Electronic Supplementary Material (ESI) for Analytical Methods.

Perylene diimide-based sensors for multiple analyte sensing (Fe^{2+}/H_2S/ dopamine and Hg^{2+}/Fe^{2+}): Cell imaging and INH, XOR, Encoder logic

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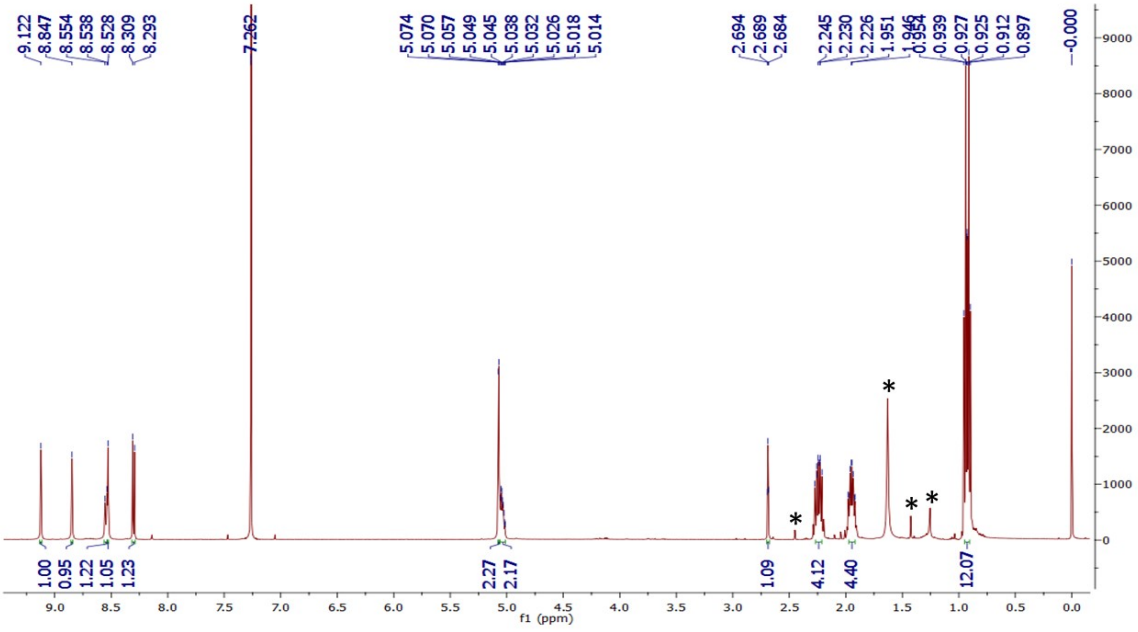

Figure S1a: ^{1}H NMR spectrum of **DNP**.

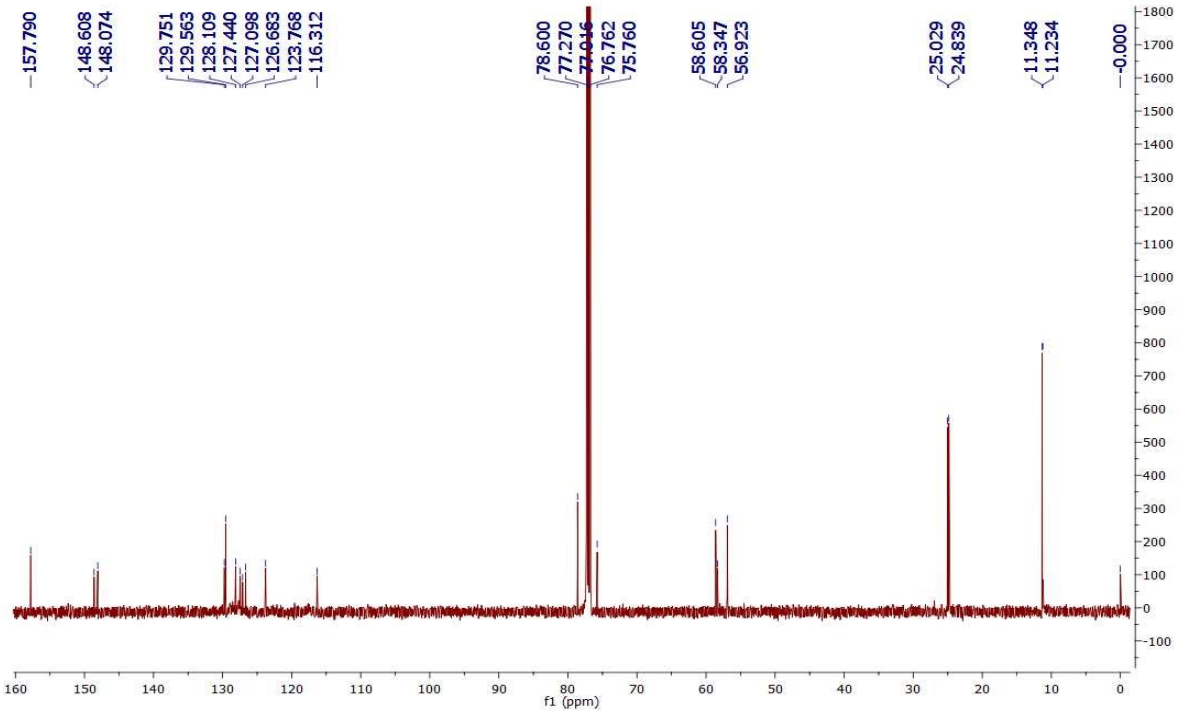

Figure S1b: ^{13}C NMR spectrum of **DNP**.

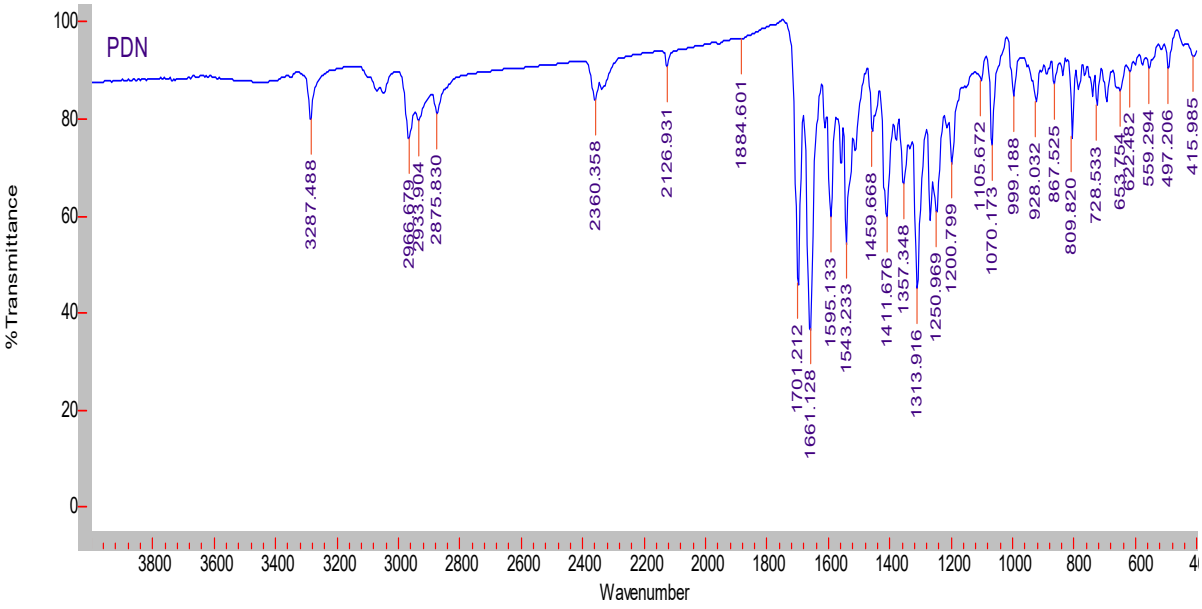

Figure S1c: IR spectrum of **DNP**.

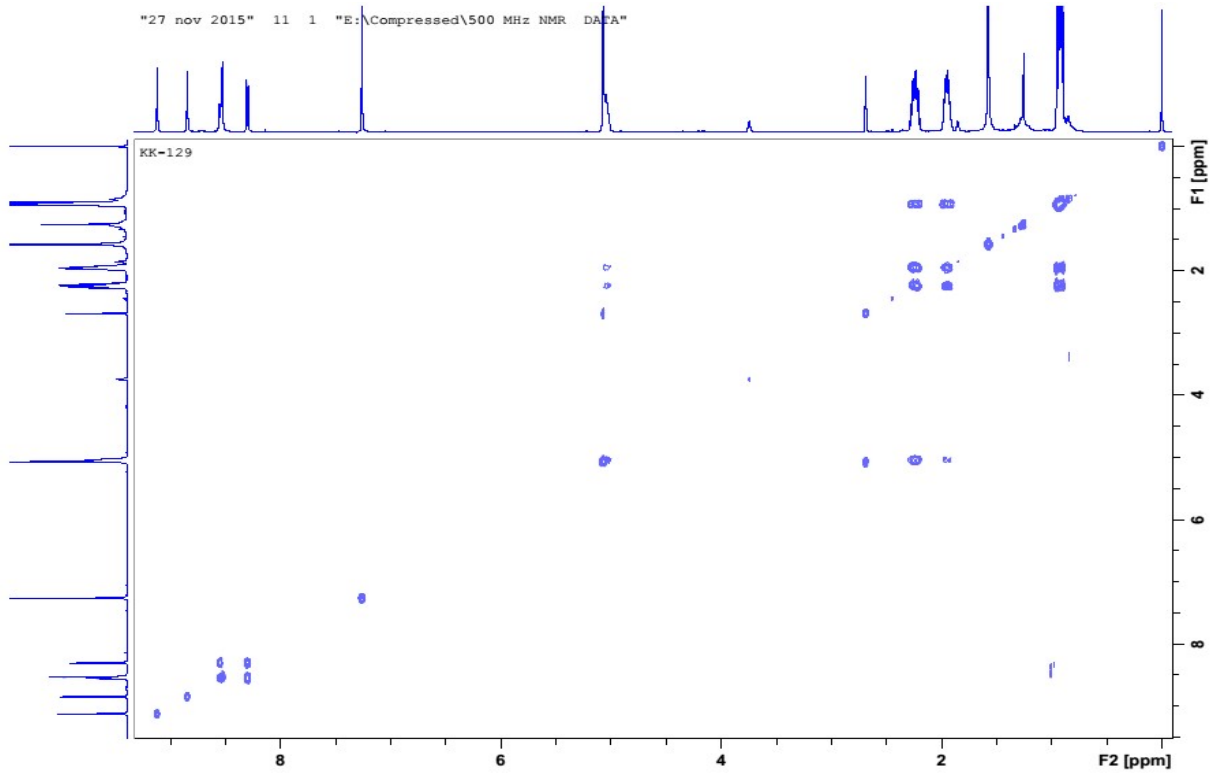

Figure S1d: ^{1}H-^{1}H COSY data of **DNP**.

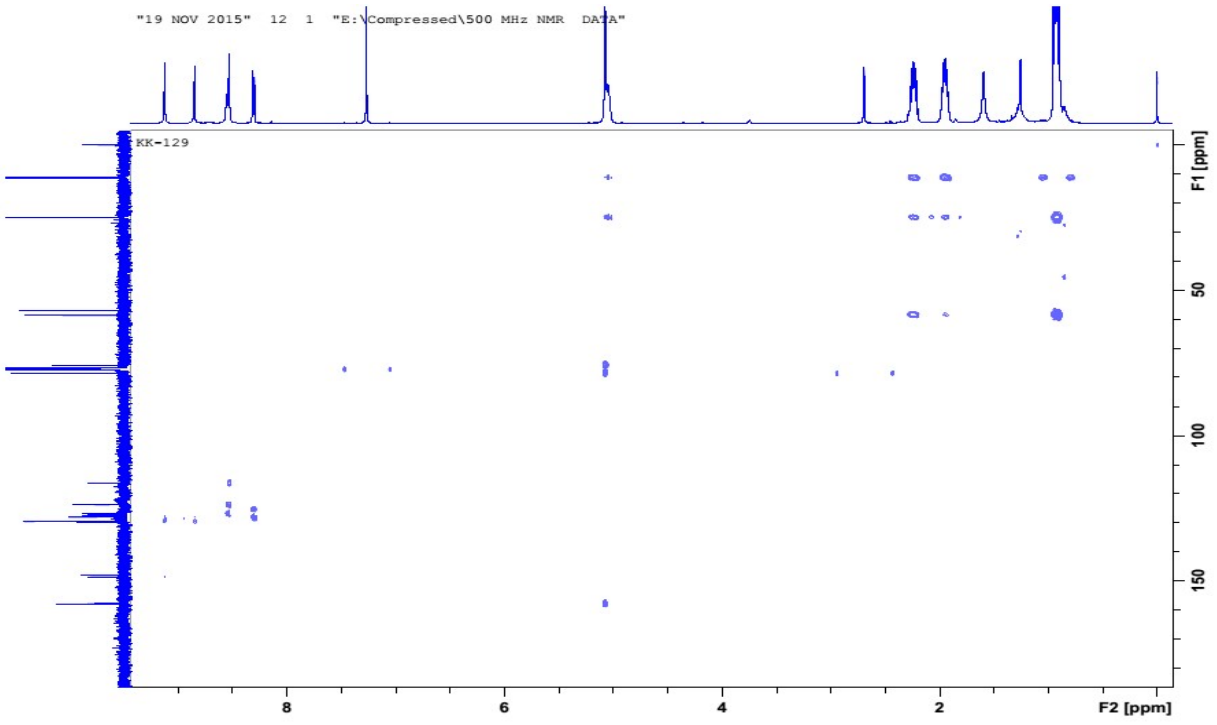

Figure S1e: HMBC data of **DNP**.

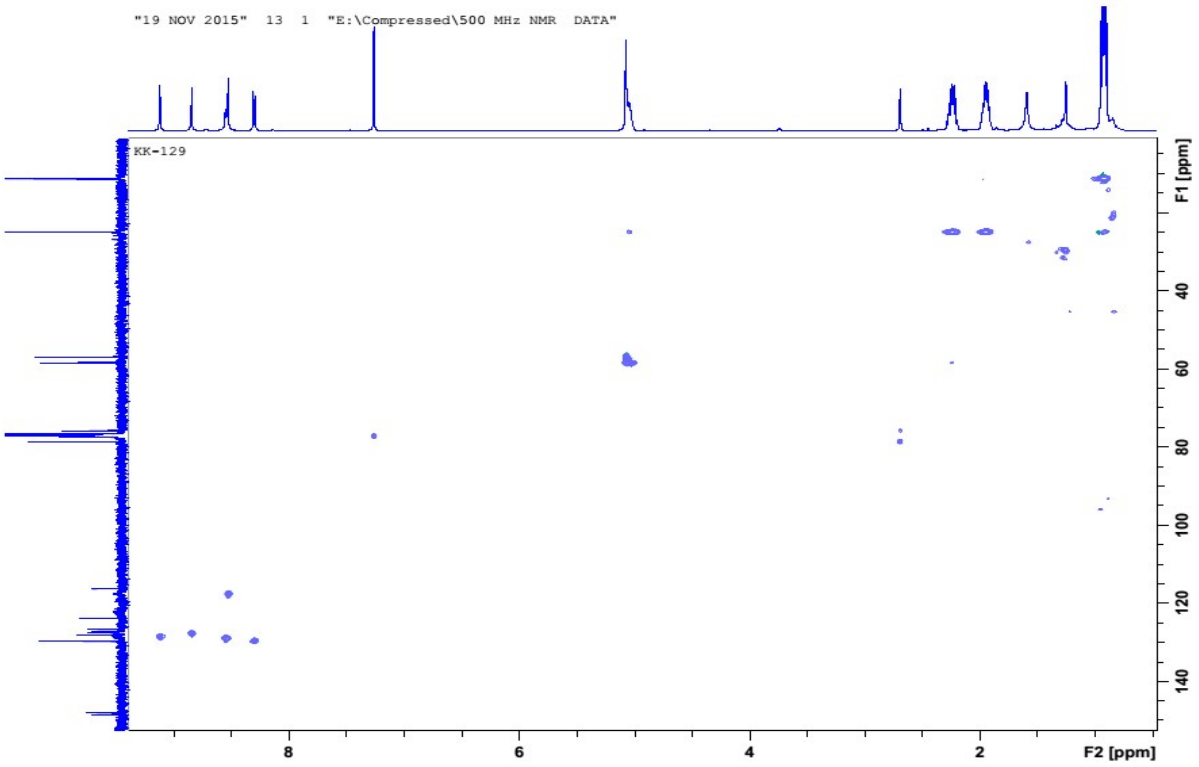

Figure S1f: HSQC data of **DNP**.

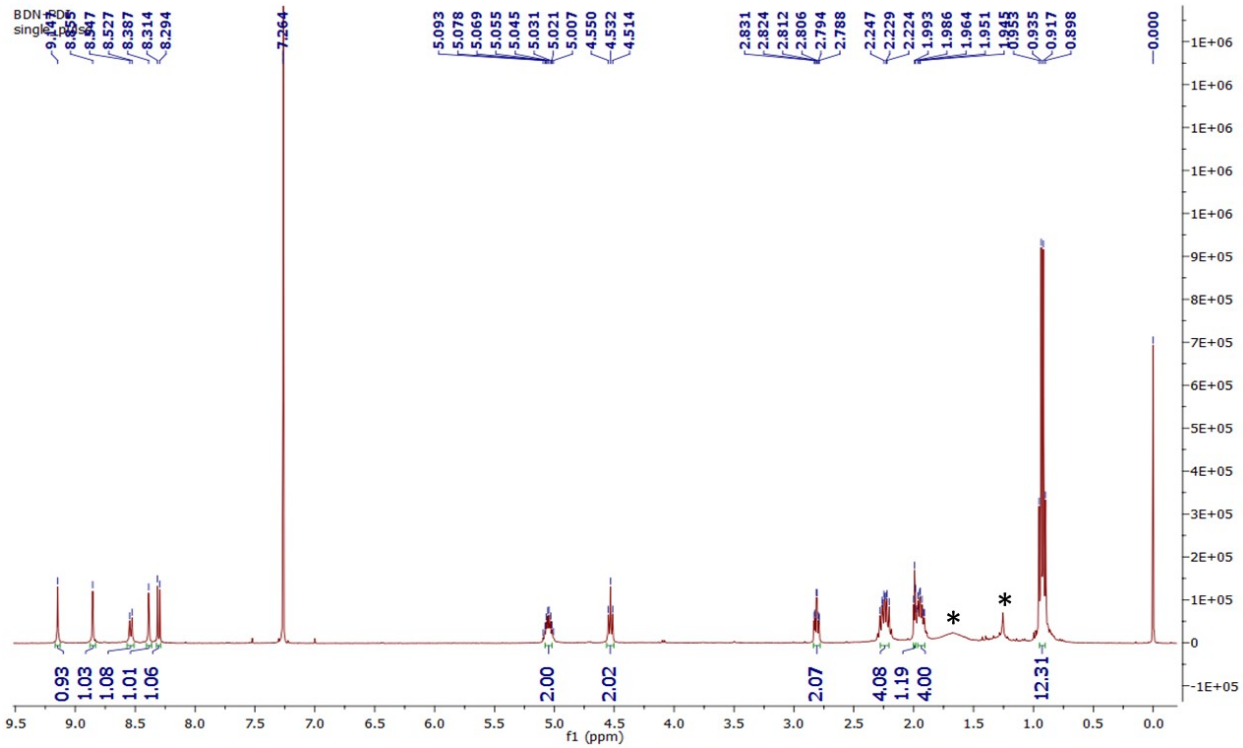

Figure S2a: ^{1}H NMR spectrum of **DNB**.

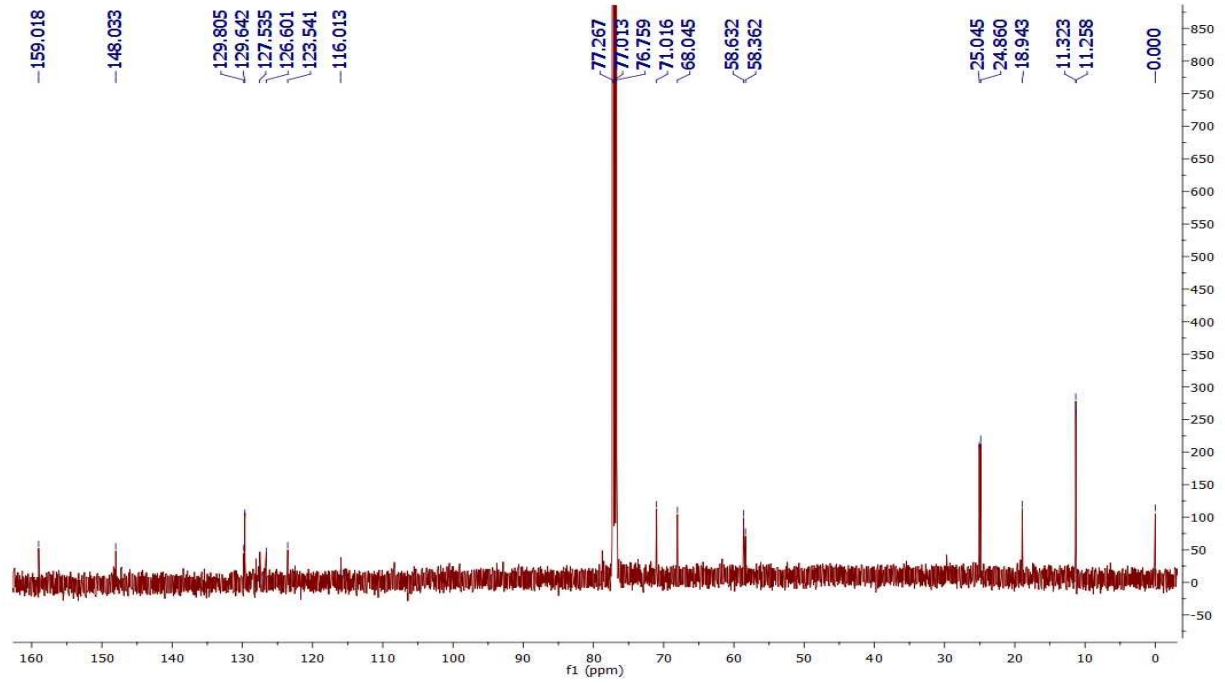

Figure S2b: ^{13}C NMR spectrum of **DNB**.

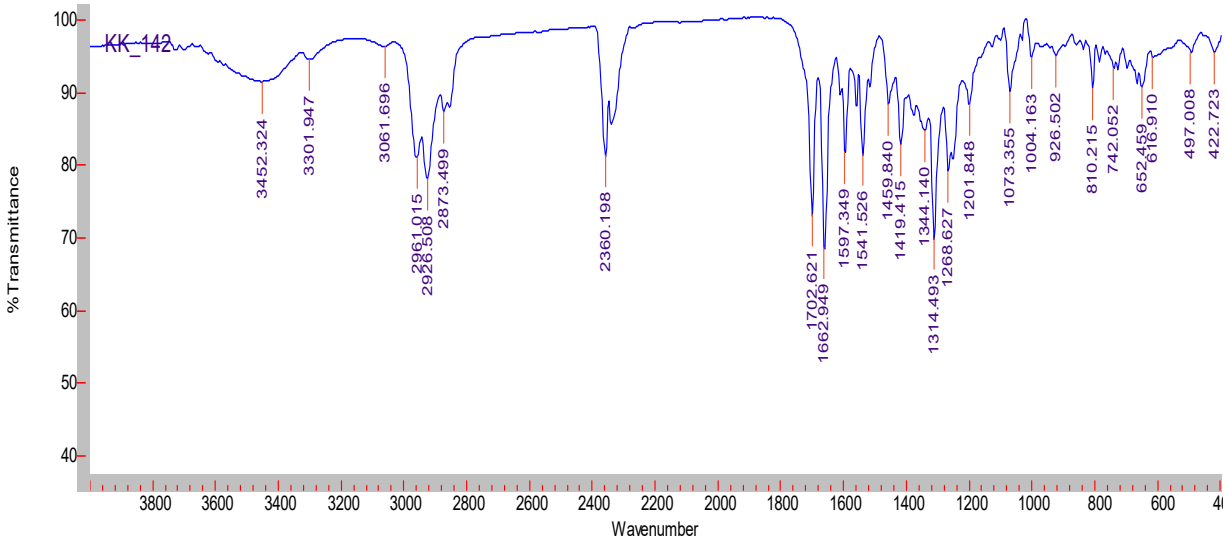

Figure S2c: IR spectrum of **DNB**.

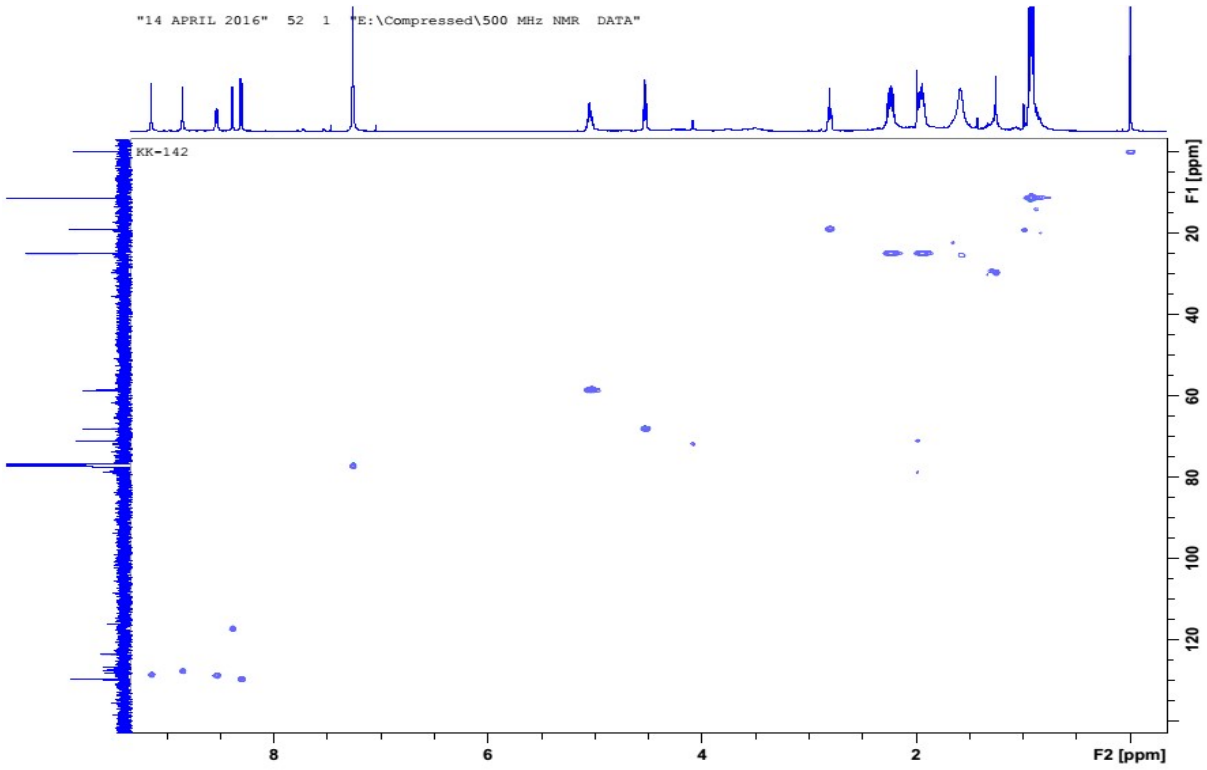

Figure S2d: HSQC spectrum of **DNB**.

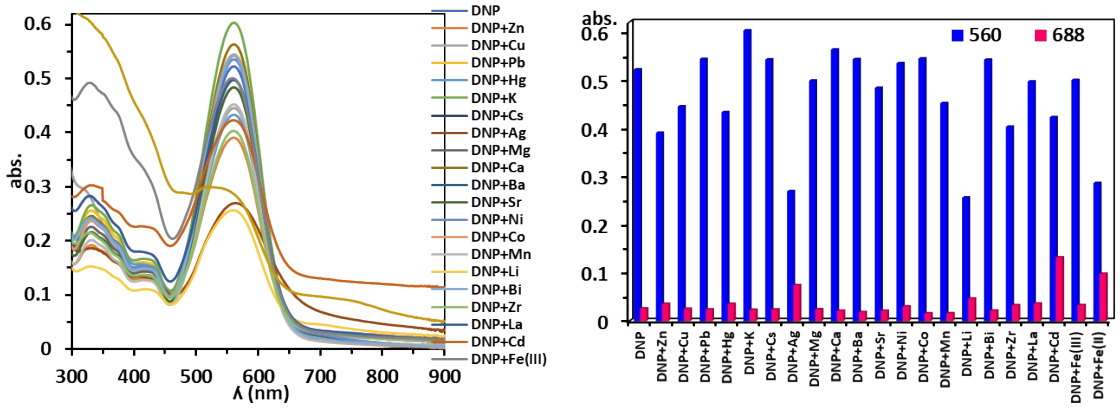

Figure S3. The absorbance spectrum of **DNP** (10 µM, 3 mL, CH_3CN-HEPES, 1:1, v/v, pH 7.2) in the presence of various anions and absorbance bar graph to investigate the competitive changes in **DNP** (10 µM at 560 nm and 688 nm in presence of various metal ions.

Figure S4: Photographs of naked eye color change in **DNP** upon addition of Fe^{2+} ions and reversal of green color back to violet with continuous increasing interval of time.

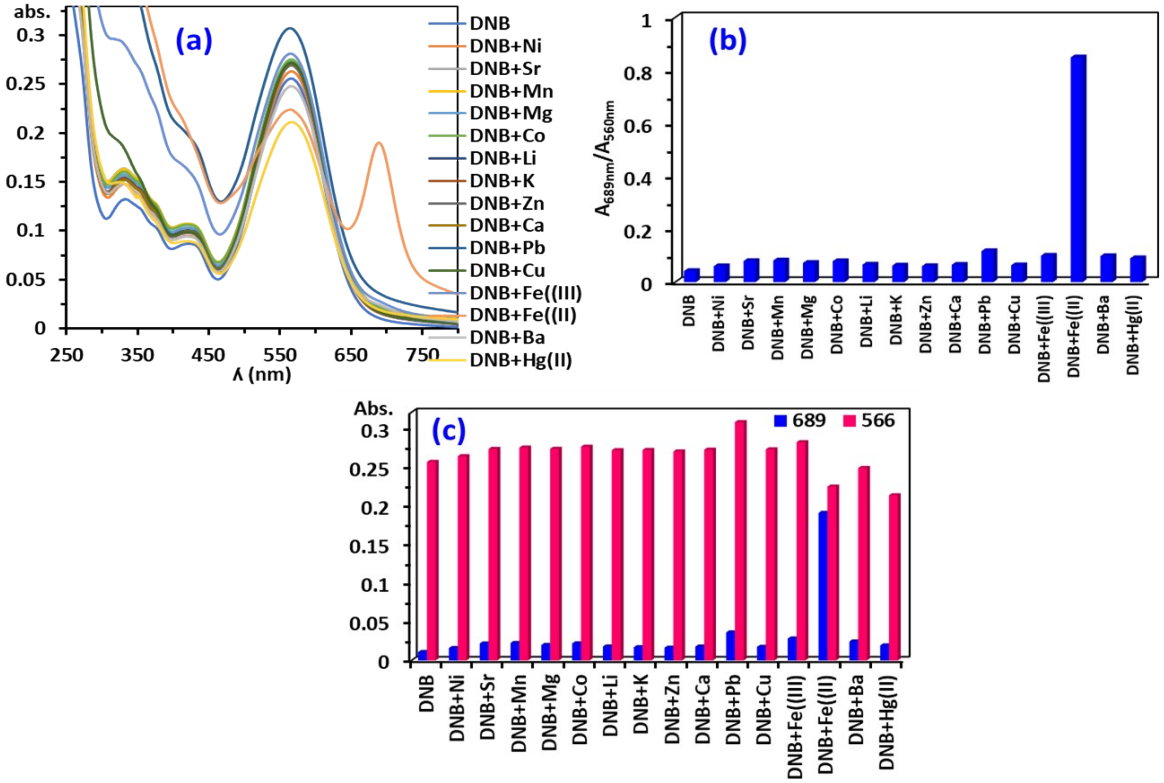

Figure S5. (a) The absorbance spectrum of **DNB** (10 µM, CH_3CN-HEPES, 1:1, v/v, pH 7.2) in the presence of various anions; (b) Ratiometric (A_{689nm}/A_{566nm}) and (c) absorbance plot to investigate the competitive changes in **DNB** (10 µM) with other anions.

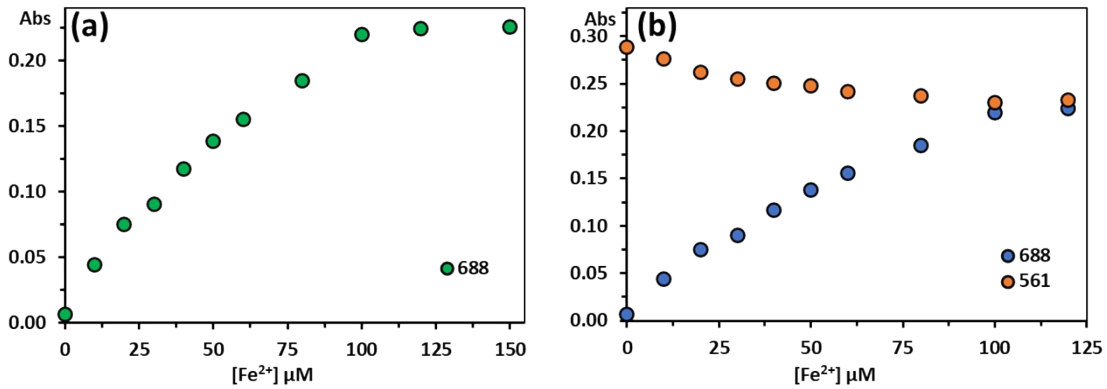

Figure S6: Plot of absorbance intensity of **DNP** (10 µM) (a) at 688 nm and (b) 688 nm and 561 nm upon addition of Fe^{2+} (0–150 µM) recorded in 50% HEPES buffer–CH_3CN (pH 7.2) solution.

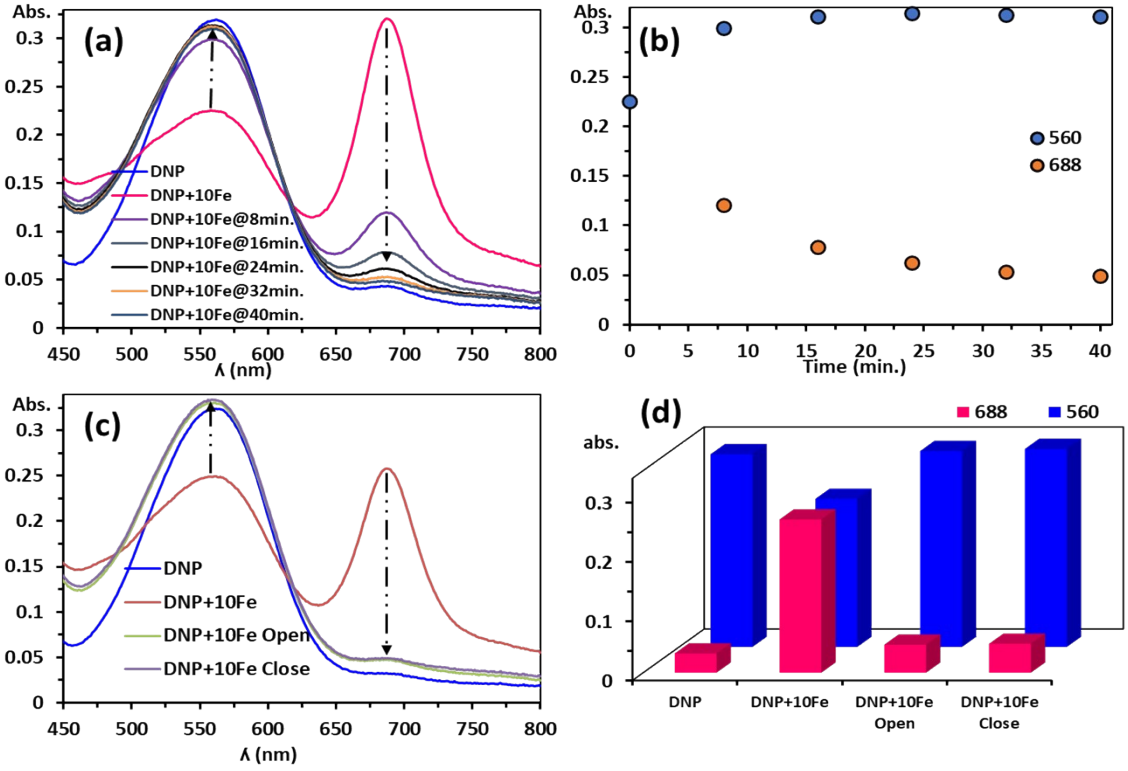

Figure S7: (a) Absorbance spectra and (b) Plot of absorbance intensity of **DNP** (10 µM) + Fe^{2+} (100 µM) assay recorded after regular interval of time; (c-d) effect of O_2 on **DNP** (10 µM) + Fe^{2+} (100 µM) assay when the vials kept open and closed. All readings have been recorded in 50% HEPES buffer–CH_3CN (pH 7.2) solution.

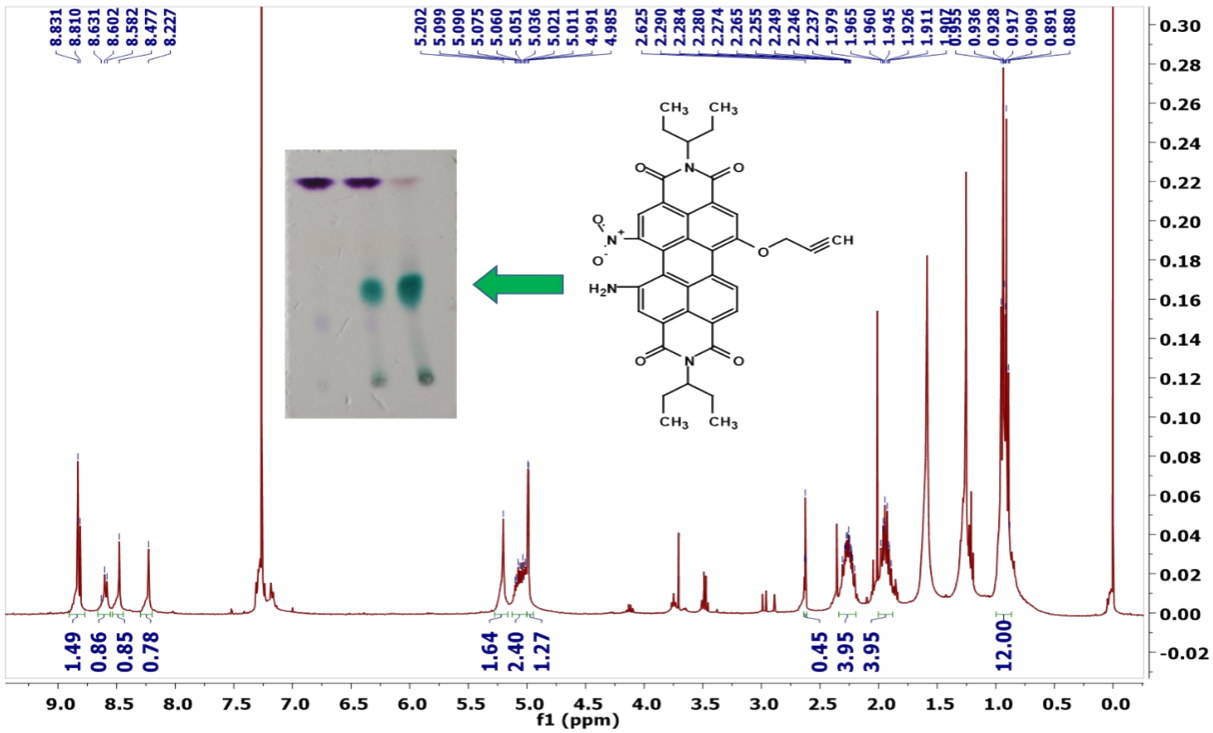

Figure S8. The proton NMR spectrum of green product (reduction of one -NO_2 group to -NH_2) isolated from model reaction.

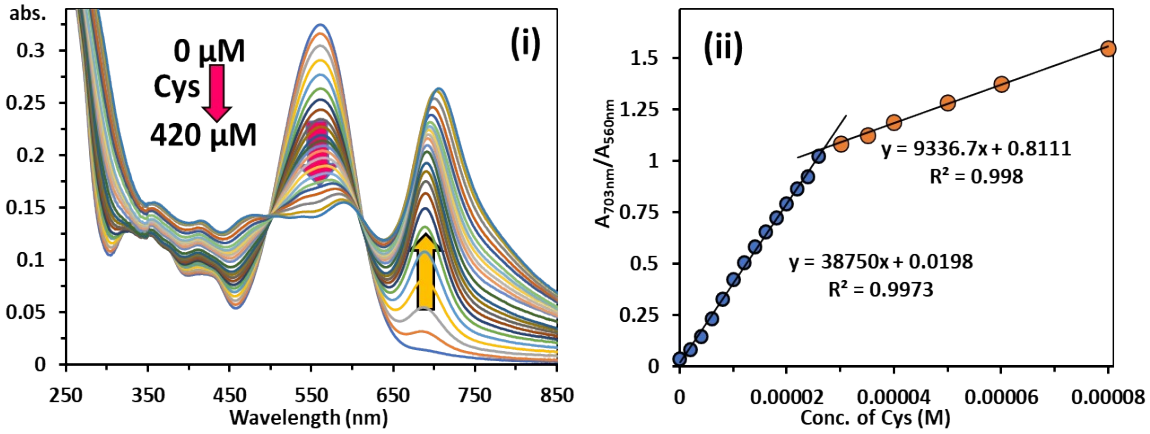

Figure S9: (i) Absorbance spectra of **DNP** (10 µM) recorded in 50% HEPES buffer–CH_3CN (pH 7.2) solution on addition of Cysteine (Cys) in concentration range of 0-420 µM; (ii) Ratiometric plot of absorbance intensity at A_{703nm}/A_{560nm} against different concentrations of Cys.

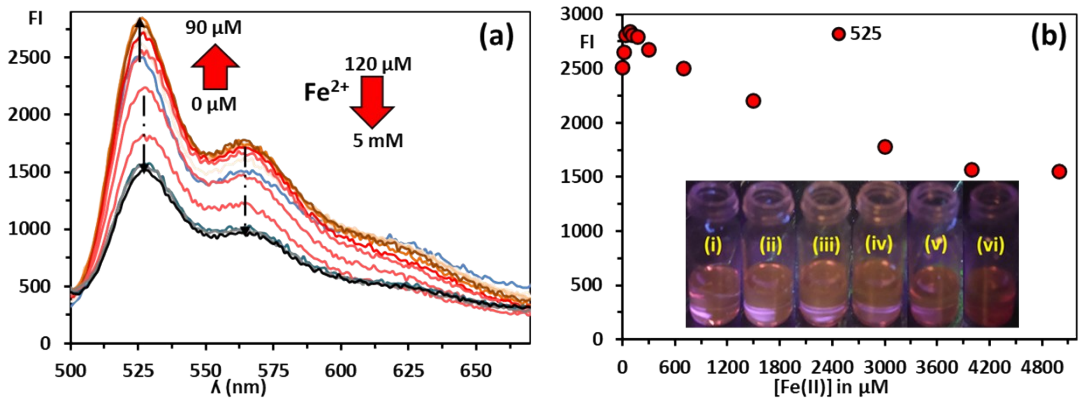

Figure S10. (a) Emission spectra of **DNP** (10 µM) recorded in HEPES buffer–CH_3CN (1:1, v/v, pH 7.2) upon addition of different concentrations of Fe^{2+} ions; (b) Plots of fluorescence intensity for **DNP** in the presence of various concentrations of Fe^{2+} ions; (Inset) Photographs of **DNP** (20 µM) under 365 nm UV illumination in the presence of (i) 0 µM (ii) 80 µM (iii) 140 µM, (iv) 200 µM, (v) 400 µM, (vi) 1 mM, concentrations of Fe^{2+} ions.

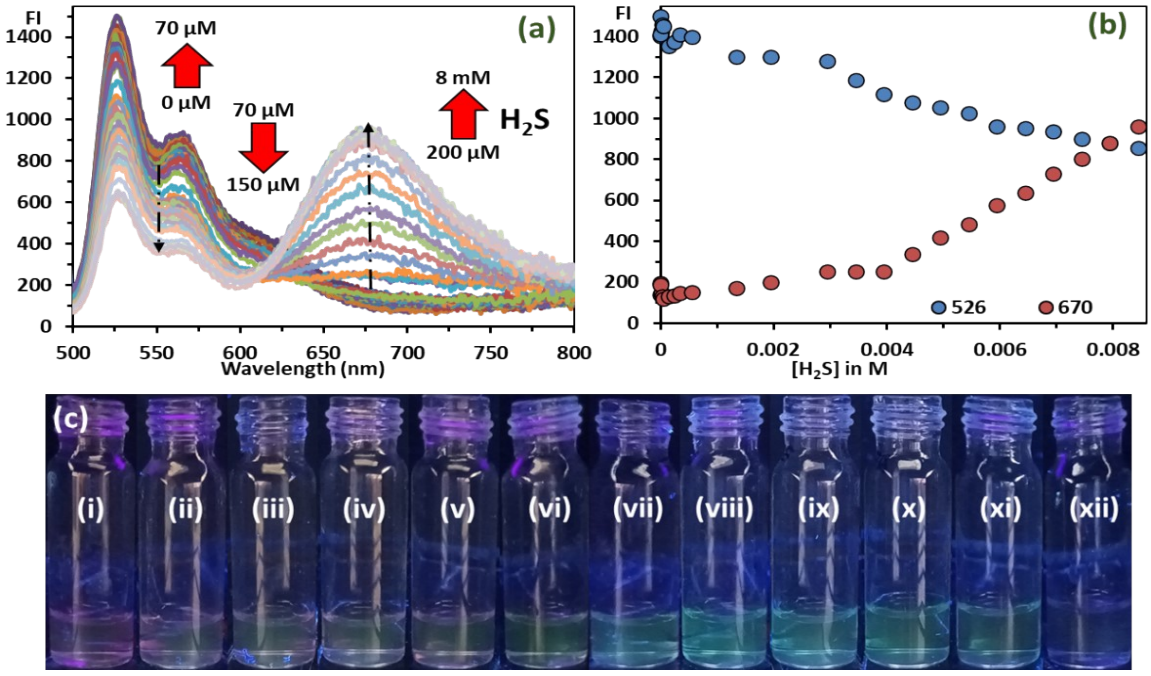

Figure S11. (a) Emission spectra of **DNP** (10 µM) recorded in HEPES buffer–CH_3CN (1:1, v/v, pH 7.2) upon gradual addition of H_2S; (b) Plot of fluorescence intensity of **DNP** (10 µM) upon addition of different concentrations of H_2S; (c) The color change photographs of **DNP** under 365 nm UV illumination in the presence of different concentrations of H_2S; labels in figure 2d (i) 0 µM (i) 10 µM, (ii) 20 µM, (iii) 40 µM,

(iv) 70 µM, (v) 100 µM, (vi) 150 µM, (vii) 200 µM, (viii) 500 µM, (ix) 750 µM, (x) 2.45 mM, (xi) 4.45 mM, (xii) 8.75 mM concentrations of H_2S.

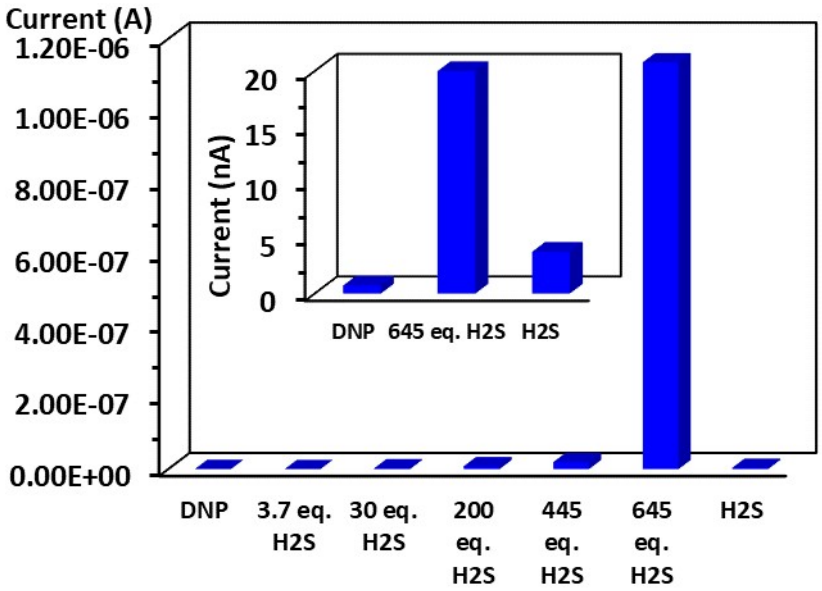

Figure S12. The bar graph for current values of **DNP** in air at different concentrations of H_2S from 37 µM to 6.45 mM; (inset) plot to show the increment in current values at high concentration of H_2S in air at working temperature of 25 °C in comparison to H_2S itself; (inset) the magnified view for current values of **DNP**, **DNP**+645eq. H_2S and H_2S alone.

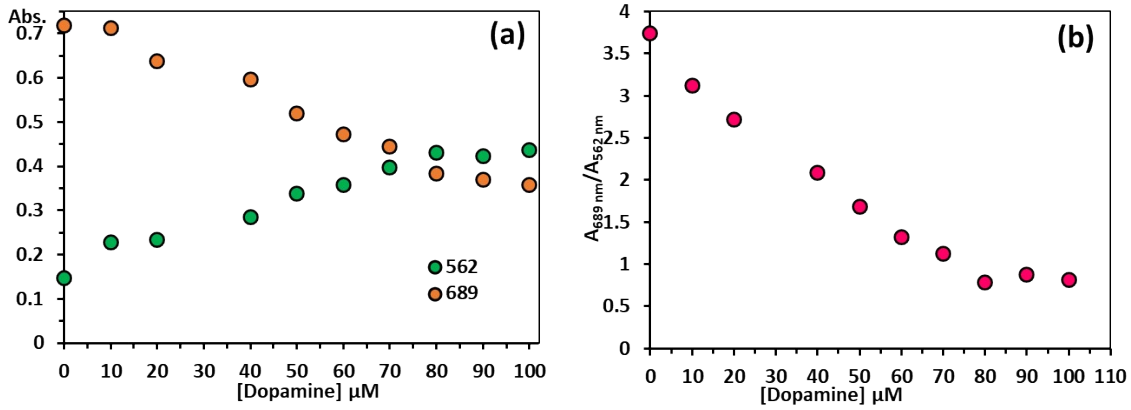

Figure S13: Plot of absorbance intensity of **DNP** (10 µM) (a) at 562 and 689 nm and (b) Ratiometric plot (A_{689nm}/A_{561nm}) versus concentration of DA (0–100 µM) recorded in 50% HEPES buffer–CH_3CN (pH 7.2) solution.

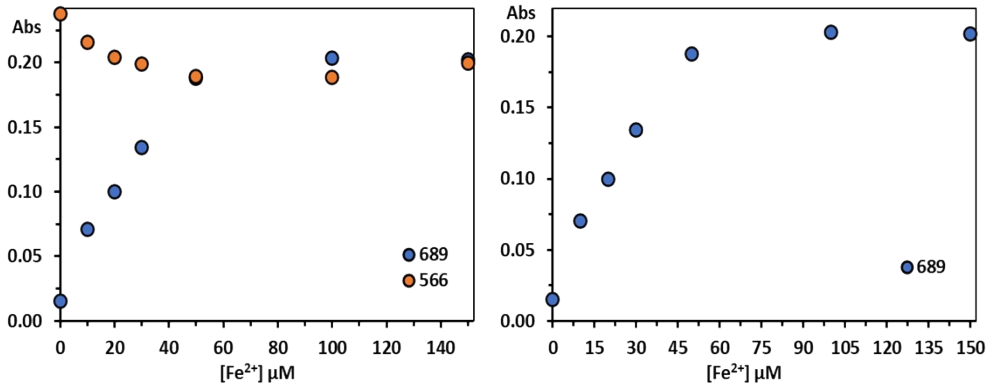

Figure S14: Plot of absorbance intensity of **DNB** (10 µM) (a) at 689 nm and 566 nm and (b) 689 nm upon addition of Fe^{2+} (0–150 µM) recorded in 50% HEPES buffer–CH_3CN (pH 7.2) solution.

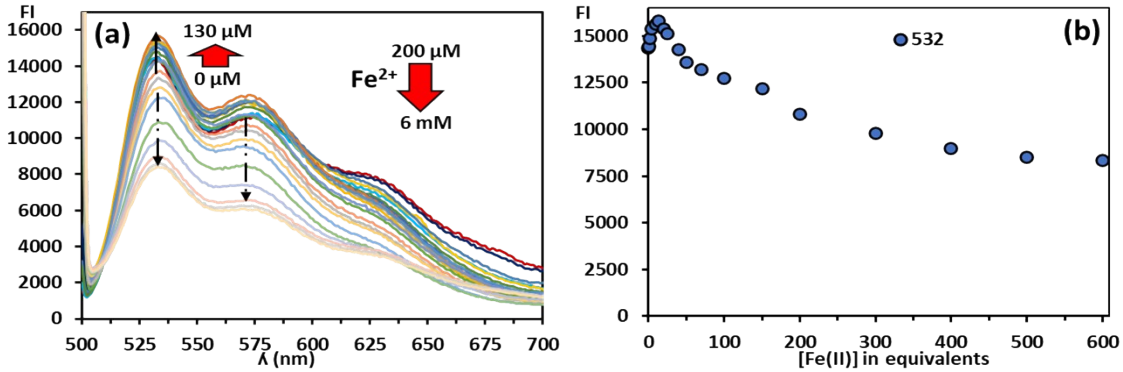

Figure S15: (a) Fluorescence spectra of **DNB** (10 µM) recorded in HEPES buffer–CH_3CN (1:1, v/v, pH 7.2) upon adding different concentrations of Fe^{2+} ions; (b) Plot of emission intensity of **DNB** (10 µM) at 532 nm upon addition of (0–600 equivalents) concentration of Fe^{2+} solution.

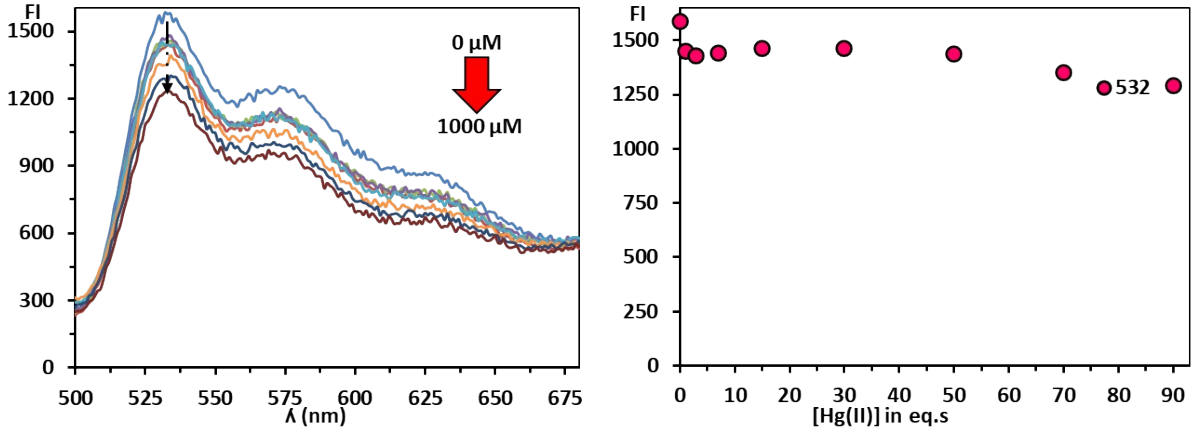

Figure S16: (a) Fluorescence spectra of **DNB** (10 µM) recorded in HEPES buffer–CH_3CN (1:1, v/v, pH 7.2) upon adding different concentrations of Hg^{2+} ions; (b) Plot of emission intensity of **DNB** (10 µM) at 532 nm upon addition of (0–100 equivalents) concentration of Hg^{2+} solution.

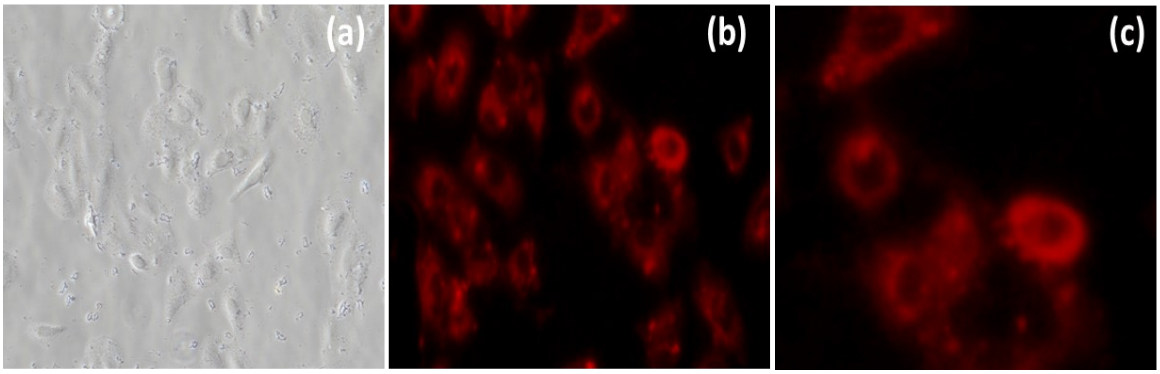

Figure S17: The Fluorescence imaging of Fe^{2+} ions in A549 cells; (a) bright field images of A549 cells (b) **DNP** (20 μM) + Fe^{2+} ions (700 μM); (c) Magnified view of cells shown in (b).