

## Supplementary Information

### Highly selective colorimetric cysteine sensor based on core-substituted naphthalenediimides

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#### Materials and Methods

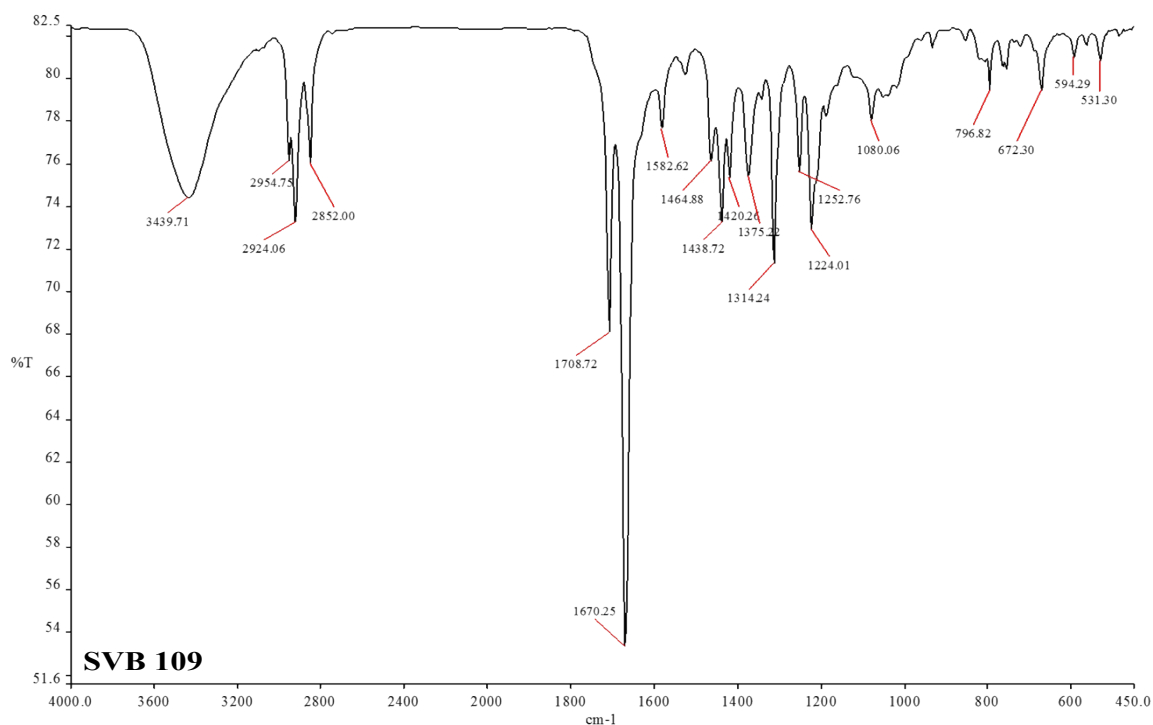
Naphthalene dianhydride, octylamine, dibromoisocyanuric acid, acetic acid, 2-tributyl stannyl thiophene, Pd (PPh<sub>3</sub>)<sub>4</sub>, DMF and chloroform-*d*, were purchased from Sigma-Aldrich, Bangalore, Karnataka, India and used without purification, unless otherwise specified. UV-vis absorption spectra were recorded UV-vis-1800 Shimadzu recording spectrophotometer. Fluorescence emission spectra were measured on Cary eclipse fluorescence spectrophotometer Agilent technologies. <sup>1</sup>H NMR, <sup>13</sup>C-NMR spectra were recorded on a Bruker spectrometer using chloroform-*d* as solvent and tetramethylsilane as an internal standard. The solvents for spectroscopic studies were of spectroscopic grade and used as received.

#### Synthesis of NDI-1

Dry DMF (0.065 mL, 0.7 mmol) in 50 mL round bottomed flask in 20 mL dry 1, 2-dichloroethane at 0 °C followed by addition of POCl<sub>3</sub> (0.0727 mL, 0.78 mmol) dropwise. Stirred the reaction mixture for 30 min at 0 °C. Warmed the reaction mixture to room temperature, **2** (510 mg, 0.78 mmol) was added in reaction mixture at room temperature. The

reaction mixture heated at 60 °C for 4 hour. The reaction mixture was cooled to room temperature, reaction mixture quenched using NaHCO<sub>3</sub>. The reaction mixture extracted with DCM (3 x 25 mL), organic layer was washed with water and brine solution. Organic layer dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and evaporated under reduced pressure. The crude product was purified via column chromatography using elutant (DCM: Hexane; 6:4) afforded reddish solid as thiophene NDIs **1** (120 mg, 35%): mp 180 -182 °C; FT-IR (KBr, cm<sup>-1</sup>)  $\nu$  2924, 2852, 1708, 1670, 1582, 1438, 1375, 1314, 1252, 1224, 1086, 786, 672, 594, 531; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) : 0.84-0.87  $\delta$  (6H, m), 1.25-1.37 (m, 20H), 1.62-1.68 (m, 4H), 4.07-4.10 (t, 4H), 7.30-7.31 (d, *J*=3.81 Hz, 2H), 7.86-7.87 (d, *J*=3.81 Hz, 2H), 8.72 (s, 2H), 10.01 (s, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  14.04, 22.57, 26.99, 27.93, 29.12, 31.72, 41.29, 124.24, 125.80, 127.67, 128.60, 135.72, 136.11, 139.14, 145.04, 150.11, 161.46, 161.61, 182.80; ESI-MS *m/z* 711 [M+H]<sup>+</sup>

### Supporting figures



**Fig. S1** FT-IR spectrum of NDI-1

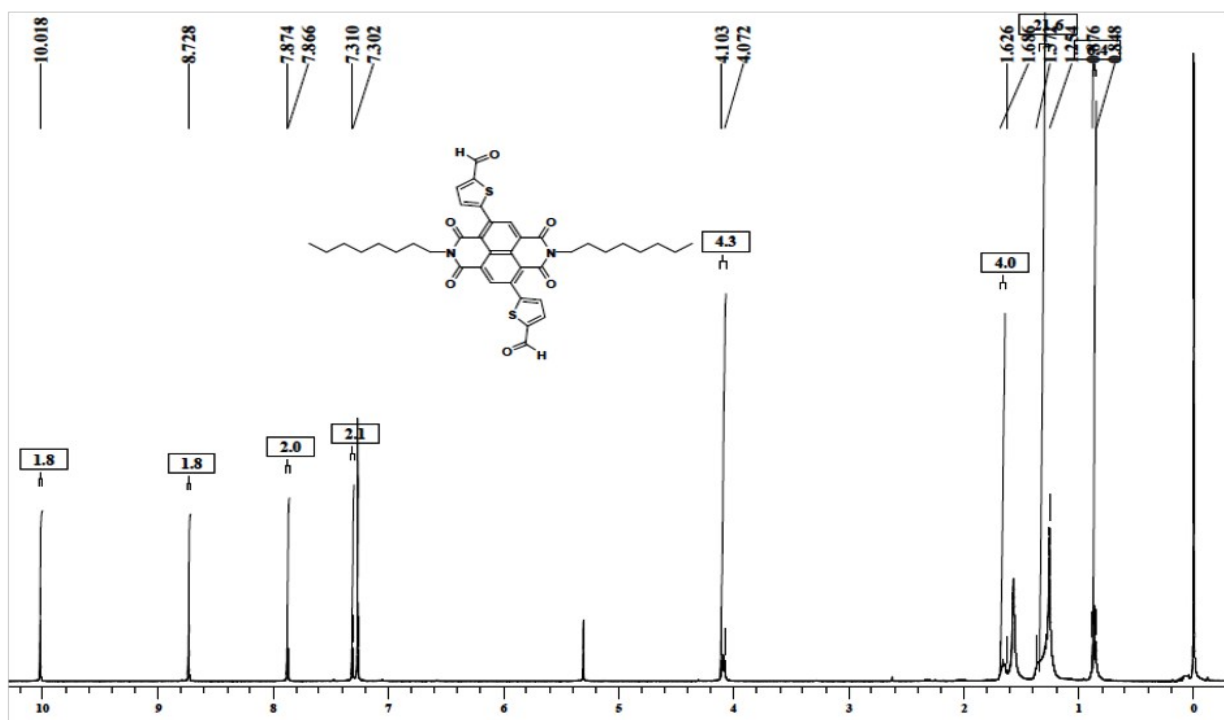


Fig. S2  $^1\text{H}$  NMR spectra of NDI-1

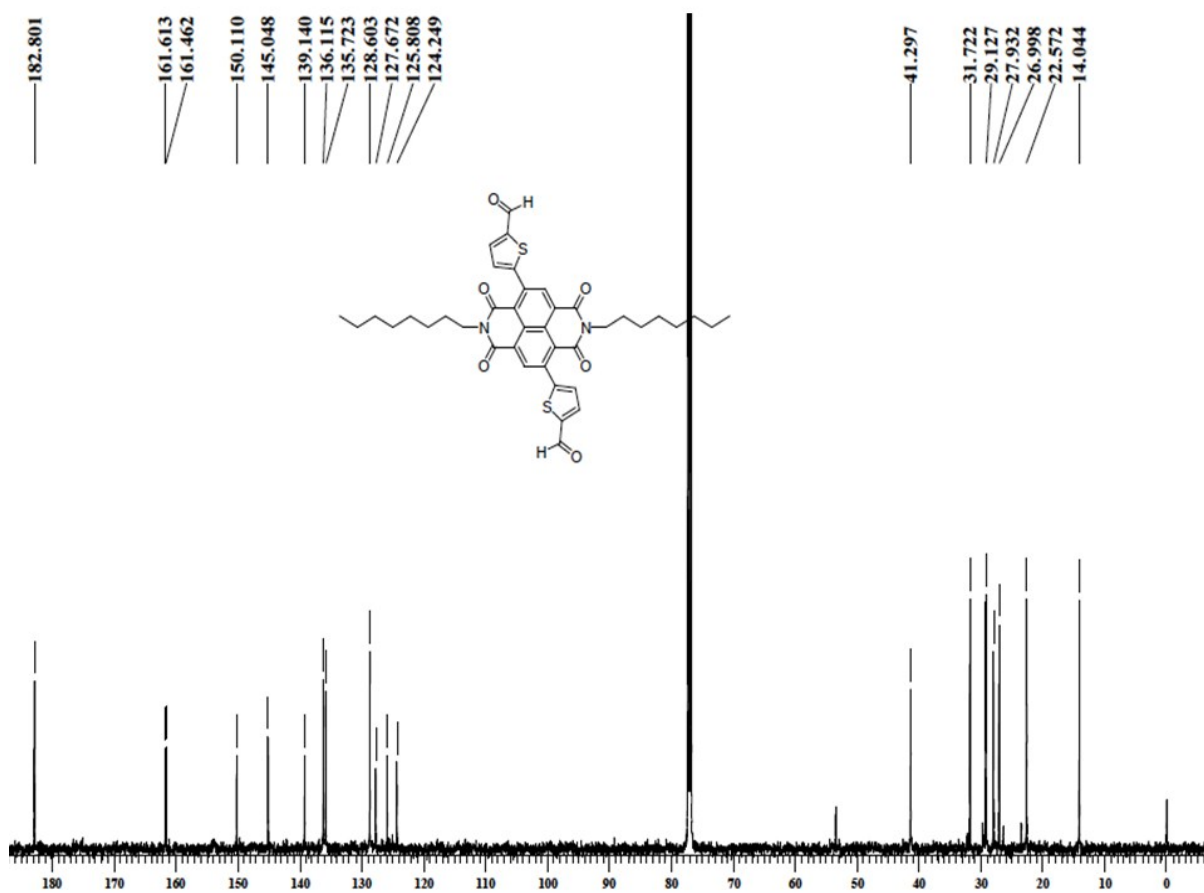
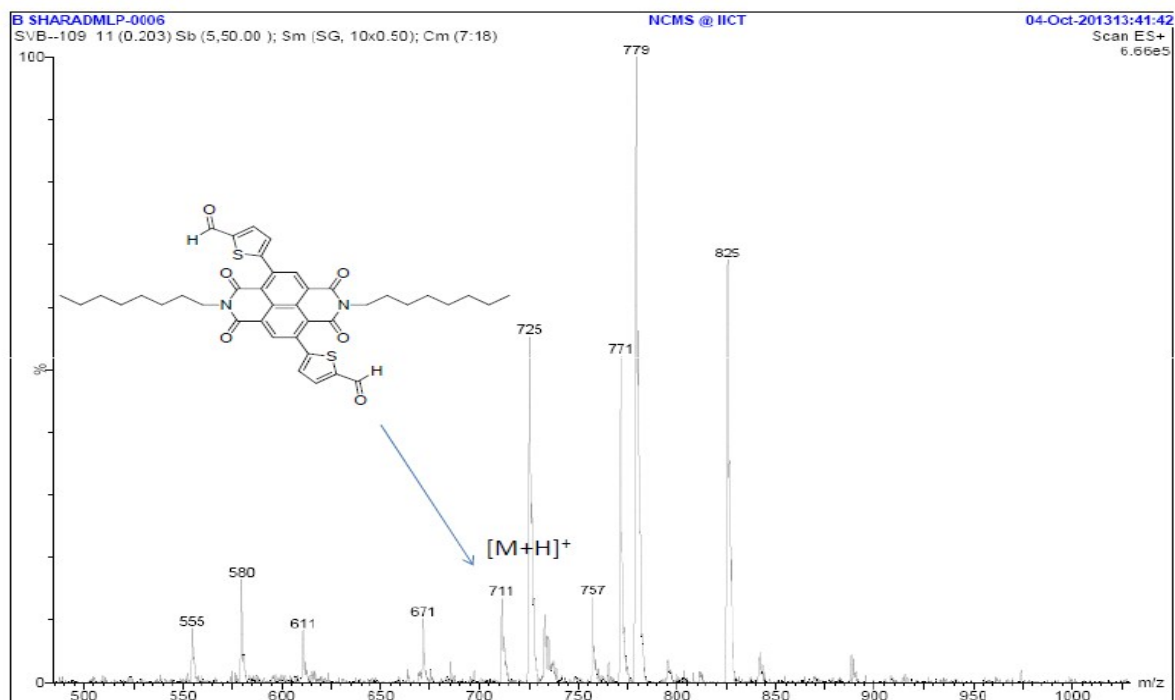
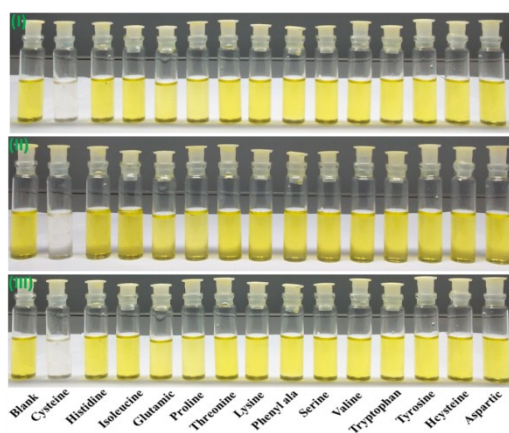


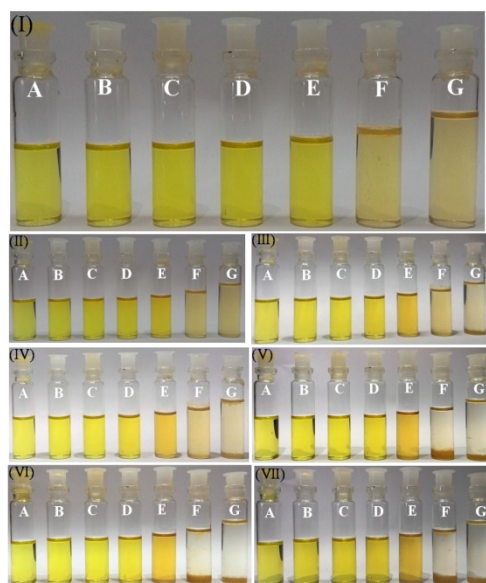
Fig. S3  $^{13}\text{C}$  NMR spectra of NDI-1



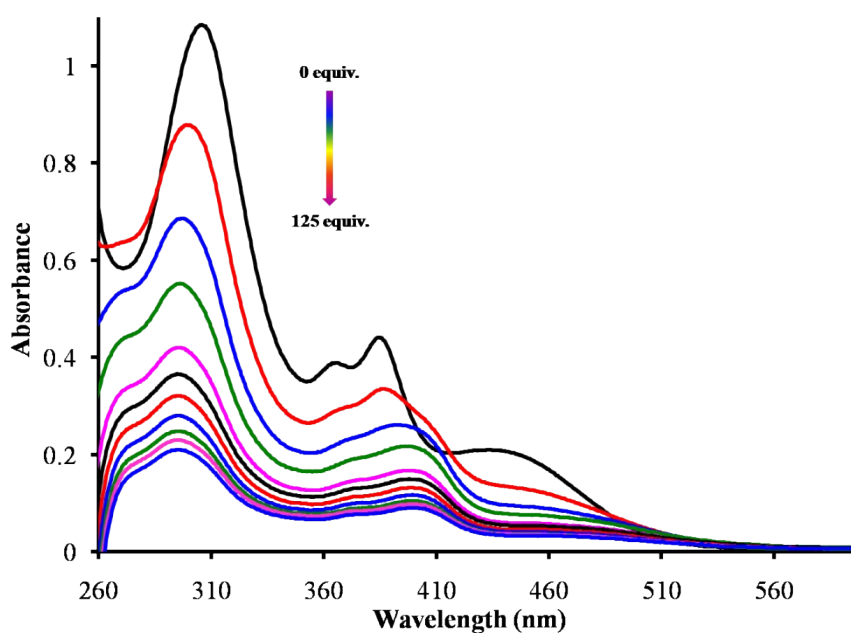
**Fig. S4** Mass spectra of NDI-1



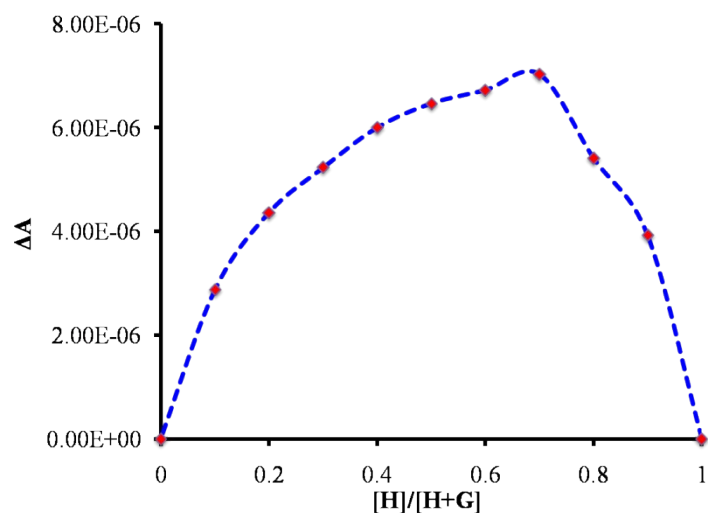
**Fig. S5** Naked-eye colorimetric changes of **1** in DMSO ( $1 \times 10^{-4}$  M) [(I) 0 h, (II) 12 h, (III) 24 h] upon addition of various amino acids (125 equiv.) in H<sub>2</sub>O (pH 7.4 ; 0.1 M HEPES) at ambient temperature.



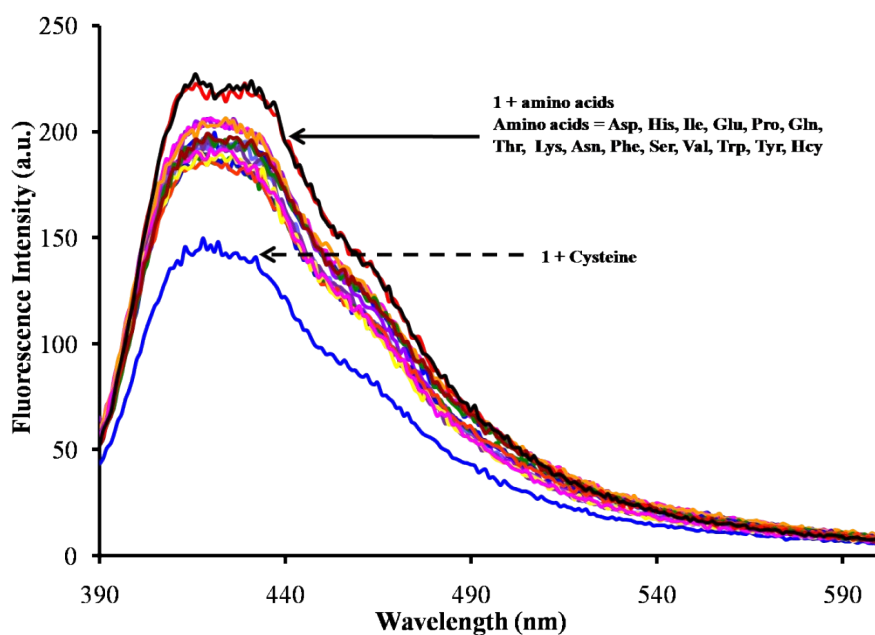
**Fig. S6** Naked-eye colorimetric changes of **1** in DMSO ( $1 \times 10^{-4}$  M) [(I) 0 h, (II) 1 h, (III) 6 h, (IV) 12 h, (V) 24 h, (VI) 36 h and (VII) 48 h] upon addition of cysteine (A = 0, B = 1, C = 2, D = 5, E = 25, F = 50 and G = 100 equiv.) in  $\text{H}_2\text{O}$  (pH 7.4 ; 0.1 M HEPES) at ambient temperature.



**Fig. S7** UV-vis absorption spectrum of **NDI-1** ( $1.0 \times 10^{-4}$  M) upon addition of cysteine (0-125 equiv.) in DMSO/ $\text{H}_2\text{O}$  (v/v, 4:1; pH 7.4; 0.1 M HEPES) at ambient temperature.



**Fig.S8** Job's plot between **NDI-1** and cysteine in DMSO/H<sub>2</sub>O (v/v, 4:1; pH 7.4; 0.1 M HEPES) at ambient temperature.



**Fig. S9** Fluorescence emission spectrum of **NDI-1** ( $1 \times 10^{-6}$  M) upon addition of various amino acids (125 equiv.) in DMSO/H<sub>2</sub>O (v/v, 4 : 1; pH 7.4 ; 0.1 M HEPES) at ambient temperature.