Supporting Information

for

A water soluble Al^{3+} selective colorimetric and fluorescent turn-on chemosensor and its application in living cell imaging

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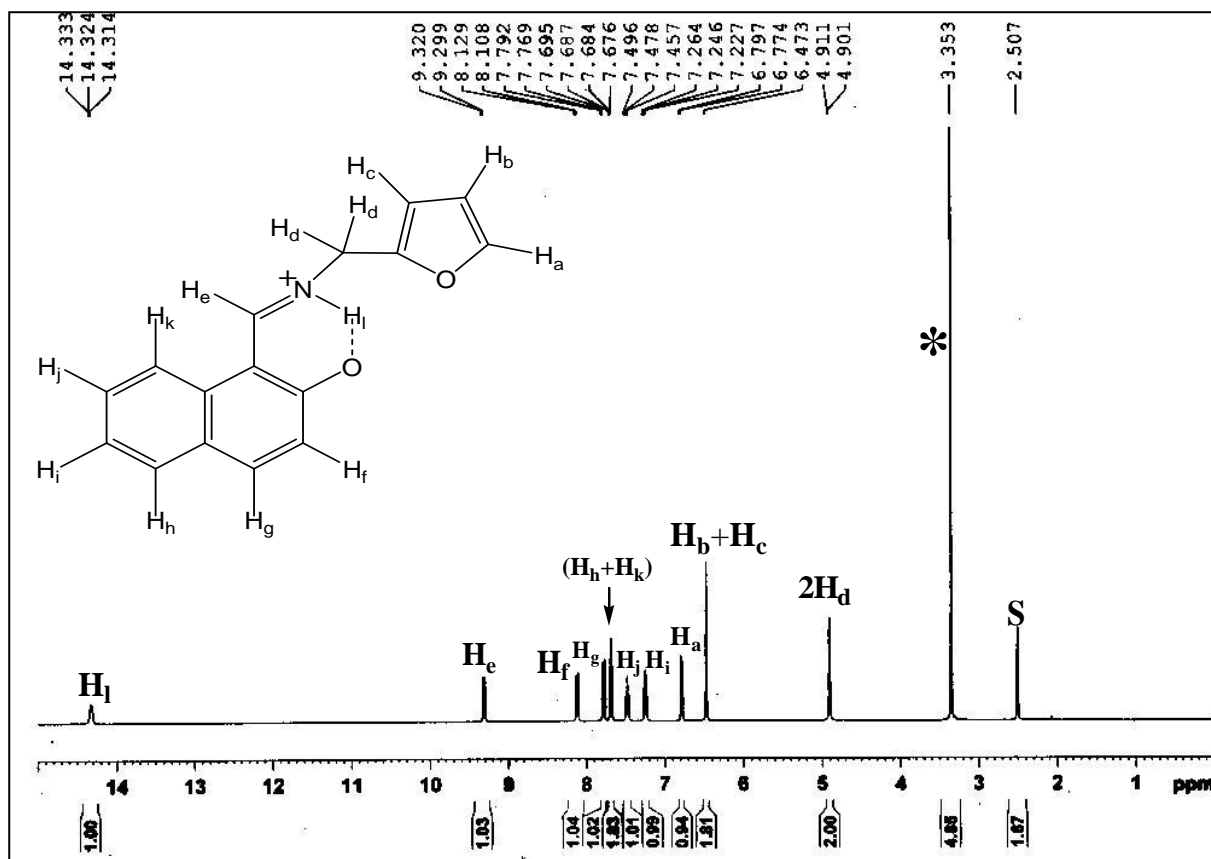
Contents

Figure S1. ^{1}H NMR spectrum of **1-H** (DMSO-d_6, 300 MHz). The signal marked with * and S are for H_2O and solvent peak(DMSO-d_6), respectively.
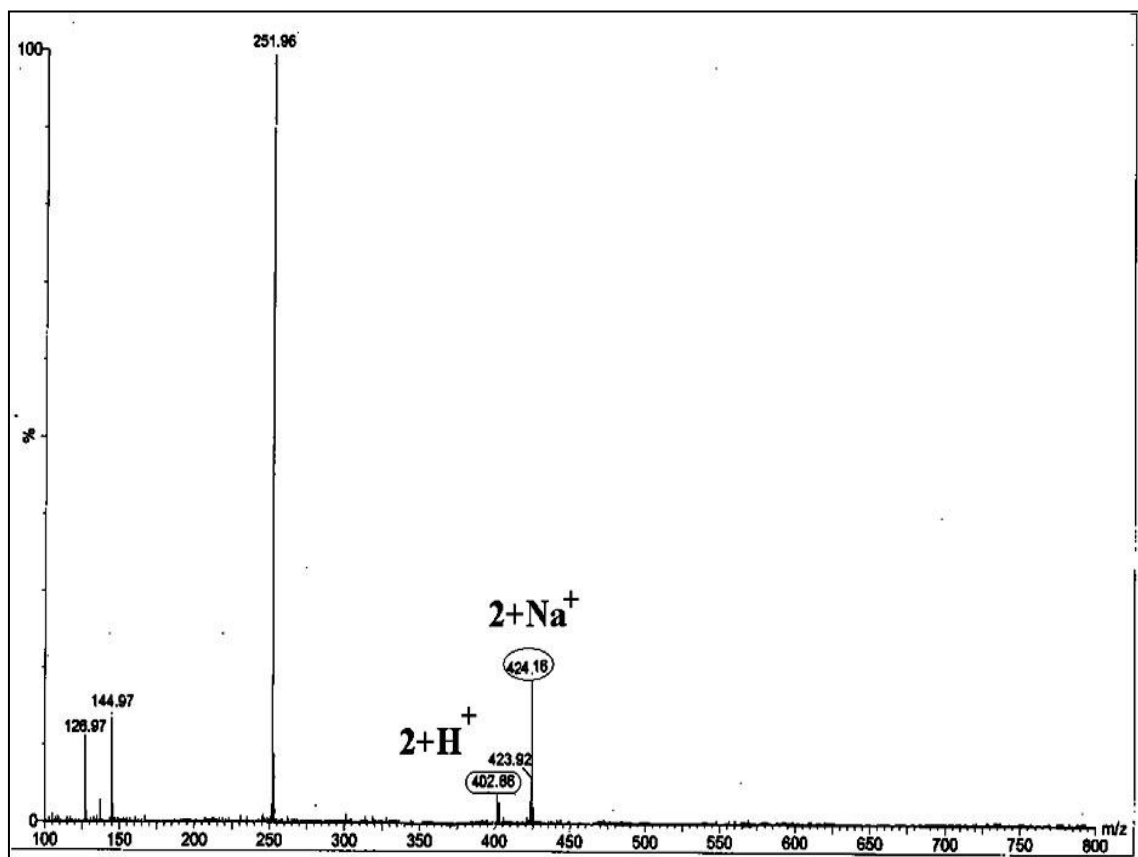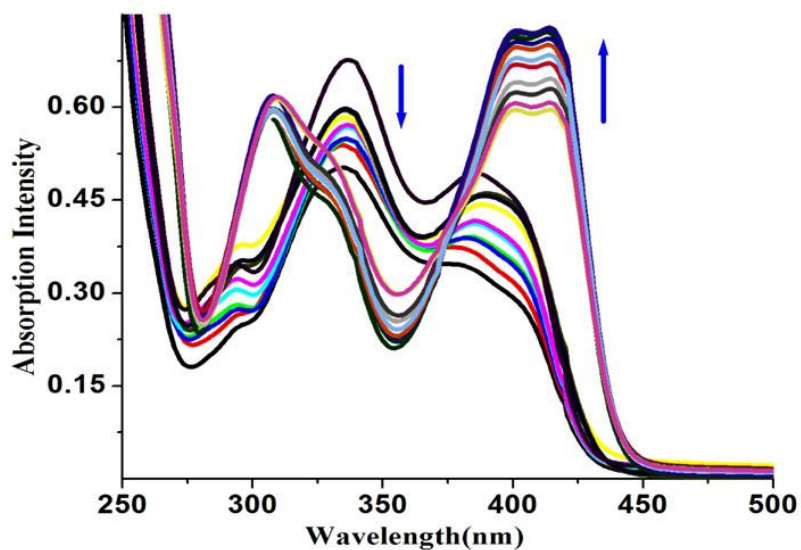
Figure S2. Mass spectrum of **2**.

Figure S3. Absorption spectra of 12.5 μM of **1-H** in presence of 0, 2.5, 5.0, 7.5, 12.5, 15, 17.5, 20, 22.5, 31.0, 62.5, 87.5 μM of Al^{3+} and at high conc. , 40, 60, 80, 100, 120, 140, 160, 180, 200 times of Al^{3+} in DMSO/water (1/100) at 25°C temperature.
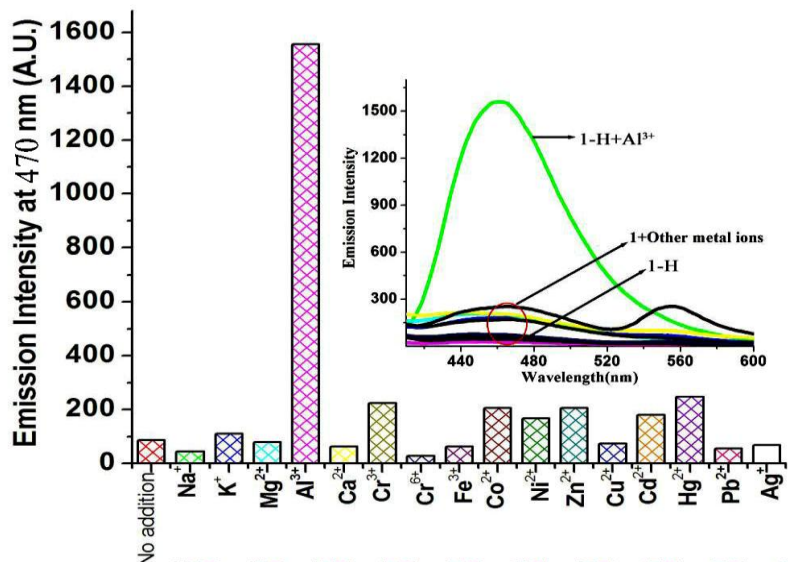

Fig.S4. Emission enhancement spectra of **1-H** (10 μM) in presence of different metal ions (200 μM) in 100 mM HEPES buffer solution.
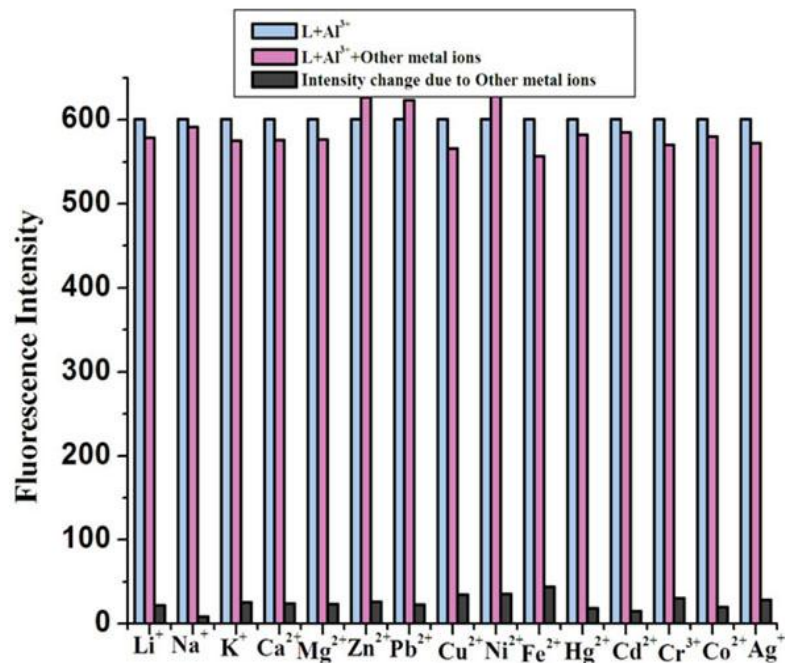
Fig.S5. Interference of different metal ions (200 µM) in presence of **1-H** (20 µM) and Al^{3+} (20 µM) in 100 mM HEPES buffer (DMSO/water : 1/100)

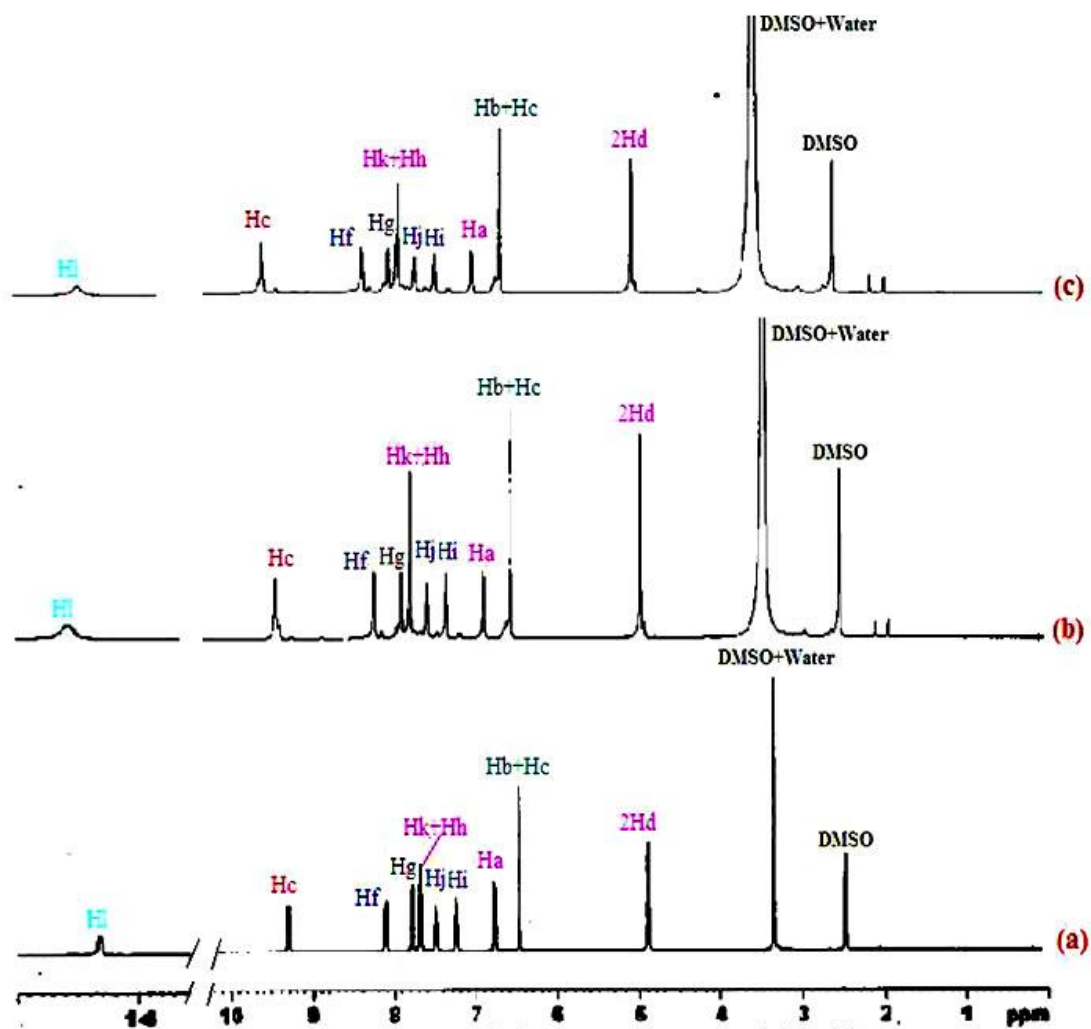**Fig.S6.** Partial ^{1}H NMR titration (DMSO-d_6, 400 MHz) (a) of **1-H**; ($coc. = 3.5\times10^{-3}$ M) (b) **1-H** + 0.5 equivalent and (c) **1-H** +1 equivalent of Al(NO$_3$)$_3$,9H$_2$O.
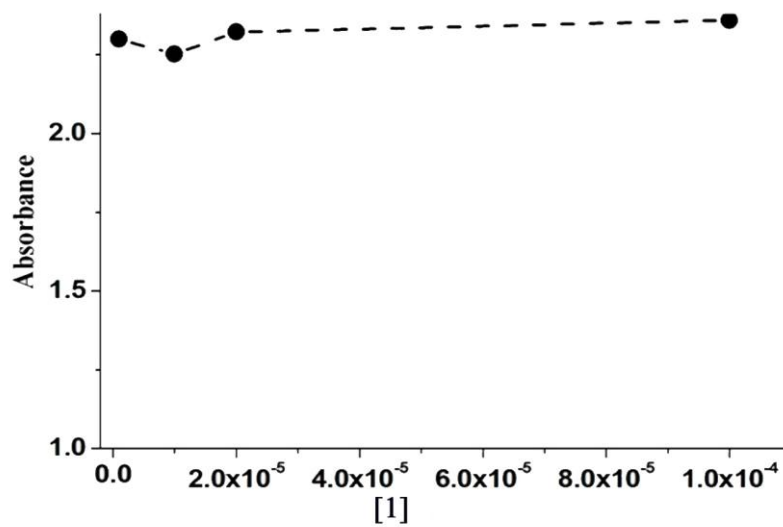
Fig.S7. MTT assay for the determining cytotoxic effect of **1-H** which was incubated with HeLa

cell for 18 hours in 24 wells plate. MTT was added and after 3 hours, absorbance was

measured at 590 nm.

Table S1. Crystal data and details of refinements for **1-H**

Empirical Formula	$C_{16}H_{13}NO_2$
Formula Weight	251.27
Crystal System	Monoclinic
Space group	P 21/c
a (Å)	9.7368(5)
b (Å)	9.5514(4)
c (Å)	13.8091(7)
α (°)	90.00
β (°)	107.501(5)
γ (°)	90.00
Volume ($Å^3$)	1224.80(11)
Temperature,K	120(2)
Z	4
ρ_{calc} (g/cm^3)	0.336
F (000)	528
μ (MoK_{α}) (mm^{-1})	0.090
Collected reflns	7887
Independent reflns	2156
R1 [$I > 2.0\ \sigma(I)$]	0.0398
wR1 [$I > 2.0\ \sigma(I)$]	0.1154
Goodness-of-fit	1.103

Table S2. Selected bond distances (Å) and bond angles (^{o}) for **1-H**

Bond distances (Å)		Bond angles (^{o})	
C14 - O15	1.348(2)	C14 - O15 - C16	105.25(15)
C11- N12	1.3098(19)	C11- N12 - C13	123.60(14)
O1- C2	1.2712(18)	O1- C2 - C3	120.08(14)
C14 - C18	1.330(2)	C9 - C10 - C1	123.82(14)

Table S3. Selectivity coefficient (k_{sc}) for Al^{3+} over competitive cations

Interfering metal ions	Selectivity coefficient (k_{sc})	$\log(k_{sc})$
Na^+	3447	3.5374
K^+	1407	3.1483
Mg^{2+}	1979	3.2964
Ca^{2+}	2476	3.3938
Cr^{3+}	991	2.9961
Cr^{6+}	5557	3.7449
Fe^{3+}	2477	3.3940
Co^{2+}	855	2.9320
Ni^{2+}	926	2.9667
Zn^{2+}	853	2.9310
Cu^{2+}	2088	3.3198
Cd^{2+}	860	2.9345
Hg^{2+}	924	2.9657
Pb^{2+}	2797	3.4467
Ag^+	2298	3.3614

[a]Selectivity coefficient (k) was calculated as $k_{B,A} = m_B/m_A$; where $m_B = d/dc$(signal of B) and $m_A = d/dc$(signal of A); dc = change of concentration of species; B = Al^{3+} and A = other interfering metal ion