

A high sensitive fluorescence turn-on probe for imaging Zn^{2+} in aqueous solution and living cells

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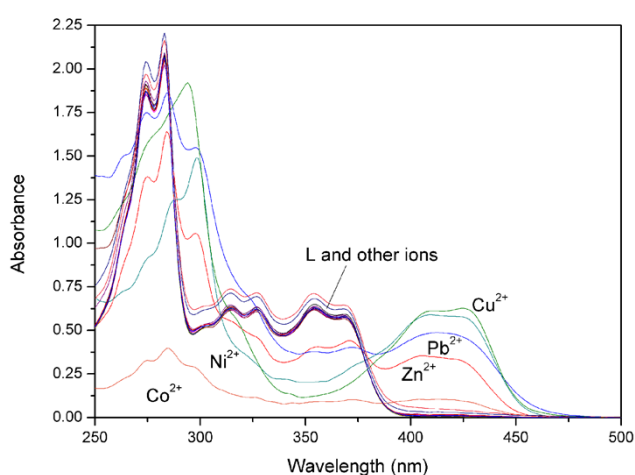


Fig. S1 UV-vis spectral changes of compound L (5×10^{-5} M) in the HEPES buffer solution (pH = 7.2, 50% CH_3CH_2OH , v/v) upon additions of various metal ions (25×10^{-5} M).

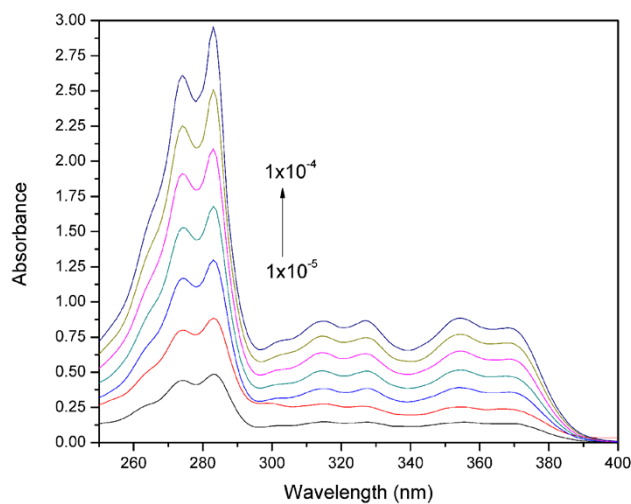


Fig. S2 UV-vis spectrum of **L** in HEPES buffer solution (20 mM HEPES, pH 7.2, EtOH : H₂O = 1 : 1) with different concentration

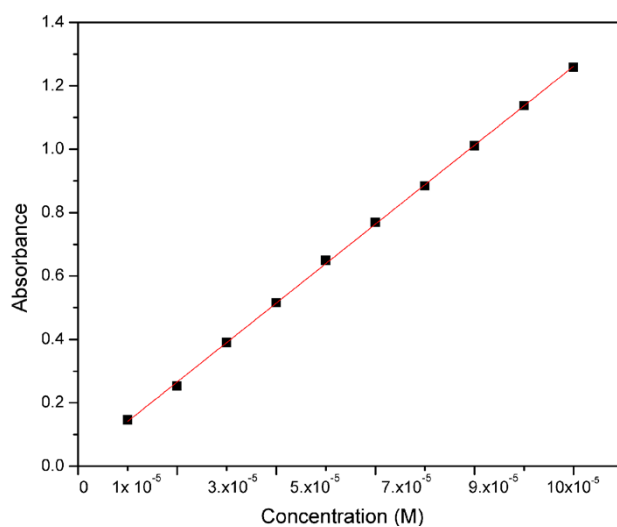


Fig. S3 Linear relation of the absorbance and **L** concentration at 355 nm. $R^2 = 0.999$

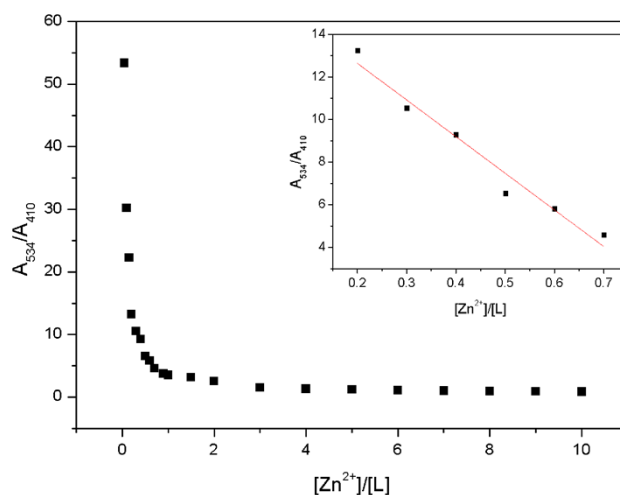


Fig. S4 The ratio of absorbance (354 nm/410 nm) of **L** (50 μM) as a function of Zn^{2+} concentration. The inset shows the ratio of absorbance at 354 nm and 410 nm (A_{354}/A_{410}). $R^2 = 0.960$.

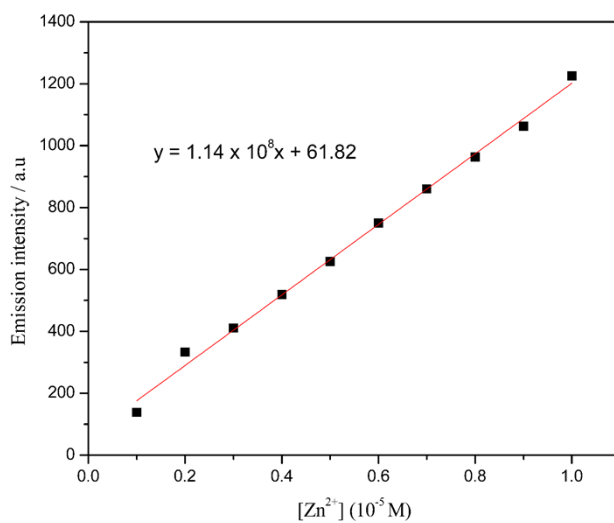


Fig. S5 Linear regression equation of **L** (10 μM) upon addition of Zn^{2+} (0.1–1.0 equiv.) in EtOH/HEPES (1:1, v/v, pH 7.2). $R^2 = 0.995$.

$$\sigma_{\text{bi}} = 4.67; \quad m = 1.14 \times 10^8; \quad \text{LOD} = 3\sigma_{\text{bi}}/m = 1.23 \times 10^{-7} \text{ M}$$

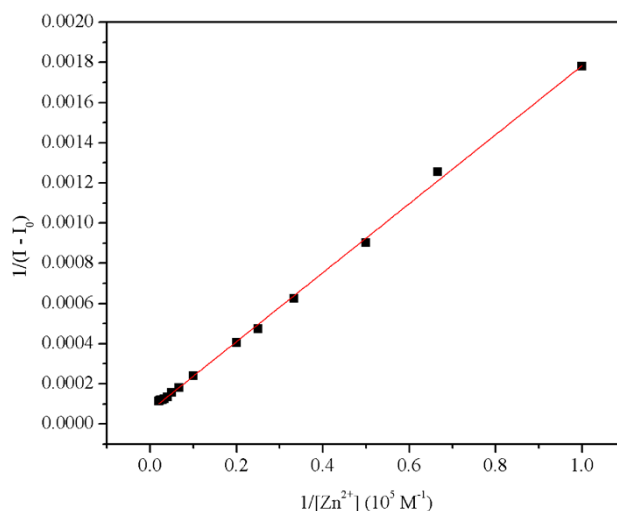


Fig. S6 Benesi–Hildebrand plot of **L** (10 μ M) in EtOH/HEPES (1:1, v/v, pH 7.2) buffered solution in the presence of Zn^{2+} (0.1–50 equiv.). $R^2 = 0.999$.

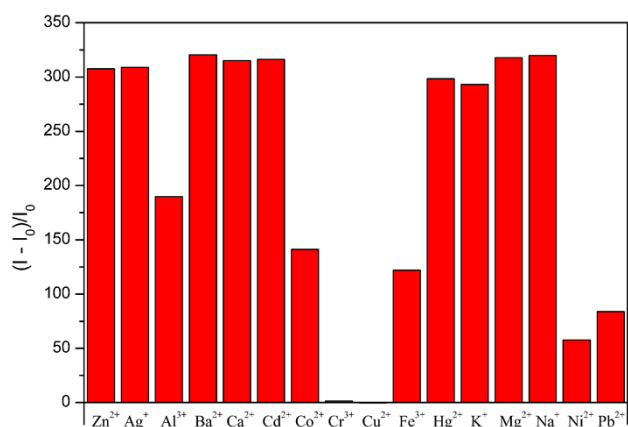


Fig. S7 Fluorescence emission spectra of **L-Zn²⁺** (1.0×10^{-5} M) in the presence of Al^{3+} , Cr^{3+} , Fe^{3+} , Co^{2+} , Cu^{2+} , Ni^{2+} , Ba^{2+} , Pb^{2+} , Na^+ , Mg^{2+} , K^+ and Ca^{2+} (50×10^{-5} M) in the HEPES buffer solution (20 mM HEPES, pH = 7.2, EtOH : H₂O = 1 : 1). (Excitation wavelength: 410 nm).

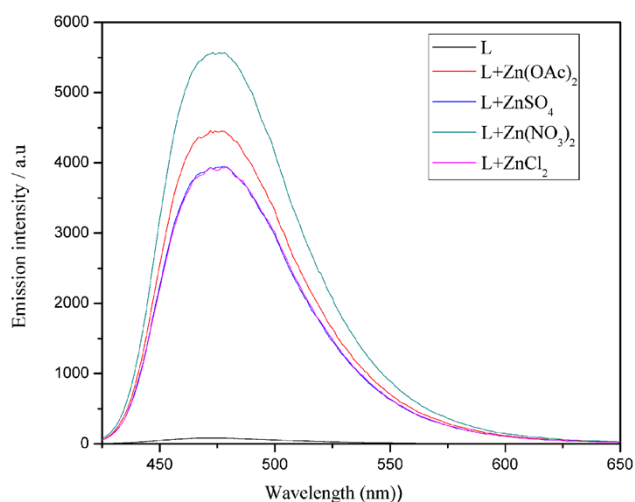


Fig. S8 Fluorescence emission spectra of free probe **L** (10 μ M) in buffered EtOH/HEPES (20 mM, pH = 7.2, 1:1, v/v) upon addition of 5 equiv. of different zinc salts.

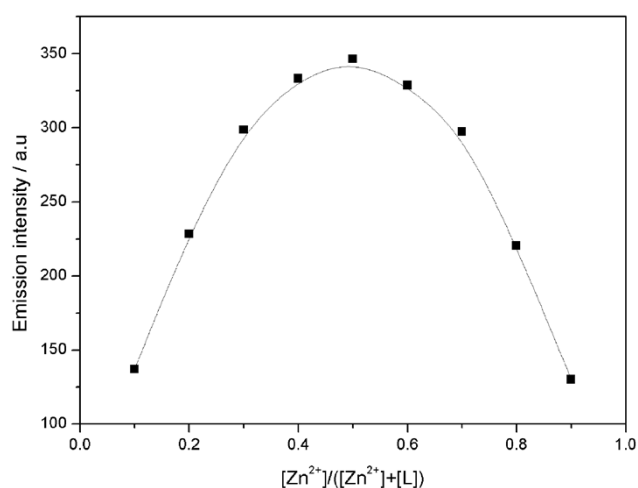


Fig. S9 Job's plot evaluated from the fluorescence spectra of **L** and Zn^{2+} at 410 nm in buffered EtOH/HEPES (1/1, v/v, pH 7.2) solution (the total concentration of **L** and Zn^{2+} is 1.0×10^{-5} M).

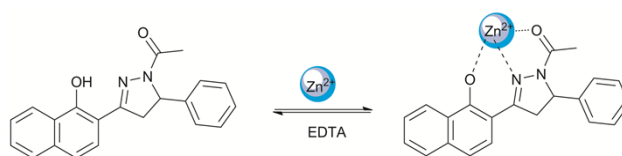


Fig. S10 Proposed complex structure of **L** with Zn^{2+} .

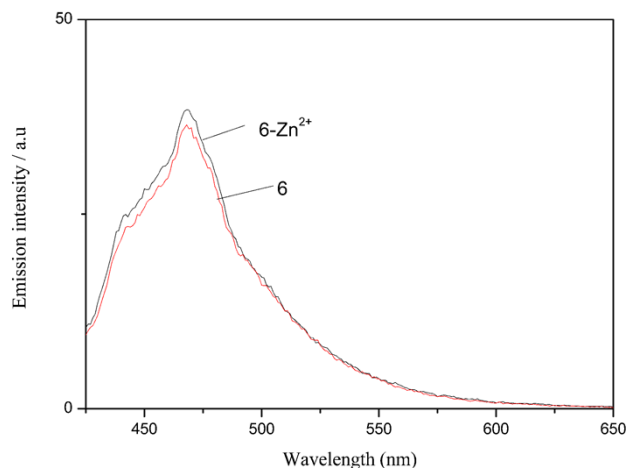


Fig. S11 Fluorescence spectra of compound **6** (1.0×10^{-5} M) in the absence and presence of 5 equiv. of Zn^{2+} in the HEPES buffer solution (20 mM HEPES, pH = 7.2, EtOH : H₂O = 1 : 1). (Excitation wavelength: 410 nm).

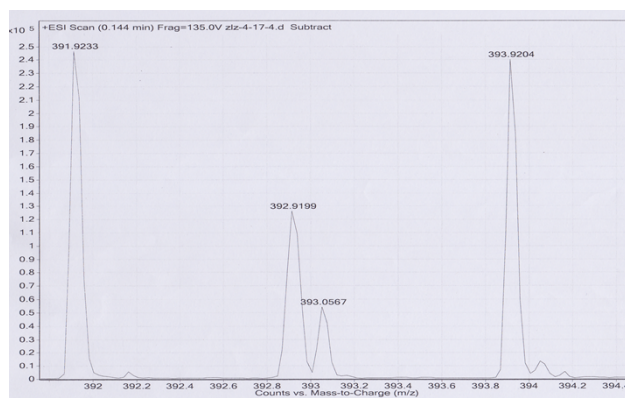


Fig. S12 HRMS spectra of **L-Zn²⁺** complex.

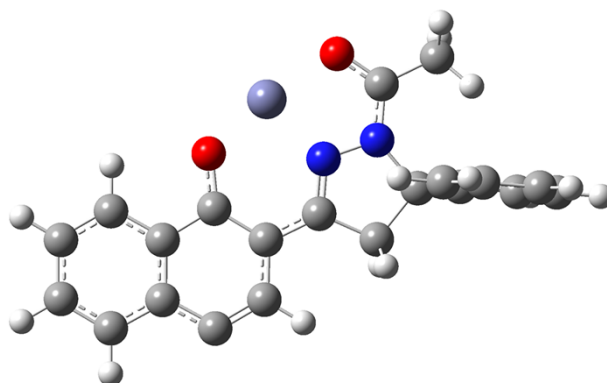


Fig. S13 Optimized structure of **L-Zn²⁺** by DFT calculation.

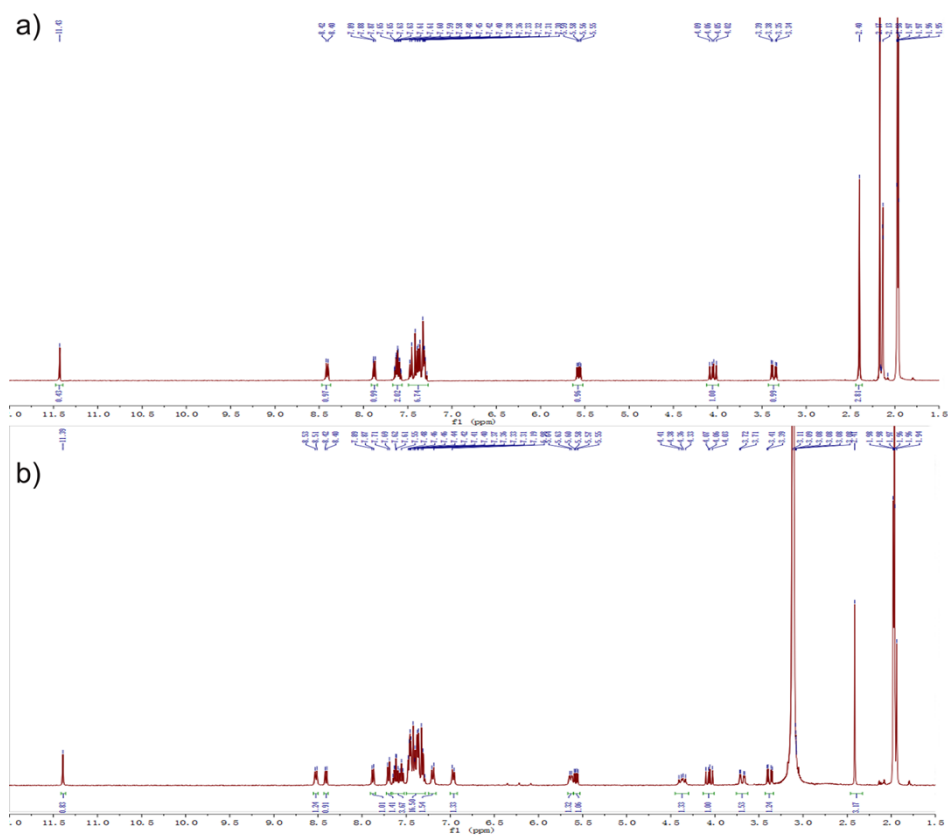


Fig. S14 ^1H NMR spectra of **L** with 0, 5.0 equiv. Zn^{2+} in $d\text{-CH}_3\text{CN}$. (a) Free probe **L**. (b) $[\text{Zn}^{2+}]/[\text{L}]$ equals 5 : 1.

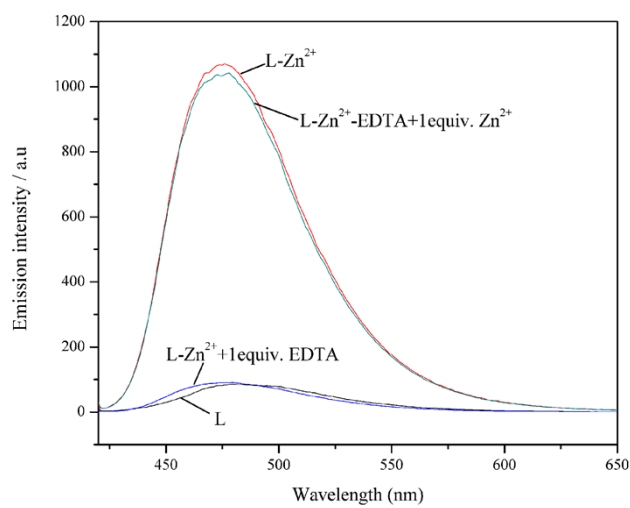


Fig. S15 Reversibility of **L-Zn** $^{2+}$ binding (Slit: 10 nm/5 nm).

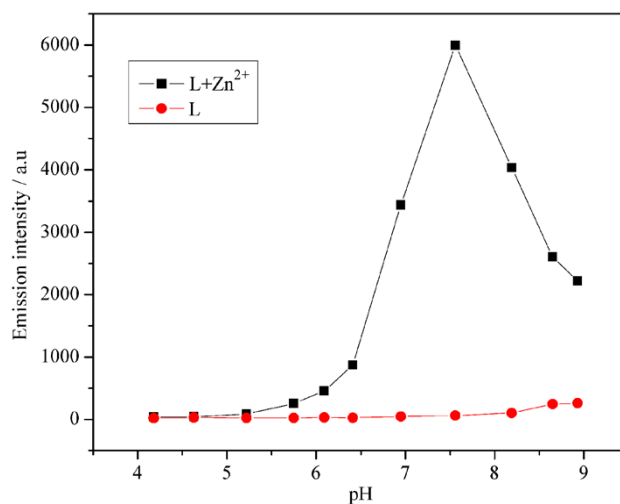


Fig. S16 Effect of pH on the fluorescence intensity ($\lambda_{\text{ex}} = 410 \text{ nm}$, $\lambda_{\text{em}} = 472 \text{ nm}$) of **L** ($10 \mu\text{M}$) in EtOH/HEPES (1/1, v/v, pH = 7.2) buffered solution measured with and without Zn^{2+} (5 equiv.).

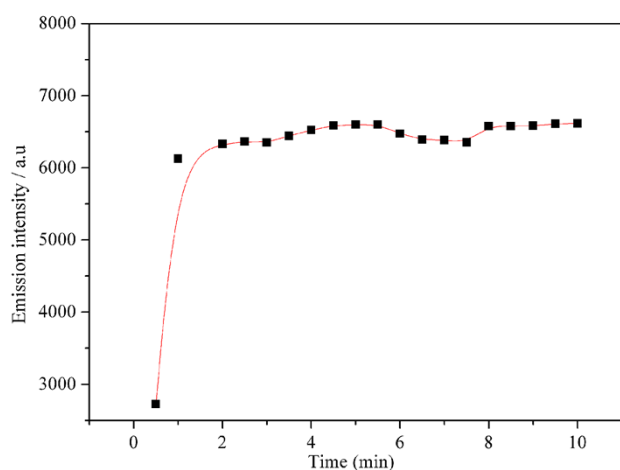


Fig.S17 Time course of the response of **L** ($10 \mu\text{M}$) in the presence of Zn^{2+} (5 equiv.) in EtOH/HEPES (1/1, v/v, pH = 7.2) buffered solution. Excitation wavelength was 410 nm.

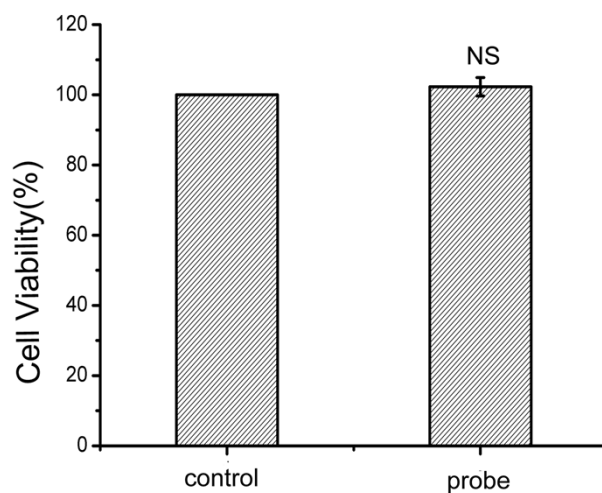


Fig. S18 SRB assay in HeLa cells with probe concentration of 5 μ M at 6 h.

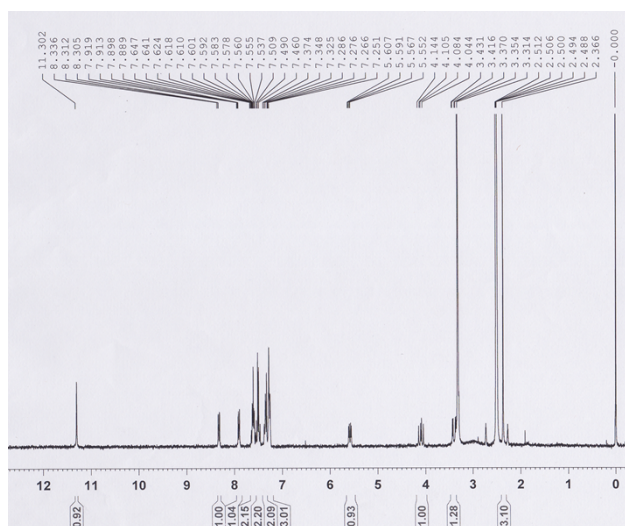


Fig. S19 ^1H NMR of 1-(3-hydroxynaphthalen-2-yl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethanone (**L**)

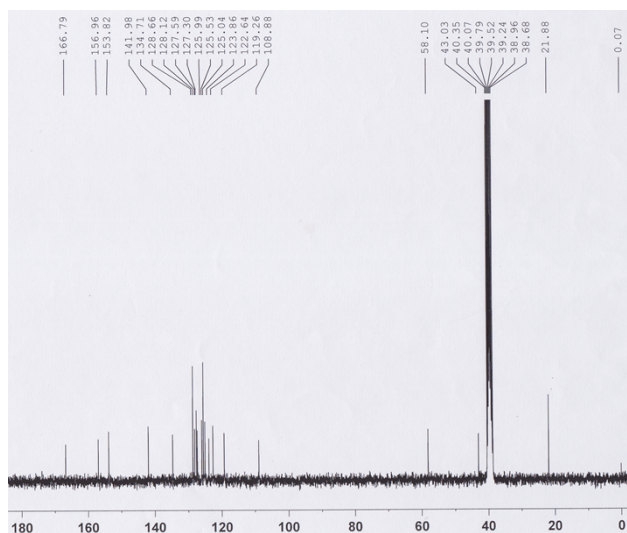


Fig. S20 ^{13}C NMR of 1-(3-hydroxynaphthalen-2-yl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethanone (**L**)

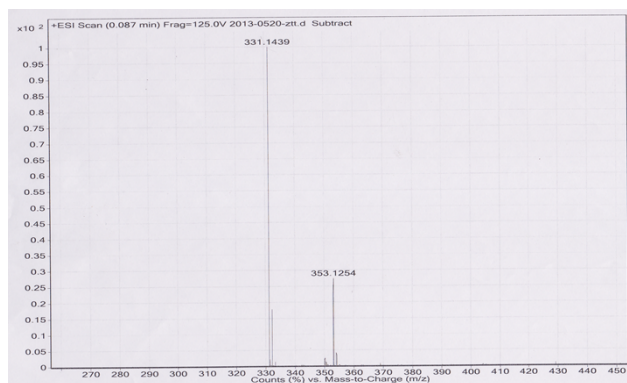


Fig. S21 HRMS of 1-(3-hydroxynaphthalen-2-yl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethanone (**L**)