

Electronic Supplementary Information

Hg²⁺ recognition by triptycene-derived heterocalixarenes: selectivity tuned by bridging heteroatoms and macrocyclic cavity

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1. Copies of ^1H NMR and ^{13}C NMR spectra of **3**, **2a** and **2b**.

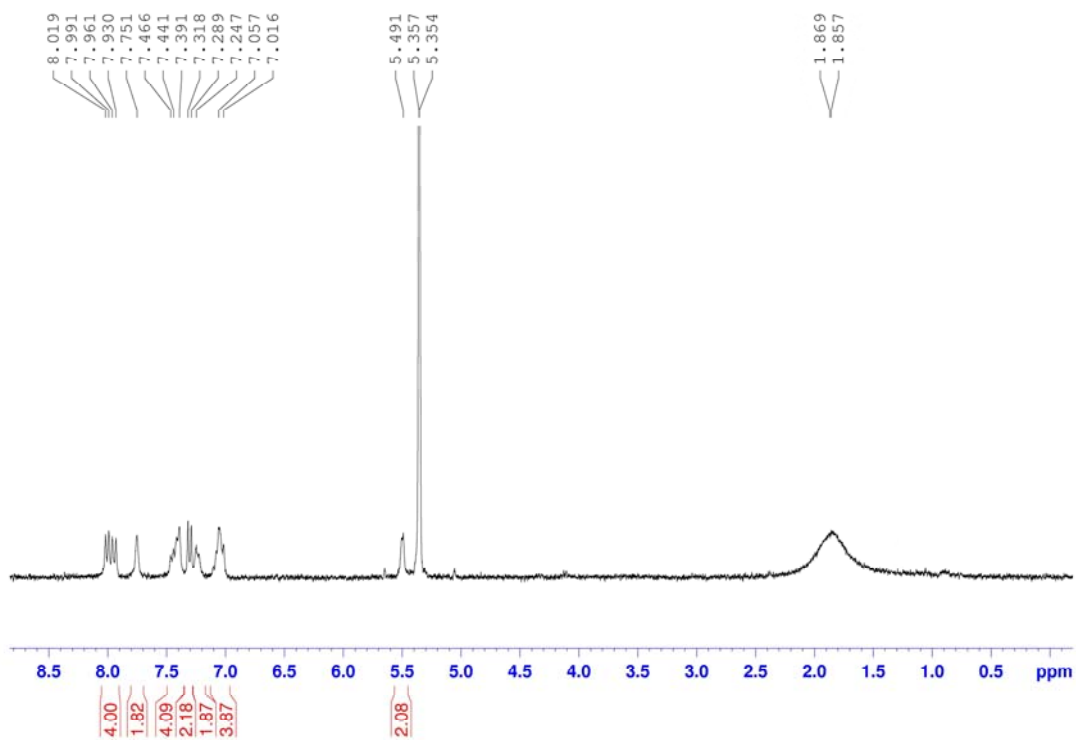


Fig. S1. ^1H NMR spectrum (CD₂Cl₂, 300 MHz, 298 K) of trimer **3**.

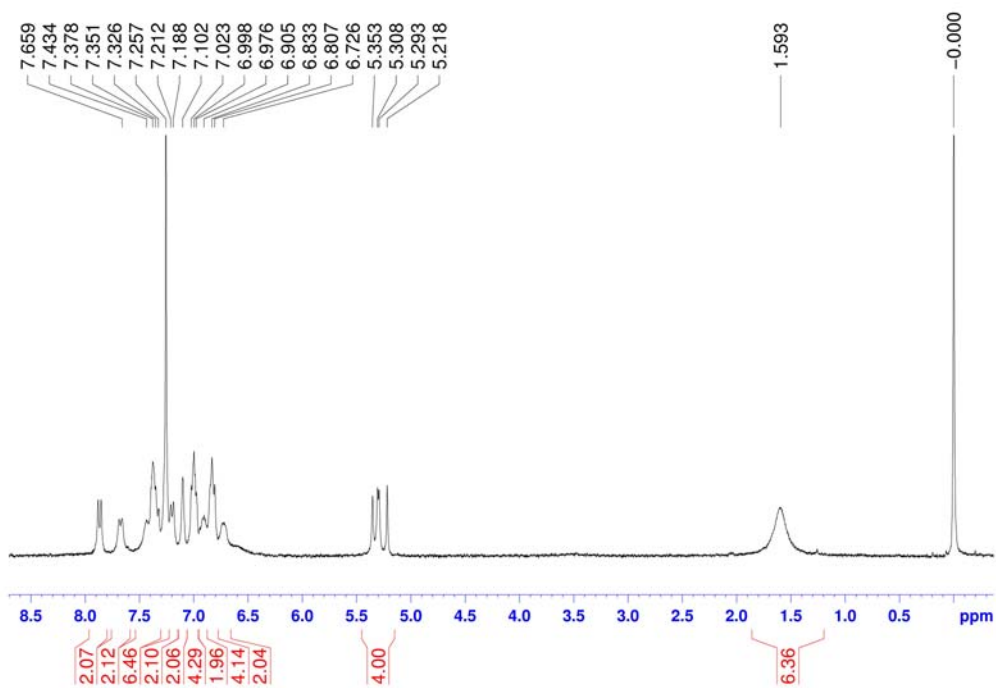


Fig. S2. ^1H NMR spectrum (CDCl₃, 300 MHz, 298 K) of **2a**.

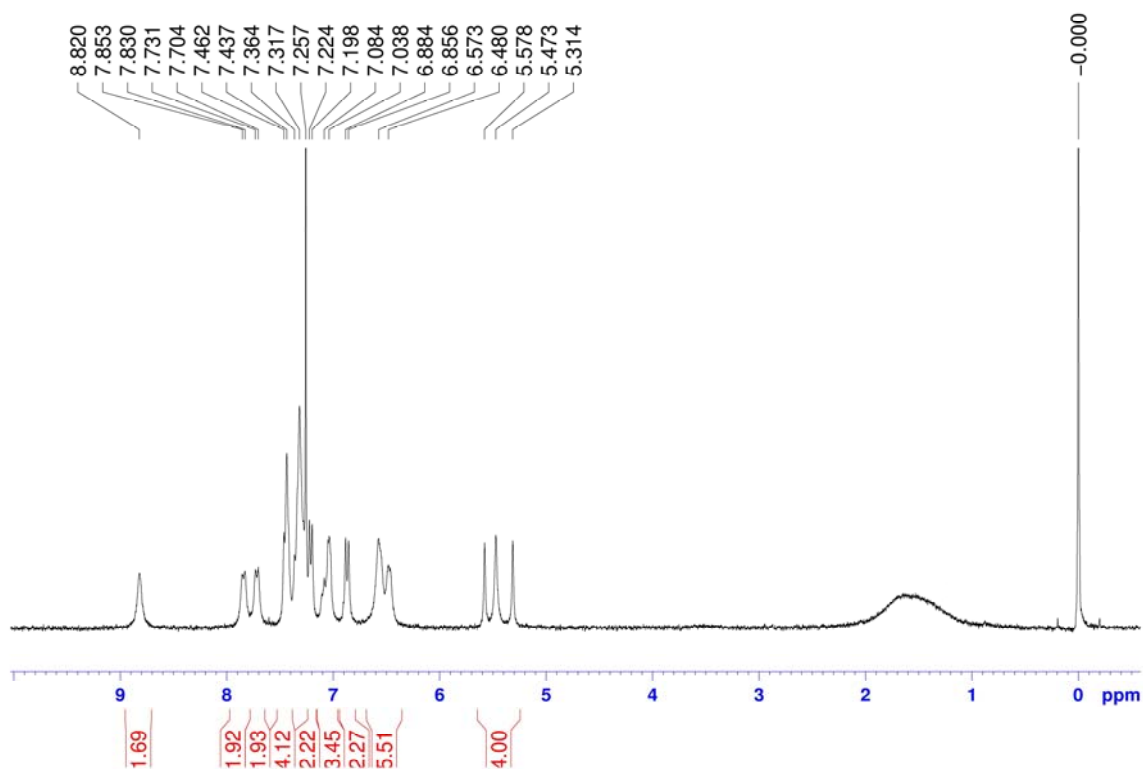


Fig. S3. ^1H NMR spectrum (CDCl_3 , 300 MHz, 298 K) of **2b**.

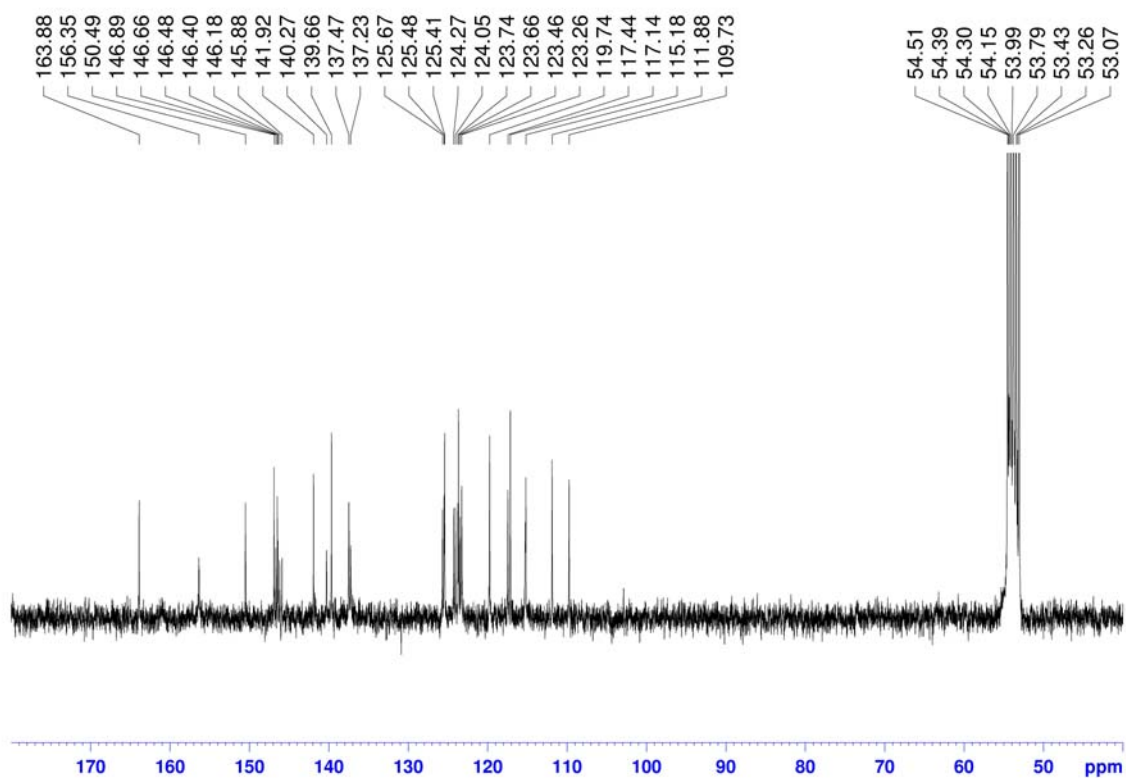


Fig. S4. ^{13}C NMR spectrum (CD_2Cl_2 , 75 MHz, 298 K) of **2b**.

2. ^1H NMR titrations of **1a** with $\text{Zn}(\text{ClO}_4)_2$

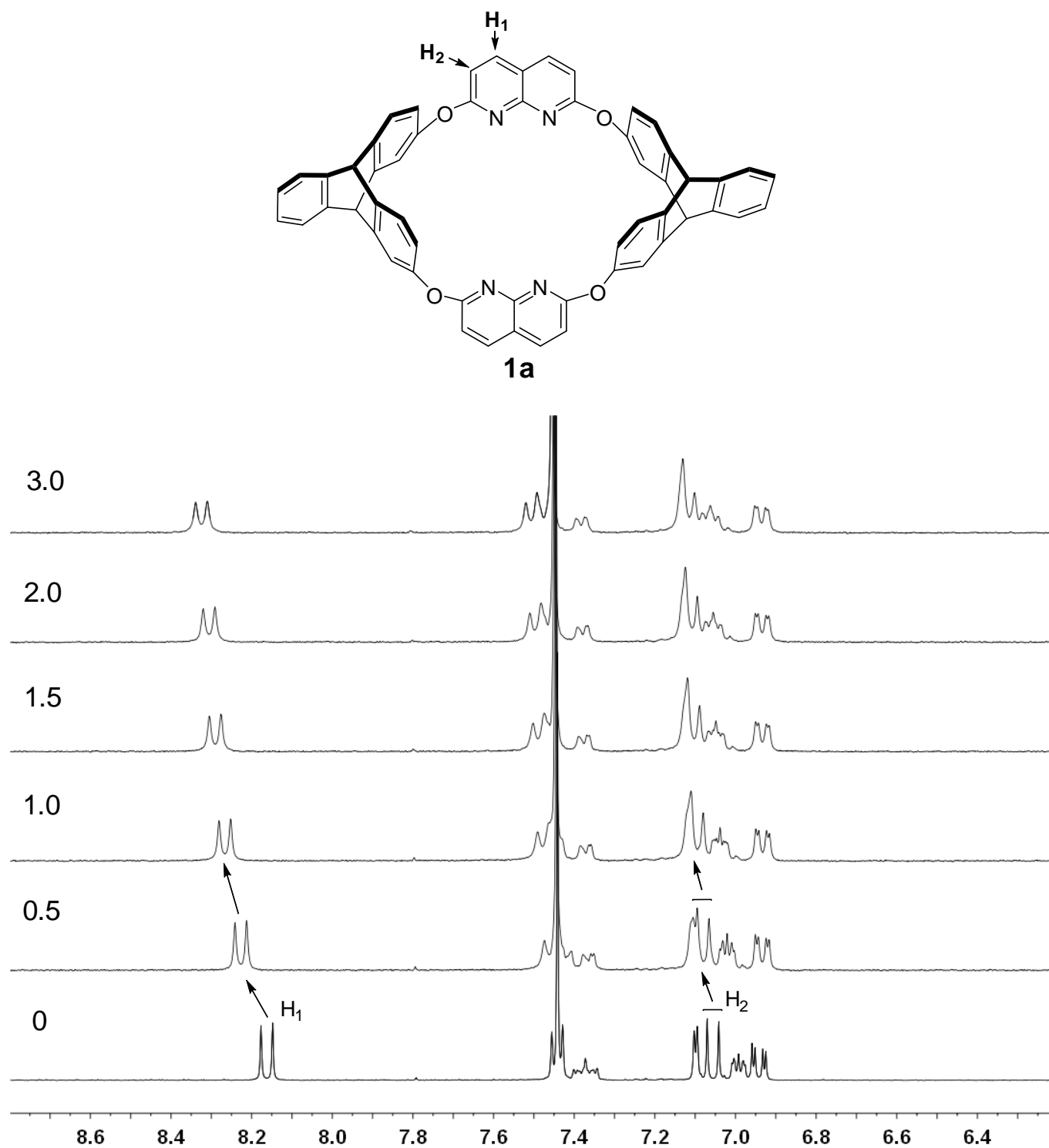


Fig. S5 ^1H NMR titrations of **1a** (2 mM in $\text{CDCl}_3/\text{CH}_3\text{CN}$, 2:1, v:v) with Zn^{2+} (0-3 equiv.) at 298 K.

3. ^1H NMR titrations of **2a** with $\text{Zn}(\text{ClO}_4)_2$

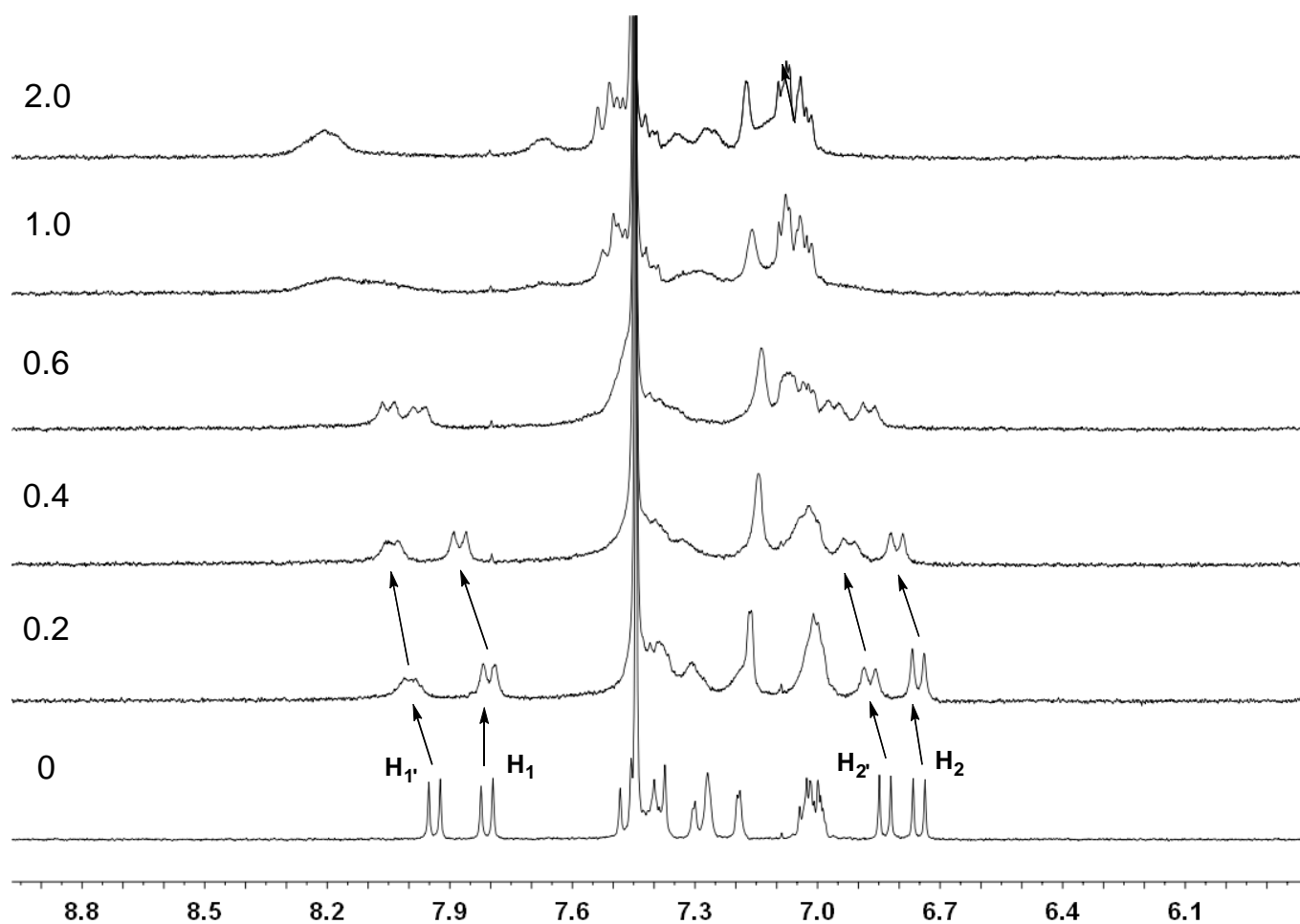
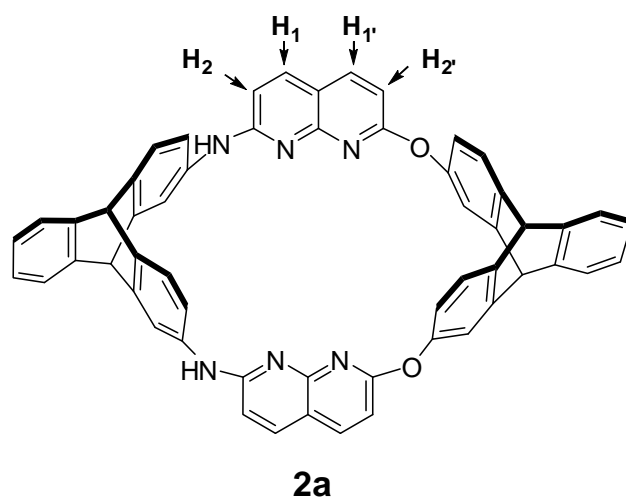


Fig. S6 ^1H NMR titrations of **2a** (2 mM in $\text{CDCl}_3/\text{CH}_3\text{CN}$, 2:1, v:v) with Zn^{2+} (0-3 equiv.) at 298 K.

4. UV-vis spectra of **1b**, **2a** and **2b** in the presence of metal ions

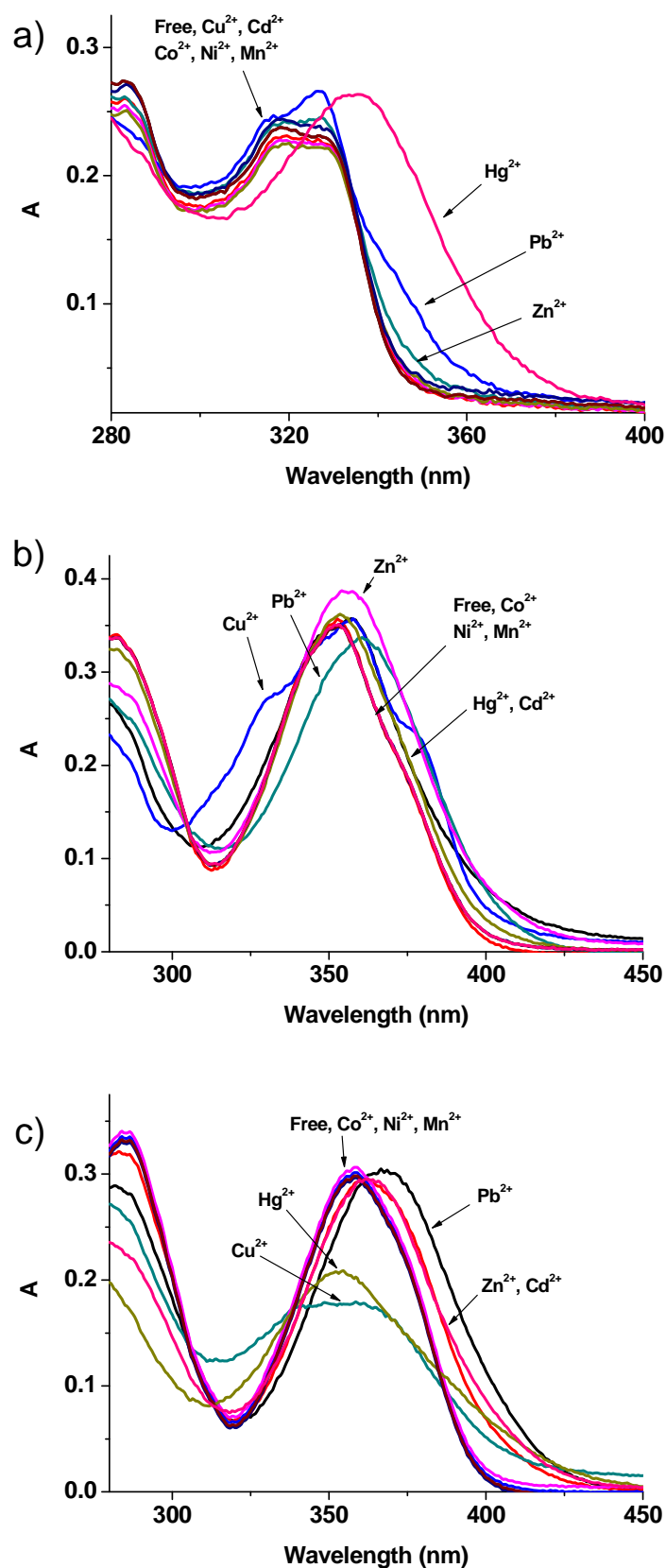


Fig. S7 Absorption spectra of a) **1b**, b) **2a**, c) **2b** (all were $10 \mu\text{M}$ in CH_3CN) in the absence and presence of 5 equiv. of metal ions.

5. Fluorescence spectra of Dmnapy in the presence of metal ions

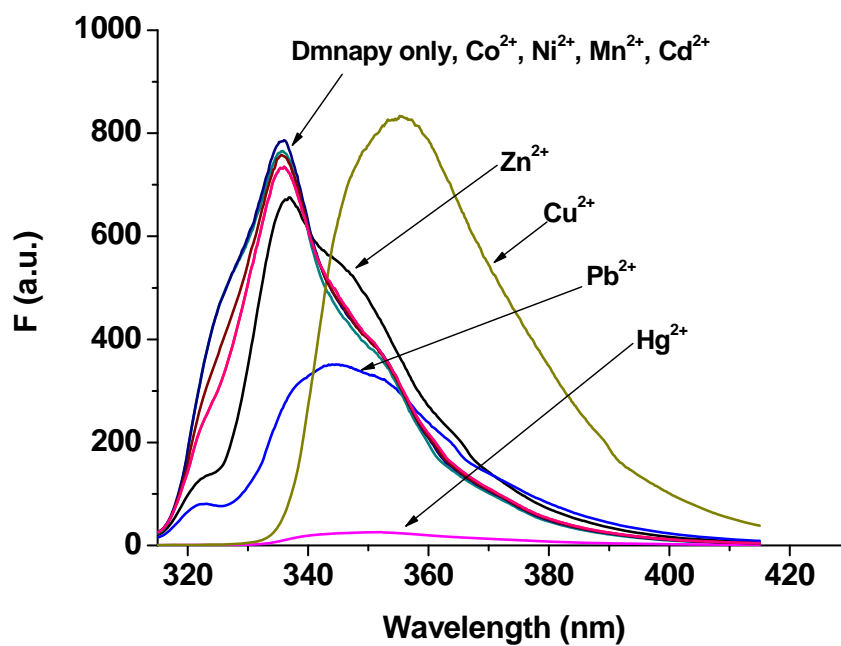


Fig. S8 Fluorescence spectra of Dmnapy (10 μ M in CH₃CN) in the absence and presence of 50 equiv. of metal ions.