Supporting Information

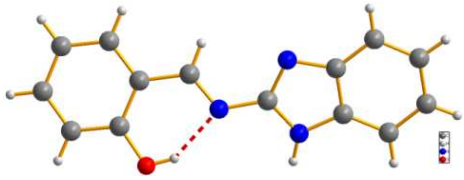
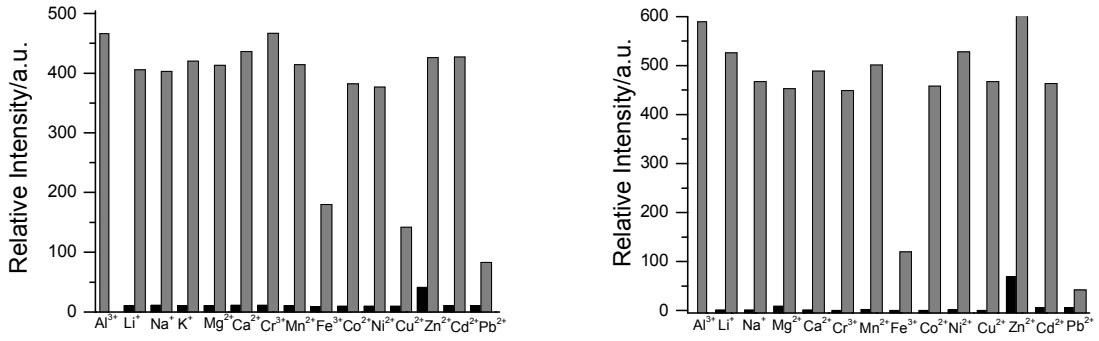
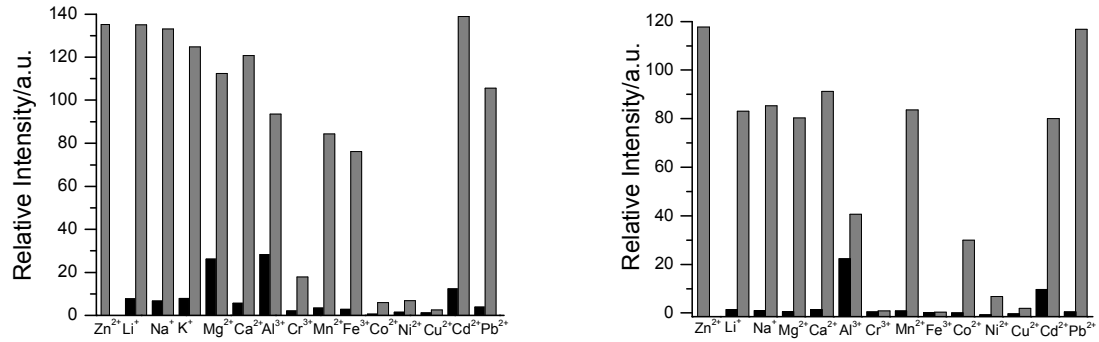


Figure S1. The intramolecular hydrogen bond in H_2L.



(a) (b)

Figure S2. (a) Relative fluorescence of H_2L with Al^{3+} in the presence of various metal ions in DMSO. 50μM of H_2L, 1 equiv of metal ions in the absence (black) and presence (gray) of 1 equiv of Al^{3+}. (b) Relative fluorescence of H_2L with Al^{3+} in the presence of various metal ions in CH_3OH. 50μM of H_2L, 10 equiv of metal ions in the absence (black) and presence (gray) of 10 equiv of Al^{3+}.



(a) (b)

Figure S3. (a) Relative fluorescence of H_2L with Zn^{2+} in the presence of various metal ions in DMF. 50μM of H_2L, 1 equiv of metal ions in the absence (black) and presence (gray) of 1 equiv of Zn^{2+}. (b) Relative fluorescence of H_2L with Zn^{2+} in the presence of various metal ions in CH_3OH. 50μM of H_2L, 10 equiv of metal ions in the absence (black) and presence (gray) of 10 equiv of Zn^{2+}.

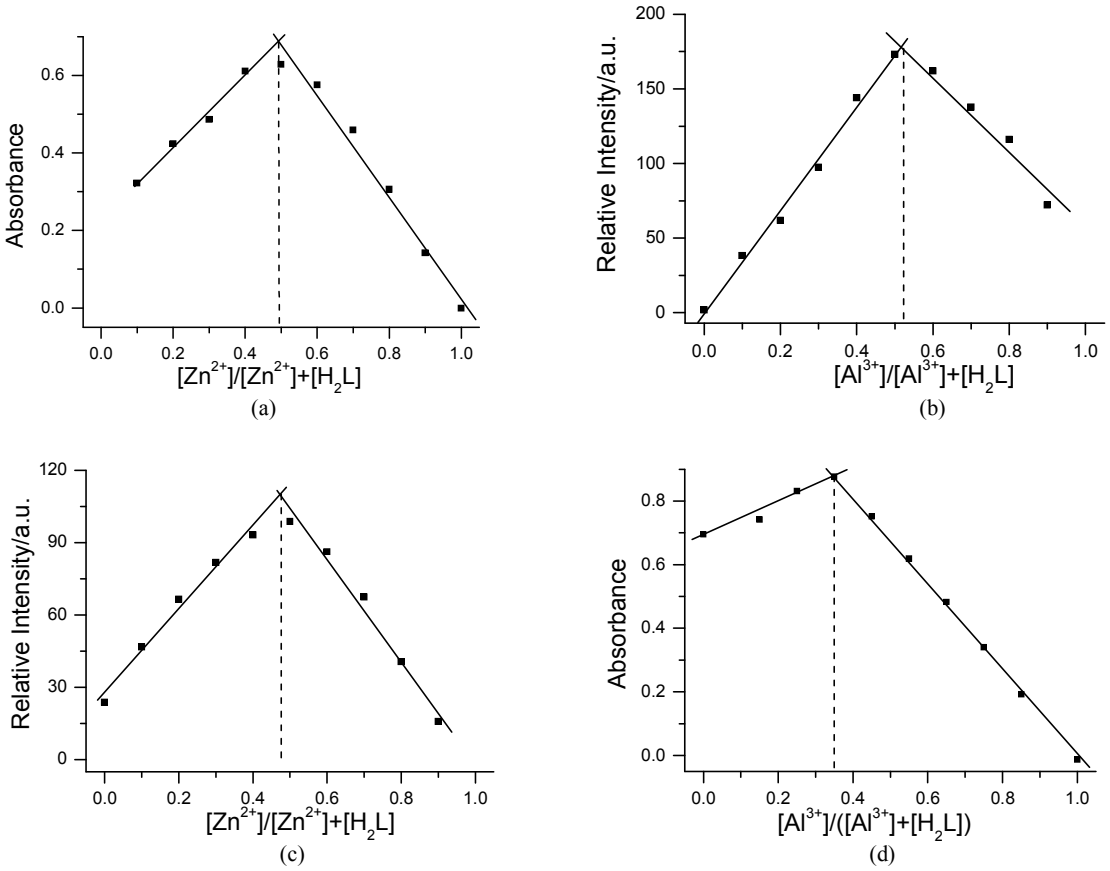
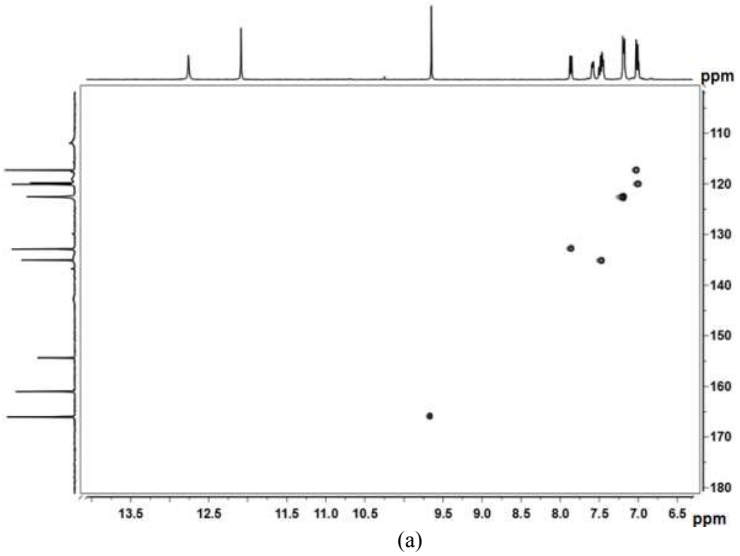
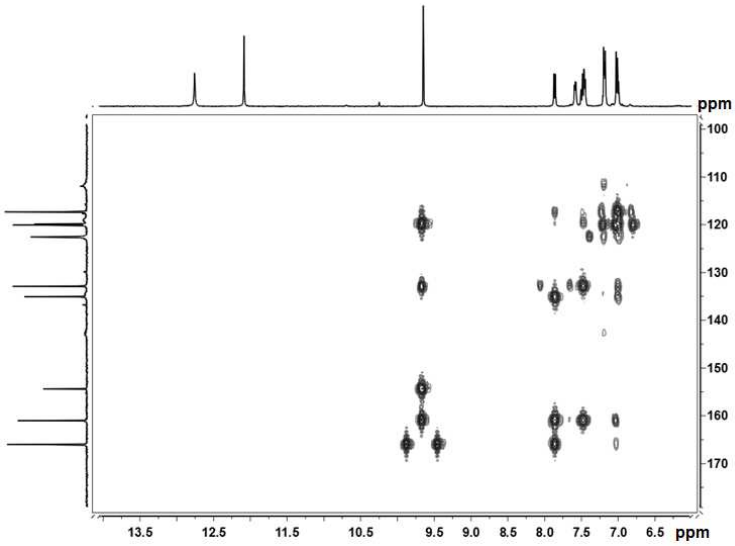
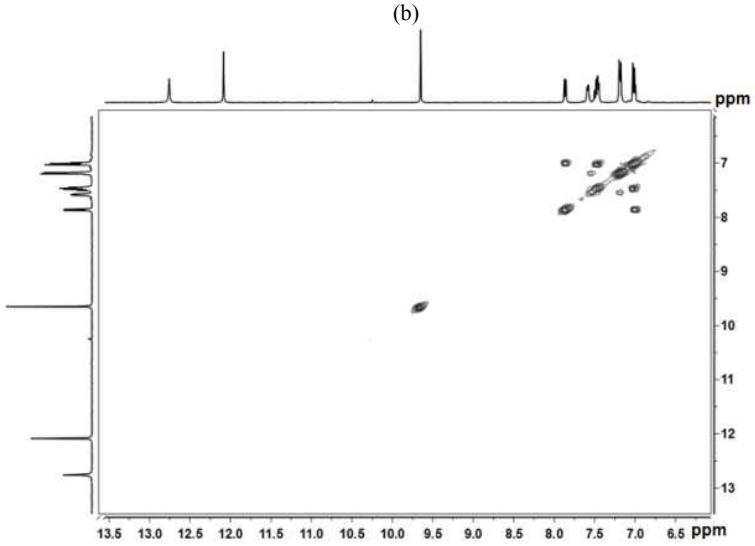


Figure S4. (a) Job's plot for the complex formed between H_2L and Zn^{2+} in DMF. Absorbance at 425 nm was plotted as function of the molar ratio $[Zn^{2+}]/([Zn^{2+}]+[H_2L])$. (b) Job's plot for the complex formed between H_2L and Al^{3+} in DMSO. Fluorescence at 500 nm was plotted as function of the molar ratio $[Al^{3+}]/([Al^{3+}]+[H_2L])$. (c) Job's plot for the binding of H_2L with Zn^{2+} in methanol. Fluorescence at 525 nm was plotted as function of the molar ratio $[Zn^{2+}]/([Zn^{2+}]+[H_2L])$. (d) Job's plot for the binding of H_2L with Al^{3+}. Absorbance at 276 nm was plotted as function of the molar ratio $[Al^{3+}]/([Al^{3+}]+[H_2L])$.



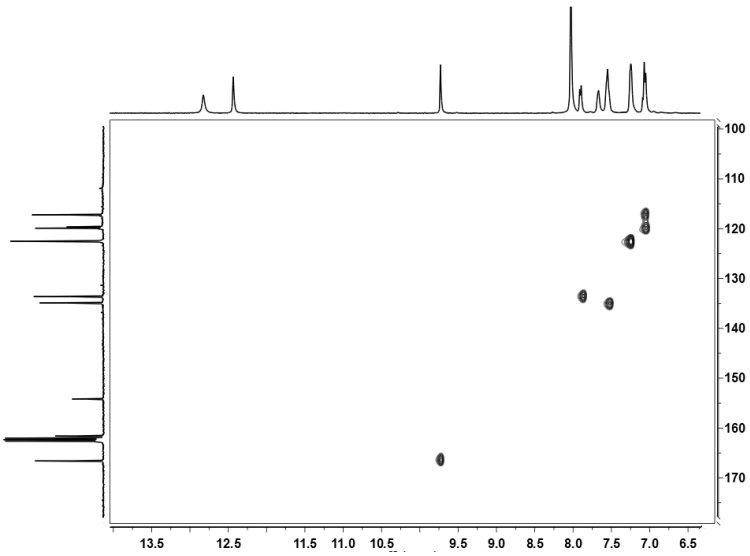


(b)

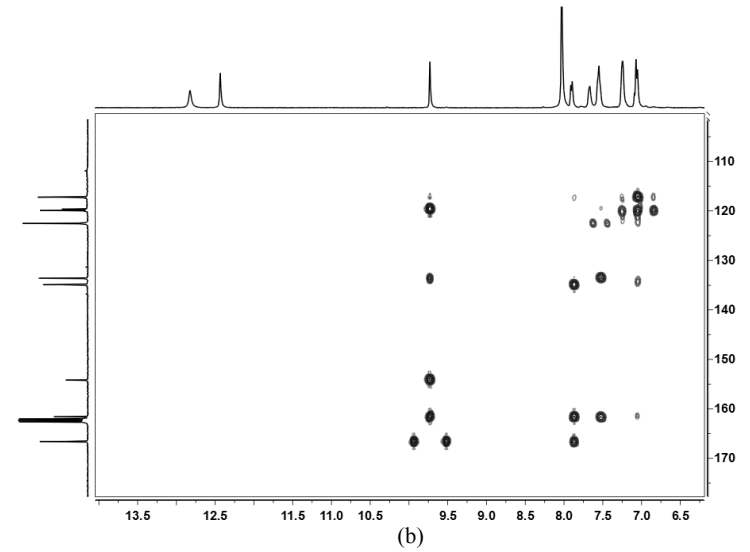


(c)

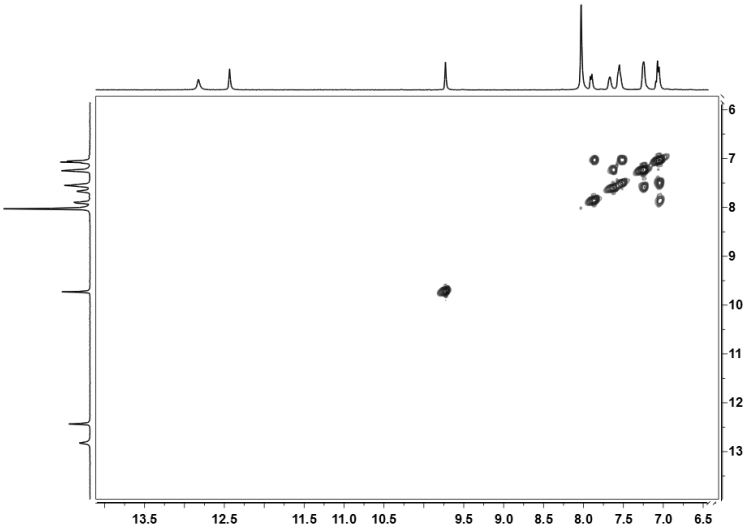
Figure S5. 2D NMR spectra of H_2L in DMSO-d_6: (a) HSQC; (b) HMBC; (c) H-H-COSY.



(a)

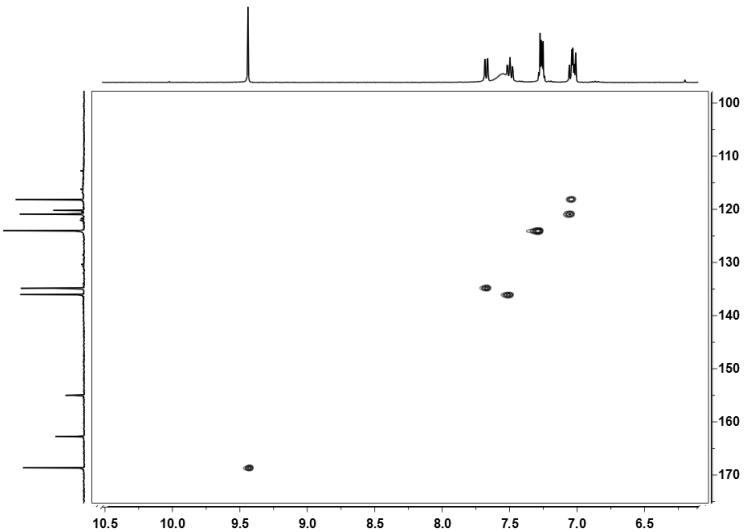


(b)



(c)

Figure S6. 2D NMR spectra of H_2L in DMF-d_7: (a) HSQC; (b) HMBC; (c) H-H-COSY.



(a)

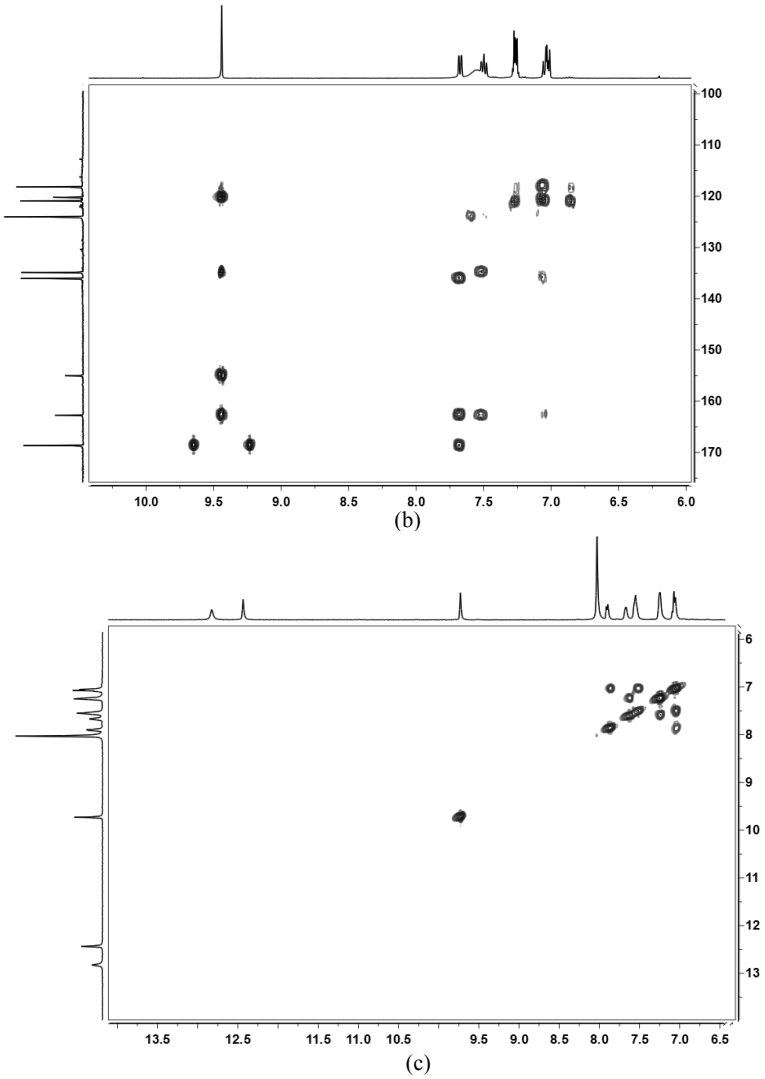


Figure S7. 2D NMR spectra of H_2L in methanol-d_4: (a) HSQC; (b) HMBC; (c) H-H-COSY.

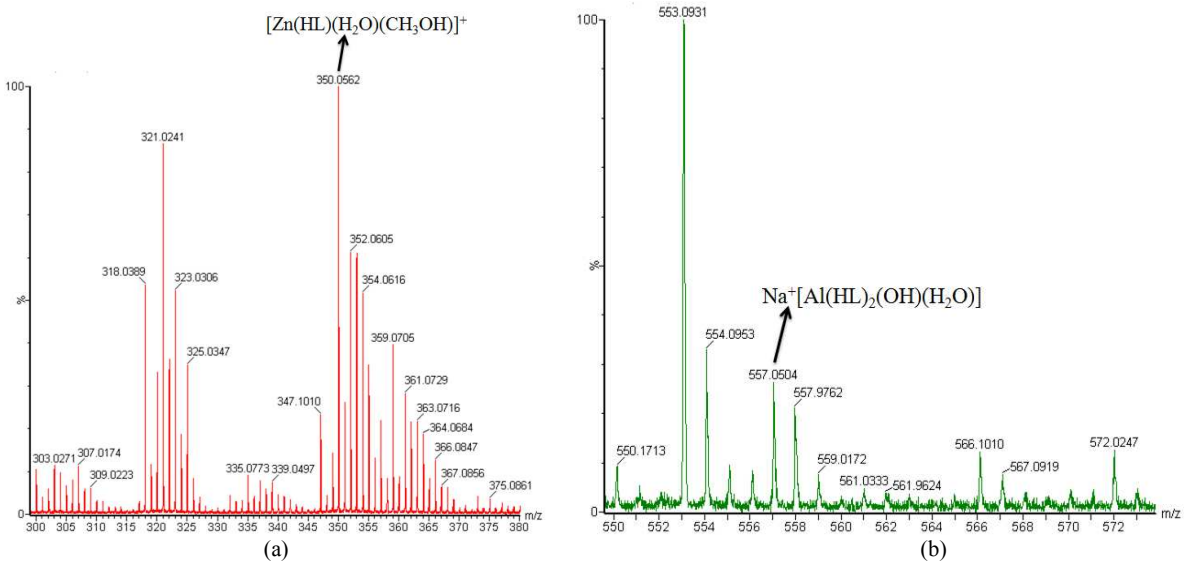


Figure S8. Positive-ion electrospray ionization mass spectra of H_2L upon addition of (a) $Zn(NO_3)_2$; (b) $Al(NO_3)_3$ in methanol.

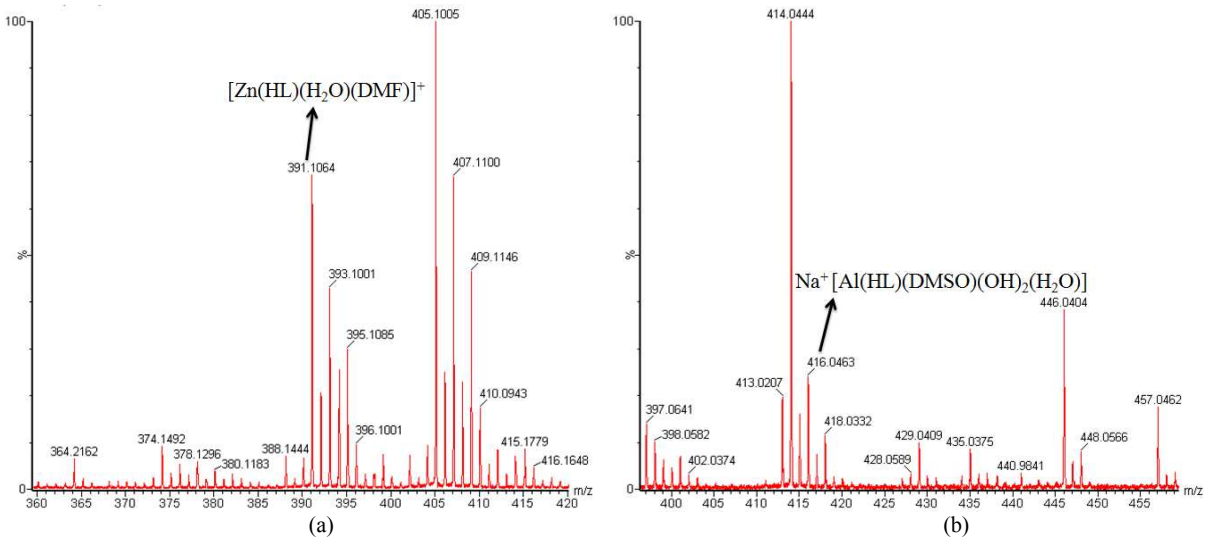


Figure S9. Positive-ion electrospray ionization mass spectra of H_2L upon addition of (a) $Zn(NO_3)_2$ in DMF; (b) $Al(NO_3)_3$ in DMSO.

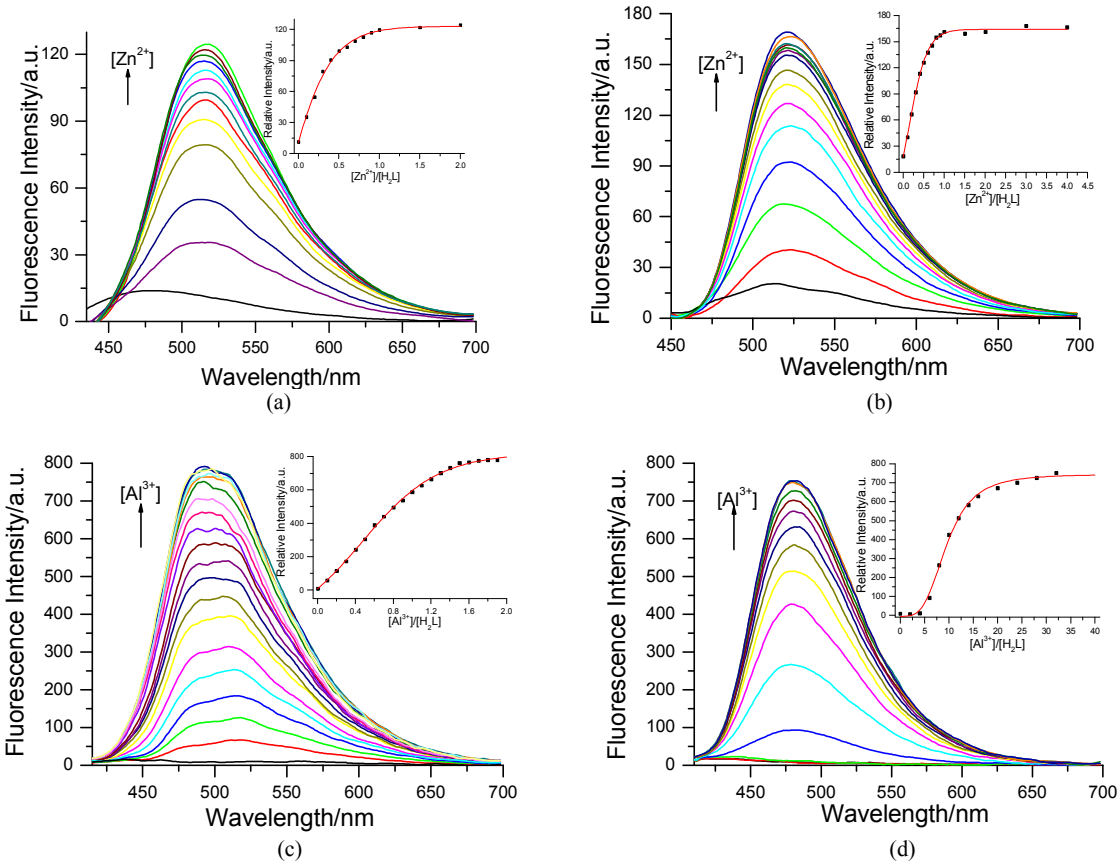


Figure S10. (a) Changes of fluorescence spectra of 0.1 mM H_2L in DMF upon addition of Zn^{2+} ions (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.5 and 2.0 equiv Zn^{2+}). Inset: Fluorescence intensity at 515 nm as a function of $[Zn^{2+}]/[H_2L]$. (b) Changes of fluorescence spectra of 0.1 mM H_2L in methanol after addition of Zn^{2+} ions (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.5, 2.0, 3.0, and 4.0 equiv Zn^{2+}). Inset: Changes in the relative intensity at 525 nm as a function of $[Zn^{2+}]/[H_2L]$. (c) Change of fluorescence spectra of 50 μM H_2L in DMSO after addition of Al^{3+} ions (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, and 1.3 equiv Al^{3+}). Inset: Fluorescence intensity at 500 nm as a function of $[Al^{3+}]/[H_2L]$. (d) Changes of fluorescence spectra of 10 μM H_2L in methanol after addition of Al^{3+} ions (0, 2, 4, 6, 8, 10, 12, 14, 16, 20, 24, 28, and 30 equiv) in CH_3OH. Inset: Changes in the relative intensity at 485 nm as a function of $[Al^{3+}]/[H_2L]$.

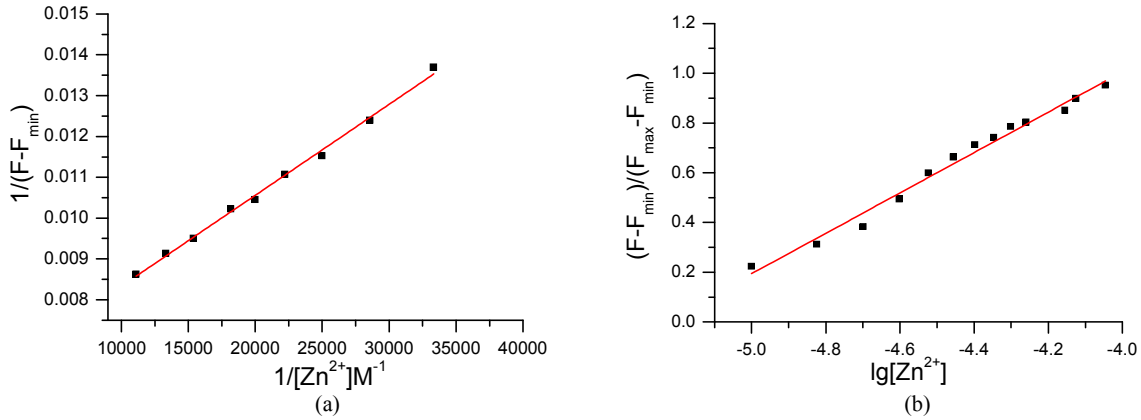


Figure S11. (a) Benesi-Hildebrand plot of H_2L, assuming 1:1 stoichiometry for association between H_2L and Zn^{2+} in DMF. (b) Normalized response of fluorescence signal at 515 nm to changing Zn^{2+} concentrations.

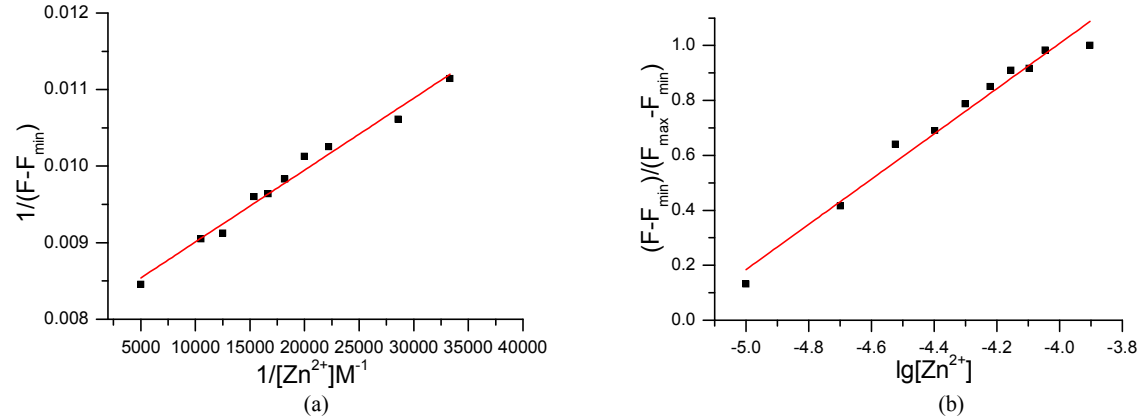


Figure S12. (a) Benesi-Hildebrand plot of H_2L, assuming 1:1 stoichiometry for association between H_2L and Zn^{2+} in methanol. (b) Normalized response of fluorescence signal at 525 nm to changing Zn^{2+} concentrations.

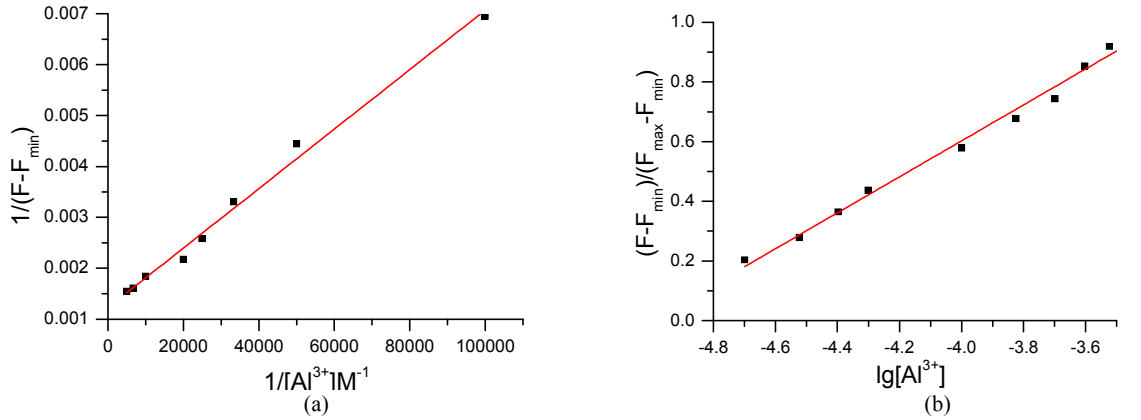


Figure S13. (a) Benesi-Hildebrand plot of H_2L, assuming 1:1 stoichiometry for association between H_2L and Al^{3+} in DMSO. (b) Normalized response of fluorescence signal at 500 nm to changing Al^{3+} concentrations.

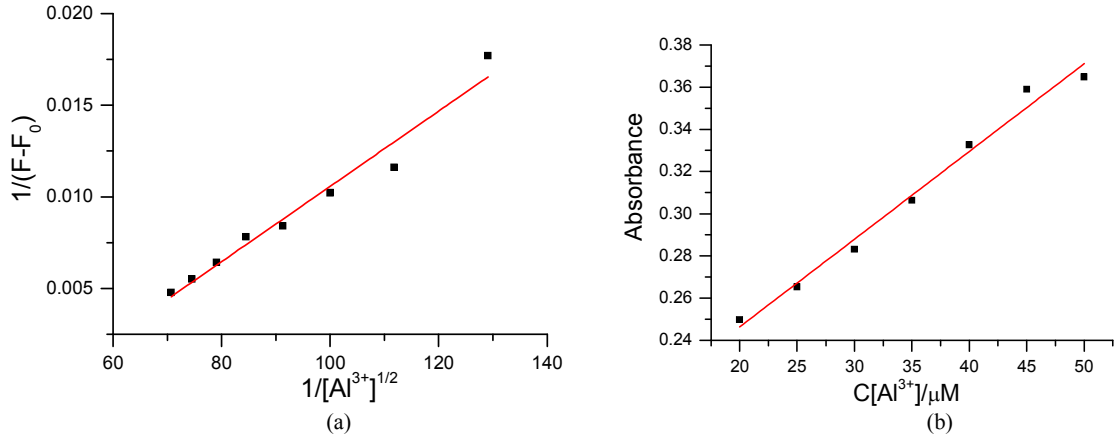


Figure S14. (a) Determination of binding constant of H_2L for Al^{3+} in methanol. (b) The absorbance of H_2L as a function of concentrations of Al^{3+}.

Table S1. Crystal Data and Structure Refinement Parameters of H_2L.

Compound	H_2L
Formula	$C_{14}H_{11}N_3O$
Fw	237.26
Crystal system, space group	Orthorhombic, Pnna
a (Å)	12.547(1)
b (Å)	15.587(1)
c (Å)	12.177(9)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	2381.5(3)
Z, calculated density (Mg/m^3)	8, 1.323
F (000)	992
Limiting indices	-16≦h≦16, -14≦k≦20, -15≦l≦15
Reflections collected/unique	13541 / 2767 [*R*(int) = 0.0347]
Goodness-of-fit on F^2	1.027
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0493, wR_2 = 0.1354
R indices (all data)	R_1 = 0.0638, wR_2 = 0.1470

R1 =$\Sigma(|Fo|- |Fc|)/|Fo|$; $wR2 = \{\Sigma[(w|F^2_o|- |F^2c|)^2/\Sigma w(F^2o)^2]\}^{1/2}$.

Table S2. Selected Bond Distances (Å) and Angles (deg) for H_2L.

C(1)-N(2)	1.377(2)	C(7)-N(1)	1.391(2)
C(1)-C(2)	1.390(2)	C(8)-N(1)	1.287(2)
C(1)-C(6)	1.397(2)	C(8)-C(9)	1.437(2)
C(2)-C(3)	1.379(3)	C(9)-C(10)	1.397(2)
C(3)-C(4)	1.386(3)	C(9)-C(14)	1.411(2)
C(4)-C(5)	1.378(3)	C(10)-C(11)	1.377(2)
C(5)-C(6)	1.394(2)	C(11)-C(12)	1.383(3)
C(6)-N(3)	1.387(2)	C(12)-C(13)	1.369(3)
C(7)-N(2)	1.328(2)	C(13)-C(14)	1.392(2)
C(7)-N(3)	1.344(2)	C(14)-O(1)	1.344(2)
N(2)-C(1)-C(2)	131.30(2)	N(2)-C(7)-N(3)	113.76(1)
N(2)-C(1)-C(6)	107.54(1)	N(2)-C(7)-N(1)	120.48(1)
C(2)-C(1)-C(6)	121.15(2)	N(3)-C(7)-N(1)	125.76(1)
C(3)-C(2)-C(1)	117.24(2)	N(1)-C(8)-C(9)	122.59(1)
C(2)-C(3)-C(4)	121.63(2)	C(10)-C(9)-C(14)	118.66(1)
C(5)-C(4)-C(3)	121.79(2)	C(10)-C(9)-C(8)	119.89(2)
C(4)-C(5)-C(6)	117.08(2)	C(14)-C(9)-C(8)	121.35(1)
N(3)-C(6)-C(5)	131.01(2)	C(11)-C(10)-C(9)	121.08(2)
N(3)-C(6)-C(1)	107.90(1)	C(10)-C(11)-C(12)	119.22(2)
C(5)-C(6)-C(1)	121.09(2)	C(13)-C(12)-C(11)	121.42(2)
C(13)-C(14)-C(9)	119.63(2)	C(12)-C(13)-C(14)	119.96(2)
C(8)-N(1)-C(7)	119.84(1)	O(1)-C(14)-C(13)	118.57(2)
C(7)-N(2)-C(1)	105.97(1)	O(1)-C(14)-C(9)	121.79(1)
C(7)-N(3)-C(6)	104.83(1)		

Table S3. The optimized Cartesian Coordinates(in Å) of species studied.

Species	Cartesian coordinates			Species	Cartesian coordinates		
a	N	1.62583	0.09455	0.09308	a^{ex}	N	-0.41018	-0.44732	0.00008
	C	0.59535	-0.69770	0.03618		C	-1.25992	0.63273	0.00009
	H	0.73393	-1.78215	0.01440		H	-0.84514	1.63873	0.00019
	C	-0.75618	-0.19440	-0.00030		C	-2.65292	0.45864	0.00004
	C	-1.03937	1.20222	0.02403		C	-3.27412	-0.85713	-0.00010
	C	-1.83376	-1.10580	-0.06190		C	-3.53048	1.59019	0.00013
	C	-2.37139	1.63883	-0.01337		C	-4.66571	-0.97964	-0.00012
	C	-3.14717	-0.66588	-0.09856		C	-4.90307	1.44319	0.00011
	C	-3.40797	0.71428	-0.07381		C	-5.47955	0.15353	-0.00002
	H	-2.56718	2.70636	0.00599		H	-5.09144	-1.97895	-0.00022
	O	-0.06369	2.12750	0.08225		O	-2.53096	-1.97695	-0.00019
	H	-1.61110	-2.16980	-0.08019		H	-3.08394	2.58140	0.00023
	C	5.11071	-0.37751	0.20707		C	3.06893	-0.71975	0.00007
	C	4.62737	-1.71305	0.15806		C	2.85078	0.70989	-0.00008
	N	3.24414	-1.72567	0.10828		N	1.53506	1.00510	-0.00012
	C	2.89502	-0.45085	0.12568		C	0.89196	-0.21206	0.00004
	N	3.97267	0.40182	0.18464		N	1.80175	-1.25681	0.00014
	H	0.80690	1.64237	0.10167		H	-1.56578	-1.69192	-0.00008
	H	-3.96468	-1.37798	-0.14581		H	-5.54289	2.32111	0.00020
	H	-4.43437	1.06961	-0.10217		H	-6.55979	0.04048	-0.00003
	H	3.91571	1.41096	0.20672		H	1.55027	-2.23579	0.00021
	C	5.53806	-2.78030	0.16568		C	3.97199	1.58013	-0.00017
	C	6.89615	-2.48181	0.22138		C	5.23664	1.01589	-0.00011
	C	6.47219	-0.07170	0.26296		C	4.33432	-1.28108	0.00014
	C	7.35638	-1.14843	0.26928		C	5.41919	-0.38995	0.00005
	H	5.18399	-3.80637	0.12886		H	3.82355	2.65518	-0.00030
	H	7.62123	-3.29083	0.22826		H	6.11272	1.65725	-0.00018
	H	6.82579	0.95419	0.29979		H	4.48709	-2.35529	0.00027
	H	8.42474	-0.95672	0.31208		H	6.42825	-0.79081	0.00010
b	N	1.61217	0.05553	0.14095	b^{ex}	N	0.41100	0.25934	-0.00008
	C	0.55039	-0.75430	0.04595		C	1.32141	-0.75294	-0.00007
	H	0.24392	-1.25314	0.96131		H	0.93475	-1.76399	-0.00008
	C	-0.12866	-0.95175	-1.15510		C	2.72318	-0.47813	-0.00005
	C	0.31025	-0.26223	-2.37684		C	3.24302	0.90188	-0.00003
	C	-1.25755	-1.83235	-1.18795		C	3.63355	-1.53699	-0.00005
	C	-0.45862	-0.53399	-3.56687		C	4.66918	1.06121	0.00008
	C	-1.94775	-2.04980	-2.34929		C	5.03410	-1.32855	-0.00001
	C	-1.53248	-1.38660	-3.54459		C	5.54478	-0.02880	0.00006
	H	-0.14991	-0.03403	-4.48037		H	5.04462	2.08079	0.00016
	O	1.30597	0.52497	-2.38676		O	2.46249	1.91275	0.00013
	H	-1.55472	-2.32596	-0.26525		H	3.25352	-2.55616	-0.00008
	C	3.87397	1.13984	2.61887		C	-3.06739	0.70526	-0.00005
	C	3.01190	0.26471	3.32772		C	-2.90849	-0.71603	0.00002
	N	2.04462	-0.25712	2.47764		N	-1.57878	-1.05859	0.00000
	C	2.31572	0.28152	1.31056		C	-0.93311	0.10873	-0.00006
	N	3.39480	1.12730	1.31782		N	-1.77954	1.20125	-0.00015
	H	-2.80293	-2.71749	-2.37158		H	5.69974	-2.18591	-0.00001
	H	-2.08827	-1.56678	-4.46205		H	6.61819	0.13746	0.00013
	H	3.76706	1.63771	0.52820		H	-1.50473	2.17436	0.00010
	C	3.21832	0.04460	4.69564		C	-4.04934	-1.53890	0.00009
	C	4.27891	0.70557	5.31104		C	-5.29735	-0.92629	0.00010
	C	4.93784	1.80546	3.22702		C	-4.31618	1.32201	-0.00004
	C	5.12490	1.57167	4.58916		C	-5.43059	0.48068	0.00004
	H	2.56634	-0.62262	5.25144		H	-3.94546	-2.61959	0.00013
	H	4.46026	0.55183	6.37103		H	-6.19392	-1.53952	0.00015
	H	5.58865	2.47226	2.66994		H	-4.42033	2.40241	-0.00009
	H	5.94156	2.06906	5.10431		H	-6.42423	0.91902	0.00005
	H	1.85620	0.50349	-0.76867		H	0.86854	1.19627	-0.00017

TSa-b					TSa-c				
	N	-0.47397	0.23072	0.00046		N	1.06618	0.40853	-0.95953
	C	-1.31903	-0.78600	0.00043		C	1.64272	-0.36239	-0.13535
	H	-0.92743	-1.80193	0.00042		H	1.05049	-1.07904	0.45875
	C	-2.70875	-0.52608	0.00037		C	3.07673	-0.41933	0.13712
	C	-3.15352	0.85388	0.00022		C	4.05263	0.34286	-0.56295
	C	-3.65609	-1.58396	0.00039		C	3.51127	-1.29079	1.15968
	C	-4.55653	1.08924	0.00010		C	5.40547	0.21396	-0.21382
	C	-5.00664	-1.31597	0.00029		C	4.84923	-1.41047	1.50147
	C	-5.44538	0.03227	0.00014		C	5.79748	-0.64650	0.80514
	H	-4.90166	2.11875	-0.00001		H	6.13324	0.80402	-0.76237
	O	-2.29309	1.82995	0.00021		O	3.77737	1.20437	-1.56683
	H	-3.29285	-2.60915	0.00050		H	2.75949	-1.87451	1.68625
	C	3.01657	0.70205	0.00050		C	-1.14219	2.42311	-2.78183
	C	2.88772	-0.71157	0.00002		C	0.08065	2.50794	-3.50511
	N	1.54956	-1.07605	-0.00011		N	1.06078	1.76796	-2.87839
	C	0.89738	0.06828	0.00033		C	0.46587	1.21031	-1.81989
	N	1.71512	1.17129	0.00053		N	-0.87073	1.57756	-1.73025
	H	-1.14783	1.22371	0.00032		H	2.82713	1.20129	-1.80886
	H	-5.73203	-2.12306	0.00031		H	5.15809	-2.08498	2.29371
	H	-6.51284	0.23912	0.00005		H	6.85120	-0.72629	1.05785
	H	1.41512	2.13691	0.00169		H	-1.50703	1.27074	-1.00726
	C	4.03769	-1.51336	-0.00030		C	0.14771	3.29372	-4.66675
	C	5.27687	-0.87890	-0.00008		C	-0.99829	3.97319	-5.06533
	C	4.25527	1.34493	0.00069		C	-2.29408	3.10852	-3.17681
	C	5.38428	0.52756	0.00041		C	-2.20137	3.88082	-4.33214
	H	3.95448	-2.59610	-0.00069		H	1.07462	3.36639	-5.22794
	H	6.18333	-1.47762	-0.00031		H	-0.97087	4.59022	-5.95904
	H	4.33738	2.42747	0.00106		H	-3.22006	3.03736	-2.61443
	H	6.36935	0.98521	0.00057		H	-3.07640	4.42371	-4.67799
c	N	-0.41943	1.98664	0.16212					
	C	-1.67448	1.67774	0.07646					
	H	-2.30054	2.57191	0.00401					
	C	-2.50847	0.46667	-0.00774					
	C	-2.32215	-0.80349	0.61386					
	C	-3.72605	0.68097	-0.70637					
	C	-3.32897	-1.78027	0.49120					
	C	-4.69295	-0.29973	-0.84506					
	C	-4.49079	-1.54266	-0.22803					
	H	-3.16000	-2.73172	0.98606					
	O	-1.27378	-1.11998	1.39408					
	H	-3.89241	1.65820	-1.15303					
	C	2.86426	0.78161	-0.02047					
	C	2.13844	-0.43401	0.05648					
	N	0.78354	-0.15975	0.13822					
	C	0.67244	1.16519	0.12819					
	N	1.90364	1.76835	0.03386					
	H	-0.41581	-0.79242	0.95616					
	H	-5.60141	-0.09894	-1.40420					
	H	-5.24517	-2.32103	-0.30482					
	H	2.03921	2.76948	-0.00979					
	C	2.81605	-1.66059	0.03712					
	C	4.20328	-1.63226	-0.06342					
	C	4.25725	0.81436	-0.12395					
	C	4.91215	-0.41417	-0.14380					
	H	2.26946	-2.59670	0.09801					
	H	4.75625	-2.56692	-0.08132					
	H	4.80236	1.75107	-0.18390					
	H	5.99518	-0.43567	-0.22235					

Table S4. The total energies(au), free energies(au) and frequencies(cm^{-1}) for the stationary points located.

species	energies	free energy	Frequencies
a	-779.62260	-779.43786	28 43 65 111 189 208 228 251 261 321 375 409 449 458 472 512 523 553 563 589 590 627 632 722 745 754 760 761 771 779 803 864 873 878 908 923 935 956 978 993 1030 1031 1056 1065 1143 1148 1179 1186 1214 1253 1261 1271 1313 1323 1343 1374 1383 1426 1462 1464 1480 1500 1525 1542 1561 1619 1633 1652 1675 1680 3128 3190 3191 3198 3201 3206 3210 3215 3216 3222 3645
b	-779.61509	-779.43045	35 39 63 107 188 189 230 255 256 346 379 407 446 448 465 487 518 531 561 588 590 615 630 713 734 752 758 769 772 784 865 867 875 888 908 919 935 960 978 1004 1010 1028 1033

			1061 1142 1155 1177 1181 1215 1245 1258 1262 1301 1327 1338 1368 1392 1420 1438 1481 1495 1514 1534 1562 1591 1602 1638 1670 1683 1685 3086 3182 3185 3192 3203 3207 3212 3218 3218 3221 3643
aex	-779.51905		
bex	-779.51940		
c	-779.60481	-779.42110	16 40 82 123 143 206 250 263 283 312 407 426 445 464 499 507 541 559 563 588 598 636 675 708 726 749 762 770 773 793 851 862 866 878 902 925 939 955 974 982 994 1029 1056 1070 1143 1148 1173 1179 1190 1226 1263 1275 1311 1316 1348 1365 1408 1443 1449 1470 1494 1510 1528 1541 1559 1606 1636 1658 1670 1675 2770 3104 3186 3195 3196 3205 3212 3215 3219 3221 3641
TSa-b	-779.61167	-779.43093	-1193i 31 40 68 115 204 239 240 258 264 354 386 430 448 458 479 532 545 560 580 587 600 629 631 719 752 759 769 770 771 813 865 868 892 909 935 943 956 979 999 1006 1034 1042 1084 1143 1148 1160 1180 1185 1234 1255 1260 1278 1311 1337 1374 1383 1407 1427 1472 1490 1509 1533 1542 1567 1582 1617 1636 1674 1678 1955 3186 3190 3191 3193 3202 3211 3212 3218 3219 3642
TSa-c	-779.58008	-779.39777	-282i 21 37 88 120 173 207 252 259 267 282 375 422 449 454 490 500 508 549 567 583 589 620 630 698 716 728 758 759 772 773 856 864 873 883 915 936 938 967 979 991 1007 1038 1062 1112 1142 1169 1177 1186 1207 1247 1261 1289 1313 1339 1345 1368 1381 1424 1433 1476 1502 1520 1535 1566 1616 1629 1666 1670 1876 2990 3184 3191 3197 3201 3211 3213 3217 3220 3565 3643

Table S5. The optimized Cartesian Coordinates(in Å) of the species studied.

Species	Cartesian coordinates			Species	Cartesian coordinates		
$[Zn(HL)(H_2O)(CH_3OH)]^+$ (ground state)	H	-4.62372	3.70899	0.36946	$[Zn(HL)(H_2O)(CH_3OH)]^+$ (excited state)	H	4.54863	-3.03371	0.90945
	C	-4.65632	2.63784	0.19782		C	4.56670	-2.01029	0.54870
	C	-5.86175	1.96044	0.02497		C	5.76846	-1.33594	0.32106
	C	-5.90140	0.56888	-0.20080		C	5.79190	-0.00400	-0.15100
	C	-4.73771	-0.19256	-0.25863		C	4.62026	0.69866	-0.40847
	C	-3.51736	0.47169	-0.08418		C	3.39834	0.04159	-0.18191
	C	-3.49460	1.86868	0.13558		C	3.39522	-1.30565	0.28885
	N	-2.15046	2.19415	0.25438		N	2.05985	-1.64843	0.39135
	N	-2.21934	-0.01666	-0.08617		N	2.11148	0.48350	-0.33703
	H	-6.79234	2.51876	0.06337		H	6.70703	-1.84800	0.51060
	H	-6.86353	0.08264	-0.33205		H	6.75068	0.47945	-0.31382
	H	-4.76719	-1.26378	-0.43194		H	4.63777	1.72282	-0.76768
	C	-1.43734	1.03346	0.11829		C	1.31069	-0.54485	0.02598
	N	-0.05756	0.91170	0.17195		N	-0.03159	-0.46025	-0.00395
	C	0.72033	1.94609	-0.07836		C	-0.82731	-1.54683	0.16812
	H	0.24403	2.89865	-0.31954		H	-0.36155	-2.51183	0.35028
	C	2.14133	1.96516	-0.11282		C	-2.26096	-1.57121	0.04670
	C	2.99178	0.80628	0.04891		C	-3.12196	-0.43830	-0.29893
	C	2.74051	3.23440	-0.37333		C	-2.89489	-2.80381	0.24533
	C	4.39485	1.00920	-0.06156		C	-4.52635	-0.65381	-0.41595
	C	4.10343	3.39160	-0.46416		C	-4.28925	-2.98267	0.12457
	C	4.93161	2.25706	-0.30489		C	-5.11005	-1.90140	-0.21005
	H	2.08472	4.09263	-0.49825		H	-2.28231	-3.66459	0.50074
	H	5.03176	0.13784	0.05636		H	-5.12676	0.21124	-0.68100
	H	4.53759	4.36669	-0.65828		H	-4.71322	-3.96754	0.29246
	H	6.01058	2.36715	-0.37759		H	-6.18313	-2.02878	-0.30885
	O	2.56010	-0.40327	0.27333		O	-2.68130	0.76512	-0.51870
	Zn	0.74988	-0.88478	0.59691		Zn	-0.86221	1.33941	-0.25359
	O	-0.59661	-2.12919	-0.27007		O	0.49315	2.28801	-1.41860
	H	-0.37821	-2.40446	-1.17665		H	0.36601	2.17704	-2.37614
	O	0.70122	-2.05370	2.26439		O	-0.96144	2.99845	0.92275
	H	0.27380	-2.90627	2.07747		H	-0.64519	3.77978	0.43882
	C	1.80765	-2.23810	3.17931		C	-2.08263	3.35231	1.76830
	H	1.43382	-2.65267	4.11803		H	-1.77600	4.13924	2.46055
	H	2.56318	-2.89711	2.74426		H	-2.93292	3.68185	1.16621
	H	2.23170	-1.25005	3.35345		H	-2.34504	2.45302	2.32435
	H	-1.78444	3.09840	0.51897		H	1.70581	-2.50463	0.79319
	H	-1.39038	-1.50038	-0.33005		H	1.30586	1.73288	-1.15536

[Al(HL)$_2$(OH)(H$_2$O)] (ground state)				
	H	-7.17834	-0.62537	-0.61568
	C	-6.50179	-1.36066	-0.19180
	C	-6.97432	-2.50420	0.45024
	C	-6.09438	-3.45944	0.99903
	C	-4.71291	-3.30163	0.92713
	C	-4.22158	-2.15672	0.28816
	C	-5.11680	-1.21103	-0.26292
	N	-4.30714	-0.22789	-0.81186
	N	-2.91786	-1.73616	0.07734
	H	-8.04589	-2.66285	0.52770
	H	-6.50591	-4.33724	1.48866
	H	-4.03393	-4.03608	1.34926
	C	-3.00163	-0.58769	-0.57510
	N	-1.89506	0.15566	-0.96631
	C	-2.03435	0.91776	-2.03161
	H	-2.96377	0.83762	-2.60017
	C	-1.09952	1.85354	-2.55293
	C	0.13683	2.17592	-1.89393
	C	-1.45620	2.53600	-3.74956
	C	0.94305	3.19283	-2.47344
	C	-0.64377	3.50520	-4.29570
	C	0.56456	3.83116	-3.63898
	H	-2.39692	2.27674	-4.23010
	H	1.87240	3.44436	-1.97104
	H	-0.92709	4.01614	-5.21012
	H	1.21032	4.59851	-4.05885
	O	0.52496	1.59506	-0.79851
	Al	0.04022	-0.05030	-0.03937
	H	3.99729	-4.37302	-0.96116
	C	4.66962	-3.53928	-0.78207
	C	6.02964	-3.62612	-1.06714
	C	6.90056	-2.54120	-0.83612
	C	6.44012	-1.33549	-0.30913
	C	5.07655	-1.25836	-0.02327
	C	4.18600	-2.33461	-0.25445
	N	2.89552	-1.97407	0.10503
	N	4.28221	-0.25080	0.49817
	H	6.43160	-4.54801	-1.47774
	H	7.95540	-2.64695	-1.07269
	H	7.11055	-0.50062	-0.12989
	H	4.56861	0.70549	0.65573
	C	2.99100	-0.73459	0.54377
	N	1.90596	0.01284	1.00906
	C	2.14949	0.89945	1.94725
	H	3.16687	0.97185	2.33848
	C	1.20904	1.77835	2.55764
	C	-0.19763	1.70952	2.28695
	C	1.69692	2.70927	3.51330
	C	-1.04899	2.59241	2.99953
	C	0.84656	3.56560	4.18103
	C	-0.53790	3.49578	3.91443
	H	2.76663	2.73808	3.70825
	H	-2.11526	2.53710	2.80097
	H	1.23189	4.27802	4.90319
	H	-1.21745	4.16320	4.43865
	O	-0.70983	0.84838	1.45069
	H	-4.62474	0.66053	-1.17445
	O	0.56032	-1.10012	-1.37045
	H	1.22499	-1.73171	-1.04928
	O	-0.48991	-1.66654	1.06503
	H	-1.40458	-1.94484	0.72278
	H	-0.66435	-1.30903	1.95350

[Al(HL)$_2$(OH)(H$_2$O)] (excited state)				
	H	-7.10087	-1.26132	-0.72629
	C	-6.36979	-1.87681	-0.21045
	C	-6.75294	-3.01322	0.51283
	C	-5.80323	-3.80559	1.17683
	C	-4.44094	-3.49164	1.14625
	C	-4.04540	-2.35773	0.43114
	C	-5.01356	-1.57097	-0.23588
	N	-4.29612	-0.54653	-0.84583
	N	-2.79142	-1.80756	0.22753
	H	-7.80387	-3.28411	0.55794
	H	-6.13337	-4.68244	1.72718
	H	-3.70883	-4.10643	1.66170
	C	-2.95929	-0.70640	-0.52770
	N	-1.95005	0.10546	-0.91712
	C	-2.23487	1.08245	-1.85063
	H	-3.18762	1.01251	-2.36858
	C	-1.39406	2.14270	-2.25665
	C	-0.06758	2.36171	-1.73916
	C	-1.88238	3.06894	-3.22635
	C	0.66189	3.47651	-2.18237
	C	-1.13750	4.15637	-3.65269
	C	0.14612	4.37003	-3.12366
	H	-2.88013	2.90582	-3.62973
	H	1.65775	3.61758	-1.76945
	H	-1.54942	4.84050	-4.39000
	H	0.74044	5.22045	-3.44664
	O	0.48806	1.53382	-0.85975
	Al	-0.05179	-0.10354	-0.25931
	H	3.85984	-4.45414	-1.03338
	C	4.57593	-3.65504	-0.86975
	C	5.92438	-3.81150	-1.15851
	C	6.85156	-2.76391	-0.94718
	C	6.46100	-1.52929	-0.43810
	C	5.10421	-1.37998	-0.14252
	C	4.15780	-2.41585	-0.35704
	N	2.89433	-1.98408	-0.01392
	N	4.36821	-0.32922	0.36665
	H	6.28082	-4.75625	-1.55786
	H	7.89763	-2.92895	-1.18752
	H	7.17484	-0.72813	-0.27676
	H	4.71236	0.61015	0.51189
	C	3.05193	-0.74373	0.41460
	N	1.99818	0.03700	0.87990
	C	2.28174	0.97400	1.73465
	H	3.30815	1.08996	2.08887
	C	1.35249	1.89679	2.33938
	C	-0.09373	1.82576	2.16094
	C	1.87136	2.86624	3.19886
	C	-0.92136	2.75738	2.88967
	C	1.03897	3.76916	3.86824
	C	-0.36352	3.70664	3.71136
	H	2.94476	2.92099	3.35128
	H	-1.99274	2.67824	2.74506
	H	1.47674	4.51647	4.51996
	H	-0.99507	4.40947	4.24381
	O	-0.65062	0.97194	1.40988
	H	-4.70091	0.27536	-1.26789
	O	0.55773	-1.18430	-1.51889
	H	1.22063	-1.79574	-1.16022
	O	-0.42381	-1.56609	0.99597
	H	-1.43655	-1.85599	0.76388
	H	-0.43945	-1.26453	1.91906

$[Zn(HL)(H_2O)(DMF)]^+$ (ground state)				
H	-4.70763	3.55800	0.84065
C	-4.81099	2.61044	0.32177
C	-6.05344	2.13695	-0.09591
C	-6.18604	0.90620	-0.77146
C	-5.08141	0.10625	-1.04939
C	-3.82553	0.56492	-0.63311
C	-3.70847	1.80491	0.03742
N	-2.35174	1.95045	0.29398
N	-2.57141	-0.01283	-0.75851
H	-6.94014	2.73136	0.10329
H	-7.17387	0.57682	-1.07992
H	-5.18200	-0.84223	-1.56783
C	-1.72395	0.83586	-0.19570
N	-0.36566	0.56857	-0.13037
C	0.50640	1.54911	-0.02316
H	0.12607	2.57276	-0.00581
C	1.92289	1.43732	0.03670
C	2.66119	0.19608	-0.04196
C	2.63930	2.66587	0.15474
C	4.08029	0.28179	0.00828
C	4.01310	2.70673	0.20306
C	4.73244	1.49226	0.12813
H	2.06605	3.58844	0.20815
H	4.63443	-0.65001	-0.05279
H	4.53708	3.65230	0.29484
H	5.81879	1.51039	0.16310
O	2.11682	-0.98188	-0.15838
Zn	0.24293	-1.37441	-0.22613
O	-1.05710	-2.04355	-1.62326
H	-0.75118	-1.94136	-2.54045
O	0.03555	-2.83897	1.09311
H	-1.93325	2.67660	0.85943
H	-1.80875	-1.37874	-1.48827
C	1.03765	-3.24431	1.74470
H	2.02397	-2.80128	1.57805
N	0.98667	-4.20545	2.65292
C	-0.26486	-4.88447	2.98772
H	-0.16598	-5.95484	2.78308
H	-0.48259	-4.74404	4.05094
H	-1.07088	-4.46669	2.38748
C	2.18766	-4.63421	3.36848
H	2.05312	-4.47970	4.44341
H	2.36958	-5.69696	3.18159
H	3.04880	-4.05743	3.02727

$[Zn(HL)(H_2O)(DMF)]^+$ (excited state)				
H	-5.37557	-1.75338	-1.91243
C	-5.20405	-0.92874	-1.22805
C	-6.23350	-0.06054	-0.85734
C	-6.01124	1.01257	0.03516
C	-4.75698	1.25724	0.58257
C	-3.70348	0.40008	0.21869
C	-3.94990	-0.68356	-0.67737
N	-2.73230	-1.32445	-0.81147
N	-2.38436	0.41110	0.58516
H	-7.22837	-0.21470	-1.26425
H	-6.84271	1.66116	0.29499
H	-4.58470	2.08426	1.26420
C	-1.80341	-0.62798	-0.05808
N	-0.49542	-0.91724	0.06646
C	0.01561	-2.09187	-0.38305
H	-0.66399	-2.82273	-0.81471
C	1.37895	-2.52833	-0.25125
C	2.46918	-1.77563	0.37079
C	1.69288	-3.80276	-0.74054
C	3.76129	-2.37284	0.44490
C	2.98303	-4.36526	-0.65092
C	4.02365	-3.64665	-0.05342
H	0.90346	-4.38620	-1.20736
H	4.53974	-1.78316	0.91980
H	3.15588	-5.36012	-1.04891
H	5.01908	-4.07200	0.02330
O	2.32679	-0.58452	0.86872
Zn	0.71495	0.49631	0.85610
O	-0.50683	1.26057	2.27166
H	-0.50641	0.77281	3.11278
O	1.36681	2.19960	0.09298
H	-2.52682	-2.05322	-1.48003
H	-1.39347	1.06267	1.81559
C	2.55872	2.32362	-0.30463
H	3.27386	1.50537	-0.18123
N	3.03241	3.41510	-0.88278
C	2.19135	4.58666	-1.12726
H	2.60107	5.44906	-0.59267
H	2.17731	4.80597	-2.19925
H	1.18090	4.38187	-0.77859
C	4.42828	3.49879	-1.31078
H	4.47435	3.66628	-2.39116
H	4.92173	4.33110	-0.79989
H	4.94749	2.57028	-1.06804

$[Al(HL)(OH)_2(H_2O)(DMSO)]$ (ground state)				
H	-14.87232	-1.15605	3.74670
C	-14.31954	-2.03301	3.42457
C	-14.22695	-3.17187	4.22301
C	-13.51076	-4.31164	3.80239
C	-12.86104	-4.34837	2.57152
C	-12.93913	-3.21166	1.75606
C	-13.66890	-2.07928	2.19097
N	-13.54764	-1.16479	1.15846
N	-12.38865	-2.97041	0.50580
H	-14.71948	-3.18127	5.19102
H	-13.46637	-5.17847	4.45553
H	-12.30890	-5.22512	2.24658
C	-12.76600	-1.74792	0.18306
N	-12.42476	-1.09166	-1.00042
C	-13.35878	-0.31828	-1.50825
H	-14.35767	-0.35383	-1.06454
C	-13.20715	0.60027	-2.58649
C	-11.91903	0.90467	-3.13707
C	-14.35448	1.30294	-3.04168
C	-11.84646	1.93323	-4.11318
C	-14.25708	2.27977	-4.01029
C	-12.98544	2.59265	-4.53927
H	-15.31950	1.05819	-2.60377
H	-10.87003	2.17656	-4.52154
H	-15.13979	2.80840	-4.35515
H	-12.89847	3.36746	-5.29693
O	-10.83778	0.28787	-2.75478
Al	-10.47604	-1.43406	-2.07050
H	-13.84193	-0.19799	1.18386
O	-11.69683	-2.21887	-3.73645
H	-10.76696	-2.21984	-4.10229
O	-10.30406	-3.06336	-1.37249
H	-10.99194	-3.30184	-0.72651
O	-9.22286	-1.69894	-3.39016
H	-9.03144	-0.84916	-3.81274
H	-12.17161	-1.54087	-4.24553
S	-8.35593	-1.43885	0.01284
O	-9.45895	-0.54795	-0.67618
C	-9.07951	-1.94593	1.59679
H	-8.30554	-2.44760	2.18379
H	-9.46233	-1.06728	2.12144
H	-9.88734	-2.63699	1.35598
C	-7.20762	-0.17158	0.61613
H	-6.74299	0.28330	-0.26077
H	-7.75472	0.57885	1.19121

$[Al(HL)(OH)_2(H_2O)(DMSO)]$ (excited state)				
H	-3.89046	-3.76609	-1.24077
C	-4.07462	-2.81910	-0.74444
C	-5.37212	-2.34801	-0.52764
C	-5.62262	-1.11156	0.12601
C	-4.59089	-0.30722	0.57695
C	-3.26398	-0.75188	0.36532
C	-3.03704	-2.01337	-0.29325
N	-1.67027	-2.15074	-0.31468
N	-2.09139	-0.16667	0.69908
H	-6.21409	-2.94398	-0.86611
H	-6.65168	-0.79693	0.27039
H	-4.77782	0.63833	1.07562
C	-1.11150	-1.01834	0.27893
N	0.19852	-0.81912	0.42597
C	1.00776	-1.93533	0.24849
H	0.57956	-2.90260	0.51104
C	2.34598	-1.92207	-0.15937
C	3.04923	-0.68231	-0.48080
C	3.06222	-3.15163	-0.28909
C	4.38028	-0.76224	-0.95303
C	4.36454	-3.18568	-0.75103
C	5.02633	-1.98425	-1.09621
H	2.55000	-4.07546	-0.03037
H	4.88170	0.17032	-1.19704
H	4.88143	-4.13629	-0.84684
H	6.04905	-2.01565	-1.46168
O	2.47248	0.47416	-0.32827
Al	1.08362	1.10520	0.84550
H	-1.14992	-2.85405	-0.82118
O	2.15540	0.08748	2.47523
H	2.57031	0.99623	2.47189
O	-0.24899	1.60712	1.92635
H	-1.06298	1.11064	1.73678
O	2.25487	2.40179	1.44162
H	3.00584	2.43333	0.83132
H	2.85246	-0.52071	2.17828
S	-0.39228	3.30837	-0.50829
O	0.36003	1.94928	-0.75368
C	-2.12563	2.94586	-0.89733
H	-2.69492	3.87736	-0.84114
H	-2.19359	2.50237	-1.89368
H	-2.46514	2.23750	-0.14069
C	0.04495	4.25175	-1.99427
H	1.10973	4.48298	-1.92534
H	-0.15951	3.65319	-2.88491

	H	-6.44512 -0.65652 1.23075		H	-0.53642 5.17737 -2.00256

Table S6. The total energies(au), free energies(au) and frequencies(cm^{-1}) for the stationary points located.

Species	energies	free energy	Frequencies
$[Zn(HL)(H_2O)(CH_3OH)]^+$ (ground state)	-2750.26490	-2750.01972	31 36 46 53 69 85 100 108 123 158 182 189 201 218 241 248 265 281 293 339 347 383 413 441 447 452 471 476 501 528 533 548 587 606 628 635 638 650 730 752 756 762 772 774 827 869 874 891 922 934 941 959 985 1002 1003 1019 1025 1036 1056 1080 1107 1144 1162 1182 1186 1189 1236 1252 1267 1278 1316 1354 1369 1386 1411 1415 1441 1466 1478 1492 1497 1504 1511 1525 1534 1562 1577 1638 1641 1667 1670 1682 2938 3082 3136 3162 3187 3194 3196 3198 3208 3212 3218 3223 3224 3646 3745 3765
$[Al(HL)_2(OH)(H_2O)]$ (ground state)	-1952.95042	-1952.54187	9 20 28 36 39 42 49 63 73 82 102 117 131 156 165 192 194 212 221 235 239 243 256 267 275 286 289 301 309 320 338 355 358 396 410 422 425 431 450 453 454 465 474 484 488 503 517 531 532 540 553 557 587 589 600 607 614 615 631 635 637 639 703 730 732 749 753 756 758 760 761 766 771 771 772 772 837 839 865 867 872 872 881 887 913 923 933 934 936 938 942 955 956 979 982 996 997 1019 1020 1027 1028 1042 1046 1055 1057 1102 1141 1143 1158 1160 1179 1181 1185 1185 1233 1243 1253 1254 1260 1268 1281 1281 1309 1318 1346 1352 1373 1377 1406 1408 1412 1415 1433 1440 1446 1460 1488 1491 1492 1495 1506 1508 1533 1535 1560 1562 1584 1584 1638 1639 1642 1643 1664 1670 1676 1677 1708 2908 3128 3128 3183 3184 3190 3190 3192 3195 3202 3206 3209 3209 3212 3216 3218 3219 3219 3222 3640 3644 3707 3734
$[Zn(HL)(H_2O)(DMF)]^+$ (ground state)	-2883.07356	-2882.78183	20 28 41 43 56 70 73 104 115 123 128 145 158 176 186 201 211 242 246 265 273 284 285 348 381 387 392 407 416 439 449 453 476 501 528 530 548 587 602 622 634 637 663 699 733 752 757 762 772 774 826 869 874 875 889 922 934 941 958 985 1002 1011 1024 1037 1045 1056 1080 1083 1139 1145 1145 1161 1182 1187 1191 1235 1252 1268 1275 1279 1316 1354 1370 1410 1415 1425 1441 1461 1466 1469 1479 1485 1493 1497 1504 1515 1517 1534 1548 1563 1577 1639 1641 1667 1672 1683 1708 2975 3070 3075 3134 3135 3137 3138 3174 3186 3193 3197 3205 3208 3211 3218 3222 3224 3643 3765
$[Al(HL)(OH)_2(H_2O)(DMSO)]$ (ground state)	-1802.94727	-1802.65192	19 26 42 52 63 68 73 85 101 122 137 157 168 185 189 200 210 215 228 239 244 258 263 287 293 304 329 346 356 368 386 402 426 452 465 486 512 527 530 541 553 589 593 603 609 618 627 635 636 671 710 720 733 752 754 761 772 772 801 841 866 871 881 902 916 916 935 937 943 957 980 982 984 996 1021 1026 1030 1050 1057 1064 1142 1158 1180 1185 1232 1255 1263 1281 1311 1346 1363 1374 1385 1406 1409 1431 1443 1464 1472 1478 1490 1494 1495 1508 1533 1560 1584 1638 1639 1667 1676 1693 3080 3081 3115 3179 3182 3185 3187 3191 3193 3204 3204 3209 3213 3219 3220 3248 3640 3648 3761 3787