

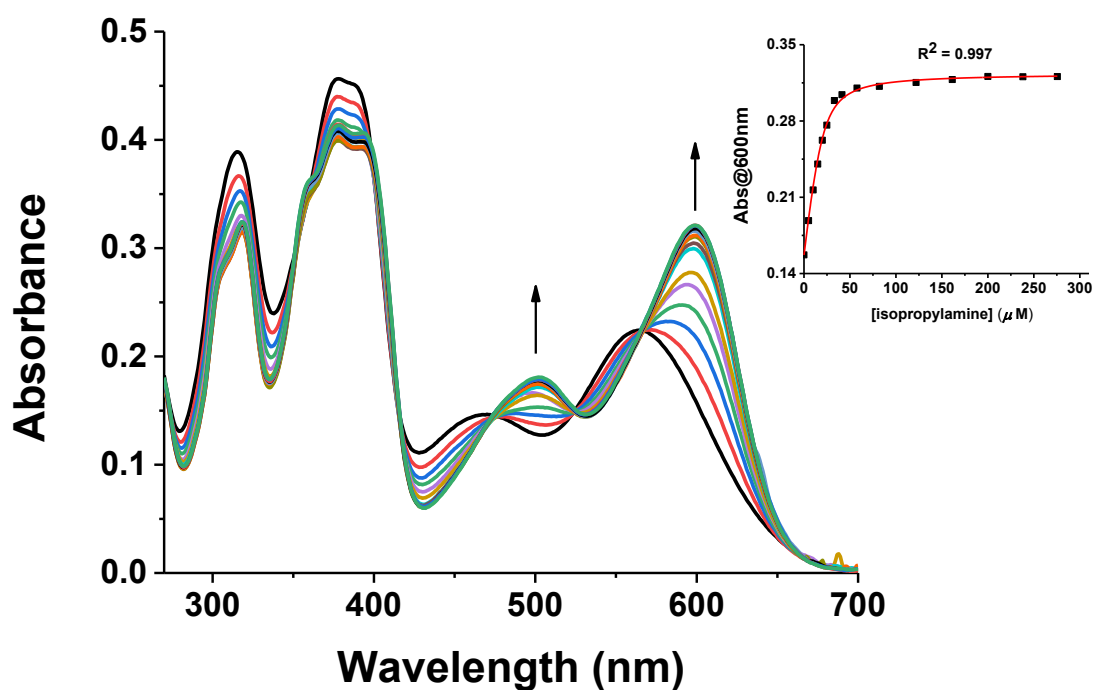
# Electronic Supplementary Information

## Deaggregation properties and transmetalation studies of a zinc(II) salen-type Schiff-base complex

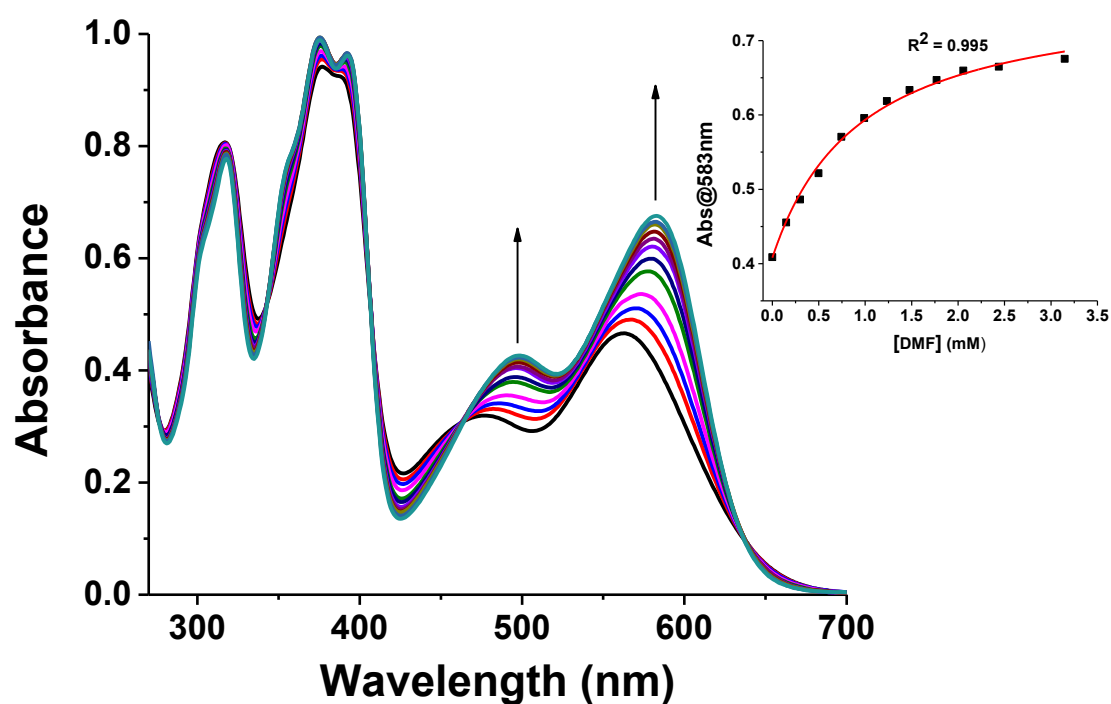
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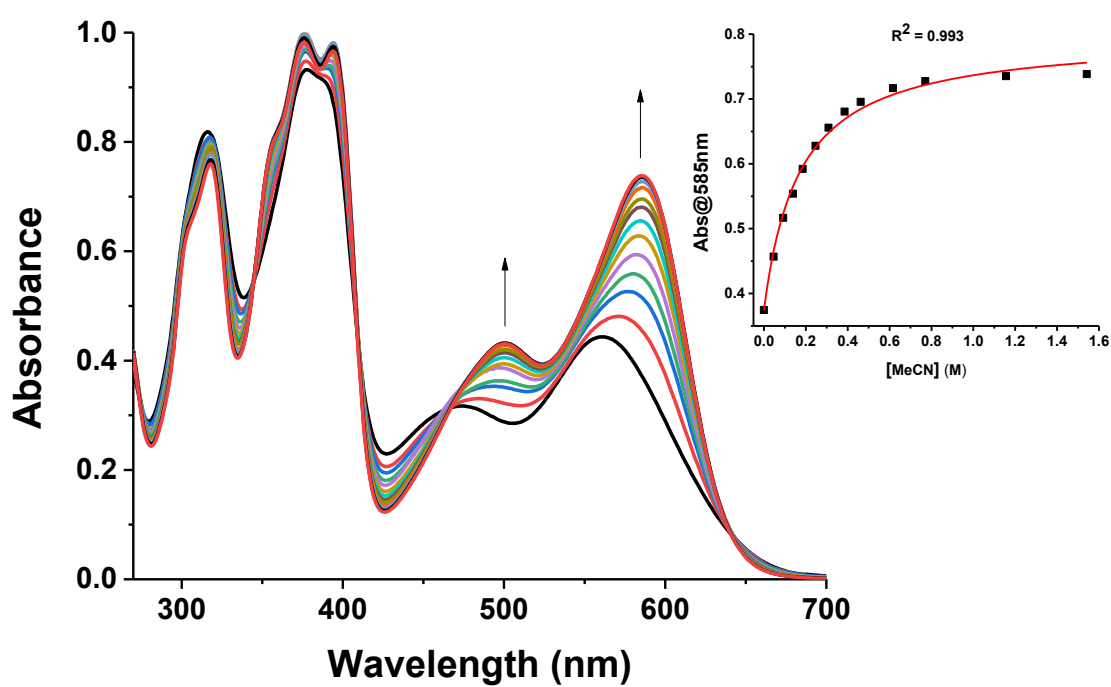
*E-mail: [sdibella@unict.it](mailto:sdibella@unict.it)*



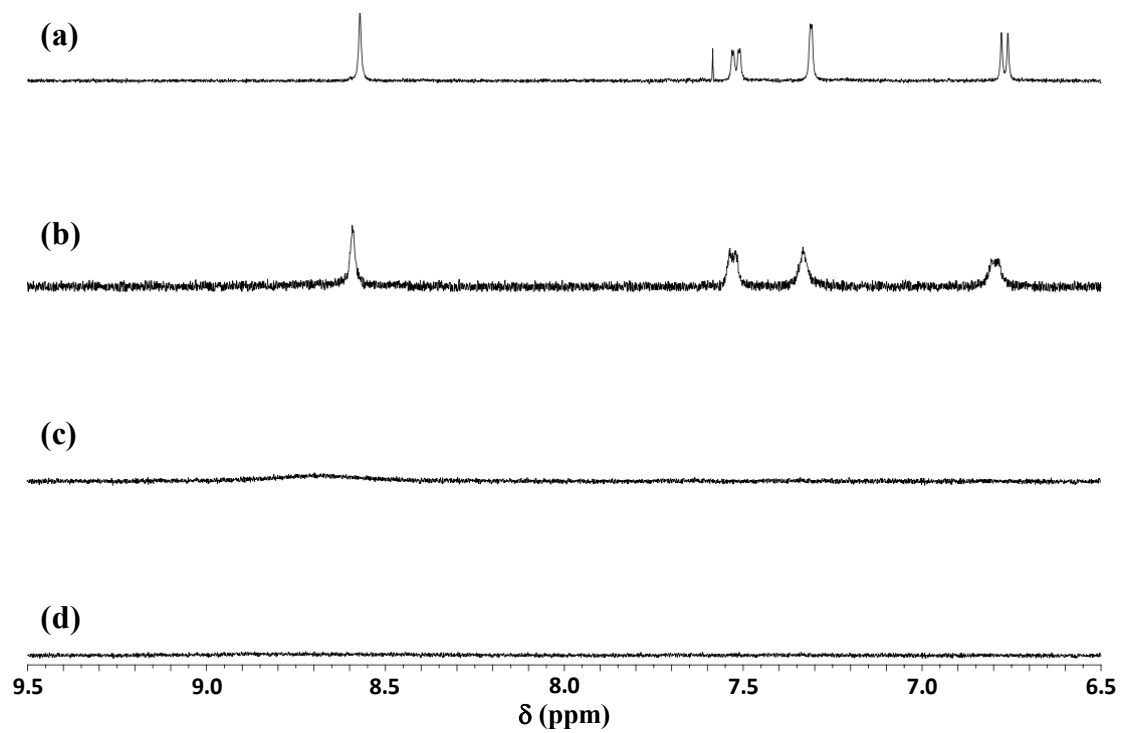
**Fig. S1** Optical absorption titration spectra of **1** (20.0 μM solution in CHCl<sub>3</sub>) upon progressive addition of isopropylamine. The concentration of isopropylamine added varied from 0 to 280 μM. Inset: variation of the absorbance at 600 nm as a function of the concentration of isopropylamine added and fit of the binding isotherm (red line). A log K value of 5.40 is achieved.



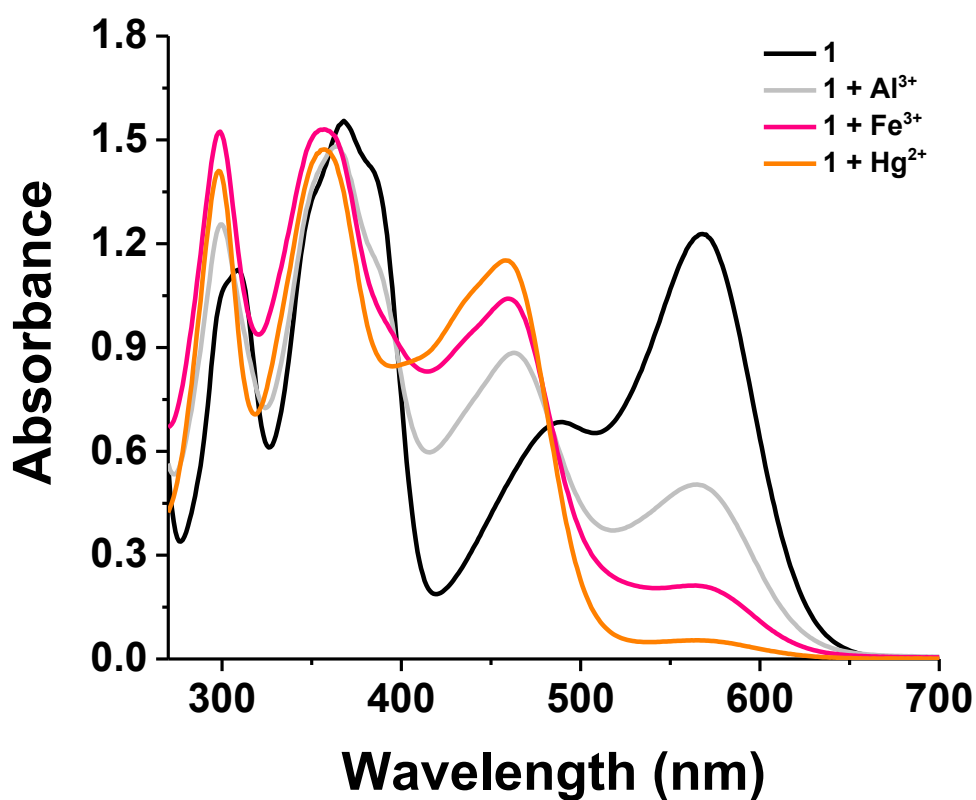
**Fig. S2** Optical absorption titration spectra of **1** (40.0 μM solution in CHCl<sub>3</sub>) upon progressive addition of DMF. The concentration of DMF added varied from 0 to 3.20 mM. Inset: variation of the absorbance at 583 nm as a function of the concentration of DMF added and fit of the binding isotherm (red line).



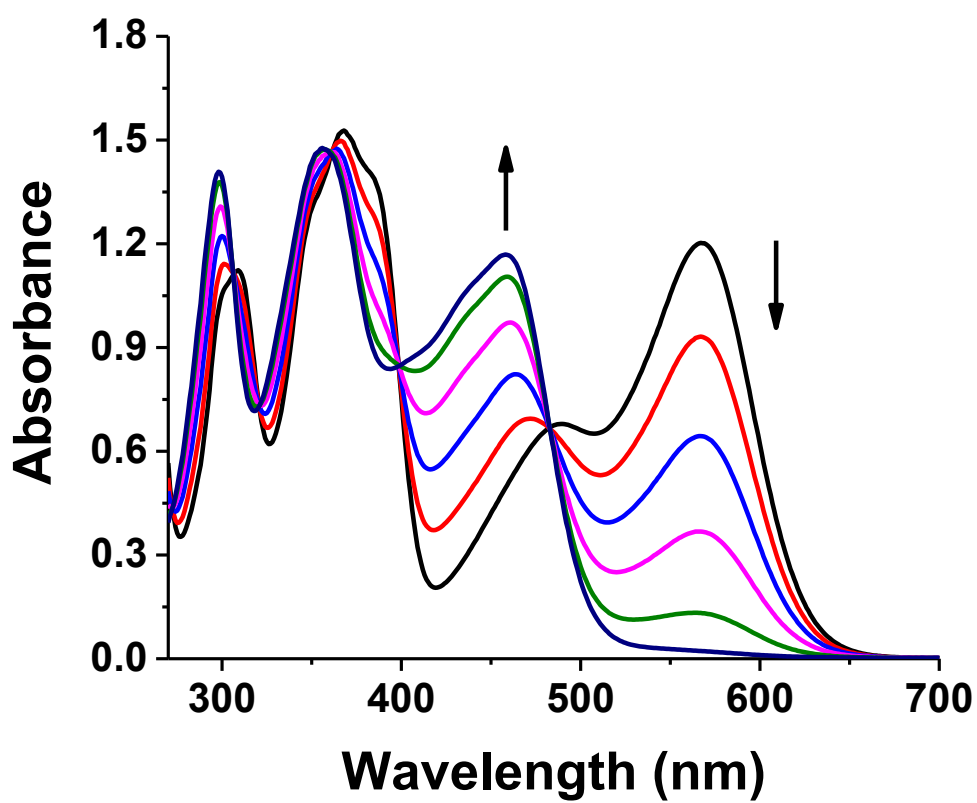
**Fig. S3** Optical absorption titration spectra of **1** (40.0 μM solution in CHCl<sub>3</sub>) upon progressive addition of MeCN. The concentration of MeCN added varied from 0 to 1.50 M. Inset: variation of the absorbance at 585 nm as a function of the concentration of MeCN added and fit of the binding isotherm (red line).



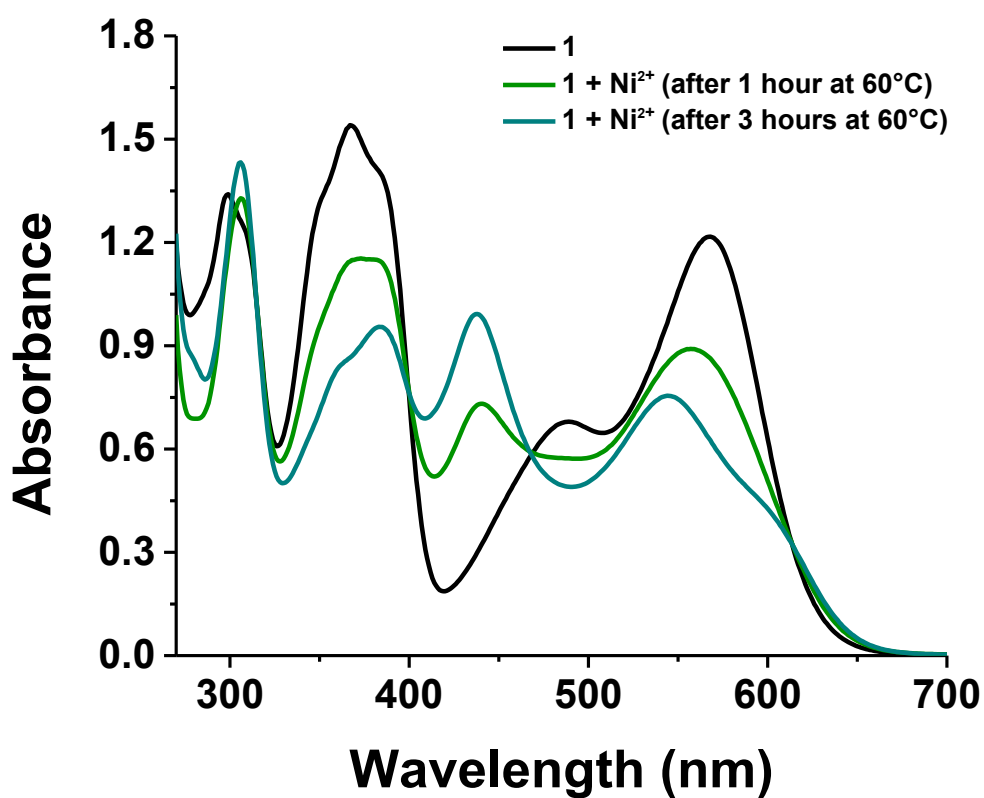
**Fig. S4** (a) <sup>1</sup>H NMR spectra of **1** ( $1.0 \times 10^{-4}$  M) in CD<sub>3</sub>CN, and upon the addition of half molar (b), an equimolar (c), and 2-fold molar excess (d) amount of a D<sub>2</sub>O solution of Cu(NO<sub>3</sub>)<sub>2</sub>.



**Fig. S5** Optical absorption spectra of **1** (40.0  $\mu\text{M}$  solution in MeCN) before and after the addition of 2-fold molar excess of  $\text{Al}^{3+}$ ,  $\text{Fe}^{3+}$ , and  $\text{Hg}^{2+}$  cations (as aqueous solutions of nitrate salts).

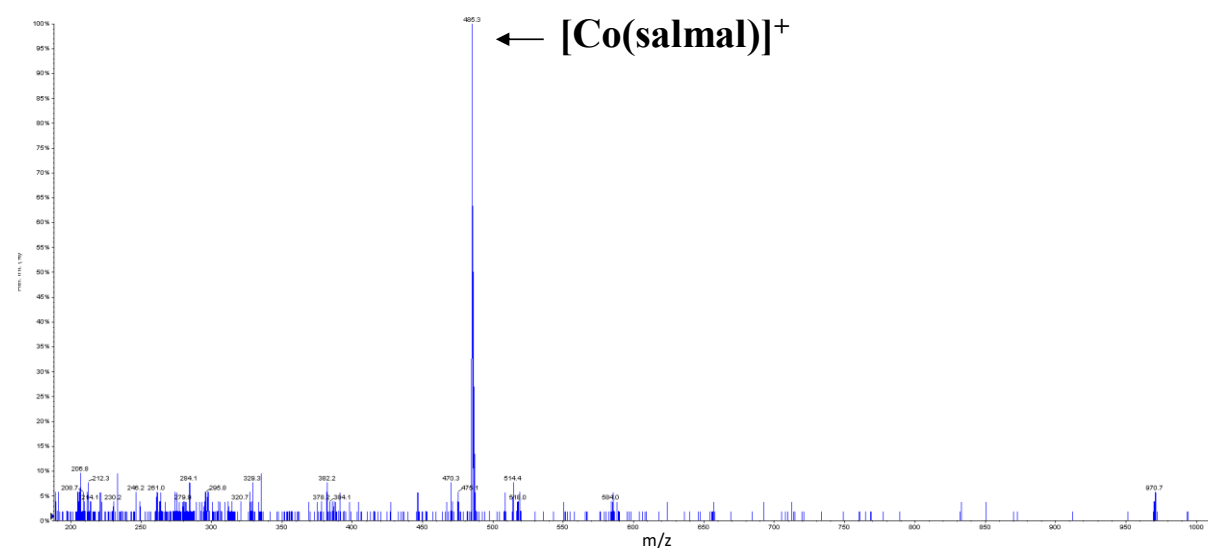
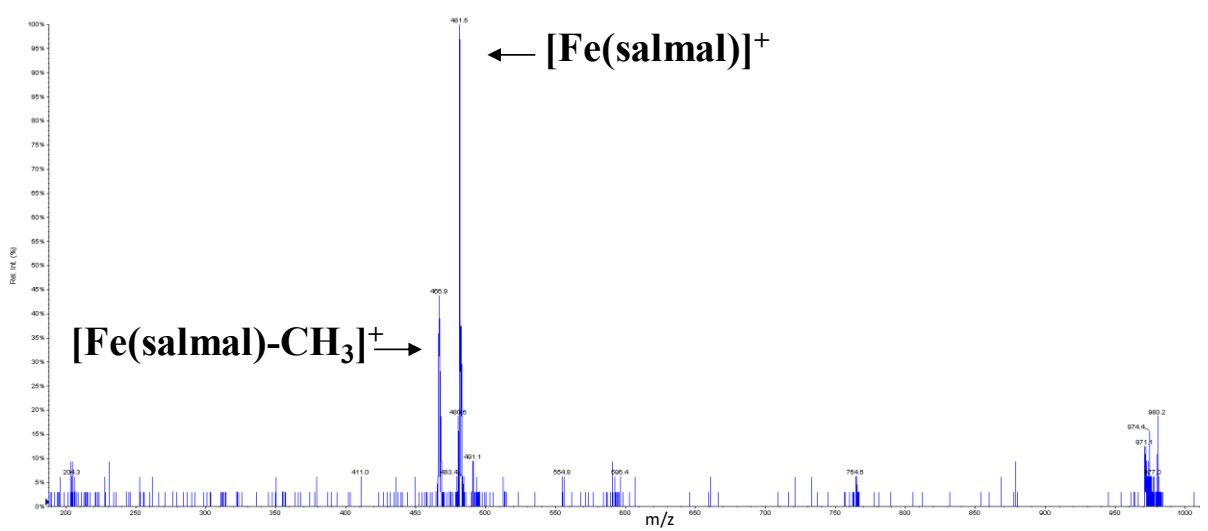
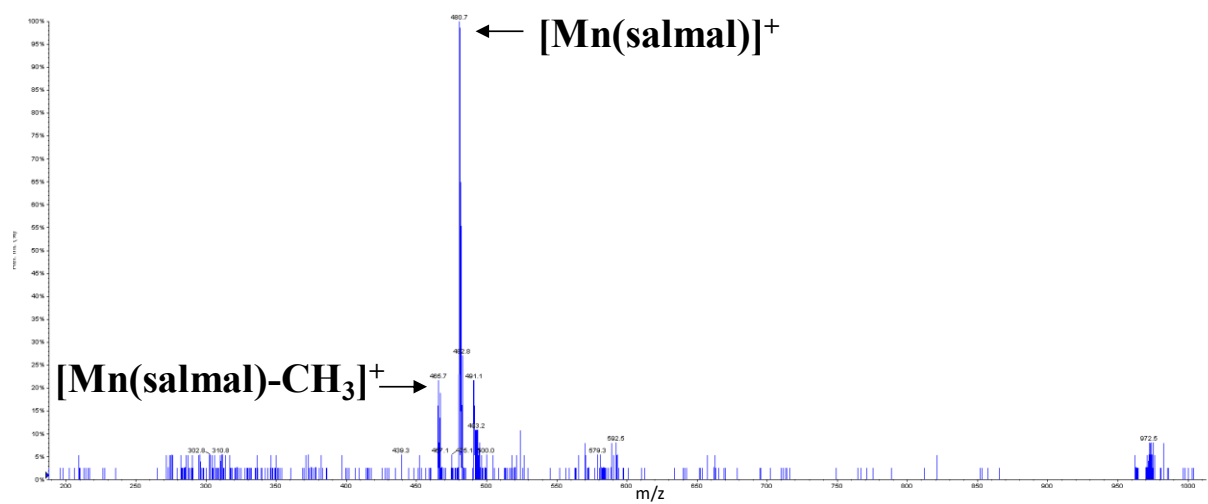


**Fig. S6** Optical absorption titration spectra of **1** (40.0  $\mu\text{M}$  solution in MeCN) upon progressive addition of an aqueous solution of  $\text{HClO}_4$ . The concentration of  $\text{HClO}_4$  added varied from 0 to 100  $\mu\text{M}$ .

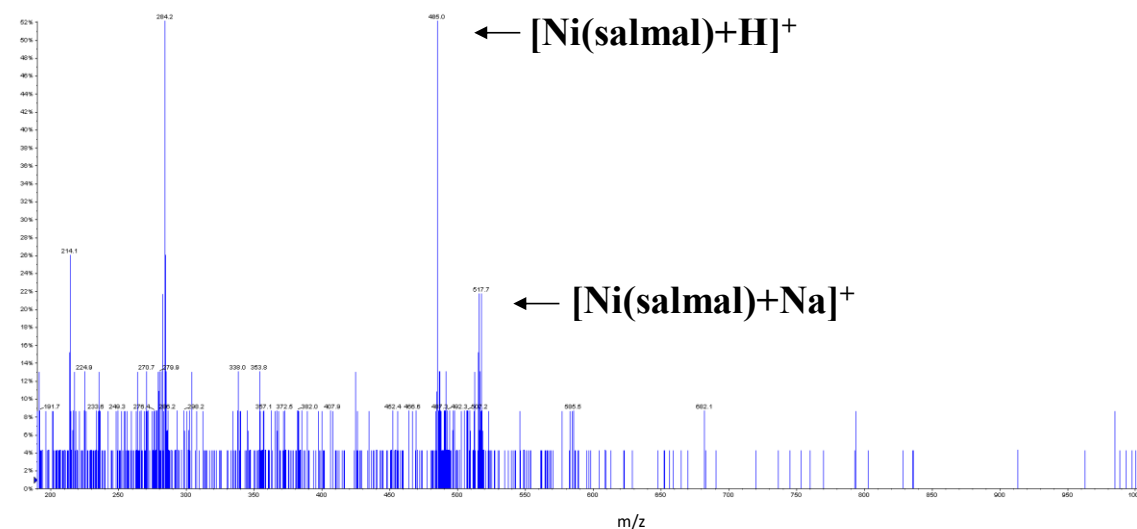
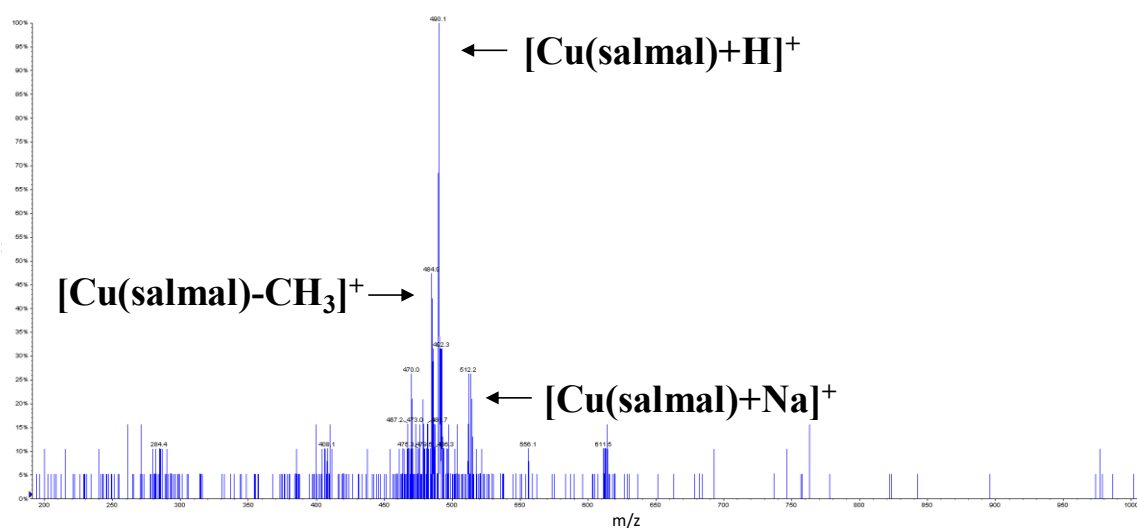
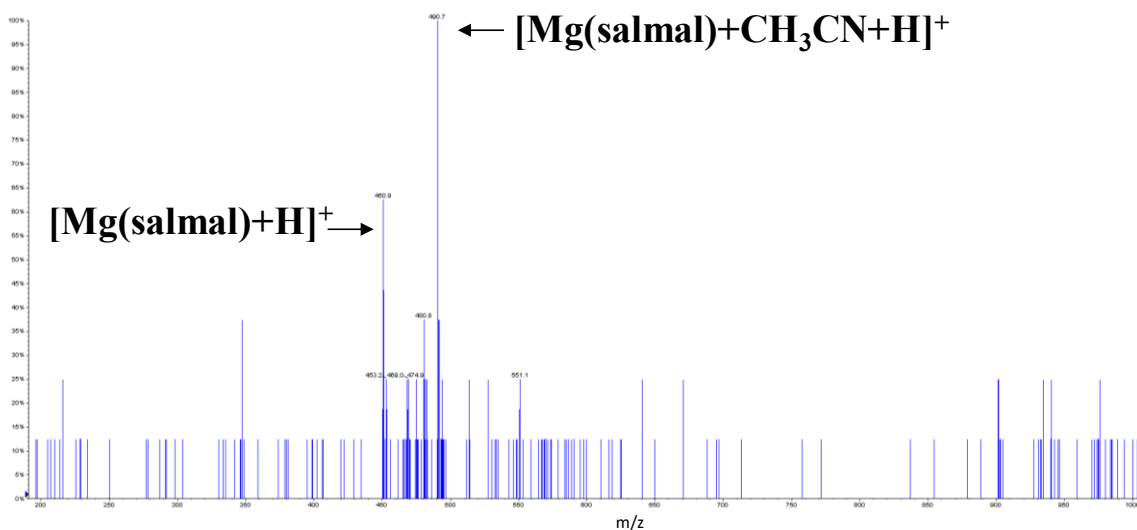


**Fig. S7** Optical absorption spectra of **1** (40.0  $\mu\text{M}$  solution in MeCN), before and after the addition of 2-fold molar excess of an aqueous solution of  $\text{Ni}^{2+}$  ions (as nitrate salt), heated at 60 °C, under stirring, recorded after 1 and 3 hours.

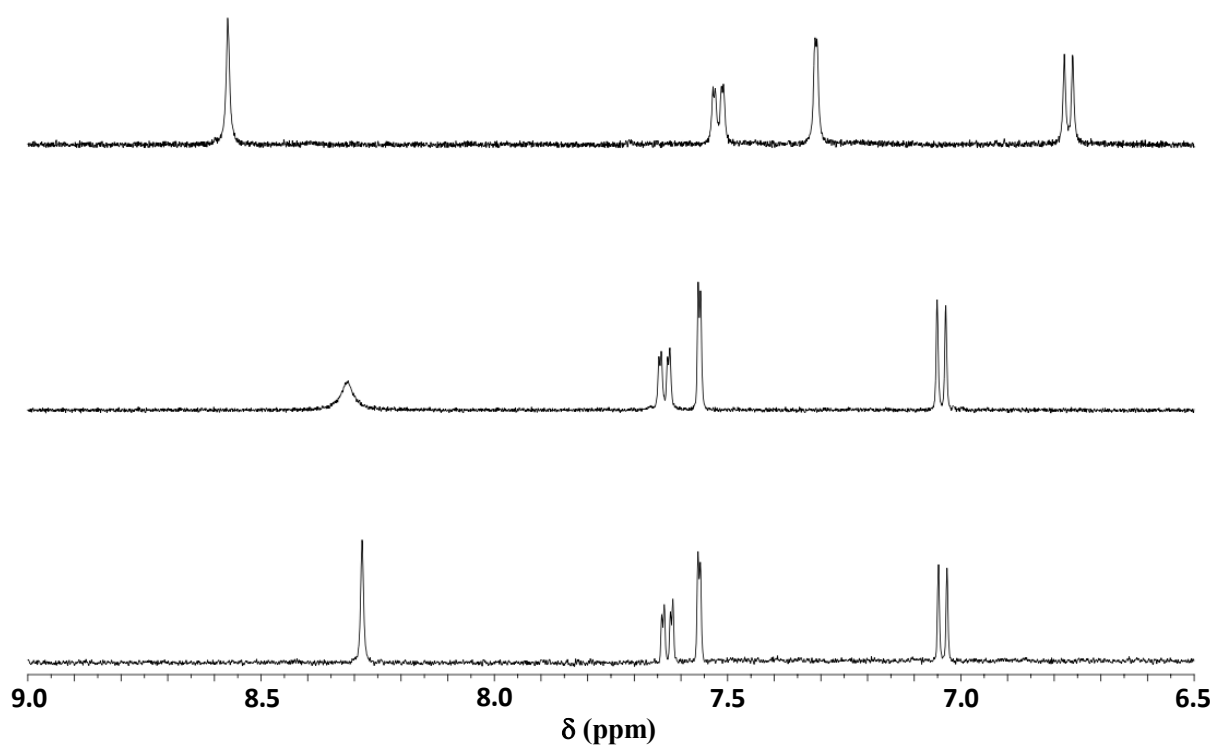




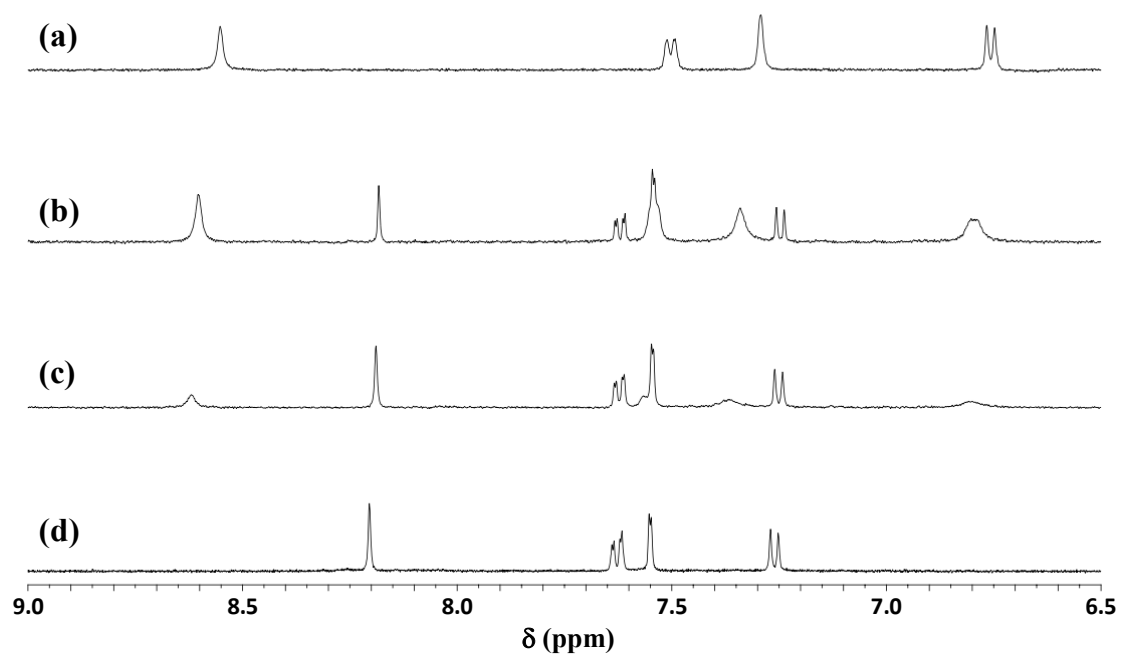
**Fig. S8** ESI-MS spectra of MeCN solutions of **1** recorded immediately after the addition of 2-fold molar excess of  $\text{MnCl}_2$  (top),  $\text{FeCl}_2$  (middle), and  $\text{CoCl}_2$ , recorded after 30 min (bottom)



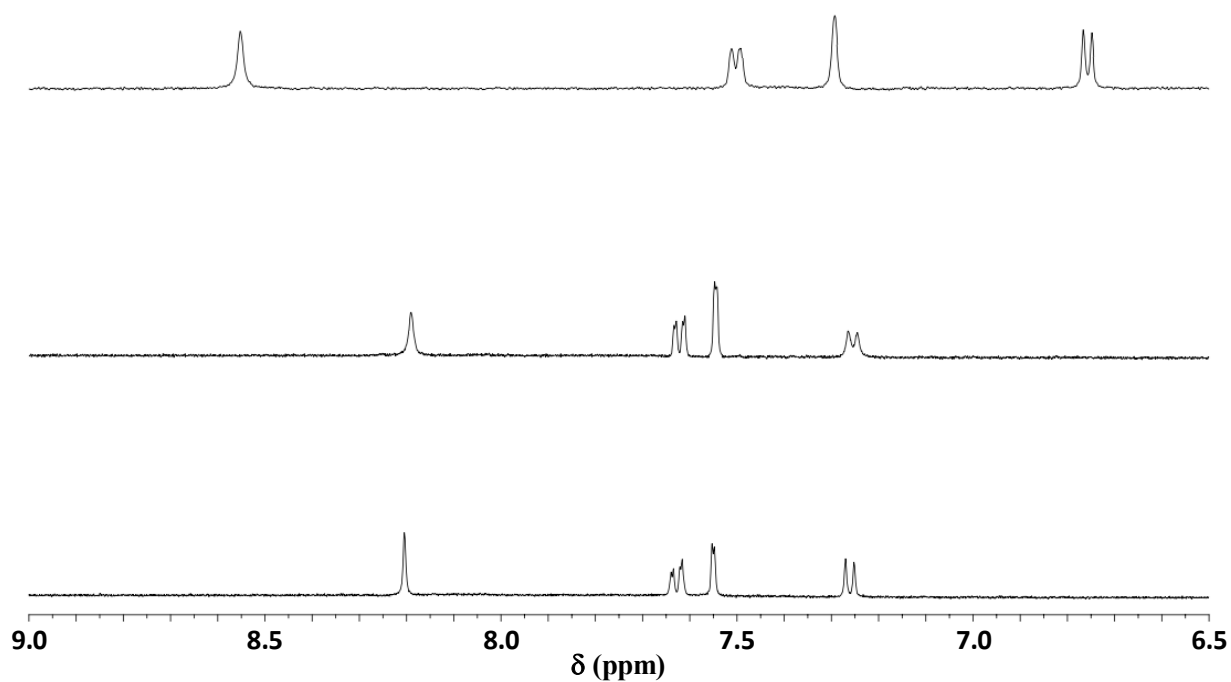
**Fig. S9** ESI-MS spectra of MeCN solutions of **1** recorded immediately after the addition of 2-fold molar excess of  $\text{MgCl}_2$  (top),  $\text{CuCl}_2$  (middle), and  $\text{NiCl}_2$ , recorded after 30 min (bottom)



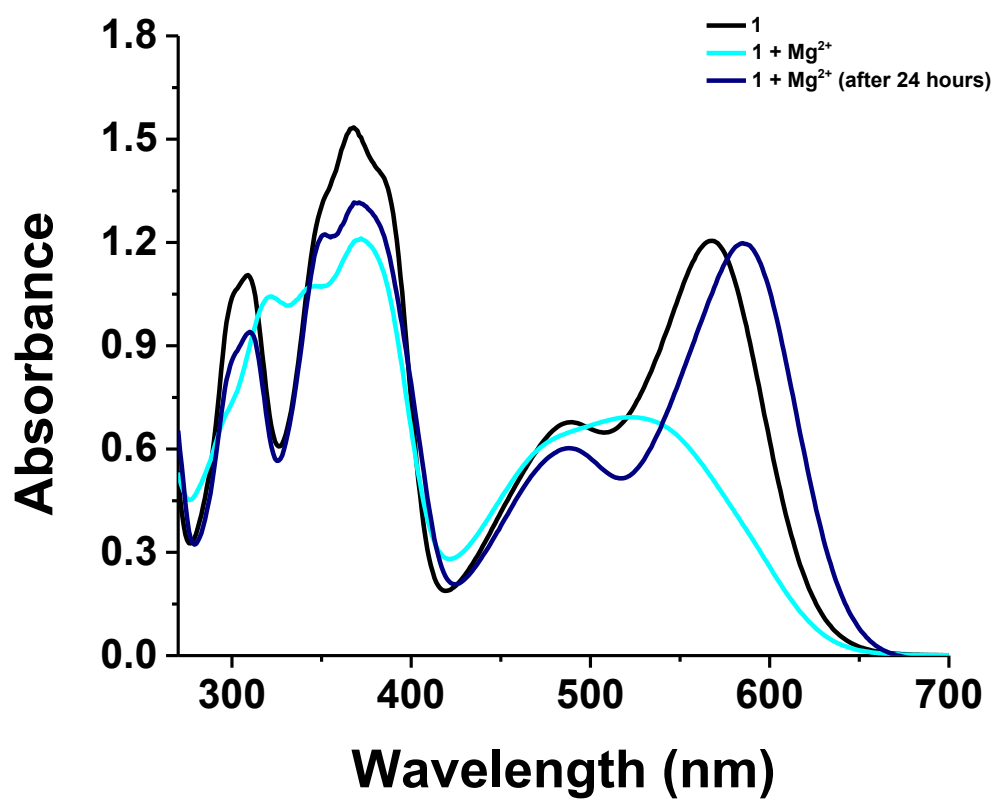
**Fig. S10**  $^1\text{H}$  NMR spectra of **1** ( $1.0 \times 10^{-4}$  M in  $\text{CD}_3\text{CN}$ ), before (top) and after (middle) the addition of 2-fold molar excess of a  $\text{D}_2\text{O}$  solution of  $\text{NiCl}_2$ . The  $^1\text{H}$  NMR spectrum of  $\text{Ni}(\text{salmal})$  (bottom) ( $1.0 \times 10^{-4}$  M solution in  $\text{CD}_3\text{CN}$ ) is reported for comparison.



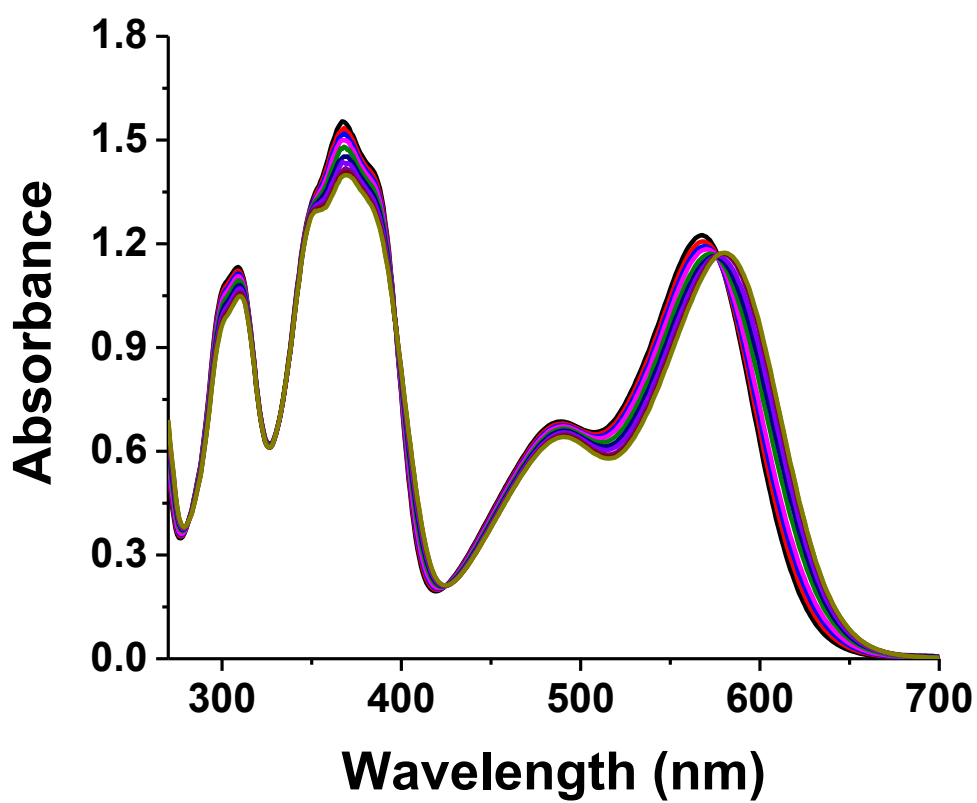
**Fig. S11** (a)  $^1\text{H}$  NMR spectra of **1** ( $1.0 \times 10^{-4}$  M) in  $\text{CD}_3\text{CN}$ , and upon the addition of half molar (b), an equimolar (c), and 2-fold molar excess (d) amount of a  $\text{D}_2\text{O}$  solution of  $\text{CoCl}_2$ .



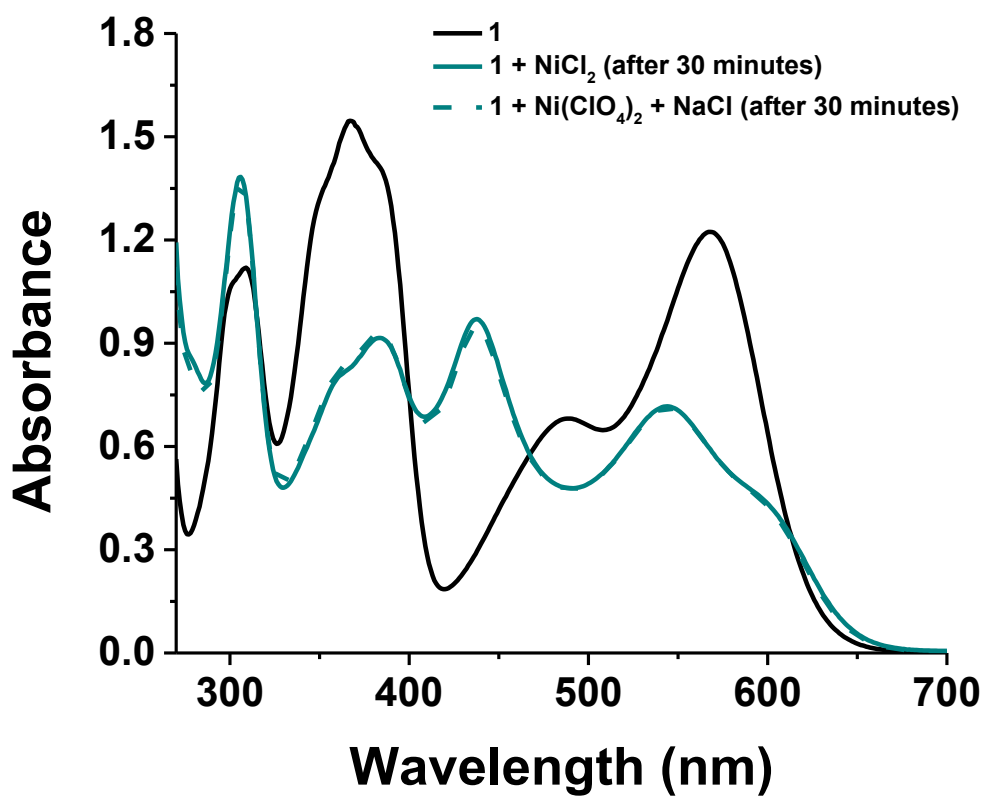
**Fig. S12** Comparison of <sup>1</sup>H NMR spectra of **1** ( $1.0 \times 10^{-4}$  M, in CD<sub>3</sub>CN) before (top), after the addition of 2-fold molar excess of a D<sub>2</sub>O solution of Co(NO<sub>3</sub>)<sub>2</sub>, recorded 24 hours later (middle), and after the addition of 2-fold molar excess of a D<sub>2</sub>O solution of CoCl<sub>2</sub>, recorded 30 min later (bottom).



**Fig. S13** Optical absorption spectra of **1** (40.0  $\mu$ M solution in MeCN) before (—), and after (—) the addition of 2-fold molar excess of an aqueous solution of MgCl<sub>2</sub>, and recorded 24 hours later (—).

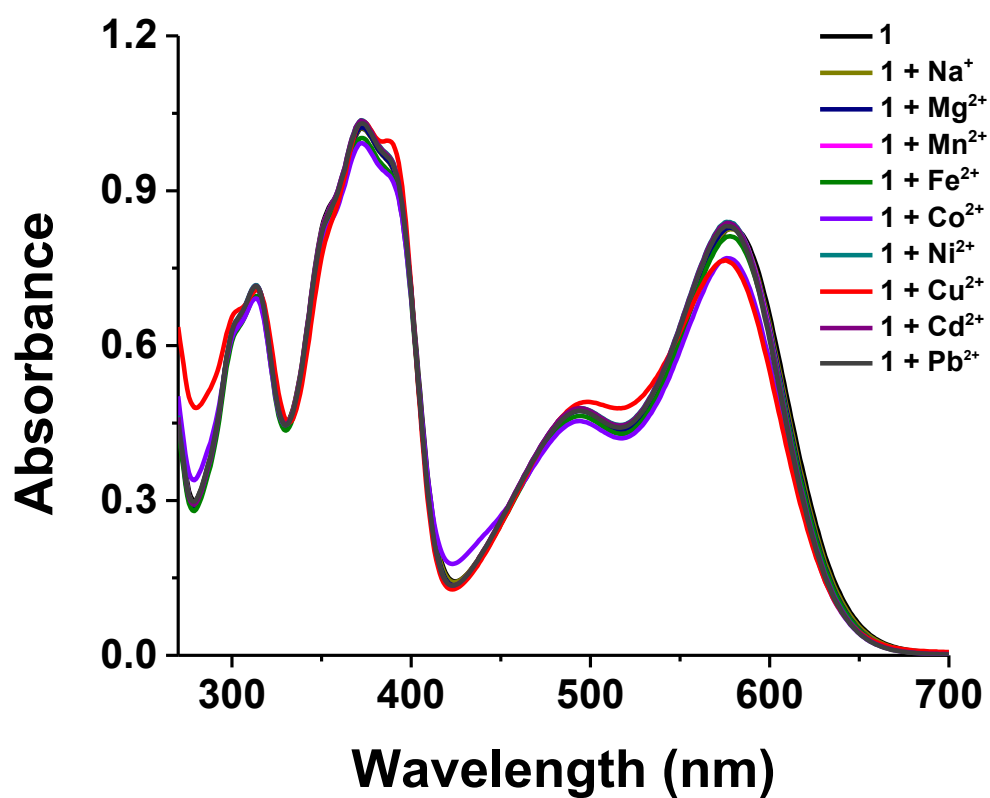


**Fig. S14** Optical absorption titration spectra of **1** (40.0 μM solution in MeCN) with addition of an aqueous solution of TBACl. The concentration of TBACl added varied from 0 to 66.0 μM.

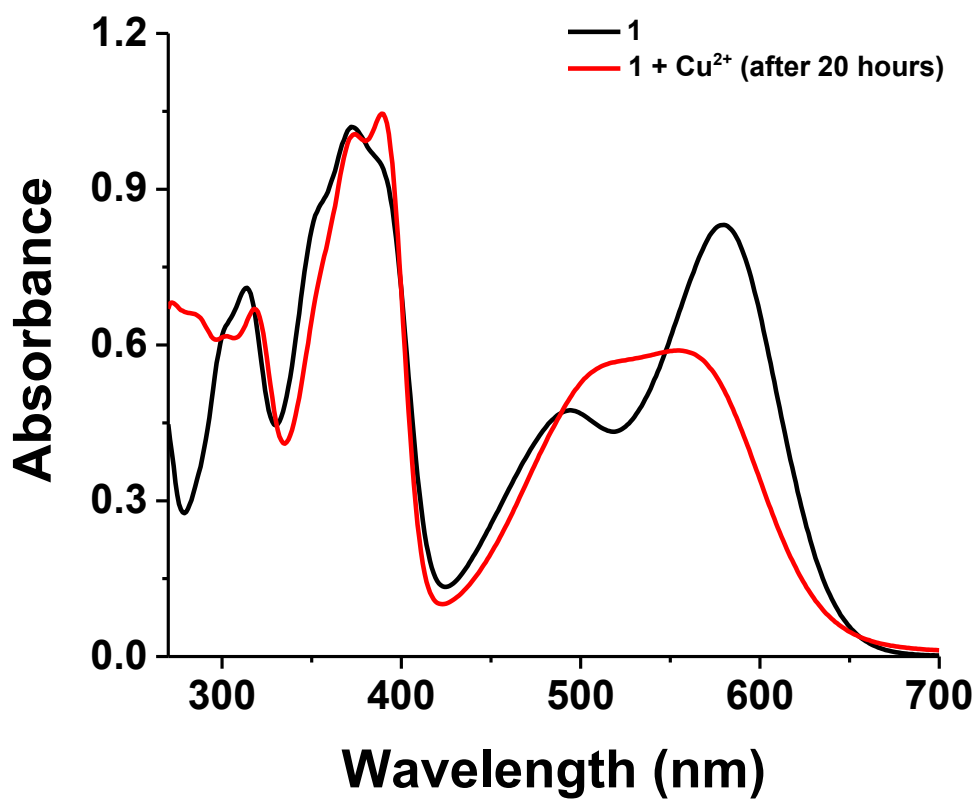


**Fig. S15** Comparison of optical absorption spectra of **1** (40.0  $\mu\text{M}$  solution in MeCN), before (—) and after the addition of 2-fold molar excess of  $\text{NiCl}_2$  (—), or after the addition of 2-fold molar excess  $\text{Ni}(\text{ClO}_4)_2$ , followed by the addition of an equimolar amount (with respect to perchlorate salt) of  $\text{NaCl}$  (---).

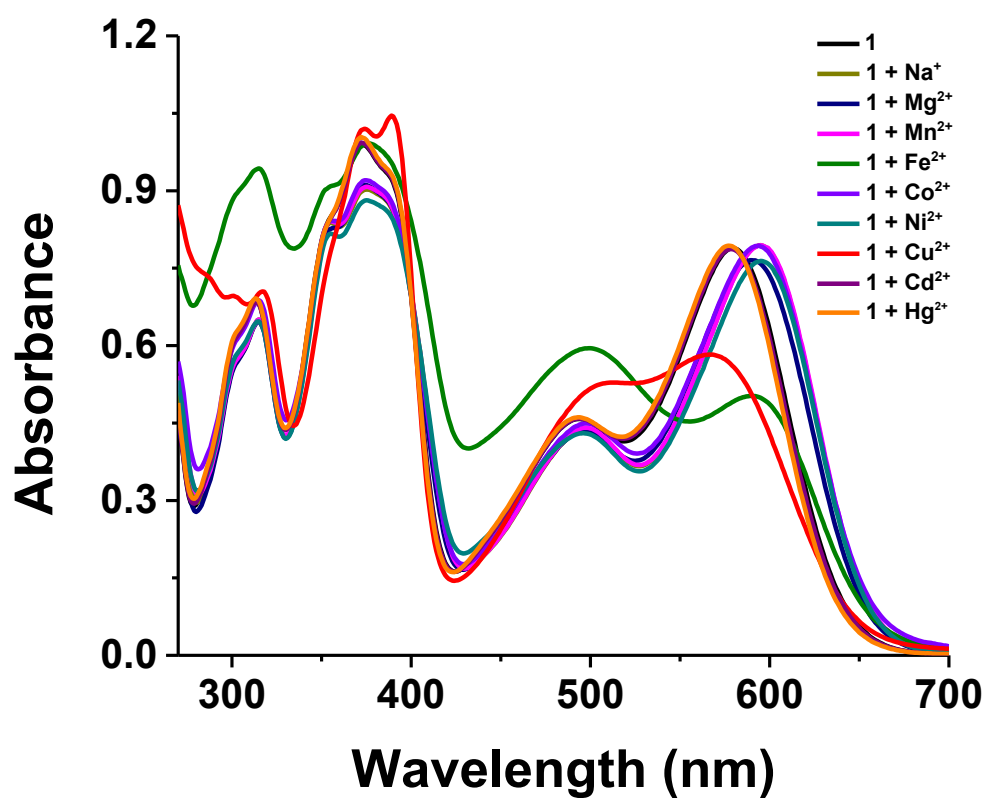




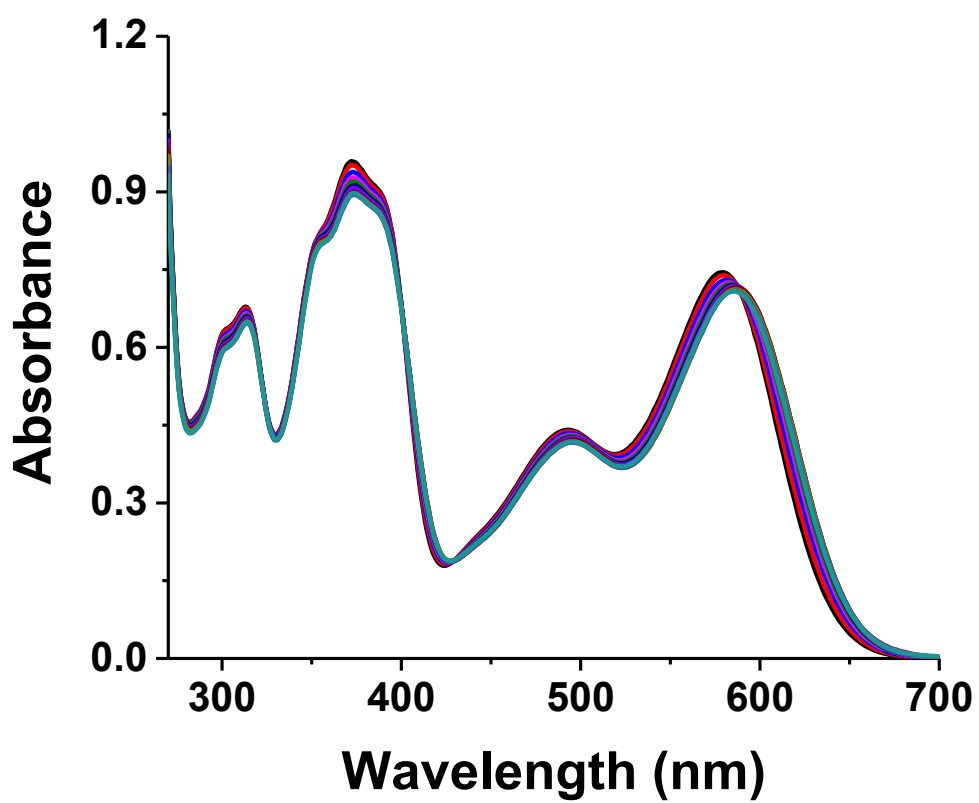
**Fig. S16** Optical absorption spectra of **1** (40.0 μM solution in DMF) before and after the addition of 2-fold molar excess of several cations (as aqueous solutions of nitrate salts).



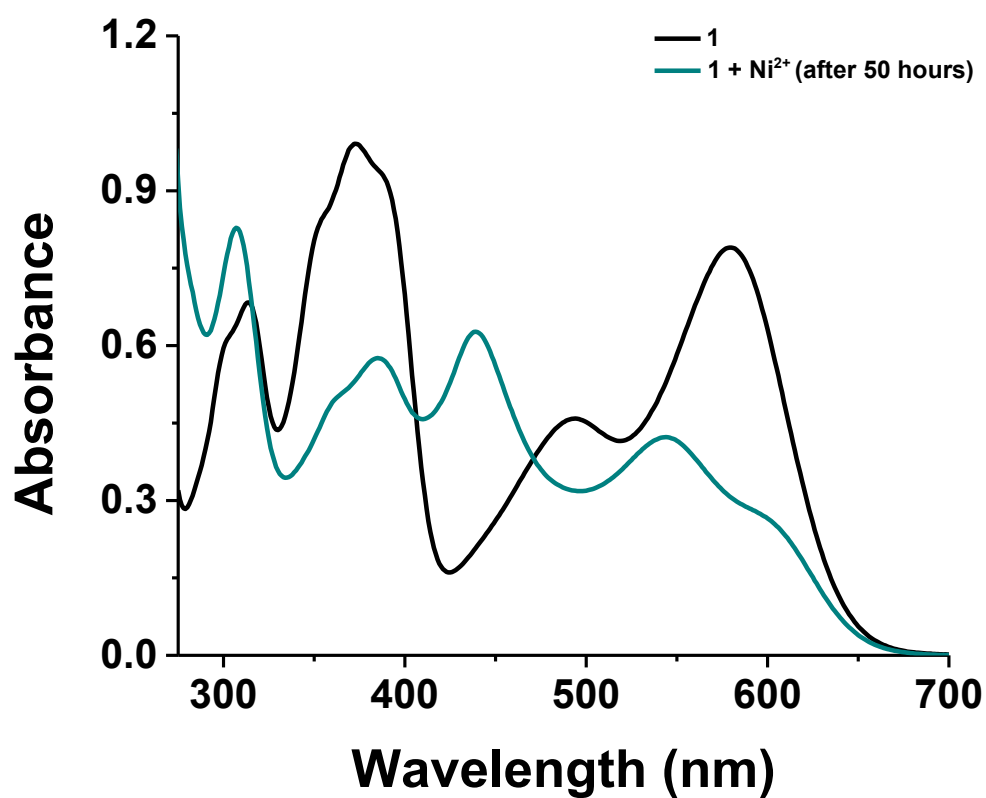
**Fig. S17** Optical absorption spectra of **1** (40.0  $\mu\text{M}$  solution in DMF) before and after the addition of 2-fold molar excess of an aqueous solution of  $\text{Cu}(\text{NO}_3)_2$ , recorded 20 hours later.



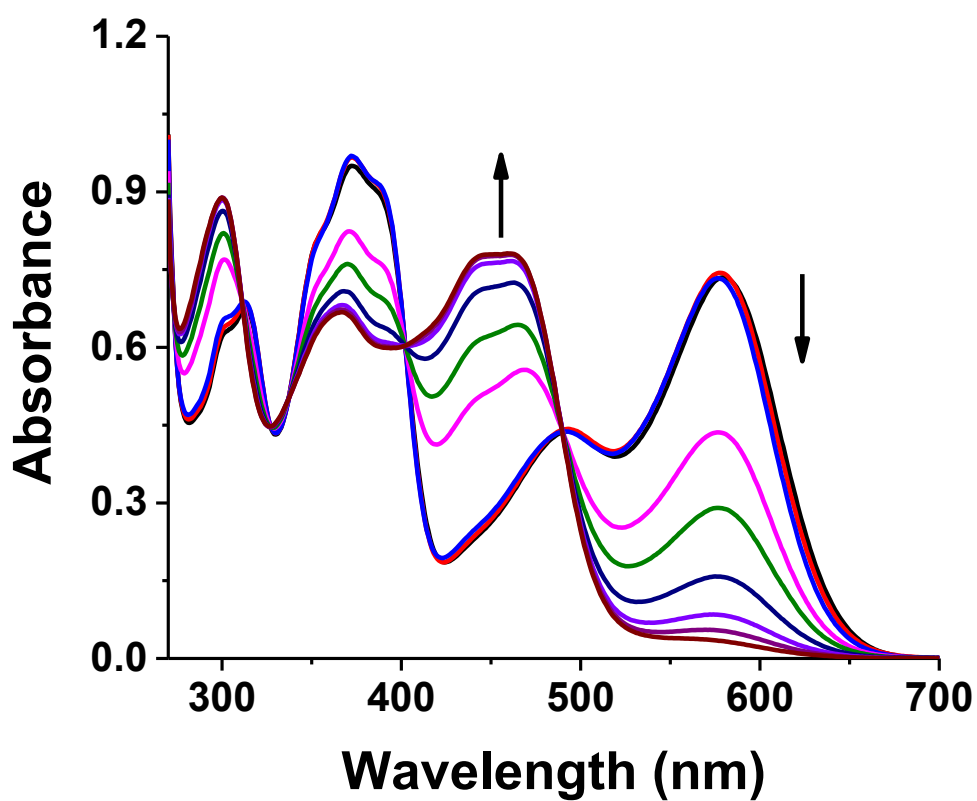
**Fig. S18** Optical absorption spectra of **1** (40.0 μM solution in DMF) before and after the addition of 2-fold molar excess of several cations (as aqueous solutions of chloride salts).



**Fig. S19** Optical absorption titration spectra of **1** (40.0 μM solution in DMF) with addition of an aqueous solution of TBACl. The concentration of TBACl added varied from 0 to 146 μM.



**Fig. S20** Optical absorption spectra of **1** (40  $\mu$ M solution in DMF) before and after the addition of 2-fold molar excess of an aqueous solution of  $\text{NiCl}_2$ , recorded 50 hours later.



**Fig. S21** Optical absorption titration spectra of **1** (40.0  $\mu\text{M}$  solution in DMF) upon progressive addition of an aqueous solution of  $\text{HClO}_4$ . The concentration of  $\text{HClO}_4$  added varied from 0 to 150  $\mu\text{M}$ .