Electronic Supplementary Information _ESI

Multi-analyte, ratiometric and relay recognition of a 2,5-diphenyl-1,3,4-oxadiazole-based fluorescent sensor through modulating ESIPT

Lijun Tang[*a], Zhuxuan Zheng[a], Zhenlong Huang[a], Keli Zhong[a], Yanjiang Bian[a], and

Raju Nandhakumar[*b]

[a]*Department of Chemistry, Liaoning Provincial Key Laboratory for the Synthesis and Application*

of Functional Compounds, Bohai University, Jinzhou 121013, China. E-mail: ljtang@bhu.edu.cn;

[b]*Department of Chemistry, Karunya University, Karunya Nagar, Coimbatore - 641114.*
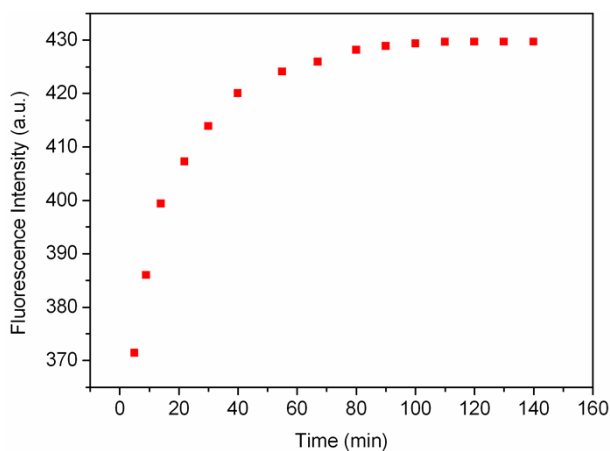
TamilNadu, India, E-mail: rajunandha@gmail.com

Fig. S1. Fluorescence intensity changes of **L** (10 μM) in HEPES buffered (10 mM, pH = 7.4) water solution against time.
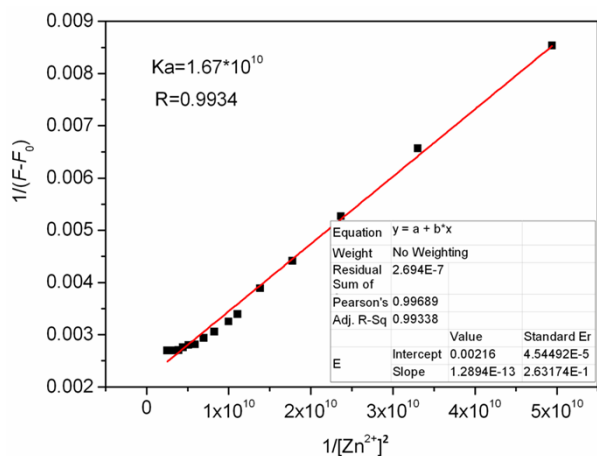
Fig. S2. Benesi-Hildebrand plot of **L** assuming 1:2 stoicheiometry with Zn^{2+}. λ_{em} = 445 nm.
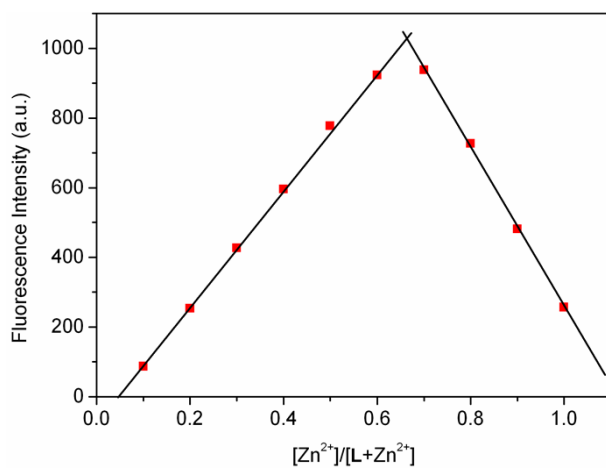

Fig. S3. Job's plot of **L** with Zn^{2+} (at 445 nm). The total concentration of **L** and Zn^{2+} is 5.0×10^{-5} M.
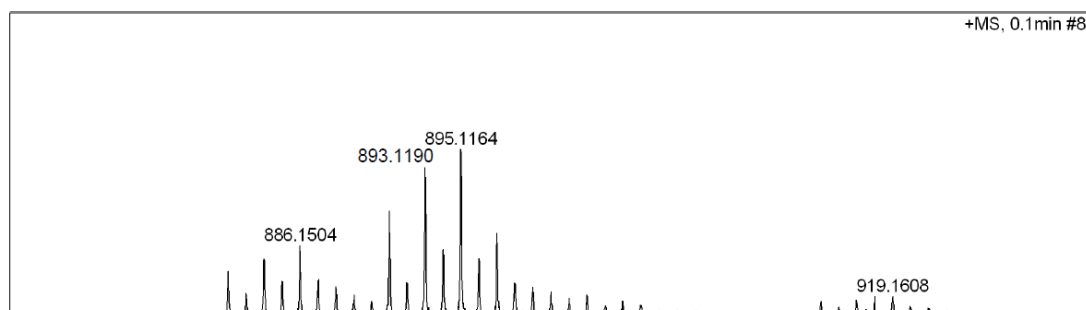

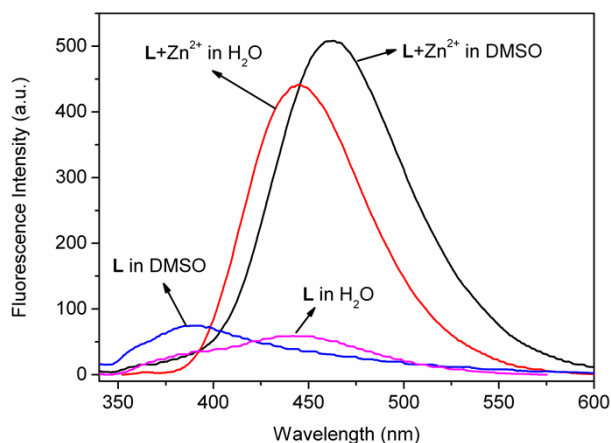**Fig. S4.** HRMS spectrum of **L** in the presence of Zn^{2+}.

Fig. S5. Fluorescence spectra of **L** with and without Zn^{2+} in DMSO and water solution (HEPES 10 mM, pH = 7.4).
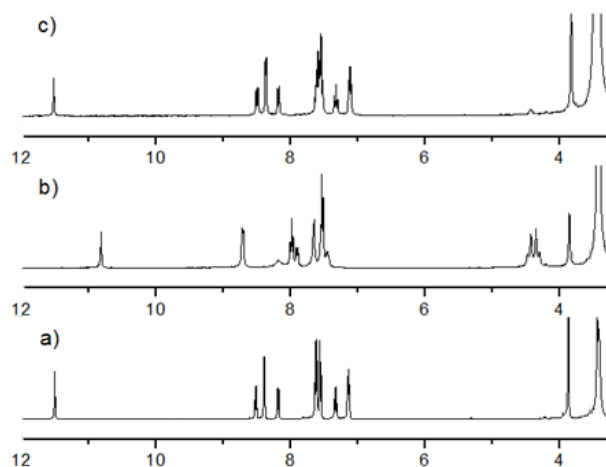

Fig. S6. ^1H NMR spectrum of **L** (a), **L**+Zn^{2+} (b) and **L**+Zn^{2+}+S^{2-} (c) in DMSO-d_6.
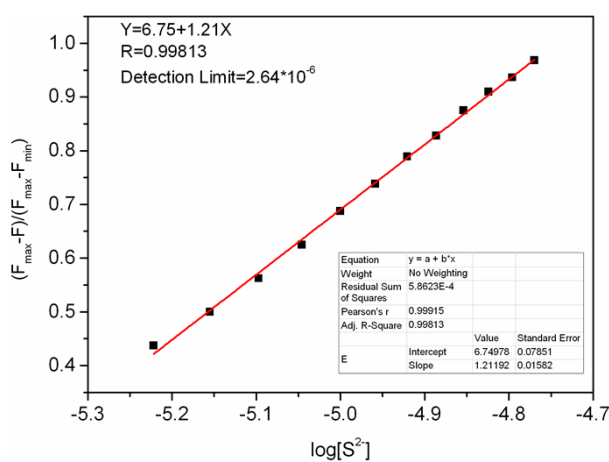

Fig. S7. Normalized fluorescence intensity $(F-F_{min})/(F_{max}-F_{min})$ of **L-2Zn^{2+}** (10 μM) to Log[S^{2-}] in water solution (HEPES 10 mM, pH = 7.4). λ_{em} = 445 nm.
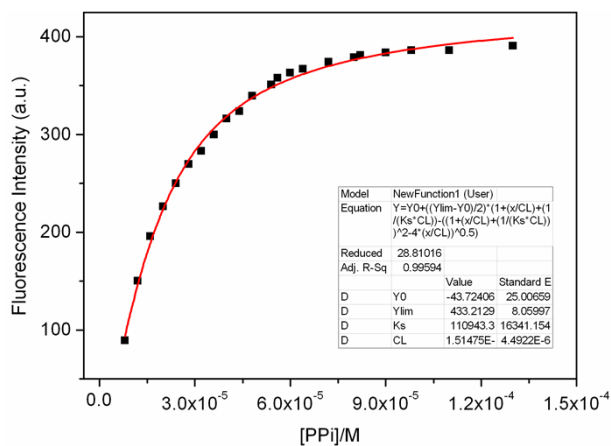
Fig. S8. Non-linear least squares fitting of fluorescence intensity of (at 396 nm) **L-2Zn^{2+}** solution with different concentrations of PPi employing a 1:1 binding equation.
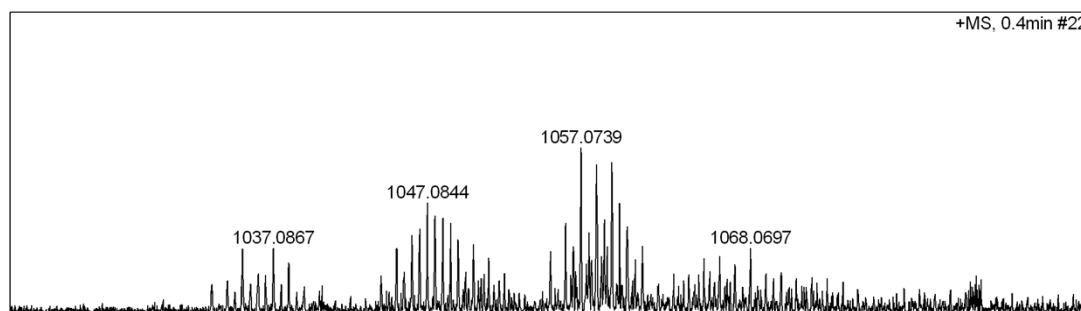

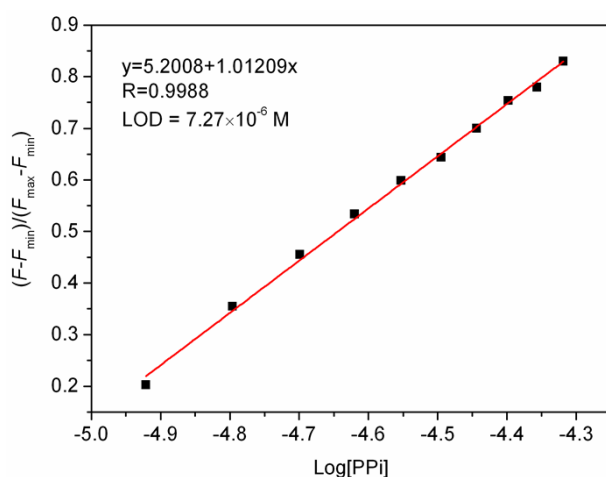**Fig. S9.** HRMS spectrum of **L**-2Zn^{2+} in the presence of PPi.

Fig. S10. Normalized fluorescence intensity $(F-F_{min})/(F_{max}-F_{min})$ of **L**-2Zn^{2+} (10 μM) to Log[PPi] in water solution (HEPES 10 mM, pH = 7.4). λ_{em} = 396 nm.
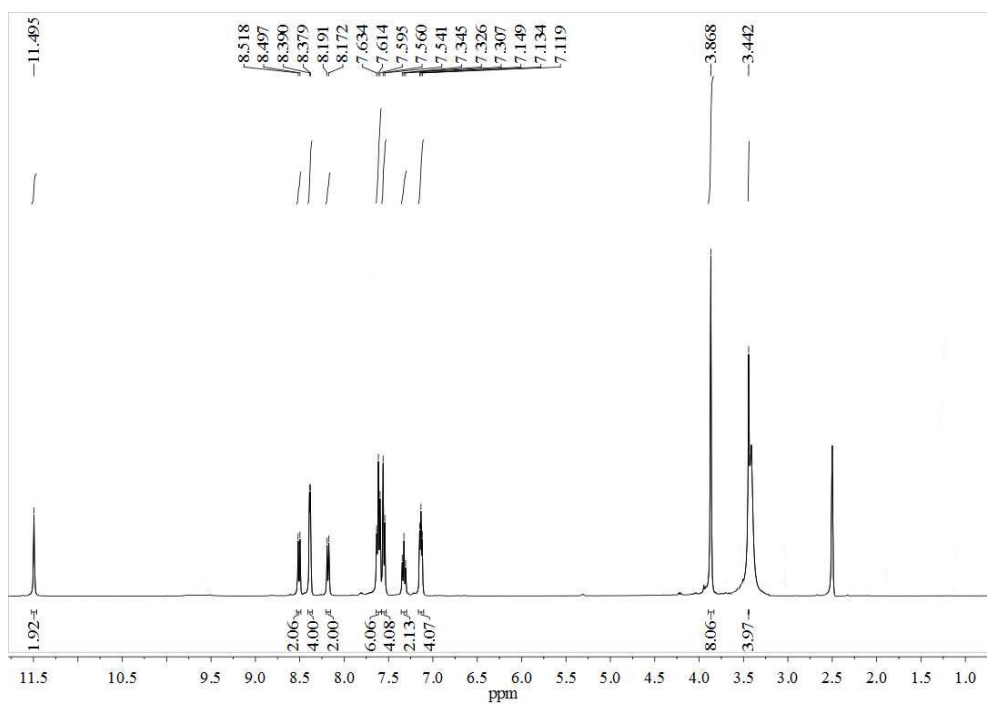
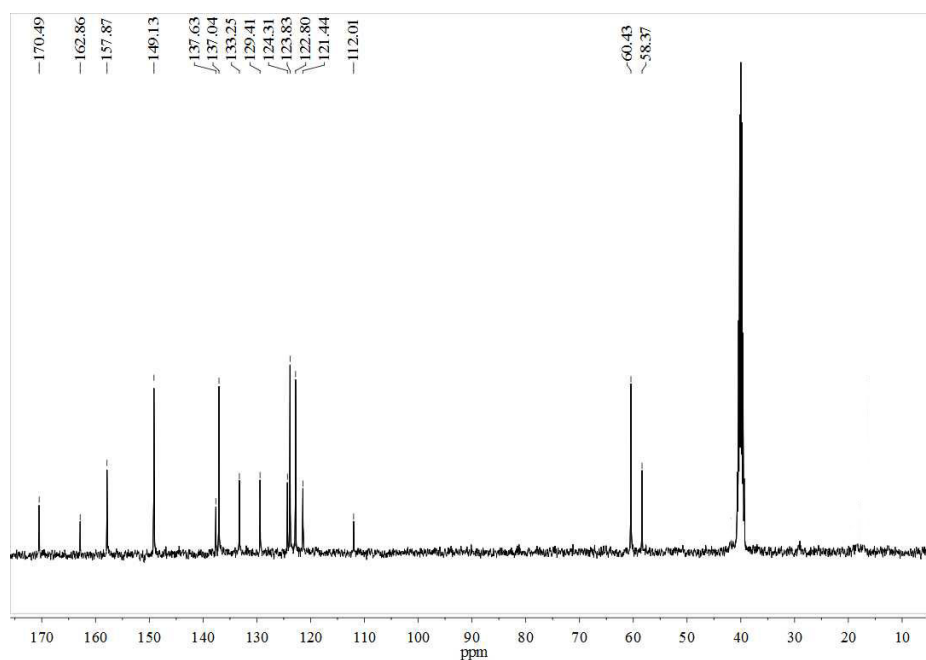**Fig. S11.** ^{1}H NMR spectrum of sensor **L** in DMSO-d_6.

Fig. S12. ^{13}C NMR spectrum of sensor **L** in DMSO-d_6.

14122601 36 (1.199) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (36:38)

TOF LD+
2.65e3

100

753.2984

M-tAi +.

729.2931

754.3029

%

755.3010

518.0790 638.2279

792.2410 844.3455

980.3376 1005.3568

1123.8596 1191.3585

1389.2821 1488.1791

m/z

0

600   700   800   900   1000   1100   1200   1300   1400

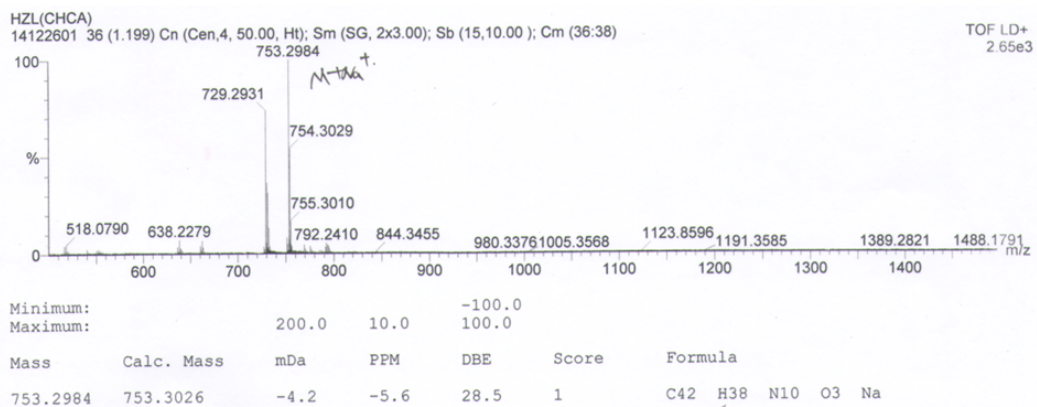|					Formula
Minimum:				-100.0	
Maximum:		200.0	10.0	100.0	
Mass	Calc. Mass	mDa	PPM	DBE	Score
753.2984	753.3026	-4.2	-5.6	28.5	1

Formula: C42 H38 N10 O3 Na

Fig. S13. MALDI-TOF-MS (positive) spectrum of sensor of **L**.