Electronic Supplementary Information

Supramolecular assembly of a 4-(1-naphthylvinyl)pyridyl appended Zn(II) coordination compound for turn-on fluorescence sensing of trivalent metal ions (Fe^{3+}, Al^{3+}, Cr^{3+}) and cell imaging application

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Table S1. Crystal data and refinement parameters for compound **1**

Formula	$C_{36}H_{26}N_4S_2Zn$
fw	644.10
Crystsyst	Monoclinic
Space group	*C*2/*c*
a (Å)	33.760(4)
b (Å)	6.1009(6)
c (Å)	17.523(2)
α(deg)	90
β(deg)	118.990(4)
γ(deg)	90
V (Å^3)	3156.9(6)
Z	4
D_{calcd}(g/cm^3)	1.355
μ(mm^{-1})	0.942
F(000)	1328.0
Crystal Size [mm]	0.12 ×0.11 ×0.10
Temperature (K)	273(2)
λ(Å)	0.71073
Data [$I > 2\sigma(I)$]/params	2257/ 195
GOF on F^2	1.040
final *R* indices ($I > 2\sigma(I)$)^{a,b}	R_1 =0.0333 wR_2 =0.0860

$^aR_1 = \Sigma||F_o| \quad |F_c||/ \Sigma|F_o|$, $^bwR_2 = [\Sigma w(F_o^2 \quad F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths and bond angles in **1**.

Zn01 - N1	2.0278(19)	N2-Zn01-N1-C1	22.1(2)
Zn01 - N2	1.915(2)	N1_a-Zn01-N1-C5	76.6(2)
Zn01 - N1_a	2.0278(19)	Zn01-N1-C1-C2	168.41(19)
Zn01 - N2_a	1.915(2)	N2_a-Zn01-N1-C1	155.0(2)
N1 - Zn01 - N2	107.73(9)	Zn01-N1-C5-H5	11
N2 - Zn01 - N1_a	107.73(9)	S1 - C18- N2	178.2(3)
Zn01 - N1 - C1	123.31(15)	N1 - C5 - C4	123.6(2)
Zn01 - N2 - C18	174.5(2)	N1-C1-H1	118.3
N1 - Zn01 - N1_a	98.38(8)	N1-C5-H5	118.2
N2 - Zn01 - N2_a	120.41(14)	N1 - C5- C4	118.9(2)
Zn01 - N1 - C5	119.23(16)	C13 - C12-C17	88.16(10)
N1 - Zn01 - N2_a	110.27(9)	C7- C8 - C13	121.2(2)
N1_a - Zn01 - N2_a	107.73(9)	C11- C12 - C17	121.6(3)

Symmetry Code: a = 1-x, y, 3/2-z

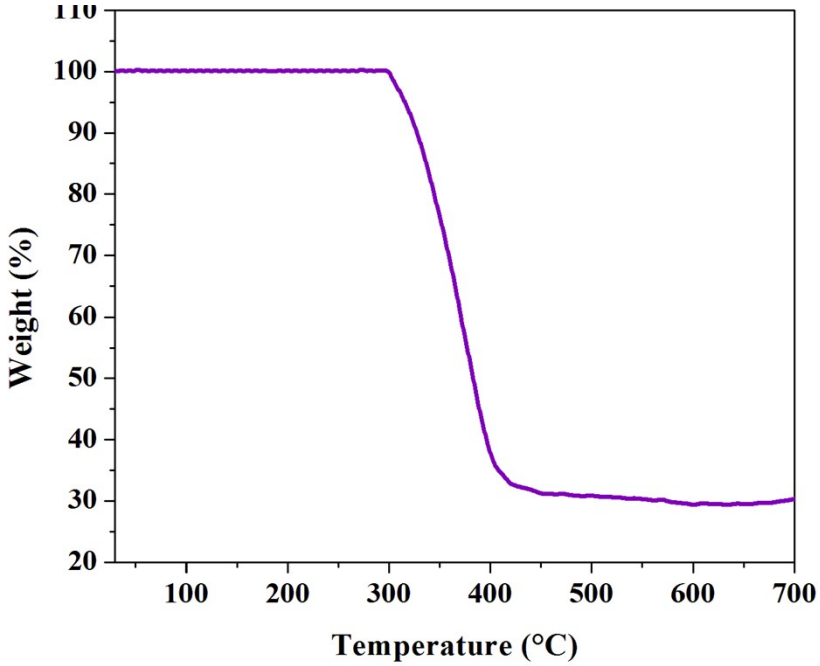


Fig. S1 TGA plot of **1**.

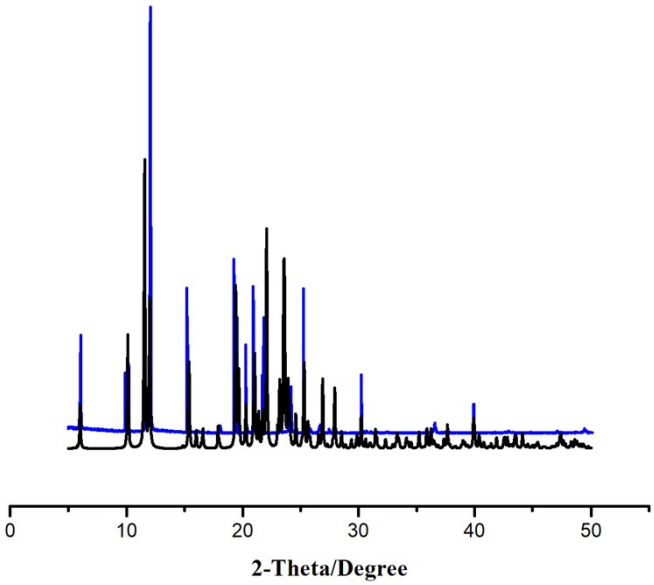


Fig. S2 Powder X-ray diffraction patterns of simulated 1 (black), as-synthesized 1 (blue).

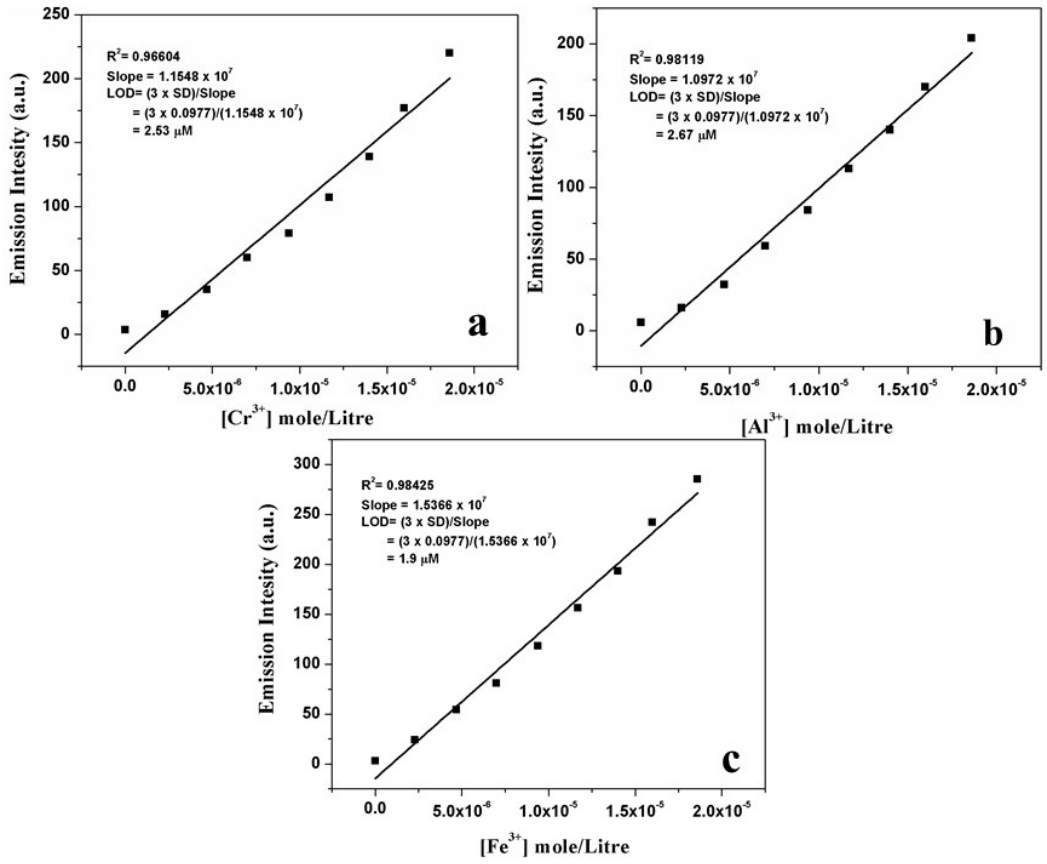


Fig. S3 Calculation of limit of detection (LOD) for M^{3+} ions (a) Cr^{3+} (b) Al^{3+} and (c) Fe^{3+}.

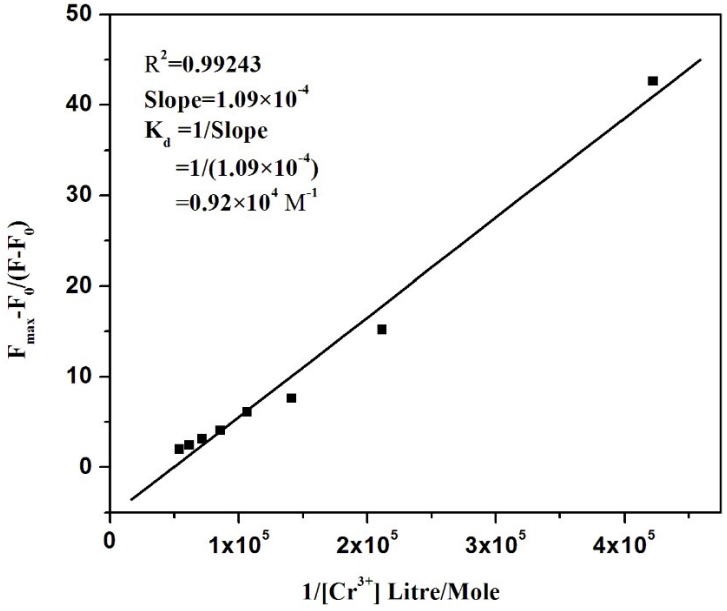


Fig. S4 Benesi–Hildebrand plot for determining the binding constant (K_d) of **1** with Cr^{3+}.

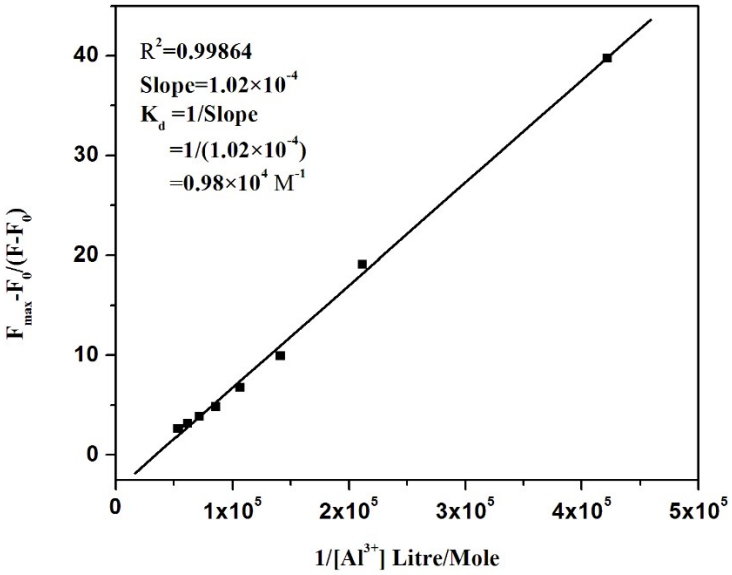


Fig. S5 Benesi–Hildebrand plot for determining the binding constant (K_d) of **1** with Al^{3+} .

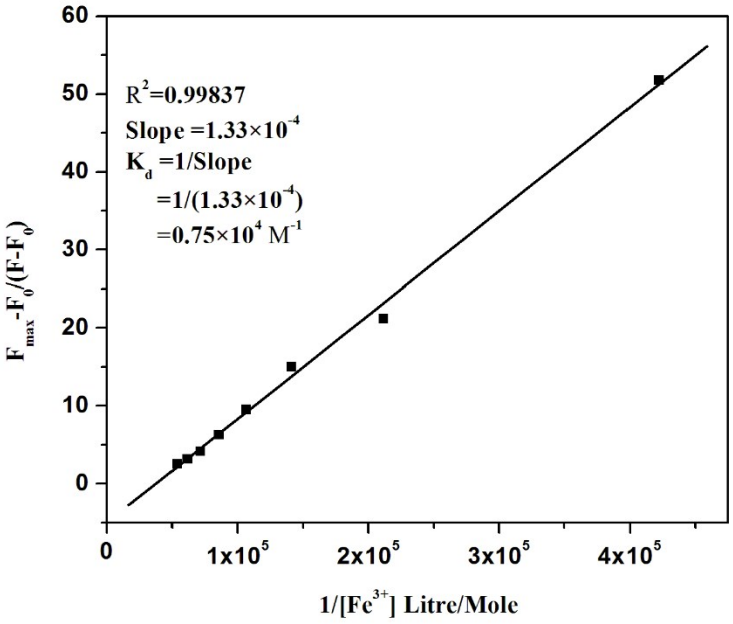


Fig. S6 Benesi–Hildebrand plot for determining the binding constant (K_d) of **1** with Fe^{3+}.

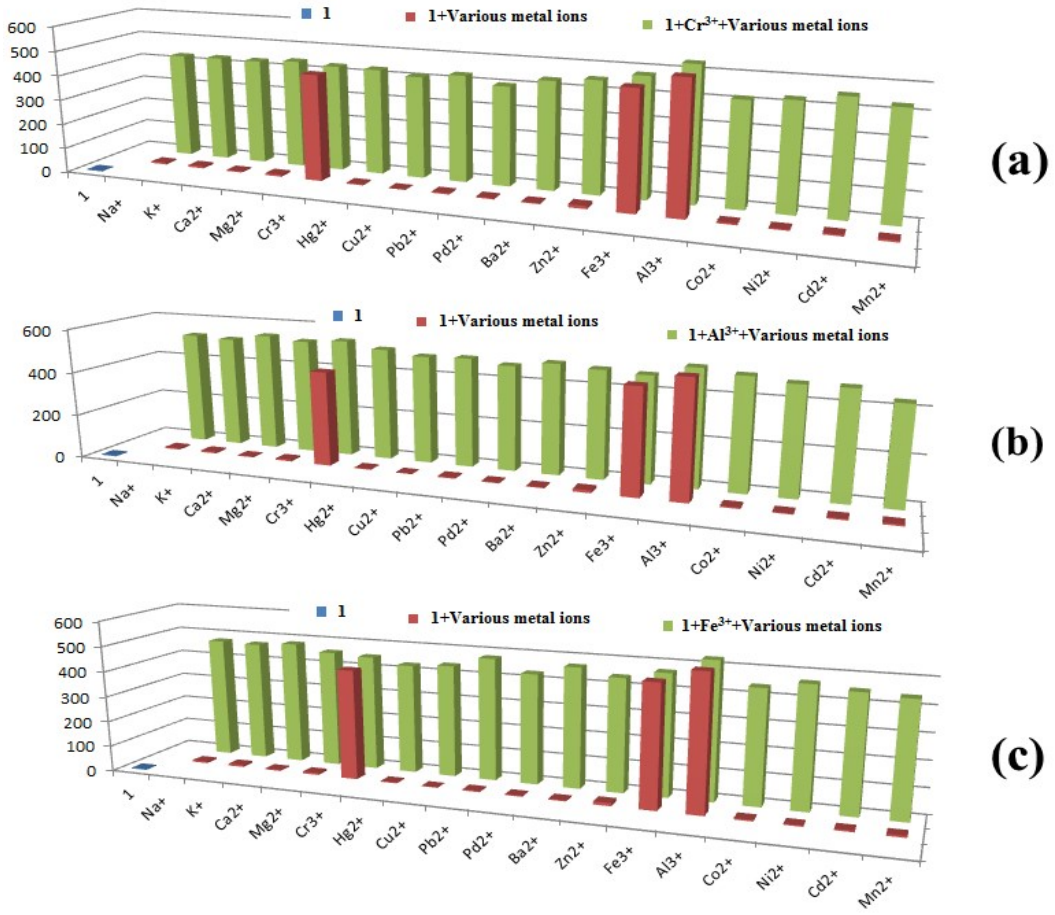


Fig. S7 Interference studies by various metal ions on M^{3+} sensitivity (a) Cr^{3+}, (b) Al^{3+} and (c) Fe^{3+}.

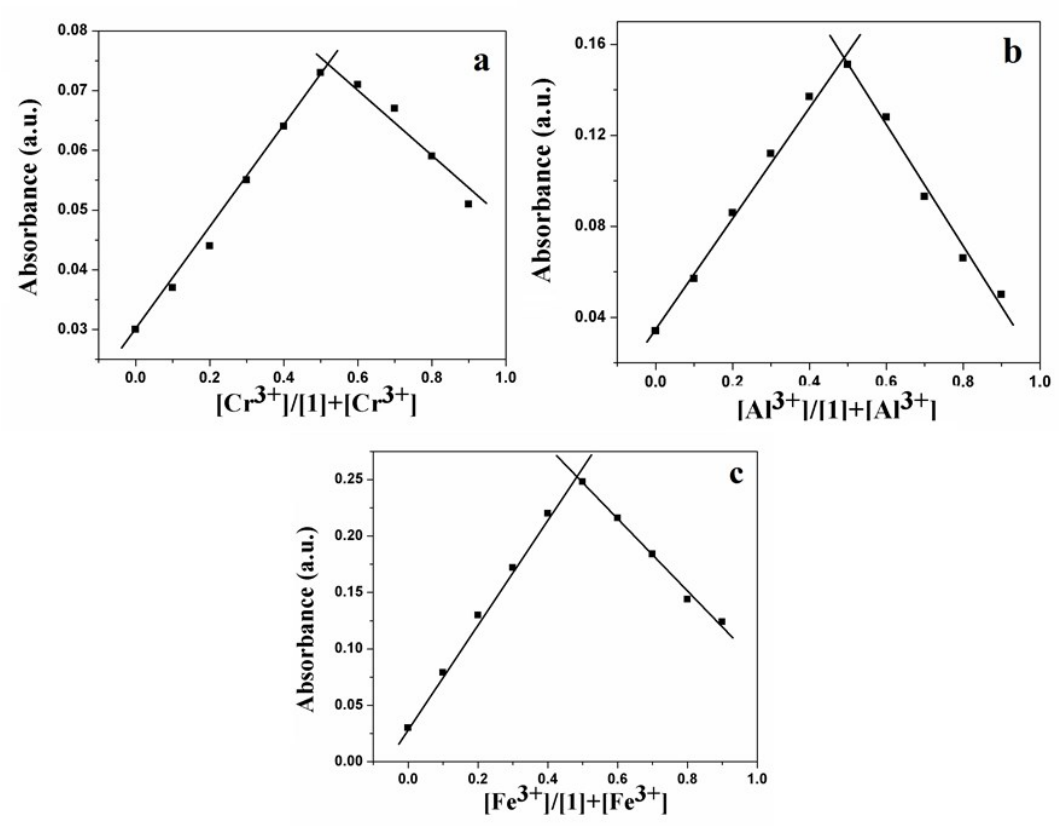


Fig. S8 Job's plots for the determination of binding stoichiometry of **1** with selective metal ions (a) Cr^{3+}, (b) Al^{3+} and (c) Fe^{3+}.

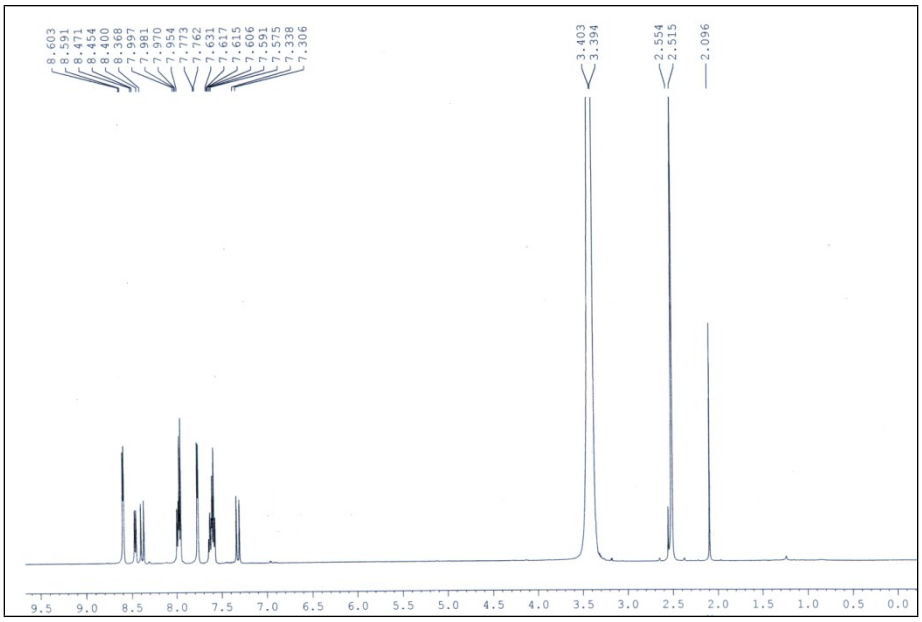


Fig. S9 ^{1}H NMR spectrum of compound **1**in DMSO-d_6.

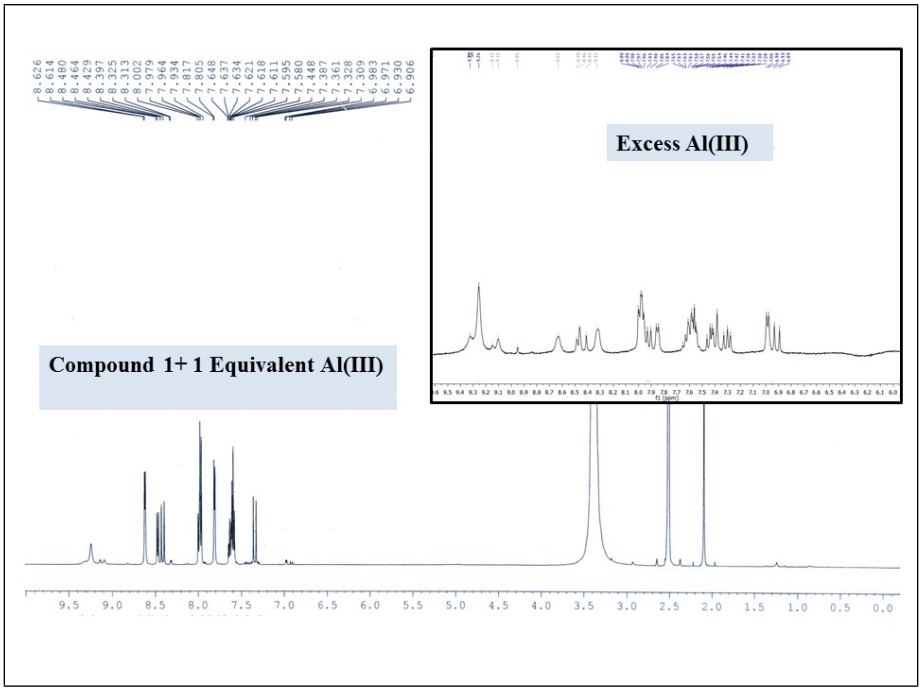


Fig. S10 ^{1}H NMR spectra (in DMSO-d_6) of compound 1 with $Al^{3+}$and partial spectra (inset)of compound 1 with excessAl^{3+}(in DMSO-d_6).

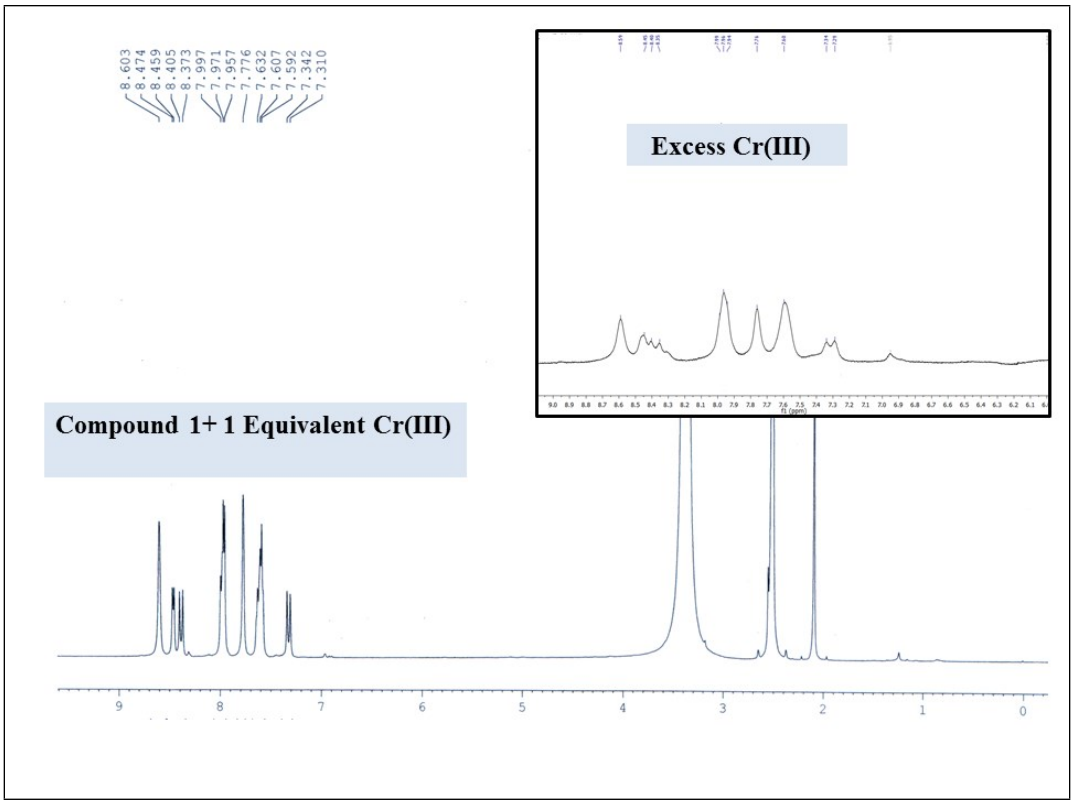


Fig. S11 ^{1}H NMR spectrum (in DMSO-d_6) of compound **1** with $Cr^{3+}$and partial spectra (inset) of compound **1** with excess Cr^{3+}(in DMSO-d_6).

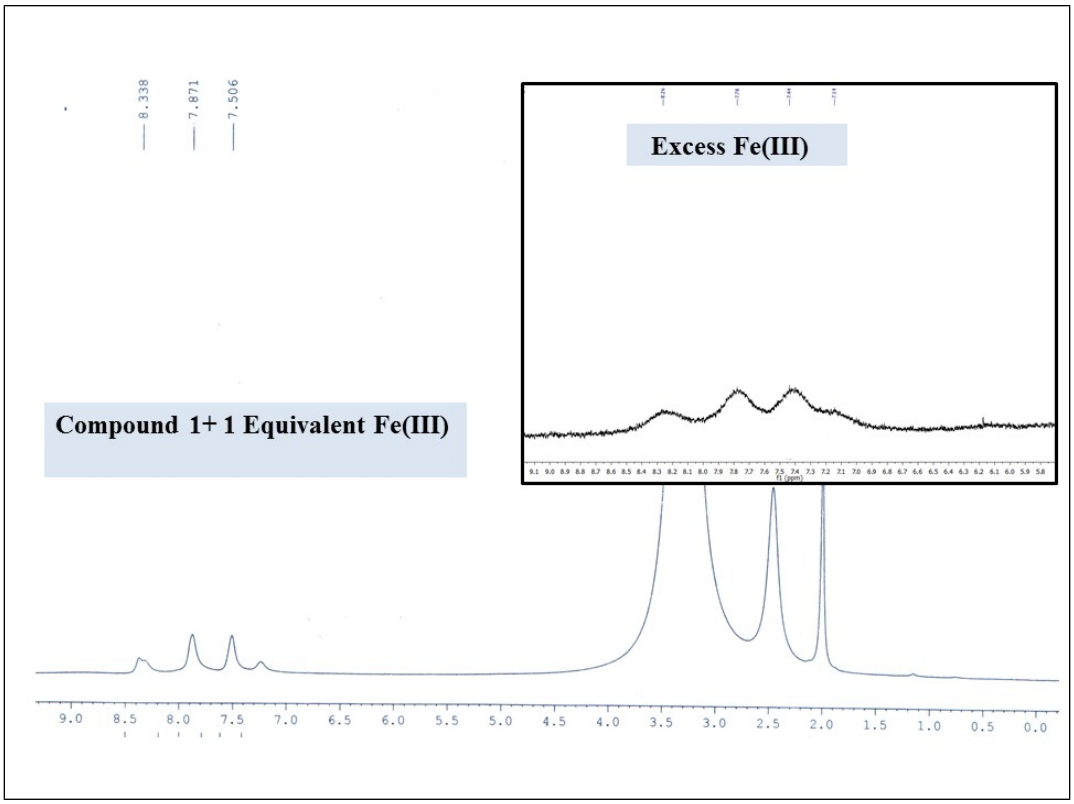


Fig. S12 ^{1}H NMR spectra (in DMSO-d_6) of compound **1** with $Fe^{3+}$and partial spectra (inset)of compound **1** with excess Fe^{3+}(in DMSO-d_6).

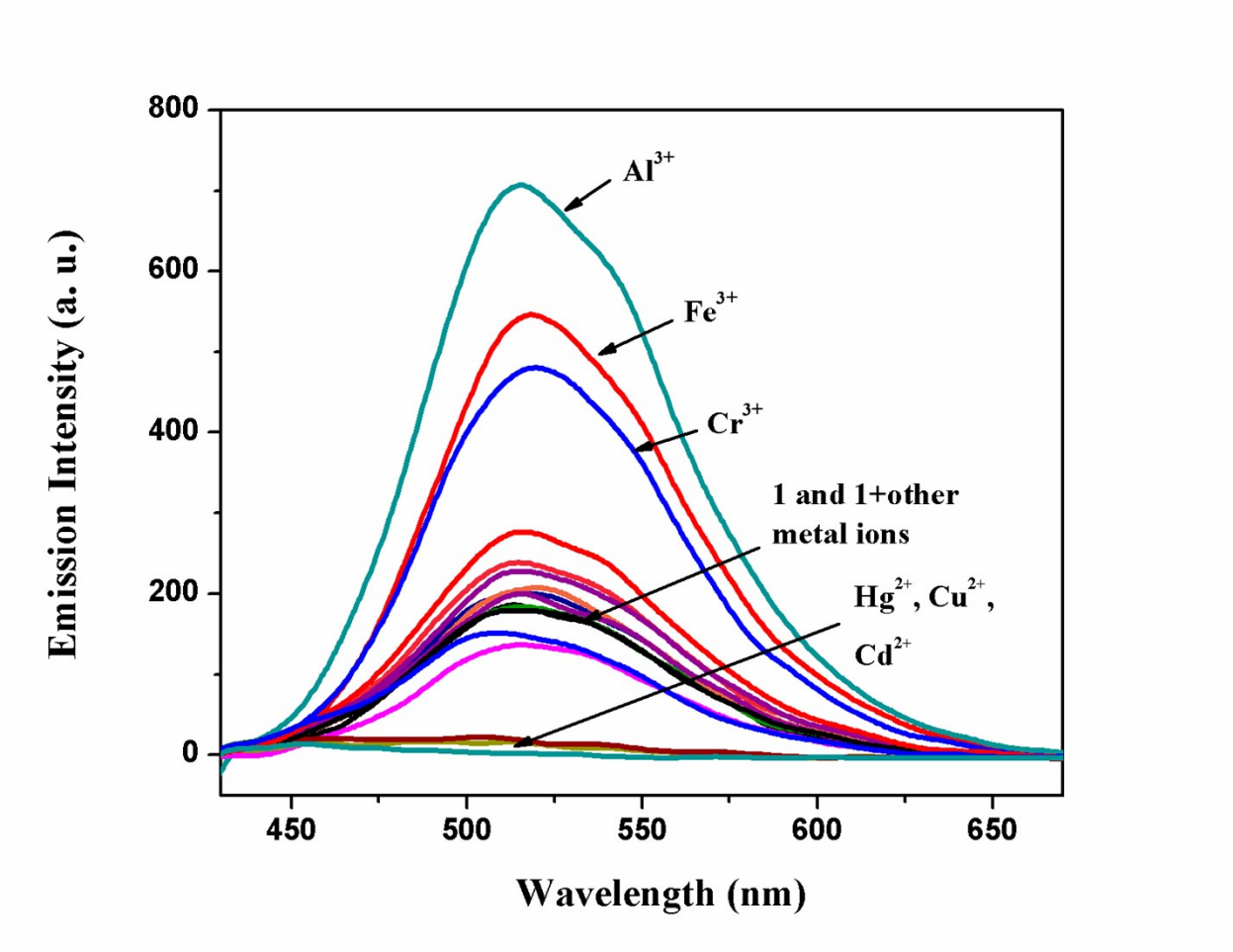


Fig. S13 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in acetone, λ_{ex}, 400 nm.

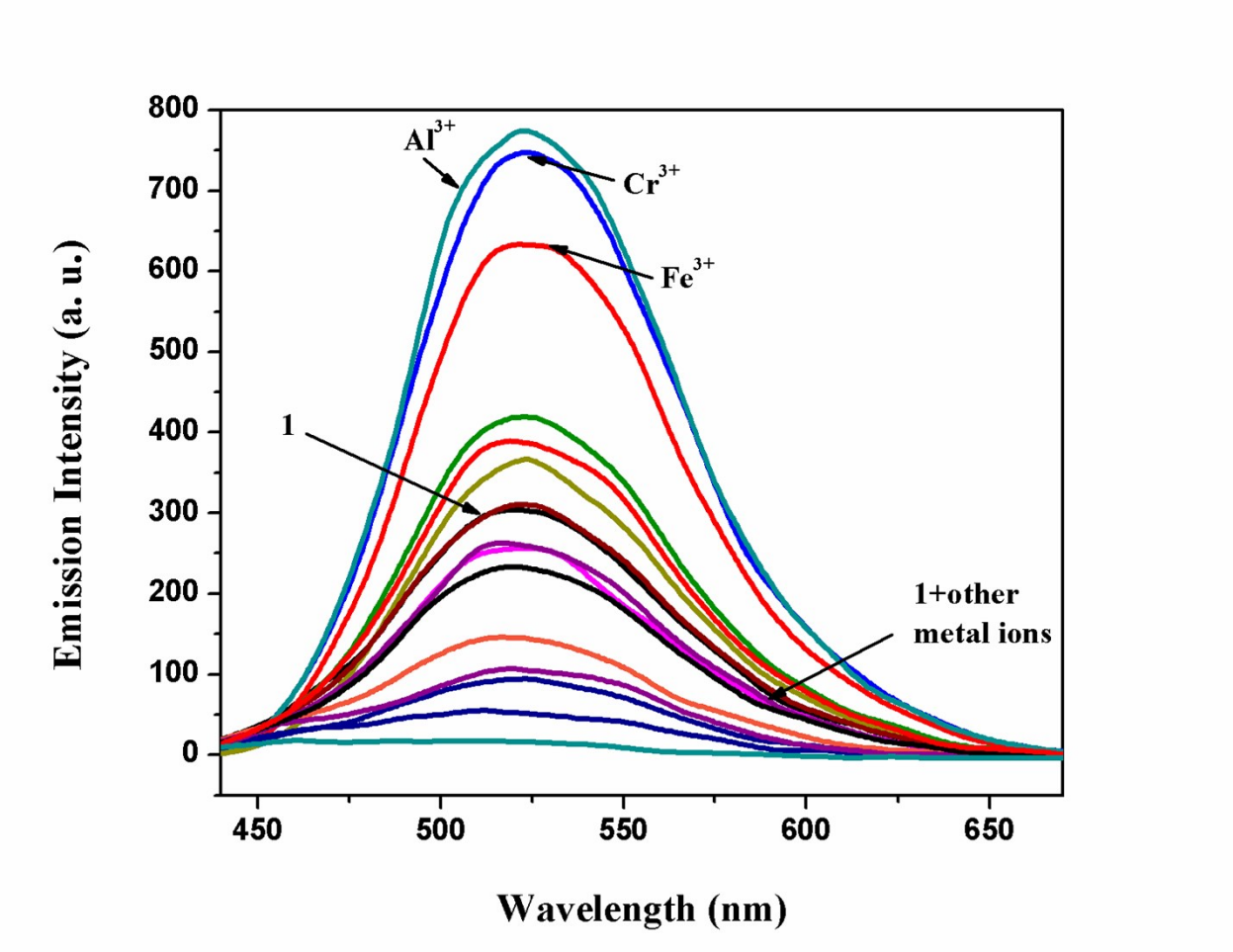


Fig. S14 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in acetonitrile, λ_{ex}, 400 nm.

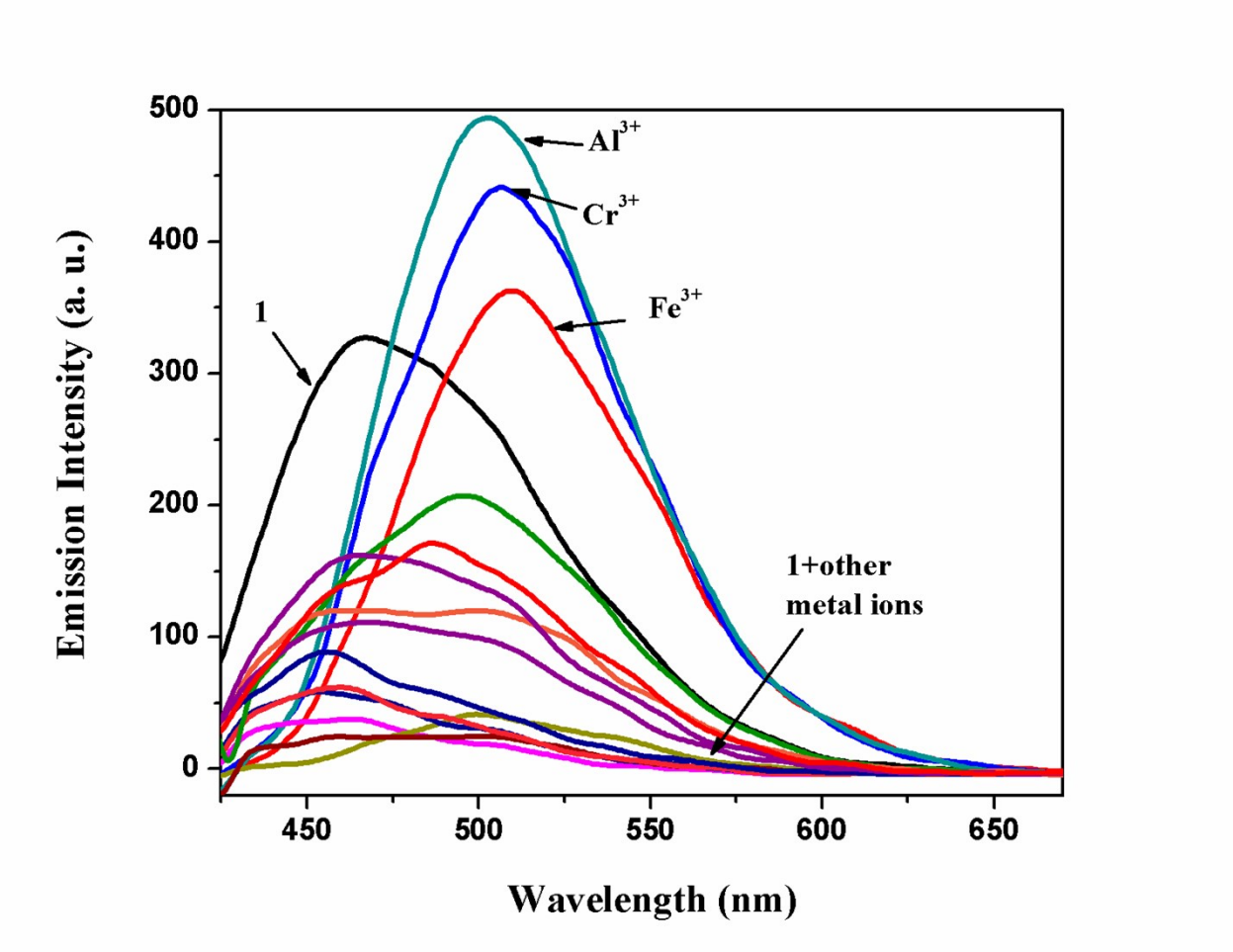


Fig. S15 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in dichloromethane, λ_{ex}, 400 nm.

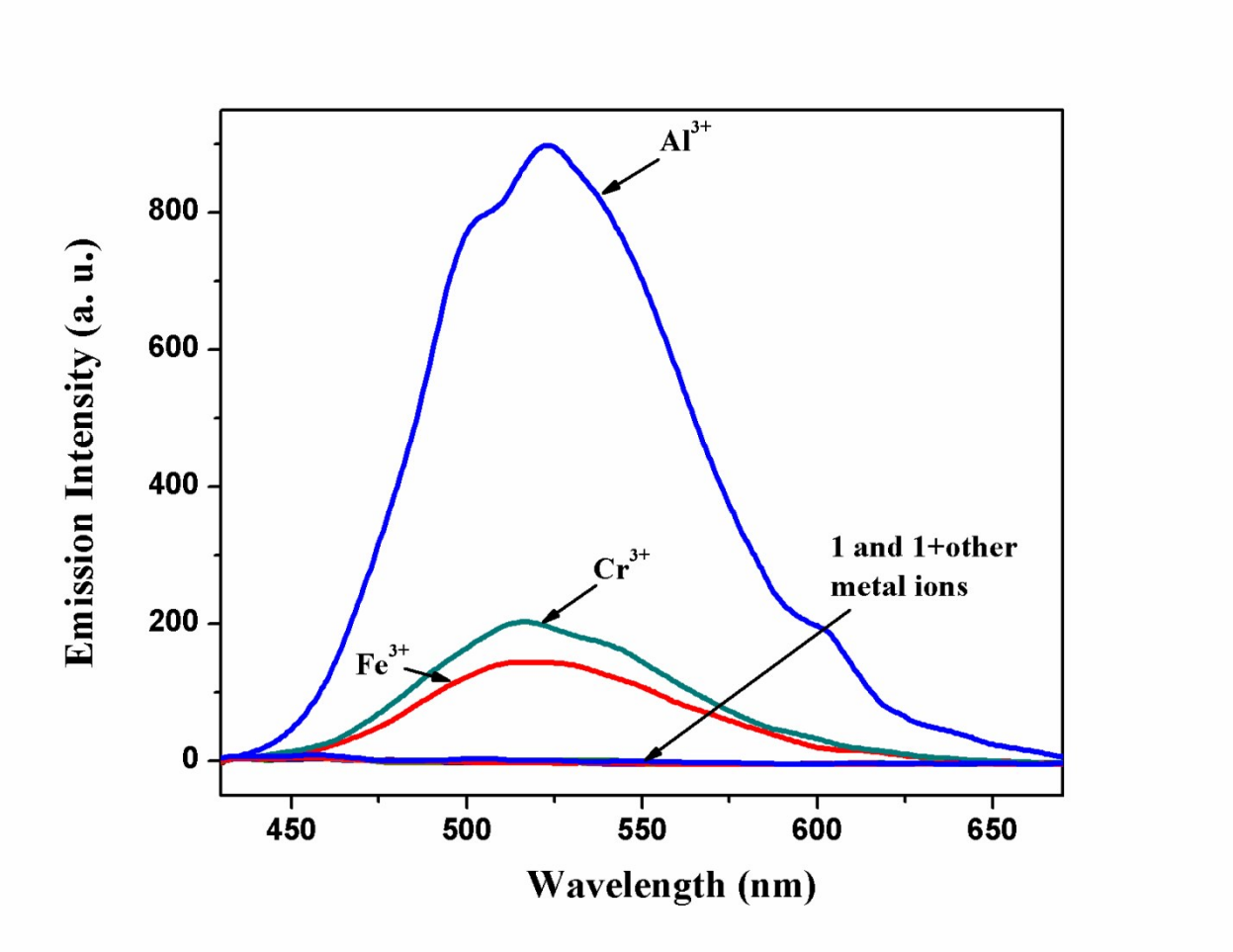


Fig. S16 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in DMF, λ_{ex}, 400 nm.

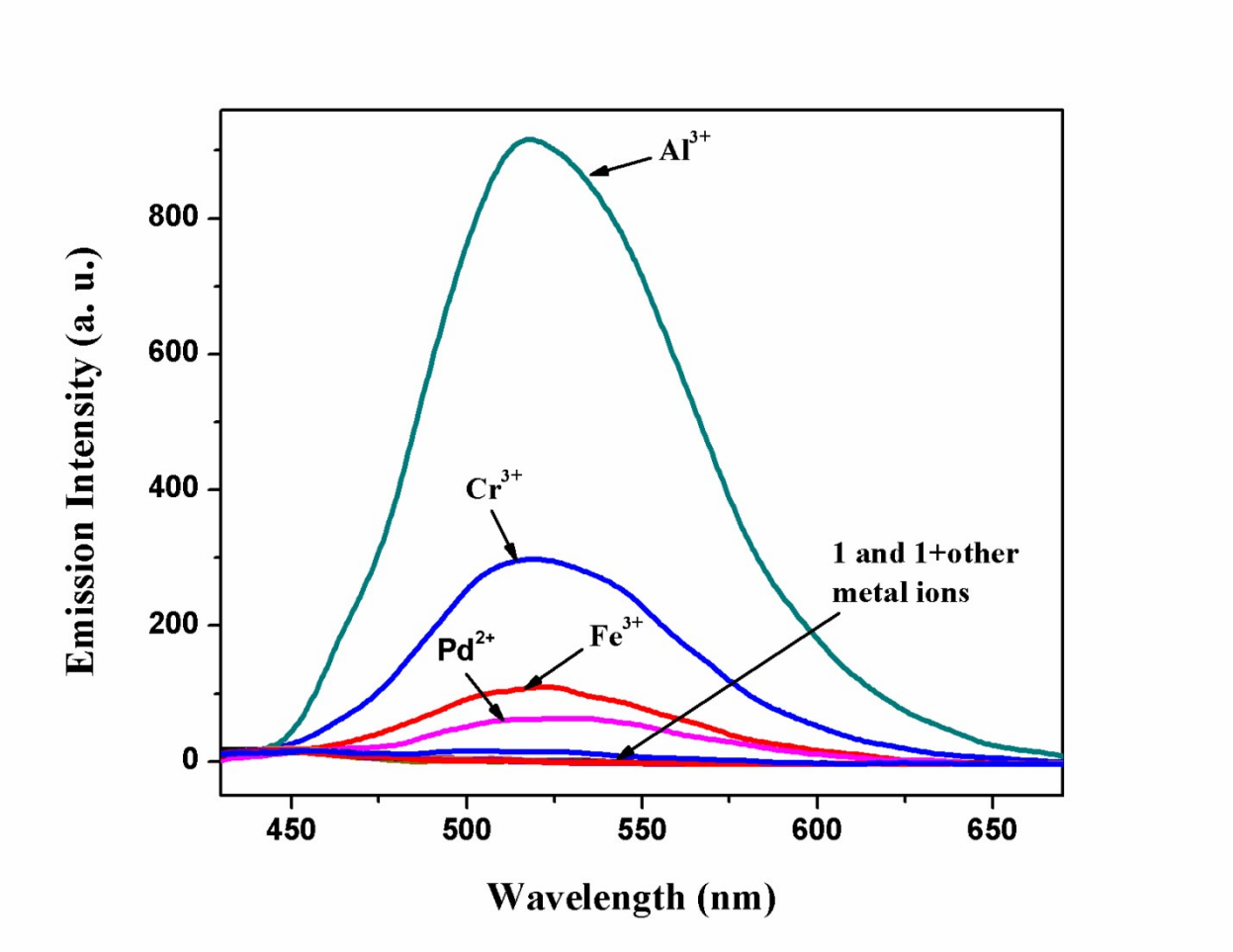


Fig. S17 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in DMSO, λ_{ex}, 400 nm.

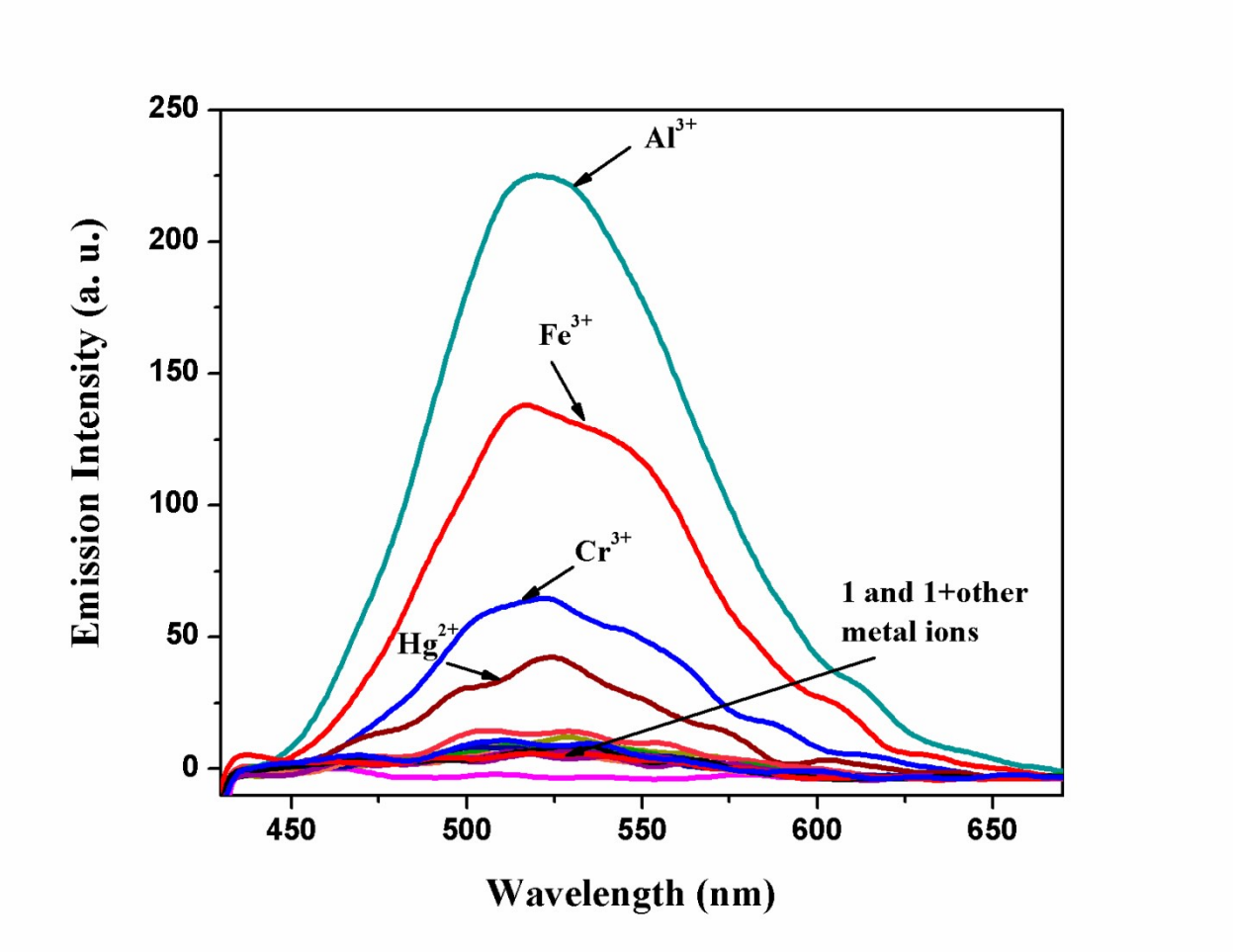


Fig. S18 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in water, λ_{ex}, 400 nm.

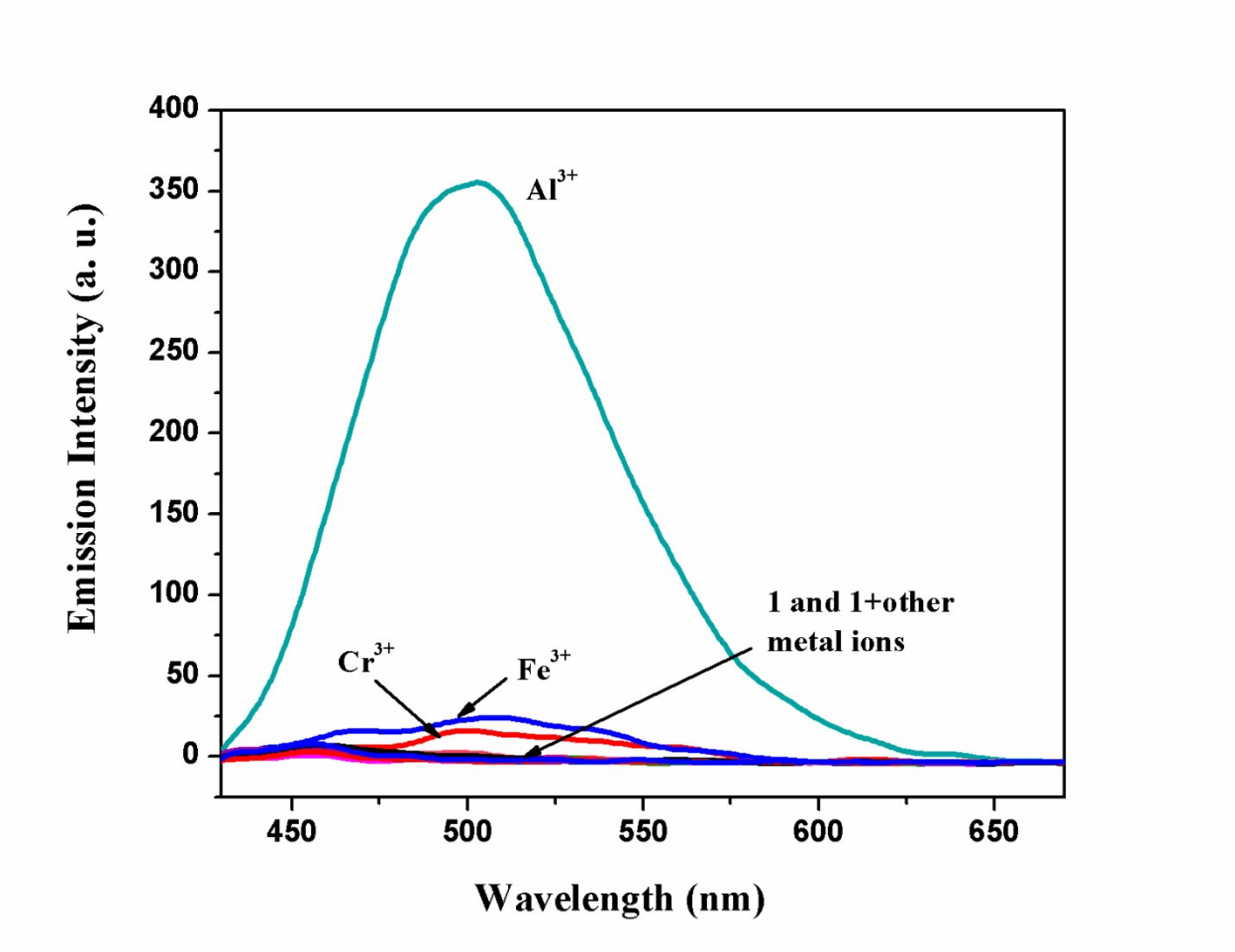


Fig. S19 Change in emission spectrum of **1** (20 μM) with addition of different metal ions (60 μM each) in THF, λ_{ex}, 400 nm.

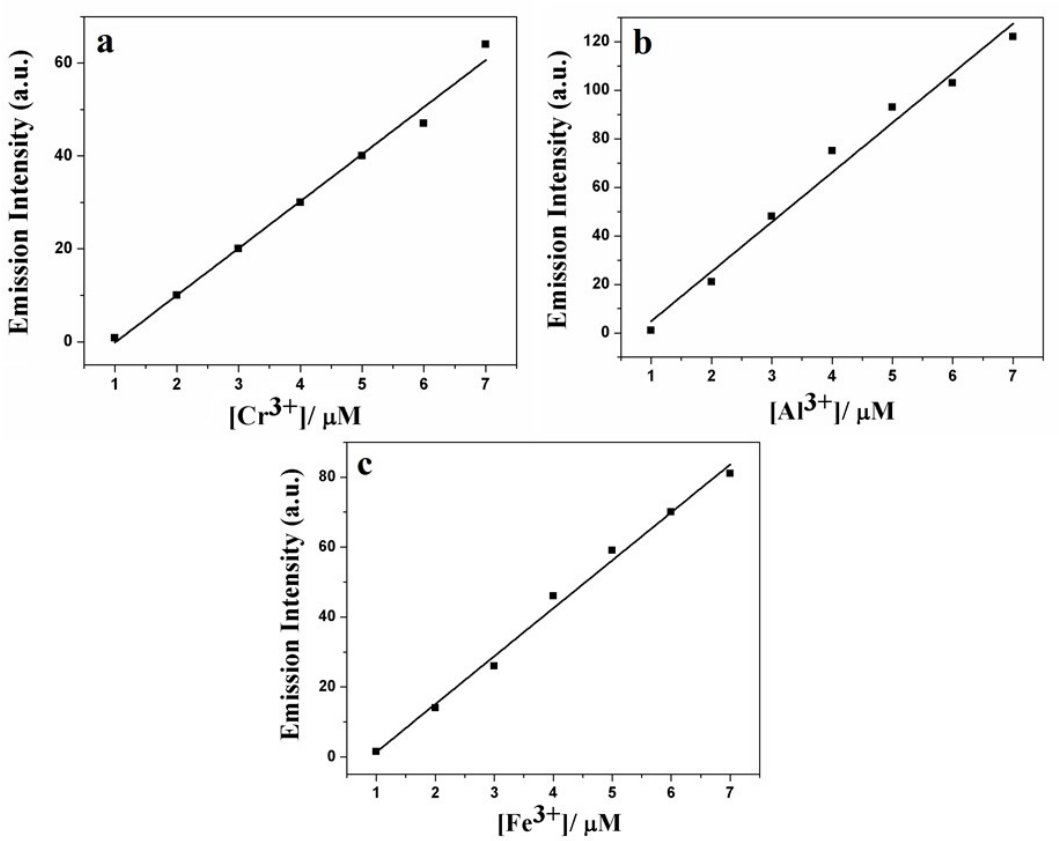
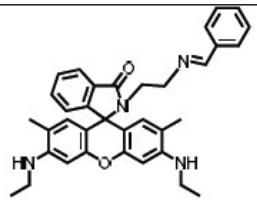
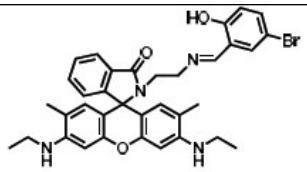
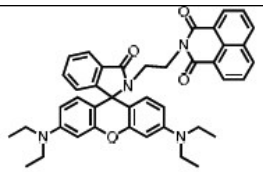
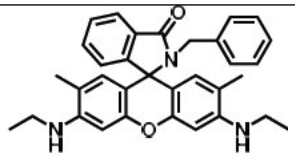
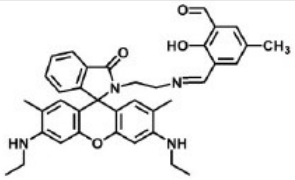
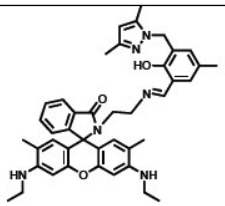
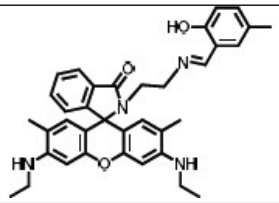
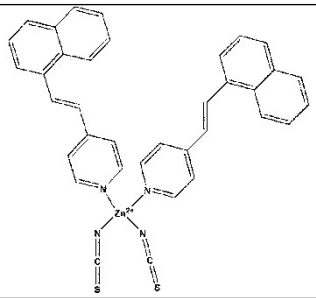


Fig. S20 Calibration plot for ion recovery (a) Cr^{3+}, (b) Al^{3+} and (c) Fe^{3+}.

Table S3. Comparison of some parameters of some recently published related research works

Entry	Sensor Molecule	Fluorescence Enhancement (fold)	Concerned Cations	LOD	Cell Imaging	Reference
1		–	Fe^{3+}	–	Yes	1
2		98 (Al^{3+}) 50 (Cr^{3+}) 38 (Fe^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	1.18 nM (Al^{3+}), 1.80 nM (Cr^{3+}), 4.04 nM (Fe^{3+})	No	2

3		62 (Al^{3+}) 1.7 (Cr^{3+}) 1.47 (Fe^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	1.74 nM (Al^{3+}), 2.36 µM (Cr^{3+}), 2.90 µM (Fe^{3+})	No	3
4		31 (Al^{3+}) 26 (Cr^{3+}) 41 (Fe^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	1.34 µM (Al^{3+}), 2.28 µM (Cr^{3+}), 1.28 µM (Fe^{3+})	Yes	4
5		1465 (Al^{3+}) 588 (Cr^{3+}) 800 (Fe^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	6.97 nM (Al^{3+}), 15.80 nM (Cr^{3+}), 14.00 nM (Fe^{3+})	Yes	5
6		14 (Al^{3+}) 10 (Cr^{3+}) 21 (Fe^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	0.34 µM (Al^{3+}), 0.31 µM (Cr^{3+}), 0.29 µM (Fe^{3+})	Yes	6
7		630	Al^{3+}	2.8 nM	Yes	7
8		117 (Fe^{3+}), 130 (Al^{3+}) , 107 (Cr^{3+})	Al^{3+}, Cr^{3+}, Fe^{3+}	2.53 µM (Cr^{3+}), 2.67 µM (Al^{3+}) , 1.9 µM (Fe^{3+})	Yes	This work

Reference:

1. M. H. Lee,H. Lee, M. J. Chang, H. S. Kim, C. Kang and J. S. Kim, *Dyes Pigm.*, **2016**, *130*, 245.
2. S. Dey, S. Sarkar, D. Maity and P. Roy, *Sens. Actuators, B*,**2017**, *246*, 518.
3. S. Paul, A. Manna and S. Goswami, *Dalton Trans.*, **2015**,*44*, 11805.
4. D. Das, R. Alam, A. Katarkar and M. Ali, *Photochem. Photobiol. Sci.*, **2019**, *18*, 242.

5. A. Roy, S. Das, S. Sacher, S. K. Mandal and P.Roy, *Dalton Trans.*, **2019**, *48*, 17594.
6. R. Alam, R. Bhowmick, A. S. M. Islam,A. Katarkar, K. Chaudhuri and M. Ali, *New J. Chem.*, **2017**,*41*, 8359.
7. A. Roy, R. Mukherjee, B. Dam, S. Dam and P. Roy, *New J.Chem.*,**2018**, *42*, 8415.