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Novel A-D-A structural imidazole derivatives with charge transfer excited states: Importance of molecular structure design in obtaining a "turn-on" type fluorescence probe

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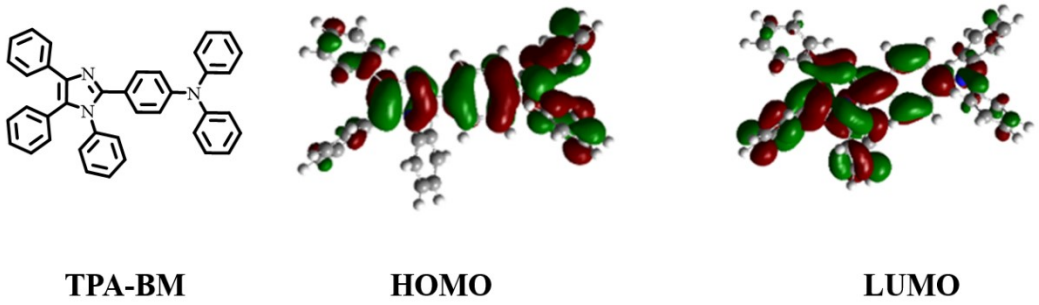

Fig. S1 The molecular structure and the electronic density distributions of the frontier molecular orbitals (HOMO and LUMO) in the ground state of **TPA-BM**.

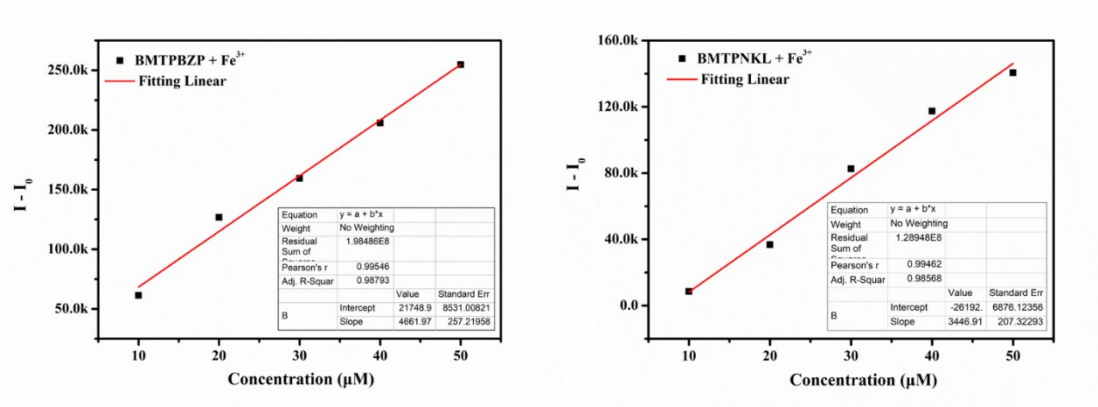

Fig. S2 The linear intensity changes of (a) **BMTPBZP** and (b) **BMTPNKL** (1×10^{-5} M) as a function of the concentration of Fe^{3+} based on their PL titration spectra.

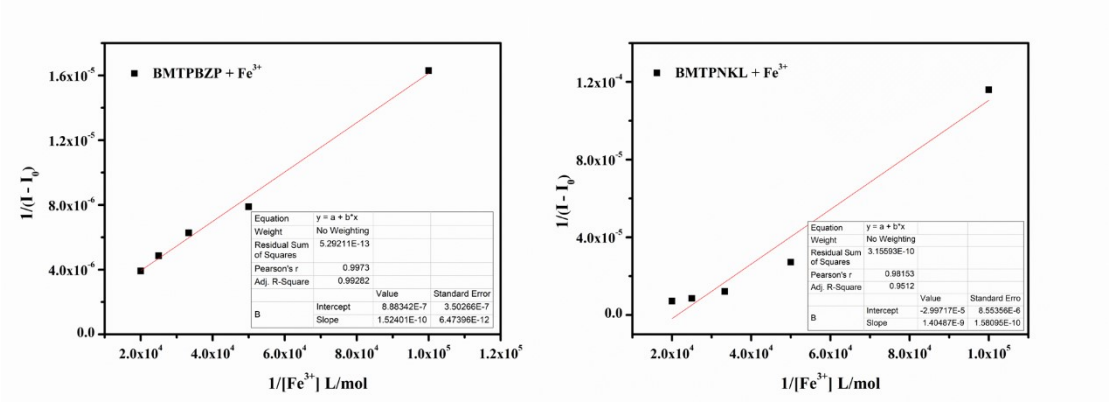

Fig. S3 The Benesi-Hildebrand linear analysis plot of (a) **BMTPBZP** and (b) **BMTPNKL** (1×10^{-5} M) at different Fe^{3+} concentrations.

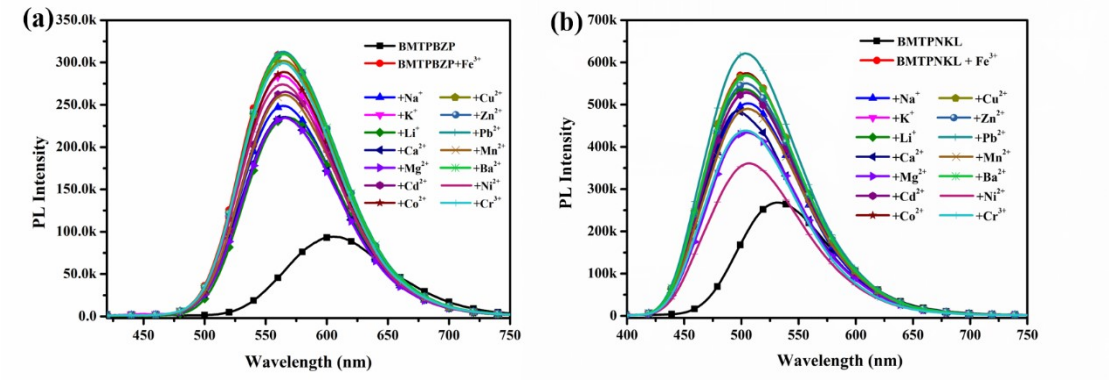

Fig. S4 The PL spectra of (a) **BMTPBZP**+Fe^{3+} and (b) **BMTPNKL**+Fe^{3+} in the

presence of different metal ions.

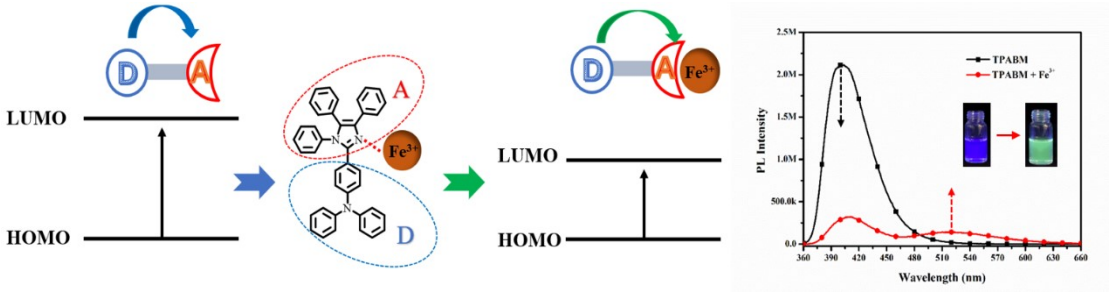

Fig. S5 The fluorescence response of the imidazole derivative **TPA-BM** with the simple D-A structure to Fe^{3+}, which showed a completely opposite fluorescence quenching and red-shifted response, and its possible response mechanism.

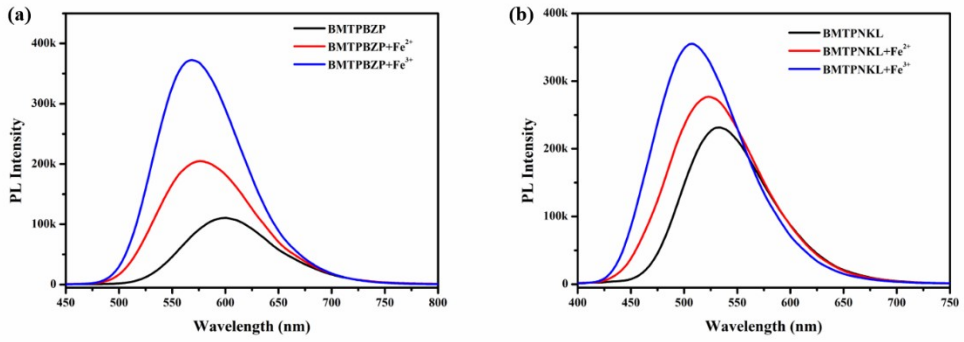

Fig. S6 The PL spectra of (a) **BMTPBZP** and (b) **BMTPNKL** (1×10-5 M) before and after adding Fe^{2+} and Fe^{3+}.

As shown in the above Fig. S6, the response behaviors of the probe molecules **BMTPBZP** and **BMTPNKL** to Fe^{2+} were also studied, and the results showed that both of they could also showed emission enhancement and blue shift response to Fe^{2+}, but the response amplitude was relatively weaker than that of Fe^{3+}.