

## SUPPORTING INFORMATION

### Cost-effective diagnostic kits for selective detection of gaseous H<sub>2</sub>S

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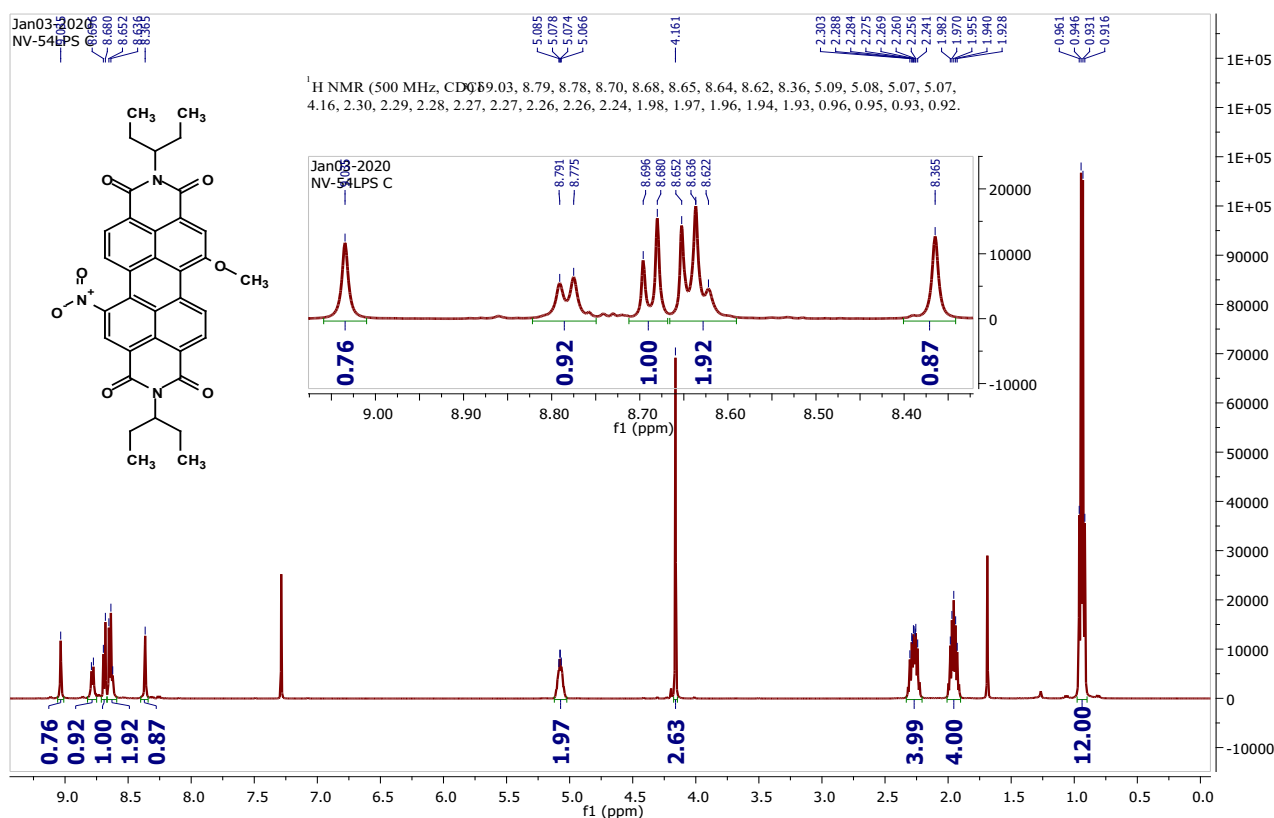
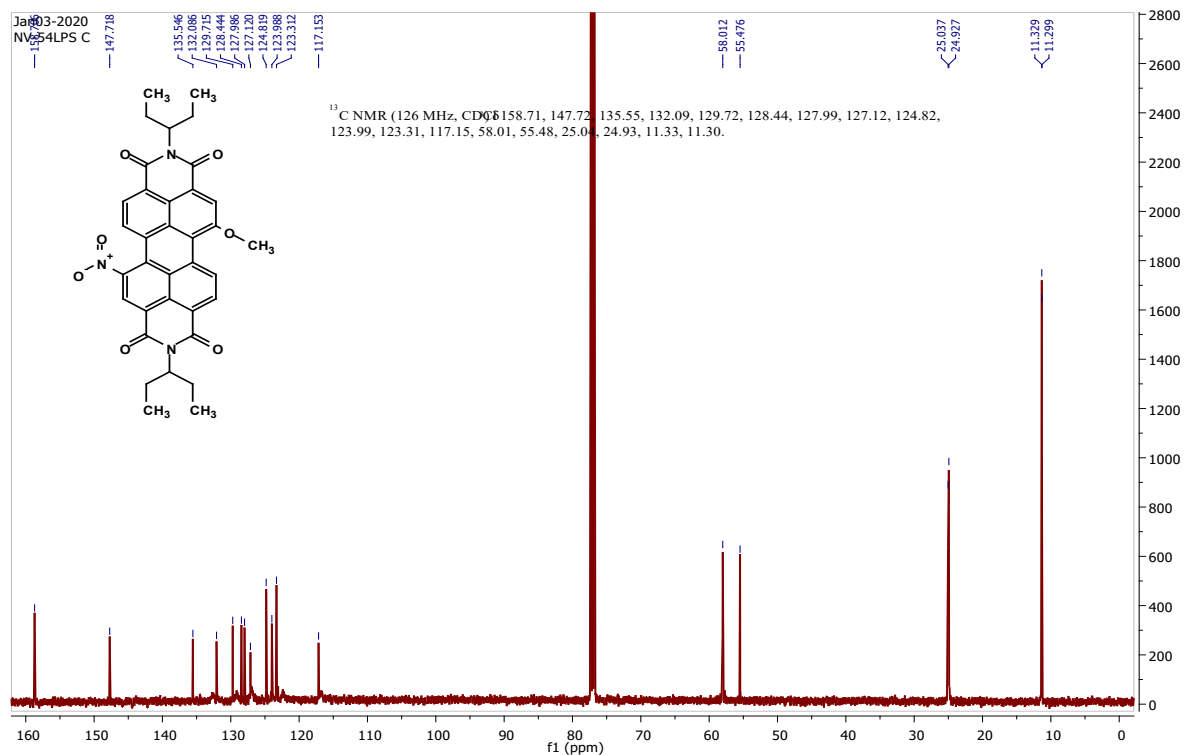
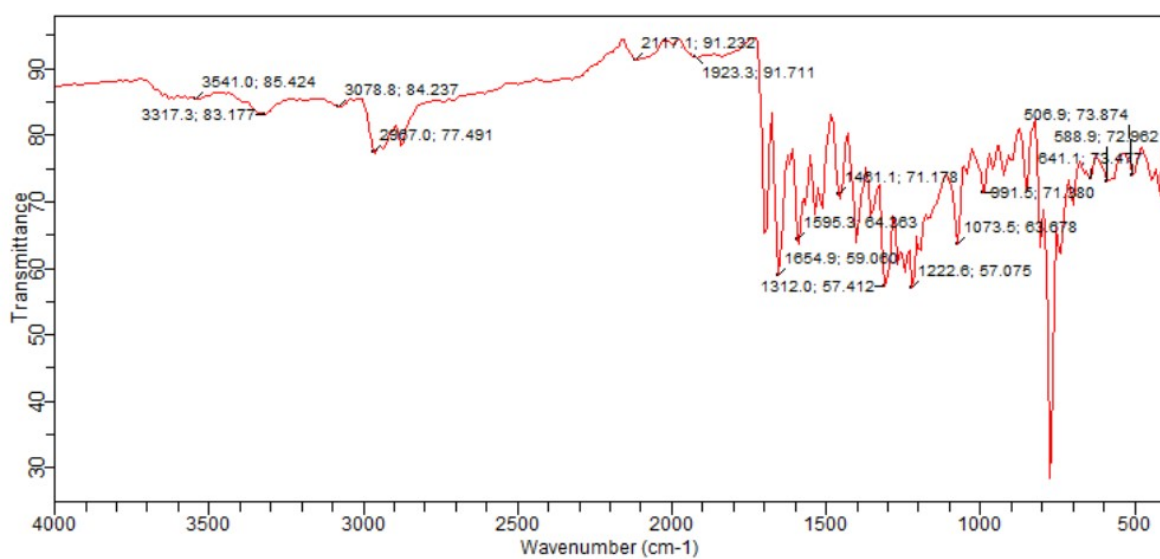


Figure S1a: The proton NMR spectrum of PDI 2.



**Figure S1b:** The carbon NMR spectrum of PDI 2.



**Figure S1c:** Infra-Red (ATR) spectrum of PDI 2.

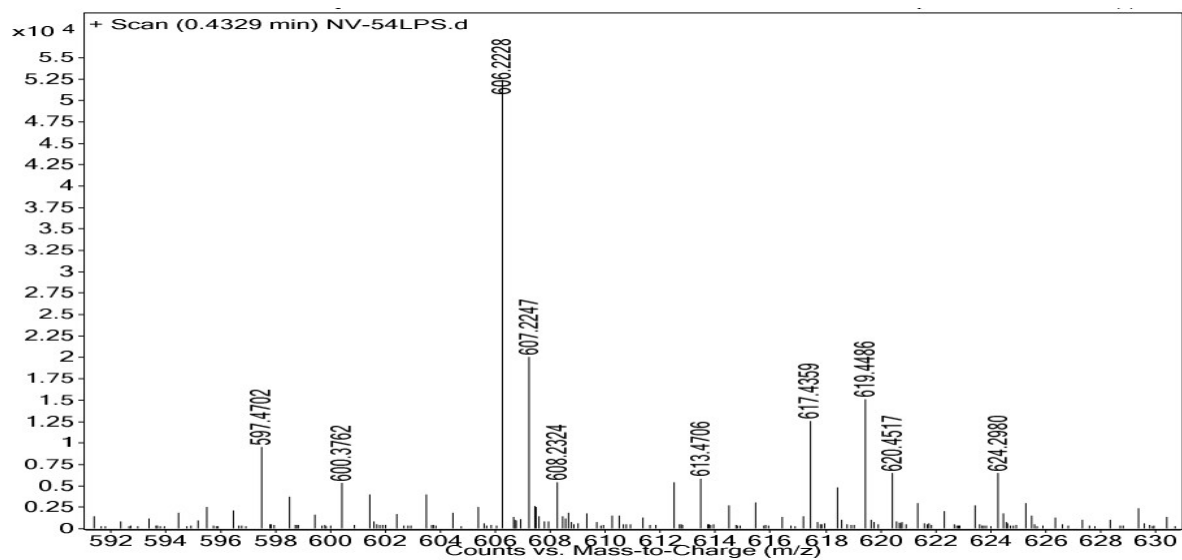
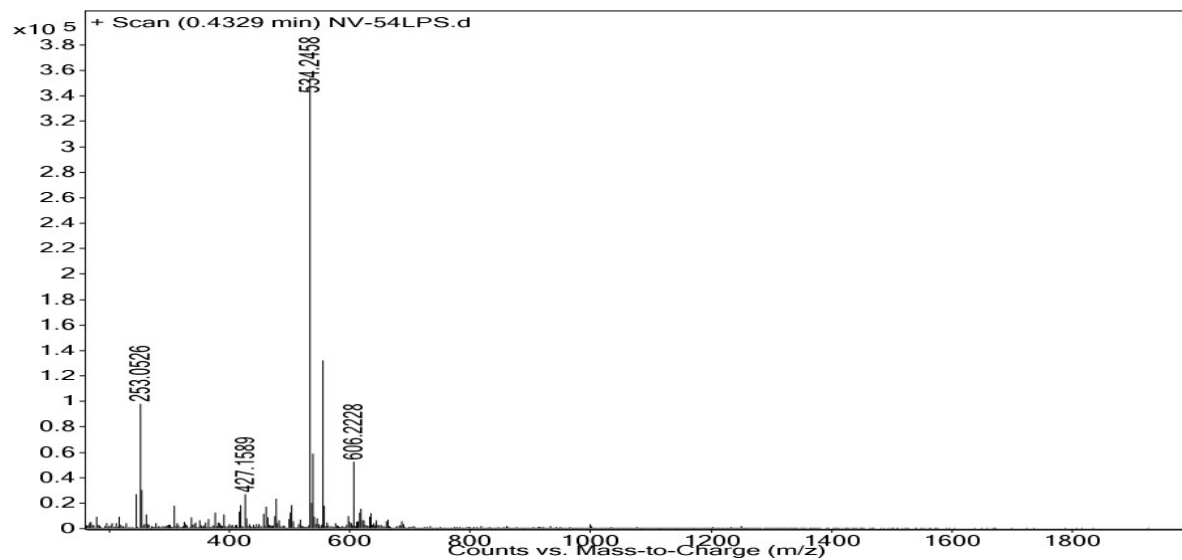


Figure S1d: Mass spectrum of PDI 2.

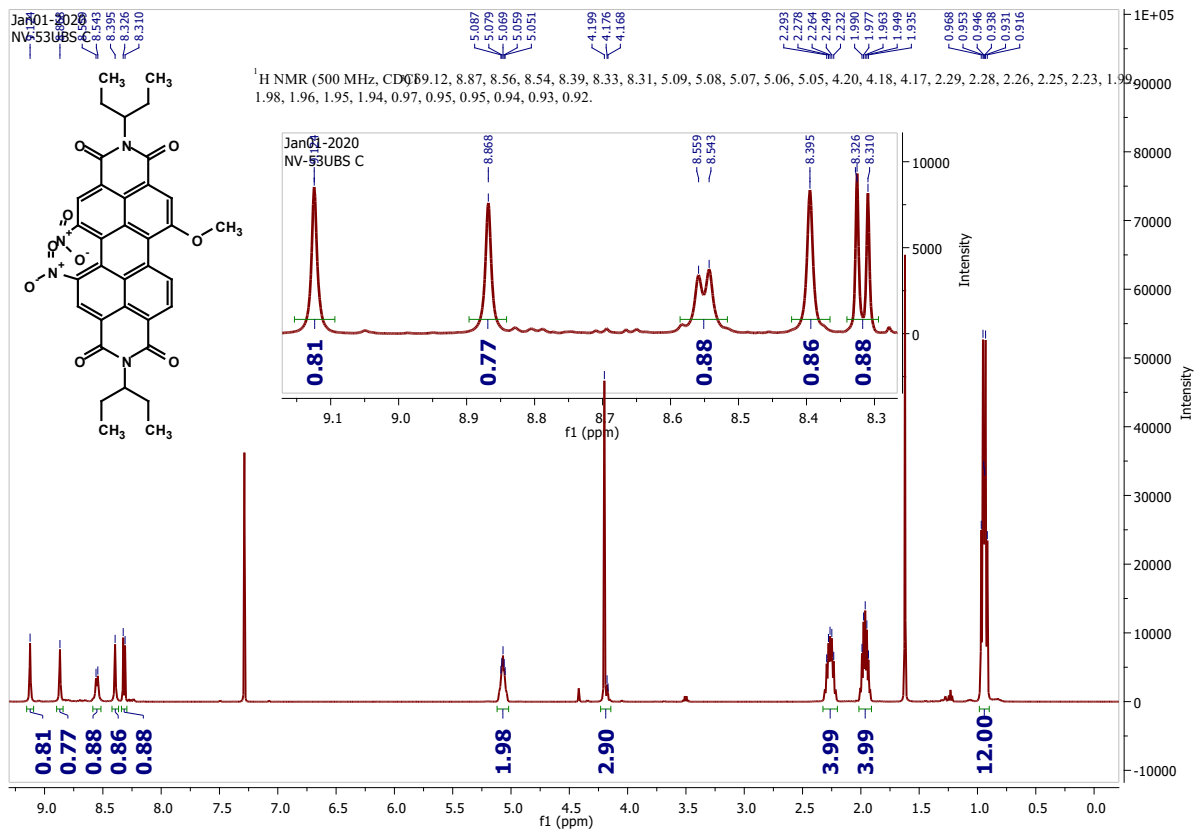


Figure S2a: The proton NMR spectrum of PDI 3.

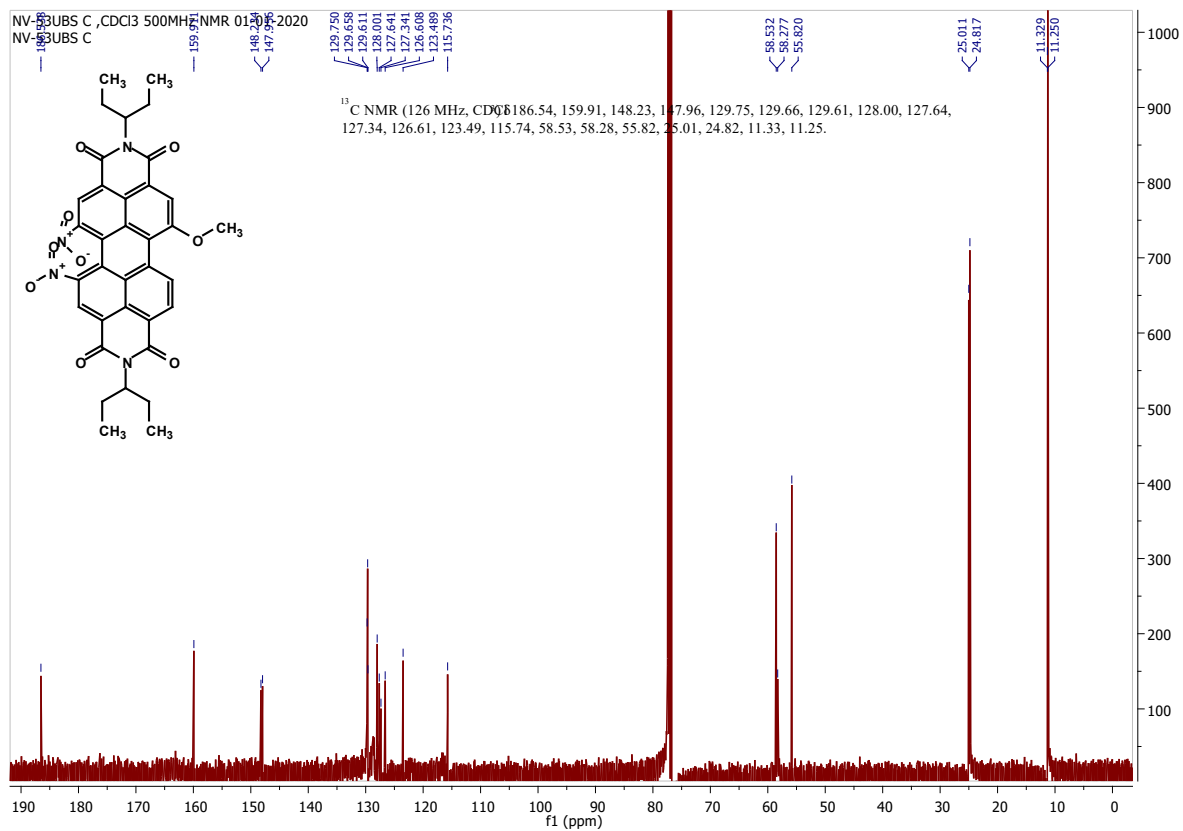


Figure S2b: The carbon NMR spectrum of PDI 3.

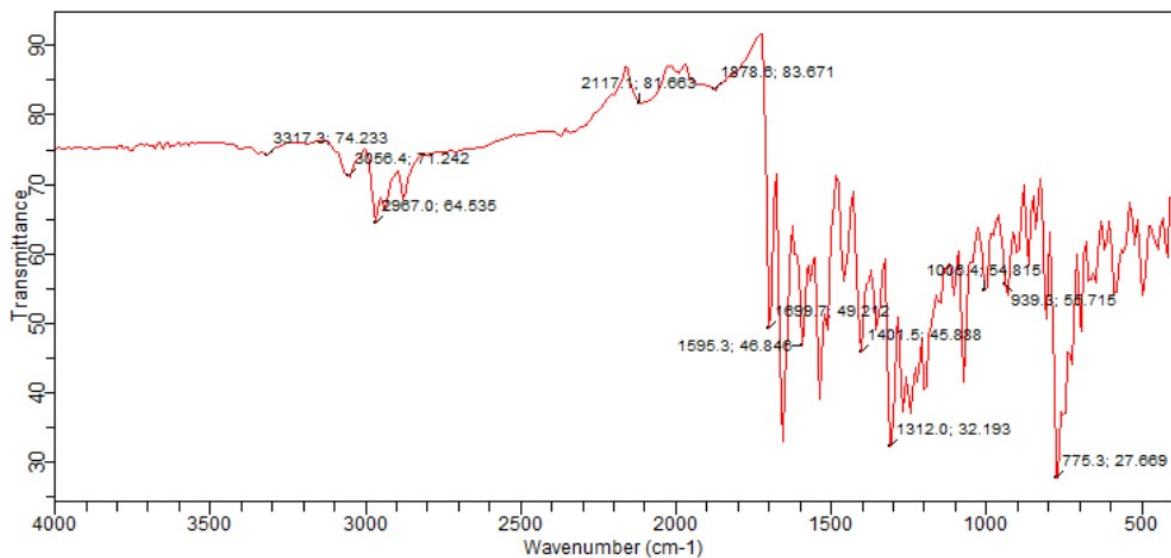
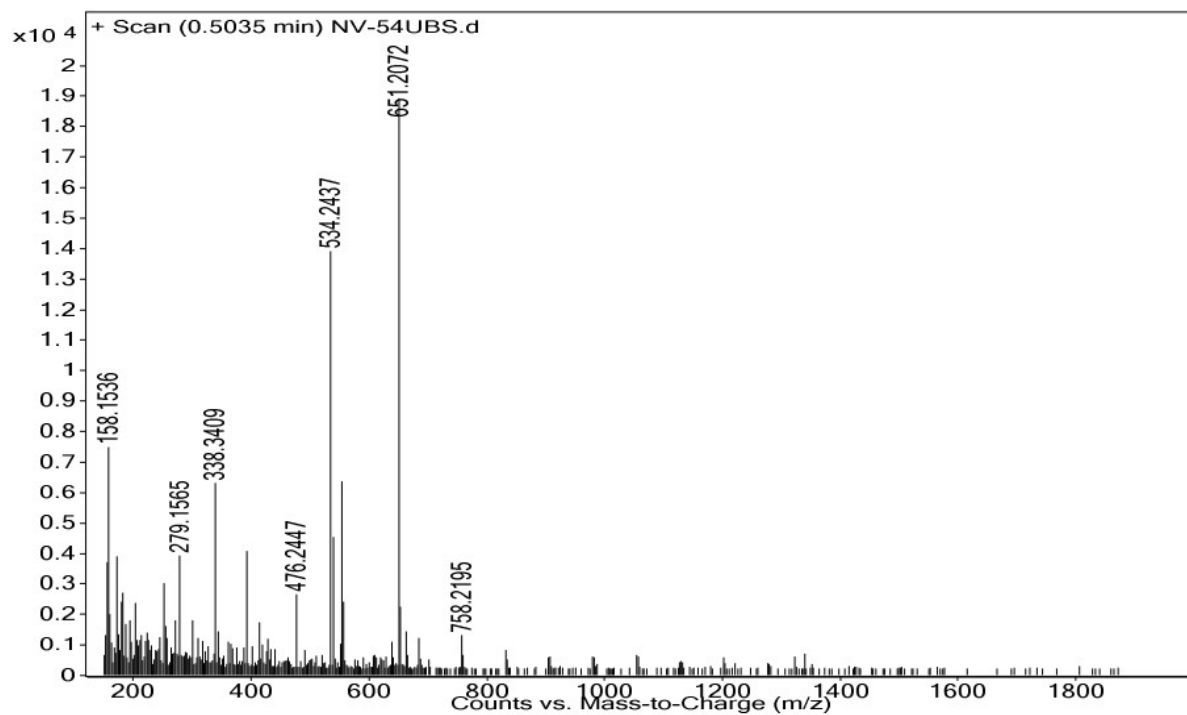


Figure S2c: Infra-Red (ATR) spectrum of PDI 3.



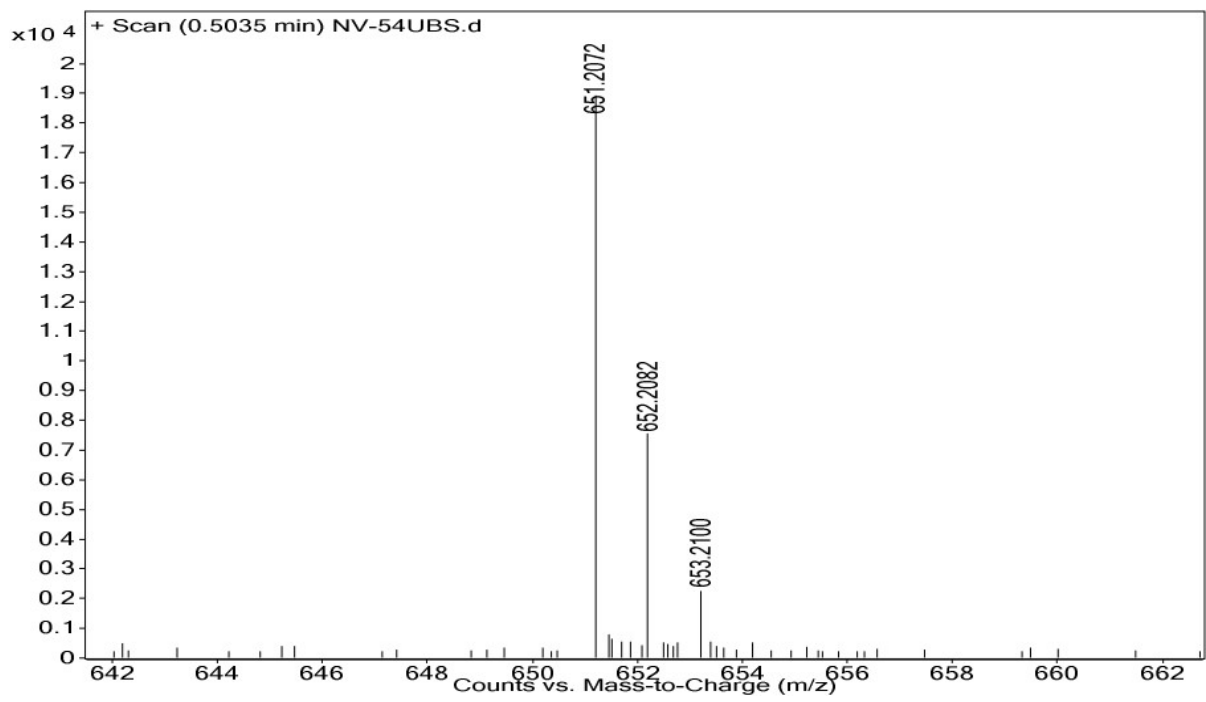
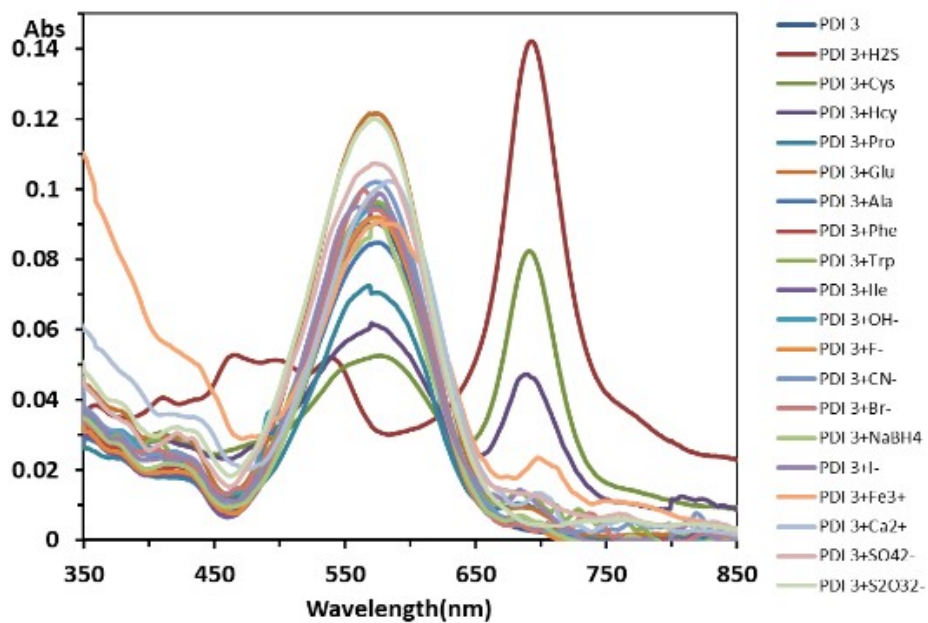
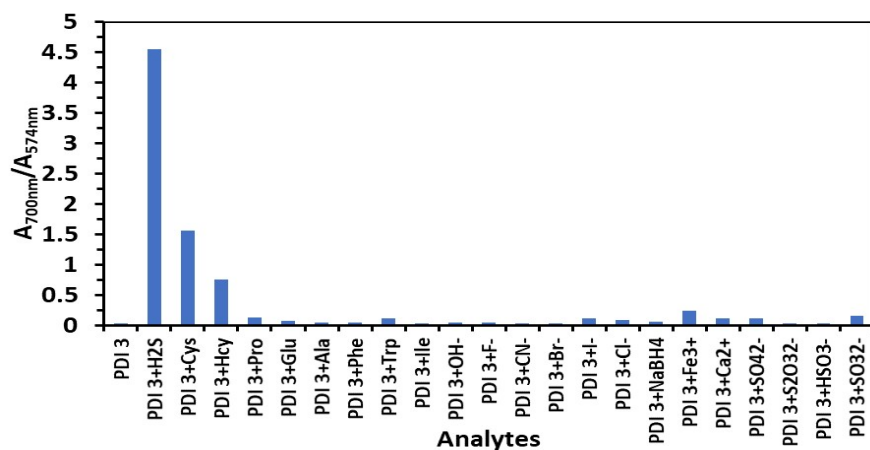
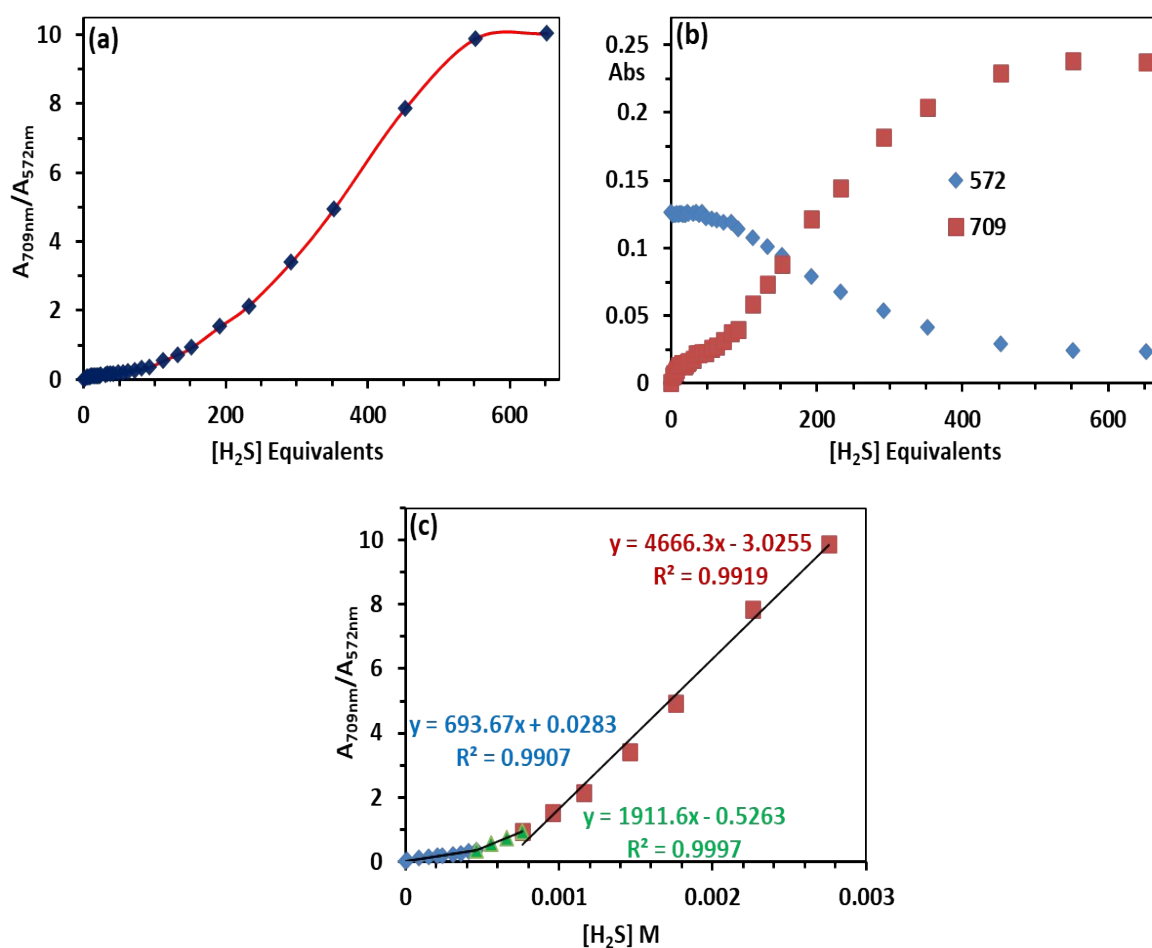


Figure S2d: Mass spectrum of PDI 3.

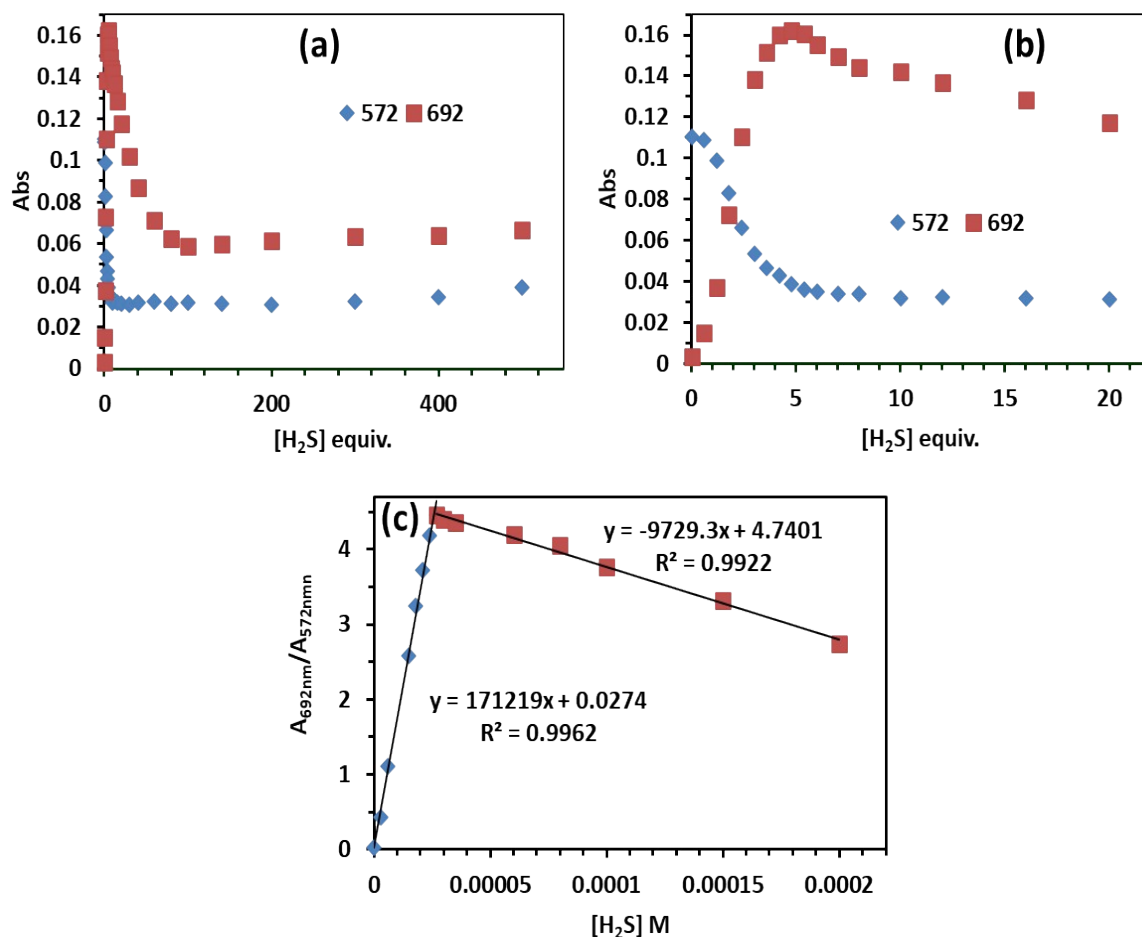




**Figure S3:** (Top) Absorbance ( $1 \times 10^{-5}$  M) changes of PDI **3** on the addition of various analytes ( $100 \mu\text{M}$ ) recorded in HEPES–THF (1:1, pH 7.2) solution; (bottom) bar graph representation.

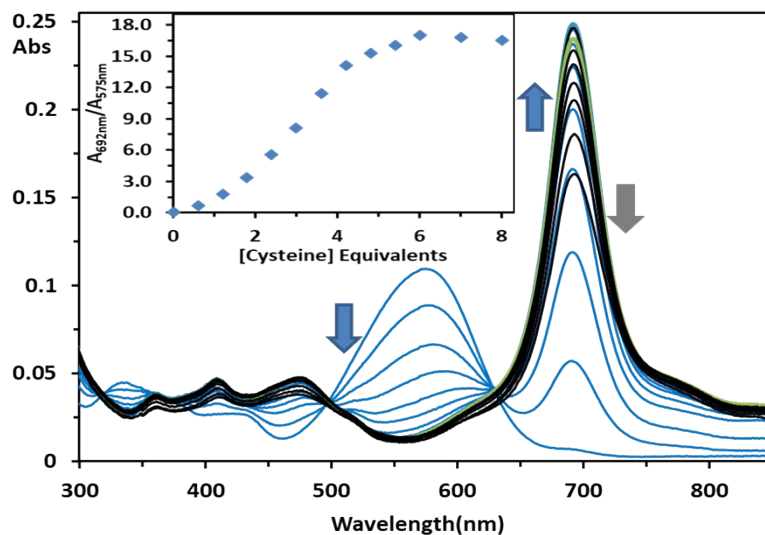


**Figure S4.** (a) Ratiometric plot of  $A_{709\text{nm}}/A_{572\text{nm}}$  of PDI **2** (b) plot of absorbance intensities at 572 nm and 709 nm of PDI **2** on addition of  $\text{H}_2\text{S}$  recorded in HEPES: THF (1:1 v/v, pH 7.2); (c) Ratiometric plot of  $A_{709\text{nm}}/A_{572\text{nm}}$  of PDI **2** on addition of  $\text{H}_2\text{S}$  recorded in HEPES:THF (1:1 v/v, pH 7.2) to determine the limit of detection.

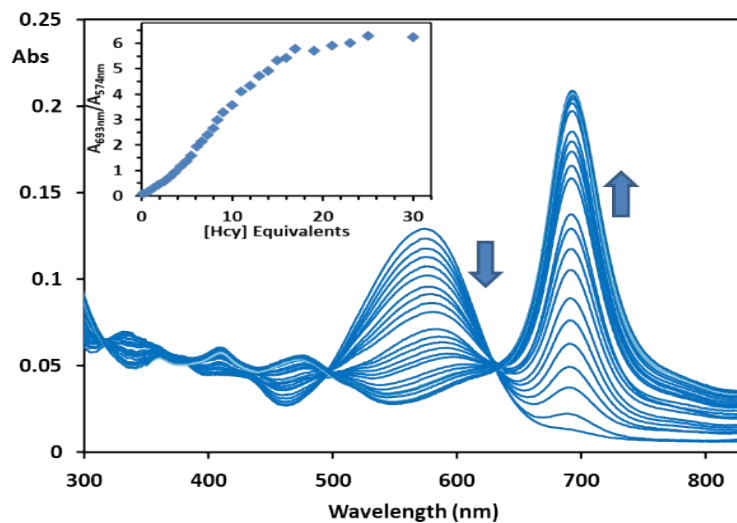


**Figure S5.** (a) Plot of absorbance intensities at 572 nm and 692 nm of PDI **3** on addition of H<sub>2</sub>S recorded in HEPES: THF (1:1 v/v, pH 7.2); (b) magnified view of absorption intensities at 572 and 692 nm given in Figure S5a (c) Ratiometric plot of  $A_{692\text{nm}}/A_{572\text{nm}}$  of PDI **3** on addition of H<sub>2</sub>S recorded in HEPES: THF (1:1 v/v, pH 7.2) to determine the limit of detection.

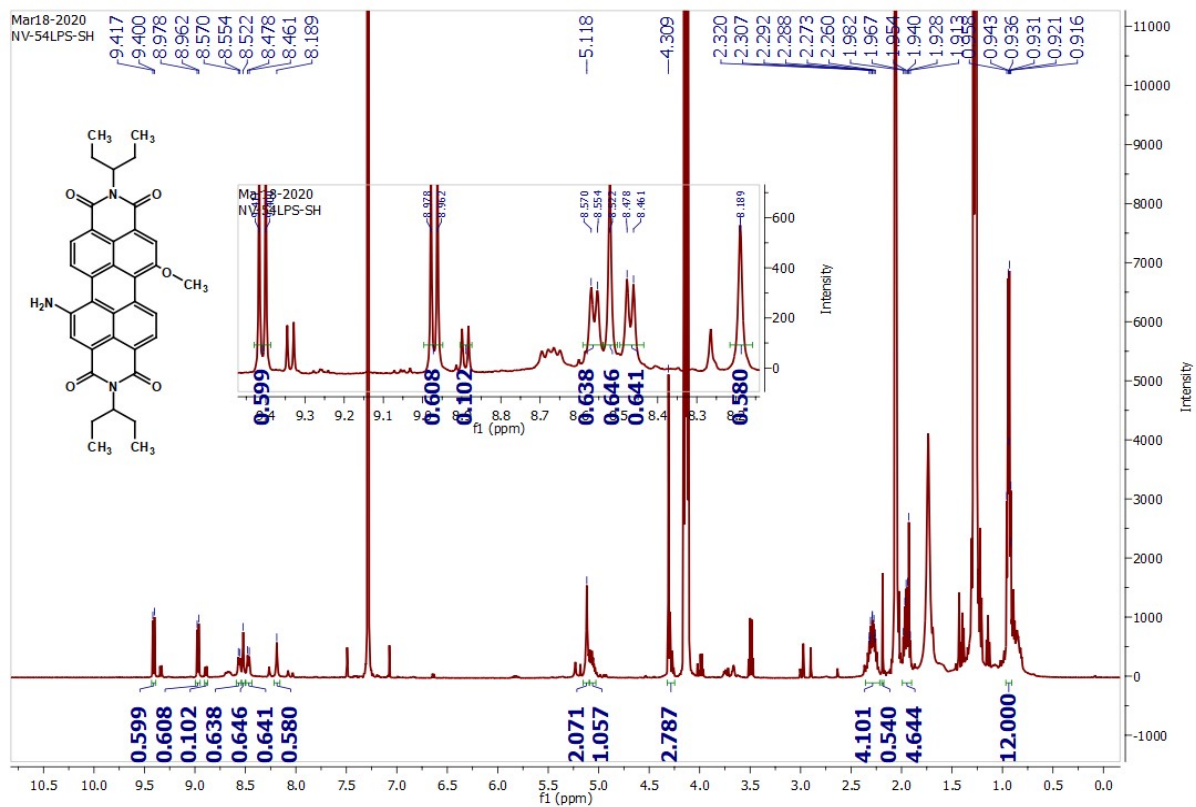




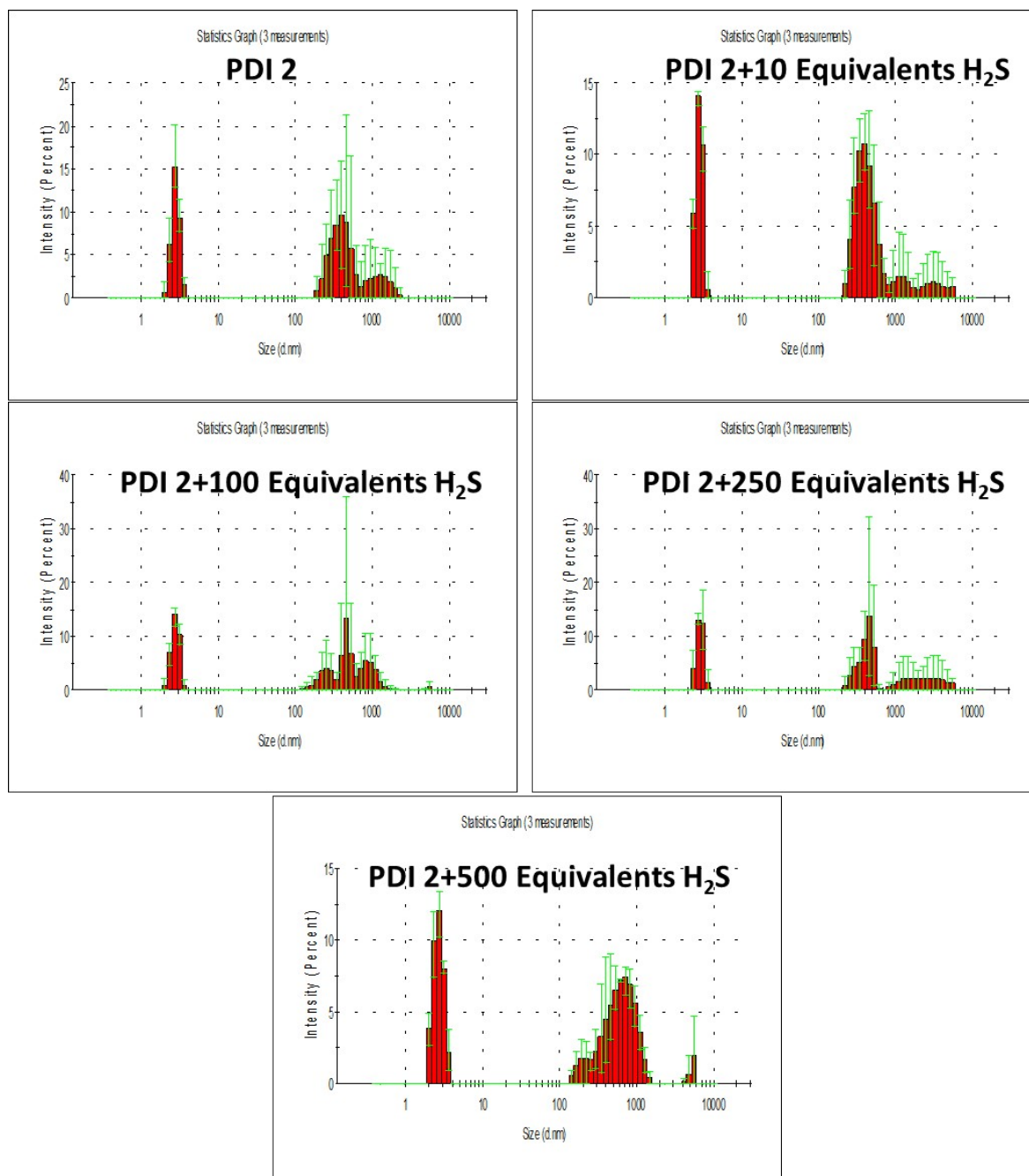
**Figure S6.** Absorbance spectrum of (a) PDI **3** (5  $\mu$ M) showing detection of Cysteine (Cys) in 50% HEPES buffer solution maintained at pH 7.2; [Inset] Ratiometric plot of absorbance intensities ( $A_{692\text{nm}}/A_{575\text{nm}}$ ) versus concentrations of Cys.



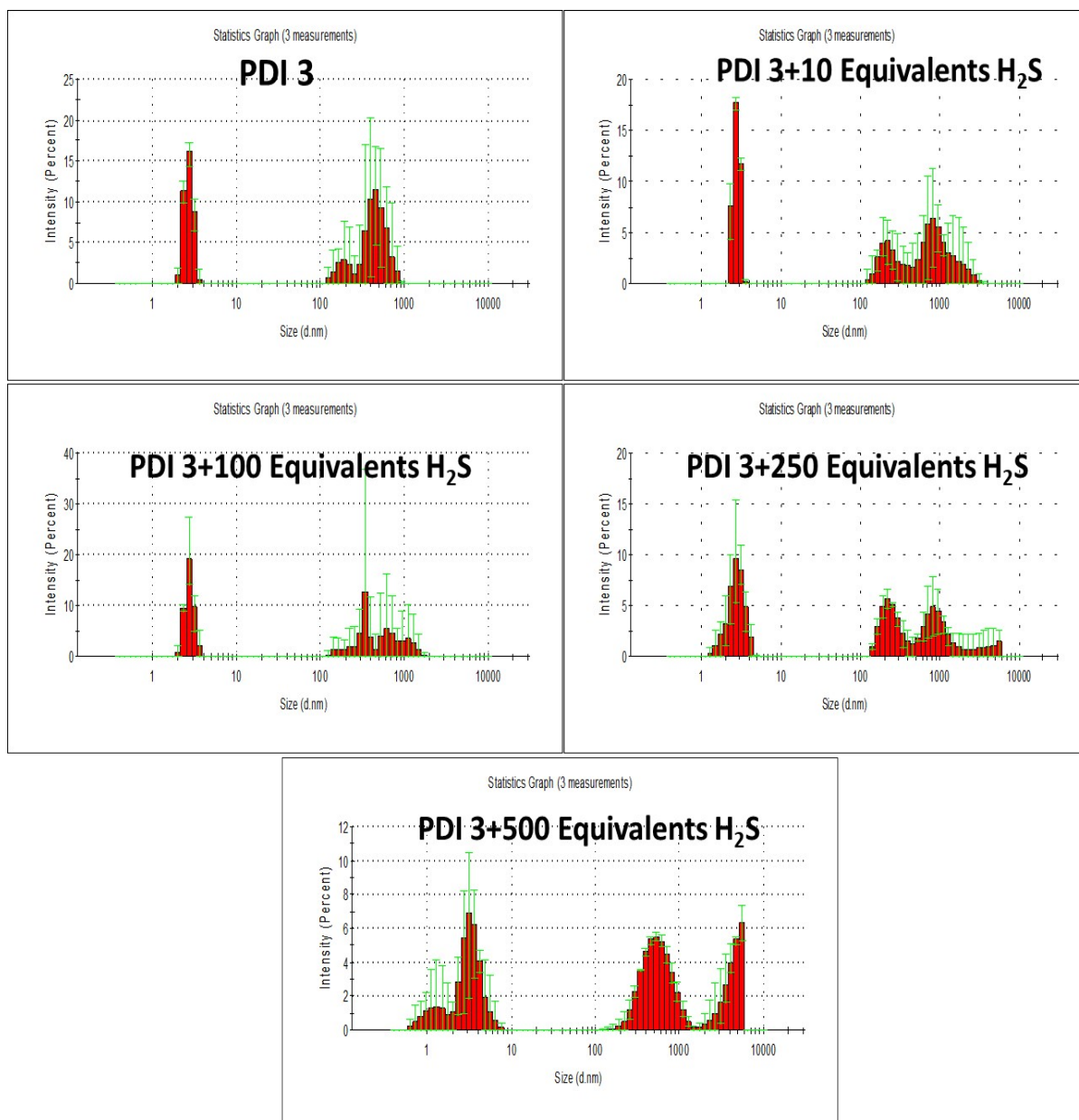
**Figure S7.** Absorbance spectrum of (a) PDI **3** (5  $\mu$ M) showing detection of Homocysteine (Hcy) in 50% HEPES buffer solution maintained at pH 7.2; [Inset] Ratiometric plot of absorbance intensities ( $A_{692\text{nm}}/A_{575\text{nm}}$ ) versus concentrations of Hcy.



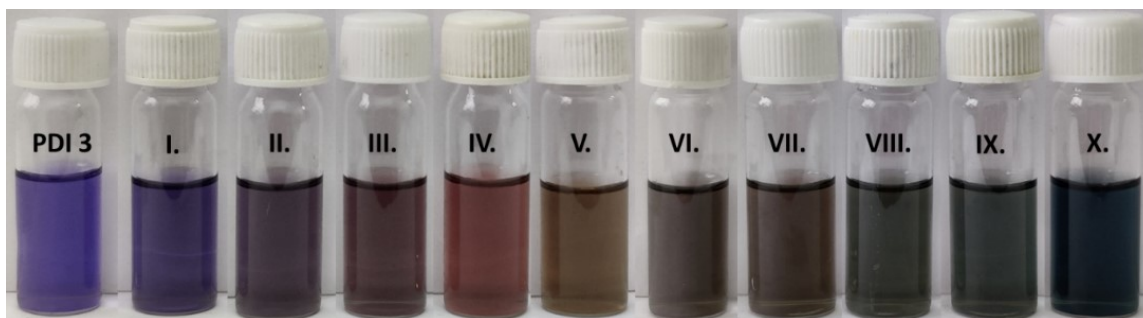
**Figure S8.**  $^1\text{H}$  NMR spectra of compound isolated from model reaction between PDI 2 + NaHS measured in  $\text{CDCl}_3$ .



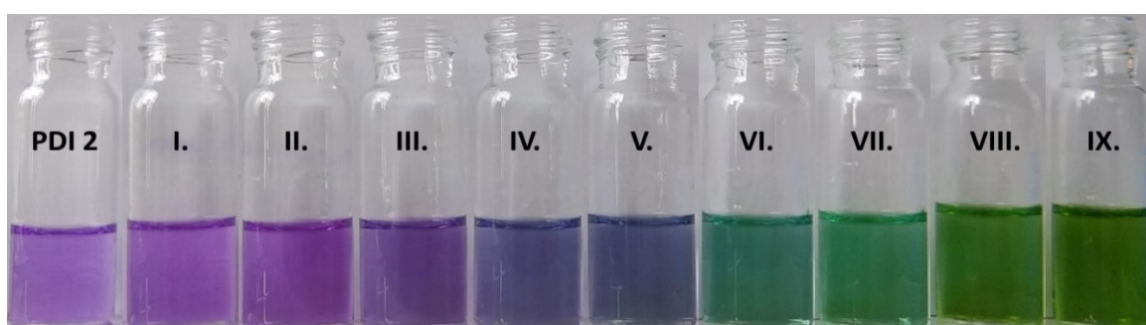
**Figure S9:** Dynamic light scattering (DLS) studies of PDI 2 on gradual addition of NaHS (used as a source of H<sub>2</sub>S) in HEPES buffer – THF (1:1, pH = 7.2) solution.



**Figure S10:** Dynamic light scattering (DLS) studies of PDI 2 on gradual addition of NaHS (used as a source of H<sub>2</sub>S) in HEPES buffer – THF (1:1, pH = 7.2) solution.



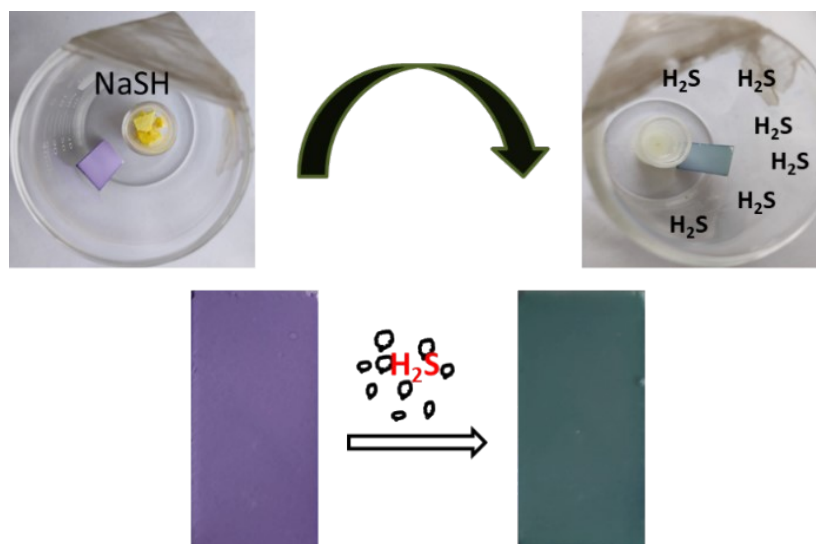
**Figure S11a:** Colour change photos of PDI 3 with gradual addition of H<sub>2</sub>S (naked eye); Images for PDI 3 (25 μM solution in THF: HEPES buffer (1:1, v/v, pH 7.2) containing I. 5, II. 10, III. 20, IV. 50, V. 100, VI. 150, VII. 200, VIII. 300, IX. 400, X. 500 equivalents of H<sub>2</sub>S solution.



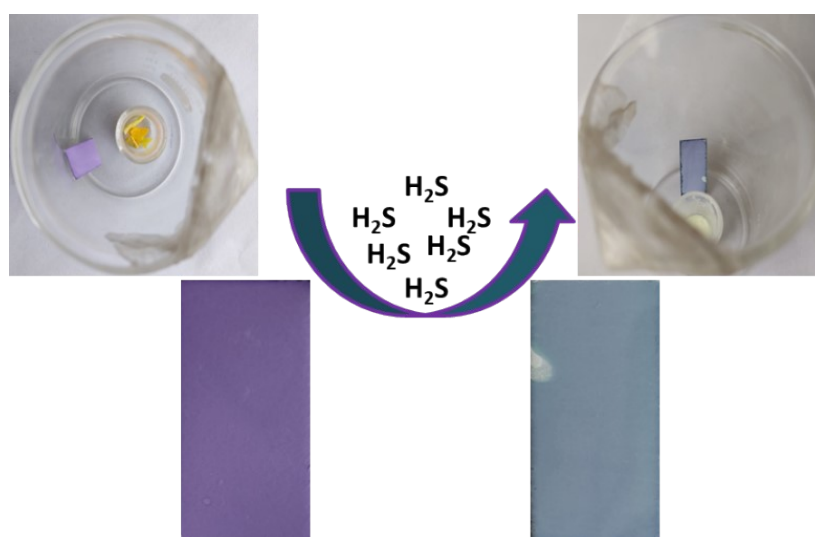
**Figure S11b:** Colour change photos of PDI 2 with gradual addition of H<sub>2</sub>S (naked eye); Images for PDI 2 (25 μM solution in THF: HEPES buffer (1:1, v/v, pH 7.2) containing I. 5, II. 10, III. 20, IV. 50, V. 100, VI. 150, VII. 200, VIII. 300, IX. 400, X. 500 equivalents of H<sub>2</sub>S solution.



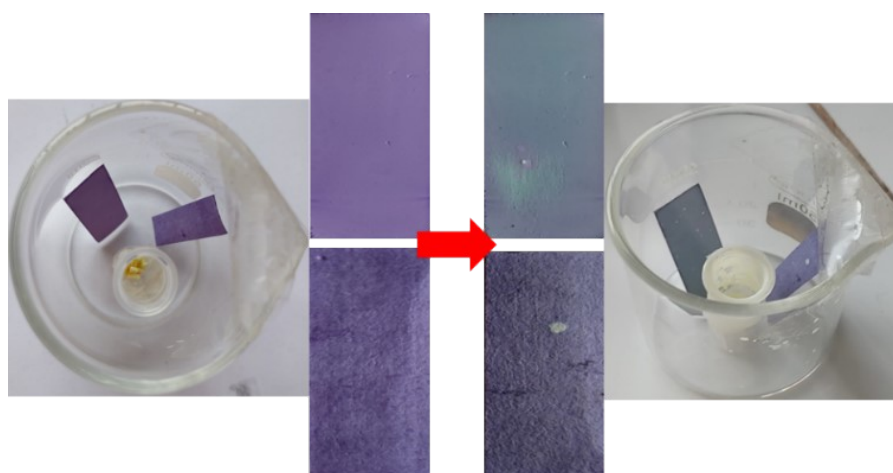
**Figure S12:** Colour change photos of PDI 3 with gradual addition of H<sub>2</sub>S (naked eye) in 30% urine sample.



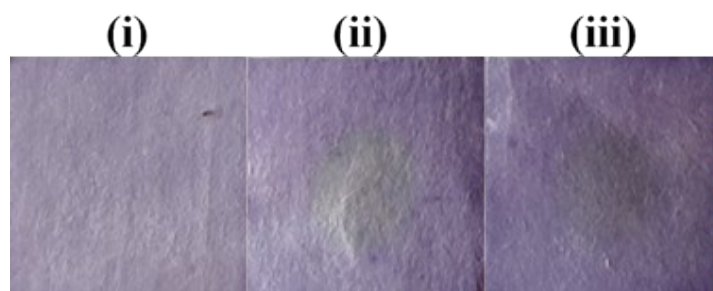
**Figure S13:** The cartoon representation of the set-up of experiment and photographs of naked eye detection of  $H_2S$  (150 mg NaSH) using PDI 3.



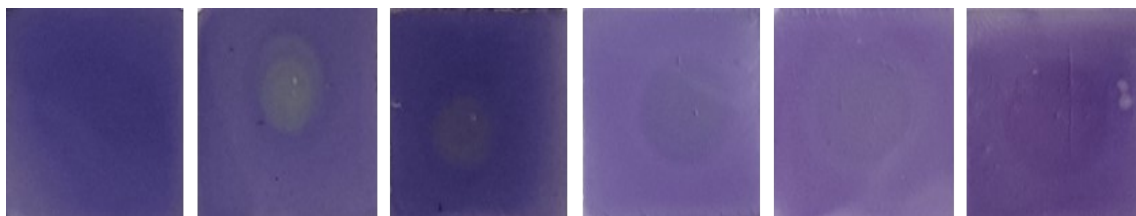
**Figure S14:** The cartoon representation of the set-up of experiment and photographs of naked eye detection of  $H_2S$  (70 mg NaSH) using PDI 3.



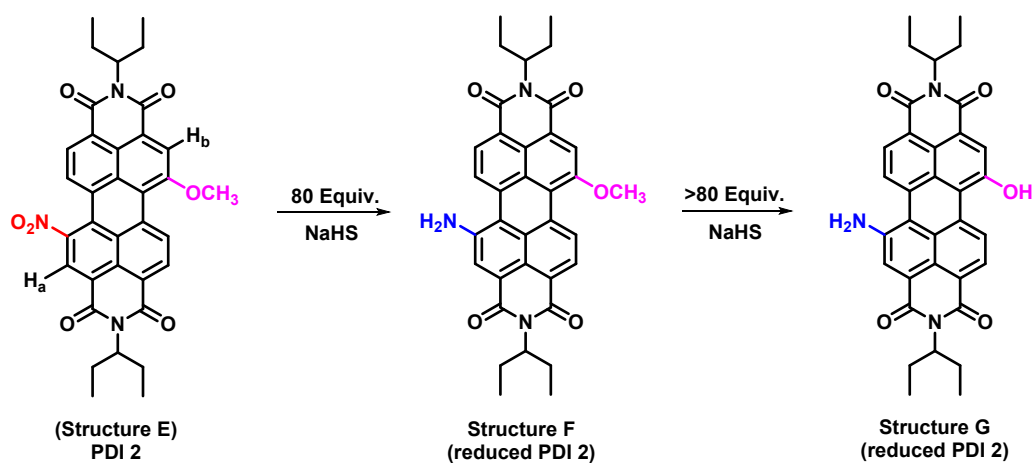
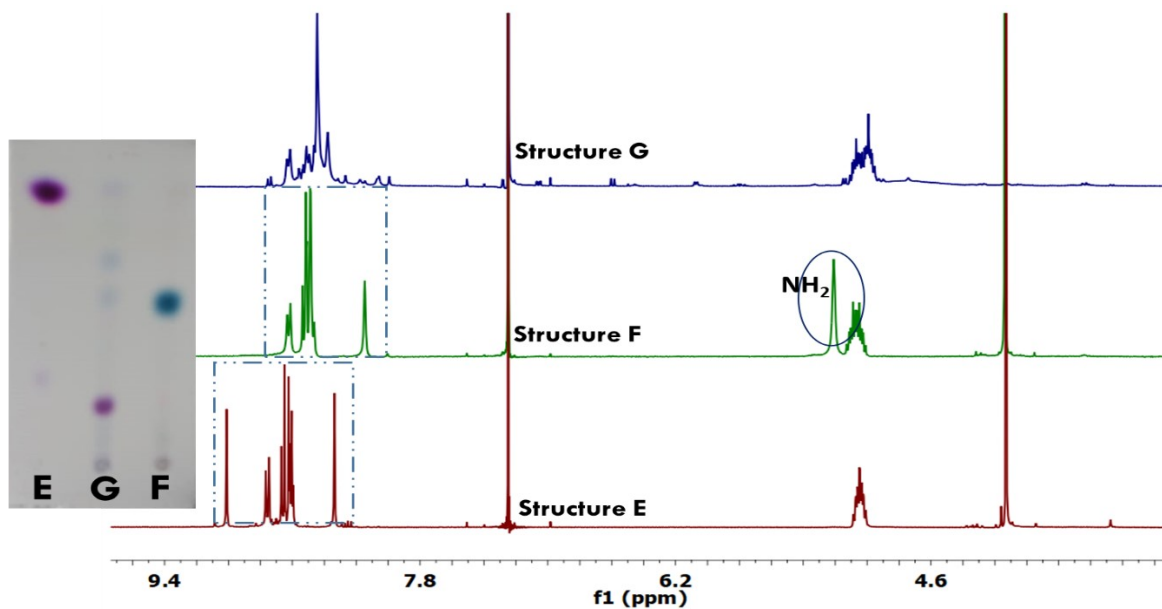
**Figure S15:** Colorimetric images of **PDI 3** ( $5 \times 10^{-4}$  M) coated Whatman filter paper showing visual detection of  $\text{H}_2\text{S}$  gas (generated using 150 mg NaHS and HCl in the flask).



**Figure S16:** The photographs of fine filter paper strips coated with **PDI 3** solution (i) with a drop of water only and after addition of  $3 \mu\text{L}$  of  $10^{-1}$  M (ii) and  $5 \times 10^{-2}$  M (iii) solution of NaHS solution.

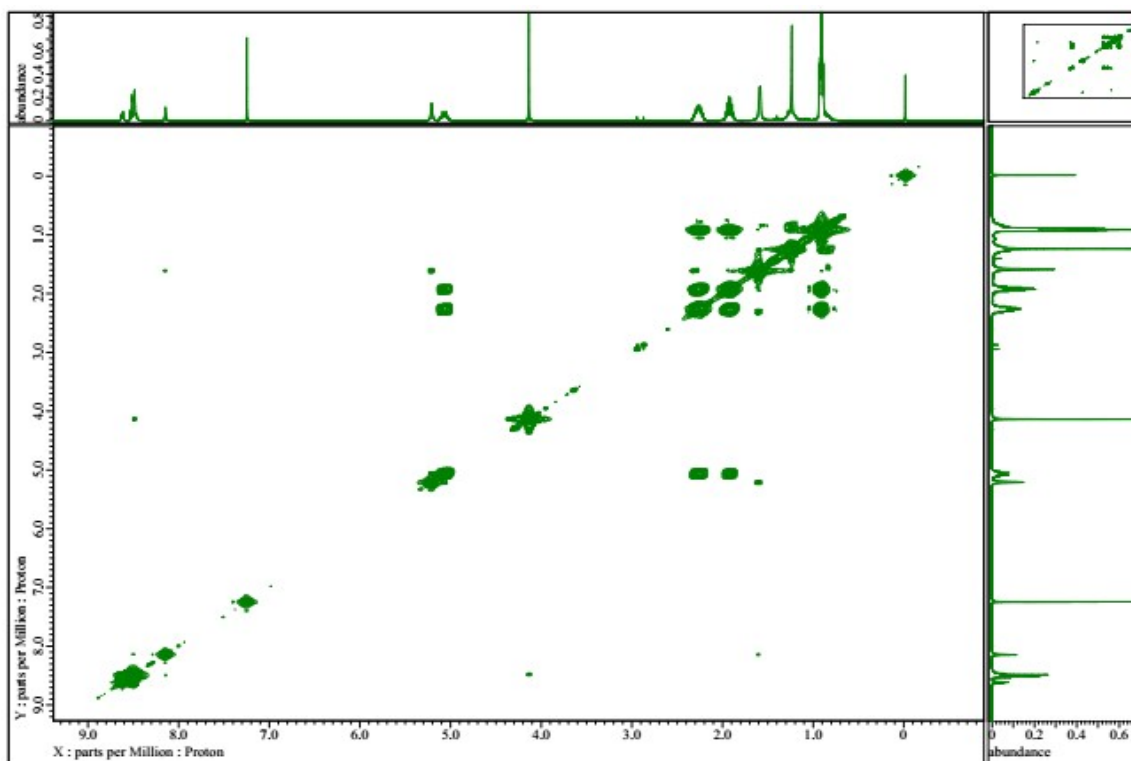


**Figure S17:** The photographs for TLC strips coated with **PDI 3** solution (i) with a drop of water only and with further addition of  $3 \mu\text{L}$  of  $10^{-1}$  M (ii) and  $5 \times 10^{-2}$  M (iii);  $6 \mu\text{L}$  of  $2.5 \times 10^{-2}$  M (iv),  $10^{-2}$  M (v) and  $10^{-3}$  M (vi) solution of NaHS solution.

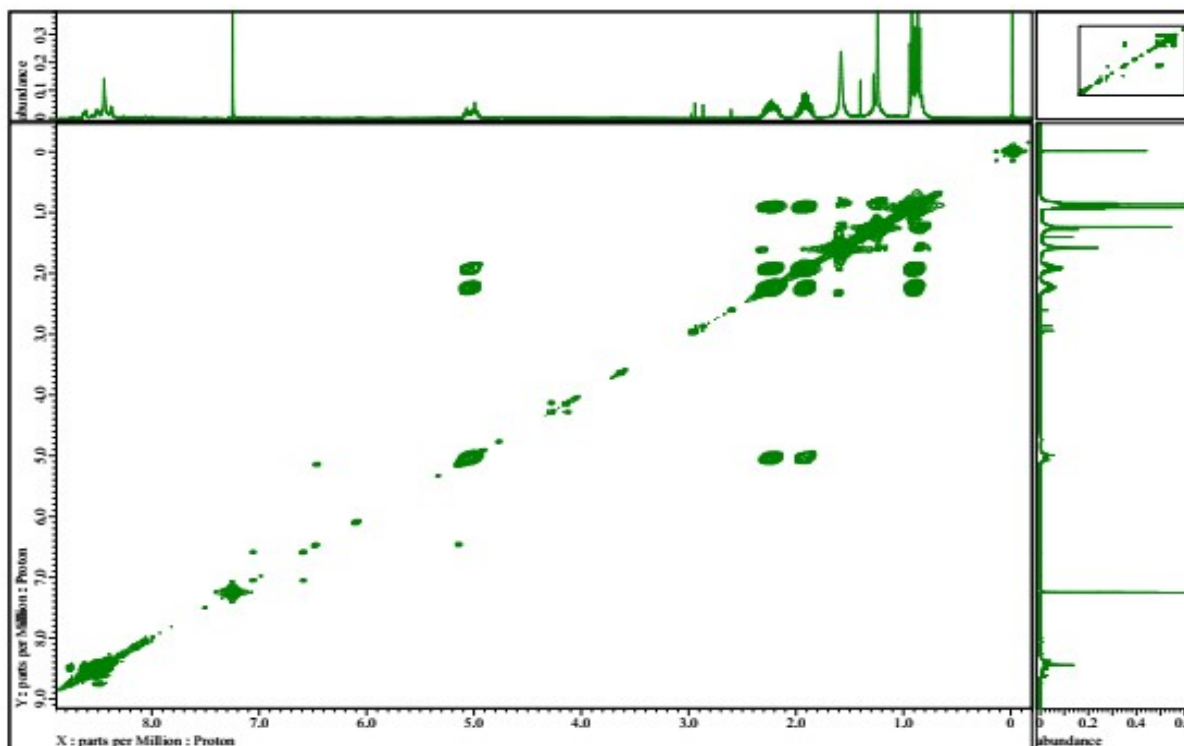


**Figure S18.** (top)  $^1\text{H}$  NMR stacked spectra of reduced products of PDI 2 isolated in model reaction after addition of NaHS; (below) Chemical structures showing reaction of PDI 2 in presence of different concentrations of NaHS.

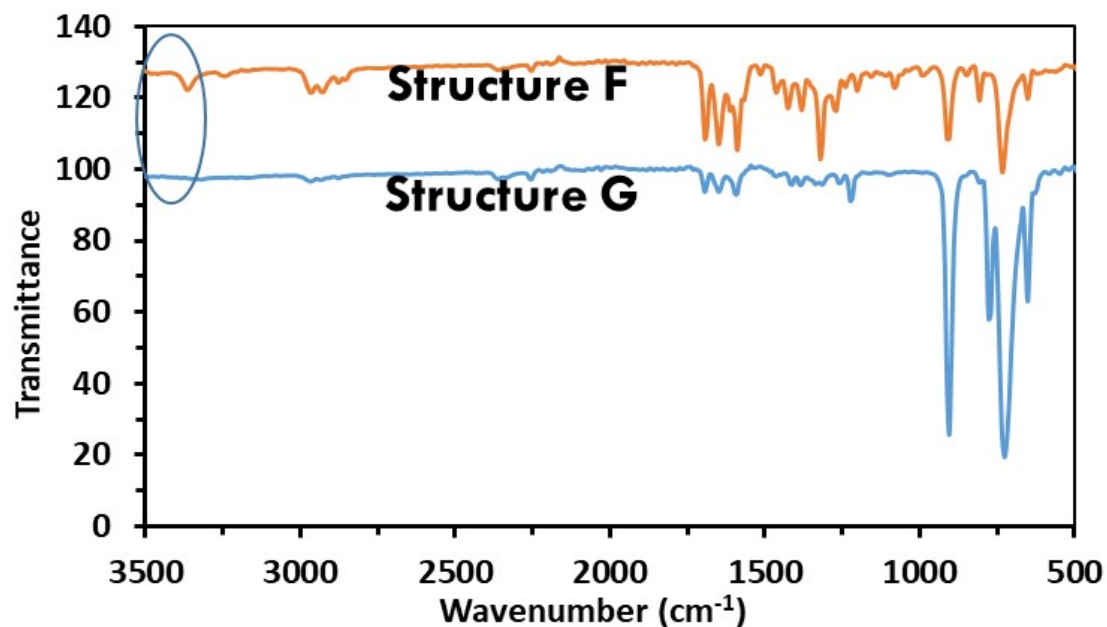




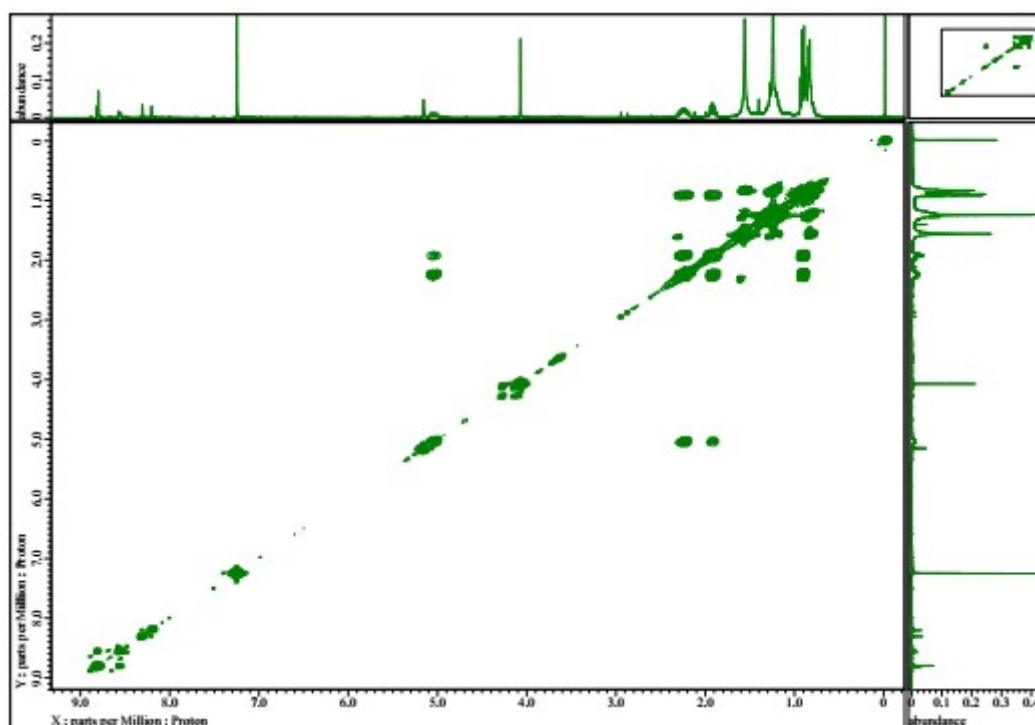
**Figure S19a.** <sup>1</sup>H-<sup>1</sup>H COSY-NMR spectrum of structure F (reduced PDI **2**) derivative isolated from model reaction of PDI **2** at 80 equivalents of NaHS, recorded in CDCl<sub>3</sub>.



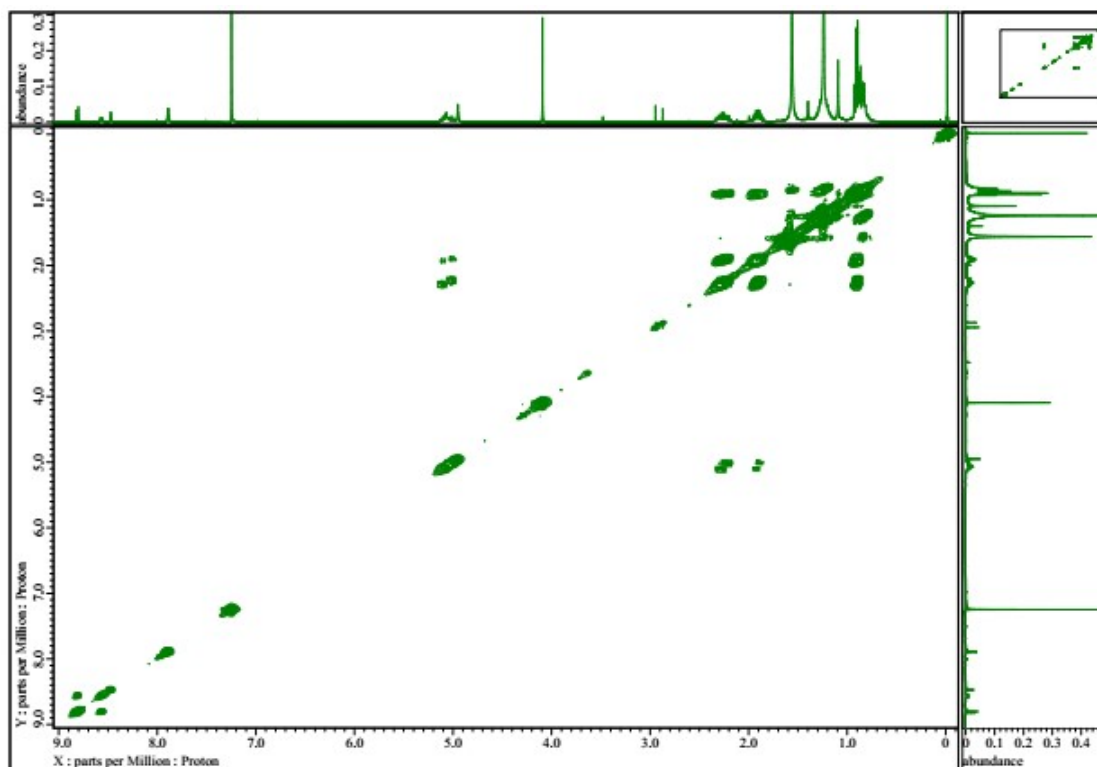
**Figure S19b.** <sup>1</sup>H-<sup>1</sup>H COSY-NMR spectrum of structure G (reduced PDI **2**) derivative isolated from model reaction of PDI **2** at 80 equivalents of NaHS, recorded in CDCl<sub>3</sub>.



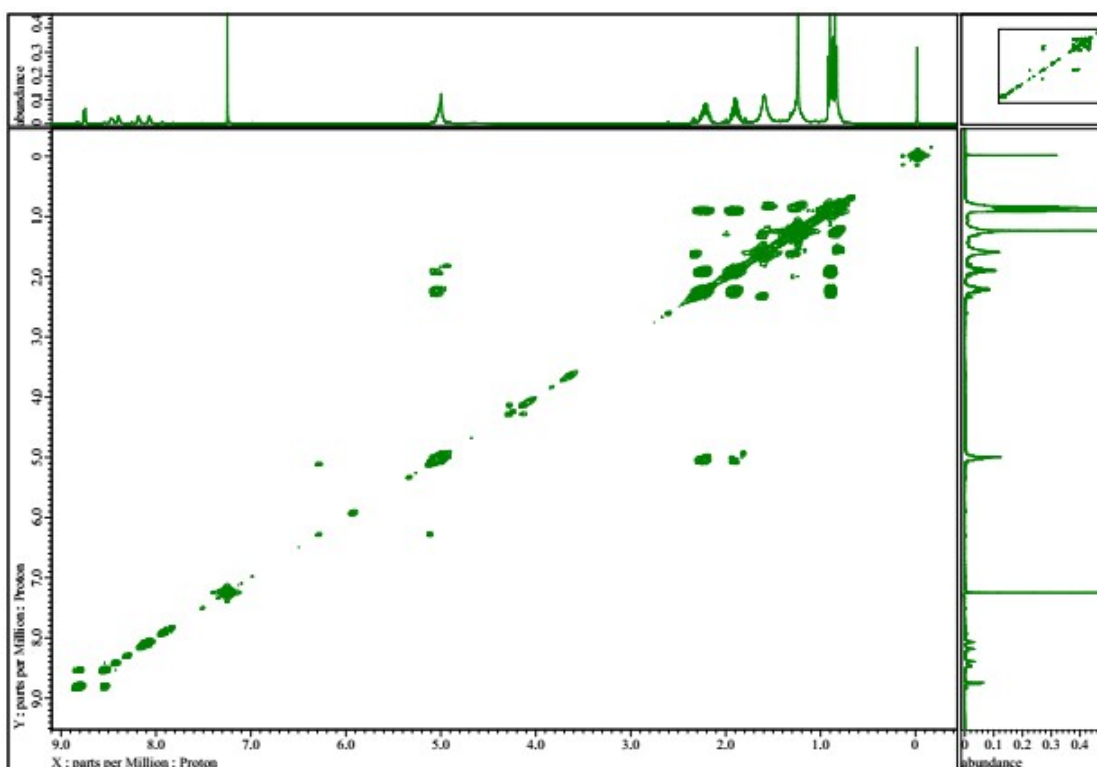
**Figure S20.** IR spectrum of structure F and G (reduced PDI 2) derivatives isolated from model reaction of PDI 2 with NaHS.



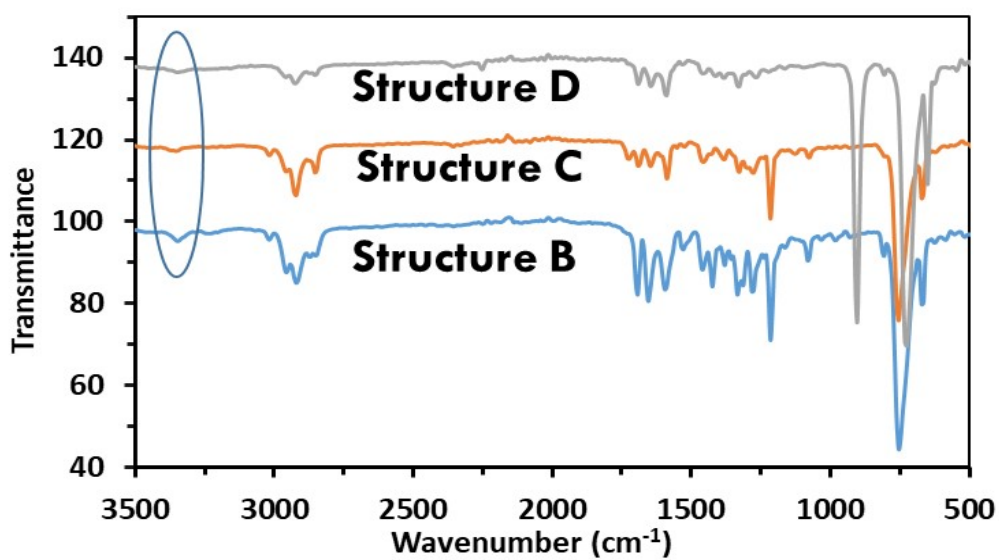
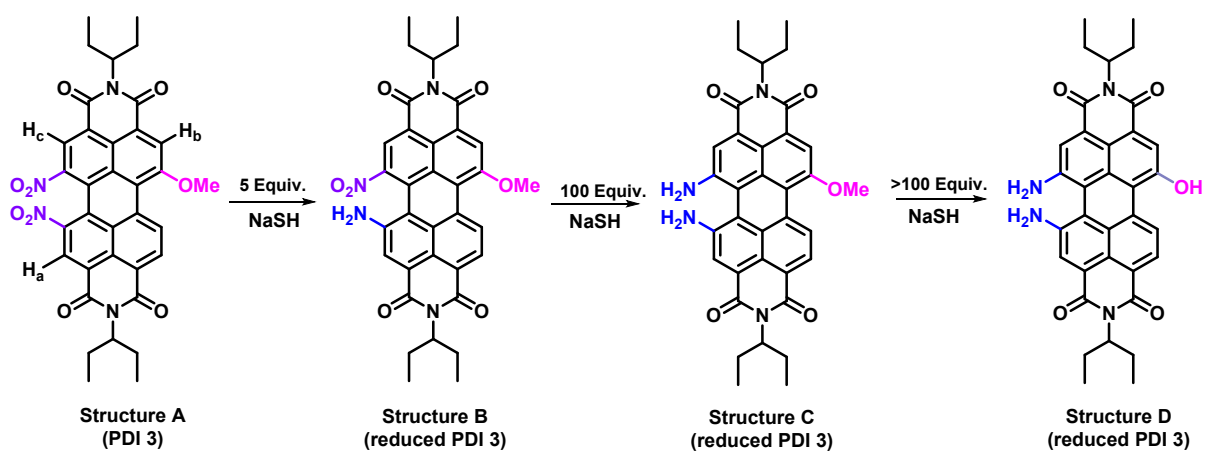
**Figure S21a.**  $^1\text{H}$ - $^1\text{H}$  COSY-NMR spectrum of structure B (reduced PDI 3) derivative isolated from model reaction of PDI 3 at 5 equivalents of NaHS, recorded in  $\text{CDCl}_3$ .



**Figure S21b.**  $^1\text{H}$ - $^1\text{H}$  COSY-NMR spectrum of structure C (reduced PDI **3**) derivative isolated from model reaction of PDI **3** at 100 equivalents of NaHS, recorded in  $\text{CDCl}_3$ .



**Figure S21c.**  $^1\text{H}$ - $^1\text{H}$  COSY-NMR spectrum of structure D (reduced PDI **3**) derivative isolated from model reaction of PDI **3** at higher equivalents of NaHS, recorded in  $\text{CDCl}_3$ .



**Figure S22.** IR spectrum of structure B-D (reduced PDI 3) derivatives isolated from model reaction of PDI 3 with NaHS.