Supporting Information

Binding sites-driving sensing properties of a quinazoline derivative with metal cations

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Table S1   Selected Bond Distances (Å) and Angles (deg) for **1** and **2**.

1					
Cd(1)-O(1)	2.586(9)	Cd(1)-O(2)	2.217(8)	Cd(1)-O(3)	2.594(6)
Cd(1)-O(4)	2.295(9)	Cd(1)-N(3)	2.295(9)	Cd(1)-N(5)	2.333(7)
O(1)-Cd(1)-O(2)	53.3(3)	O(1)-Cd(1)-O(3)	82.26(11)	O(1)-Cd(1)-O(4)	97.9(3)
O(1)-Cd(1)- N(3)	94.7(3)	O(1)-Cd(1)- N(5)	158.8(3)	O(2)-Cd(1)-O(3)	96.6(3)
O(2)-Cd(1)-O(4)	143.67(12)	O(2)-Cd(1)-N(3)	98.9(3)	O(2)-Cd(1)-N(5)	106.0(3)
O(3)-Cd(1)-O(4)	53.6(3)	O(3)-Cd(1)- N(3)	158.1(3)	O(3)-Cd(1)- N(5)	97.0(3)
O(4)-Cd(1)-N(3)	105.9(3)	O(4)-Cd(1)-N(5)	98.6(3)	N(3)-Cd(1)-N(5)	93.50(11)

2					
Cd(1)-N(2)	2.329(16)	Cd(1)-N(4)	2.199(14)	Cd(1)-Cl(2)	2.430(5)
Cd(1)-Cl(3)	2.421(6)	N(2)-Cd(1)-Cl(2)	106.6(4)	N(2)-Cd(1)-Cl(3)	118.8(4)
N(2)-Cd(1)-N(4)	96.5(2)	N(4)-Cd(1)-Cl(2)	119.0(4)	N(4)-Cd(1)-Cl(3)	108.3(4)
Cl(3)-Cd(1)-Cl(2)	107.93(8)				

Table S2 Comparison of the chemosensors for Al^{3+}, Cr^{3+} and Fe^{3+} ions

Chemosensor	Detected cation	Detection limit	Differentiation of one from another	Reference
Chromo-fluorogenic probe	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-8} M	√	8a
Pyridinyl-functionalized tetraphenylethene	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-6} M		8b
Spirobenzopyran-quinoline dyad	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-6} M	√	8c
ESIPT based sensor	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-6} M		8d
Chemodosimetric probe	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-8} M		8g
RhB-based probe	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-5}-10^{-7} M		8e
Rhodamine-naphthalimide dyad	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-5} M		8f
6-furan-2-yl-5,6-dihydrobenzo(4,5) imidazo[1,2-c]quinazoline	Al^{3+}, Cr^{3+}, Fe^{3+}	10^{-6} M	√	Our paper

Figure S1 Crystal structure of L.

Figure S2 Fluorescence properties of L (100 μM) in CH$_3$OH with HCl (0, 0.4, 0.8, 1.2, 1.6, 2.0, 2.4, 2.8 equiv.)
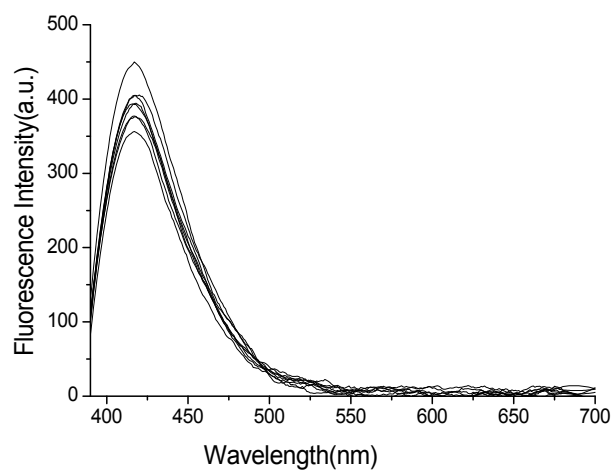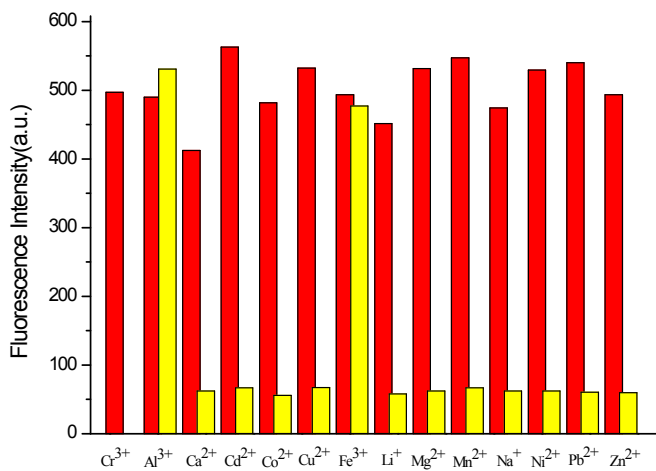
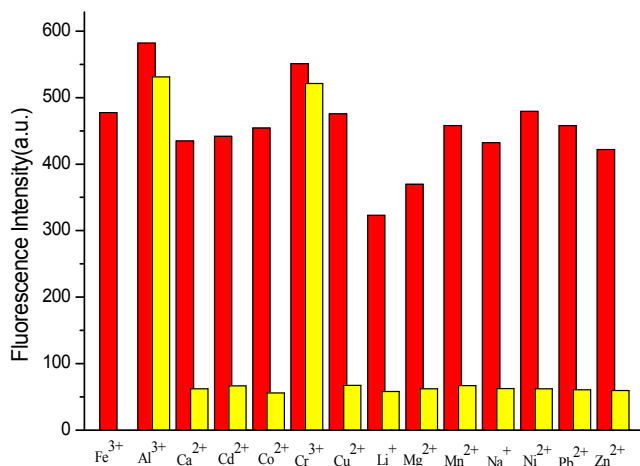**Figure** S3 Fluorescence properties of L (100 μM) in CH$_3$OH with NaOH (0, 0.4, 0.8, 1.2, 1.6, 2.0, 2.4, 2.8 equiv.)
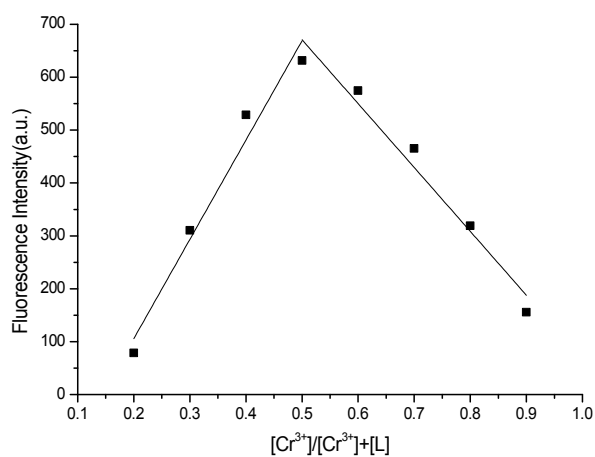
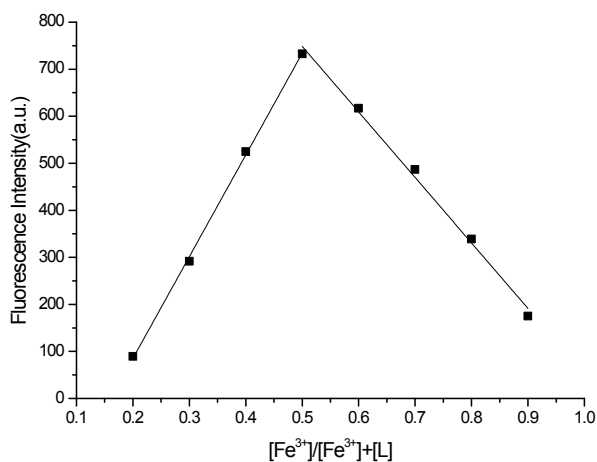(a)   (b)

Figure S4 (a) Fluorescence intensity of complexes of L and Cr^{3+} in the presence of various metal ions in CH_3OH. λ_{ex}=390 nm and λ_{em}=471 nm. Red bars: L(30μM) with 1.0 equiv. of Cr^{3+} and 1.0 equiv. of other metal ionsstated.Yel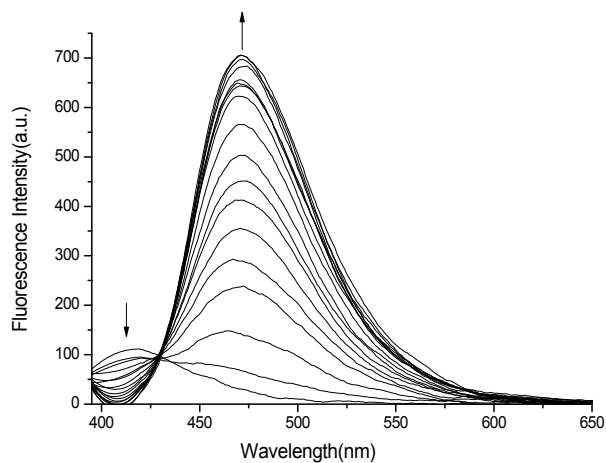low bars: L(30μM) with 1.0 equiv. of other metal ions stated; (b) Fluorescence intensity of complexes of L and Fe^{3+} in the presence of various metal ions in CH_3OH. λ_{ex}=388 nm and λ_{em}=470 nm. Red bars: L(30μM) with 1.0 equiv.of Fe^{3+} and 1.0 equiv. of other metal ions stated.Yellow bars: L(30μM) with 1.0 equiv. of other metal ions stated.

(a)   (b)
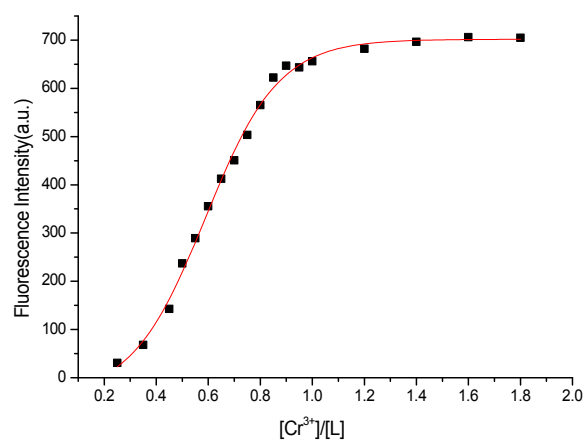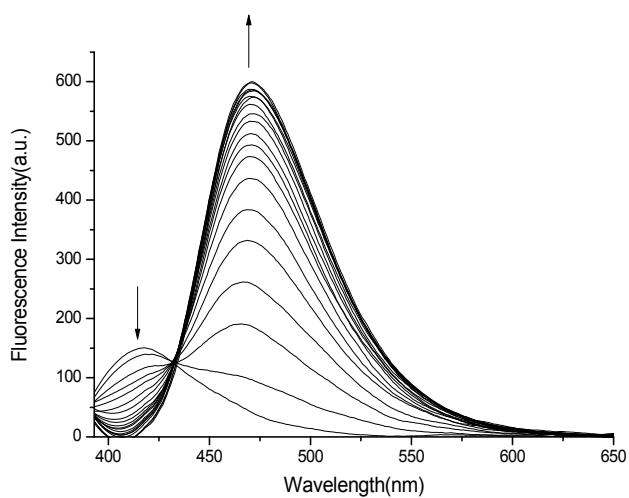
Figure S5 (a) Job's plot for the determination of the stoichiometry of L and Cr^{3+} in the complexation; (b) Job's plot for the determination of the stoichiometry of L and Fe^{3+} in the complexation.
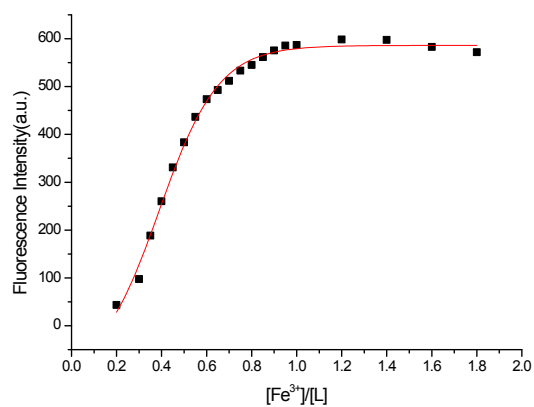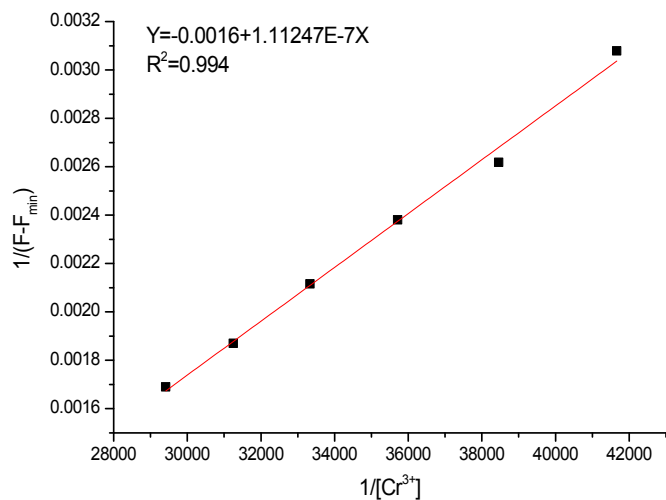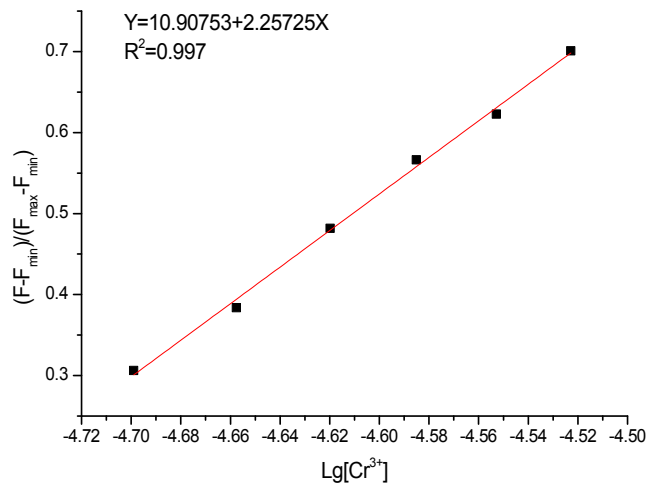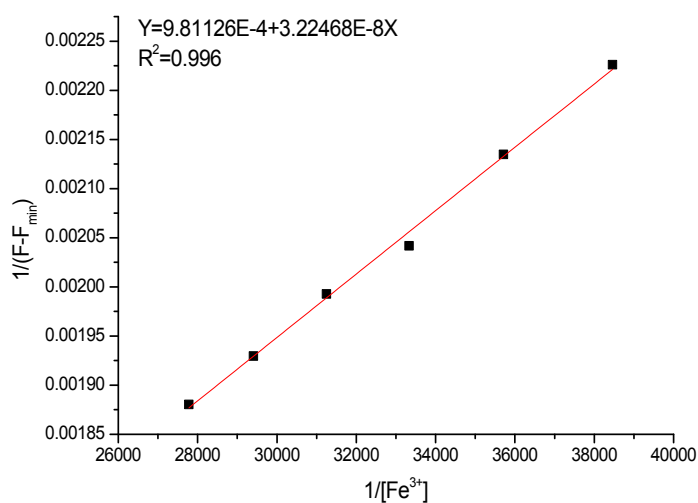
(a)

(b)

(c)

(d)

Figure S6 (a) Fluorescence emission spectra(λ_{ex}=390nm) of L(40μM) in the presence of increasing amounts of Cr^{3+} (0.25, 0.35, 0.45, 0.50...0.80, 0.85, 0.90, 0.95, 1.00, 1.20, 1.40, 1.60, 1.80 equiv.) in CH_3OH; (b) Spectrofluorimetric titration curve at λ_{em}=471nm; (c) Fluorescence emission spectra(λ_{ex}=388nm) of L(40μM) in the presence of increasing amounts of Fe^{3+} (0.20, 0.30,0.35, 0.45, 0.50...0.80, 0.85, 0.90, 0.95, 1.00, 1.20, 1.40, 1.60, 1.80 equiv.) in CH_3OH; (d) Spectrofluorimetric titration curve at λ_{em}= 471nm.

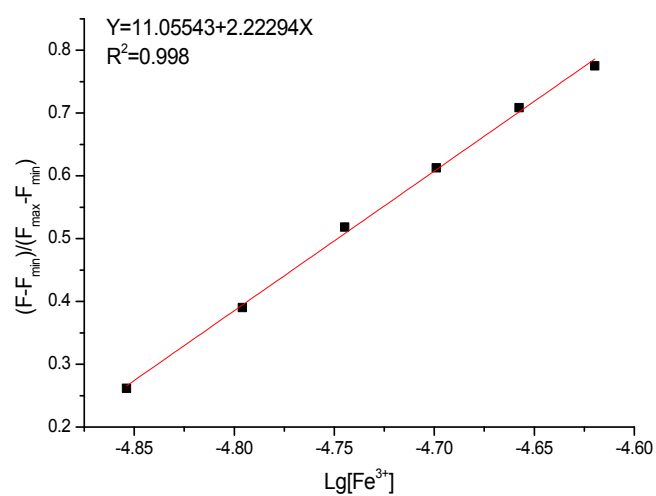**Figure** S7 (a) Benesi-Hildebrand plot of L with Cr^{3+} in CH_3OH (λ_{em}=471 nm); (b) Normalized response of emission signal changing Cr^{3+} concentrations at 471 nm; (c) Benesi-Hildebrand plot of L with Fe^{3+} in CH_3OH (λ_{em}=470 nm); (d) Normalized response of emission signal changing Fe^{3+} concentrations at 470 nm.
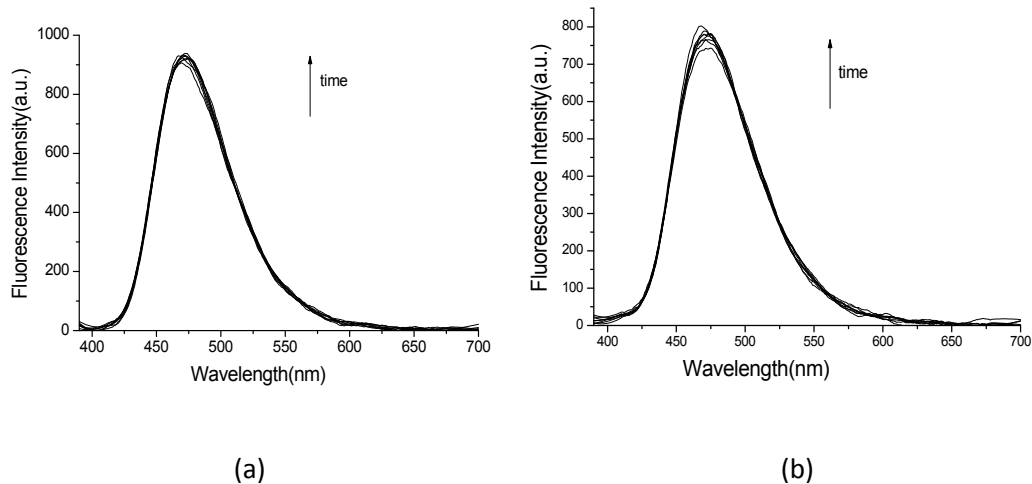
(a)

(b)

Figure S8 Fluorescence spectra variation of L (67 μM) upon addition of 1.0 equiv. of Al^{3+} (a) and Fe^{3+} (b) in CH_3OH after 1 , 2 , 3, 4 , 5, 10, 15 , and 20 min, λ_{ex}=383 nm.
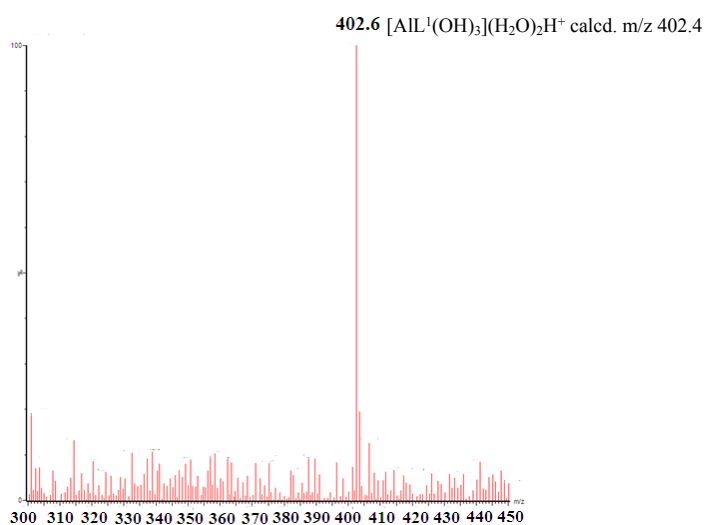

402.6 $[AlL^1(OH)_3](H_2O)_2H^+$ calcd. m/z 402.4

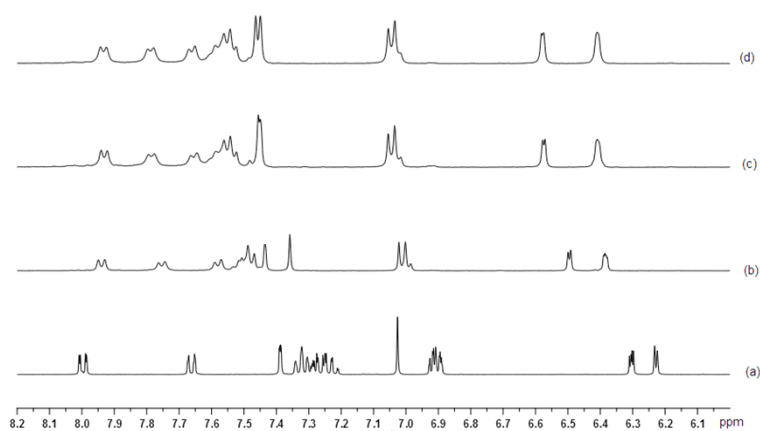**Figure** S9 ESI-MS of L-Al^{3+}(1:1) in CH_3OH/H_2O (1:9).

Figure S10 ^1H NMR spectra in CH_3OH-d_6: (a) L only; (b) L and 0.5 equiv. of Cr^{3+}; (c) L and 1.0 equiv. of Cr^{3+}; (d) L and 1.5 equiv. of Cr^{3+}.
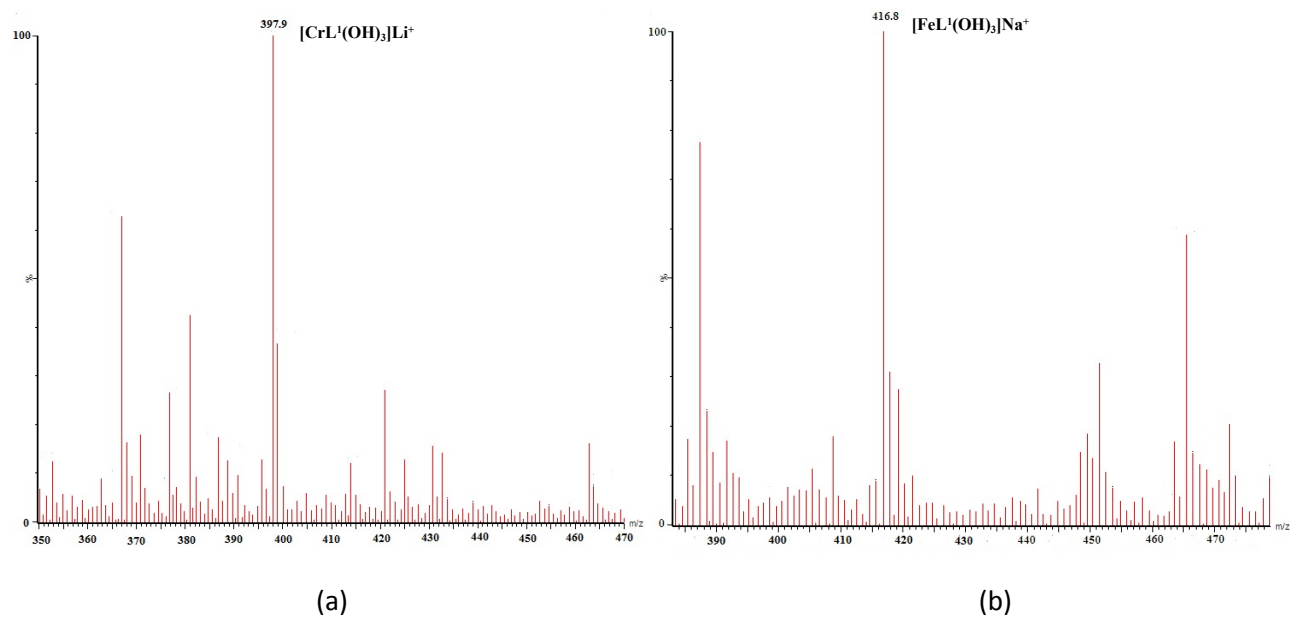
7

(a)

(b)

Figure S11 (a) Positive-ion electrospray ionization mass spectra of L upon addition of 1.0 equiv. Cr^{3+} in CH_3OH; (b) Positive-ion electrospray ionization mass spectra of L upon addition of 1.0 equiv. Fe^{3+} in CH_3OH.
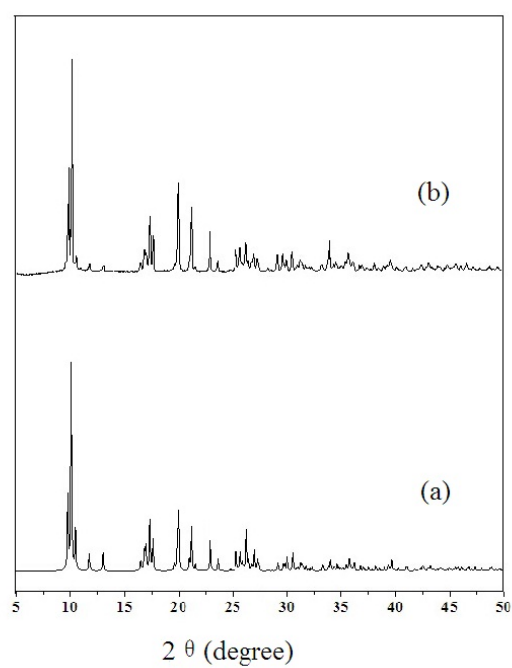

Figure S12 (a) Simulated Powder X-ray diffraction for $[CdL_2(OAc)_2]$; (b)Powder X-ray diffraction for sample **1'**.

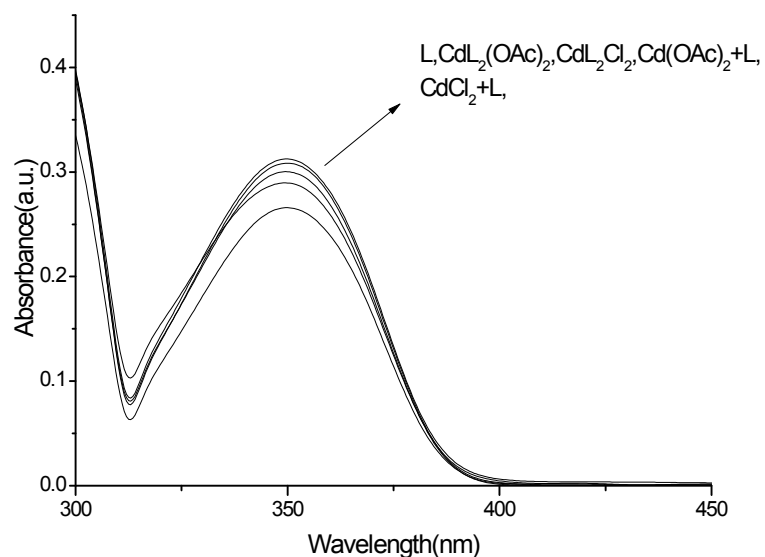**Figure** S13 UV-Vis absorptionspectra of $CdL_2(OAc)_2$(15 μM), CdL_2Cl_2(15 μM), L(30 μM) and L(30 μM) with 1.0 equiv. of $CdCl_2$, $Cd(OAc)_2$ in CH_3OH, respectively.

Figure S14 Fluorescence spectra of $CdL_2(OAc)_2$(15 μM), CdL_2Cl_2(15 μM), L(30 μM) , and L(30 μM) with 1.0 equiv. of $CdCl_2$, $Cd(OAc)_2$ in CH_3OH, respectively.

Figure S15 ^{1}HNMR spectra in $CH_3OH\text{-}d_6$: (a) L; (b) $CdL_2(OAc)_2$.