Supporting Material

for

Easily synthesizable naphthalene-based sensing platform for Al^{3+} and Zn^{2+} ions: Theoretical insight and live cells imaging

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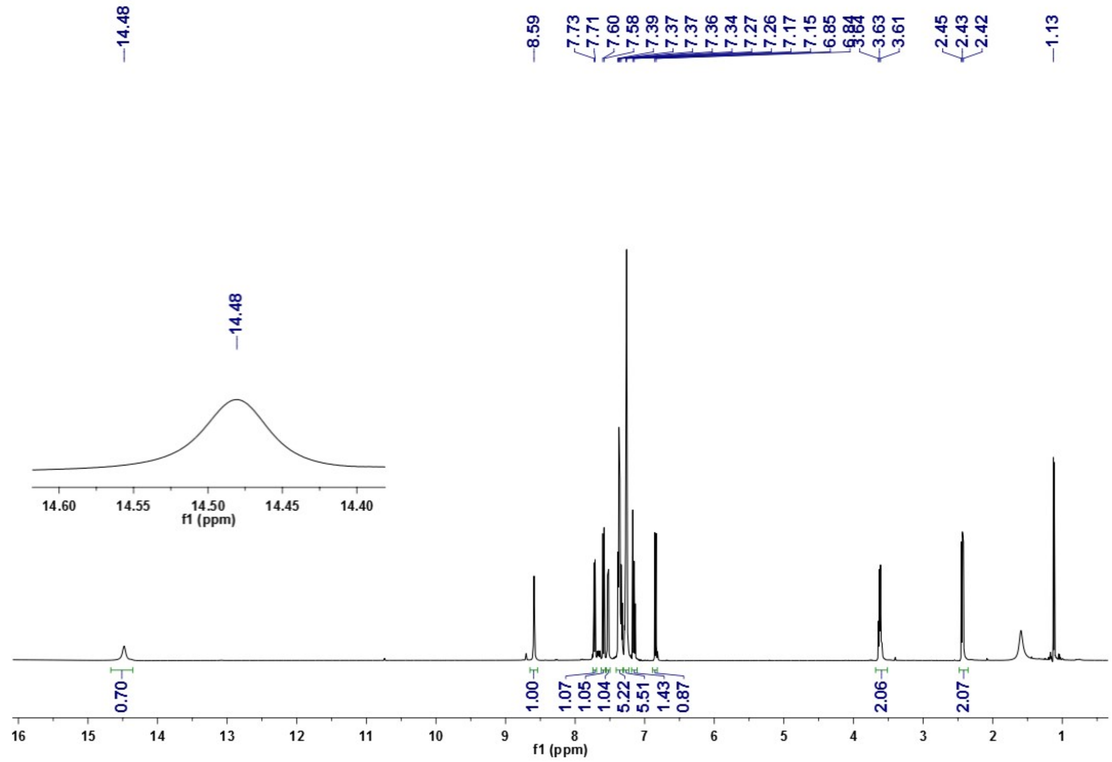


Fig. S1. ^{1}H NMR spectrum of **HL** in $CDCl_3$ at room temperature. ^{1}H NMR ($CDCl_3$, 500 MHz, TMS), δ (ppm): 14.48 (s, 1H, broad, -OH), 8.59 (s, 1H, -CH=N-), 7.72 (d, 1H), 7.59 (d, 1H), 7.52 (d, 1H), 7.39-7.34 (m, 5H), 7.28-7.25 (m, 6H), 7.17-7.14 (m, 1H), 6.84 (d, 1H), 3.63 (t, 2H, -CH_2-N-), 2.43 (t, 2H, -CH_2-P<).

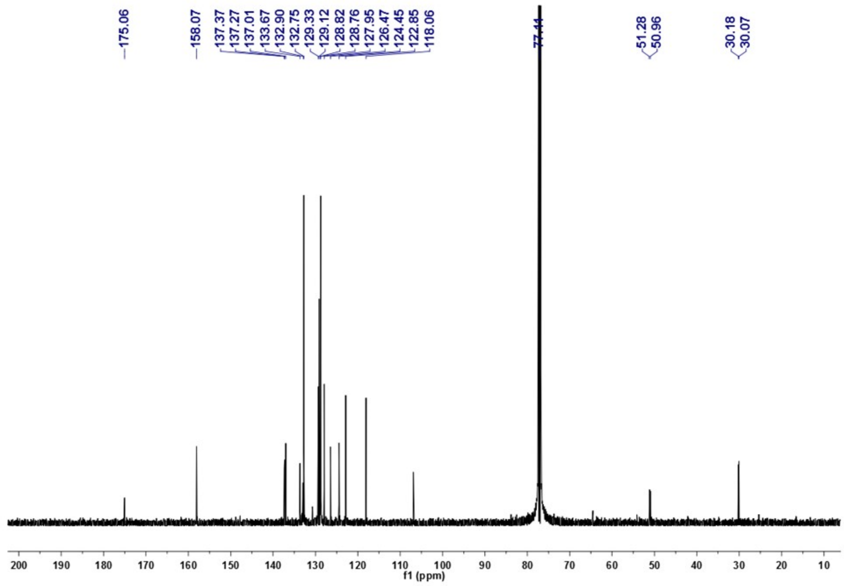


Fig. S2. ^{13}C NMR spectrum of **HL** in $CDCl_3$ at room temperature. ^{13}C NMR ($CDCl_3$, 500 MHz), δ (ppm): 175.06, 158.07, 137.37, 137.27, 137.01, 133.67, 132.90, 132.75, 129.33, 129.12, 128.82, 128.76, 127.95, 126.47, 124.45, 122.85, 118.06, 50.62, 30.12.

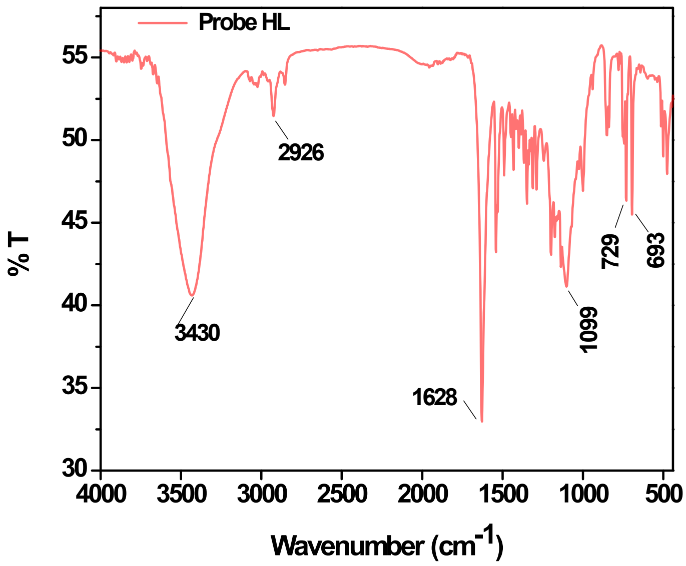


Fig. S3. FT-IR spectrum of **HL**. IR data (KBr disk): 3430, 2926, 1628 ($\nu_{C=N}$), 1480, 1430, 1099, 729, 693, 514 (ν_{PPh2}) cm^{-1}.

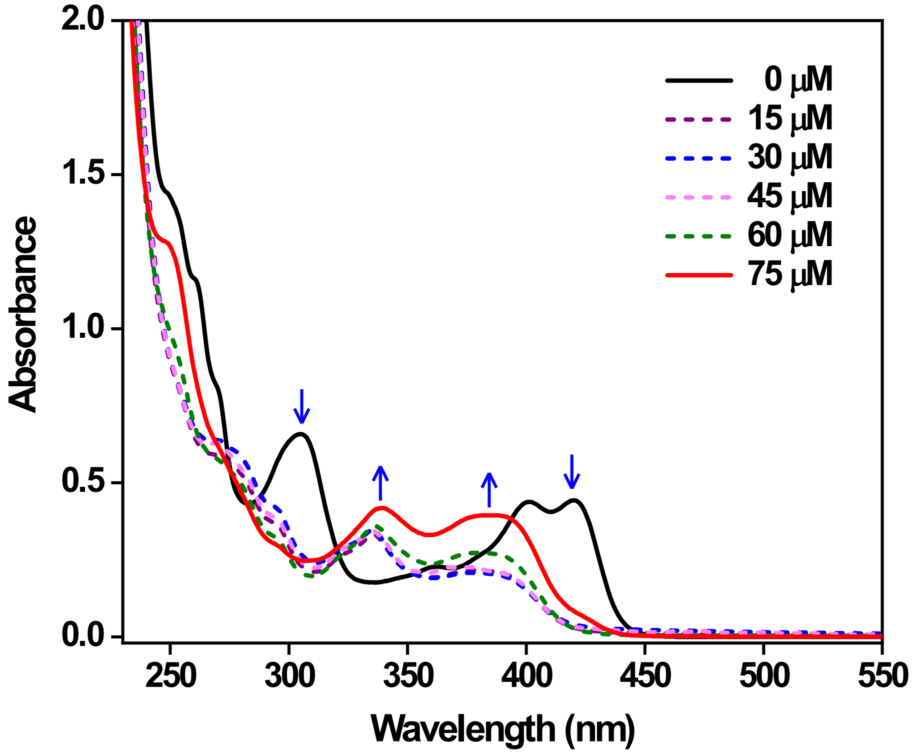


Fig. S4. Changes observed in UV-visible spectra of **HL** (3.3×10^{-5} M) in the presence of 0–75 μM of Al^{3+} ions in CH_3CN solution.

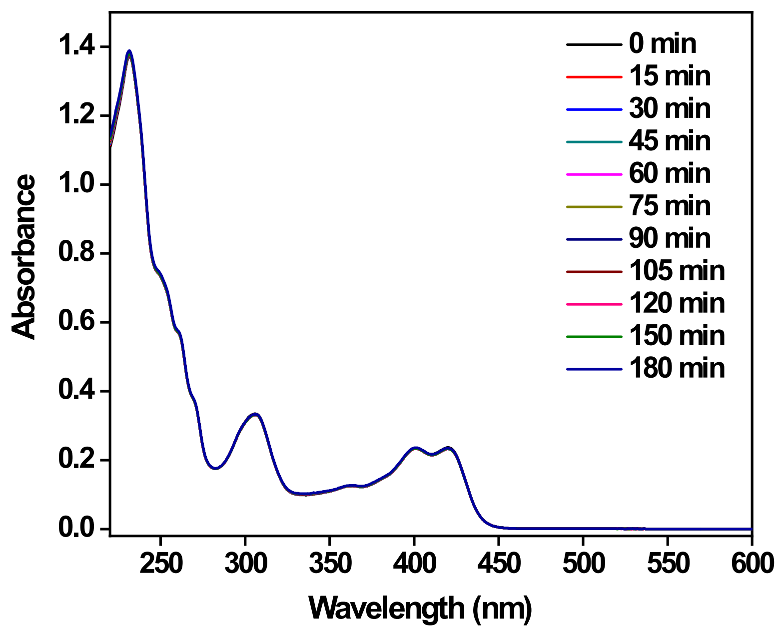


Fig. S5. The stability of fluorescent probe **HL**. UV-visible spectral changes observed for **HL** in CH_3CN solution with different intervals of time.

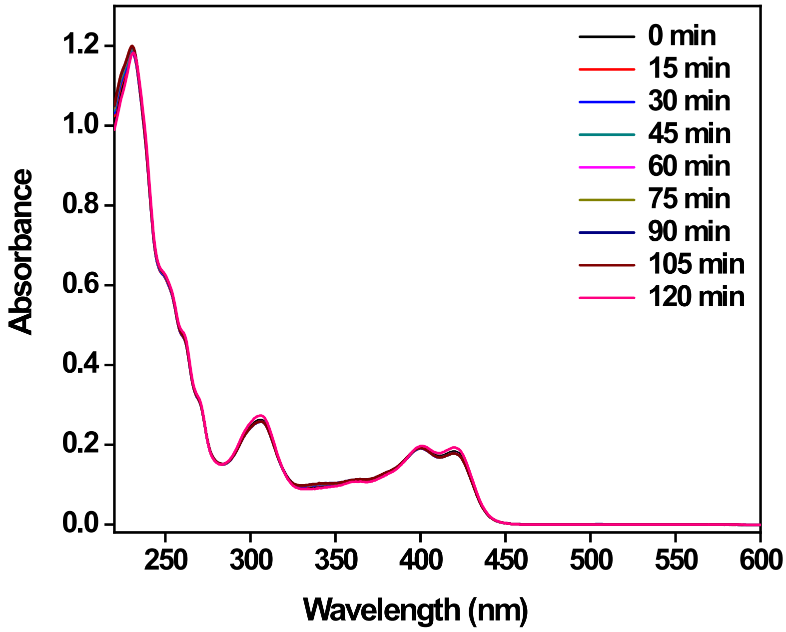


Fig. S6. The stability of fluorescent probe **HL**. UV-visible spectral changes observed for **HL** in CH_3CN-H_2O (4:1, v/v) mixture with different intervals of time.

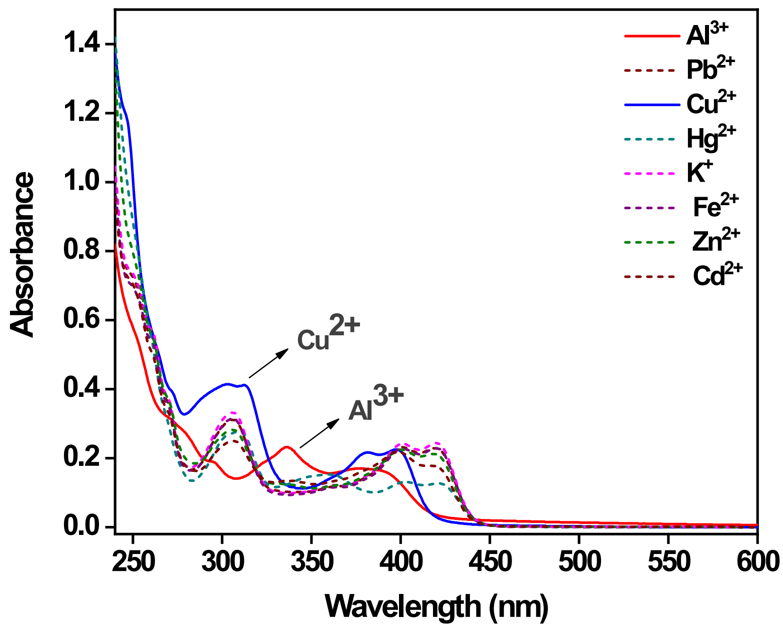


Fig. S7. Absorption spectra of **HL** (3.3×10^{-5} M) on exposure to 3.0 equivalents (i.e., 100 μM) of selected metal ions in CH_3CN-H_2O (4:1, v/v) mixture.

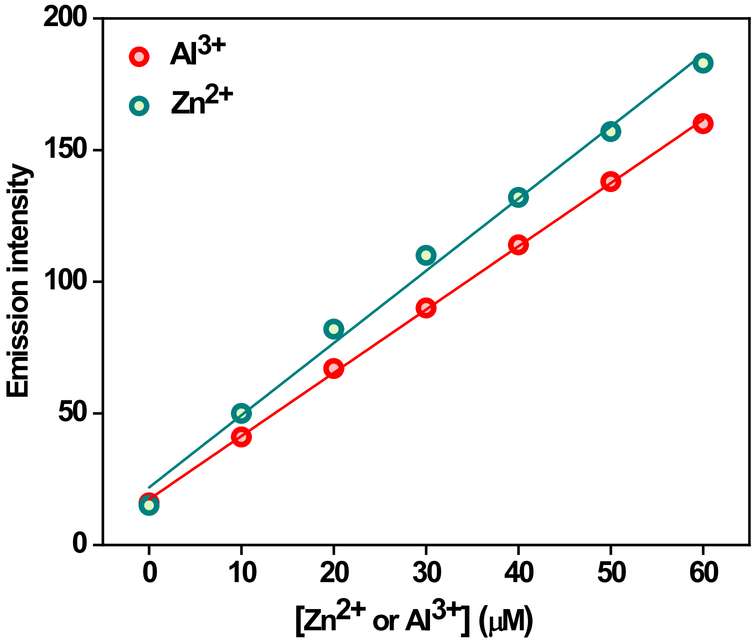


Fig. S8. Detection limits for Al^{3+} (red circles) and Zn^{2+} ions (green circles).

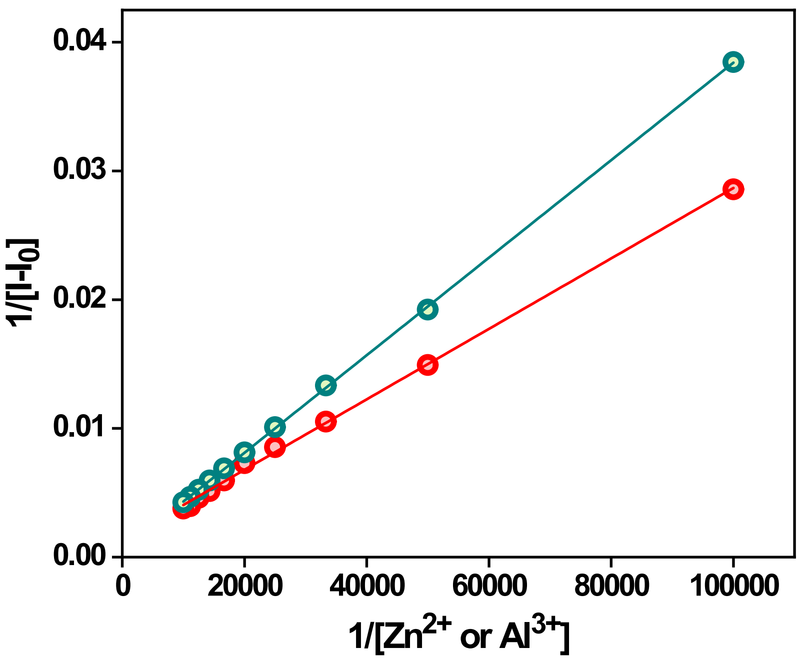


Fig. S9. Benesi-Hildebrand plots of **HL** for Al^{3+} (red circles) and Zn^{2+} ions (green circles).

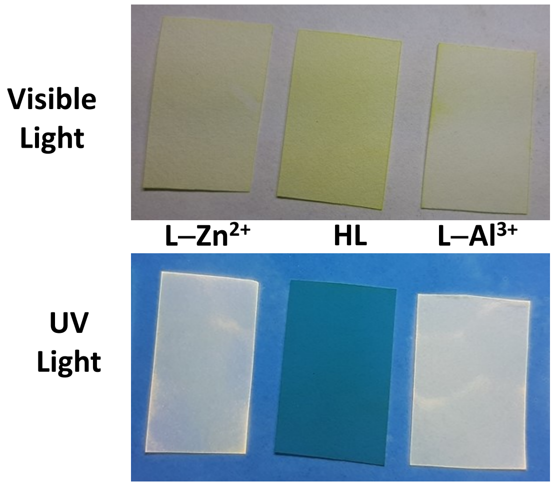
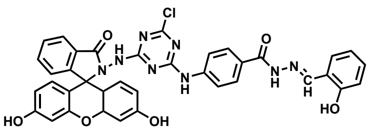
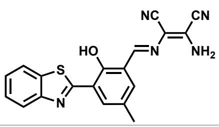


Fig. S10. Detection using paper strips, showing color changes of probe **HL** with Zn^{2+} and Al^{3+} ions under visible light (top) and ultraviolet light (bottom).

Table S1. Changes in the emission quantum yield of **HL** upon addition of Al^{3+} and Zn^{2+}.

Compound	Emission quantum Yield (*Φem*)
HL	0.06
HL-Al^{3+}	0.35
HL-Zn^{2+}	0.28

Table S2. Comparative sensing performance of previously reported Al^{3+}/Zn^{2+} responsive probes with this work.

S.No	Structure of probe	Target ion	LoD (μM)	Binding constant (M^{-1})	Applications	Ref.
1.		Al^{3+} Zn^{2+}	0.053 0.079	1.5 x 10^5 6.0 x10^5	Industry wastewater Live cell imaging	[1]
2.		Al^{3+}	7.06	1.32 x 10^7	Live cell imaging	[2]

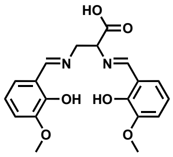
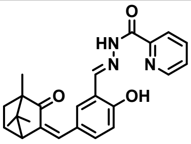
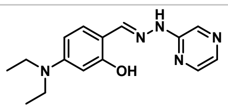
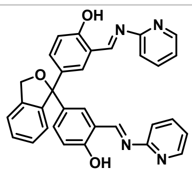
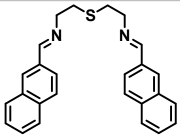
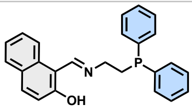
		Zn^{2+}	2.98	1.92 x 10^4		
3.		Al^{3+} Zn^{2+}	0.0018 0.0076	5.83 x 10^4 7.71 x 10^4	Live cell imaging Paper strips	[3]
4.		Al^{3+} Zn^{2+}	0.012 0.014	3.77 x 10^4 6.58 x 10^4	Live cell imaging Paper strips Distilled water Tap water Lake water	[4]
5.		Al^{3+} Zn^{2+}	0.233 0.168	2.03 x 10^4 1.15 x 10^4	Cotton swabs Potable water Drug sample	[5]
6.		Al^{3+} Zn^{2+}	0.085 0.188	2.01 x 10^4 6.84 x 10^4	Live cell imaging	[6]
7.		Al^{3+} Zn^{2+}	0.038 0.043	1.18 x 10^6 3.5 x 10^5	Paper strips Distilled water Tap water Soil samples	[7]
8.		Al^{3+} Zn^{2+}	0.62 0.54	1.39 × 10^3 4.78 × 10^3	Paper strips Live cell imaging Tap water Distilled water	**This work**

Table S3. Changes in HOMO-LUMO gaps of **HL** in presence and absence of Al^{3+} and Zn^{2+}.

Compound	**E_{HOMO} (eV)**	**E_{LUMO} (eV)**	**ΔE (eV)**
HL	-5.548	-1.513	4.035
HL + Al^{3+}	-6.289	-2.943	3.346
HL + Zn^{2+}	-5.689	--2.037	3.652

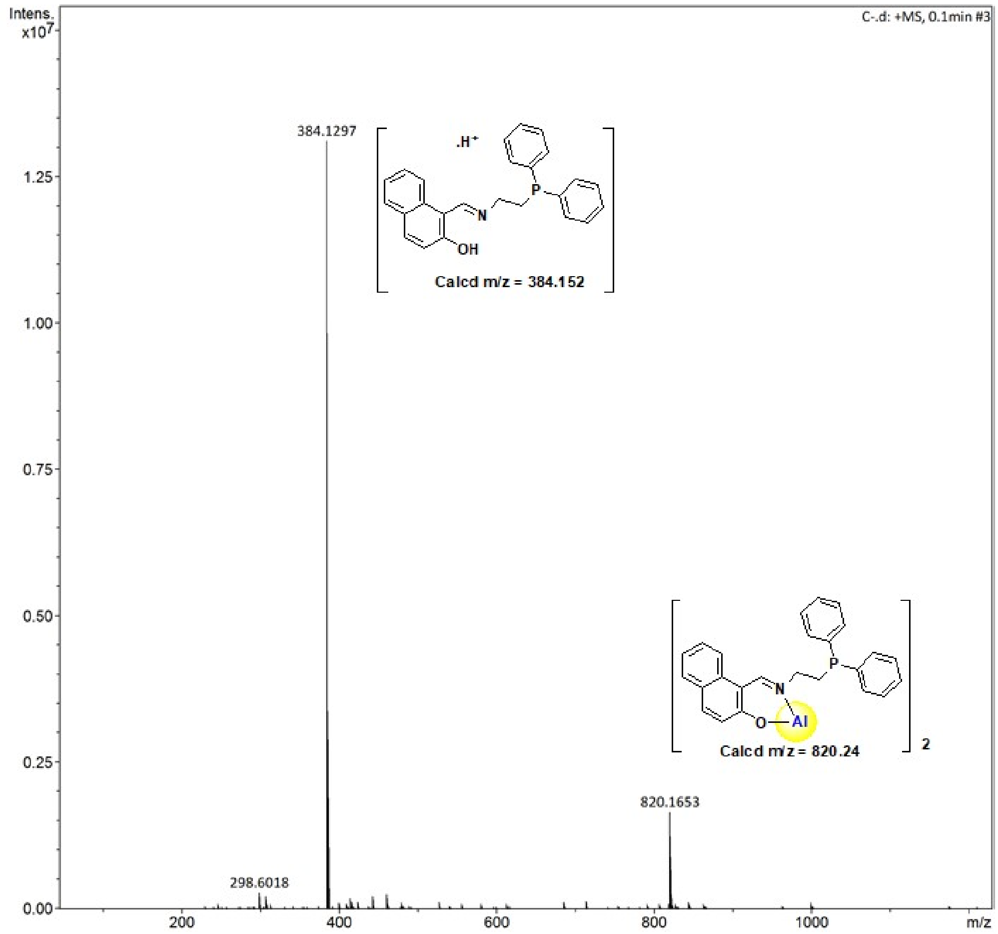


Fig. S11 ESI-mass spectrum of probe **HL** treated with 3.0 equiv. of Al^{3+} ions in methanol at room temperature.

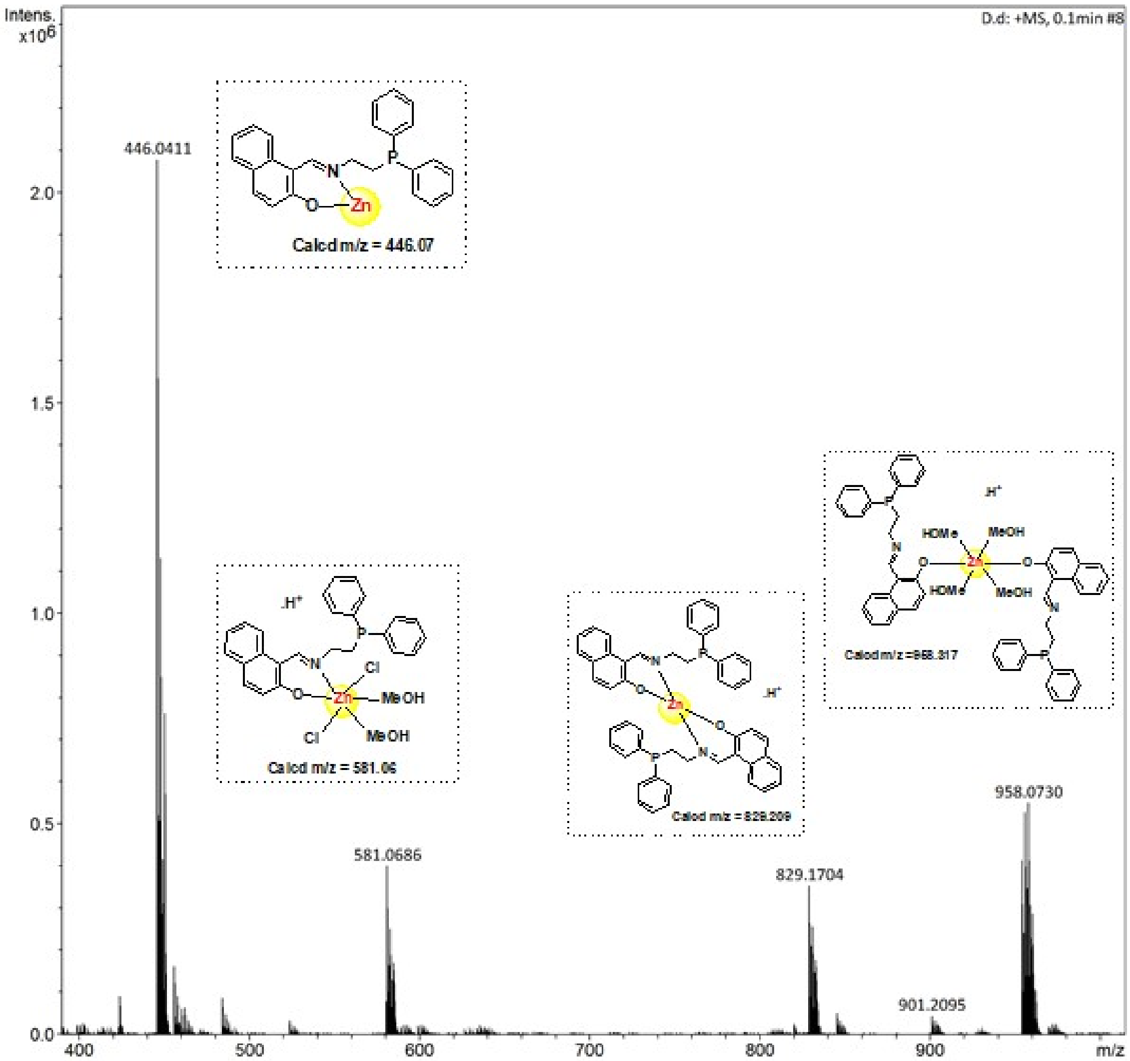


Fig. S12 ESI-mass spectrum of probe **HL** treated with 3.0 equiv. of Zn^{2+} ions in methanol at room temperature.

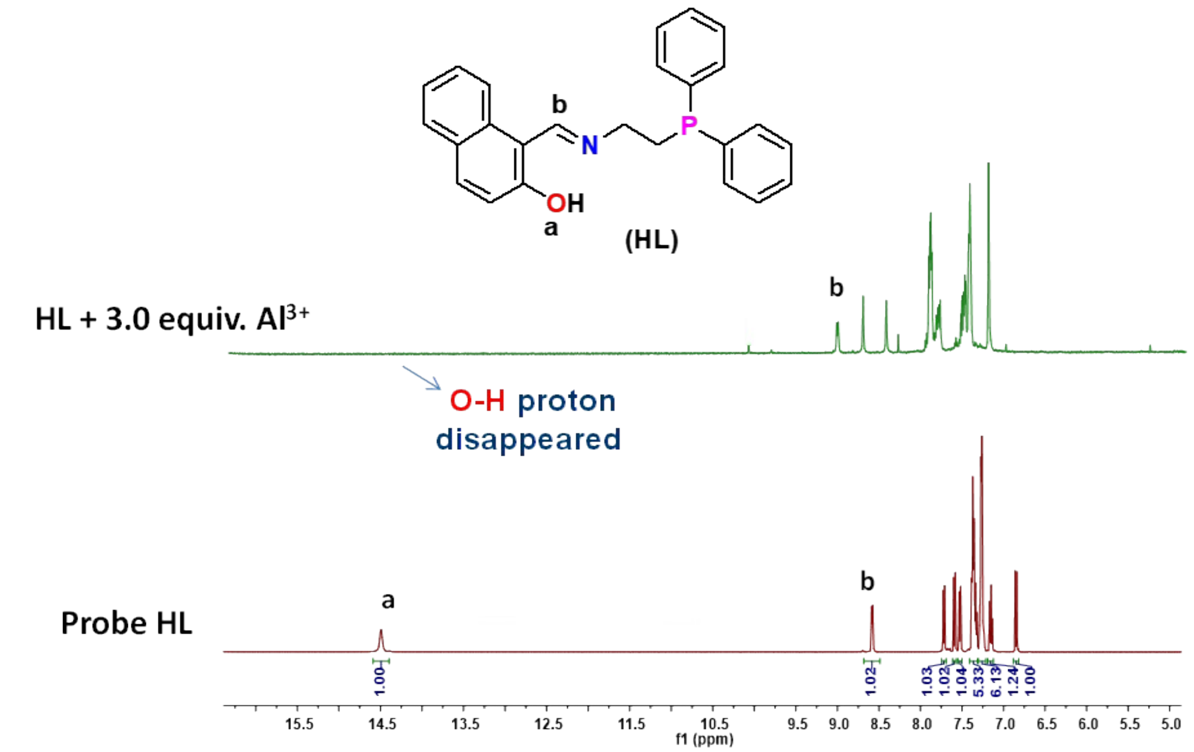


Fig. S13. ^{1}H NMR titrations of probe **HL** with 3.0 equiv. of Al^{3+} ions in DMSO-d^6at room temperature.

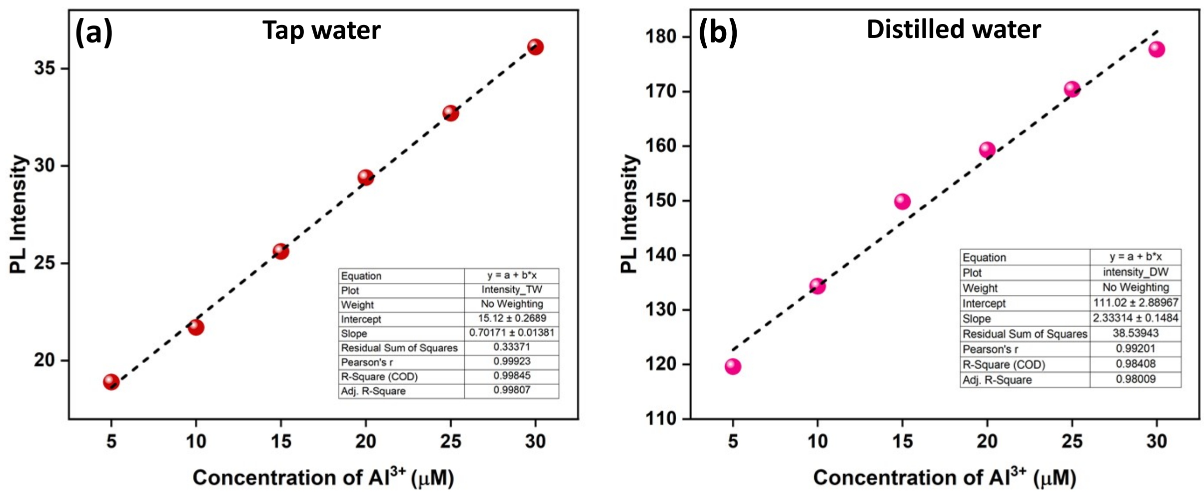


Fig. S14 Variation in emission intensity of **HL** upon gradual addition of Al^{3+} in (a) tap water and (b) distilled water.

Table S4. Detection of Al^{3+} in real samples.

Real Samples	Al^{3+} added (μM)	Al^{3+} detected (μM)	% Recovery
Tap water	5	5.4	108
	10	9.38	93.8
	15	14.97	99.8
	20	20.7	103.5
	25	25.11	100.4
	30	29.9	99.6
Distilled water	5	3.69	73.8
	10	10	100
	15	16.65	111
	20	20.7	103.5
	25	25.4	101.6
	30	28.6	95.3

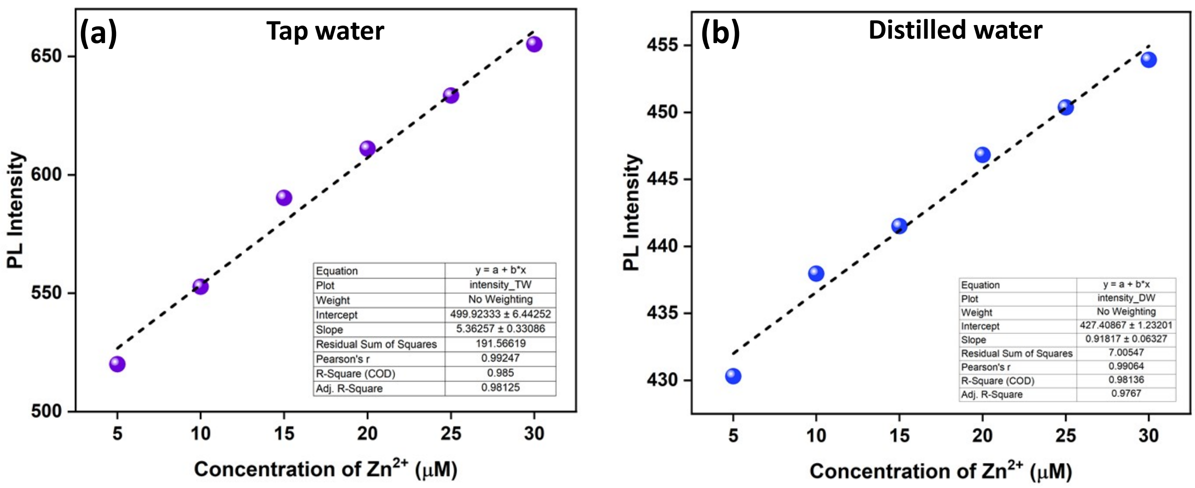


Fig. S15 Variation in emission intensity of **HL** upon gradual addition of Zn^{2+} in (a) tap water and (b) distilled water.

Table S5. Detection of Zn^{2+} in real samples.

Real Samples	Zn^{2+} added (μM)	Zn^{2+} detected (μM)	% Recovery
Tap water	5	3.91	78.35
	10	10.02	100.27
	15	17.03	113.5
	20	20.89	104.47
	25	25.08	100.3
	30	29.13	97.10
Distilled water	5	4.8	96
	10	11.49	114.92
	15	15.35	102.39
	20	21.15	105.77
	25	25.02	100.08
	30	28.8	96.29

References

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5. Y. Liu, M. Wu, J. Zhao, Y. Wang, and Y. Zhang. Rev Anal. Chem., 2022, 41, 217-227.
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7. S. Naithani, N. Goswami, S. Singh, V. Yadav, S. Kumar, P. Kumar, A. Kumar, T. Goswami and S. Kumar, Anal. Methods, 2023, 15, 6021–6030.