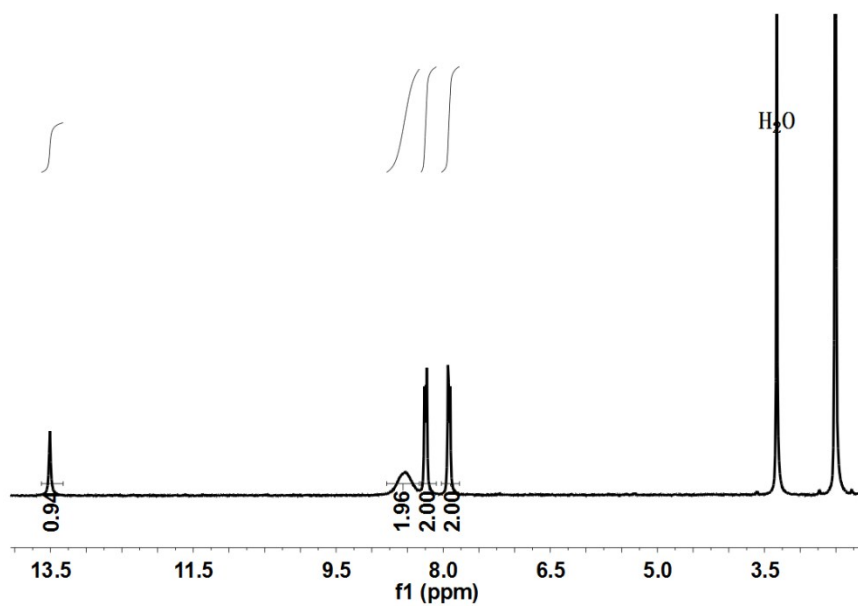


Figure S1 ^1H NMR spectrum of compound **PFIPZ** in $\text{DMSO-}d_6$.

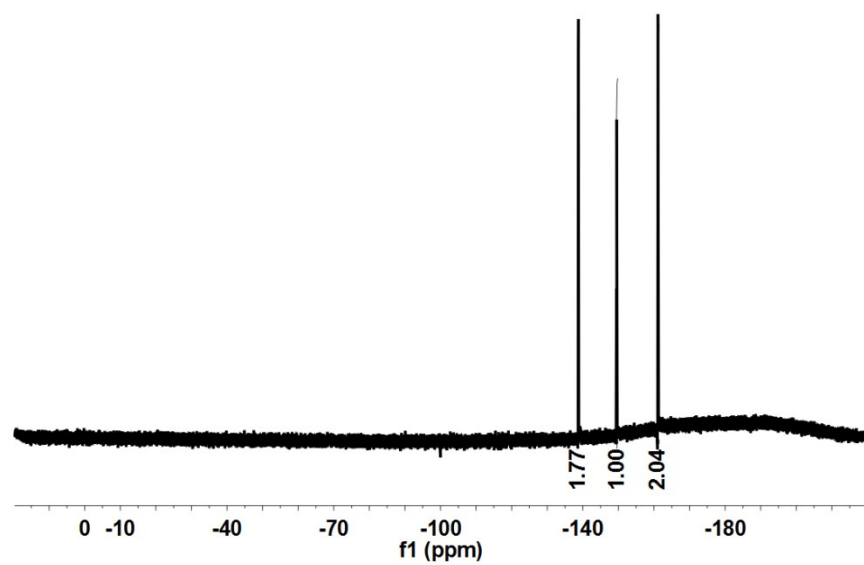


Figure S2 ^{19}F NMR spectrum of compound PFIPZ in $\text{DMSO-}d_6$.

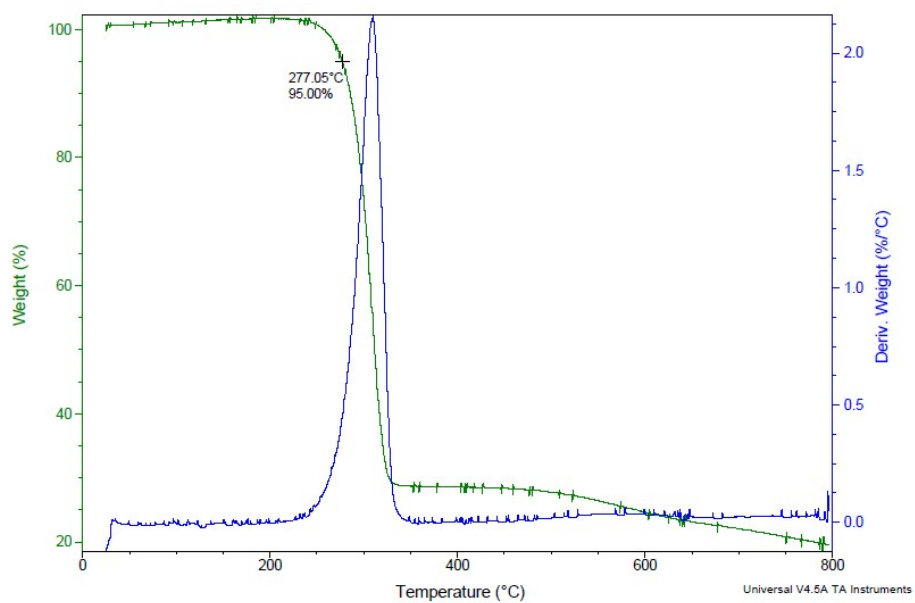


Figure S3 TGA spectrum of compound PFIPZ.

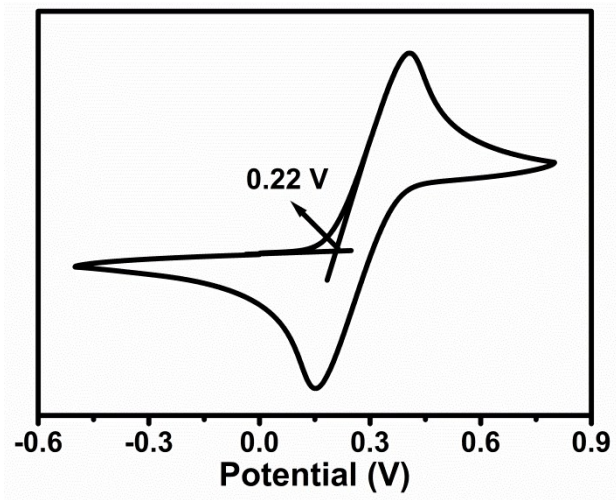


Figure S4 Cyclic voltammogram of the ferrocene standard in acetonitrile solution at the scan rate of 100 mV S⁻¹.

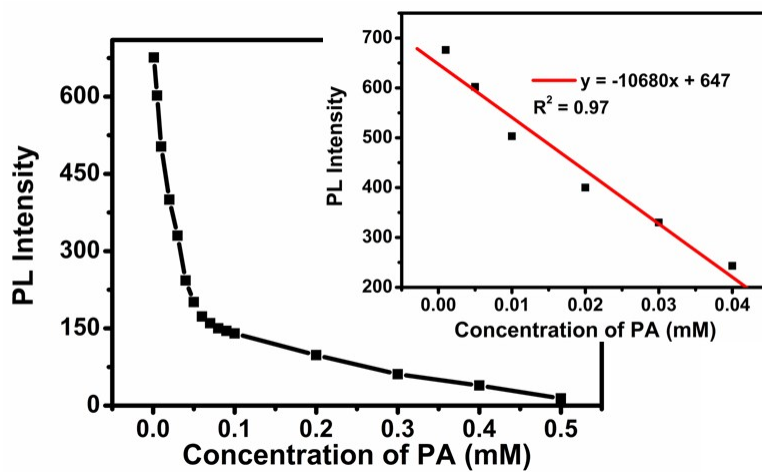


Figure S5 Change in PL intensity of compound PFIPZ (10 uM) upon titration with picric acid