

Supporting Information

A Quinazolin-based Schiff-base chemosensor for colourimetric detection of Ni²⁺ and Zn²⁺ ions and 'turn-on' fluorometric detection of Zn²⁺ ion

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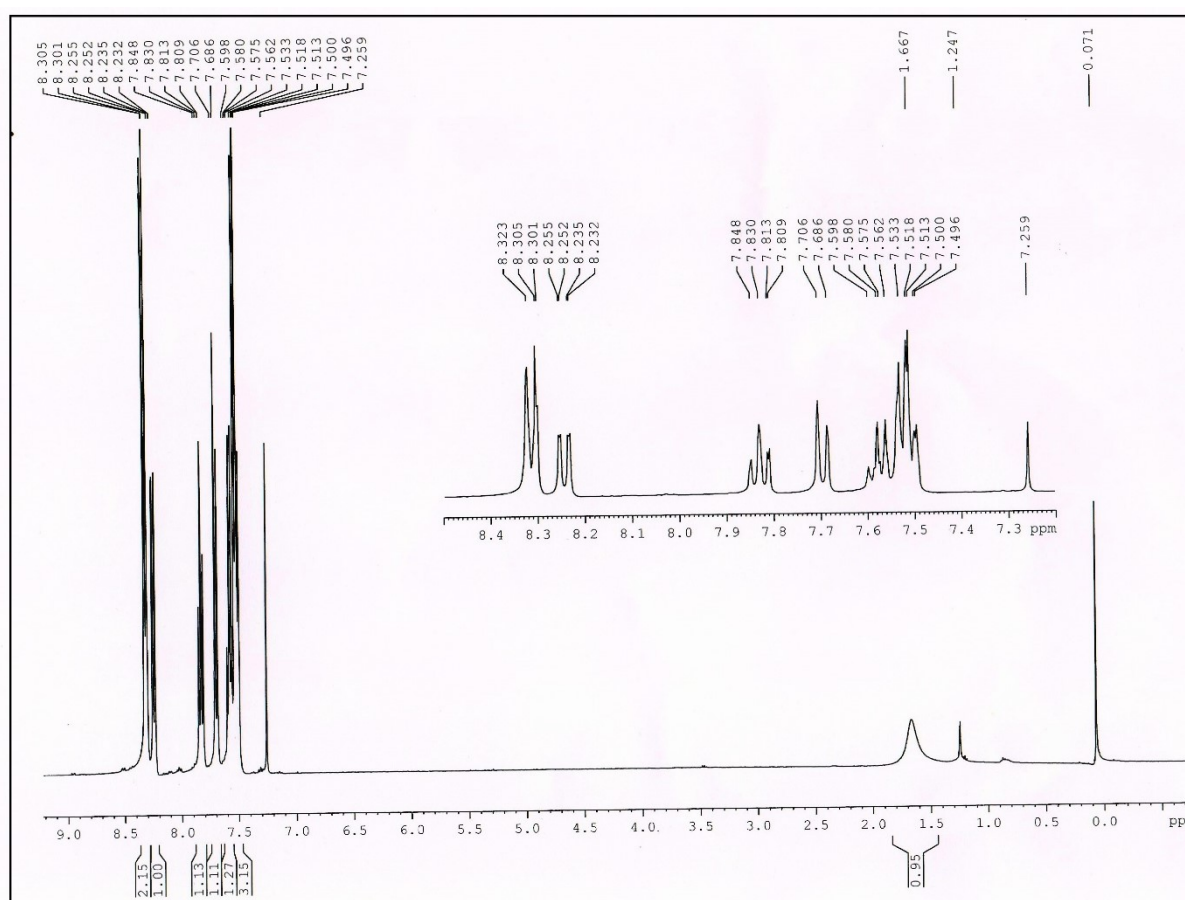


Fig.S1. ¹H NMR spectra of 1 in CDCl₃.

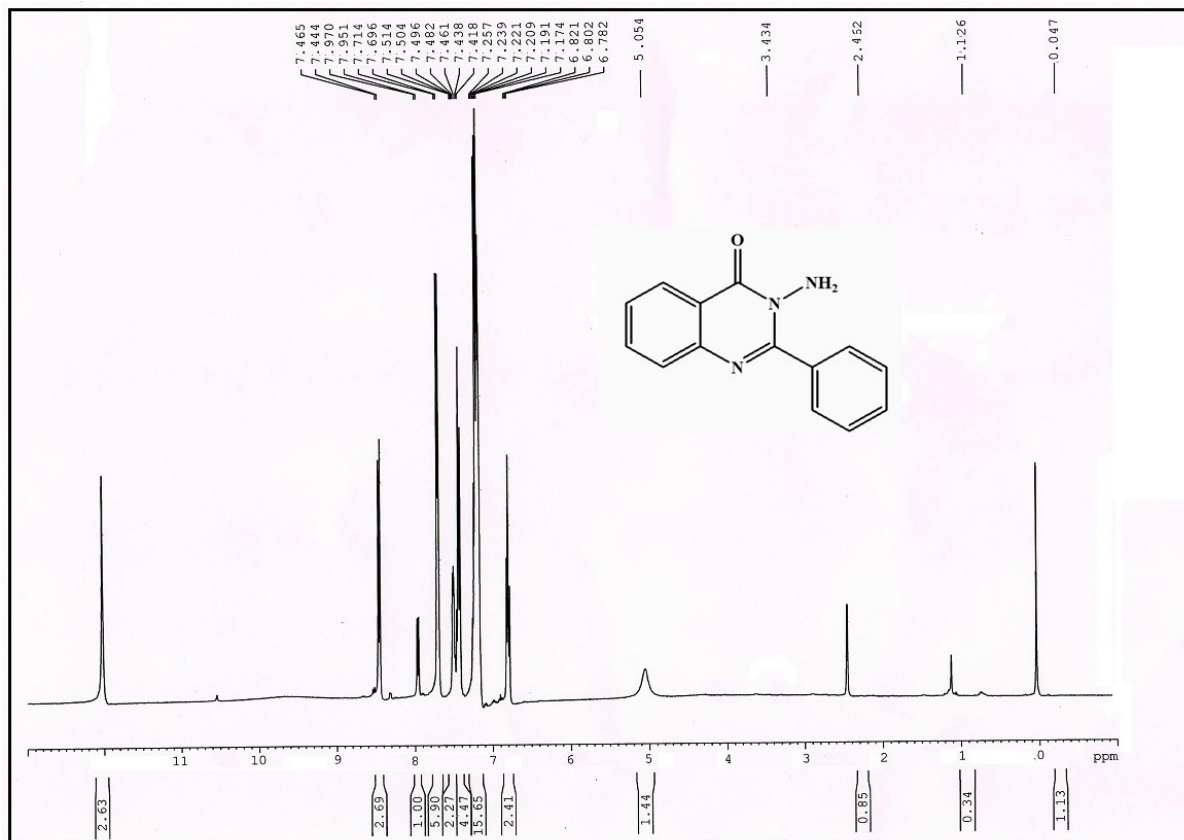


Fig.S2. ¹H NMR spectra of 2 in CDCl₃.

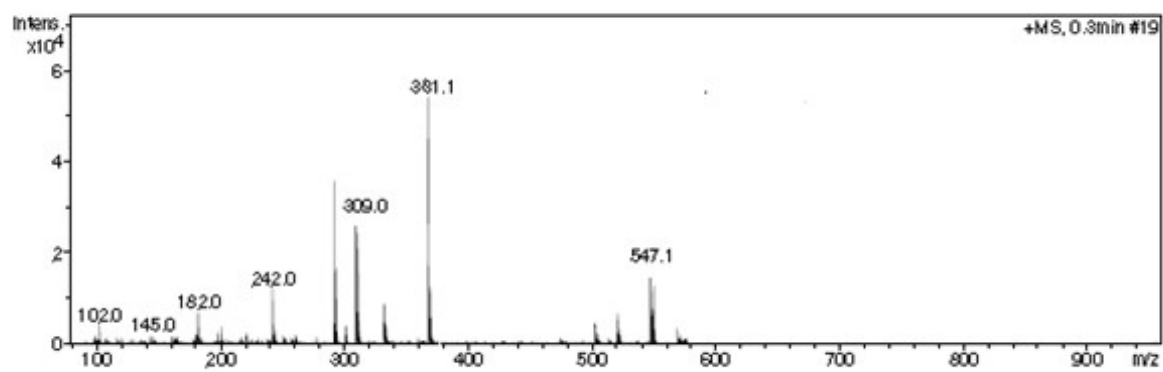


Fig. S3. ESI-mass spectra of L

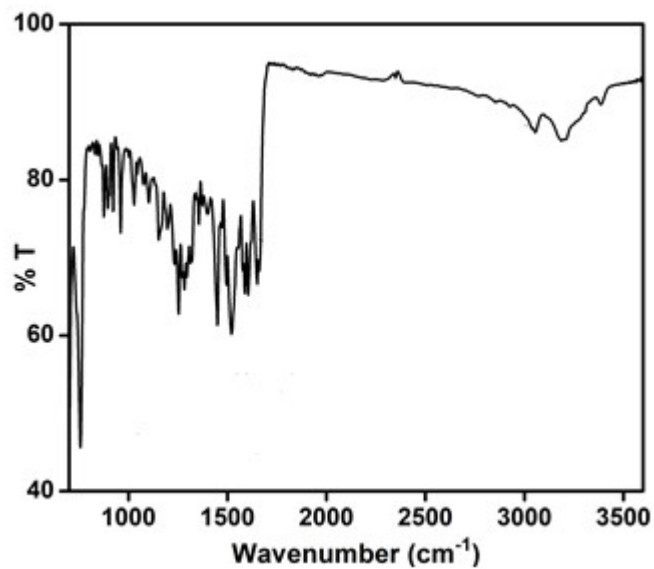


Fig. S4. FTIR spectra of **L**

AC-B-PYal-1H-(ND)-400

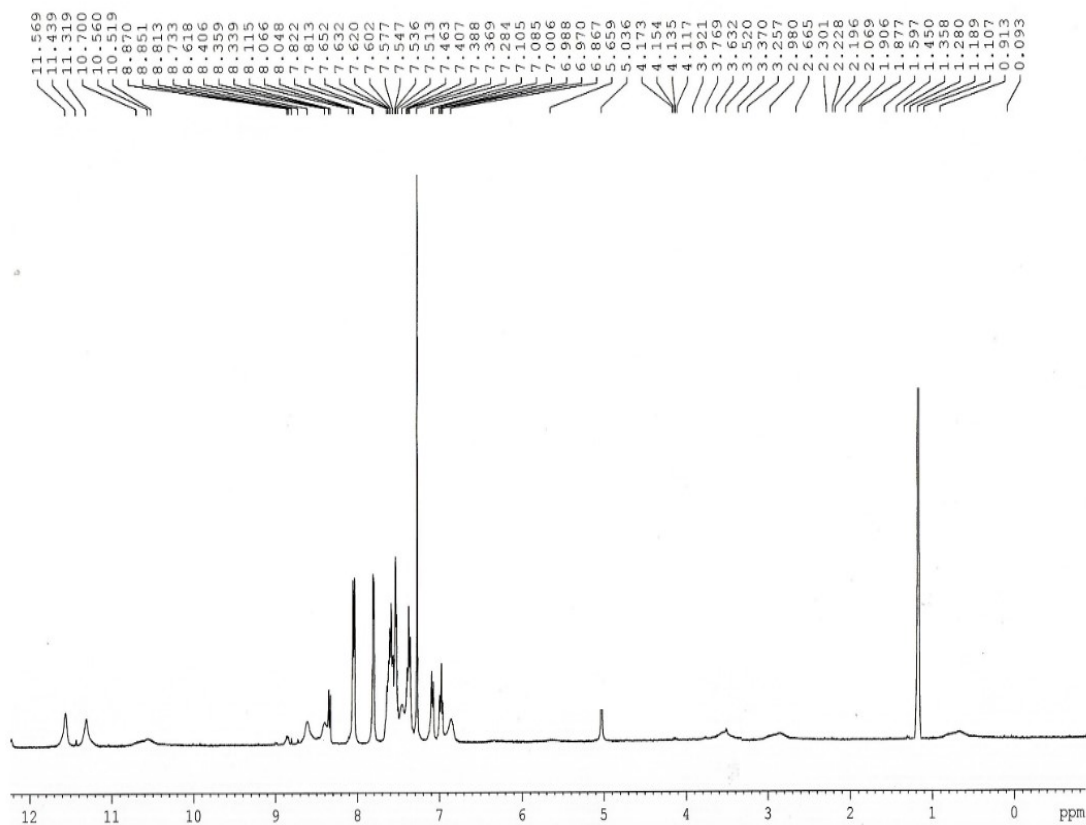


Fig.S5. ^1H NMR spectra of **L** in CDCl_3

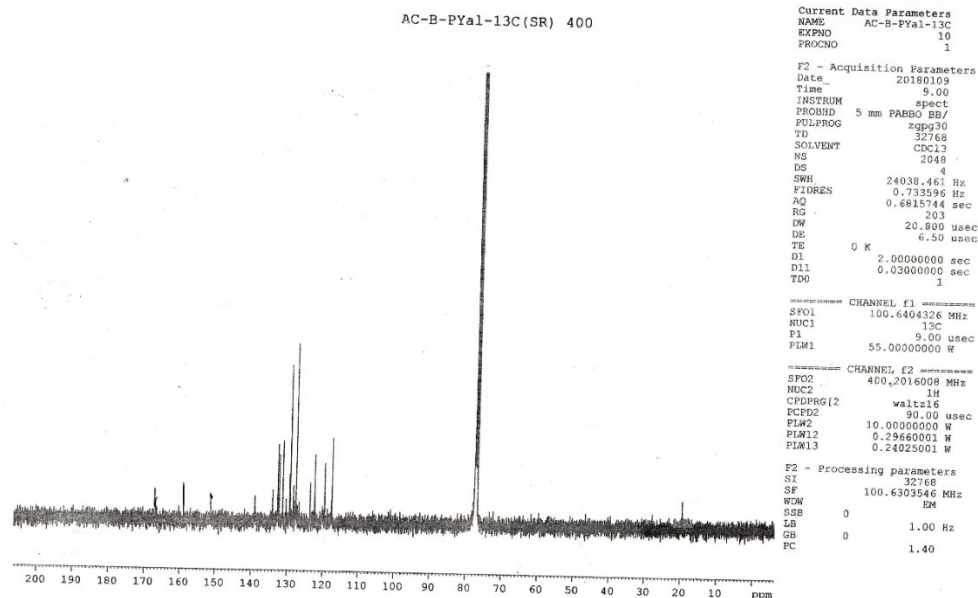


Fig.S6. ^{13}C NMR spectra of **L** in CDCl_3

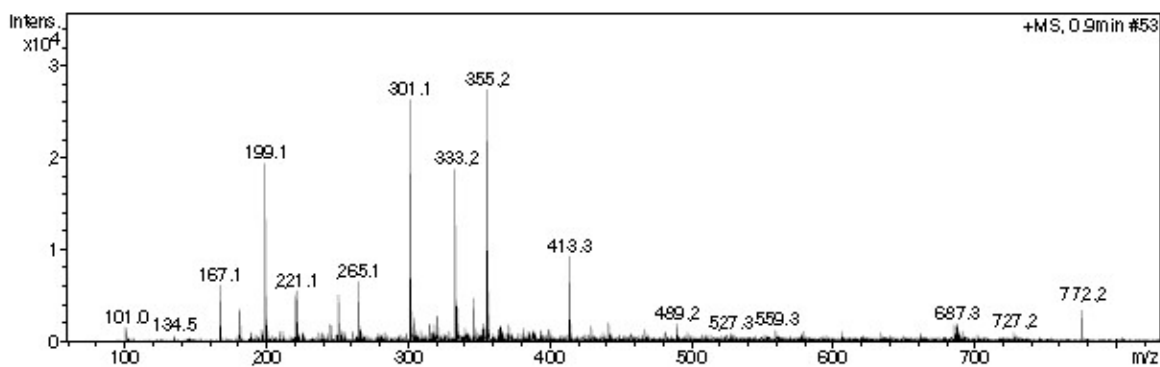


Fig. S7. ESI-mass spectra of NiL_2 (**3**)

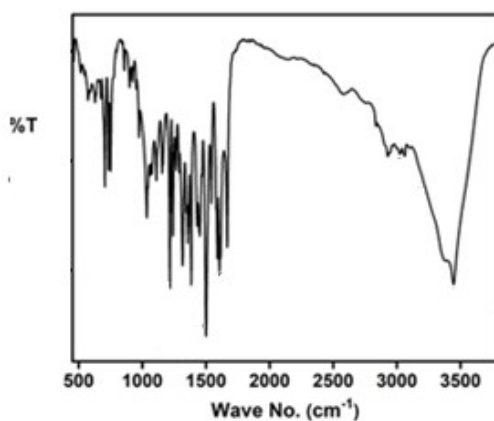


Fig. S8. FTIR spectra of NiL_2 (**3**)

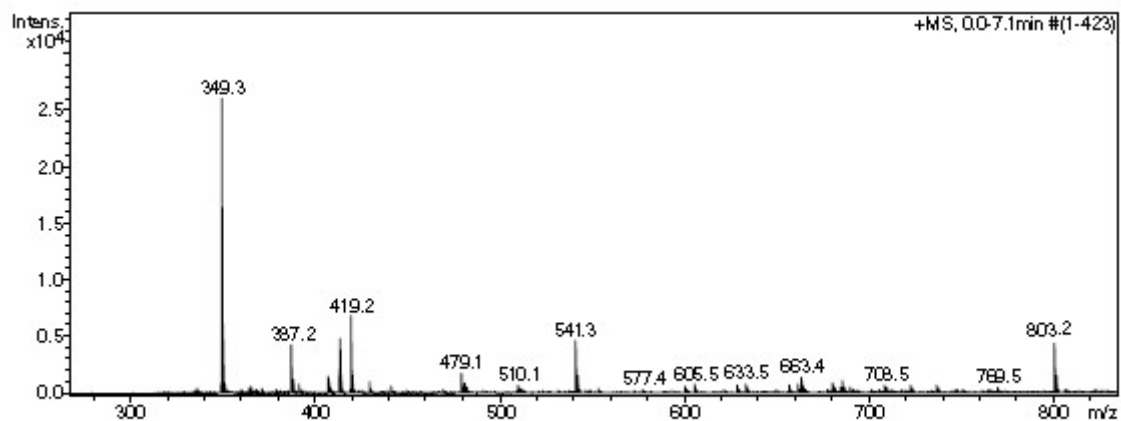


Fig. S9. ESI-mass spectra of ZnL₂ (4)

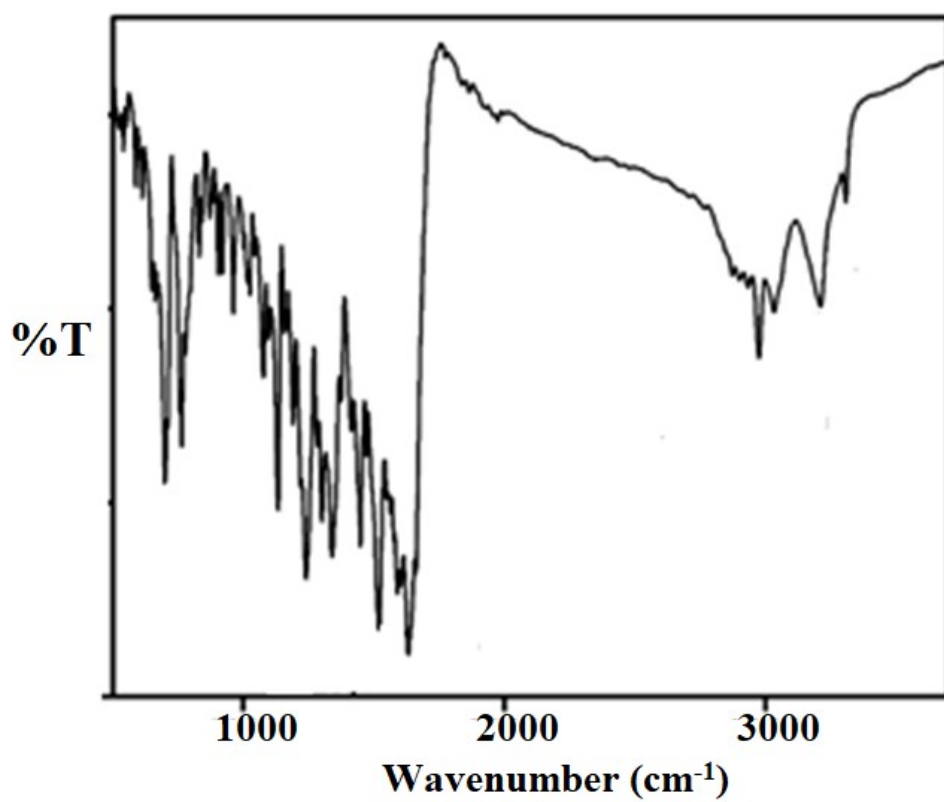


Fig. S10. FTIR spectra of ZnL₂ (4)

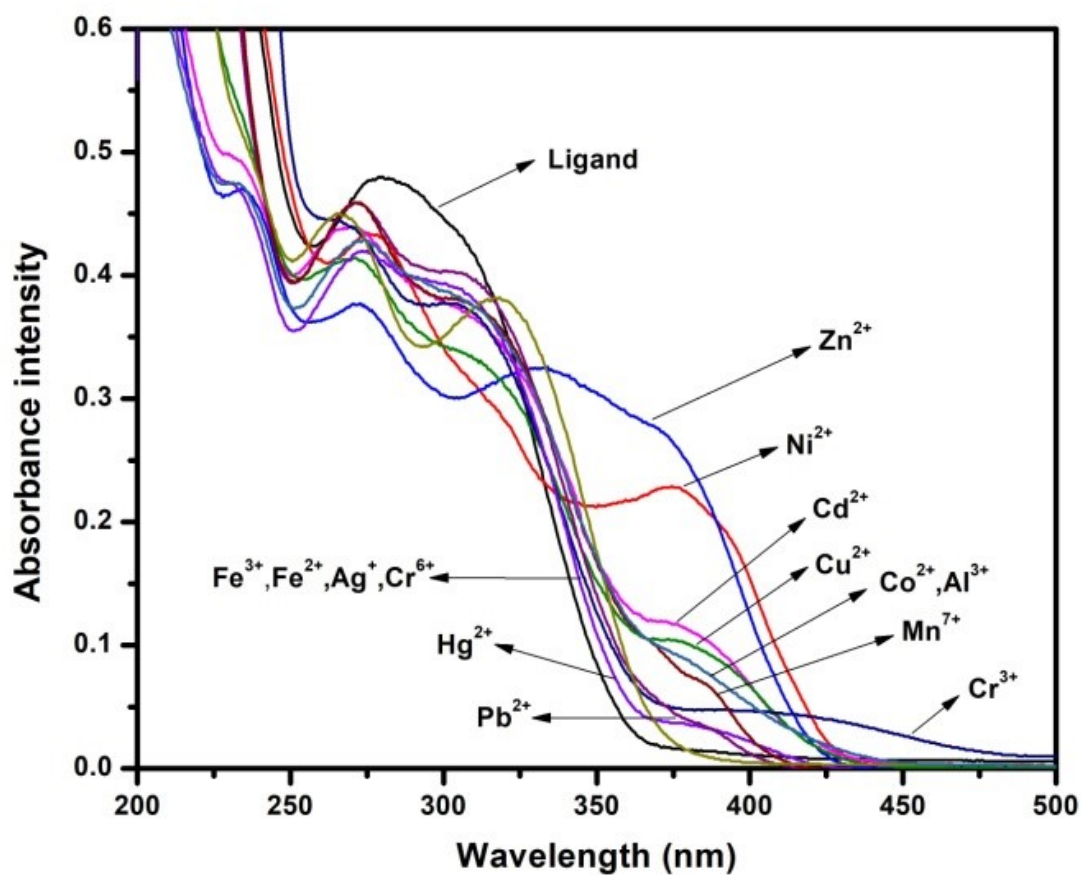


Fig. S11. Change in absorption spectra of L (10 μM) in presence of 2 equiv. of different metal ions in methanol-tris-HCl buffer (1:1 v/v, pH 7.2) at room temperature.

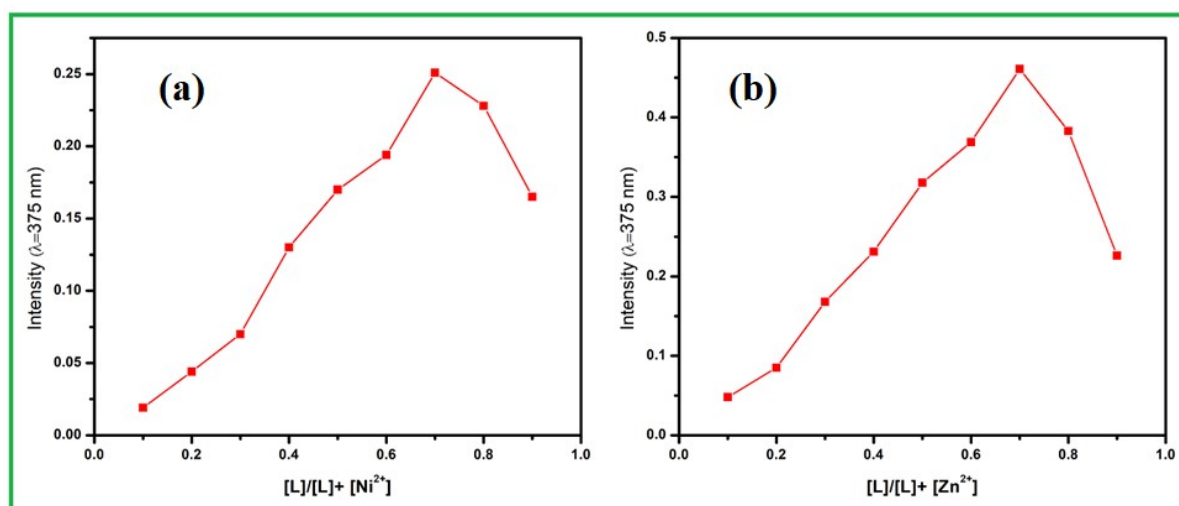


Fig. S12. Job's plot for (a) Ni²⁺ and (b) Zn²⁺.

Table S1. Selected Bond Lengths for **3**

Atom	Atom	Length/Å
Ni(1)	O(2) ¹	2.053(5)
Ni(1)	O(2)	2.053(5)
Ni(1)	N(1) ¹	2.112(6)
Ni(1)	N(1)	2.112(6)
Ni(1)	N(2)	1.979(5)
Ni(1)	N(2) ¹	1.979(5)

¹1-X,+Y,3/2-Z**Table S2.** Selected Bond Angles for **3**

Atom	Atom	Atom	Angle/°
O(2) ¹	Ni(1)	O(2)	89.3(3)
O(2) ¹	Ni(1)	N(1) ¹	154.73(18)
O(2)	Ni(1)	N(1) ¹	96.3(2)
O(2)	Ni(1)	N(1)	154.73(18)
O(2) ¹	Ni(1)	N(1)	96.3(2)
N(1)	Ni(1)	N(1) ¹	89.1(3)
N(2) ¹	Ni(1)	O(2) ¹	75.8(2)
N(2)	Ni(1)	O(2)	75.8(2)
N(2) ¹	Ni(1)	O(2)	104.2(2)
N(2)	Ni(1)	O(2) ¹	104.2(2)
N(2) ¹	Ni(1)	N(1) ¹	79.0(2)
N(2)	Ni(1)	N(1) ¹	101.1(2)
N(2) ¹	Ni(1)	N(1)	101.1(2)
N(2)	Ni(1)	N(1)	79.0(2)
N(2)	Ni(1)	N(2) ¹	179.9(4)
C(8)	O(2)	Ni(1)	111.1(4)
C(5)	N(1)	Ni(1)	111.6(5)
C(1)	N(1)	Ni(1)	127.6(5)
N(3)	N(2)	Ni(1)	120.4(4)
C(6)	N(2)	Ni(1)	118.1(5)

¹1-X,+Y,3/2-Z