Simple Fluorescence Sensing Approach for Selective Detection of Fe^{3+} Ion: Live Cell Imaging and Logic Gate Functioning

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1. Synthetic Procedure and Spectral Data of Sensor APSB

A solution of pyrene-1- carboxaldehyde (0.230g, 1mmol) in hot ethanol (25 mL), was added dropwise to a solution of 2-amino anthracene (0.193g, 1mmol) in ethanol (5 mL), 4-5 drops of glacial acetic acid was added to the reaction. Then the reaction mixture was further refluxed for 8 h. Finally, the precipitate formed was filtered, washed well with cold ethanol, and dried. Yield 92%; IR (ATR) υmax/cm-1 3037,1577. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.72 (s, 1H), 8.52 (s, 1H), 8.50 (s, 2H), 8.37 (d, *J* = 9.2 Hz, 2H), 8.34 (d, *J* = 9.6 Hz, 3H), 8.32 – 8.29 (m, 6H), 8.15 (d, *J* = 4.8 Hz, 2H), 8.3 (s, 1H), 7.71 (d, *J* = 9.1 Hz, 1H) ppm.

^{13}C NMR (126 MHz) δ 193.08, 158.64, 135.58, 132.22, 131.40, 130.86, 130.74, 129.71, 129.15, 128.27, 128.02, 127.53, 127.23, 127.07, 126.86, 126.59, 126.28, 126.27, 126.26, 126.00, 125.65, 125.35, 125.14, 124.58, 123.85, 123.82, 123.06, 122.63, 122.51, 120.04, 117.34 ppm. (HR-MS) m/z: calcd for $C_{31}H_{19}N$: 405.15, found: 406.04 $[M+H]^+$

2. ^{1}H NMR and 13C NMR Spectra of APSB

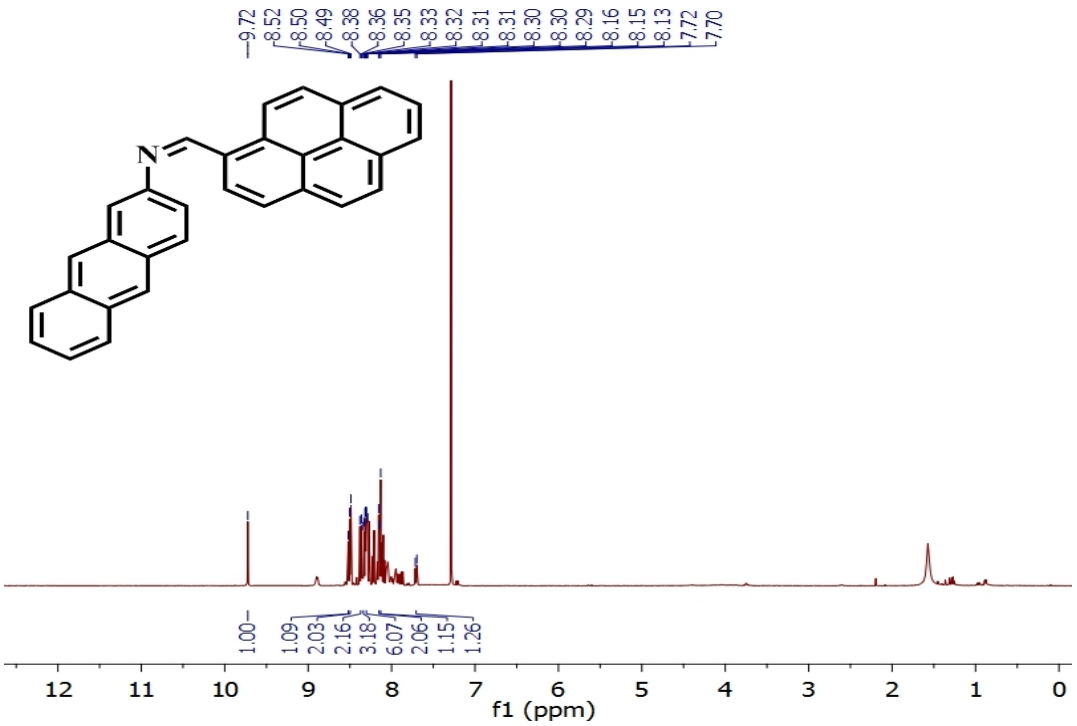


Figure S1: ^{1}H NMR spectra of APSB

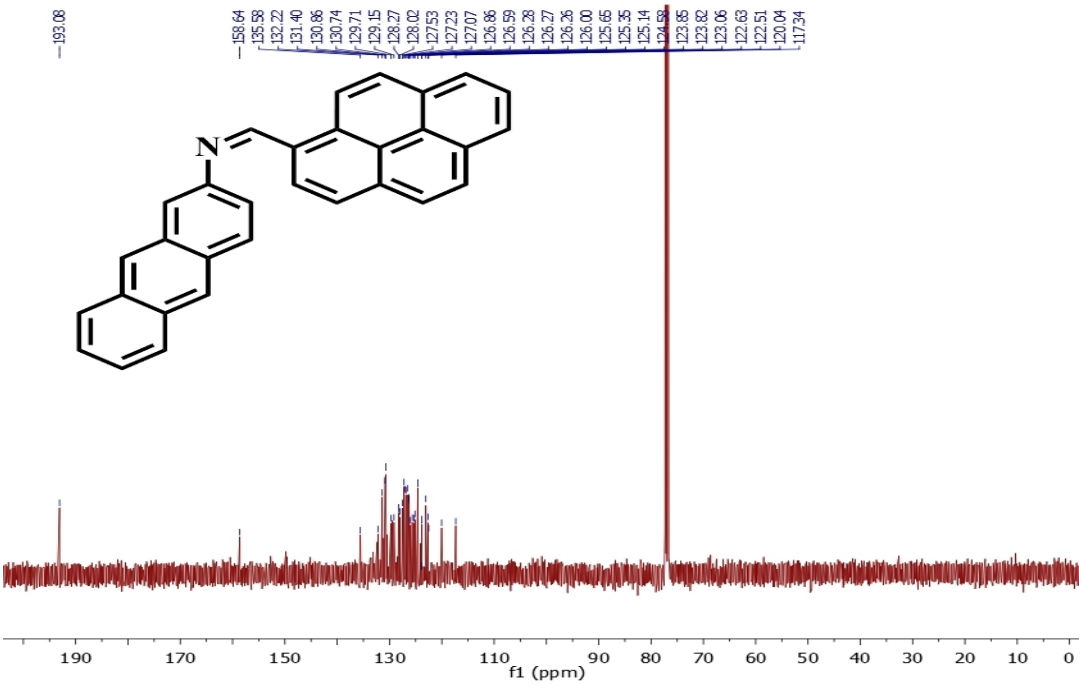
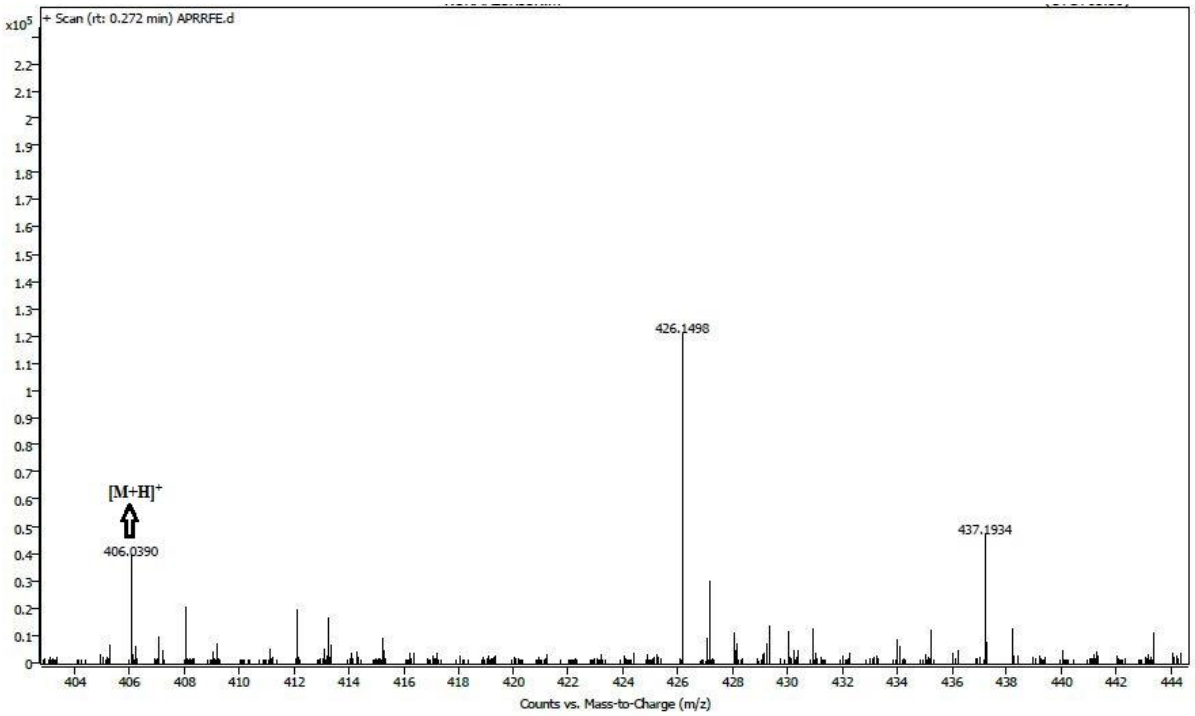
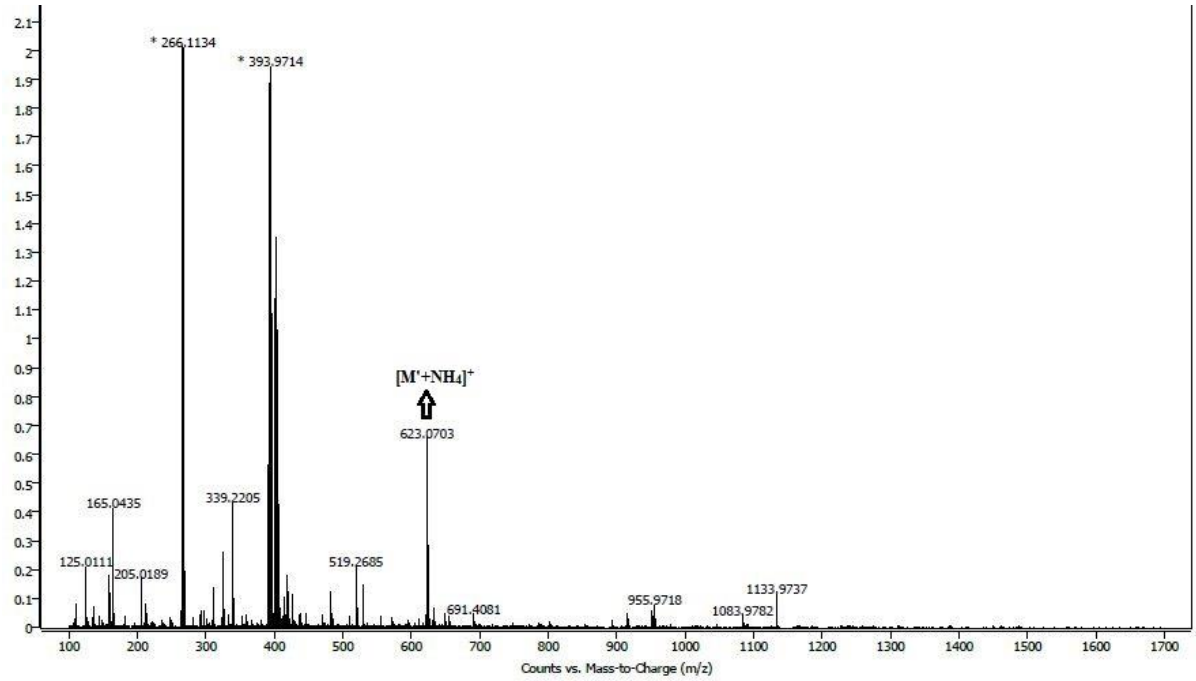


Figure S2: ^{13}C NMR spectra of APSB

3. HR-MS spectra of APSB and its Fe^{3+} Complex



(A)



Where M'= APSB-Fe^{3+}

(B)

Figure S3: HR-MS spectra of chemosensor APSB (A) and APSB-Fe^{3+} complex (B)

4. Linear Response of Fluorescence Titration of APSB

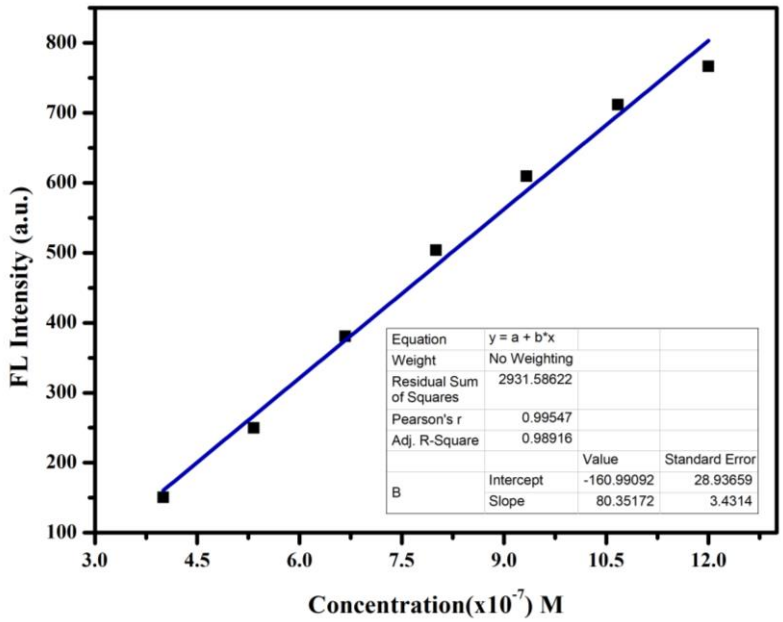


Figure S4: Linear response of fluorescence titration of APSB (1×10^{-5} M) in the presence of the increasing amount of Fe^{3+} (0-1.5 Equiv.) in CH3CN/H2O (95/5 v/v,) medium, λem = 520 nm

5. Solvatochromic study of APSB

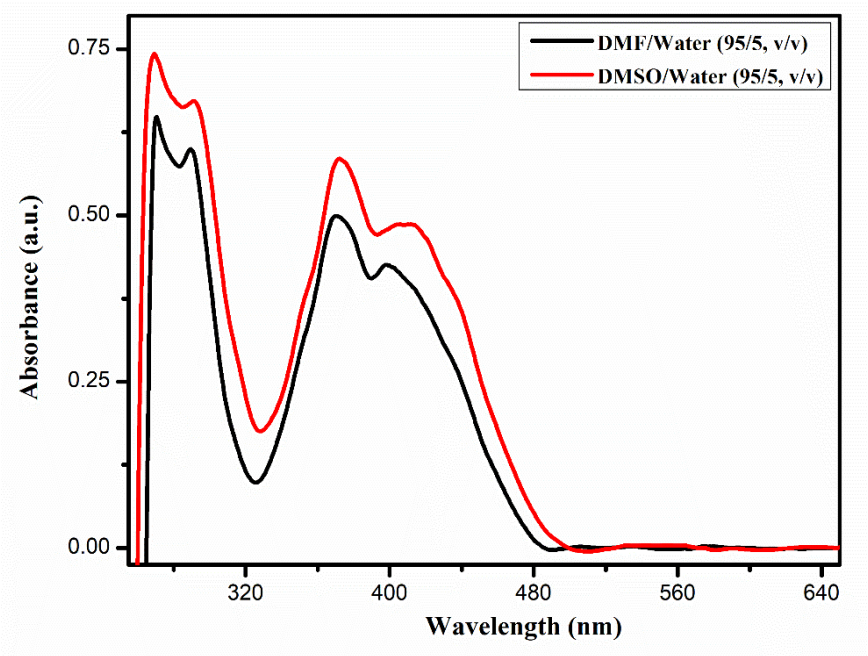


Figure S5: Solvatochromic studies of APSB in DMF and DMSO solvents and water mixture (solvent/H2O, 95/5 v/v) medium.

6. Time-dependence study

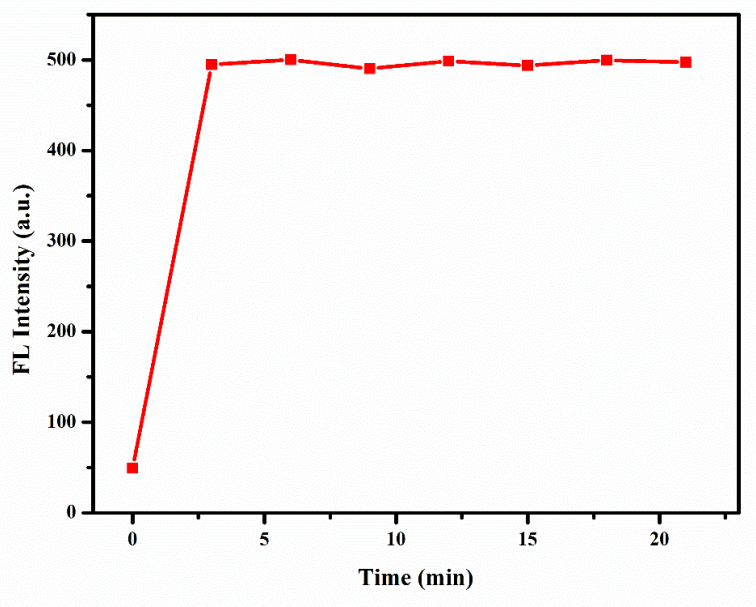


Figure S6: Fluorescent Intensity of APSB-Fe^{3+} complex at different time intervals (λ_{em}=520 nm, λ_{ex}=413 nm)

7. Effect of pH on receptor APSB

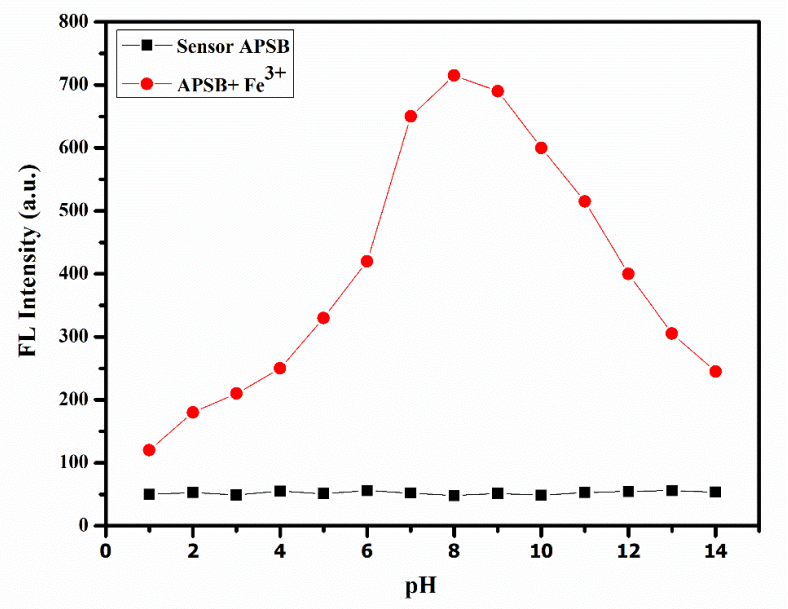


Figure S7: Fluorescence intensity (520 nm) of free receptor APSB (Black) (1×10^{-5} M) and after the addition of Fe^{3+} (1×10^{-3} M) (Red circles) in DMSO/Water (95/5, v/v) solutions as a The function of pH.

8. UV/vis Spectral Responses of APSB

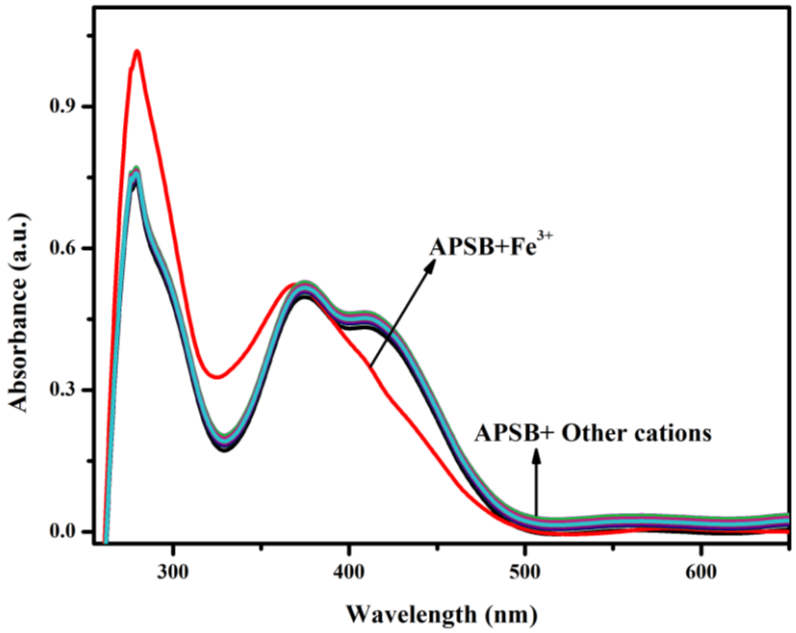


Figure S8: UV/vis absorption spectra of APSB (1×10^{-5} M) in DMSO/H2O (95/5 v/v) medium with various metal ions (1×10^{-3} M, λabs= 290 and 375 nm).

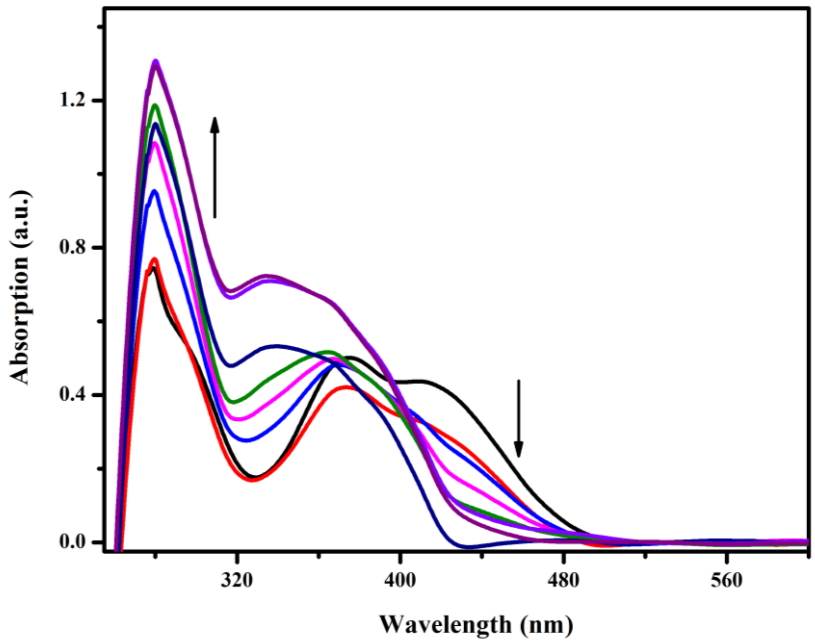


Figure S9: UV/vis absorption spectra of APSB (1×10^{-5} M) with the increasing amount of Fe^{3+} (0–1.5 Equiv.) in DMSO/H2O (95/5 v/v) medium.

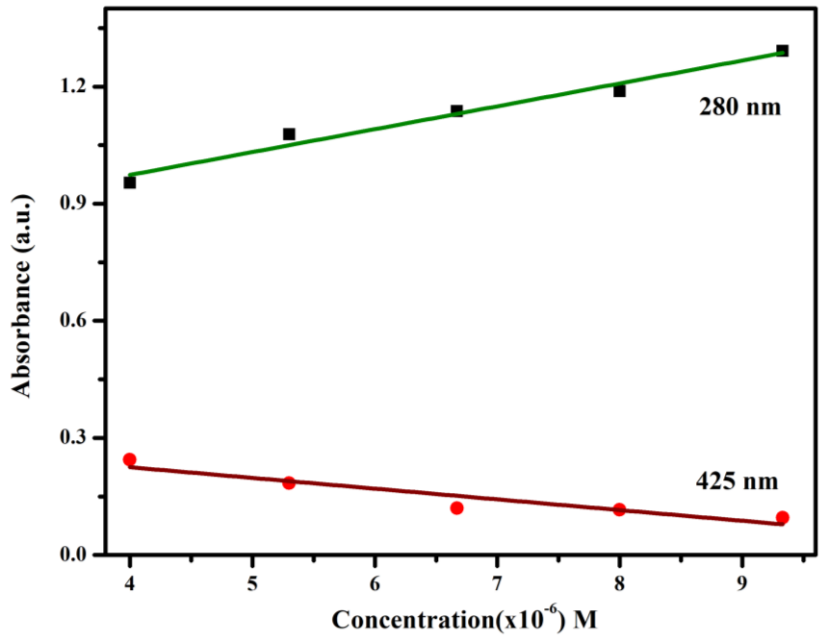


Figure S10: Linear response of UV/vis titration of APSB (1×10^{-5} M) in the presence of the increasing amount of Fe^{3+} (0–1.5 Equiv.) in DMSO/H2O (95/5 v/v) medium

9. Job's Plot for 1:1 Complexation of APSB and Fe^{3+}

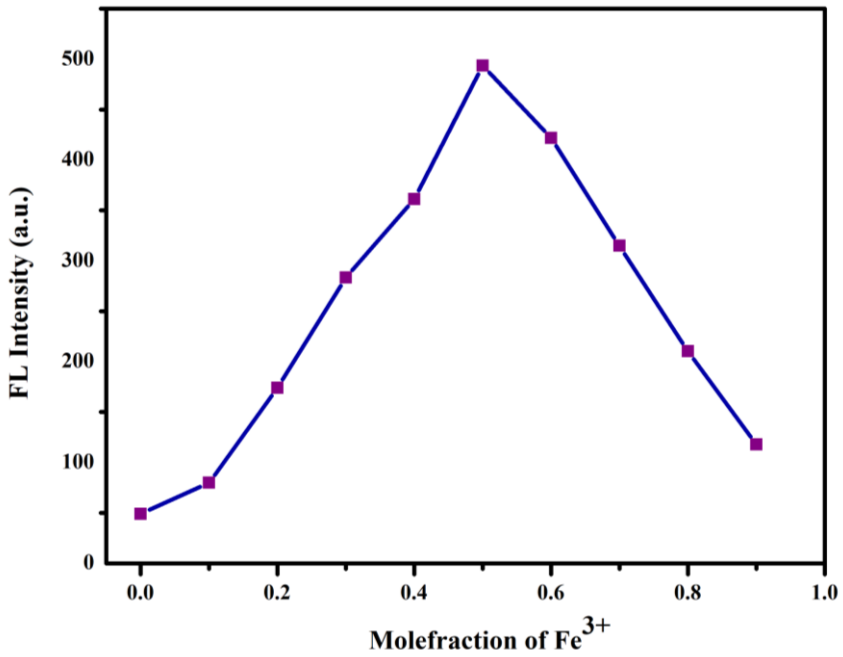


Figure S11: Job's plot for 1:1 complexation of APSB and Fe^{3+} (λem = 520 nm) in DMSO/H2O (95/5 v/v) medium.

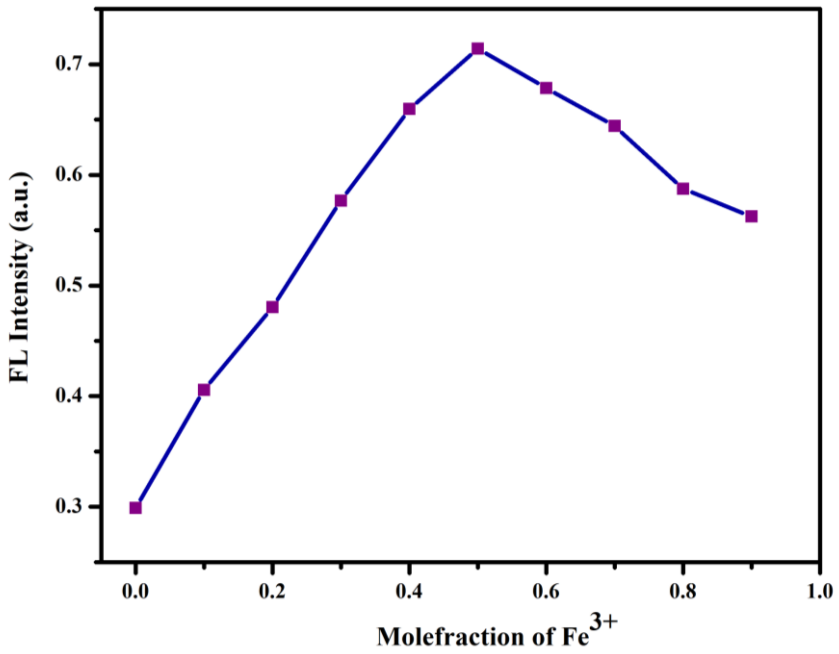


Figure S12: Job's plot for 1:1 complexation of APSB and Fe^{3+} (λabs = 413 nm) in DMSO/H2O (95/5 v/v) medium.

10. Cyclic Voltammetry of APSB

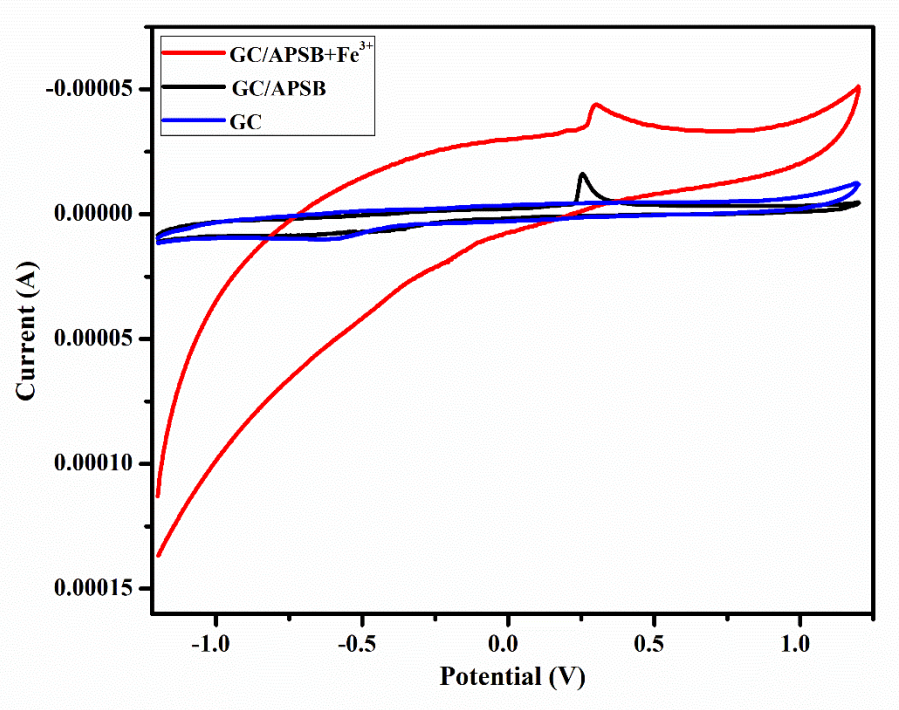
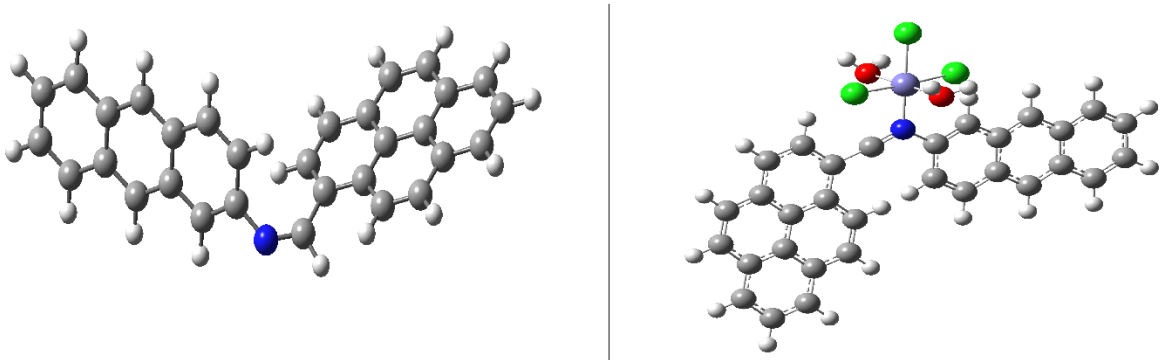


Figure S13: Cyclic voltammetry of APSB (1×10^{-5} M) with Fe^{3+} (1×10^{-3} M) in PBS (7) potential range: -1.5 V up to 1.5 V, v = 0.1 V s-1.

11. Proposed Optimized Geometries of APSB and its Fe^{3+} Complex



A B

Figure S14: Proposed optimized geometries of APSB (A) and APSB with the Fe^{3+} complex (B)