Electronic Supporting Information

A novel 2-(2'-aminophenyl)benzothiazole derivative displays ESIPT and permits selective detection of Zn^{2+} ions: Experimental and theoretical studies

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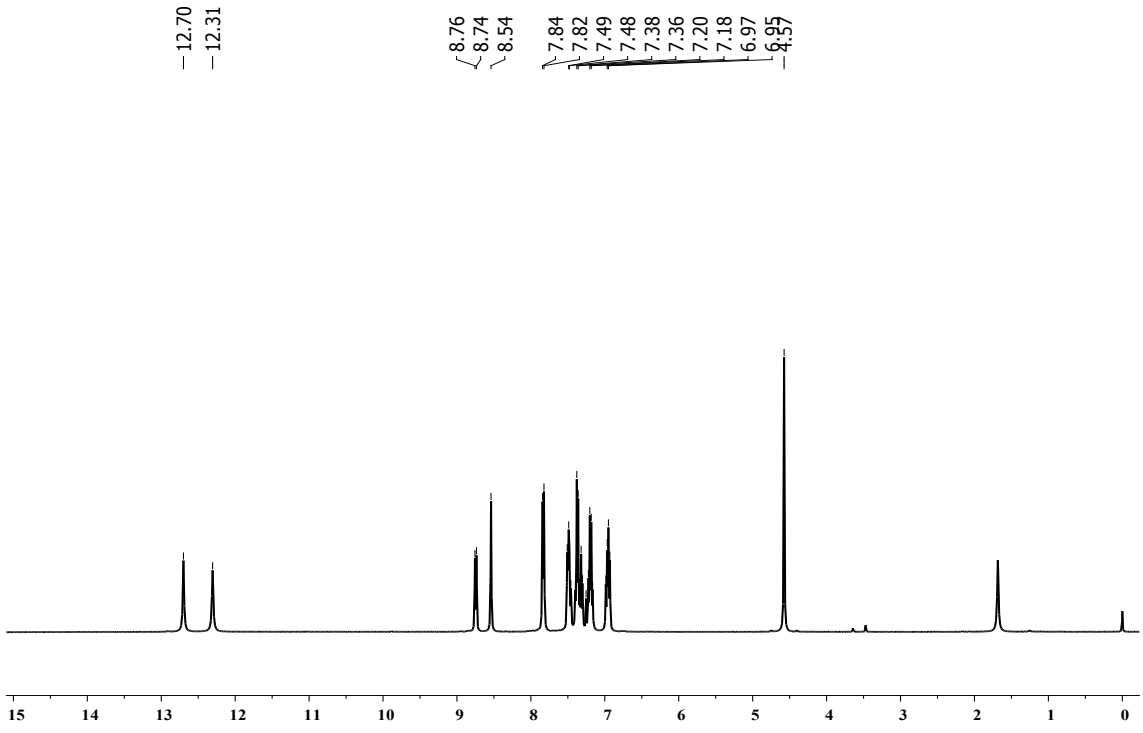

Fig. S1 ^{1}H NMR spectrum of **1** in $CDCl_3$

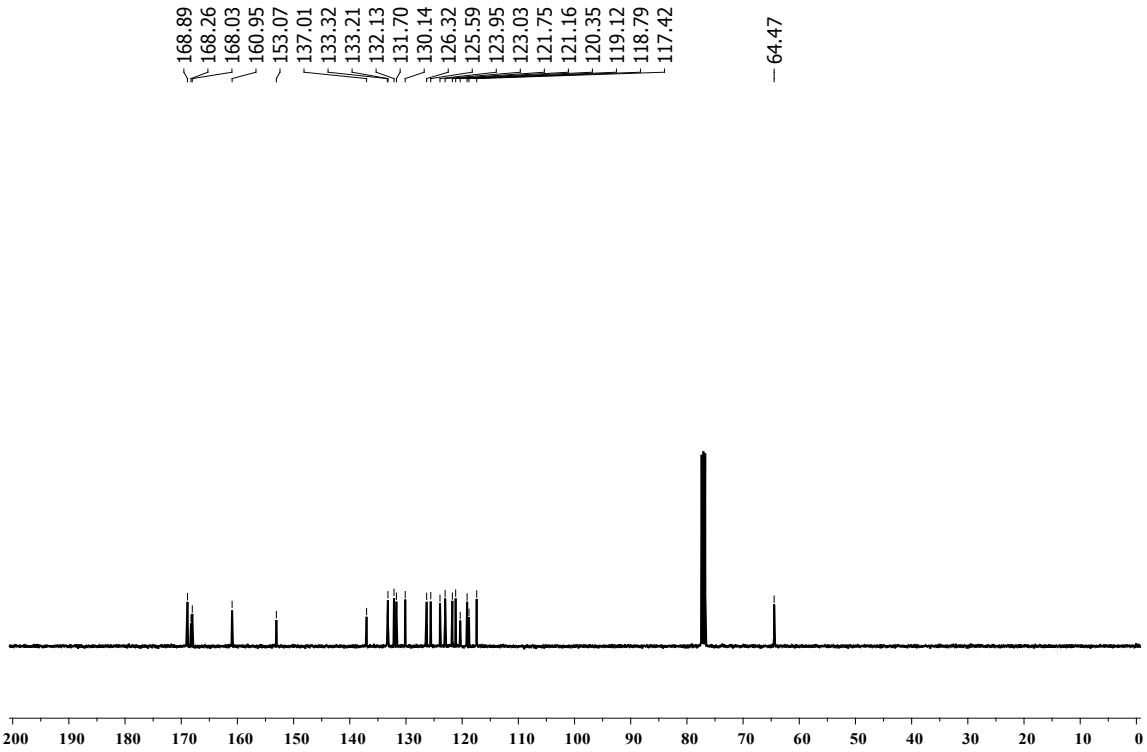

Fig. S2 ^{13}C NMR spectrum of **1** in $CDCl_3$

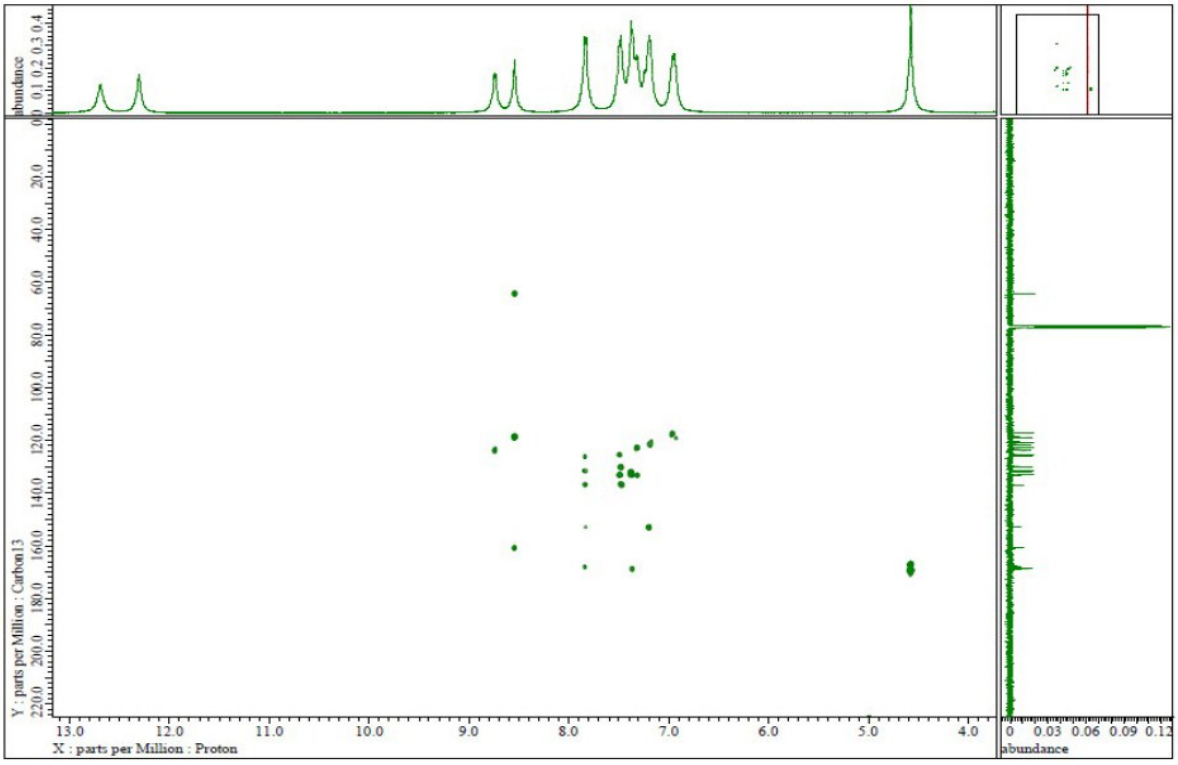

Fig. S3 HMBC spectrum of **1** in $CDCl_3$

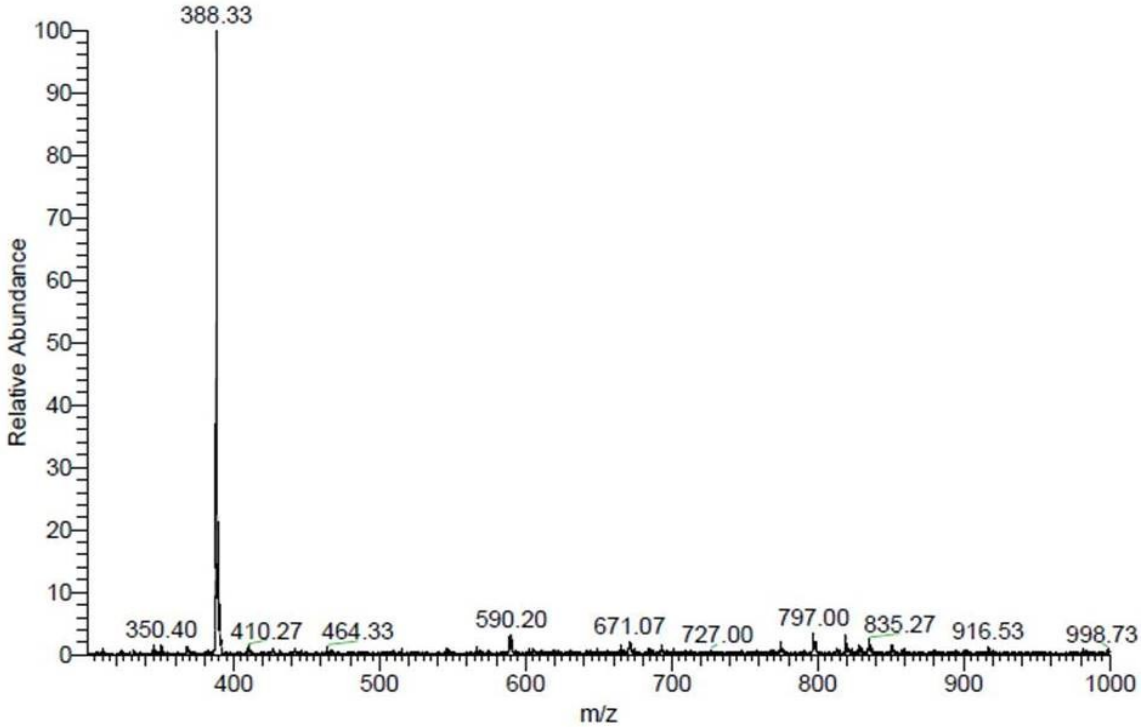

Fig. S4 ESI-MS spectrum of **1**

(a)

Solvent	Excitation energy (eV)	Nature of S1 transition	Wavelength (nm)	Oscillator strength
Acetonitrile	3.9653	HOMO→LUMO (91%)	312.66	0.6549
Chloroform	3.9381	HOMO→LUMO (87%)	314.82	0.6655
Dimethyl sulfoxide	3.9567	HOMO→LUMO (91%)	313.34	0.6724
Methanol	3.9671	HOMO→LUMO (91%)	312.52	0.6509
Tetrahydrofuran	3.9485	HOMO→LUMO (91%)	313.99	0.6615
Toluene	3.9197	H-1→LUMO (91%)	316.30	0.6645

(b)

Solvent	Excitation energy (eV)	Nature of S1 transition	Wavelength (nm)	Oscillator strength
Acetonitrile	4.0074	HOMO→LUMO (92%)	309.37	0.6477
Chloroform	3.9830	H-1→LUMO (92%)	311.27	0.6616
Dimethyl sulfoxide	3.9990	HOMO→LUMO (92%)	310.02	0.6638
Methanol	4.0092	HOMO→LUMO (92%)	309.23	0.6441
Tetrahydrofuran	3.9924	H-1→LUMO (79%), HOMO→LUMO (13%)	310.54	0.6563
Toluene	3.9672	H-1→LUMO (93%)	312.51	0.6640

Table S1. Photophysical parameters of **1** in different solvents calculated using Gaussian 09 at B3LYP/6-31++ G level (**a**) and B3LYP/6-31G** level (**b**)

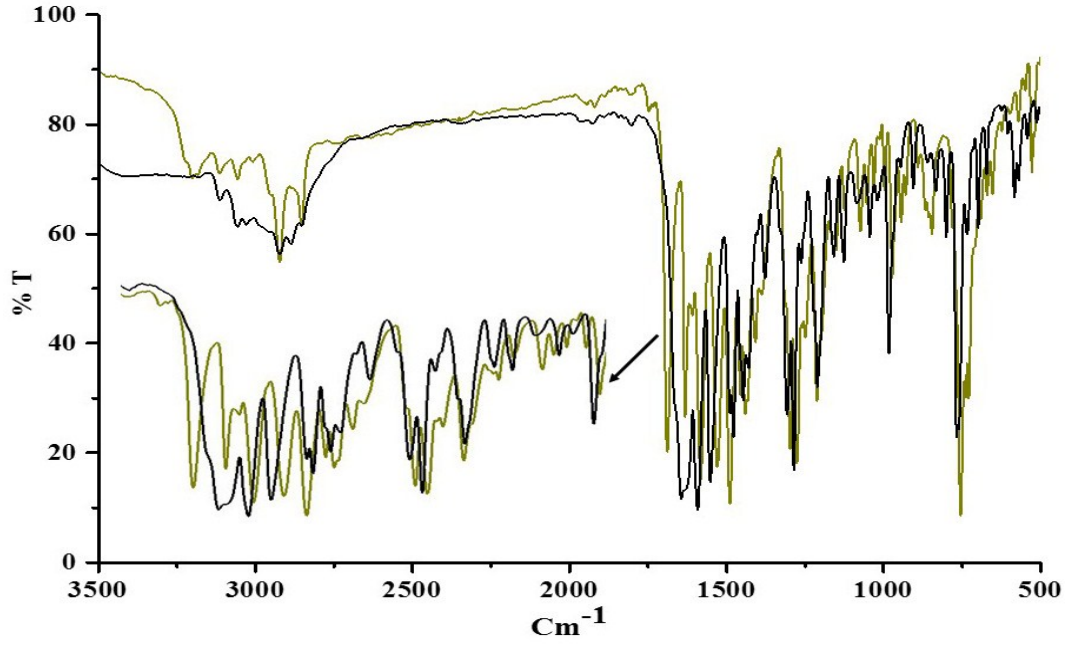

Fig. S5 FT-IR spectra of **1** (green line) and **1-Zn^{2+}** complex (block line). Inset: Expanted spectra

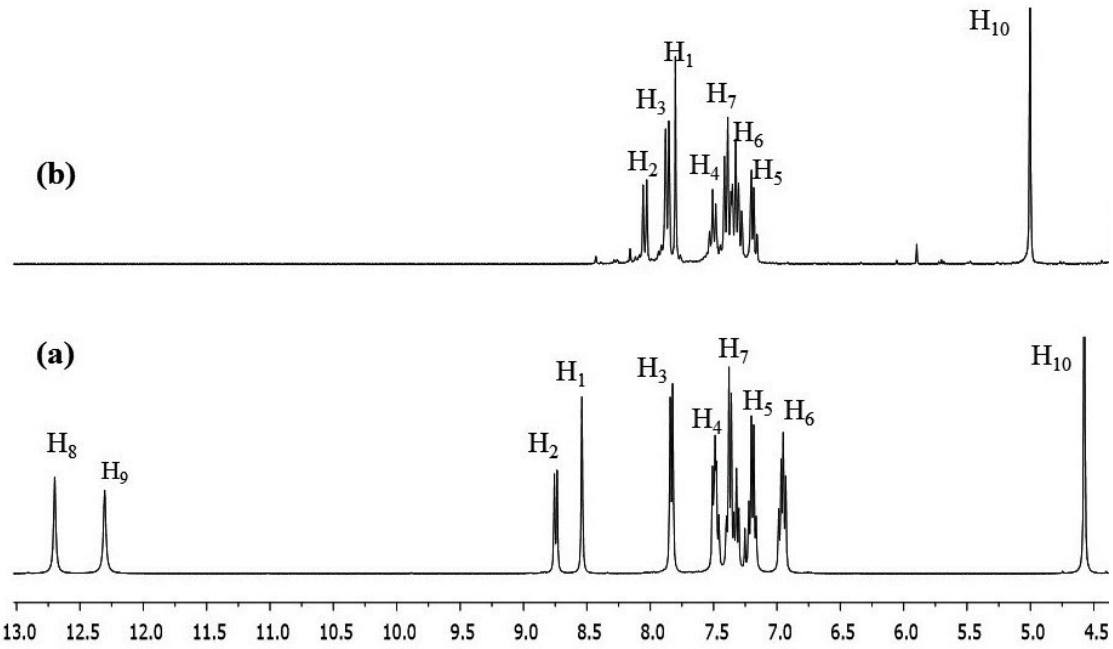

Fig. S6 Change in the ^{1}H-NMR spectra of **1** (**a**) in the presence of Zn^{2+} ions (**b**) in $CDCl_3$

(a)

Solvent	Excitation energy (eV)	Nature of S1 transition	Wavelength (nm)	Oscillator strength
Acetonitrile	3.867727	HOMO→L+1 (78%)	320.55	0.2862
	3.595932	H-1→LUMO (60%), HOMO→LUMO (28%)	344.78	0.2650
Chloroform	3.821928	HOMO→L+1 (77%)	324.39	0.2935
	3.553133	H-1→LUMO (57%), HOMO→LUMO (32%)	348.93	0.2720
Dimethyl sulfoxide	3.861627	HOMO→L+1 (79%)	321.05	0.2954
	3.591232	H-1→LUMO (60%), HOMO→LUMO (28%)	345.23	0.2783
Methanol	3.868827	HOMO→L+1 (78%)	320.46	0.2841
	3.596732	H-1→LUMO (60%), HOMO→LUMO (28%)	344.70	0.2620
Tetrahydrofuran	3.839328	HOMO→L+1 (77%)	322.92	0.2910
	3.570133	H-1→LUMO (58%), HOMO→LUMO (30%)	347.27	0.2690
Toluene	3.788929	HOMO→L+1 (75%)	327.21	0.2927
	3.516834	H-1→LUMO (53%), HOMO→LUMO (35%)	352.53	0.2727

(b)

Solvent	Excitation energy (eV)	Nature of S1 transition	Wavelength (nm)	Oscillator strength
Acetonitrile	3.8423	HOMO→L+1 (76%),	322.67	0.2688
	3.6097	H-1→LUMO (62%), HOMO→LUMO (24%)	343.46	0.2503
Chloroform	3.8040	HOMO→L+1 (76%)	325.92	0.2749
	3.5703	H-1→LUMO (61%), HOMO→LUMO (26%)	347.25	0.2591
Dimethyl sulfoxide	3.8364	HOMO→L+1 (77%),	323.16	0.2771
	3.6052	H-1→LUMO (62%), HOMO→LUMO (24%)	343.89	0.2616
Methanol	3.8434	HOMO→L+1 (76%)	322.57	0.2669
	3.6104	H-1→LUMO (62%), HOMO→LUMO (24%)	343.39	0.2477
Tetrahydrofuran	3.8186	HOMO→L+1 (76%)	324.67	0.2728
	3.5858	H-1→LUMO (61%), HOMO→LUMO (25%)	345.75	0.2555
Toluene	3.7763	HOMO→L+1 (76%),	328.31	0.2740
	3.5373	H-1→LUMO (60%), HOMO→LUMO (27%)	350.49	0.2617

Table S2. Photophysical parameters of **1-Zn^{2+}** complex in different solvents calculated using Gaussian 09 at B3LYP/6-31++ G level (**a**) and B3LYP/6-31G** level (**b**)

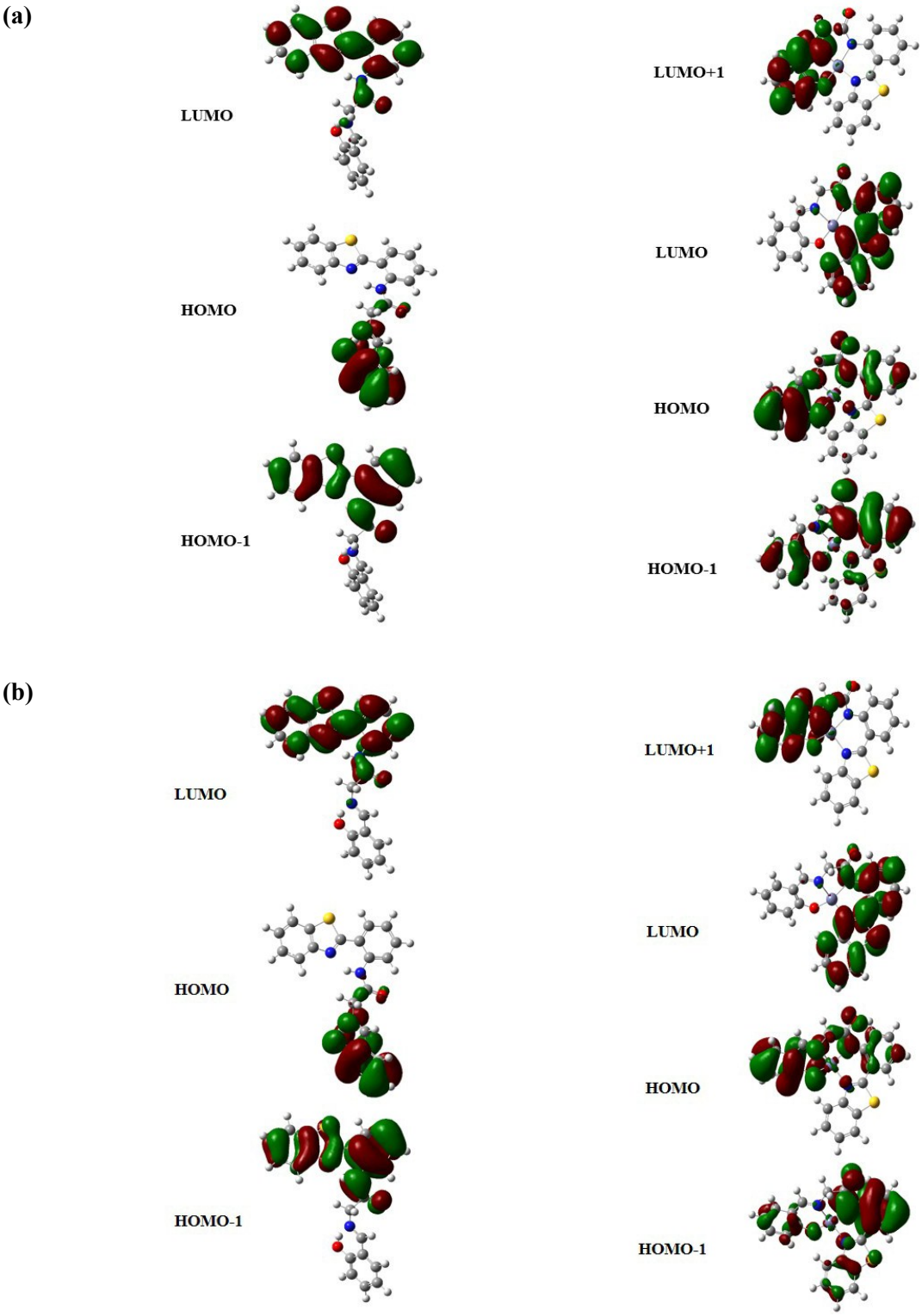

Fig. S7 Frontier molecular orbitals involved in the excitation of **1** (Left Panel) and **1-Zn**$^{2+}$ complex (Right Panel). The calculations were based on the energetically optimized structures using Gaussian 09 at B3LYP/6-31++ G level (**a**) and B3LYP/6-31G** level (**b**)

(a)

Orbitals	Probe 1	1-Zn^{2+} Complex
LUMO +1	−1.42	−1.62
LUMO	−2.09	−2.12
HOMO	−5.82	−5.54
HOMO −1	−6.18	−5.80

(b)

Orbitals	Probe 1	1-Zn^{2+} Complex
LUMO +1	−1.26	−1.5
LUMO	−1.95	−2.02
HOMO	−5.74	−5.44
HOMO −1	−6.08	−5.73

Table S3. Calculated energy values of molecular orbitals of **1** and **1-Zn^{2+}** complex using Gaussian 09 at B3LYP/6-31++ G level (**a**) and B3LYP/6-31G** level (**b**)

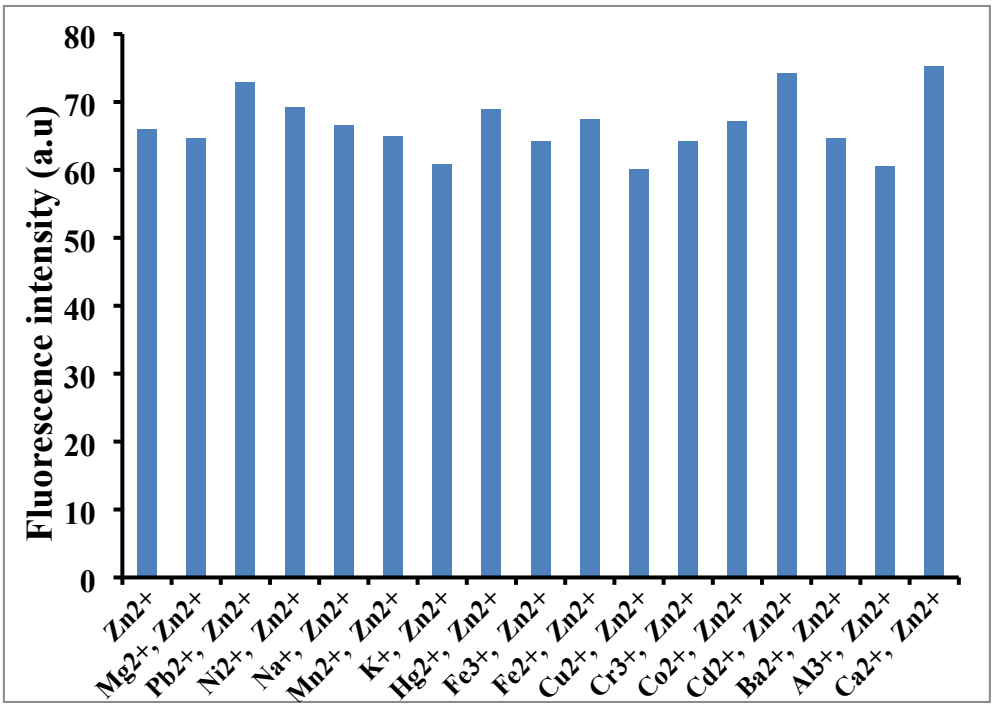

Fig. S8 Change in fluorescence intensity of **1** (10 μM) in H_2O:CH_3CN (3:7, v/v) medium upon addition of 3 equiv. of Zn^{2+} ions along with 5 equiv. of other metal ions

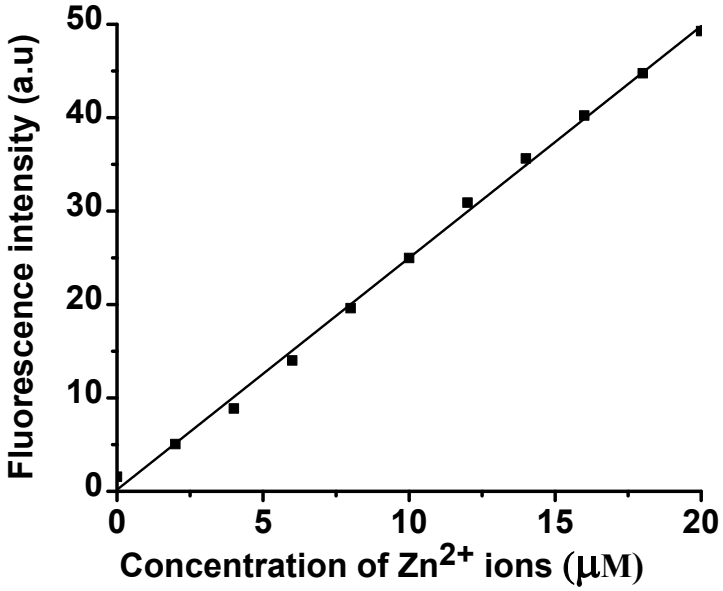

Fig. S9 Linear response of **1** (10 μM) in the presence of Zn^{2+} ions (0−20 μM) in H_2O:CH_3CN (3:7, v/v) medium. The detection limits was calculated using the equation, DL = 3σ /slope.

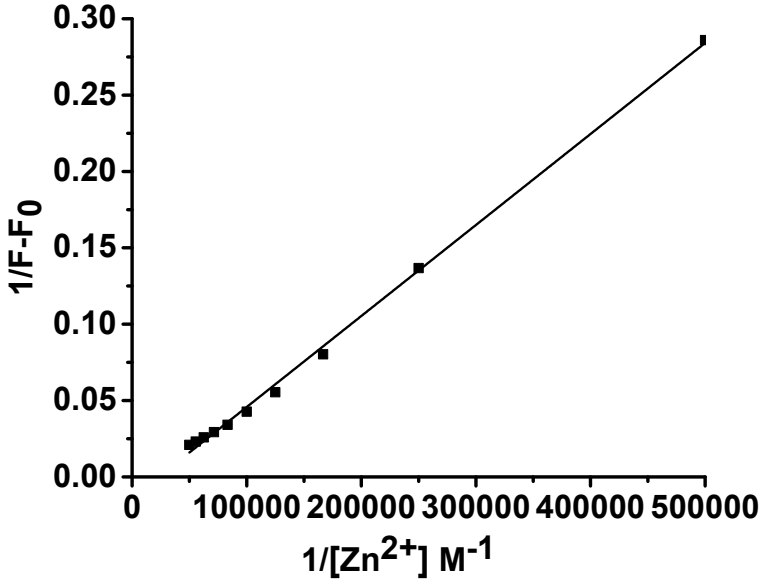

Fig. S10 Benesi–Hildebrand plot obtained from the titration of **1** with Zn^{2+} ions in H_2O:CH_3CN (3:7, v/v) medium

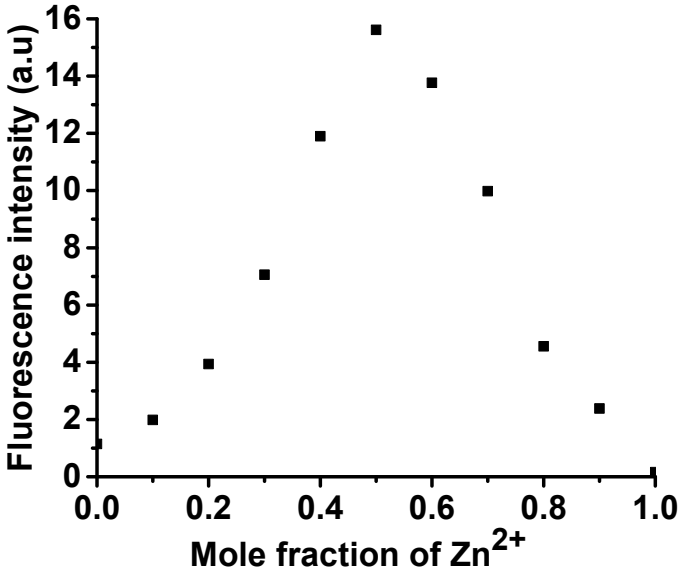

Fig. S11 Job plot showing 1:1 stoichiometry for **1-Zn^{2+}** complex in H_2O:CH_3CN (3:7, v/v) medium

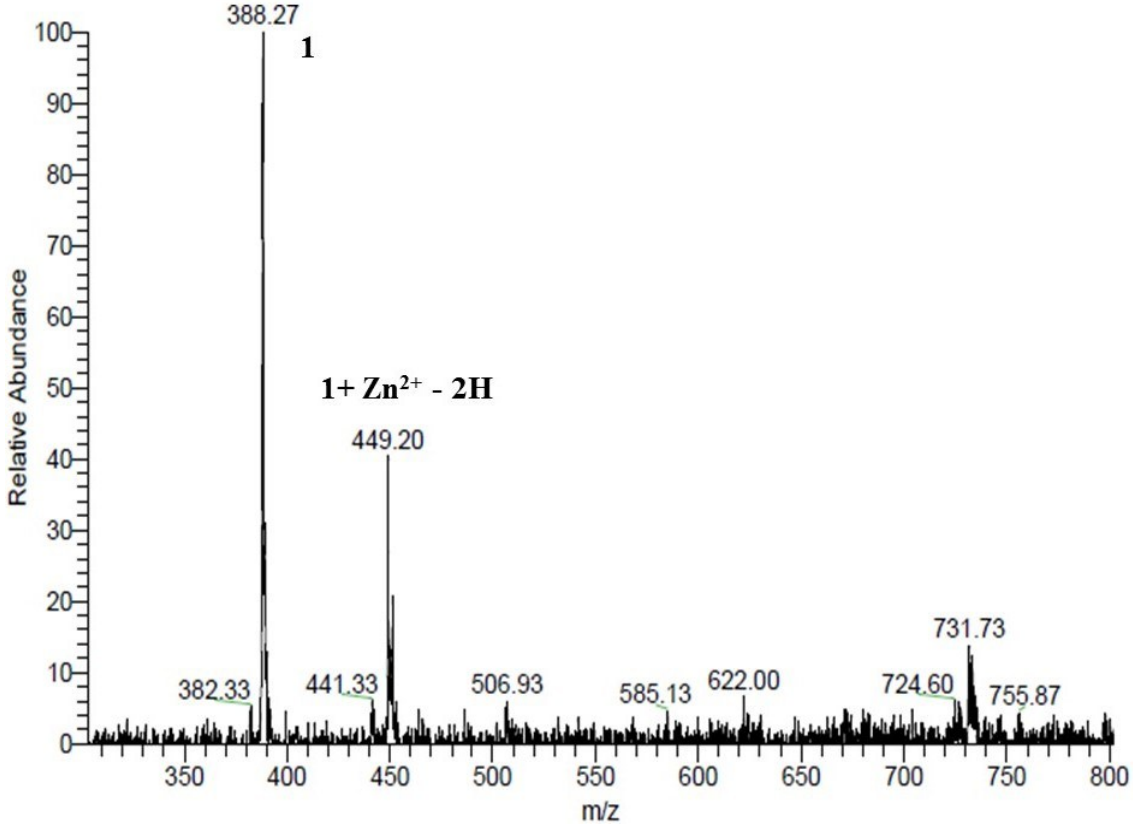

Fig. S12 ESI-MS spectrum of **1-Zn^{2+}** complex

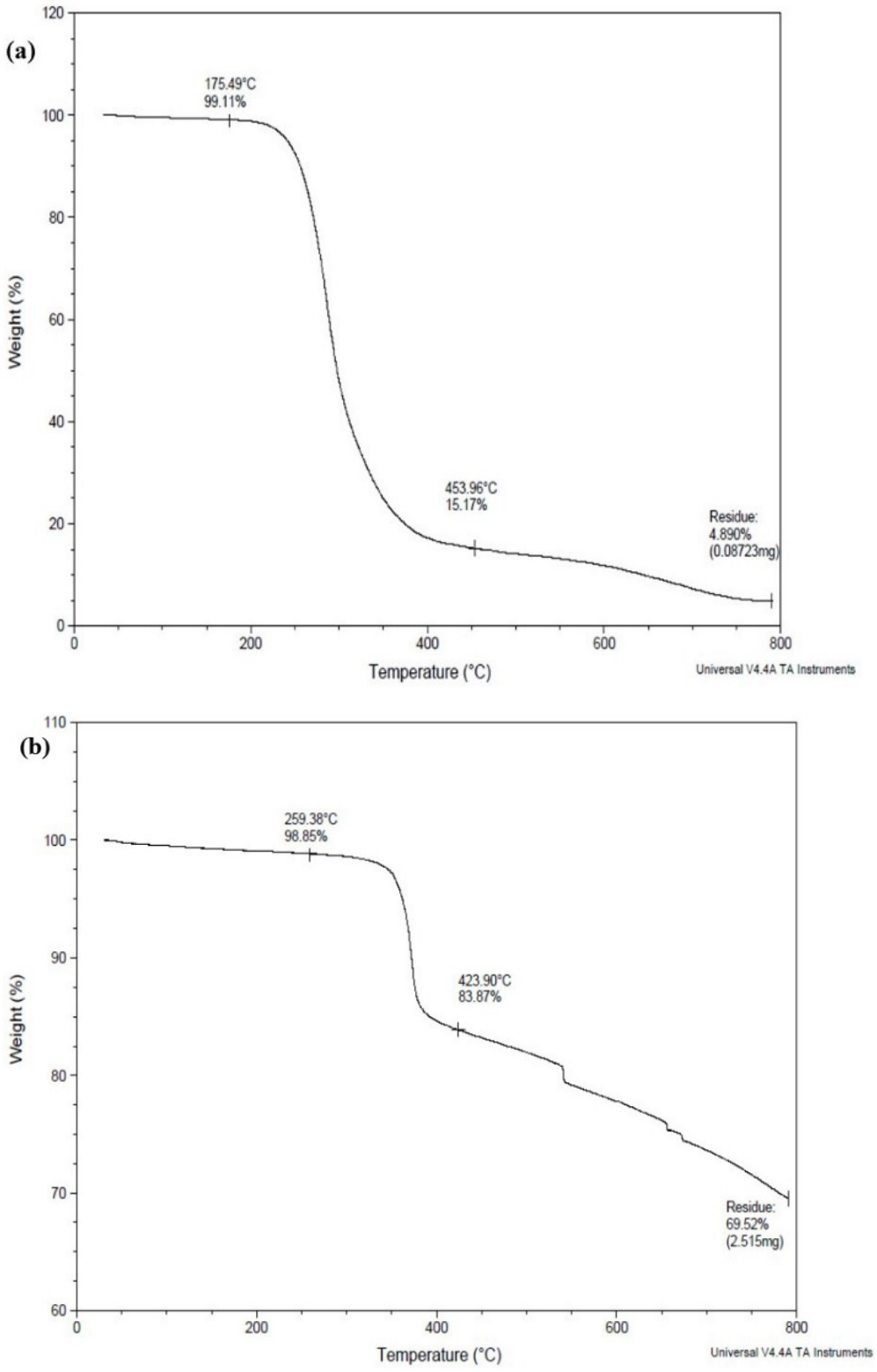

Fig. S13 TGA curve of **1 (a)** and **1-Zn^{2+}** complex **(b)**