Electronic Supplementary Material (ESI) for RSC Advances

A ratiometric fluorescent sensor for selective recognition of Al^{3+} ions based on a simple benzimidazole platform

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SUPPLEMENTARY INFORMATION

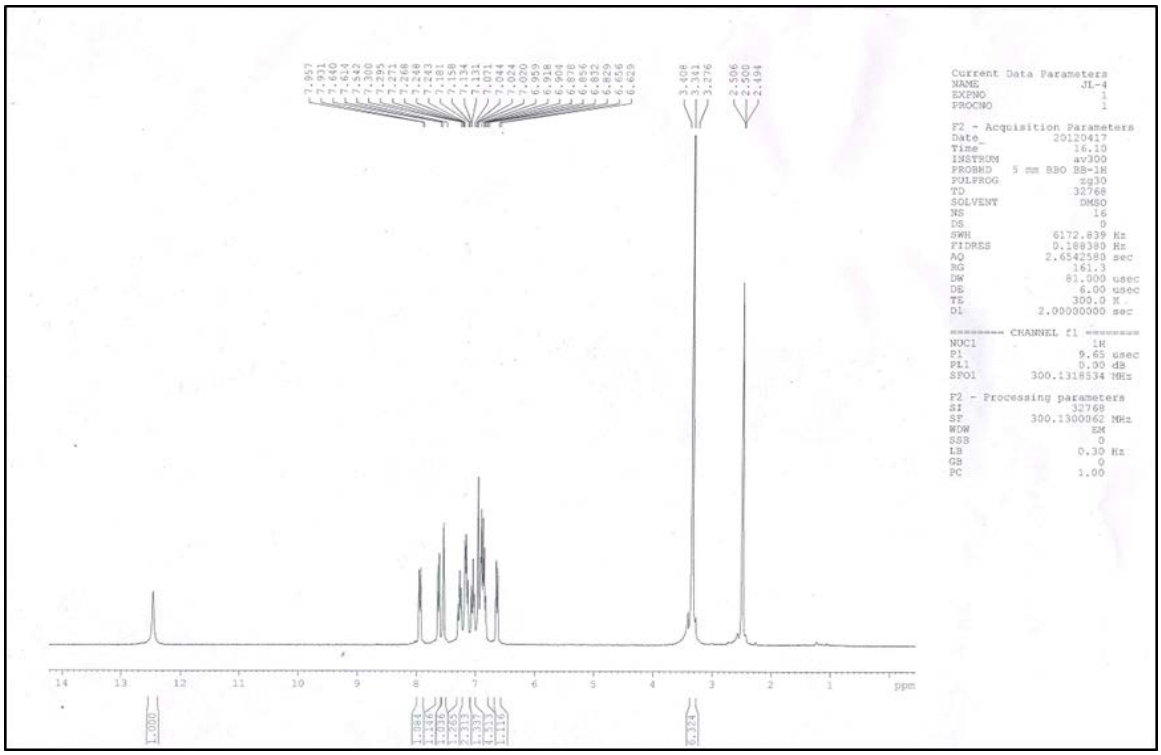

Fig S1.^{1}H NMR spectrum of PB

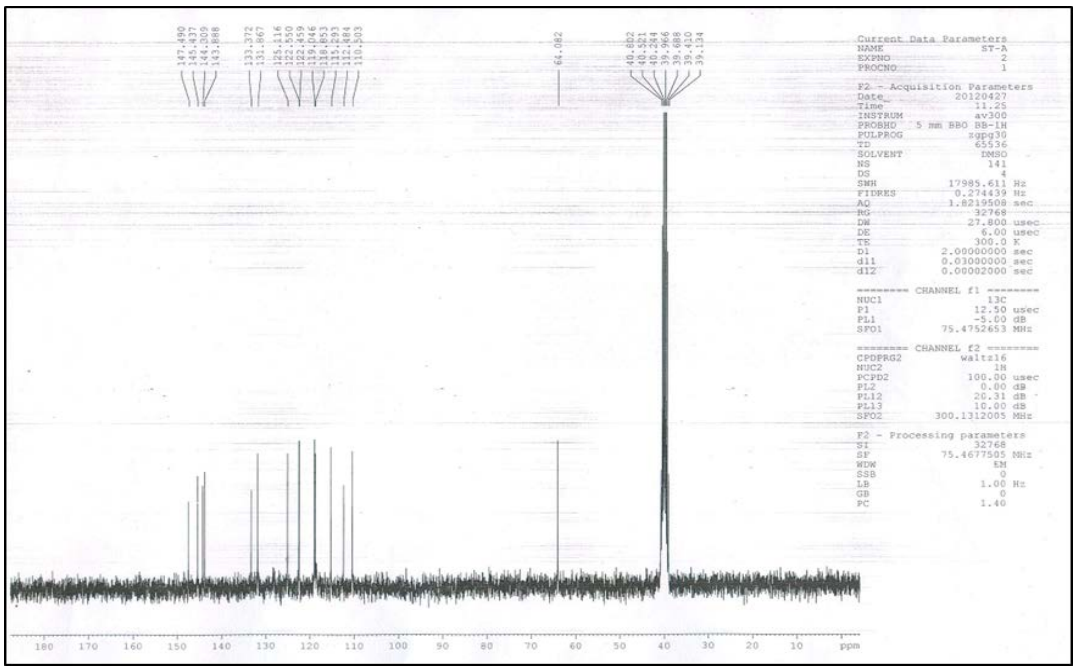

Fig S2.^{13}C NMR spectrum of PB

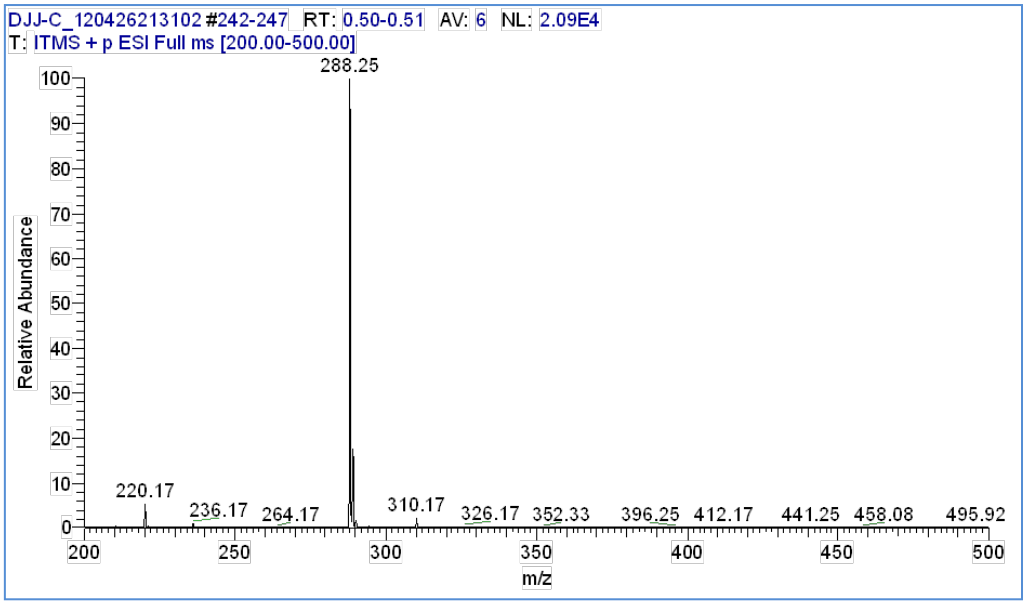

Fig S3. ESI-MS spectrum of PB

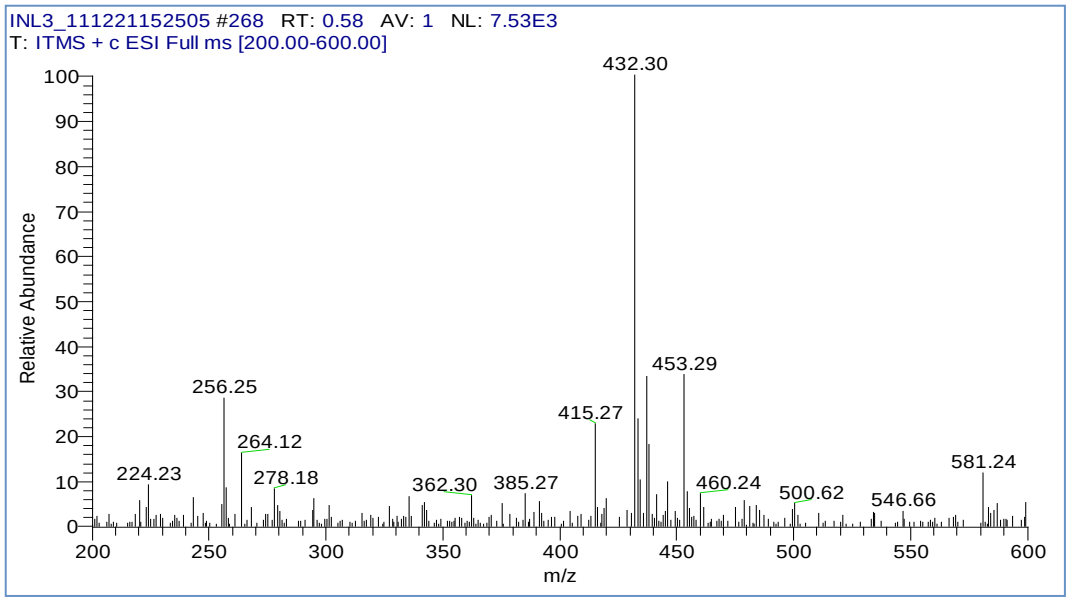

Fig S4. ESI-MS spectrum of PB-Al^{3+}

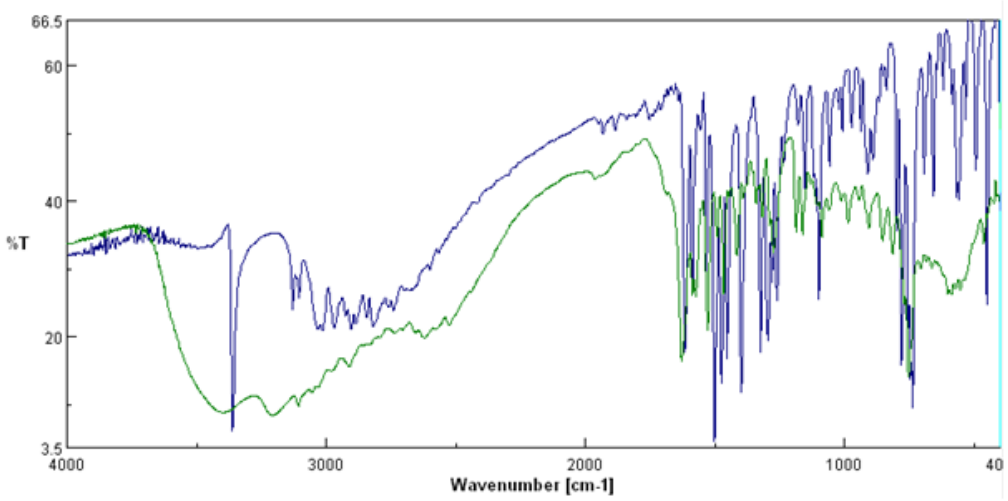

Fig S5. IR spectrum of PB and PBI.Al^{3+}

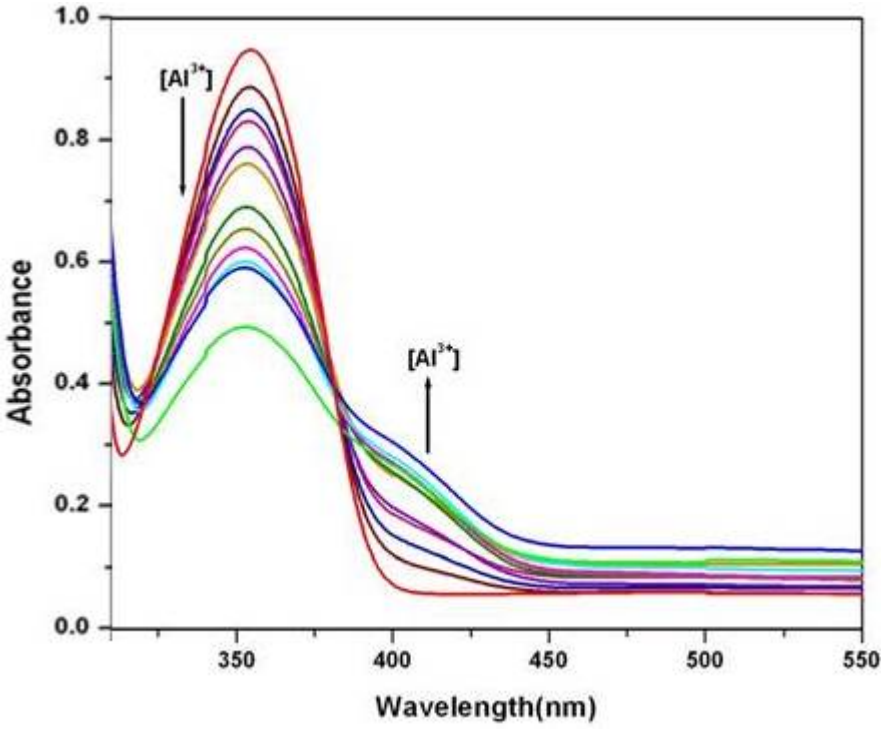

Fig S6. UV-visible spectral changes of PB(10μM) upon the successive addition of Al^{3+} (0-1 equivalents) at 25˚C in DMSO/H2O (1:9, v/v, phosphate buffer, 100mM: pH = 7.54)

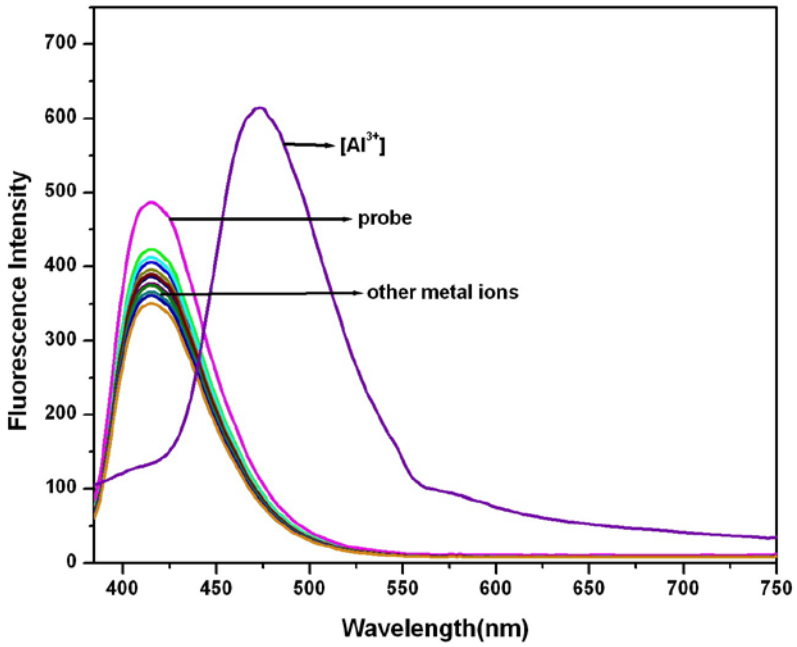

Fig S7. Changes in the fluorescence spectra of PB(10μM) upon addition of various metal ions($1x10^{-5}$M) in 100mM phosphate buffer (DMSO/H_2O, 1:9) of pH 7.54 at 25°C (λ_{ex} = 350nm, slit = 5nm)

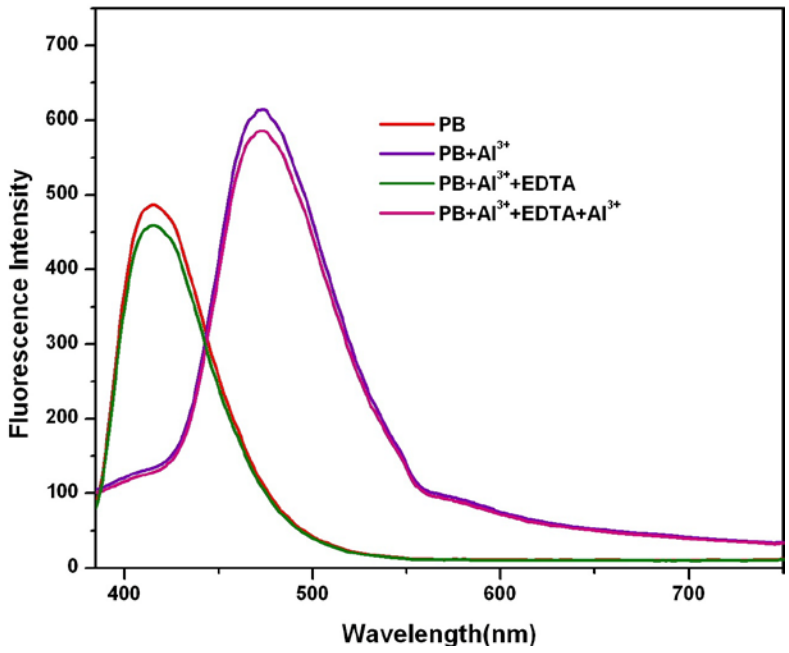

Fig S8.Fluorescence responses of PB to Al^{3+} (1eq) and EDTA (1eq) at 25°C in DMSO/H_2O (1:9, v/v). Excitation at 350nm (slit: 5nm)

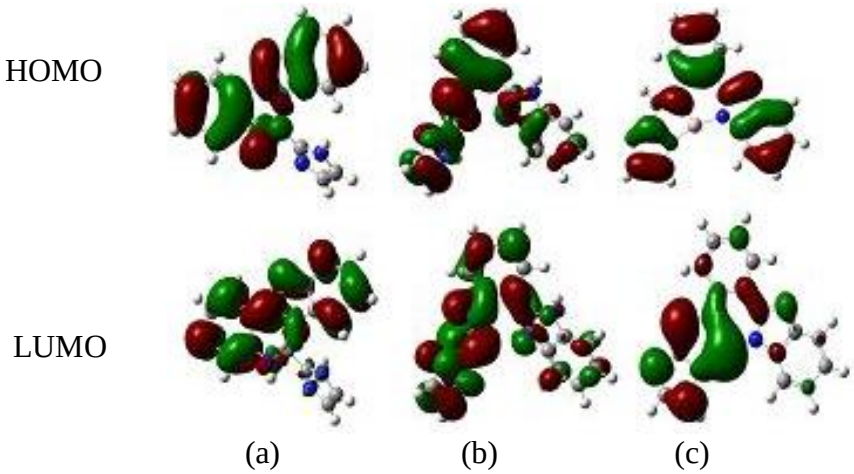

Fig S9. HOMO, LUMO plot of PB(a), PBI(b) and PBI.Al^{3+}(c) respectively

Calculation of Binding constant:

The binding constant K was determined from the plot of the linear regression of log [(F - F_0) / (F_m - F)] vs. log [M] in equation to obtain the intercept as log K and the slope as n.

$$\log \frac{F - F_0}{F_m - F} = \log K + n \log [M]$$

Calculation of Detection limit:

LOD was calculated based on the standard deviation of the response (SD) and the slope of the calibration curve (S) at levels approximating the LOD according to the formula:

$$LOD = 3.3\ (SD/S)$$

Calculation of Quantum Yield

Fluorescence quantum yields (Φ) were estimated by integrating the area under the fluorescence curves using the equation,

$$\phi_{\text{sample}} = \frac{\text{OD}_{\text{standard}} \times A_{\text{sample}}}{\text{OD}_{\text{sample}} \times A_{\text{standard}}} \times \phi_{\text{standard}}$$

where A was the area under the fluorescence spectral curve and OD was optical density of the compound at the excitation wavelength. Anthracene was used as quantum yield standard (quantum yield is 0.27 in ethanol) for measuring the quantum yields of ligand and its Al^{3+} complex.