Electronic Supplementary Information (ESI)

Bipyridine bisphosphonate-based fluorescent optical sensor and optode for selective detection of Zn^{2+} ions and its applications

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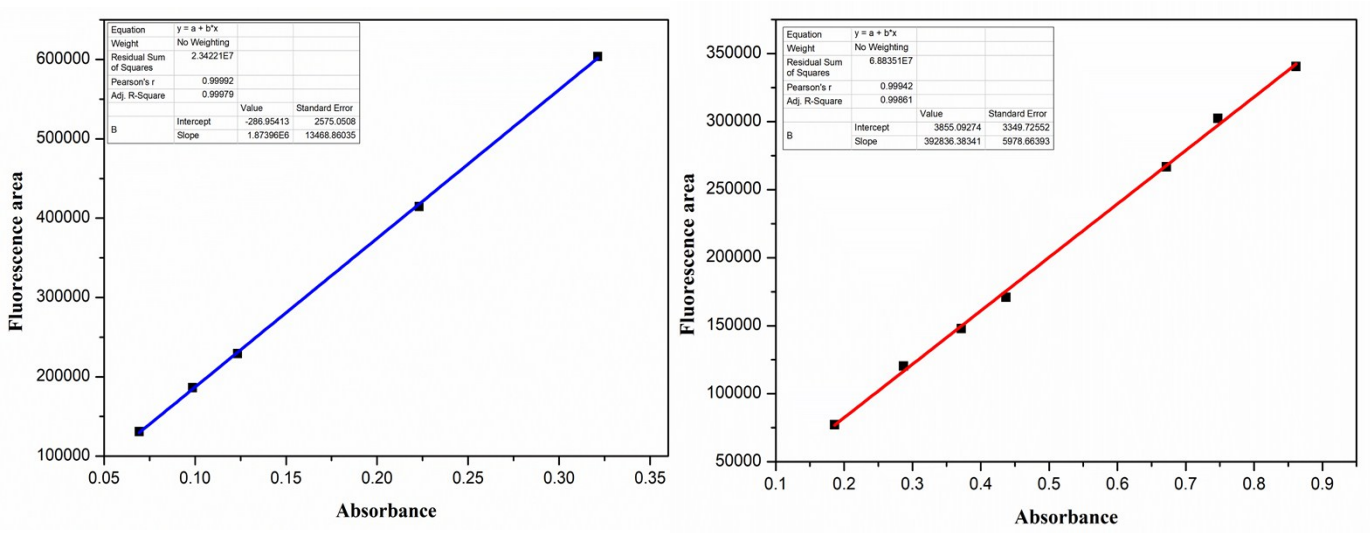

Figure 1S: Absorbance *verses* fluorescence of (a) 2-Amino pyridine in 1N H_2SO_4 (b) **L**-Zn^{2+} in acetonitrile.

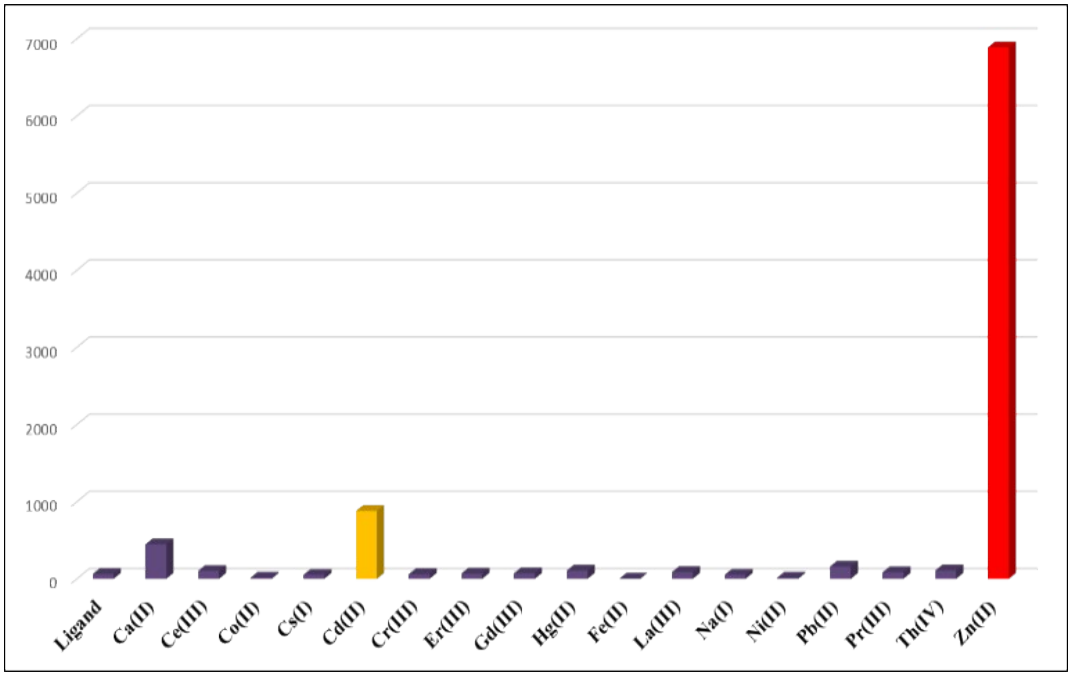

Figure 2S: Bar diagram of fluorescence intensity of alone **L** ($1x10^{-5}$ M) and **L** in the presence of various metal ions of interest ($1x10^{-4}$ M) in CH_3CN-H_2O (9:1, v/v).

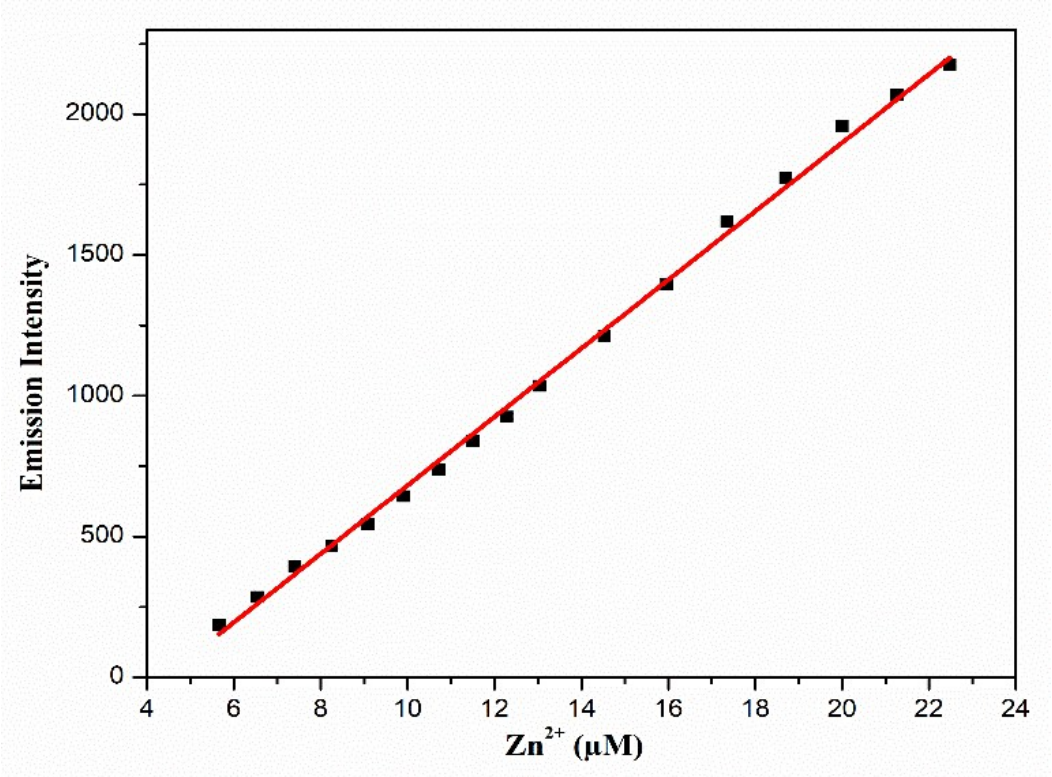

Figure 3S: Calibration plot of **L**-Zn^{2+} in acetonitrile

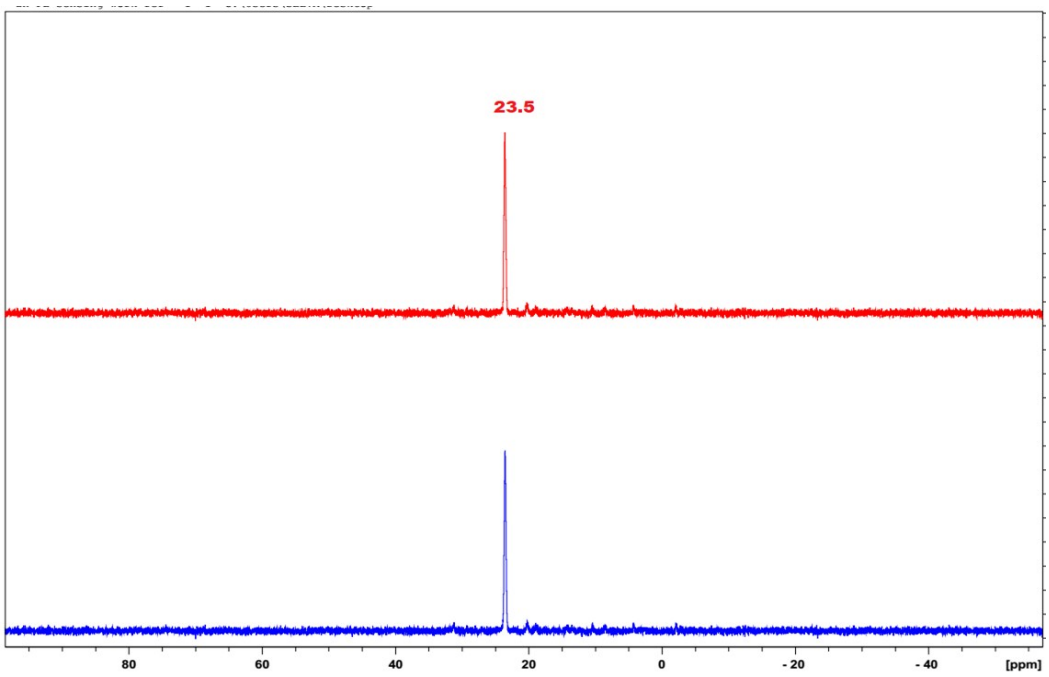

Figure 4S: ^{31}P NMR for **L** and **L**-Zn^{2+} in DMSO-d_6.

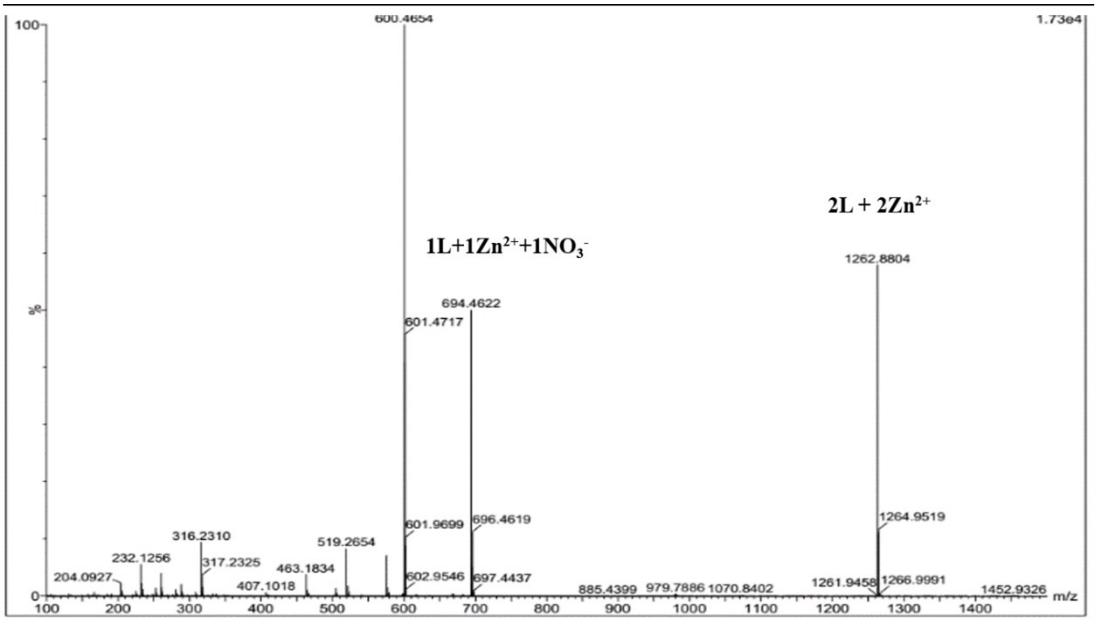

Figure – 5S (b) ESI-TOF mass spectrum for **L**-Zn^{2+} complex (ESI-MS exhibited the formation of a complex between **L** and Zn^{2+} [m/z 694.46 (1**L**+1Zn^{2+}+1NO_3^-) m/z 1262.88 (2**L** + 2Zn^{2+})]).

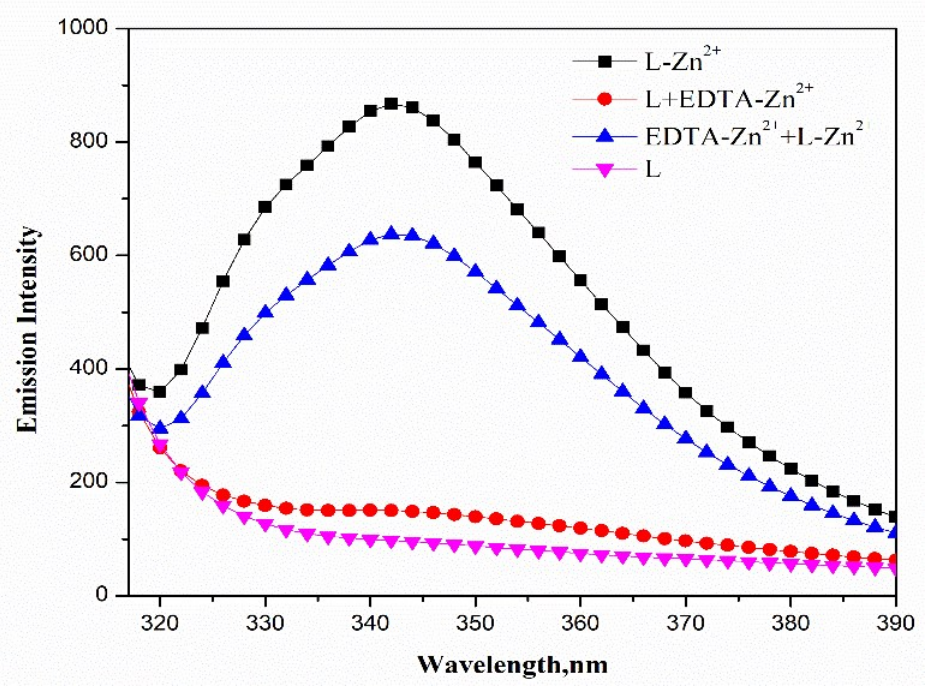

Figure 6S: Reversible changes of optode probe with sequential addition Zn^{2+} and EDTA

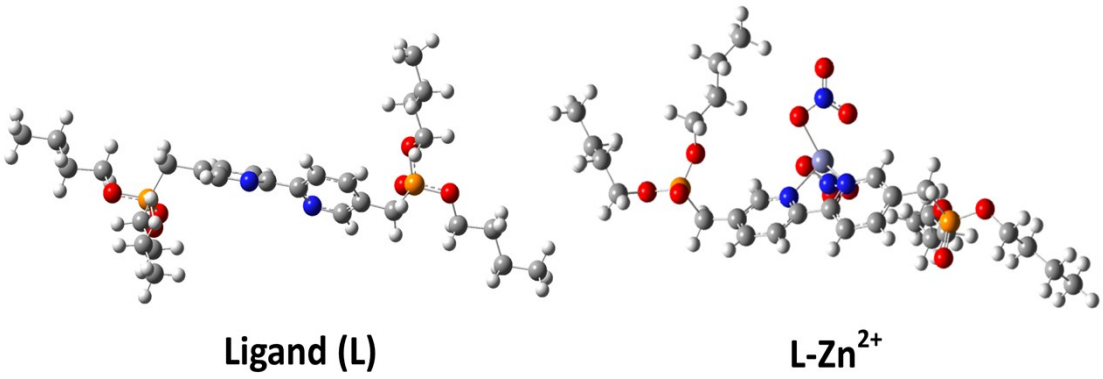

Figure 7S: Optimized structure of **L** and **L**-Zn^{2+} complex by DFT/B3LYP method

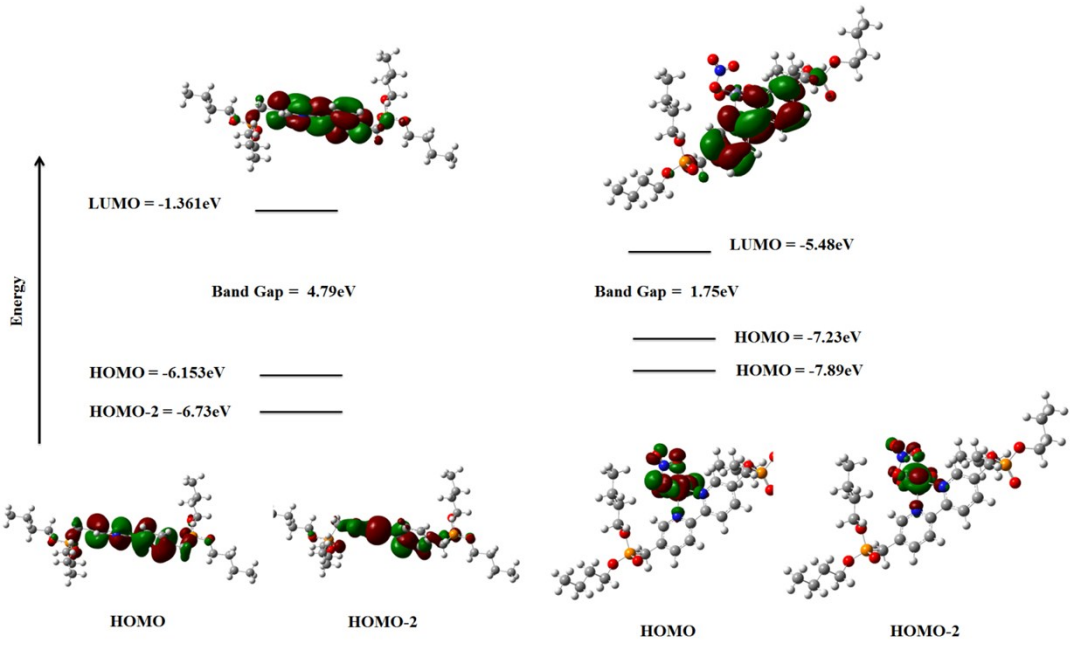

Figure 8S: Calculated HOMO-LUMO of **L** and **L**-Zn^{2+} by DFT/B3LYP method.

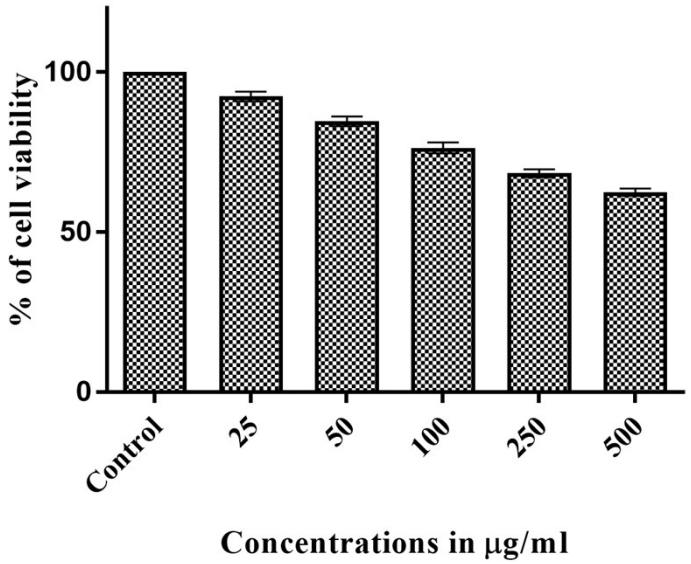

Figure 9S: Cell viability estimated by MTT assay *versus* incubation concentration of cells.

Table 1S: Comparison of optode performance towards Zn^{2+} with previously reported work

S.No	Reagent	Support	Output Signal measured	Limit of Detection (M)	pH	Interference
1	1-octadecyloxy-4-(2-pyridylazo) resorcinol[29]	PVC	absorbance	1×10^{-5}	4.8	Cu^{2+}, Co^{2+}
2	1-(2-pyridylazo)-2-naphthol[30]	PVC	diffuse reflectance	1.53×10^{-6}	3.9	Cd^{2+}, Cu^{2+}, Mn^{2+}, Ni^{2+}
3	1-(2-pyridylazo)-2-naphthol[31]	Sol-gel	absorbance	2×10^{-6}	5.5	Pb^{2+}, Fe^{2+}, Cu^{2+}, Cd^{2+}
4	1-(6-(tert-butyl)-1',3',3'-trimethylspiro[chromene-2,2'-indolin]-8-yl)-N,N'-dimethylmethanamine[32]	PVC	fluorescence	1.51×10^{-7}	7.4	***
5	Zincon[33]	Triacetyl cellulose	absorbance	1.6×10^{-7}	9.0	Cu^{2+}, Ni^{2+}, Mn^{2+}
6	4-Benzoxazol-2'-yl-3hydroxyphenyl allyl ether[34]	Silanized glass	fluorescence	4×10^{-5}	7.24	Cu^{2+}, Co^{2+}, Ni^{2+}
7	2-(2-hydroxy-5-chloro) benzaldehyde-[4-(3-methyl-3-mesitylcyclobutyl)-1,3-thiazol-2yl] hydrazone[35]	PVC	fluorescence	2.2×10^{-7}	6.0	Fe^{2+}, Cd^{2+}, Cu^{2+},
8	1-methyl-1-phenyl-3-[1-hydroxyimino-2-(succinimido) ethyl]cyclobutane[36]	PVC	fluorescence	2.5×10^{-8}	6.0	Co^{2+}, Ni^{2+}
9	Dithizone[37]	PVC	fluorescence	8.0×10^{-9}	5.0	Hg^{2+}, Ag^{+}
10	1-(p-Nitrophenylazo)-2-naphthol[38]	PVC	absorbance	8.0×10^{-7}	9.0	Cu^{2+}, Co^{2+}, Ni^{2+}
11	1,5-Diphenylcarbazone[39]	Sol-gel	absorbance	1.6×10^{-5}	9.0	Cu^{2+}, Co^{2+}, Ni^{2+}
12	**tetra butyl 2,2'-bipyridine-5,5'-diybis(methylene)diphosphonate (Present work)**	**PVC**	**fluorescence**	**1.27×10^{-9}**	**7.0**	**No interference**