1,3-Di-amidoquinoline conjugate of calix[4]arene (L) as a ratiometric and colorimetric sensor for Zn2+: Spectroscopy, microscopy and computational studies

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1,3-Di-amidoquinoline conjugate of calix[4]arene (L) as ratiometric and colorimetric sensor for Zn^{2+}: Spectroscopy, microscopy and computational studies

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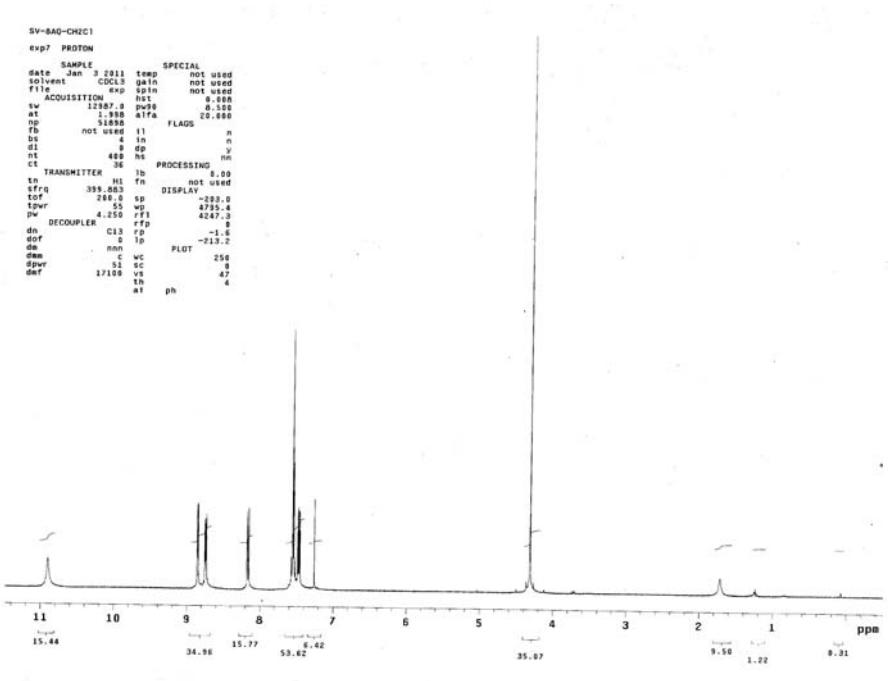
Electronic Supporting Information

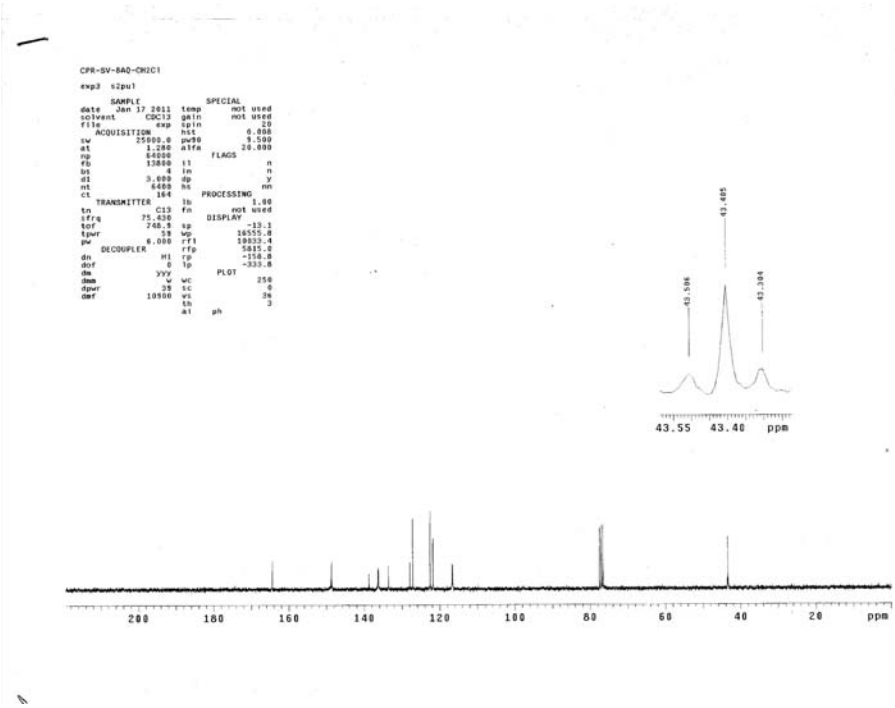
S01. Synthesis and characterization of (iii)

2-chloro-*N*-(quinolin-8-yl)acetamide (iii): To a vigorously stirred solution of 8-Amino quinoline (0.5 g, 3.4 mmol) and triethylamine (0.48 mL) in a 50 mL dry methylene dichloride, chloroacetyl chloride (0.27 mL) was added at 0°C. The reaction mixture was stirred at room temperature for 6 h. After the reaction is over, excess chloroacetyl chloride was quenched with distilled water and then extracted with CH_2Cl_2 (2 × 50 ml). The organic layer was washed with 10 % aqueous HCl solution (50 mL) and water (50 mL), dried over Na_2SO_4, and evaporated to afford solid product which was purified by recrystallization from the C_2H_5OH. ^{1}H NMR: ($CDCl_3$, δ ppm), 4.2 (s, 2H, CH_2-Cl), 7.4 (m, 2H, Ar-H), 7.5 (m, 1H, Ar-H), 8.2 (d, 1H, Ar-H, *J*=8.4), 8.7 (d, 1H, Ar-H, *J*=7.6), 8.8 (d, 1H, Ar-H, *J*=8), 10.9 (broad, 1H, CO-NH); ^{13}C- NMR: ($CDCl_3$, δ ppm): 43.4 (*C*H_2-Cl), 116.8, 121.8, 122.5, 127.1, 127.9, 133.5, 136.3, 138.7, 148.6, Quinoline *Ar*-H, 164.3 (*C*O-NH).

(a) ^{1}H-NMR spectrum of **1** recorded in $CDCl_3$

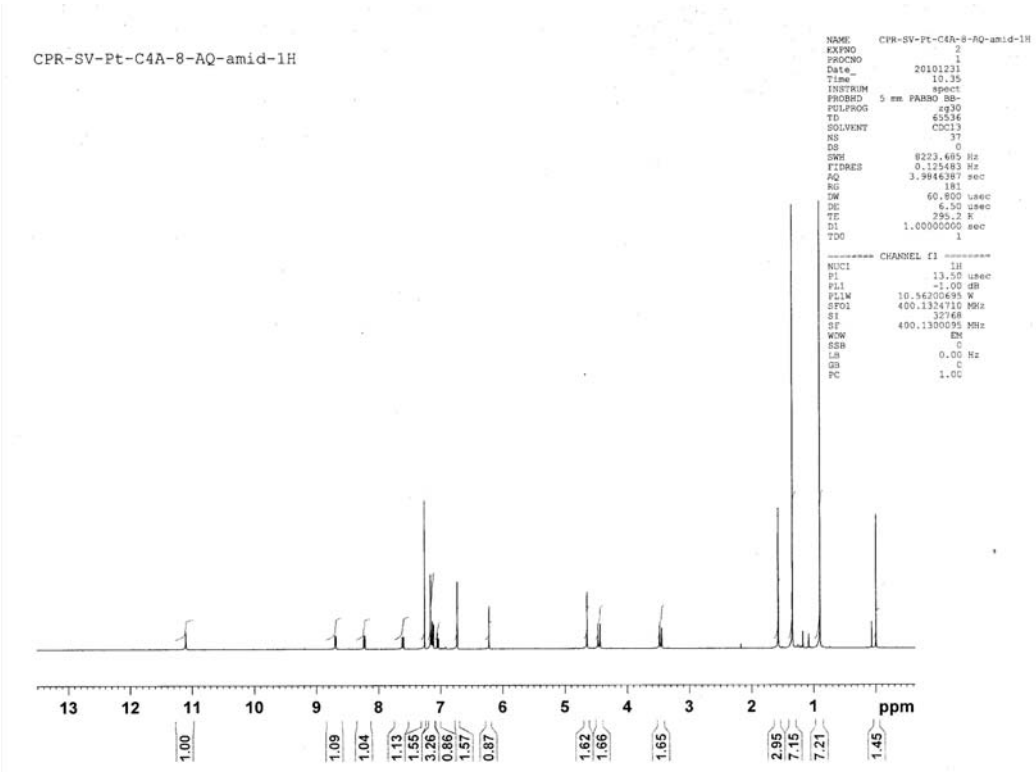


(b) ^{13}C-NMR spectrum of **1** recorded in $CDCl_3$

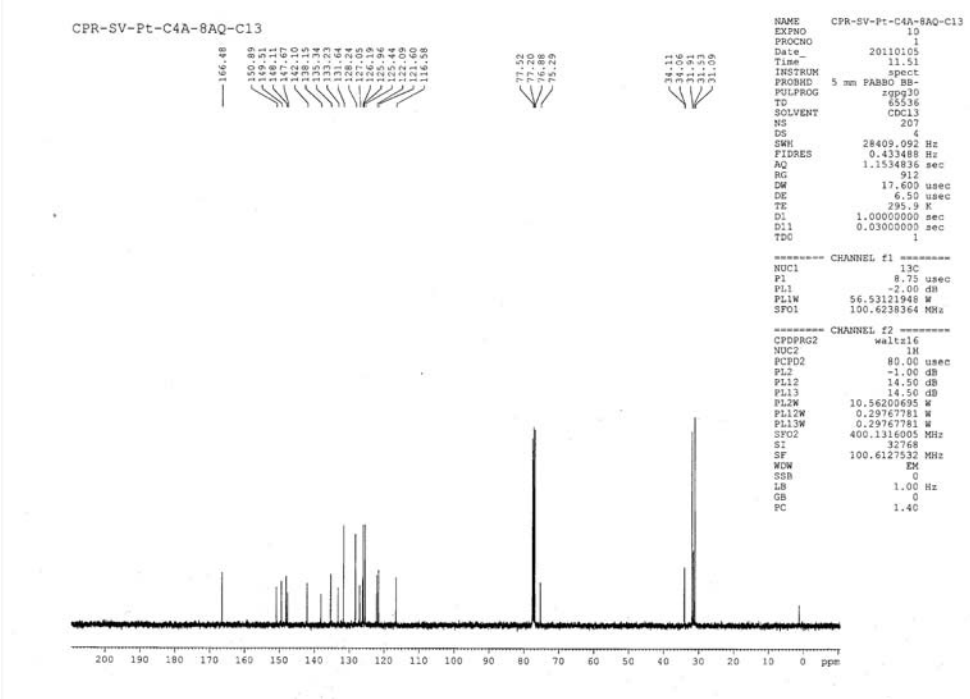


S02. **Synthesis and characterization of L**:

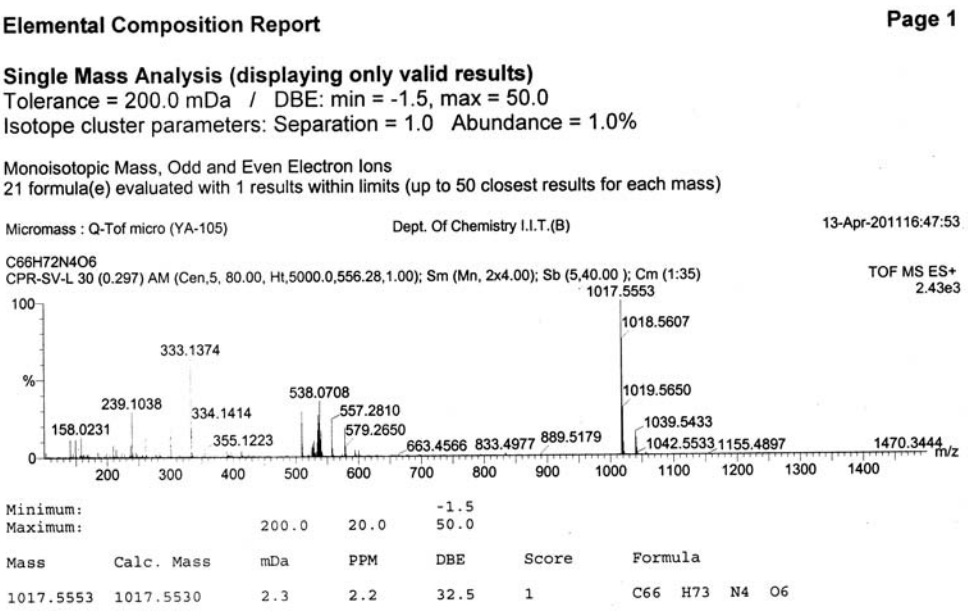
(a) ^{1}H-NMR spectrum of **L**



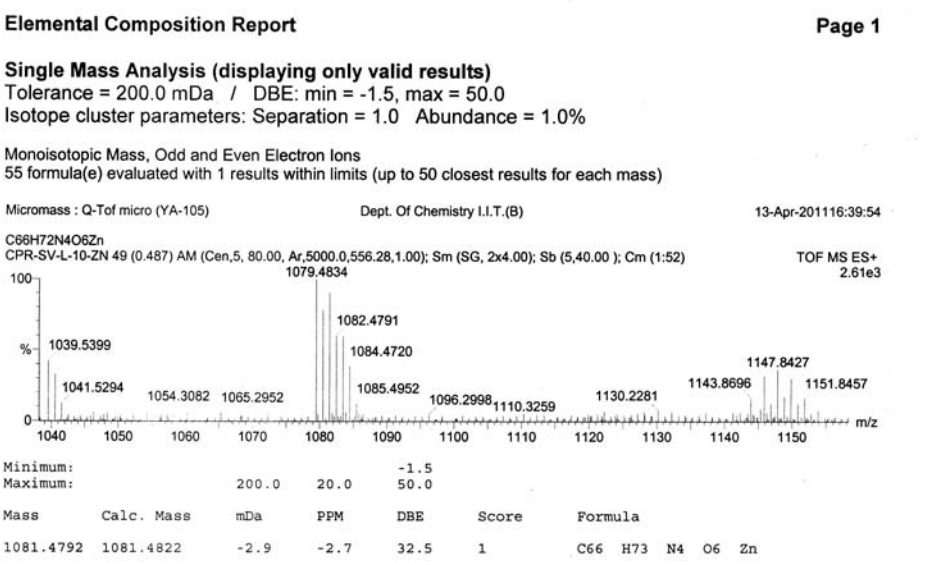
(b) ^{13}C-NMR spectrum of **L**



(c) HRMS spectrum of **L**



S03. HRMS spectrum of *in situ* prepared Zn(II) complex of **L**

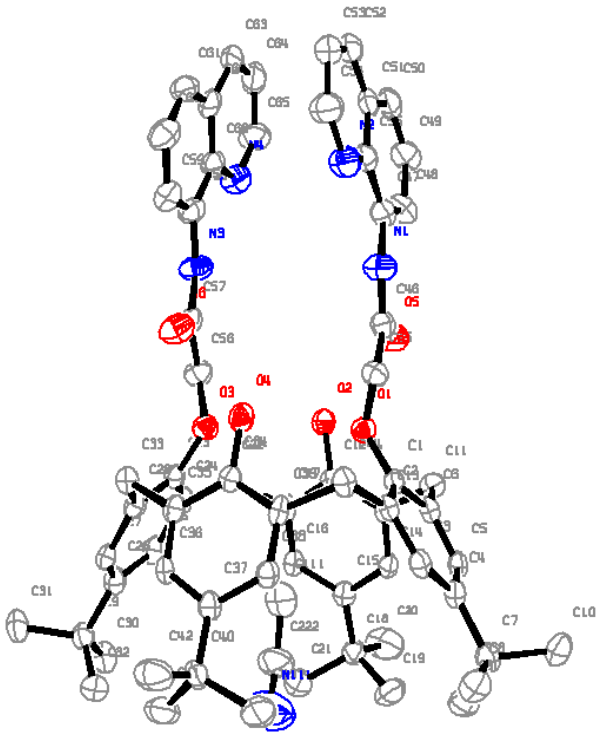


S04. Fluorescence and absorption details

Bulk solutions of **L** and the metal salts were prepared in MeOH by initially dissolving **L** in 50 μL of $CHCl_3$. The concentration of the bulk solution of **L** has been maintained as 6 x 10^{-4} M throughout the titration. All the fluorescence titrations were carried out by exciting **L** at 320 nm of the solutions taken in 1 cm quartz cells by maintaining a final [**L**] at 10 μM in a total volume of 3 mL achieved by diluting with MeOH. All the metal ions used for the fluorescence and absorption titrations were used as their perchlorate salts. Absorption studies were carried out in a similar manner as in fluorescence studies.

S05. Preliminary crystallographic data for **L**

(a) ORTEP diagram of **L**



(b) Bond lengths (Å)

O1 - C1	1.384(5)	C13 - C14	1.375(6)	C33 - C35	1.511(6)
O1 - C45	1.403(5)	C14 - C15	1.395(6)	C33 - H33A	0.99
O2 - C12	1.351(5)	C14 - H14	0.95	C33 - H33B	0.99
O2 - H2	0.84	C15 - C16	1.399(6)	C34 - C35	1.400(6)
O3 - C23	1.384(5)	C15 - C18	1.518(6)	C34 - C39	1.412(6)
O3 - C56	1.417(5)	C16 - C17	1.384(6)	C35 - C36	1.376(5)
O4 - C34	1.356(5)	C16 – H16	0.95	C36 - C37	1.395(6)
O4 - H4	0.84	C17 - C 22	1.489(6)	C36 - H36	0.95
O5 - C46	1.237(5)	C18 - C21	1.525(6)	C37 - C38	1.412(6)
O6 - C57	1.244(5)	C18 - C19	1.527(6)	C37 - C40	1.524(6)
N1 - C46	1.333(6)	C18 - C20	1.528(6)	C38 - C39	1.396(5)
N1 - C47	1.398(5)	C19 - H19A	0.98	C38 - H38	0.95
N1 - H1	0.88	C19 - H19B	0.98	C39 - C44	1.513(6)
N2 - C54	1.329(6)	C19 - H19C	0.98	C40 - C42	1.501(6)
N2 - C55	1.372(6)	C20 - H20A	0.98	C40 - C43	1.523(7)
N4 - C65	1.313(5)	C20 - H20B	0.98	C40 - C41	1.524(7)
N4 - C66	1.380(6)	C20 - H20C	0.98	C41 - H41A	0.98
C1 - C2	1.402(5)	C21 - H21A	0.98	C41 - H41B	0.98
C1 - C6	1.411(6)	C21 - H21B	0.98	C41 - H41C	0.98
C2 - C3	1.384(6)	C21 - H21C	0.98	C42 - H42A	0.98
C2 - C44	1.520(6)	C22 - C24	1.539(5)	C42 - H42B	0.98
C3 - C4	1.381(6)	C22 - H22A	0.99	C42 - H42C	0.98
C3 - H3	0.95	C22 - H22B	0.99	C43 - H43A	0.98
C4 - C5	1.392(5)	C23 - C24	1.390(6)	C43 - H43B	0.98
C4 - C7	1.541(6)	C23 - C28	1.401(6)	C43 -H43C	0.98
C5 - C6	1.384(6)	C24 - C25	1.392(6)	C44 - H44A	0.99
C5 - H5	0.95	C25 - C26	1.413(6)	C44 - H44B	0.99
C6 - C11	1.517(5)	C25 - H25	0.95	C45 - C46	1.480(6)
C7 - C8	1.515(6)	C26 - C27	1.388(6)	C45 - H45A	0.99
C7 - C9	1.517(6)	C26 - C29	1.531(6)	C45 - H45B	0.99
C7 - C10	1.528(6)	C27 - C28	1.382(6)	C47 - C48	1.361(6)
C8 - H8A	0.98	C27 – H27	0.95	C47 - C55	1.416(6)
C8 - H8B	0.98	C28 - C33	1.516(6)	C48 - C49	1.384(6)
C8 - H8C	0.98	C29 - C30	1.529(6)	C48 - H48	0.95
C9 - H9A	0.98	C29 - C31	1.530(6)	C49 - C50	1.355(7)
C9 - H9B	0.98	C29 - C32	1.557(6)	C49 - H49	0.95
C9 - H9C	0.98	C30 - H30A	0.98	C50 - C51	1.444(7)
C10 - H10A	0.98	C30 - H30B	0.98	C50 - H50	0.95
C10 - H10B	0.98	C30 - H30C	0.98	C51 - C52	1.381(7)
C10 - H10C	0.98	C31 - H31A	0.98	C51 - C55	1.385(6)
C11 - C13	1.510(6)	C31 - H31B	0.98	C52 - C53	1.378(7)
C11 - H11A	0.99	C31 - H31C	0.98	C52 - H52	0.95
C11 - H11B	0.99	C32 - H32A	0.98	C53 - C54	1.388(6)
C12 - C13	1.411(6)	C32 - H32B	0.98	C53 - H53	0.95
C12 - C17	1.416(6)	C32 - H32C	0.98	C54 - H54	0.95

C56 - C57	1.484(6)	C65 - H65	0.95		
C56 - H56A	0.99	C111 - C222	1.406(8)		
C56 - H56B	0.99	C111 - H11C	0.98		
C57 - N3	1.339(5)	C111 - H11D	0.98		
N3 -C58	1.389(6)	C111 - H11E	0.98		
N3 - H3A	0.88	C222 - N111	1.135(7)		
C58 - C59	1.372(6)				
C58 - C66	1.414(6)				
C59 - C60	1.394(7)				
C59 - H59	0.95				
C60 - C61	1.347(6)				
C60 - H60	0.95				
C61 - C62	1.419(7)				
C61 - H61	0.95				
C62 - C66	1.402(6)				
C62 - C63	1.413(6)				
C63 - C64	1.393(7)				
C63 - H63	0.95				
C64 - C65	1.376(7)				
C64 - H64	0.95				

(C) Bond angles

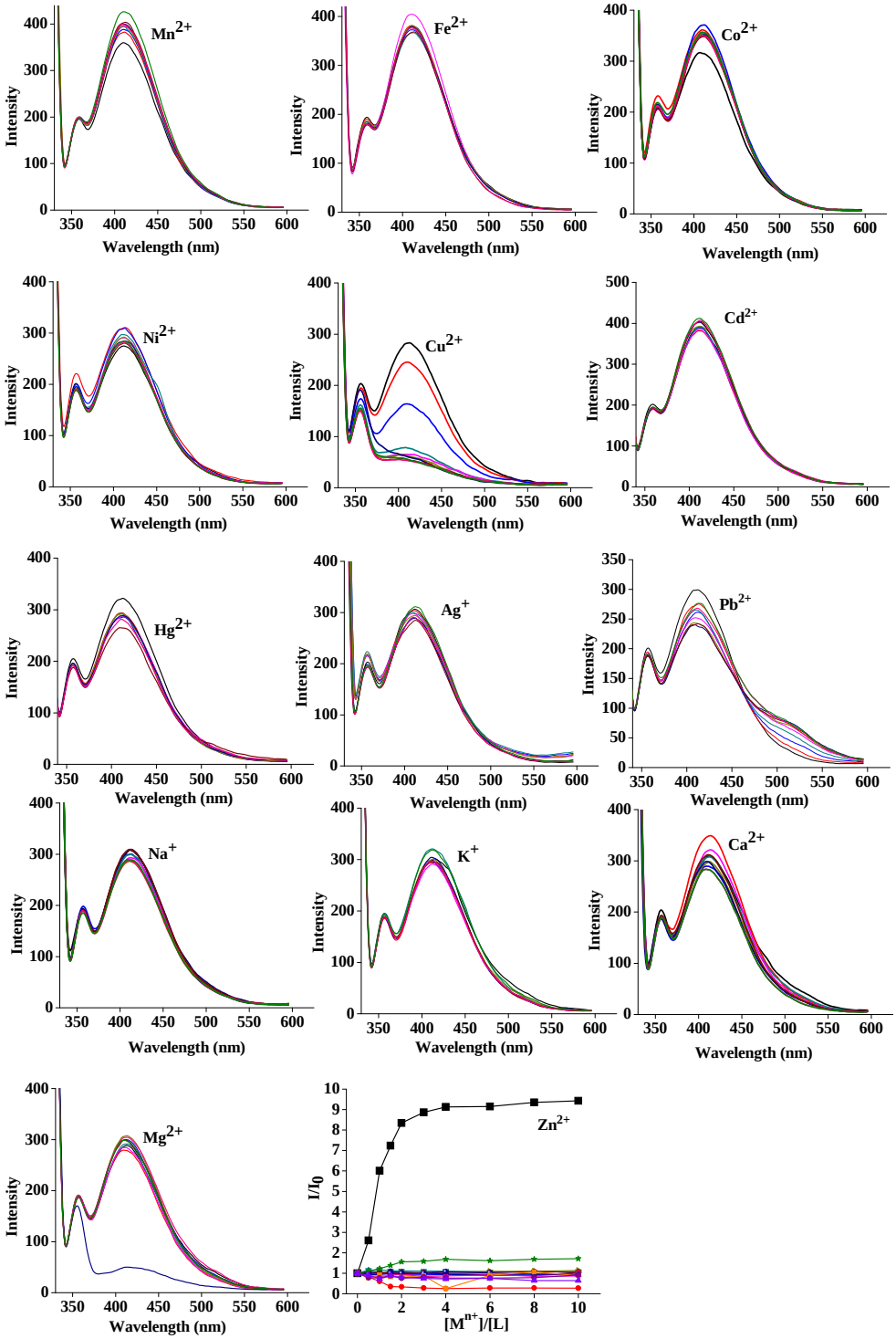
C1 - O1 - C45	118.4(3)	C7 - C10 - H10A	109.5
C12 - O2 - H2	109.5	C7 - C10 - H10B	109.5
C23 - O3 - C56	118.7(3)	H10A - C10 H10B	109.5
C34 - O4 - H4	109.5	C7 - C10 - H10C	109.5
C46 - N1 - C47	130.9(4)	H10A - C10 - H10C	109.5
C46 - N1 - H1	114.6	H10B - C10 - H10C	109.5
C47 - N1 - H1	114.6	C13 - C11 - C6	110.6(3)
C54 - N2 - C55	117.7(4)	C13 - C11 - H11A	109.5
C65 - N4 - C66	117.0(4)	C6 - C11 - H11A	109.5
O1 - C1 - C2	123.7(4)	C13 - C11 - H11B	109.5
O1 - C1 - C6	115.5(3)	C6 - C11 - H11B	109.5
C2 - C1 - C6	120.7(4)	H11A - C11 - H11B	108.1
C3 - C2 - C1	117.3(4)	O2 - C12 - C13	124.3(4)
C3 - C2 - C44	119.1(3)	O2 - C12 - C17	116.0(4)
C1 - C2 - C44	123.3(4)	C13 - C12 - C17	119.6(4)
C4 - C3 - C2	124.7(4)	C14 - C13 - C12	118.7(4)
C4 - C3 - H3	117.6	C14 - C13 - C11	119.2(4)
C2 - C3 - H3	117.6	C12 - C13 - C11	121.8(4)
C3 - C4 - C5	115.7(4)	C13 - C14 - C15	124.1(4)
C3 - C4 - C7	124.1(3)	C13 - C14 -H14	117.9
C5 - C4 - C7	120.2(4)	C15 - C14 - H14	117.9
C6 - C5 - C4	123.6(4)	C14 - C15 - C16	115.3(4)
C6 - C5 - H5	118.2	C14 - C15 - C18	121.1(4)
C4 - C5 - H5	118.2	C16 - C15 - C18	123.6(4)
C5 - C6 - C1	117.9(4)	C17 - C16 - C15	124.0(4)
C5 - C6 - C11	120.3(4)	C17 - C16 - H16	118
C1 - C6 - C11	121.6(4)	C15 - C16 - H16	118
C8 - C7 - C9	108.4(4)	C16 - C17 - C12	118.2(4)
C8 - C7 - C10	107.6(4)	C16 - C17 - C22	120.4(4)
C9 - C7 - C10	110.8(4)	C12 - C17 - C22	121.2(4)
C8 - C7 - C4	110.8(4)	C15 - C18 - C21	111.7(4)
C9 - C7 - C4	109.5(4)	C15 - C18 - C19	111.9(4)
C10 - C7 - C4	109.6(3)	C21 - C18 - C19	107.5(4)
C7 - C8 - H8A	109.5	C15 - C18 - C20	108.4(4)
C7 - C8 - H8B	109.5	C21 - C18 - C20	109.0(4)
H8A - C8 - H8B	109.5	C19 - C18 - C20	108.3(4)
C7 - C8 - H8C	109.5	C18 - C19 - H19A	109.5
H8A - C8 - H8C	109.5	C18 - C19 - H19B	109.5
H8B - C8 - H8C	109.5	H19A - C19 - H19B	109.5
C7 - C9 - H9A	109.5	C18 - C19 - H19C	109.5
C7 - C9 - H9B	109.5	H19A - C19 - H19C	109.5
H9A - C9 - H9B	109.5	H19B - C19 - H19C	109.5
C7 - C9 - H9C	109.5	C18 - C20 - H20A	109.5
H9A - C9 - H9C	109.5	C18 - C20 - H20B	109.5
H9B - C9 - H9C	109.5	H20A - C20 - H20B	109.5

C18 - C20 - H20C	109.5	C29 - C31 - H31A	109.5
H20A - C20 - H20C	109.5	C29 - C31 - H31B	109.5
H20B - C20 - H20C	109.5	H31A - C31 - H31B	109.5
C18 - C21 - H21A	109.5	C29 - C31 - H31C	109.5
C18 - C21 - H21B	109.5	H31A - C31 - H31C	109.5
H21A - C21 - H21B	109.5	H31B - C31 - H31C	109.5
C18 - C21 - H21C	109.5	C29 - C32 - H32A	109.5
H21A - C21 - H21C	109.5	C29 - C32 - H32B	109.5
H21B - C21 - H21C	109.5	H32A - C32 - H32B	109.5
C17 - C22 - C24	111.8(3)	C29 - C32 – H32C	109.5
C17 - C22 - H22A	109.3	H32A - C32 - H32C	109.5
C24 - C22 - H22A	109.3	H32B - C32 - H32C	109.5
C17 - C22 - H22B	109.3	C35 - C33 - C28	111.2(3)
C24 - C22 - H22B	109.3	C35 - C33 - H33A	109.4
H22A - C22 - H22B	107.9	C28 - C33 - H33A	109.4
O3 - C23 - C24	122.4(3)	C35 - C33 - H33B	109.4
O3 - C23 - C28	117.1(4)	C28 - C33 - H33B	109.4
C24 - C23 - C28	120.4(4)	H33A - C33 - H33B	108
C23 - C24 - C25	118.1(4)	O4 - C34 - C35	123.8(4)
C23 - C24 - C22	124.2(4)	O4 - C34 - C39	115.8(4)
C25 - C24 - C22	117.2(4)	C35 - C34 - C39	120.4(4)
C24 - C25 - C26	122.7(4)	C36 - C35 - C34	118.6(4)
C24 - C25 - H25	118.7	C36 - C35 - C33	119.0(4)
C26 - C25 - H25	118.7	C34 - C35 - C33	122.1(4)
C27 - C26 - C25	117.2(4)	C35 - C36 - C37	124.2(4)
C27 - C26 - C29	120.4(4)	C35 - C36 - H36	117.9
C25 - C26 - C29	122.5(4)	C37 - C36 - H36	117.9
C28 - C27 - C26	121.5(4)	C36 - C37 - C38	115.5(4)
C28 - C27 - H27	119.3	C36 - C37 - C40	122.1(4)
C26 - C27 - H27	119.3	C38 - C37 - C40	122.3(4)
C27 - C28 - C23	120.2(4)	C39 - C38 - C37	122.9(4)
C27 - C28 - C33	119.9(4)	C39 - C38 - H38	118.5
C23 - C28 - C33	119.8(4)	C37 - C38 - H38	118.5
C30 - C29 - C31	108.0(4)	C38 - C39 - C34	118.3(4)
C30 - C29 - C26	112.3(4)	C38 - C39 - C44	119.3(4)
C31 - C29 - C26	110.2(4)	C34 - C39 - C44	122.3(4)
C30 - C29 - C32	107.8(4)	C42 - C40 - C43	109.3(4)
C31 - C29 - C32	108.6(4)	C42 - C40 - C37	109.5(4)
C26 - C29 - C32	109.7(4)	C43 - C40 - C37	111.6(4)
C29 - C30 - H30A	109.5	C42 - C40 - C41	109.4(4)
C29 - C30 - H30B	109.5	C43 - C40 - C41	106.4(4)
H30A - C30 - H30B	109.5	C37 - C40 - C41	110.5(4)
C29 - C30 - H30C	109.5	C40 - C41 - H41A	109.5
H30A - C30 - H30C	109.5	C40 - C41 -H41B	109.5
H30B - C30 - H30C	109.5	H41A - C41 - H41B	109.5

C40 - C41 - H41C	109.5	C53 - C52 - C51	119.2(4)
H41A - C41 - H41C	109.5	C53 - C52 - H52	120.4
H41B - C41 - H41C	109.5	C51 - C52 - H52	120.4
C40 - C42 - H42A	109.5	C52 - C53 - C54	118.4(5)
C40 - C42 - H42B	109.5	C52 - C53 - H53	120.8
H42A - C42 - H42B	109.5	C54 - C53 - H53	120.8
C40 - C42 - H42C	109.5	N2 - C54 - C53	123.7(5)
H42A - C42 - H42C	109.5	N2 - C54 - H54	118.1
H42B - C42 - H42C	109.5	C53 - C54 - H54	118.1
C40 - C43 - H43A	109.5	N2 C55 C51	121.4(4)
C40 - C43 - H43B	109.5	N2 - C55 - C47	117.3(4)
H43A - C43 - H43B	109.5	C51 - C55 - C47	121.3(4)
C40 - C43 - H43C	109.5	O3 - C56 - C57	110.7(4)
H43A - C43 - H43C	109.5	O3 - C56 - H56A	109.5
H43B - C43 - H43C	109.5	C57 - C56 - H56A	109.5
C39 - C44 - C2	110.3(3)	O3 - C56 - H56B	109.5
C39 - C44 - H44A	109.6	C57 - C56 - H56B	109.5
C2 - C44 - H44A	109.6	H56A - C56 - H56B	108.1
C39 - C44 - H44B	109.6	O6 - C57 - N3	122.5(4)
C2 - C44 - H44B	109.6	O6 - C57 - C56	121.7(4)
H44A - C44 - H44B	108.1	N3 - C57 - C56	115.8(4)
O1 - C45 - C46	111.0(4)	C57 - N3 - C58	130.7(4)
O1 - C45 - H45A	109.4	C57 - N3 - H3A	114.6
C46 - C45 - H45A	109.4	C58 - N3 - H3A	114.6
O1 - C45 - H45B	109.4	C59 - C58 - N3	124.1(4)
C46 - C45 - H45B	109.4	C59 - C58 - C66	118.7(4)
H45A - C45 - H45B	108	N3 - C58 - C66	117.2(4)
O5 - C46 – N1	122.1(4)	C58 - C59 - C60	120.5(4)
O5 - C46 - C45	121.7(4)	C58 - C59 - H59	119.8
N1 - C46 - C45	116.2(4)	C60 - C59 - H59	119.8
C48 - C47 - N1	124.4(4)	C61 - C60 - C59	121.8(5)
C48 - C47 - C55	118.2(4)	C61 - C60 - H60	119.1
N1 - C47 - C55	117.4(4)	C59 - C60 - H60	119.1
C47 - C48 - C49	121.8(5)	C60 - C61 - C62	119.8(4)
C47 - C48 - H48	119.1	C60 - C61 - H61	120.1
C49 - C48 - H48	119.1	C62 - C61 - H61	120.1
C50 - C49 - C48	121.2(5)	C66 - C62 - C63	119.2(5)
C50 - C49 - H49	119.4	C66 - C62 - C61	118.6(4)
C48 - C49 - H49	119.4	C63 - C62 - C61	122.3(5)
C49 - C50 - C51	119.2(4)	C64 - C63 - C62	118.0(5)
C49 - C50 - H50	120.4	C64 - C63 - H63	121
C51 - C50 - H50	120.4	C62 - C63 - H63	121
C52 - C51 - C55	119.7(4)	C65 - C64 - C63	118.2(4)
C52 - C51 - C50	122.1(4)	C65 - C64 - H64	120.9
C55 - C51 - C50	118.2(4)	C63 - C64 - H64	120.9

N4 - C65 - C64	126.1(5)		
N4 - C65 - H65	117		
C64 - C65 - H65	117		
N4 - C66 - C62	121.5(4)		
N4 - C66 - C58	117.9(4)		
C62 - C66 - C58	120.6(4)		
C222 - C111 - H11C	109.5		
C222 - C111 - H11D	109.5		
H11C - C111 - H11D	109.5		
C222 - C111 - H11E	109.5		
H11C - C111 - H11E	109.5		
H11D - C111 - H11E	109.5		
N111 - C222 - C111	174.9(8)		

S06. Fluorescence studies of **L** with metal ions



S07. Competitive metal ion titrations

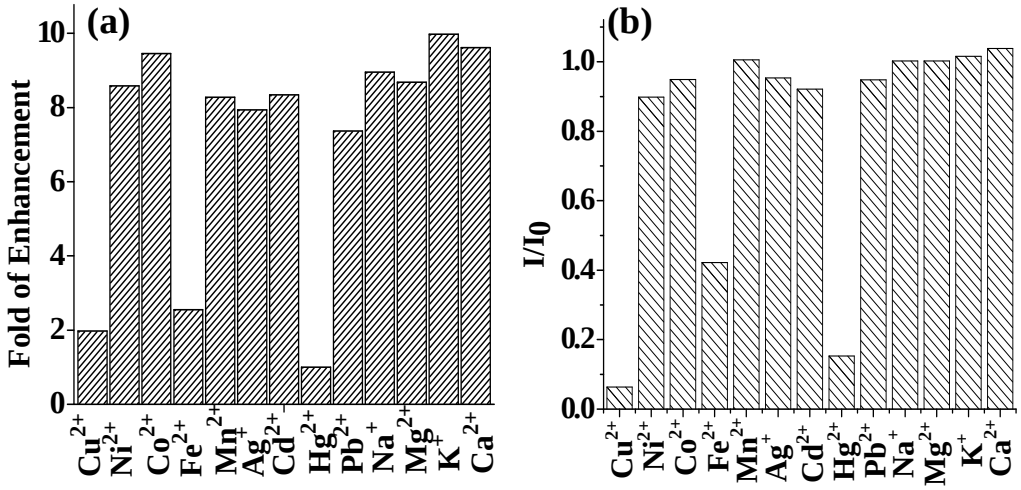
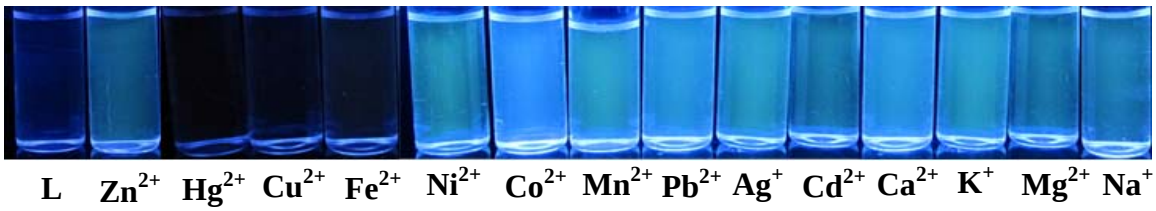


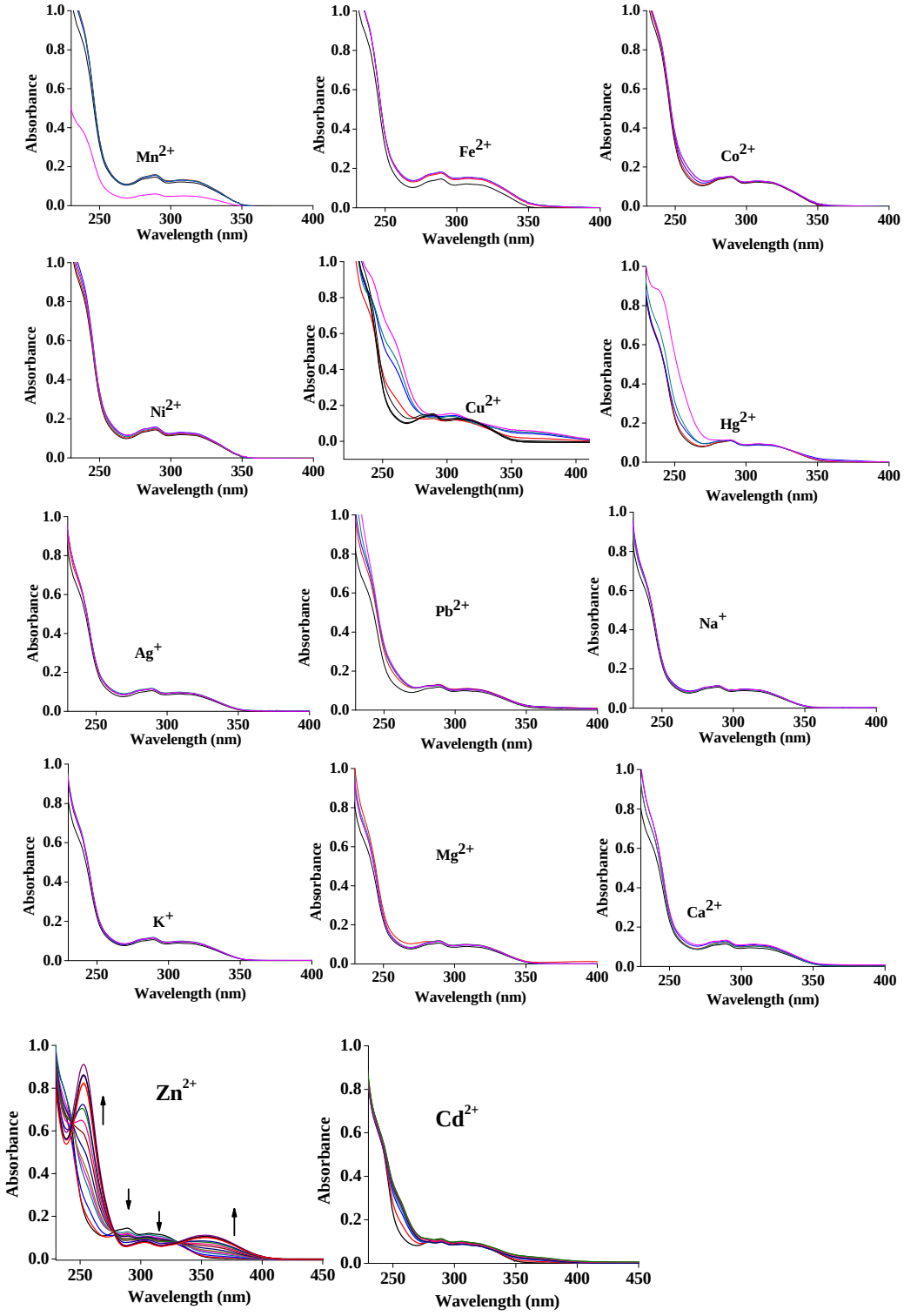
Fig. S8. Plot of relative fluorescence intensity of, (a) [L+M^{n+}] *vs.* Zn^{2+}; (b) [L+Zn^{2+}] *vs.* M^{n+}

S08. Competitive colour change titration

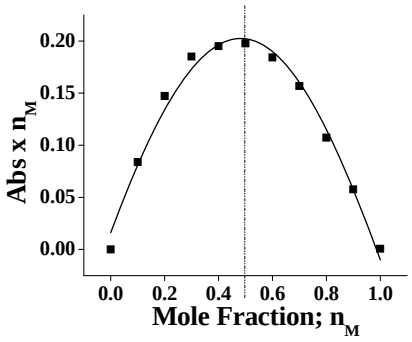


Competitive colorimetric titration of {**L**+Zn^{2+} as (1:2)} with 2 equivalents of various other metal ions. First one from the left is only L, second one from the left is {L+Zn^{2+}} and third onwards it is in the presence addition of other metal ion solution into a solution of {L+Zn^{2+}}.

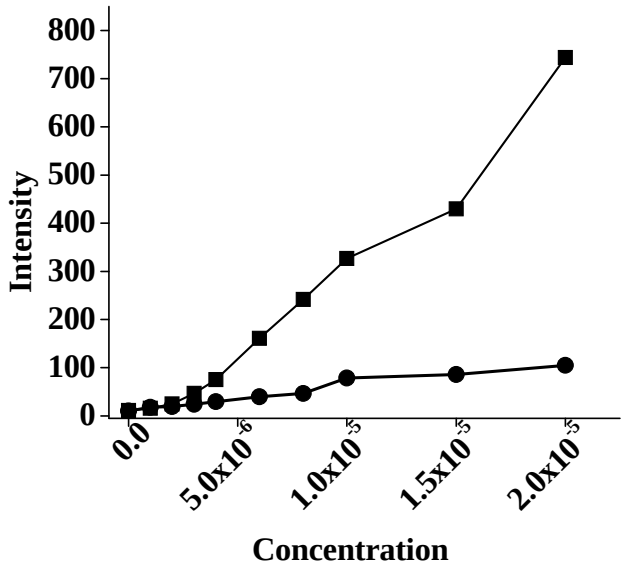
S09. Absorption studies of L with metal ions



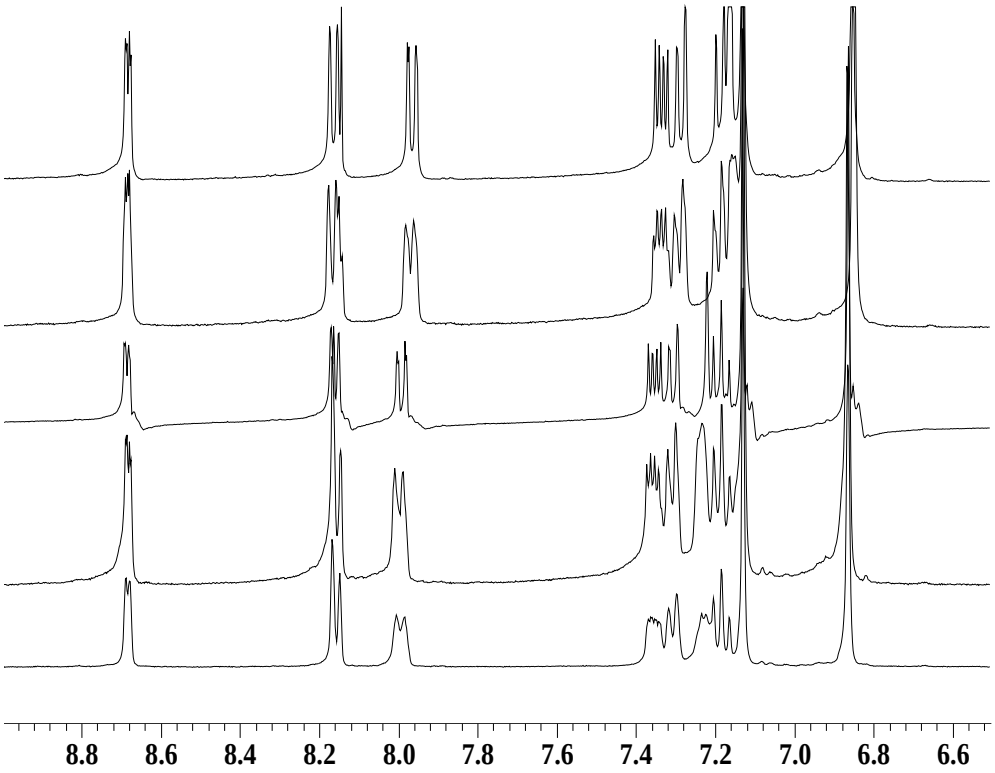
S10. Job's plot obtained from the absorption titration of L with Zn^{2+}



S11. Dilution experiment by maintaining the ratio of **L**:Zn^{2+} as 1:1



S12. 1H NMR titration of **L** with Zn^{2+}



S13. Computational data

(a) Cartesian coordinates of B3LYP/6-31G optimized structure of **L**

8	0.194893	2.067638	-0.029024	7	5.885305	2.596124	-1.844865
6	-1.049966	2.698984	-0.271220	6	7.424102	3.223287	-0.038111
6	1.390979	2.477452	-0.722603	1	-4.656376	5.406283	-2.733449
6	-1.612386	2.817438	-1.553121	1	-6.328878	5.371640	-2.153946
6	-1.727638	3.138777	0.883390	1	-5.519357	3.858241	-2.587877
1	1.198979	3.401109	-1.282737	1	-6.094714	2.914454	-0.270701
1	1.669119	1.680977	-1.419944	1	-6.946768	4.439711	0.059815
6	2.501120	2.745321	0.295303	1	-5.721769	3.839875	1.192561
6	-2.848852	3.484574	-1.654225	1	-4.463105	6.114404	0.987188
6	-1.027189	2.211958	-2.834108	1	-5.721396	6.670854	-0.131476
6	-2.962234	3.773870	0.721848	1	-4.011716	6.721025	-0.615146
6	-1.167248	2.884956	2.281773	1	0.189640	-0.915224	-1.221163
8	2.272102	2.994890	1.496759	6	-1.176872	-2.866437	-2.293637
7	3.752391	2.720366	-0.265941	6	-2.820463	-1.600557	-3.751088
1	-3.273358	3.590488	-2.645204	6	-4.599686	-0.561176	-5.262235
6	-3.542112	3.978886	-0.542995	1	0.188166	0.929999	1.199095
6	-1.634989	0.858909	-3.189173	6	-2.729507	-0.750712	4.036557
1	0.053493	2.101821	-2.768988	6	-1.022731	-2.192925	2.822634
1	-1.231639	2.909350	-3.655627	6	-4.554583	0.511117	5.305499
1	-3.475468	4.118141	1.614409	1	6.590817	3.905128	3.197242
1	-0.073445	2.887307	2.249795	6	7.581901	3.575309	1.330584
1	-1.472054	3.716065	2.927357	6	6.918283	2.518976	-2.680353
6	-1.686419	1.589287	2.905228	6	8.499669	3.131196	-0.964325
1	3.865426	2.470897	-1.247865	6	-1.734018	-3.118100	-0.893607
6	4.983128	3.015460	0.340868	1	-1.484900	-3.697151	-2.938154
6	-4.896217	4.711798	-0.658767	1	-0.083042	-2.869809	-2.265479
6	-1.097306	-0.321173	-2.645034	1	-3.268655	-2.568801	-3.956909
6	-2.750799	0.776244	-4.033189	6	-5.789150	-1.174842	-4.472975
6	-1.091735	0.342337	2.632222	6	-4.262488	-1.476495	-6.471152
6	-2.802908	1.626703	3.757522	6	-5.049018	0.812186	-5.812219
6	5.168249	3.359040	1.672648	1	-3.117540	-1.670009	4.466836
6	6.115684	2.941628	-0.536920	1	-1.226114	-2.891838	3.643095
6	-5.370699	4.840271	-2.124431	1	0.057914	-2.084240	2.754941
6	-5.979317	3.927140	0.131810	6	-1.612445	-2.794616	1.541942
6	-4.762638	6.141434	-0.065799	6	-5.086511	1.946065	5.526564
8	0.051098	-0.188063	-1.884564	6	-4.144344	-0.068156	6.687388
6	-1.698058	-1.570196	-2.913929	6	-5.710271	-0.344017	4.716076
6	-3.369062	-0.446205	-4.336518	1	8.574311	3.791416	1.713692
1	-3.135262	1.698438	-4.453972	6	8.251675	2.781157	-2.277283
8	0.048371	0.201690	1.861228	1	6.695855	2.241115	-3.705539
6	-1.626880	-0.839836	3.183329	1	9.509887	3.339112	-0.624551
1	-3.240495	2.597085	3.963267	6	-1.051890	-2.679476	0.258848

6	-3.343598	0.476529	4.348705	6	-2.970922	-3.747658	-0.729129
1	4.314291	3.408987	2.332110	1	-5.543171	-2.168328	-4.082615
6	6.473526	3.637430	2.152236	1	-6.668060	-1.275147	-5.122664
1	-6.059556	-0.537734	-3.623091	1	4.314057	-3.404847	-2.344846
1	-3.433645	-1.058149	-7.053682	6	6.471536	-3.646088	-2.160189
1	-5.133852	-1.573375	-7.131244	7	5.879999	-2.606149	1.836760
1	-3.971623	-2.481180	-6.146484	6	7.419385	-3.240201	0.032910
1	-5.332469	1.497425	-5.004805	1	6.589744	-3.913226	-3.205232
1	-5.923354	0.680880	-6.460380	6	7.578318	-3.591505	-1.335841
1	-4.260314	1.286872	-6.407348	6	6.911397	-2.536150	2.674828
6	-2.851887	-3.455833	1.645961	6	8.493244	-3.155649	0.961832
1	-4.321785	2.596654	5.966323	1	8.570332	-3.813037	-1.716864
1	-5.939602	1.920699	6.214547	6	8.244167	-2.805769	2.274632
1	-5.427733	2.399446	4.588594	1	6.688153	-2.258246	3.699827
1	-3.792158	-1.101783	6.601934	1	9.503029	-3.369165	0.624254
1	-4.999450	-0.058578	7.375323	1	9.047145	-2.735145	2.999413
1	-3.337954	0.526324	7.132086				
1	-6.025220	0.049780	3.742983				
1	-6.576187	-0.332860	5.390280				
1	-5.407094	-1.387093	4.574333				
1	9.055965	2.704821	-3.000026				
8	0.194481	-2.053536	0.011694				
6	-3.549662	-3.948320	0.536870				
1	-3.487487	-4.090464	-1.620293				
1	-3.275151	-3.558230	2.637834				
6	1.389797	-2.462805	0.706574				
6	-4.907571	-4.673541	0.655634				
1	1.196751	-3.384743	1.269204				
1	1.669180	-1.664883	1.401792				
6	2.499711	-2.734987	-0.310419				
6	-5.378738	-4.800849	2.122488				
6	-4.784096	-6.103222	0.060681				
6	-5.988175	-3.881235	-0.130770				
8	2.271101	-2.982356	-1.512372				
7	3.750206	-2.716396	0.252861				
1	-4.665334	-5.370502	2.729241				
1	-6.339172	-5.328003	2.154073				
1	-5.522203	-3.818418	2.586728				
1	-4.034734	-6.687784	0.606906				
1	-4.487979	-6.076938	-0.993299				
1	-5.745676	-6.627158	0.128954				
1	-6.958178	-4.388828	-0.057949				
1	-5.732598	-3.792255	-1.191883				
1	-6.097304	-2.869038	0.274581				
1	3.862663	-2.468644	1.235302				

6	4.980573	-3.017594	-0.351598				
6	5.166773	-3.360614	-1.683353				
6	6.111476	-2.951396	0.528936				

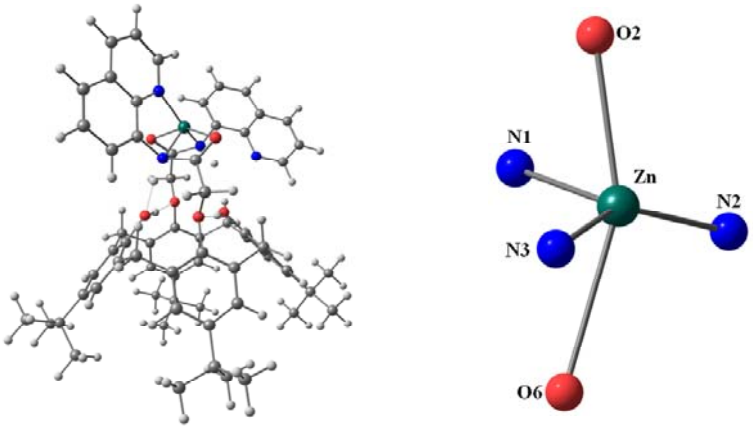
(b) Cartesian coordinates of B3LYP/6-31G* optimized structure of [Zn**L**] in deprotonated form.

8	-0.411178	0.579440	1.788012	6	-5.453650	3.713363	-1.169314
6	0.702325	0.716251	2.616583	1	4.959516	-0.796743	4.827902
6	-1.696311	0.344595	2.404080	1	6.139912	0.350479	5.478414
6	1.212168	-0.397197	3.307833	1	5.614017	0.474838	3.787047
6	1.333083	1.966212	2.672515	1	5.066981	2.943087	4.254906
1	-1.569343	0.198985	3.478876	1	5.551451	2.703833	5.938250
1	-2.105830	-0.562187	1.950249	1	3.955884	3.372378	5.571656
6	-2.553447	1.599271	2.187781	1	2.901708	1.530396	7.015731
6	2.311060	-0.190284	4.146858	1	4.543115	0.956009	7.373313
6	0.687181	-1.817729	3.109247	1	3.324212	-0.167282	6.750462
6	2.445152	2.107075	3.512324	1	-0.514986	-1.535639	-0.300715
6	0.879031	3.144646	1.817319	6	0.879055	-3.144648	-1.817316
8	-2.419147	2.529031	2.987509	6	2.731402	-3.711102	-0.183063
7	-3.336339	1.583540	1.062958	6	4.709950	-4.371927	1.342920
1	2.688100	-1.045824	4.701553	1	-0.515015	1.535627	0.300710
6	2.944718	1.052807	4.282339	6	2.626282	3.127927	-2.128441
6	1.377147	-2.533183	1.951475	6	0.687171	1.817725	-3.109247
1	-0.389692	-1.824803	2.940644	6	4.709924	4.371940	-1.342910
1	0.872919	-2.379639	4.032207	1	-4.480303	6.088284	1.050841
1	2.912431	3.084669	3.562004	6	-5.336501	4.988632	-0.566164
1	-0.211953	3.176434	1.771254	6	-5.602566	1.161738	-2.238250
1	1.195055	4.065031	2.320580	6	-6.206998	3.475242	-2.344115
6	1.473125	3.140225	0.411054	6	1.333105	-1.966210	-2.672507
6	-3.980588	2.740889	0.607941	1	1.195083	-4.065030	-2.320581
6	4.142864	1.208043	5.237642	1	-0.211929	-3.176438	-1.771254
6	0.790785	-2.562256	0.673468	1	3.237153	-4.160340	-1.031896
6	2.626300	-3.127927	2.128447	6	5.317679	-4.999121	0.073855
6	0.790767	2.562248	-0.673466	6	4.570430	-5.486608	2.406540
6	2.731380	3.711099	0.183070	6	5.690739	-3.292767	1.860198
6	-3.911003	4.019195	1.163946	1	3.063222	3.104281	-3.124067
6	-4.784924	2.595888	-0.580245	1	0.872908	2.379637	-4.032206
6	5.278776	0.250534	4.805895	1	-0.389703	1.824791	-2.940648
6	4.705008	2.642324	5.244635	6	1.212170	0.397197	-3.307830
6	3.699608	0.858948	6.678379	6	5.317670	4.999083	-0.073829
8	-0.471192	-2.047309	0.534816	6	4.570369	5.486667	-2.406478
6	1.473146	-3.140231	-0.411050	6	5.690718	3.292815	-1.860253
6	3.333860	-3.732695	1.078743	1	-5.842983	5.840480	-1.010832

1	3.063241	-3.104274	3.124072	6	-6.283318	2.208990	-2.884157
8	-0.471211	2.047300	-0.534819	1	-5.632235	0.146518	-2.625160
6	1.377130	2.533183	-1.951472	1	-6.722893	4.308912	-2.814420
1	3.237127	4.160342	1.031903	6	0.702336	-0.716253	-2.616578
6	3.333843	3.732688	-1.078733	6	2.445180	-2.107063	-3.512310
1	-3.331007	4.159506	2.063010	1	4.683227	-5.796556	-0.329823
6	-4.578463	5.115734	0.575804	1	6.293594	-5.439708	0.308800
7	-4.889052	1.351833	-1.136410	1	5.473203	-4.253501	-0.714134
1	4.175955	-5.099589	3.352023	7	-4.889092	-1.351823	1.136368
1	5.545717	-5.944726	2.614534	6	-5.453671	-3.713358	1.169317
1	3.891114	-6.273838	2.059777	1	-4.480246	-6.088325	-1.050754
1	5.821252	-2.496206	1.118906	6	-5.336496	-4.988641	0.566201
1	6.674809	-3.733039	2.065924	6	-5.602636	-1.161707	2.238184
1	5.332773	-2.828219	2.785050	6	-6.207053	-3.475213	2.344091
6	2.311072	0.190294	-4.146845	1	-5.842982	-5.840482	1.010878
1	4.683185	5.796448	0.329936	6	-6.283397	-2.208948	2.884100
1	6.293545	5.439752	-0.308787	1	-5.632322	-0.146478	2.625068
1	5.473279	4.253416	0.714100	1	-6.722953	-4.308875	2.814404
1	4.175885	5.099681	-3.351971	1	-6.852448	-2.008047	3.785475
1	5.545644	5.944811	-2.614466	30	-3.848061	-0.000006	-0.000019
1	3.891044	6.273869	-2.059669				
1	5.821258	2.496226	-1.118997				
1	6.674776	3.733111	-2.065982				
1	5.332741	2.828299	-2.785116				
1	-6.852344	2.008106	-3.785552				
8	-0.411176	-0.579453	-1.788018				
6	2.944755	-1.052786	-4.282306				
1	2.912461	-3.084656	-3.561992				
1	2.688096	1.045832	-4.701554				
6	-1.696306	-0.344635	-2.404100				
6	4.142881	-1.208022	-5.237634				
1	-1.569333	-0.199045	-3.478898				
1	-2.105836	0.562151	-1.950288				
6	-2.553429	-1.599317	-2.187777				
6	5.278842	-0.250574	-4.805880				
6	3.699598	-0.858845	-6.678342				
6	4.704976	-2.642322	-5.244704				
8	-2.419135	-2.529084	-2.987497				
7	-3.336322	-1.583572	-1.062955				
1	4.959636	0.796719	-4.827854				
1	6.139962	-0.350542	-5.478415				
1	5.614091	-0.474921	-3.787043				
1	3.324228	0.167401	-6.750358				
1	2.901668	-1.530251	-7.015706				
1	4.543082	-0.955894	-7.373305				

1	5.551379	-2.703839	-5.938368				
1	3.955810	-3.372341	-5.571710				
1	5.066990	-2.943130	-4.255004				
6	-3.980573	-2.740915	-0.607926				
6	-3.910963	-4.019233	-1.163897				
6	-4.784941	-2.595891	0.580236				
1	-3.330945	-4.159562	-2.062945				
6	-4.578427	-5.115764	-0.575744				

(c) B3LYP/6-31G* optimized structure of [Zn**L**] in neutral form and the coordination geometry around Zn^{2+}



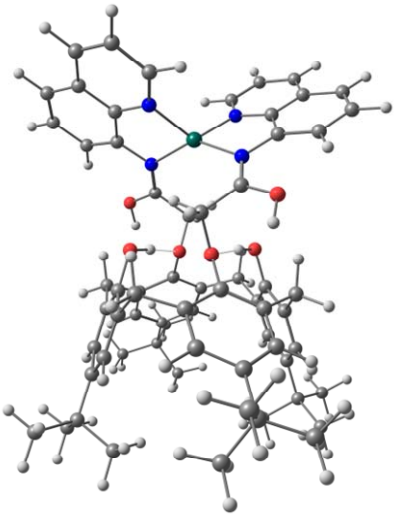
(d) Cartesian coordinates of B3LYP/6-31G* optimized structure of [Zn**L**] in neutral form.

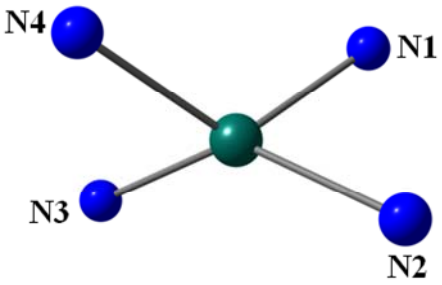
8	0.307030	-0.983573	-2.114132	7	5.414724	-1.816617	-0.378090
6	-1.035831	-1.101174	-2.554932	6	5.681668	-4.192987	-0.838211
6	1.336826	-1.334141	-3.028917	1	-5.316373	-3.539451	-3.961440
6	-1.736319	-2.270484	-2.257346	1	-6.865659	-2.706431	-3.823090
6	-1.627670	0.013366	-3.162443	1	-5.853814	-2.900421	-2.390296
1	1.404178	-0.656297	-3.885906	1	-5.972325	-0.362713	-2.005038
1	1.228572	-2.367672	-3.385246	1	-7.034698	-0.272275	-3.421857
6	2.568490	-1.183954	-2.164729	1	-5.605518	0.762360	-3.323076
6	-3.073195	-2.336874	-2.670662	1	-4.826322	-0.169303	-5.627059
6	-1.122567	-3.415694	-1.457104	1	-6.272586	-1.184035	-5.674951
6	-2.963451	-0.109834	-3.548333	1	-4.670059	-1.918845	-5.856485
6	-0.891415	1.341143	-3.337887	1	0.315985	-1.082745	1.123058
8	3.468860	-0.382072	-2.369442	6	-0.800055	-1.597647	3.320795
7	2.644646	-1.920004	-0.913412	6	-2.493218	-3.348433	2.631667
1	-3.624412	-3.244144	-2.451362	6	-4.299229	-5.120741	2.105029

6	-3.710398	-1.279151	-3.330149	1	0.251162	0.583338	-1.232173
6	-1.542408	-3.419688	0.008926	6	-1.838524	4.273799	-0.319194
1	-0.032709	-3.374642	-1.536513	6	-0.379630	3.148393	1.418951
1	-1.436597	-4.363618	-1.907284	6	-3.423068	5.533391	-1.875422
1	-3.433649	0.744154	-4.026888	1	3.261235	-6.469717	-1.614084
1	0.191168	1.178039	-3.391898	6	5.081100	-5.437062	-1.164197
1	-1.179231	1.768803	-4.303116	6	6.724832	-1.721702	-0.151603
6	-1.200360	2.370524	-2.253108	6	7.071052	-4.049598	-0.596986
1	1.705570	-2.093697	-0.493136	6	-1.312741	-0.164673	3.181359
6	3.468928	-3.131605	-0.998116	1	-1.064741	-1.968290	4.315732
6	-5.176039	-1.350013	-3.796722	1	0.293891	-1.625116	3.266661
6	-0.918277	-2.608323	0.969668	1	-2.844807	-3.299834	3.656464
6	-2.618830	-4.211854	0.414059	6	-4.700145	-4.968781	3.584667
6	-0.604124	2.316549	-0.983635	6	-3.904906	-6.597155	1.860476
6	-2.111743	3.402150	-2.520670	6	-5.527404	-4.766122	1.232627
6	2.917473	-4.358547	-1.301781	1	-2.076313	5.004690	0.449409
6	4.866821	-3.026443	-0.738687	1	-0.485504	4.123088	1.908064
6	-5.829924	-2.705783	-3.468814	1	0.689641	2.932833	1.372475
6	-5.990051	-0.236989	-3.093506	6	-1.106047	2.104432	2.260864
6	-5.233917	-1.141094	-5.329249	6	-3.993314	5.464008	-3.304804
8	0.212176	-1.890775	0.581681	6	-2.685119	6.884225	-1.714806
6	-1.399695	-2.543753	2.284265	6	-4.607311	5.475656	-0.880878
6	-3.118719	-4.208656	1.724511	1	5.707706	-6.320779	-1.236866
1	-3.082600	-4.854341	-0.329546	6	7.594073	-2.817994	-0.263805
8	0.342186	1.363810	-0.655415	1	7.100121	-0.743434	0.132204
6	-0.938274	3.257753	0.005792	1	7.715227	-4.920874	-0.675864
1	-2.554284	3.435486	-3.510536	6	-0.587763	0.833716	2.516352
6	-2.445936	4.380482	-1.580262	6	-2.579797	0.174787	3.658243
1	1.849573	-4.441422	-1.478358	6	4.313249	2.158821	1.097338
6	3.724424	-5.517764	-1.377310	6	5.449914	1.949181	1.847569
1	-5.027740	-3.949089	3.818694	6	4.032598	3.424134	0.512158
1	-3.649512	-6.785540	0.811994	1	-3.879158	-5.232522	4.261256
1	-4.738089	-7.259459	2.120946	1	-5.536167	-5.638886	3.809325
1	-3.042233	-6.881649	2.473554	1	5.647748	0.988930	2.315822
1	-5.834538	-3.725689	1.388329	6	6.364602	3.015721	2.035362
1	-6.374201	-5.411418	1.491876	7	2.880915	3.550664	-0.194660
1	-5.325699	-4.901985	0.164341	6	4.967945	4.484268	0.698171
6	-2.381633	2.387559	2.767745	1	7.251589	2.845817	2.636810
1	-3.206631	5.533005	-4.064969	6	6.135319	4.251754	1.471400
1	-4.679053	6.301651	-3.468281	6	2.618254	4.724324	-0.742171
1	-4.559047	4.540731	-3.475516	6	4.648323	5.725469	0.086243
1	-2.287119	7.015443	-0.702589	1	6.843472	5.062078	1.618523
1	-3.369691	7.717078	-1.911267	6	3.480027	5.844308	-0.631473
1	-1.848785	6.962173	-2.419271	1	1.682526	4.801421	-1.290433
1	-5.152197	4.529284	-0.972748	1	5.327446	6.566648	0.194352

1	-5.310537	6.291888	-1.081143	1	3.206623	6.779685	-1.108172
1	-4.276166	5.574336	0.158642	30	4.009228	-0.458545	-0.205643
1	8.653219	-2.681619	-0.077504	6	2.971974	0.349143	2.047967
8	0.696150	0.492178	2.017276	6	-4.976350	3.209445	3.748315
6	-3.137127	1.451335	3.482244	6	-4.506469	1.580867	5.589587
1	-3.148796	-0.590474	4.178023	6	-5.569400	0.799034	3.434137
1	-2.787895	3.374499	2.577982	8	3.608149	-0.667097	2.233070
6	1.790941	0.798307	2.879825	7	3.312457	1.100713	0.830908
6	-4.531934	1.766424	4.053341	1	-4.297201	3.949329	4.187288
1	1.768325	0.222020	3.810473	1	-5.968864	3.384585	4.175798
1	1.836103	1.870833	3.103718	1	-5.046344	3.398734	2.670877
1	-3.781831	2.256947	6.057184				
1	-4.244582	0.556615	5.875625				
1	-5.493656	1.800182	6.011254				
1	-6.567301	1.013354	3.832528				
1	-5.342104	-0.248326	3.659911				
1	-5.608855	0.907811	2.344378				
1	2.491627	1.583645	0.401712				

(e) B3LYP/6-31G* optimized structure of [Zn**L**] in tautomeric form and the coordination geometry around Zn^{2+}





(f) Cartesian coordinates of B3LYP/6-31G* optimized structure of [Zn**L**] in tautomeric form.

8	-0.22697	-1.68423	-0.50107	7	-5.05223	-0.03965	1.732827
6	0.781849	-2.62282	-0.82885	6	-5.72586	-1.58031	3.484831
6	-1.52722	-1.89418	-1.05071	1	4.797124	-4.26637	-3.36042
6	1.2624	-2.67672	-2.15033	1	5.810912	-5.57513	-2.74447
6	1.334957	-3.3924	0.206855	1	5.503815	-4.14722	-1.7396
1	-1.48563	-2.58493	-1.89955	1	4.767894	-5.76929	0.11771

1	-1.89898	-0.93221	-1.40679	1	5.030957	-7.12311	-0.98196
6	-2.39008	-2.49044	0.037489	1	3.465608	-6.94157	-0.18748
6	2.228549	-3.64376	-2.43489	1	2.344388	-7.04355	-2.50396
6	0.868002	-1.67024	-3.23029	1	3.957343	-7.26094	-3.20399
6	2.314885	-4.33464	-0.14897	1	2.897526	-5.98478	-3.81332
6	1.010543	-3.18822	1.688737	1	-0.34353	0.968336	-1.15804
8	-2.04815	-3.71032	0.436649	6	1.010291	3.188303	-1.68903
7	-3.36139	-1.8283	0.593373	6	3.016406	2.046801	-2.75168
1	2.589122	-3.70858	-3.45732	6	5.122259	1.032066	-3.85351
6	2.764471	-4.50332	-1.46131	1	-0.34318	-0.96828	1.157537
6	1.59992	-0.33892	-3.08546	6	2.923227	0.214748	3.513154
1	-0.20727	-1.48214	-3.24842	6	0.868133	1.670301	3.230109
1	1.121503	-2.10881	-4.20103	6	5.122189	-1.03209	3.854033
1	2.732749	-4.94251	0.645451	1	-4.80376	-4.83377	3.863297
1	-0.06594	-3.10783	1.861205	6	-5.65208	-2.8809	4.044507
1	1.340931	-4.0858	2.221238	6	-5.82611	0.901144	2.272944
6	1.687372	-1.97474	2.319773	6	-6.53191	-0.5538	4.03465
6	-4.11397	-2.26988	1.726032	6	1.334533	3.392625	-0.20712
6	3.820046	-5.55213	-1.85572	1	1.340846	4.0858	-2.22157
6	0.985204	0.774662	-2.49662	1	-0.06618	3.108024	-1.86165
6	2.92319	-0.21473	-3.51313	1	3.544928	2.984035	-2.61303
6	0.985436	-0.77461	2.496284	6	5.759722	2.413347	-3.61088
6	3.016535	-2.04683	2.75182	6	5.166992	0.740845	-5.37254
6	-4.0905	-3.53431	2.300834	6	5.964651	-0.02652	-3.1019
6	-4.96923	-1.27865	2.314006	1	3.391321	1.07963	3.975835
6	5.052359	-4.83717	-2.46124	1	1.122019	2.10891	4.200722
6	4.290592	-6.3881	-0.6507	1	-0.20714	1.48223	3.248683
6	3.214268	-6.5127	-2.90745	6	1.262174	2.676848	2.150047
8	-0.34355	0.684272	-2.09212	6	5.759735	-2.41334	3.611446
6	1.687144	1.974758	-2.31992	6	5.166622	-0.74096	5.373087
6	3.664642	0.96685	-3.36064	6	5.96469	0.026577	3.10266
1	3.391361	-1.07962	-3.97571	1	-6.23025	-3.1101	4.934422
8	-0.34327	-0.68428	2.091641	6	-6.57952	0.688478	3.437197
6	1.600057	0.338985	3.085184	1	-5.85262	1.859424	1.761991
1	3.545052	-2.98409	2.613333	1	-7.11204	-0.75983	4.929886
6	3.664674	-0.96687	3.360867	6	0.781712	2.622773	0.828538
1	-3.47957	-4.31665	1.879336	6	2.313947	4.335366	0.148778
6	-4.85823	-3.832	3.449919	1	5.229795	3.208902	-4.14729
1	6.793493	2.408662	-3.97142	1	-3.48083	4.316468	-1.87837
1	5.785986	2.671401	-2.54579	6	-4.85936	3.831789	-3.44909
1	4.76878	-0.25083	-5.61213	7	-5.05196	0.038872	-1.73309
1	6.200498	0.778125	-5.73501	6	-5.72613	1.579777	-3.48469
1	4.584542	1.480608	-5.93308	1	-4.80529	4.833715	-3.86216
1	5.964606	0.16438	-2.02258	6	-5.65284	2.880565	-4.04397
1	7.003321	-0.0016	-3.45071	6	-5.82547	-0.90206	-2.27348

1	5.585805	-1.04164	-3.26254	6	-6.53177	0.553112	-4.03481
6	2.227815	3.644385	2.434675	1	-6.23109	3.109805	-4.93382
1	5.229521	-3.20898	4.147428	6	-6.57893	-0.68935	-3.43771
1	6.793328	-2.40875	3.972487	1	-5.85167	-1.86048	-1.76278
1	5.786519	-2.67118	2.546311	1	-7.11197	0.759174	-4.93
1	4.768588	0.250797	5.612649	1	-7.1875	-1.49145	-3.83963
1	6.200032	-0.7785	5.73581	30	-4.057650	-0.00036	-4.8E-05
1	4.583869	-1.48063	5.933455	1	-1.19814	3.986839	-0.03273
1	5.964583	-0.16405	2.023288	1	-1.19807	-3.98746	0.032407
1	7.003369	0.001446	3.451422				
1	5.585968	1.041708	3.263567				
1	-7.18841	1.490449	3.83888				
8	-0.22687	1.683976	0.500688				
6	2.763368	4.504239	1.461149				
1	2.731566	4.943456	-0.6456				
1	2.588304	3.709356	3.457129				
6	-1.52717	1.8935	1.050425				
6	3.818424	5.55353	1.855649				
1	-1.48575	2.583977	1.899492				
1	-1.89867	0.931328	1.406203				
6	-2.39021	2.48986	-0.03756				
6	5.051762	4.83898	2.459567				
6	3.212751	6.512726	2.908703				
6	4.287368	6.390908	0.650979				
8	-2.04836	3.709751	-0.43675				
7	-3.36165	1.827753	-0.59325				
1	4.797765	4.267598	3.358728				
1	5.810181	5.577234	2.742378				
1	5.502875	4.149639	1.737124				
1	2.897062	5.983773	3.814337				
1	2.342193	7.043319	2.506342				
1	3.955517	7.261228	3.205357				
1	5.027341	7.126285	0.98232				
1	3.461571	6.944056	0.188825				
1	4.764643	5.773148	-0.11829				
6	-4.11446	2.269414	-1.72572				
6	-4.09149	3.534039	-2.30012				
6	-4.96939	1.27806	-2.31395				

(g) Dihedral angles of crystal structure of **L**, and the optimized structures of **L** & [Zn**L**]

	L (Crystal structure)	**L**	[**ZnL**] (Deprotonated)	[**ZnL**] (neutral	[**ZnL**] (Tautomeric)
C1-O1-C2-C5	135.6	128.4	111.4	-175.6	101.8
O1-C2-C5-N1	165.3	160.5	92.0	55.4	110.3
C2-C5-N1-C13	-177.7	175.0	-168.3	100.8	-172.4
C5-N1-C13-C20	166.7	-177.9	-179.5	88.6	169.2
N1-C13-C20-N2	-1.4	-0.1	2.0	1.9	2.9
C48-O5-C52-C54	134.7	128.6	111.4	-178.7	101.8
O5-C52-C54-N3	165.6	160.8	92.0	68.7	110.4
C52-C54-N3-C58	-179.1	174.9	-168.3	92.5	-172.4
C54-N3-C58-C60	166.6	-177.7	-179.5	-134.7	169.2
N3-C58-C60-N4	-0.9	-0.2	2.0	1.5	2.9

(h) Metric data for zinc coordination center in [ZnL]: bond lengths in Å, bond angles in °.

	[**ZnL**] (Deprotonated)	[**ZnL**] (neutral)	[**ZnL**] (Tautomeric)
Zn-N1	1.975	2.121	2.044
Zn-N2	2.050	1.962	1.998
Zn-N3	1.975	1.998	2.044
Zn-N4	2.050	-	1.998
Zn-O2	-	2.232	-
Zn-O6	-	2.480	-
N1-Zn-N2	84.3	87.4	84.3
N1-Zn-N3	149.9	119.1	140.2
N1-Zn-N4	111.2	-	116.0
N2-Zn-N3	111.2	146.7	116.0
N2-Zn-N4	118.9	-	120.3

N3-Zn-N4	84.3	-	84.3
N1-Zn-O2	-	62.9	-
N1-Zn-O6	-	99.6	-
N2-Zn-O2	-	96.4	-
N2-Zn-O6	-	98.3	-
N3-Zn-O2	-	113.1	-
N3-Zn-O6	-	59.3	-
O2-Zn-O6	-	156.5	-

S14. AFM data

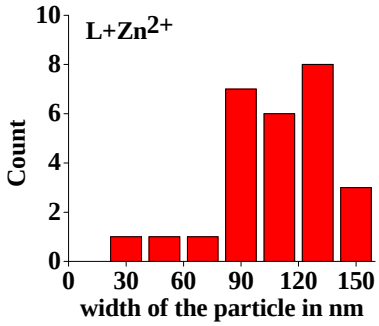


Figure S14: Particle size distribution of **L** in absence and in presence of zinc ion from the AFM data.

S15. TEM data

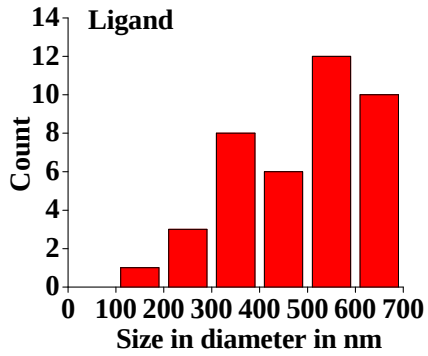


Figure S15: Particle size distribution of **L** from TEM analysis.

S16. **Gaussian 03 reference**

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, Jr. J. A. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, *Gaussian 03*, revision C.02; Gaussian, Inc.: Wallingford, CT, 2004.