

## Electronic Supplementary Information (ESI)

### **AIE active Schiff base compounds as fluorescent probes for highly sensitive and selective detection of Fe<sup>3+</sup> ions**

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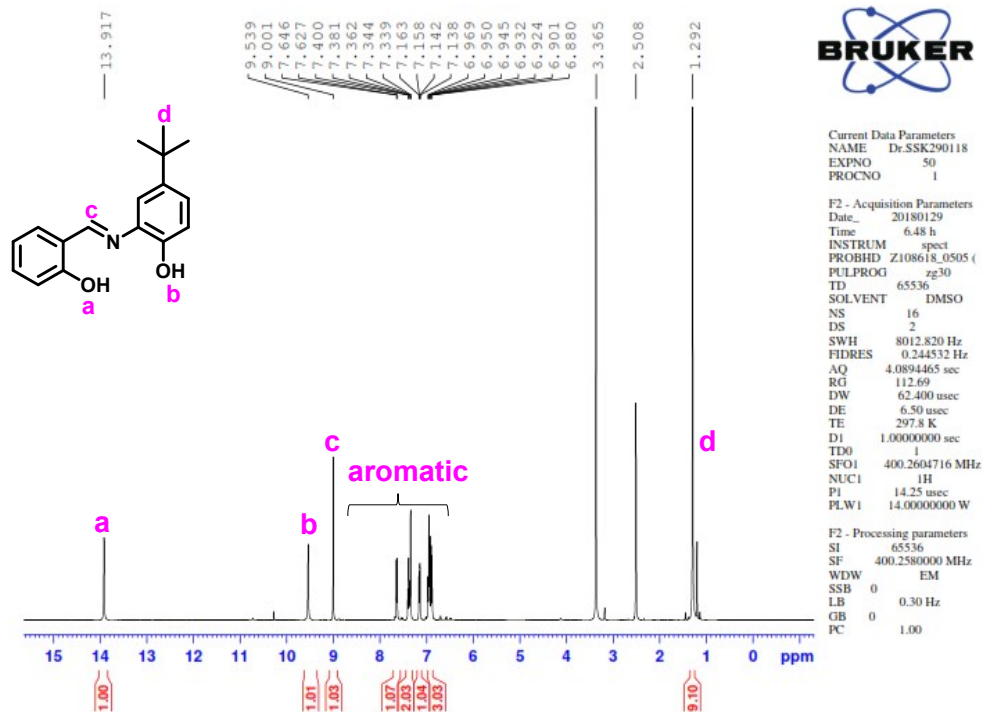


Fig. S1 <sup>1</sup>H NMR spectrum of L1

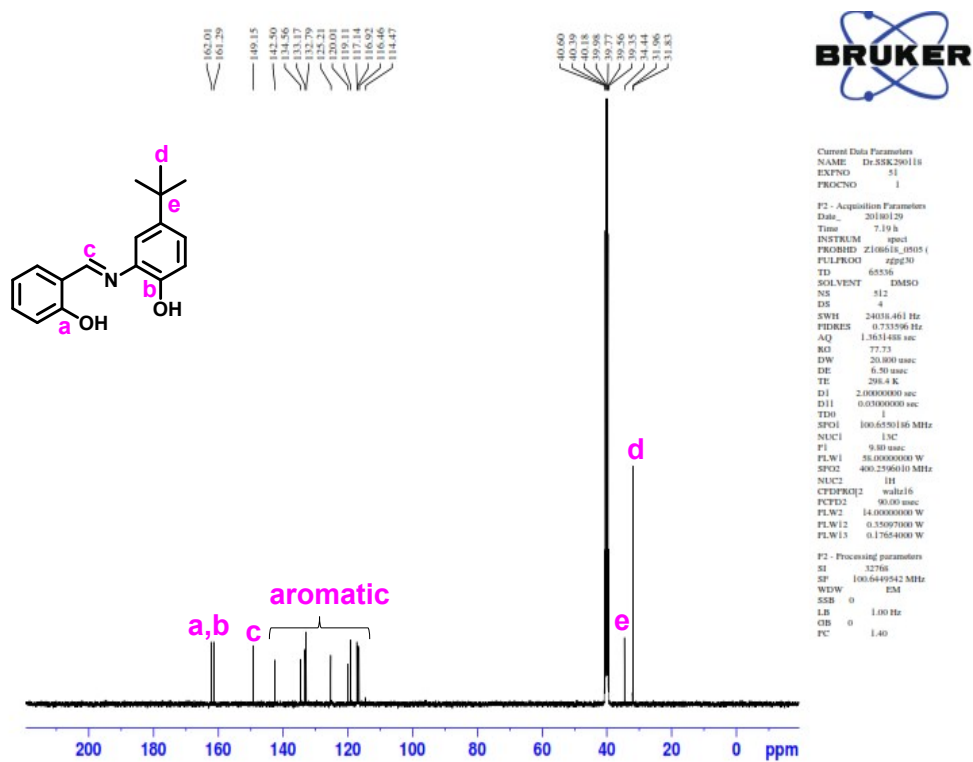


Fig. S2 <sup>13</sup>C NMR spectrum of L1

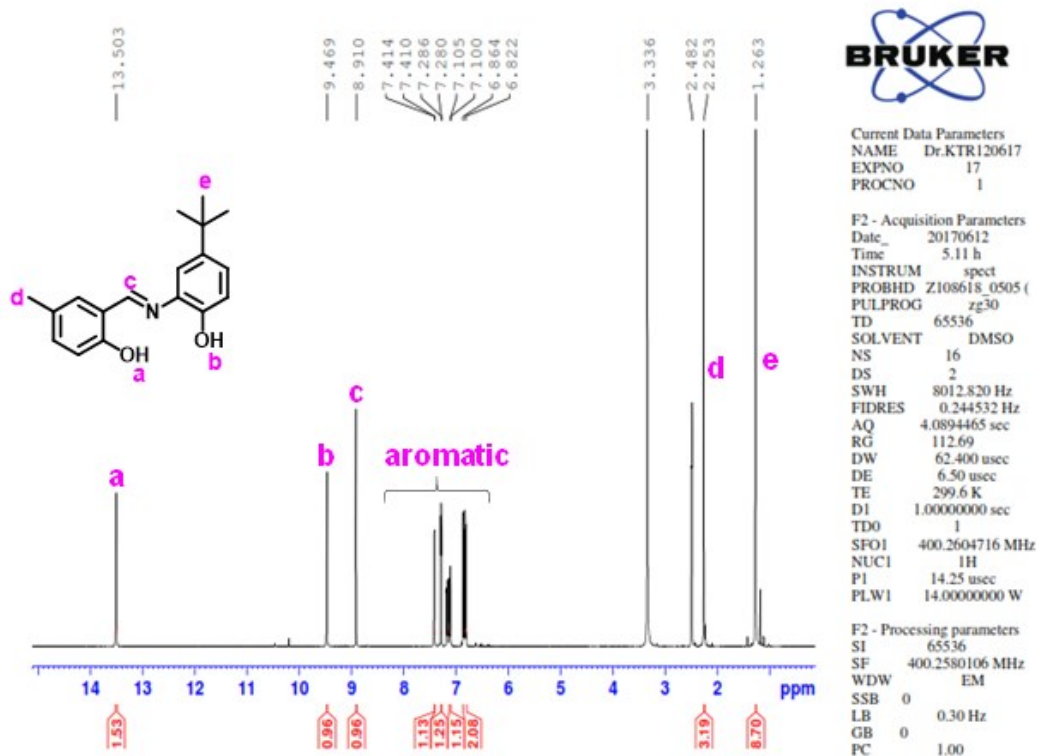


Fig. S3  $^1\text{H}$  NMR spectrum of L2

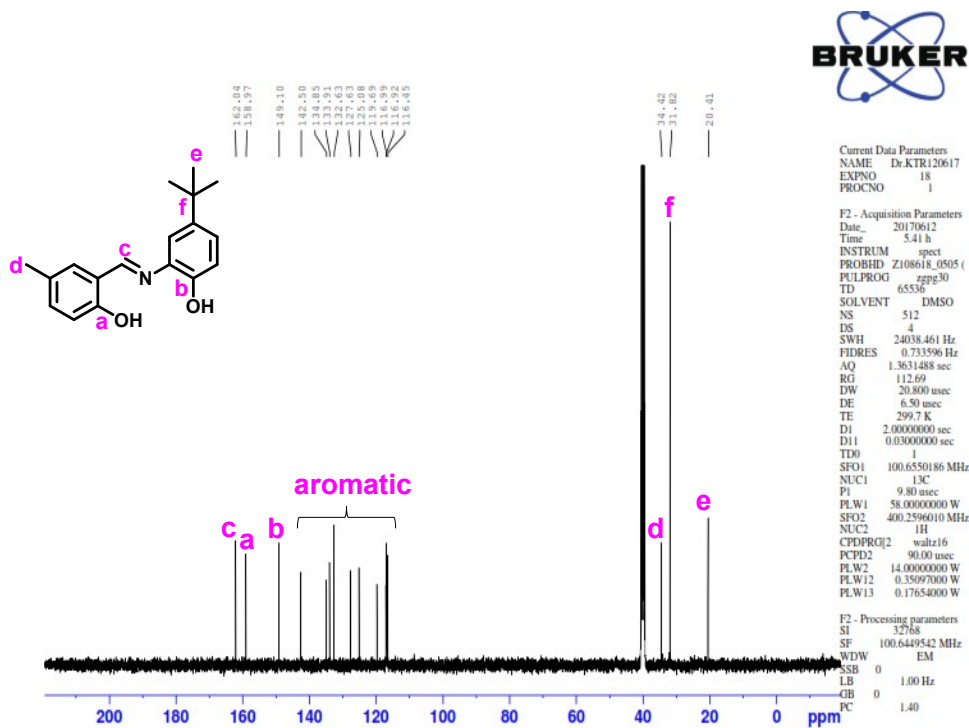


Fig. S4  $^{13}\text{C}$  NMR spectrum of L2

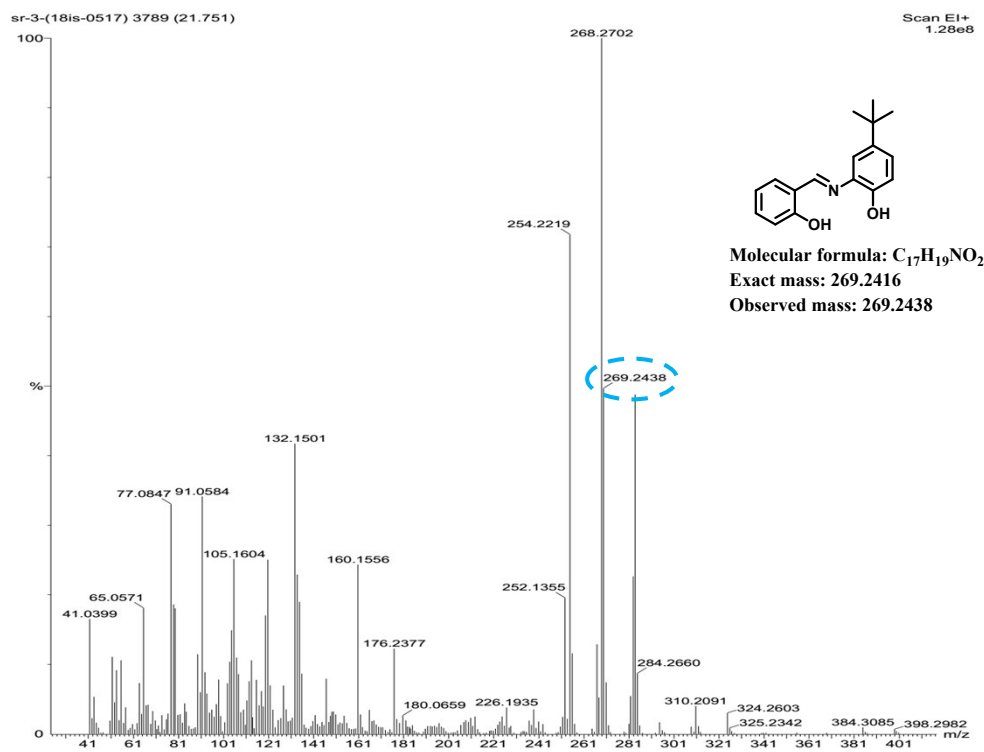


Fig. S5 GC-MS spectrum of L1

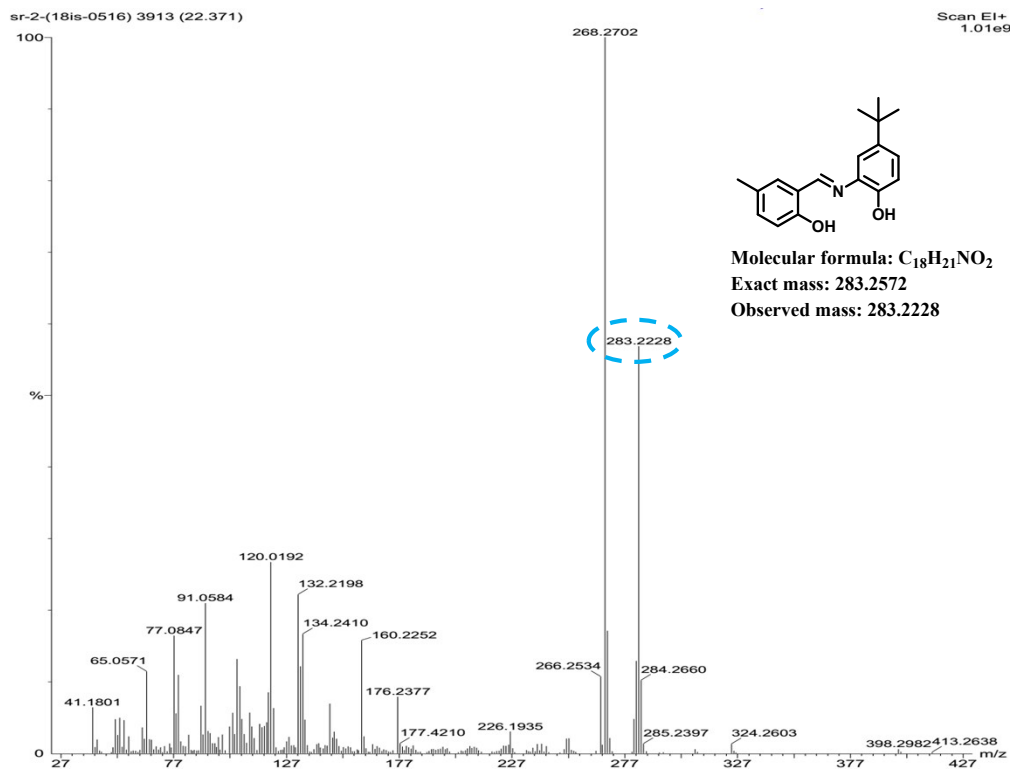


Fig. S6 GC-MS spectrum of L2

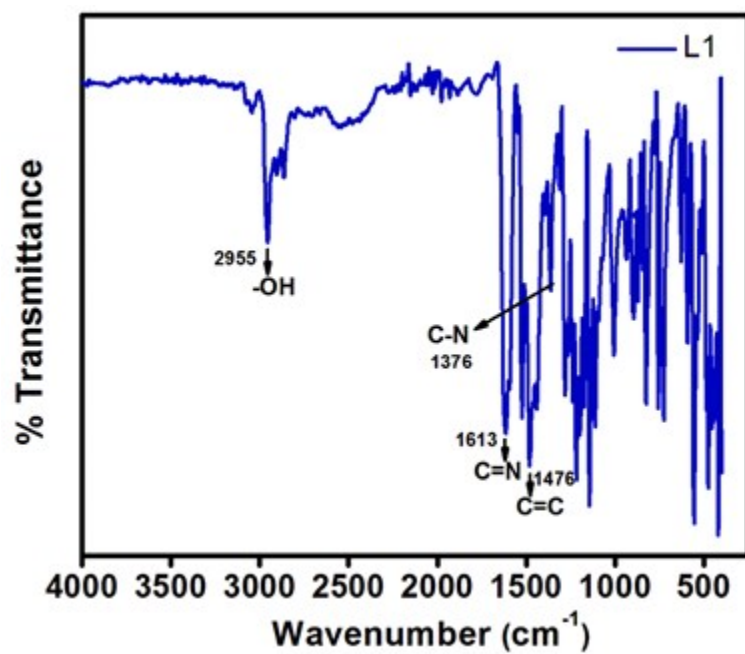


Fig. S7 FT-IR spectrum of L1

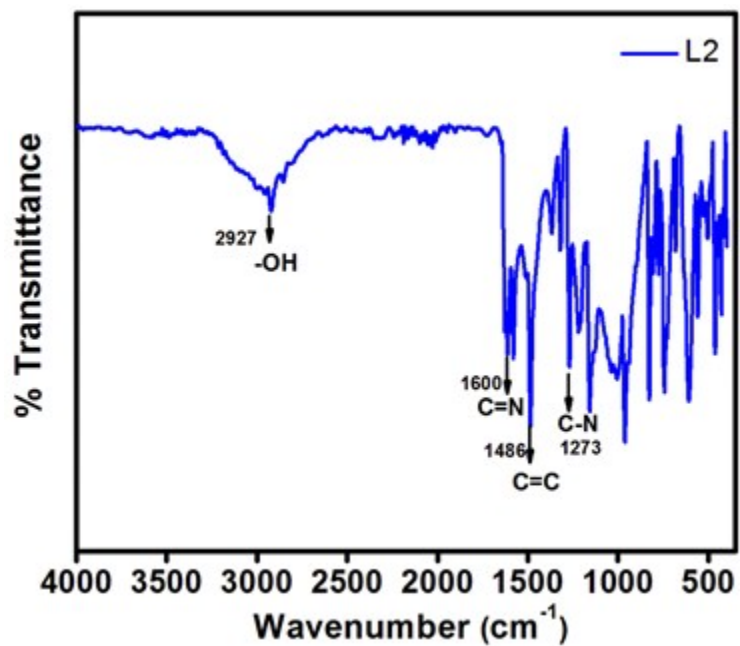
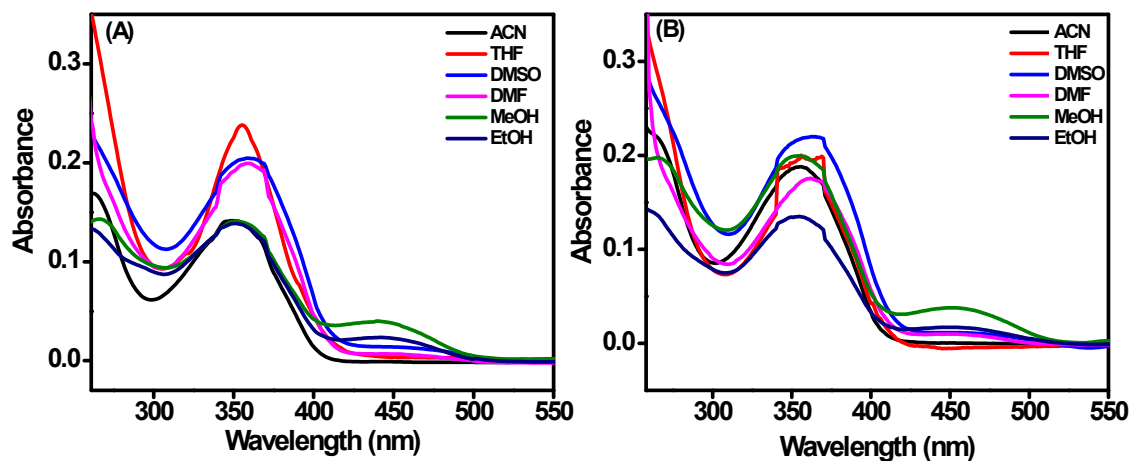
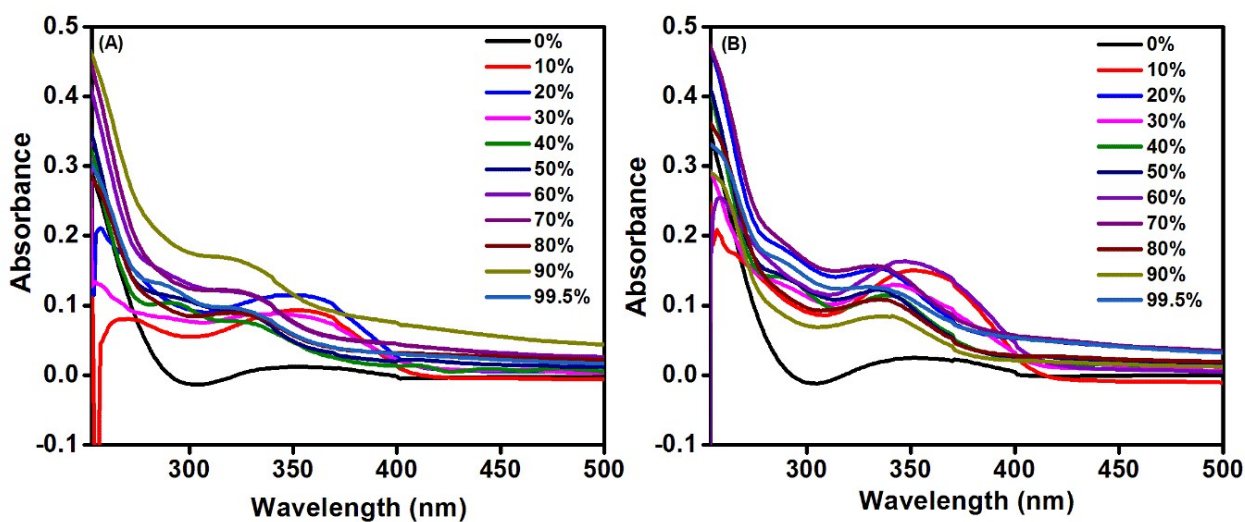


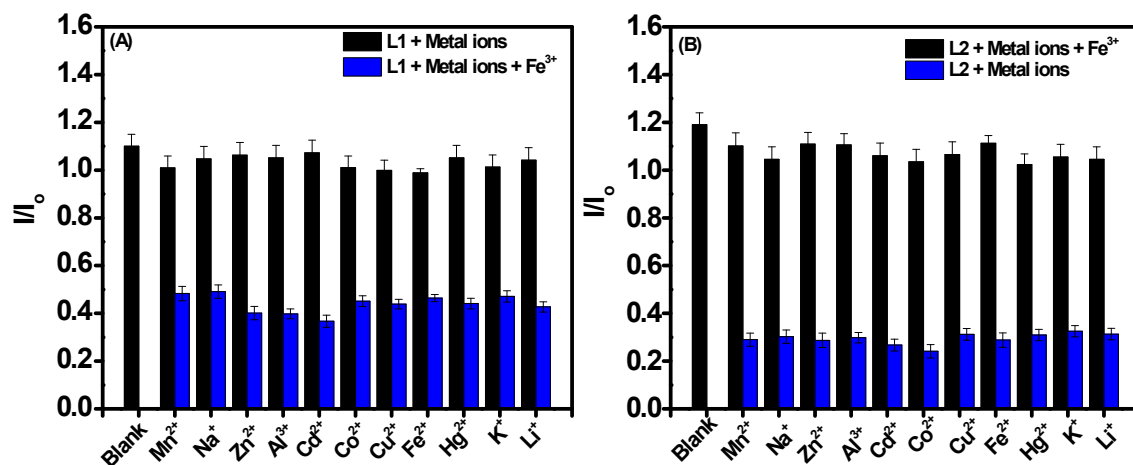
Fig. S8 FT-IR spectrum of L2



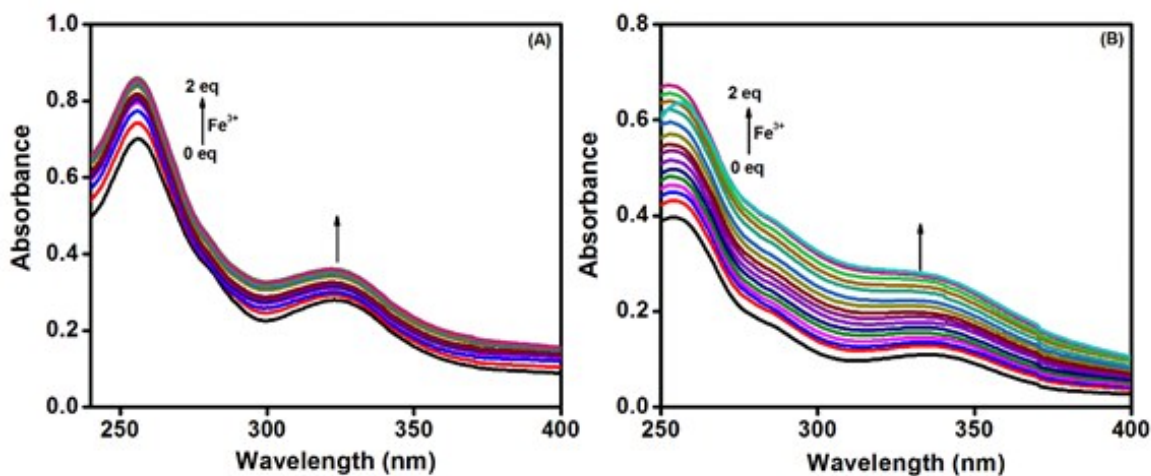
**Fig. S9** UV-visible absorption spectra of (A) L1 and (B) L2 using different solvents at  $1 \times 10^{-5}$  M concentration.



**Fig. S10** UV-visible absorption spectra of (A) L1 and (B) L2 in THF-H<sub>2</sub>O using various water fractions at  $1 \times 10^{-5}$  M concentration.



**Fig. S11** Selectivity graph of (A) L1 and (B) L2 towards the addition of different coexisting metal ions in THF-H<sub>2</sub>O (10:90% (L1) and 40:60% (L2)) mixture at  $1 \times 10^{-5}$  M concentration.



**Fig. S12** UV titration spectra of (A) L1 and (B) L2 at  $1 \times 10^{-5}$  M in THF-H<sub>2</sub>O (10:90% and 40:60% ) upon successive addition of Fe<sup>3+</sup>.

**Table S1.** Molar absorptivity values of L1 and L2 in different solvents at  $1 \times 10^{-5}$  M concentrations.

| Solvent            | L1                                                                                      |                                                                                         | L2                                                                                      |                                                                                         |
|--------------------|-----------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
|                    | $\lambda_{\text{max}}$ , abs(254 nm)<br>$\epsilon(10^4 \text{ M}^{-1} \text{ cm}^{-1})$ | $\lambda_{\text{max}}$ , abs(355 nm)<br>$\epsilon(10^4 \text{ M}^{-1} \text{ cm}^{-1})$ | $\lambda_{\text{max}}$ , abs(256 nm)<br>$\epsilon(10^4 \text{ M}^{-1} \text{ cm}^{-1})$ | $\lambda_{\text{max}}$ , abs(356 nm)<br>$\epsilon(10^4 \text{ M}^{-1} \text{ cm}^{-1})$ |
| THF                | 3.36                                                                                    | 2.39                                                                                    | 2.97                                                                                    | 1.99                                                                                    |
| DMSO               | 2.19                                                                                    | 2.05                                                                                    | 2.63                                                                                    | 2.23                                                                                    |
| DMF                | 2.12                                                                                    | 2                                                                                       | 2.40                                                                                    | 1.77                                                                                    |
| CH <sub>3</sub> CN | 1.68                                                                                    | 1.43                                                                                    | 2.19                                                                                    | 1.90                                                                                    |
| MeOH               | 1.45                                                                                    | 1.4                                                                                     | 1.97                                                                                    | 2.01                                                                                    |
| EtOH               | 1.33                                                                                    | 1.38                                                                                    | 1.39                                                                                    | 1.36                                                                                    |

**Table S2.** Quantum yield ( $\Phi$ ) values of  $1 \times 10^{-5}$  M of L1 and L2 in different THF-water mixtures.

| S. No. | Water fraction<br>( $f_w$ ) | Quantum yield<br>( $\Phi$ ) |       |
|--------|-----------------------------|-----------------------------|-------|
|        |                             | L1                          | L2    |
| 1      | 0%                          | 0.046                       | 0.017 |
| 2      | 10%                         | 0.065                       | 0.049 |
| 3      | 20%                         | 0.073                       | 0.06  |
| 4      | 30%                         | 0.092                       | 0.091 |
| 5      | 40%                         | 0.102                       | 0.122 |
| 6      | 50%                         | 0.116                       | 0.129 |
| 7      | 60%                         | 0.135                       | 0.136 |
| 8      | 70%                         | 0.139                       | 0.1   |
| 9      | 80%                         | 0.151                       | 0.058 |
| 10     | 90%                         | 0.174                       | 0.053 |
| 11     | 99.5%                       | 0.149                       | 0.035 |

**Table S3.** Association constant ( $K_a$ ) values of L1/L2 with  $\text{Fe}^{3+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Cu}^{2+}$  and  $\text{Co}^{2+}$  in THF and THF-water mixture.

| Metal ions       | Association constants ( $K_a$ )<br>( $\text{M}^{-1}$ ) |                    |                           |                    |
|------------------|--------------------------------------------------------|--------------------|---------------------------|--------------------|
|                  | THF                                                    |                    | THF- $\text{H}_2\text{O}$ |                    |
|                  | L1                                                     | L2                 | L1                        | L2                 |
| $\text{Fe}^{3+}$ | $3.12 \times 10^5$                                     | $9.21 \times 10^5$ | $1.31 \times 10^5$        | $2.93 \times 10^5$ |
| $\text{Fe}^{2+}$ | $1.36 \times 10^5$                                     | $1.01 \times 10^5$ | $1.43 \times 10^6$        | $1.21 \times 10^6$ |
| $\text{Cu}^{2+}$ | $3.42 \times 10^5$                                     | $8.81 \times 10^5$ | $1.12 \times 10^6$        | $1.01 \times 10^6$ |
| $\text{Co}^{2+}$ | $3.31 \times 10^5$                                     | $3.71 \times 10^5$ | $1.20 \times 10^6$        | $1.0 \times 10^6$  |