Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A dual functional fluorescence sensor for detection of Al^{3+} and Zn^{2+} in different solvent.

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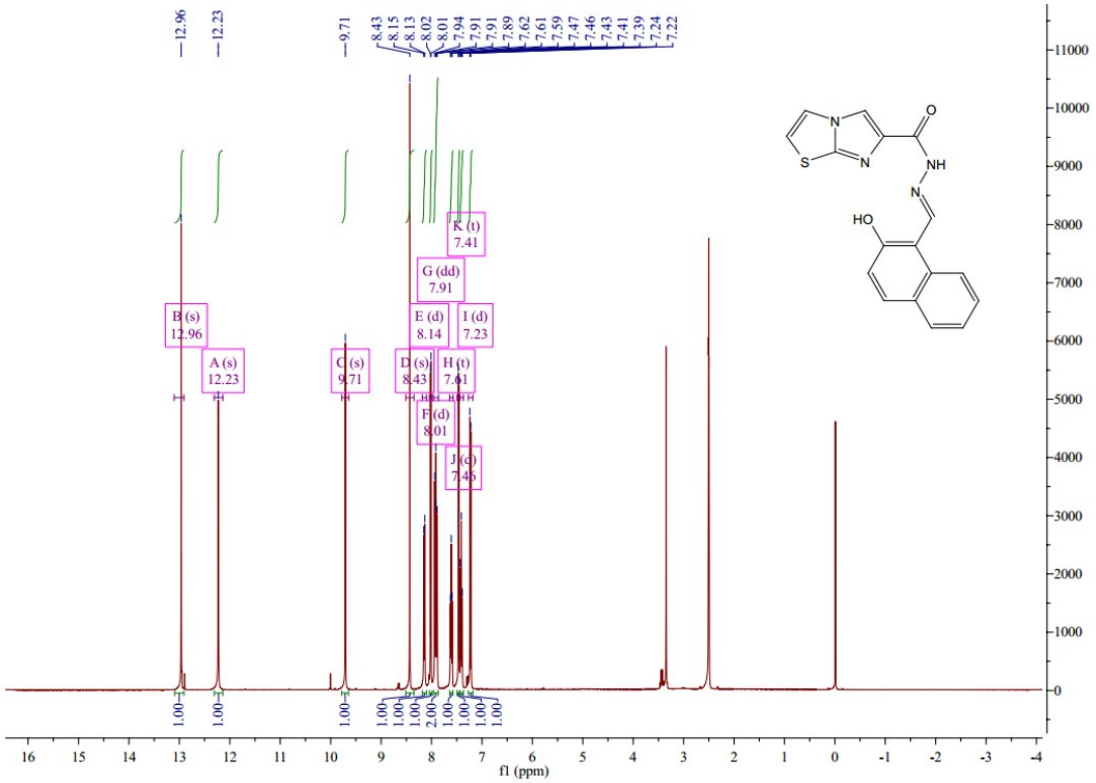


Fig. S1. ^{1}H NMR spectrum of **X**.

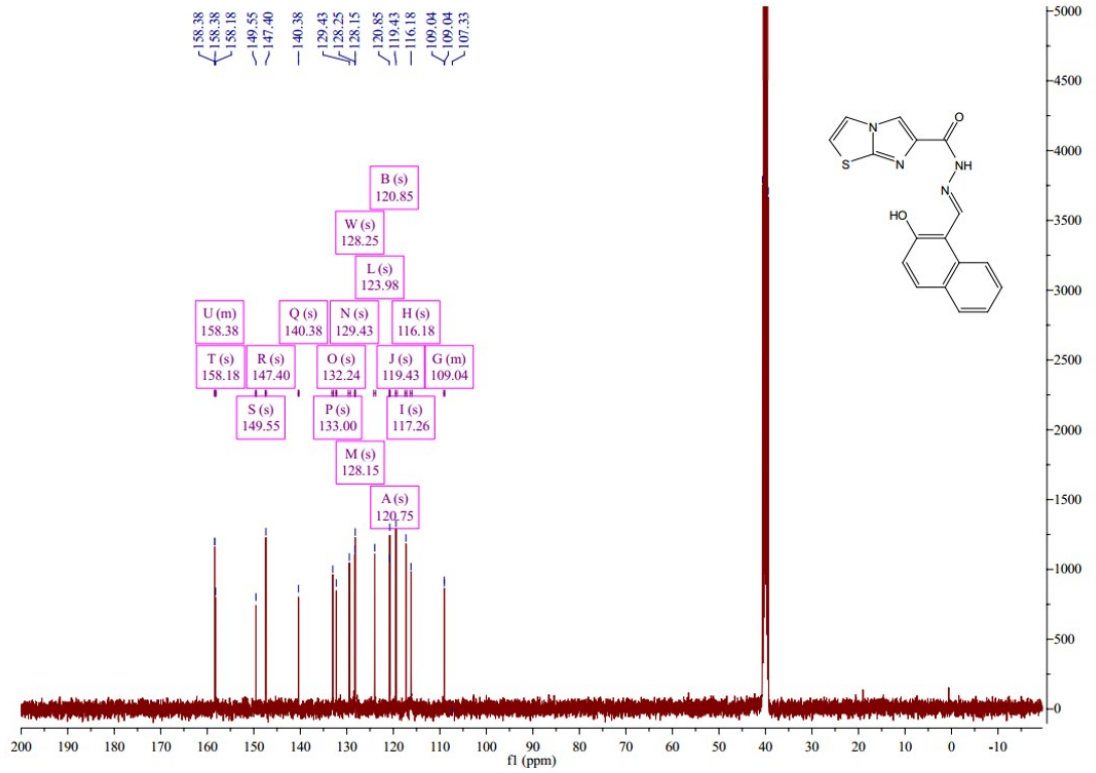


Fig. S2. ^{13}C NMR spectrum of **X.**

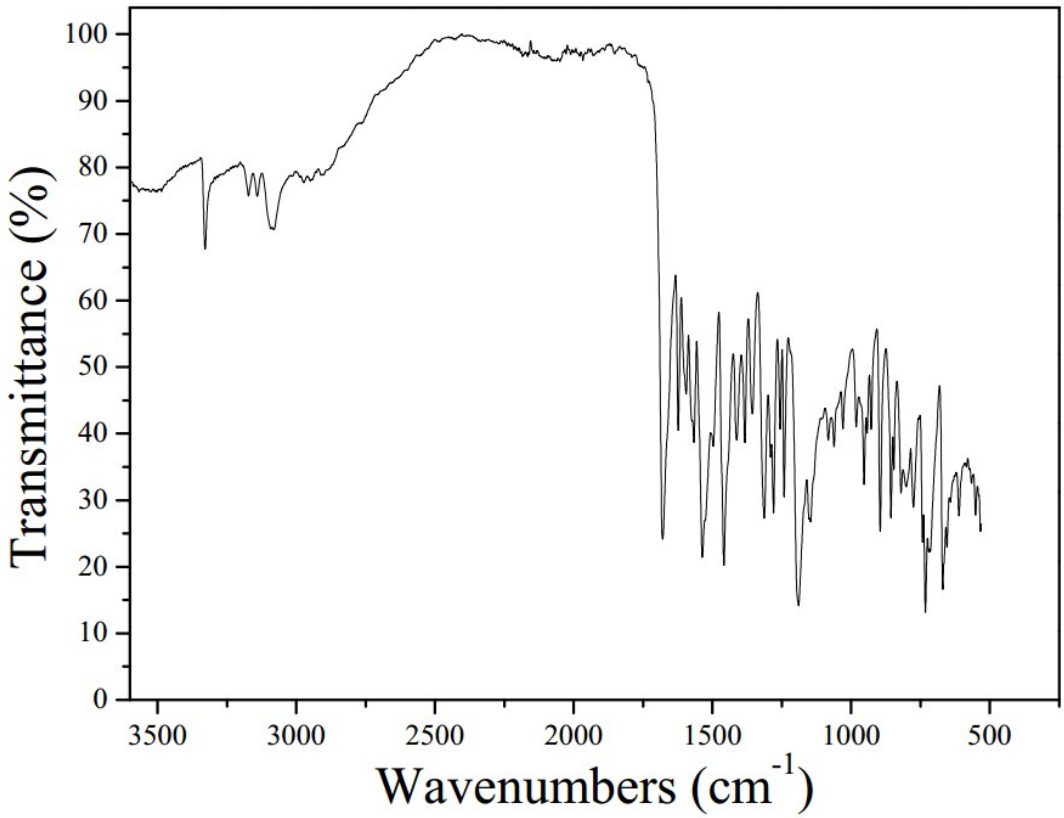


Fig. S3. The FTIR spectra of **X**.

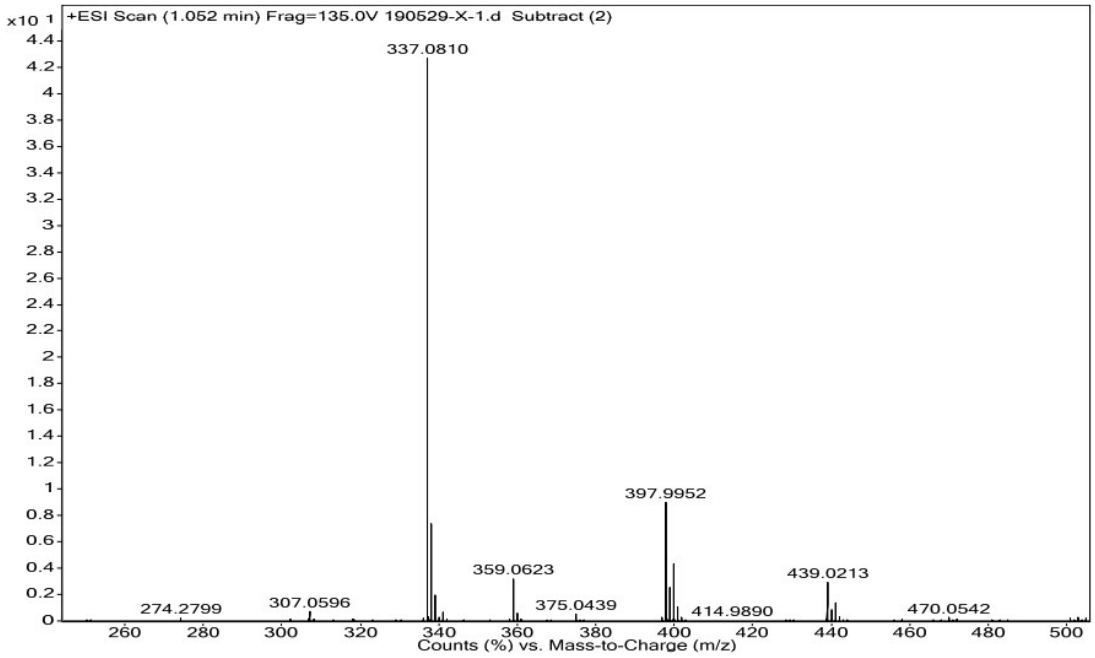


Fig. S4. ESI mass spectrum of **X**.

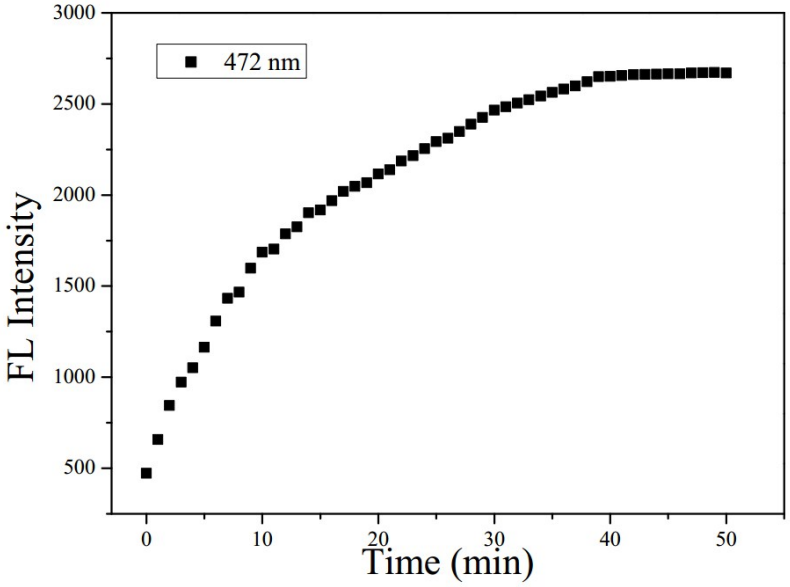


Fig. S5. Time course for the fluorescence response of **X** (1×10^{-5} M) at 472 nm upon the addition of Al^{3+} (10 equiv.) in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

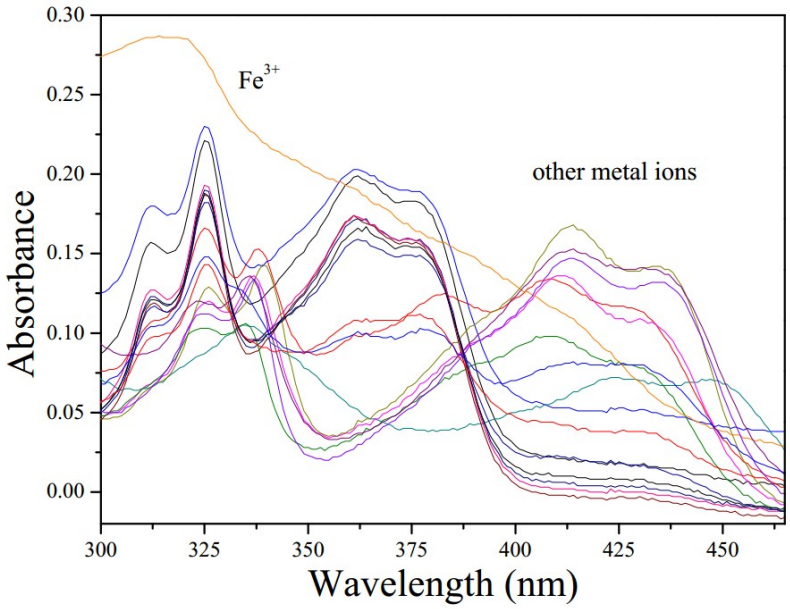


Fig. S6. Absorption spectra of **X** (1×10^{-5} M) upon the addition of various metal ions (10 equiv.) in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

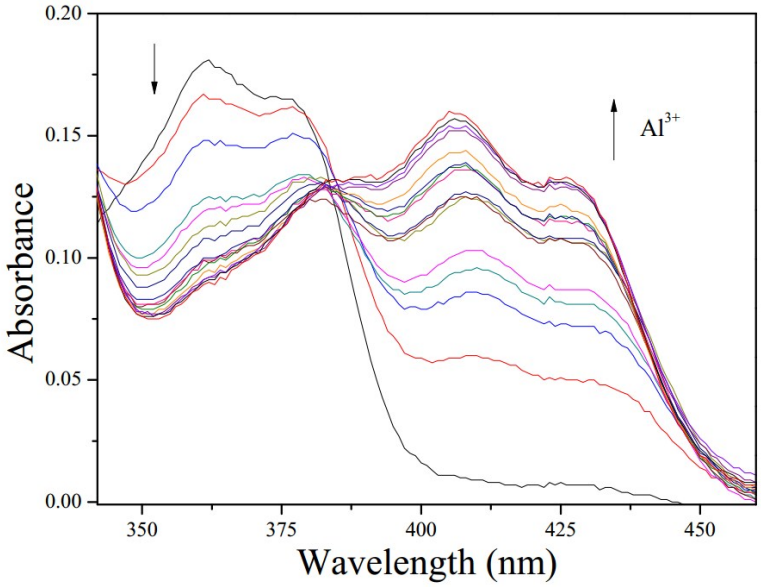


Fig. S7. Absorption titration spectra of **X** (1 × 10^{-5} M) upon the addition of Al^{3+} (0 - 15 equiv.) in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

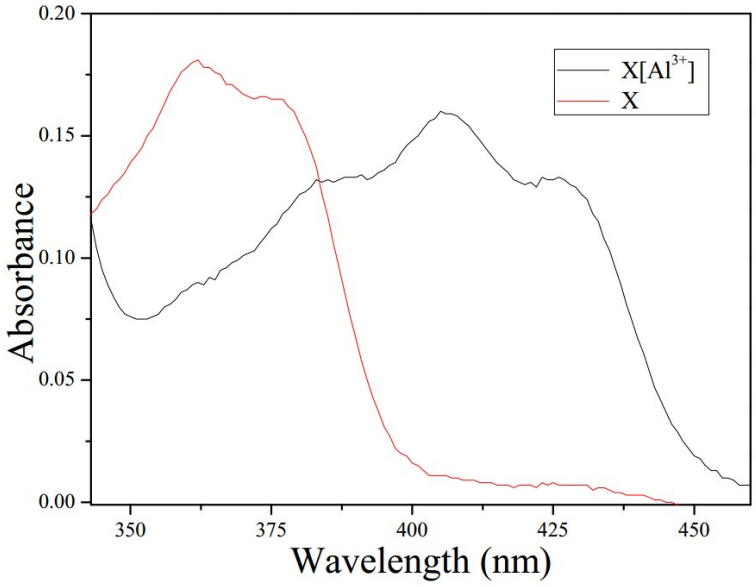


Fig. S8. Absorption spectra of **X** and **X**[Al^{3+}] in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

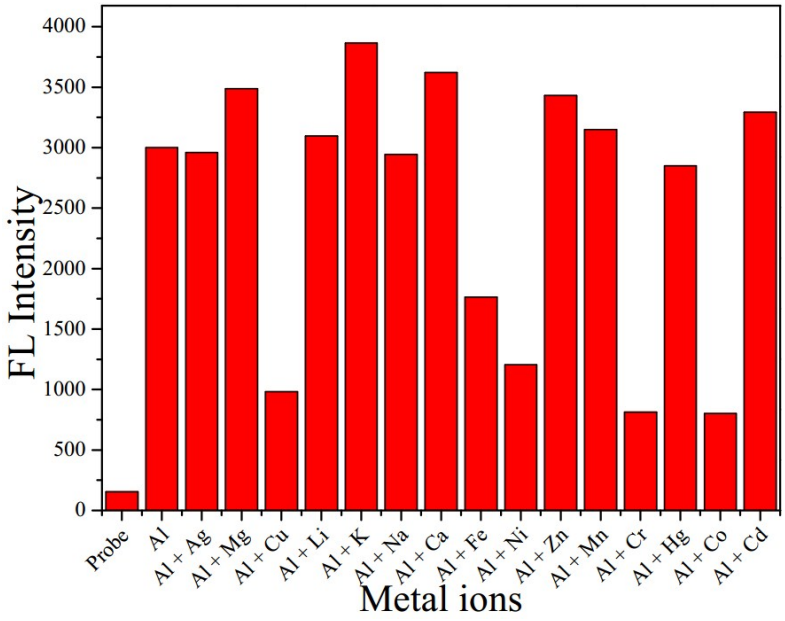


Fig. S9. Fluorescence intensity of **X** and its complexation with Al^{3+} in the presence of other metal ions (Ag^{+}, Mg^{2+}, Cu^{2+}, Li^{+}, K^{+}, Na^{+}, Ca^{2+}, Fe^{3+}, Ni^{2+}, Zn^{2+}, Mn^{2+}, Cr^{3+}, Hg^{2+}, Co^{2+} and Cd^{2+}) in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

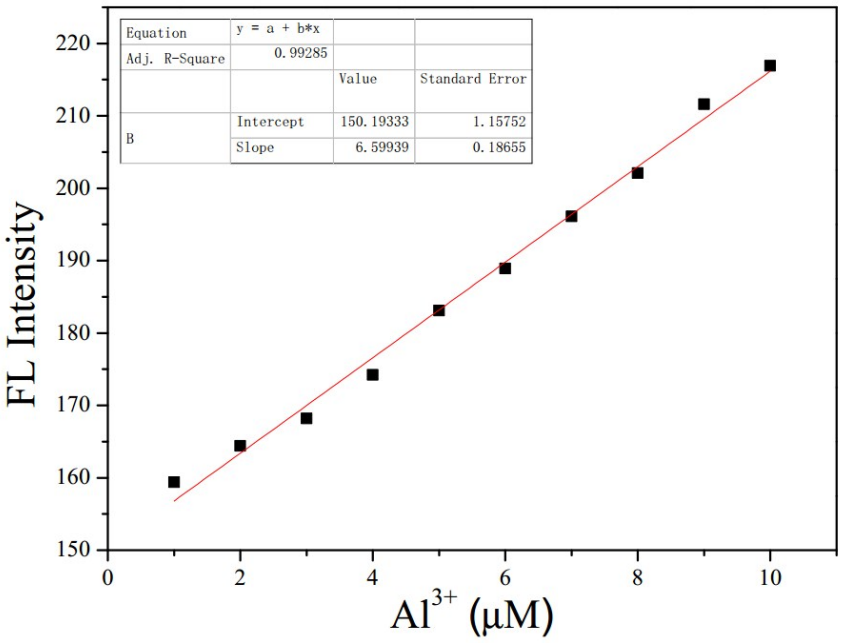


Fig. S10. Fluorescence intensity of **X** at 472 nm with the addition of Al^{3+} (0 - 1 equiv.)

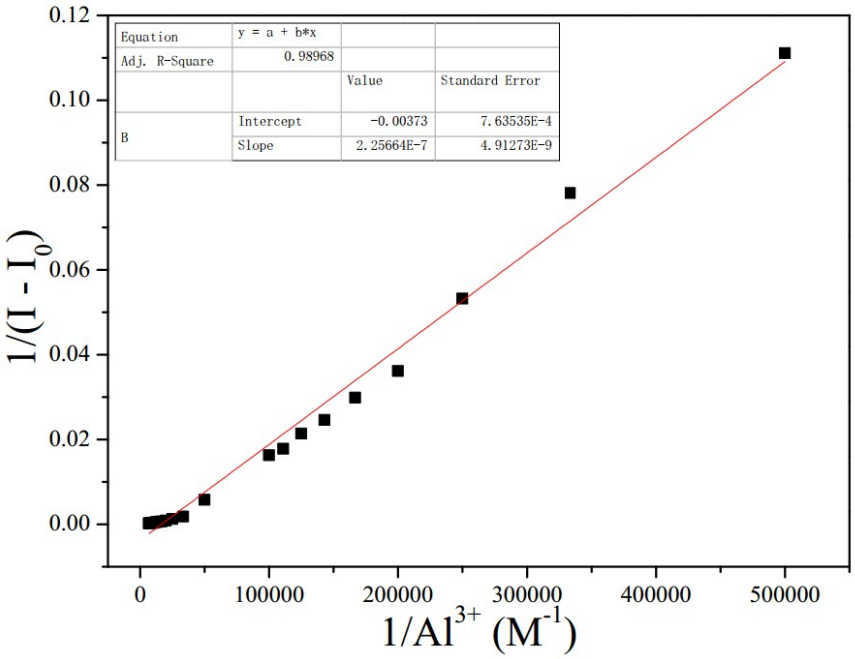


Fig. S11. Benesi-Hilderbrand plot of **X** with Al^{3+}.

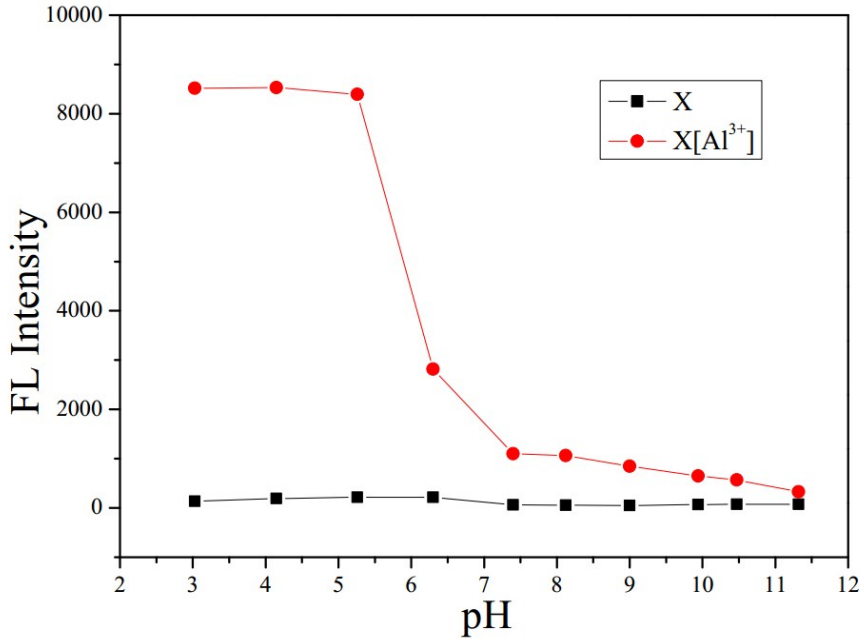


Fig. S12. The influence of pH value of solution on the fluorescence of X and X[Al^{3+}] at the slits of excitation and emission were 10 nm and 10 nm, respectively.

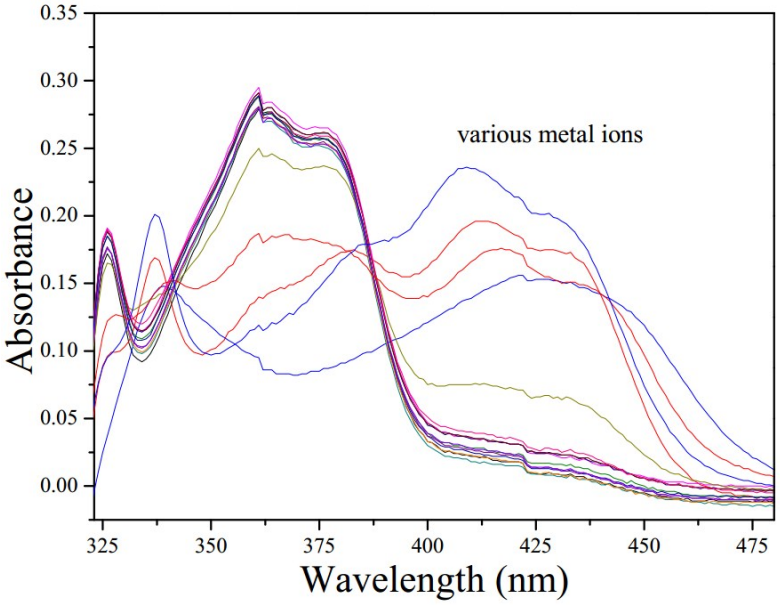


Fig. S13. Absorption spectra of **X** (1×10^{-5} M) upon the addition of various metal ions (5 equiv.) in ethanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

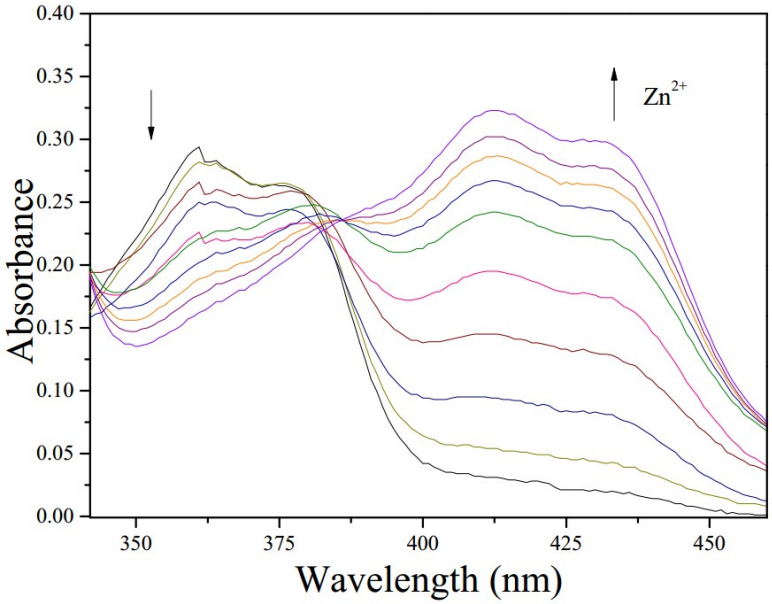


Fig. 14. Absorption titration spectra of **X** (1×10^{-5} M) upon the addition of Zn^{2+} (0 - 5 equiv.) in ethanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

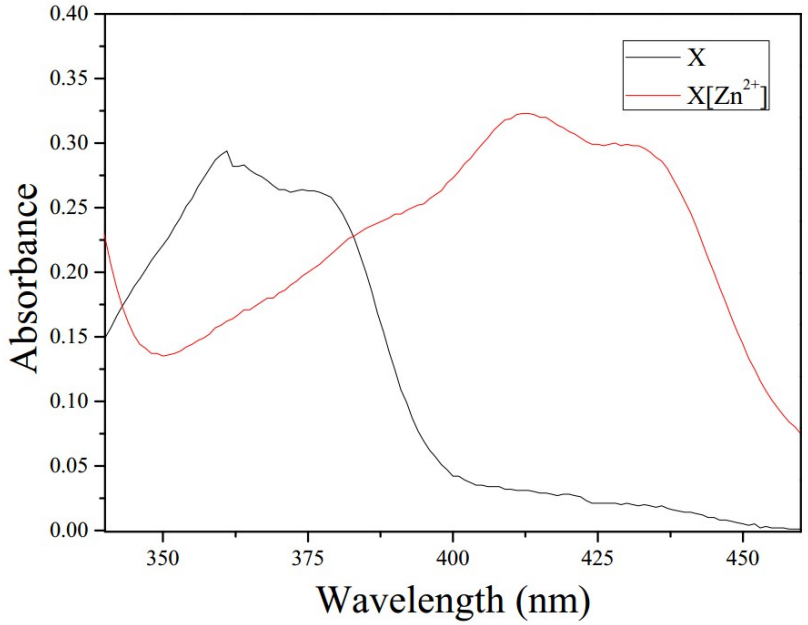


Fig. S15. Absorption spectra of **X** and **X**[Zn^{2+}] in ethanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

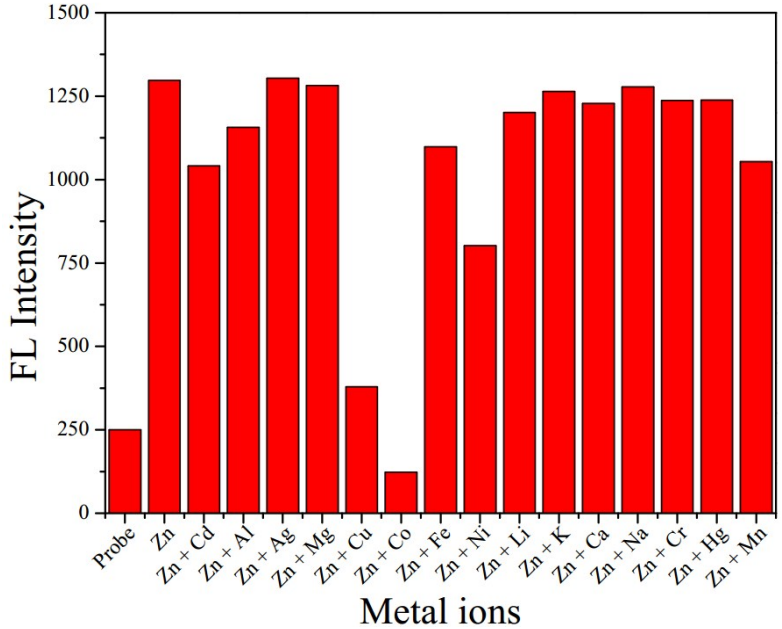


Fig. S16. Fluorescence intensity of **X** and its complexation with Zn^{2+} in the presence of other metal ions (Cd^{2+}, Al^{3+}, Ag^{+}, Mg^{2+}, Cu^{2+}, Co^{2+}, Fe^{3+}, Ni^{2+}, Li^{+}, K^{+}, Ca^{2+}, Na^{+}, Cr^{3+}, Hg^{2+} and Mn^{2+}) in ethanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

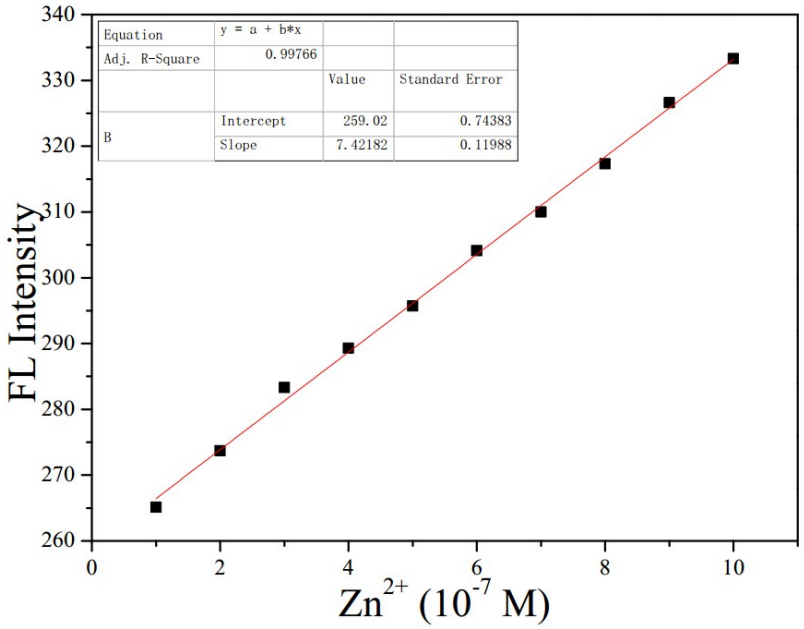


Fig. S17. Fluorescence intensity of **X** at 484 nm with the addition of Zn^{2+} (0 - 1 × 10^{-6} M)

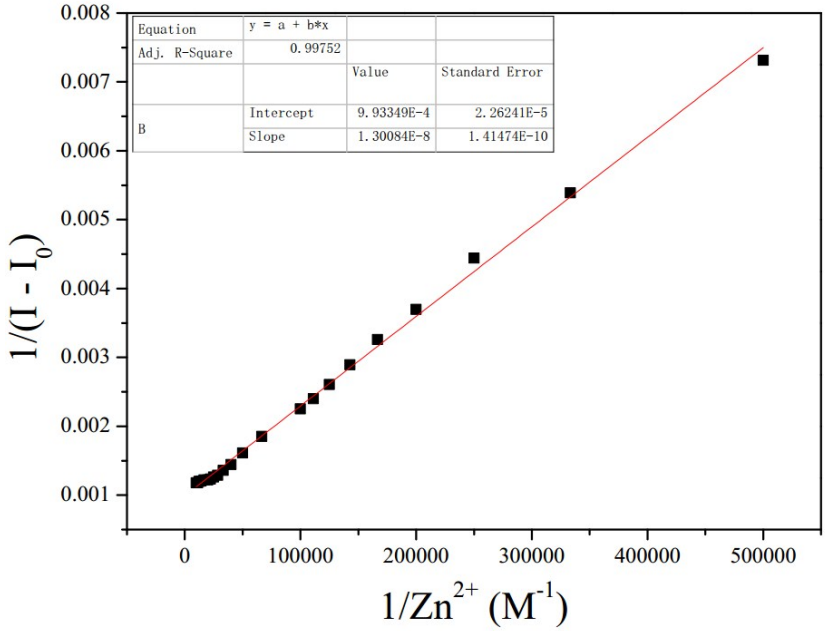


Fig. S18. Benesi-Hilderbrand plot of **X** with Zn^{2+}.

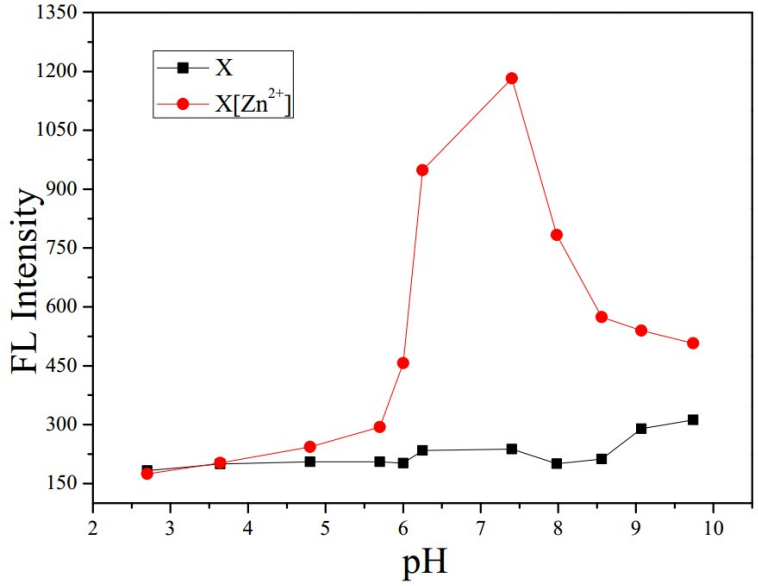


Fig. S19. The influence of pH value of solution on the fluorescence of X and X[Zn^{2+}] at the slit width value of 20 nm.

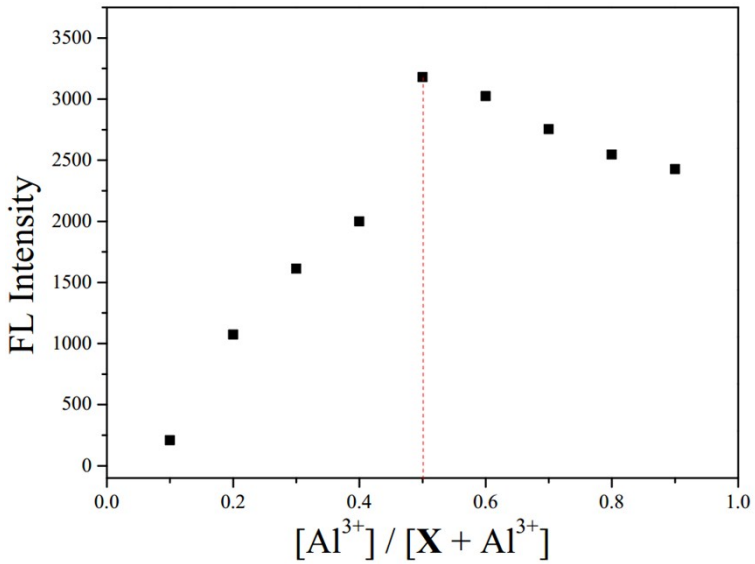


Fig. S20. Job's plot of **X** with Al^{3+} complexation in methanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

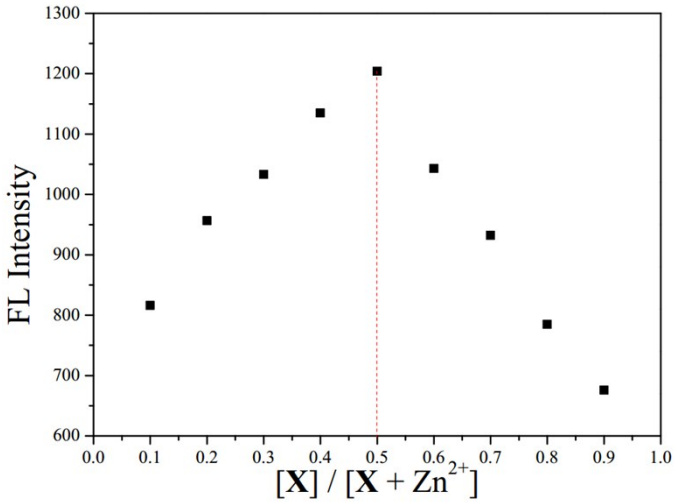


Fig. S21. Job's plot of **X** with Zn^{2+} complexation in ethanol/H_2O buffer solution (v/v = 9:1, tris = 10 mM, pH = 7.4).

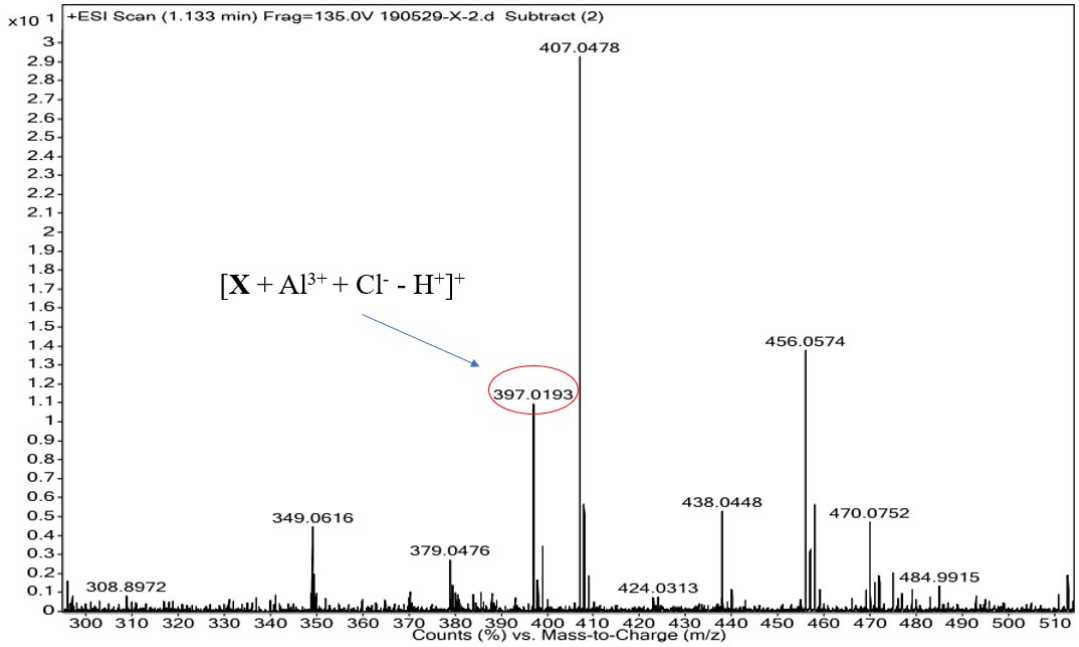


Fig. S22. ESI mass spectrum of complex **X**[Al^{3+}].

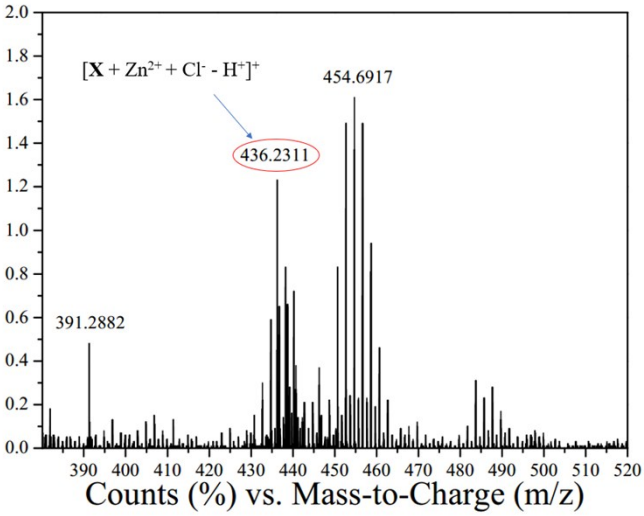


Fig. S23. ESI mass spectrum of complex **X**[Zn^{2+}].

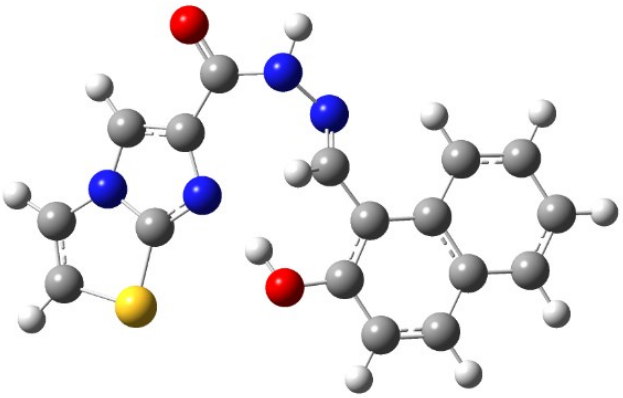
Table S1. Determination of Al^{3+} concentrations in tap water samples

sample	Al^{3+} added (M)	Al^{3+} recovered (M)	Recovery (%)	RSD (%)
1	1.0×10^{-5}	9.04×10^{-6}	90.4	0.57
2	5.0×10^{-5}	4.73×10^{-5}	94.7	1.70
3	1.0×10^{-4}	9.97×10^{-5}	99.7	1.13

Table S2. Determination of Zn^{2+} concentrations in tap water samples

sample	Zn^{2+} added (M)	Zn^{2+} recovered (M)	Recovery (%)	RSD (%)
1	1.0×10^{-5}	1.10×10^{-5}	110.1	1.38
2	2.0×10^{-5}	2.28×10^{-5}	114.3	0.64
3	3.0×10^{-5}	3.10×10^{-5}	103.4	0.46

Table S3. XYZ coordinate of the optimized structure of **X**.

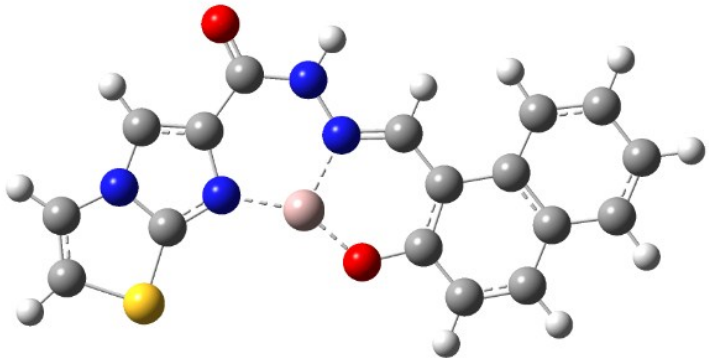


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.380763	-0.299407	-1.336343
2	6	0	6.022813	0.738092	-0.598627
3	6	0	3.635847	0.464107	0.024297
4	6	0	2.264502	-1.277847	0.066319
5	6	0	3.189357	-1.511402	-0.969431
6	6	0	1.147241	-2.244796	0.500301
7	6	0	-0.829322	0.091960	0.994782
8	6	0	-2.051928	0.846892	0.440767
9	6	0	-2.018713	2.242837	0.321801
10	6	0	-3.241363	2.997710	-0.232207
11	6	0	-4.387182	2.288701	-0.617351
12	6	0	-4.423671	0.754698	-0.486605
13	6	0	-3.311049	0.067764	0.017503
14	6	0	-3.347501	-1.466249	0.148205
15	6	0	-4.493308	-2.175268	-0.236932
16	6	0	-5.715995	-1.420392	-0.790856
17	6	0	-5.682815	-0.024443	-0.909809
18	16	0	4.847619	1.692710	0.347532
19	7	0	3.905610	-0.261500	-1.193034
20	7	0	2.550310	0.042058	0.687144
21	7	0	0.251323	-1.883030	1.608170
22	7	0	-0.860050	-1.196613	1.104491
23	8	0	1.001230	-3.344653	-0.093468
24	8	0	-0.849519	2.966308	0.714828
25	1	0	5.904746	-1.029406	-1.917238
26	1	0	7.078873	0.910229	-0.596684
27	1	0	3.341390	-2.433687	-1.490172

28	1	0	-0.053182	-2.713148	2.075264
29	1	0	0.045522	0.633258	1.288943
30	1	0	-2.497971	-1.990739	0.533080
31	1	0	-4.518635	-3.241106	-0.146126
32	1	0	-6.590854	-1.961744	-1.084898
33	1	0	-6.532341	0.500049	-1.294682
34	1	0	-5.236691	2.813194	-1.002265
35	1	0	-3.216005	4.063545	-0.323061
36	1	0	-0.256844	3.048816	-0.035853

Table S4. XYZ coordinate of the optimized structure of **X**[Al^{3+}].



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.589017	0.303986	0.181609
2	6	0	6.760004	-1.071839	0.539538
3	6	0	4.472762	-0.571591	-0.210221
4	6	0	3.132250	1.319098	-0.133185
5	6	0	4.491148	1.730106	-0.237834
6	6	0	1.831080	2.363416	-0.003442
7	6	0	-1.892358	0.984997	0.166953
8	6	0	-2.824243	-0.414988	0.052073
9	6	0	-2.674665	-1.987812	-0.033015
10	6	0	-3.977018	-2.818086	-0.093574
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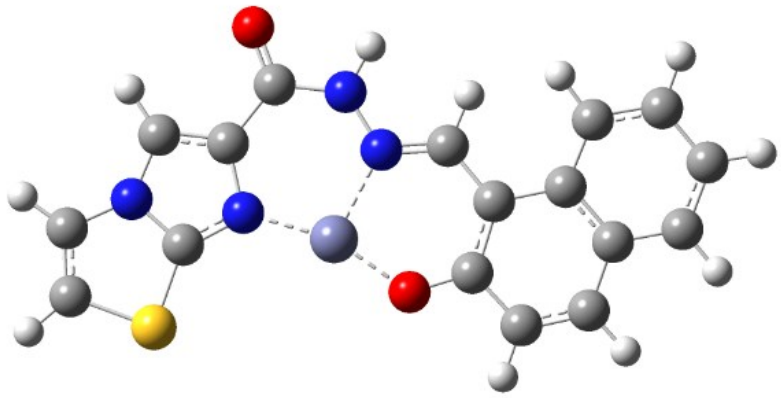
12	6	0	-5.404898	-0.734156	-0.029890
13	6	0	-4.286821	0.103336	0.036552
14	6	0	-4.496902	1.630752	0.100378
15	6	0	-5.787321	2.174347	0.091251
16	6	0	-7.009162	1.246929	0.017515
17	6	0	-6.826067	-0.138105	-0.039996
18	16	0	5.344223	-2.062987	0.073173
19	7	0	5.326680	0.538073	-0.559693
20	7	0	3.225803	-0.173611	-0.157052
21	7	0	0.274645	2.303159	0.425731
22	7	0	-0.572352	1.128550	0.221386
23	8	0	2.168126	3.538710	-0.301190
24	8	0	-1.508522	-2.964108	-0.077125
25	1	0	7.287102	1.075966	0.429849
26	1	0	7.621831	-1.457303	1.043098
27	1	0	4.853351	2.727628	-0.101238
28	1	0	-0.176289	3.038714	-0.079855

29	1	0	-2.449368	1.897595	0.209438
30	1	0	-3.648460	2.280655	0.152071
31	1	0	-5.921947	3.234916	0.135617
32	1	0	-7.996615	1.658976	0.010215
33	1	0	-7.675714	-0.786473	-0.091176
34	1	0	-6.107688	-2.870129	-0.136321
35	1	0	-3.900770	-3.884362	-0.139870
36	13	0	0.647090	-1.256619	-0.074091

Table S5. XYZ coordinate of the optimized structure of **X**[Zn^{2+}].



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	6.709804	-0.936416	0.549329
3	6	0	4.420584	-0.447771	-0.202046
4	6	0	3.071918	1.437293	-0.129658
5	6	0	4.429053	1.853913	-0.234984
6	6	0	1.766229	2.476288	-0.002595
7	6	0	-1.951267	1.082225	0.170241
8	6	0	-2.877083	-0.322027	0.058415
9	6	0	-2.720708	-1.894384	-0.023000
10	6	0	-4.019456	-2.730404	-0.081899
11	6	0	-5.285948	-2.161886	-0.082205
12	6	0	-5.456321	-0.652509	-0.023329
13	6	0	-4.341879	0.189948	0.041400
14	6	0	-4.558556	1.716588	0.101646
15	6	0	-5.851305	2.254591	0.091000
16	6	0	-7.069121	1.321745	0.019165
17	6	0	-6.880043	-0.062616	-0.035101
18	16	0	5.298408	-1.934736	0.084976
19	7	0	5.269785	0.664753	-0.553914
20	7	0	3.171910	-0.055049	-0.150050
21	7	0	0.209979	2.410314	0.426403
22	7	0	-0.631904	1.231594	0.224607
23	8	0	2.098269	3.652333	-0.302996
24	8	0	-1.550357	-2.865742	-0.064614
25	1	0	7.227660	1.213383	0.434774
26	1	0	7.573178	-1.316993	1.053954
27	1	0	4.786923	2.853302	-0.100626

28	1	0	-0.244016	3.142746	-0.080976
29	1	0	-2.512215	1.992509	0.210501
30	1	0	-3.712935	2.370261	0.152005
31	1	0	-5.990512	3.314670	0.132884
32	1	0	-8.058340	1.729513	0.010713
33	1	0	-7.726876	-0.714758	-0.084951
34	1	0	-6.149873	-2.791732	-0.124954
35	1	0	-3.938601	-3.796445	-0.125711
36	30	0	0.597874	-1.148971	-0.065101