

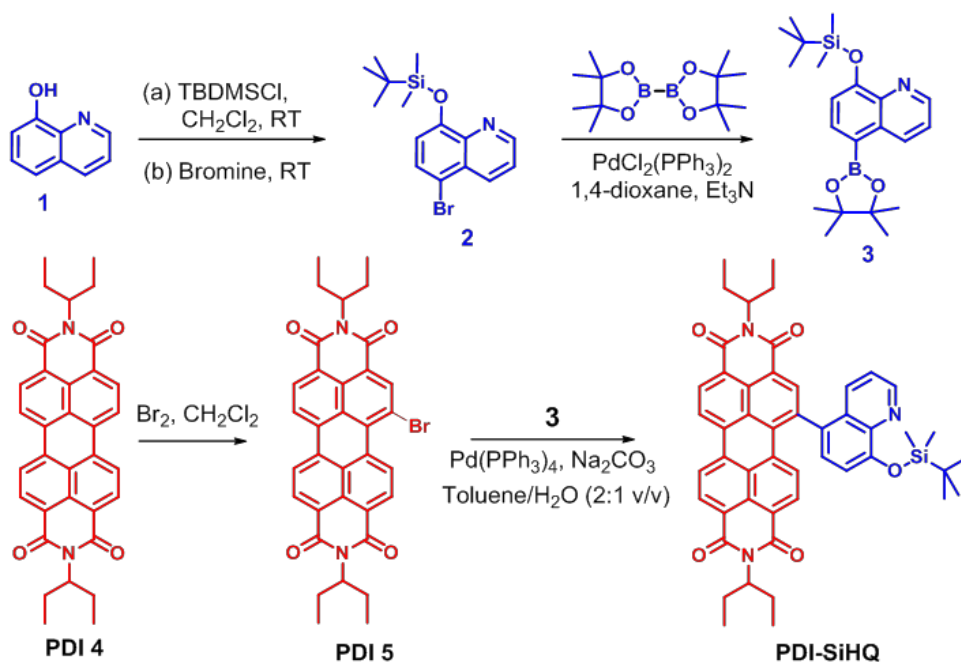
# Perylene diimide-based organic $\pi$ -motif for differentiating $\text{CN}^-$ and $\text{F}^-$ ions by encounter of electron-transfer vs. desilylation mechanisms: Applications to complex logic circuits

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## 1. Experimental Section



### Synthesis of compound 2

Compound 8-Hydroxyquinoline (1) (5.0 g, 0.034 mol) was taken in dichloromethane (150 mL, dry) and *tert*-butyl dimethylsilyl chloride (5.7 g, 0.038 mol), imidazole (2.46 g, 0.036 mol) were added all at once. The reaction mixture was stirred for 24 hour at RT. After this time interval, the reaction mixture was quenched with 0.1 N HCl solution washed with

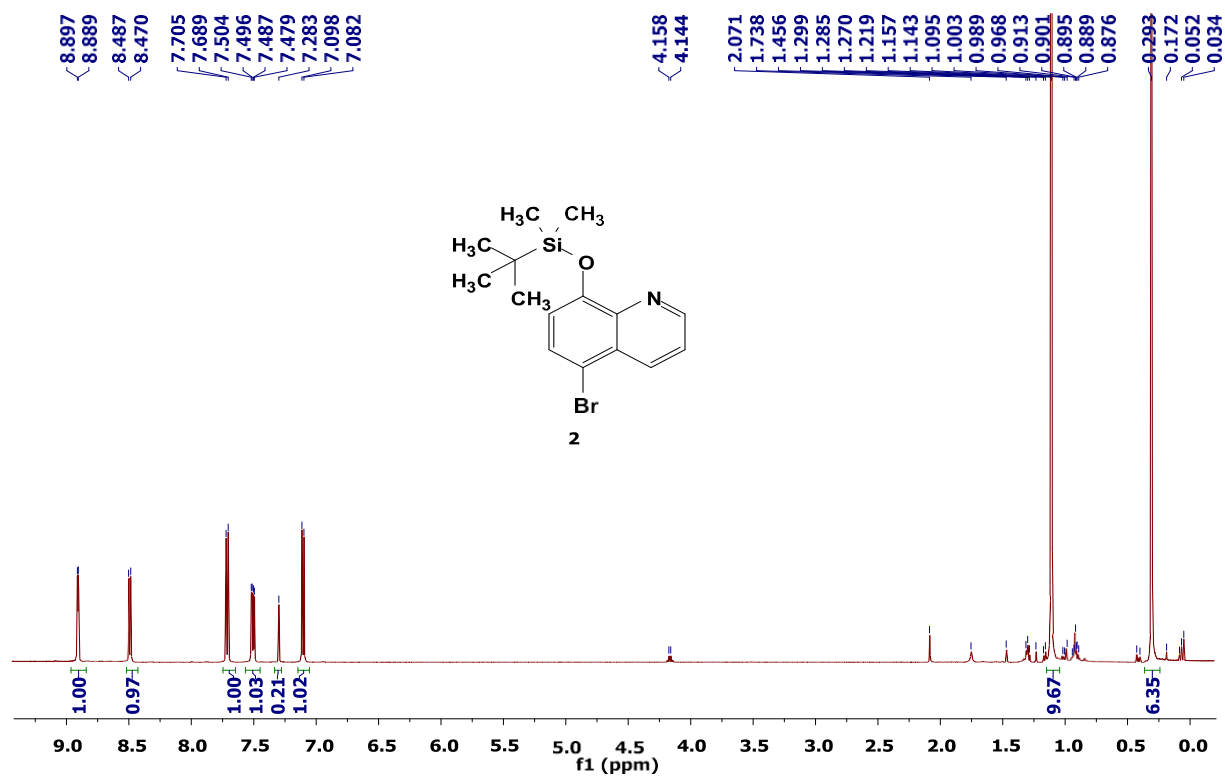
brine and crude product was concentrated under high vacuum. Isolated as colourless liquid and subsequently used without purification; Yield is 80.1% (7.2 g, 0.025 mol);  $R_f = 0.3$  (Et<sub>2</sub>O:hexane 2:98 v/v). Crude product (5.0 g, 0.019 mol) was dissolved in dichloromethane (120 mL, dry) under nitrogen atmosphere. Bromine (0.49 mL, 0.019 mol) in dichloromethane (20 mL, dry) was added drop-wise at RT under nitrogen atmosphere. The reaction mixture was stirred for 10 h at RT. After this interval, quenched the reaction mixture with saturated solution of sodium thiosulfate, washed with brine and crude product was concentrated under high vacuum. The crude product was purified by column chromatography (ethyl acetate:hexane, 1:99 v/v) to obtained compound **2** as pale yellow liquid; Yield is 92% (6.0 g, 0.017 mol);  $R_f = 0.6$  (Ethyl acetate:hexane 1:99); HRMS (TOF, ESI)  $m/z$  found 339.04; calcd. 340.06 for C<sub>12</sub>H<sub>20</sub>BrNOSi; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta$  0.27 (s, 6H), 1.07 (s, 9H), 7.07 (d,  $J = 8.0$  Hz, HQ-H7, 1H), 7.47 (dd,  $J_1 = 8.5$  Hz,  $J_2 = 4.0$  Hz, HQH-3, 1H), 7.67 (d,  $J = 8$  Hz, HQH-6, 1H), 8.45(d,  $J = 8.5$  Hz, HQH-4, 1H), 8.87(d,  $J = 4$  Hz, HQH-2, 1H) ppm; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 25 °C):  $\delta = -3.8, 19.0, 26.0, 112.4, 118.4, 122.4, 128.6, 130.6, 135.4, 143.0, 149.1, 153.0$  ppm.

**NMR titration studies:** <sup>1</sup>H NMR titration of **PDI-SiHQ** against CN<sup>-</sup> was performed in THF(*d*<sub>8</sub>) on Bruker-AVANCE-II FT-NMR AL400 spectrometer. All the data were then processed in Top Spin software to draw the stacking spectra of **PDI-SiHQ** and **PDI-SiHQ**+CN<sup>-</sup> complex at different concentrations.

**Theoretical calculations:** All the calculations were carried out using density functional theory (DFT) at B3LYP/6-31G\* basis set.

**Cyclic voltametry studies.** Electrochemical measurements were made using CHI660D electrochemical workstation using three electrodes- platinum as working as well as counter electrode, glassy as reference electrode and ferrocene as standard. The experiments were carried at  $25 \times 10^{-6}$  M solution of the compound in Tetrahydrofuran using  $2 \times 10^{-2}$  M tetrabutylammonium hexafluorophosphate as supporting electrolyte. The solutions were purged with nitrogen for 10 min before performing the experiment. The working electrode as well as the

reference electrode was cleaned after each reading. The experiments were carried out at scan rate of  $100 \text{ mVs}^{-1}$ .



**Fig S1a:**  $^1\text{H}$  NMR spectrum of compound 2.

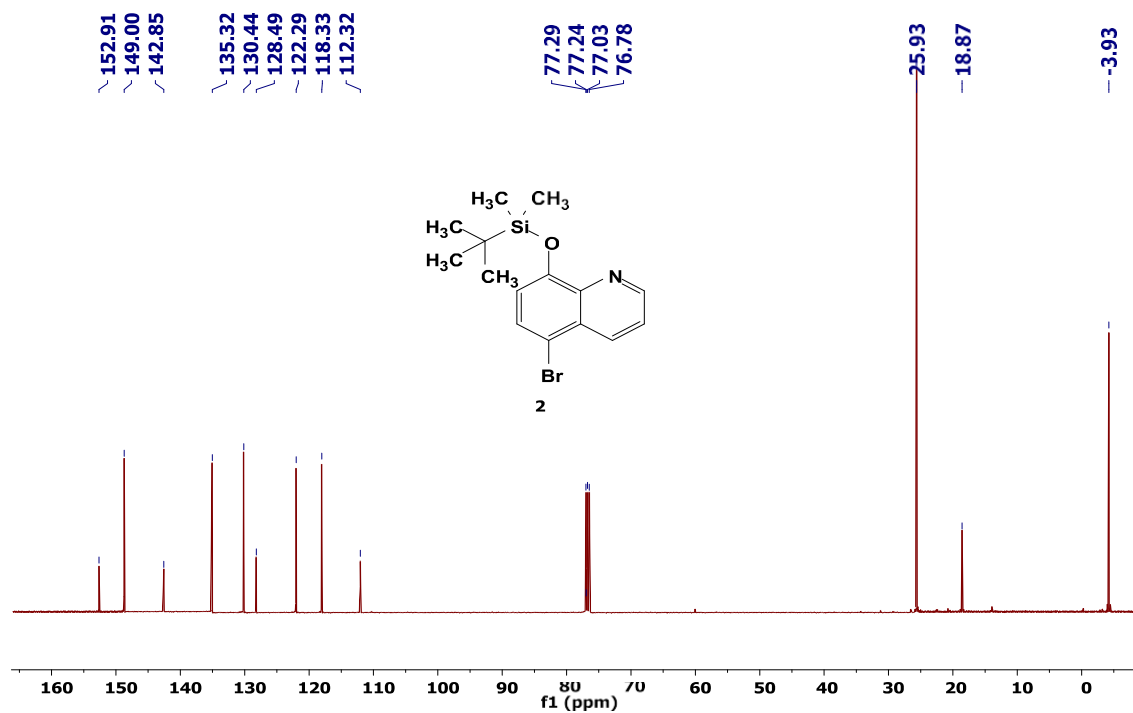


Fig S1b:  $^{13}\text{C}$  NMR spectrum of compound 2.

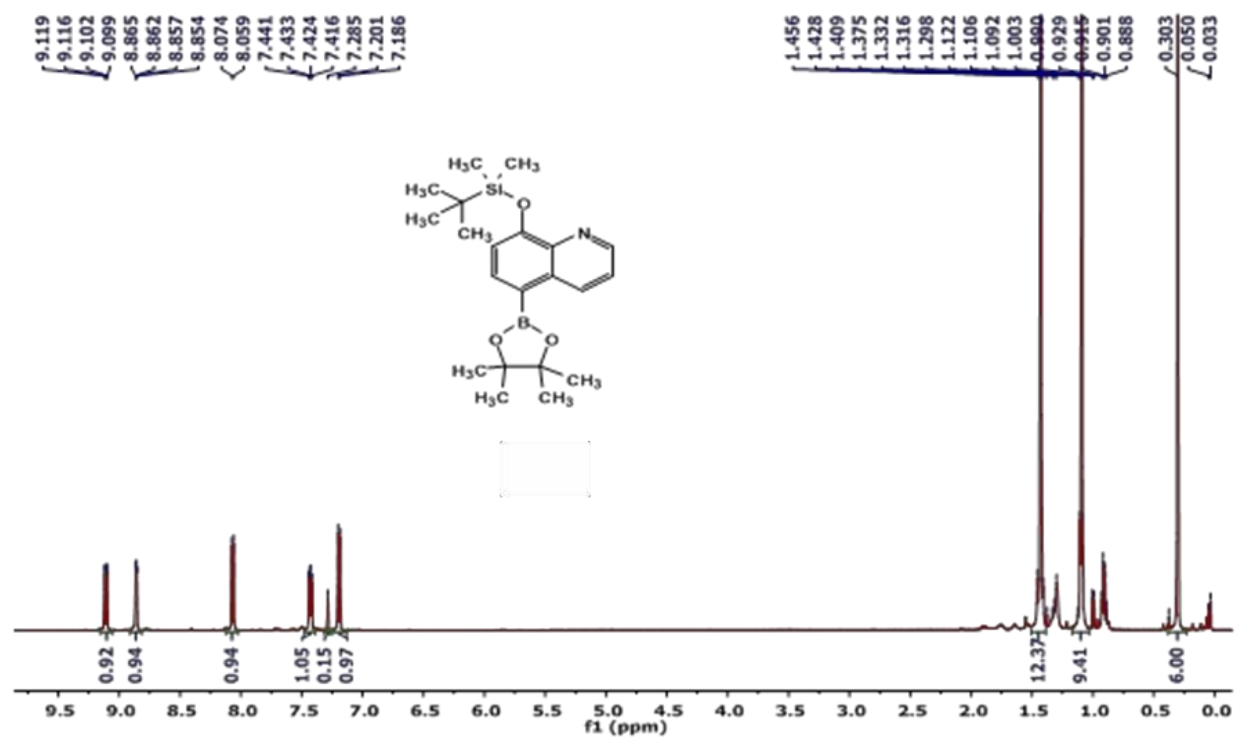


Fig S2a:  $^1\text{H}$  NMR spectrum of derivative 3.

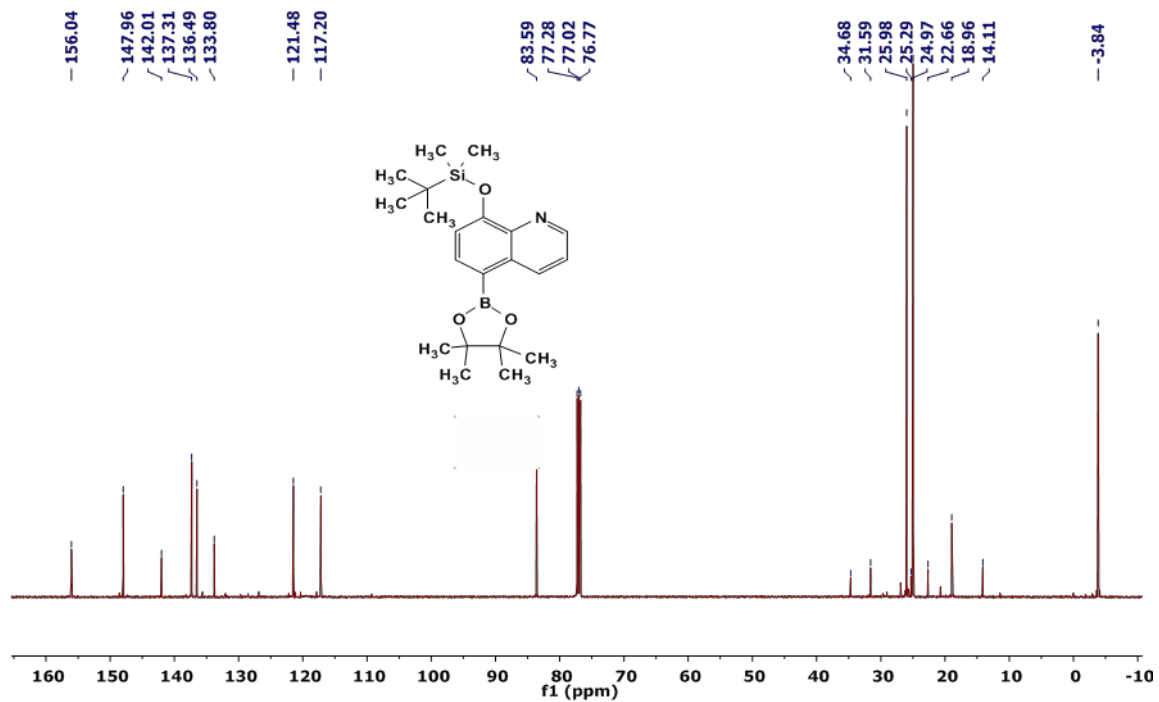


Fig S2b:  $^{13}\text{C}$  NMR spectrum of compound 3.

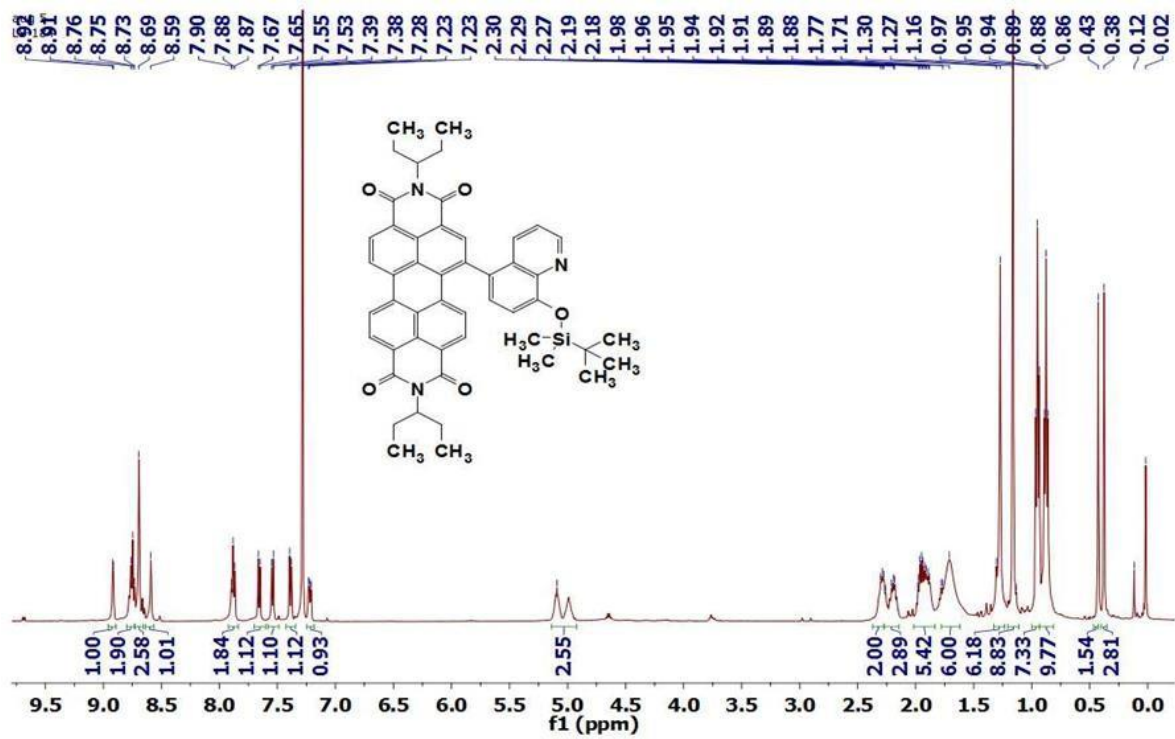


Fig S3a:  $^1\text{H}$  NMR spectrum of PDI-SiHQ.

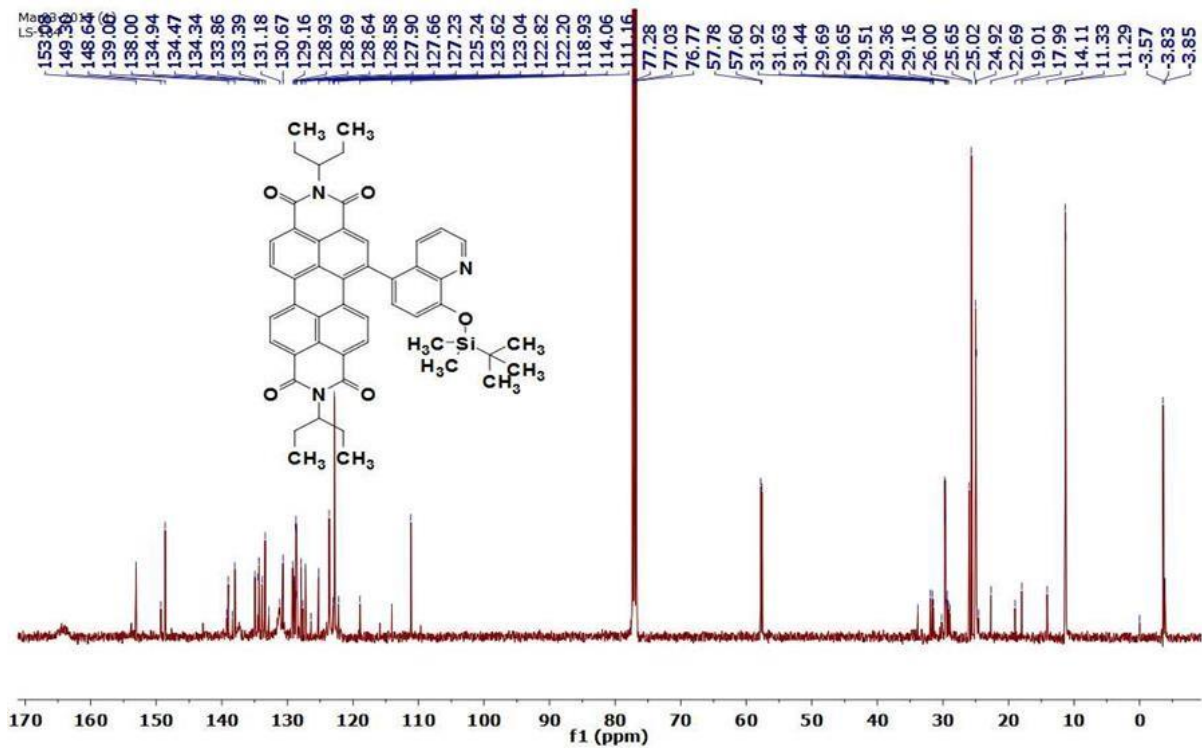
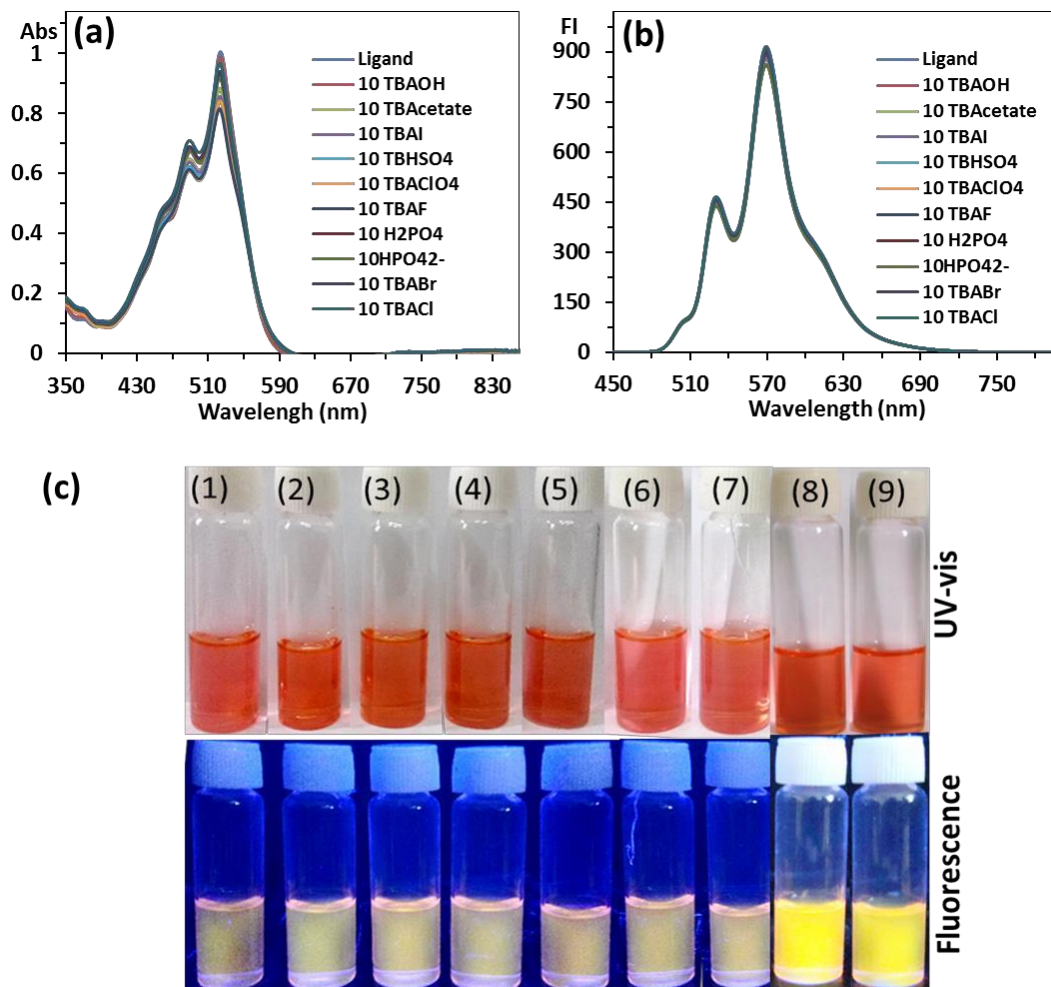
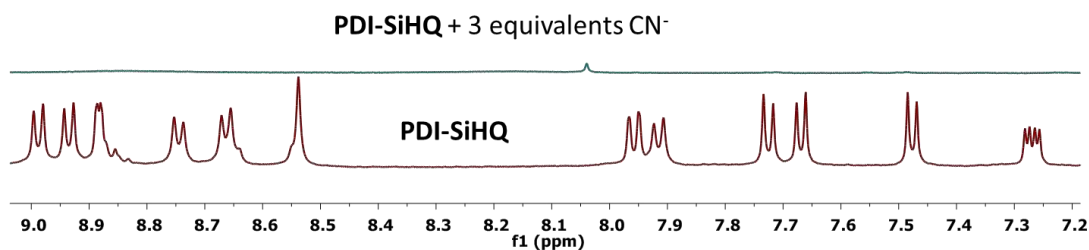


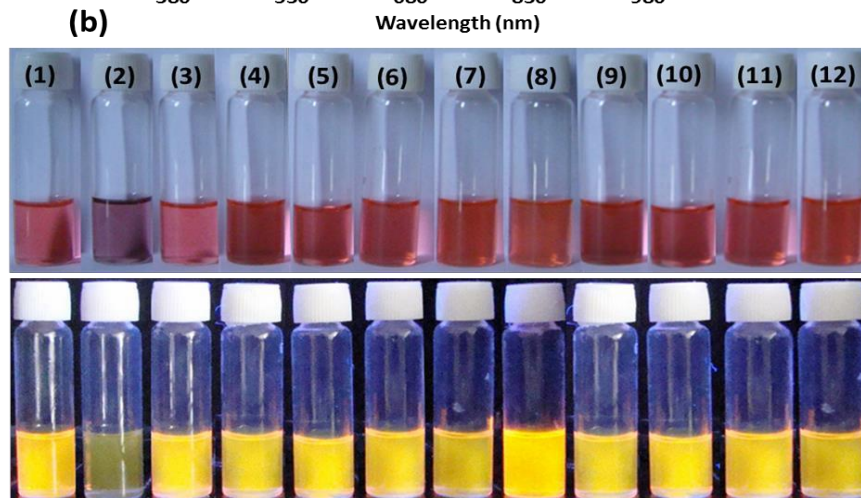
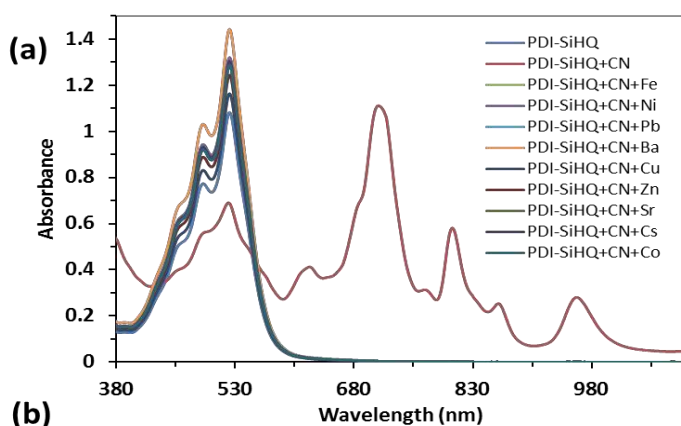
Fig S3b: <sup>13</sup>C NMR spectrum of PDI-SiHQ.



**Figure S4:** (a) UV-vis-NIR absorption and (b) emission spectra of **PDI-SiHQ** (25  $\mu\text{M}$ ) after addition of different anions recorded in a THF solvent; (c) Photographs showing visible colorimetric (upper panel) and fluorescence (under 365 nm UV illumination) changes in **PDI-SiHQ** after interaction with different anions in THF; (1) **PDI-SiHQ**; tetrabutylammonium salts of (2)  $\text{OH}^-$ ; (3)  $\text{CH}_3\text{COO}^-$ ; (4)  $\text{I}^-$ ; (5)  $\text{HSO}_4^-$ ; (6)  $\text{ClO}_4^-$ ; (7)  $\text{Br}^-$ ; (8)  $\text{H}_2\text{PO}_4^-$  and (9)  $\text{H}_2\text{PO}_4^{2-}$ .



**Figure S5.** Partial <sup>1</sup>H NMR spectra (aromatic region) of **PDI-SiHQ** (1 mM) with CN<sup>-</sup> ions recorded in THF (d<sub>8</sub>) solvent.



**Figure S6:** (a) UV-vis-NIR absorption titration spectra of **PDI-SiHQ**<sup>•-</sup> radical anion after addition of different metal ions recorded in a THF solvent; (b) Photographs showing the naked-eye color (upper panel) and fluorescence (lower panel) changes in **PDI-SiHQ**<sup>•-</sup> radical anion solution on addition of different metal ions in THF; (1) **PDI-SiHQ**; (2) **PDI-SiHQ**<sup>•-</sup> radical anion (generated by mixing **PDI-SiHQ** and CN<sup>-</sup> 1:10); **PDI-SiHQ**<sup>•-</sup> radical anion+tetrabutylammonium salts of (3) Ni<sup>2+</sup>; (4) Pb<sup>2+</sup>; (5) Fe<sup>3+</sup>; (6) Ba<sup>2+</sup>; (7) Cu<sup>2+</sup>; (8) Sr<sup>2+</sup>; (9) Zn<sup>2+</sup>; (10) Cs<sup>+</sup>; (11) Co<sup>2+</sup>; (12) Hg<sup>2+</sup>.