Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis and characterization of a Novel Ditopic, Reversible and Highly Selective "Turn-On" Fluorescent Chemosensor for Al^{3+} ion

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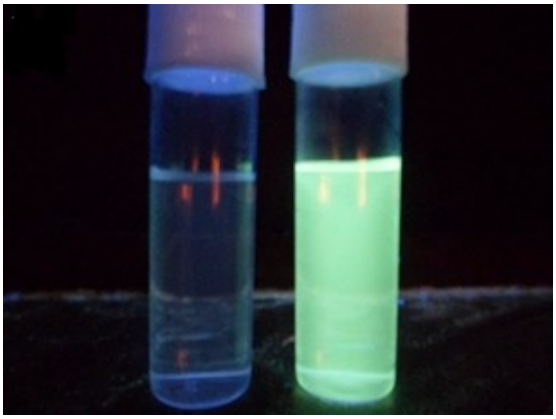

Fig. S1 Naked eye image of free ligand and its 1:2 aluminium complex in UV light.

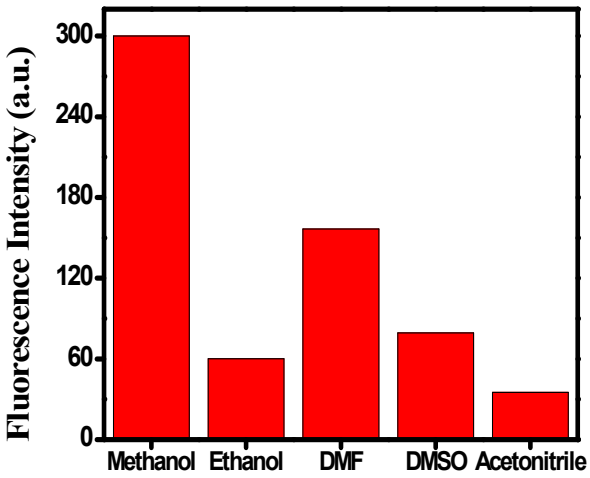

Fig. S2 Solvent effect on fluorescent intensity of L + Al^{3+} probe in different solvent methanol, ethanol, DMF, DMSO and acetonitrile.

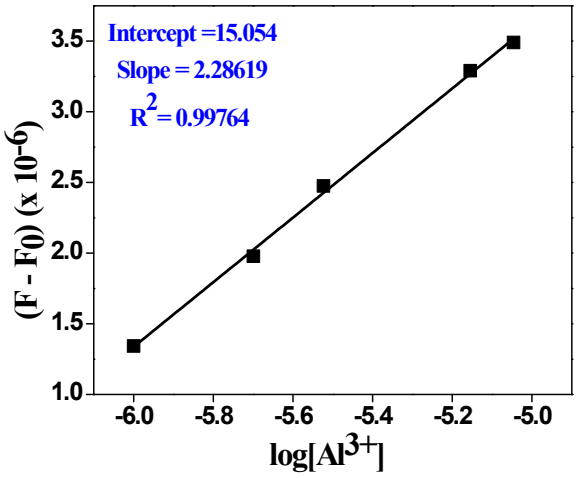

Fig. S3 The detection limit of L for Al^{3+} was estimated from plot of normalized fluorescence change of L vs. log[Al^{3+}]

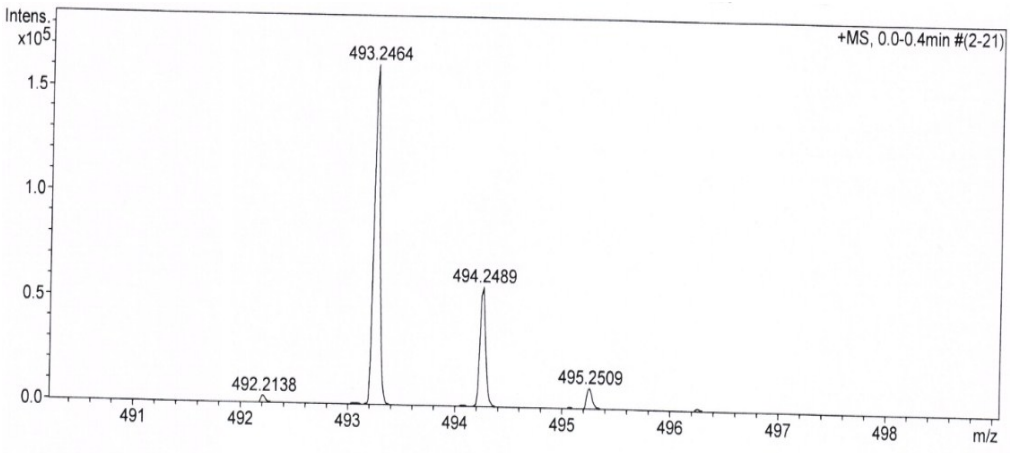

Fig. S4 ESI-MS spectrum of L in MeOH.

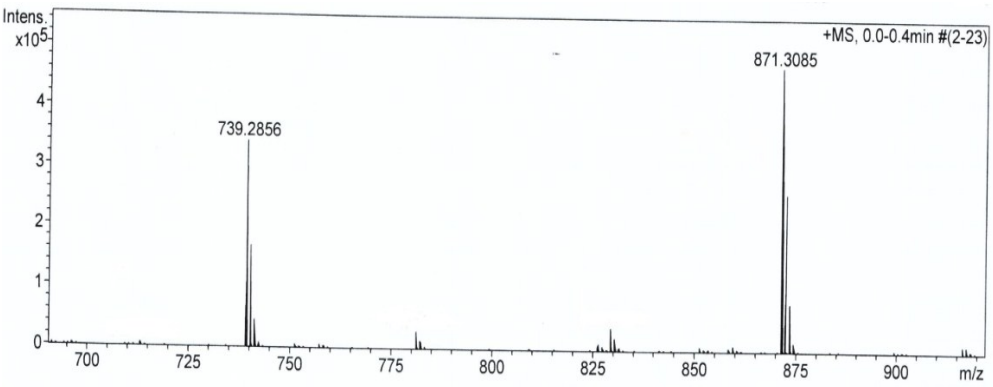

Fig. S5 ESI-MS spectrum of L-Al^{3+} complex in MeOH.

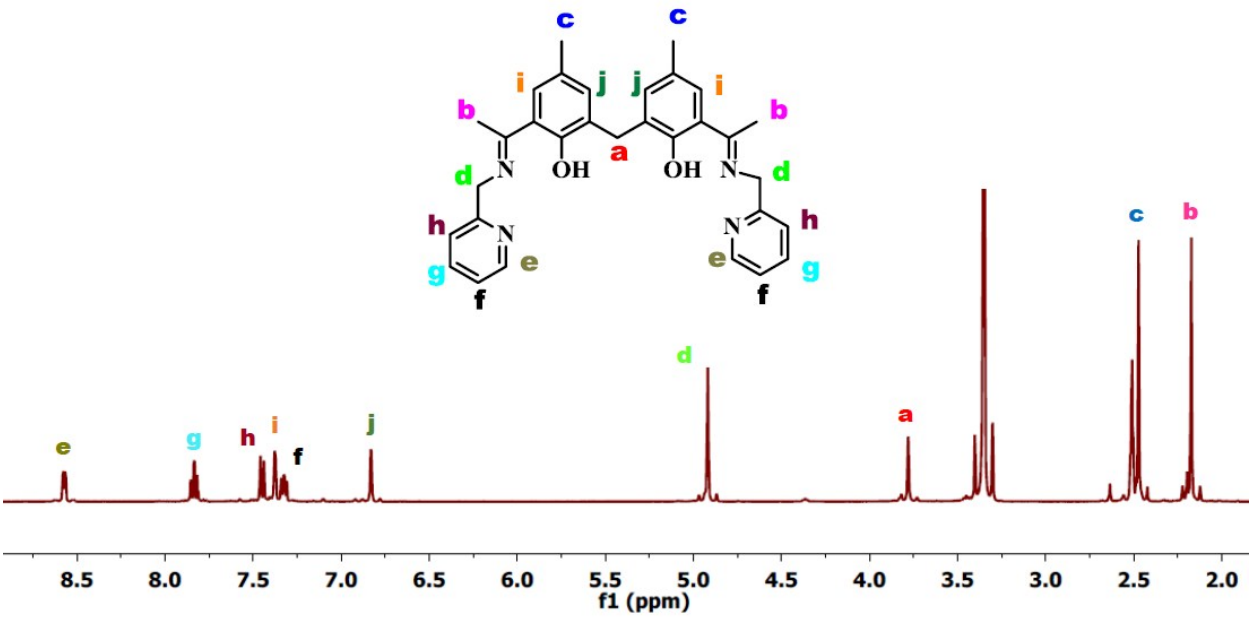

Fig. S6 ^{1}H NMR spectrum of L in DMSO-d_6.

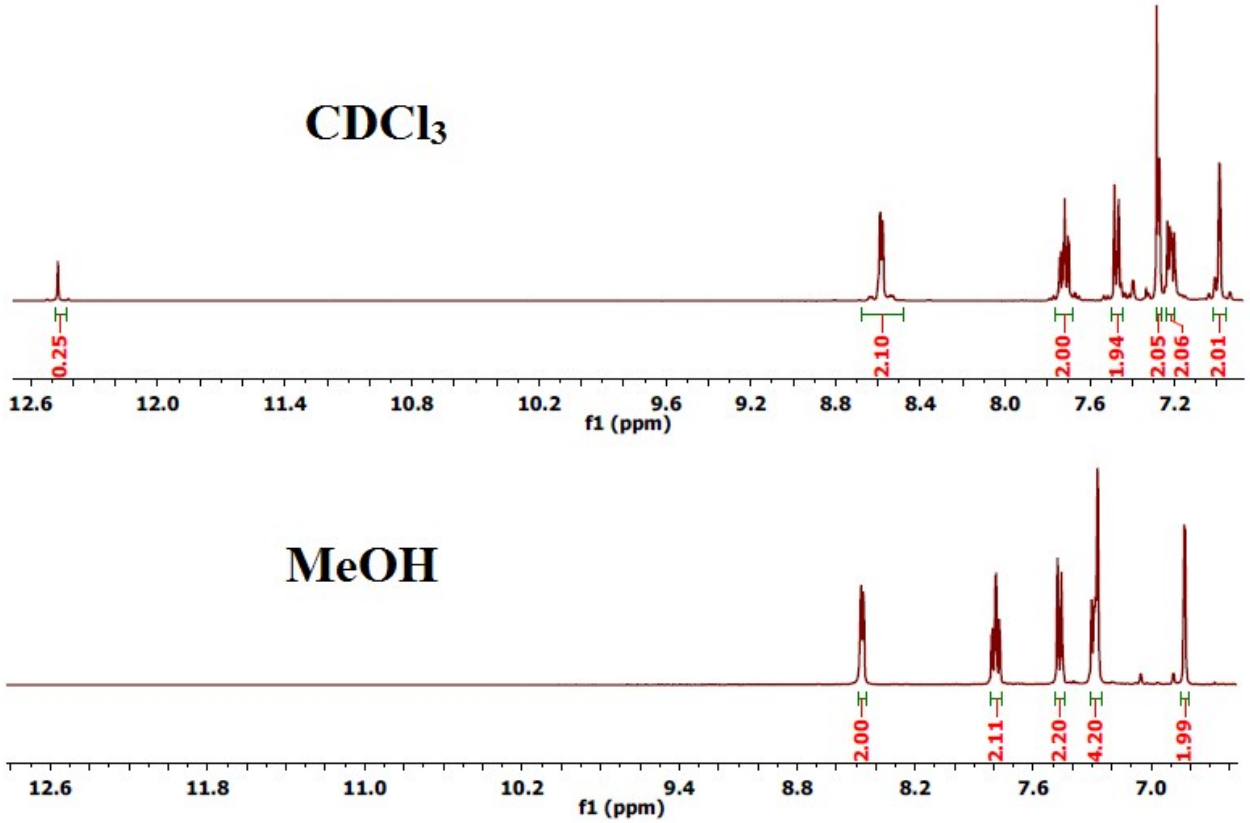

Fig. S7 ^{1}HNMR of L in both aprotic ($CDCl_3$) and protic (methanol-d_4).

Table S1. Crystal data and structure refinement parameters of L.

Identification code	L	
Empirical formula	$C_{31}H_{32}N_4O_2$	
Formula weight	492.61	
Temperature	110(0) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 13.0342 (16)Å, b = 11.9408 (15)Å, c = 16.232 (2)Å,	α = 90.0° α = 96.921(3)° α = 90.0°
Volume	2507.8(5) $Å^3$	
Z, Calculated density	4, 1.305 mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1048	
Crystal size	0.4 x 0.2 x 0.4 mm^3	
Theta range for data collection	2.32 to 27.00˚	
Limiting indices	$-16 \leq h \leq 16$, $-15 \leq k \leq 15$, $-20 \leq l \leq 20$	
Reflections collected / unique	41229 / 5475 [$R_{(int)} = 0.0608$]	
Completeness to theta = 27.00°	100.0 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5475 / 0 / 344	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2σ (I)]	$R_1 = 0.0546$, $wR_2 = 0.1418$	
R indices (all data)	$R_1 = 0.0850$, $wR_2 = 0.1574$	
Largest diff. peak and hole	0.317 and -0.248 $e.A^{-3}$	

Table S2. Selected Bond Distances (in Å) and Angles (deg) for L from X-ray.

O(1)-C(15)	1.354(2)	C(12)-H(13)	0.980(0)
O(1)-H(31)	0.940(3)	C(13)-C(14)	1.384(2)
O(2)-C(23)	1.354(2)	C(13)-H(14)	0.950(0)
O(2)-H(32)	0.940(3)	C(14)-C(15)	1.401(2)
N(1)-C(5)	1.350(2)	C(14)-C(16)	1.518(2)
N(1)-C(1)	1.357(3)	C(16)-C(17)	1.518(2)
N(2)-C(7)	1.285(2)	C(16)-H(15)	0.990(0)
N(2)-C(6)	1.461(2)	C(16)-H(16)	0.990(0)
N(3)-C(27)	1.339(3)	C(17)-C(18)	1.381(2)
N(3)-C(31)	1.342(3)	C(17)-C(23)	1.397(2)
N(4)-C(25)	1.277(2)	C(18)-C(19)	1.395(2)
N(4)-C(26)	1.465(2)	C(18)-H(17)	0.950(0)
C(1)-C(2)	1.364(3)	C(19)-C(21)	1.379(3)
C(1)-H(1)	0.950(0)	C(19)-C(20)	1.507(2)
C(2)-C(3)	1.381(3)	C(20)-H(18)	0.980(0)

C(2)-H(2)	0.950(0)	C(20)-H(20)	0.980(0)
C(3)-C(4)	1.359(3)	C(20)-H(19)	0.980(0)
C(3)-H(3)	0.950(0)	C(21)-C(22)	1.391(2)
C(4)-C(5)	1.364(3)	C(21)-H(21)	0.950(0)
C(4)-H(4)	0.950(0)	C(22)-C(23)	1.421(2)
C(5)-C(6)	1.509(3)	C(22)-C(25)	1.482(2)
C(6)-H(6)	0.990(0)	C(24)-C(25)	1.505(2)
C(6)-H(5)	0.990(0)	C(24)-H(22)	0.980(0)
C(7)-C(9)	1.480(2)	C(24)-H(24)	0.980(0)
C(7)-C(8)	1.504(2)	C(24)-H(23)	0.980(0)
C(8)-H(7)	0.980(0)	C(26)-C(27)	1.499(3)
C(8)-H(9)	0.980(0)	C(26)-H(26)	0.990(0)
C(8)-H(8)	0.980(0)	C(26)-H(25)	0.990(0)
C(9)-C(10)	1.396(2)	C(27)-C(28)	1.370(3)
C(9)-C(15)	1.415(2)	C(28)-C(29)	1.360(3)
C(10)-C(11)	1.382(3)	C(28)-H(27)	0.950(0)
C(10)-H(10)	0.950(0)	C(29)-C(30)	1.363(3)
C(11)-C(13)	1.395(2)	C(29)-H(28)	0.950(0)
C(11)-C(12)	1.506(2)	C(30)-C(31)	1.362(3)
C(12)-H(11)	0.980(0)	C(30)-H(29)	0.950(0)
C(12)-H(12)	0.980(0)	C(31)-H(30)	0.950(0)
C(15)-O(1)-H(31)	105.20(17)	C(14)-C(16)-C(17)	112.46(14)
C(23)-O(2)-H(32)	102.90(17)	C(14)-C(16)-H(15)	109.10(0)
C(5)-N(1)-C(1)	117.60(19)	C(17)-C(16)-H(15)	109.10(0)
C(7)-N(2)-C(6)	121.47(15)	C(14)-C(16)-H(16)	109.10(0)
C(27)-N(3)-C(31)	116.90(2)	C(17)-C(16)-H(16)	109.10(0)
C(25)-N(4)-C(26)	120.12(16)	H(15)-C(16)-H(16)	107.80(0)
N(1)-C(1)-C(2)	122.62(19)	C(18)-C(17)-C(23)	119.19(15)
N(1)-C(1)-H(1)	118.70(0)	C(18)-C(17)-C(16)	120.70(15)
C(2)-C(1)-H(1)	118.70(0)	C(23)-C(17)-C(16)	120.10(15)
C(1)-C(2)-C(3)	118.03(19)	C(17)-C(18)-C(19)	122.22(16)
C(1)-C(2)-H(2)	121.00(0)	C(17)-C(18)-H(17)	118.90(0)
C(3)-C(2)-H(2)	121.00(0)	C(19)-C(18)-H(17)	118.90(0)
C(4)-C(3)-C(2)	120.40(2)	C(21)-C(19)-C(18)	117.64(16)
C(4)-C(3)-H(3)	119.80(0)	C(21)-C(19)-C(20)	121.21(16)
C(2)-C(3)-H(3)	119.80(0)	C(18)-C(19)-C(20)	121.15(17)
C(3)-C(4)-C(5)	118.91(18)	C(19)-C(20)-H(18)	109.50(0)
C(3)-C(4)-H(4)	120.50(0)	C(19)-C(20)-H(20)	109.50(0)
C(5)-C(4)-H(4)	120.50(0)	H(18)-C(20)-H(20)	109.50(0)
N(1)-C(5)-C(4)	122.43(18)	C(19)-C(20)-H(19)	109.50(0)
N(1)-C(5)-C(6)	116.90(19)	H(18)-C(20)-H(19)	109.50(0)
C(4)-C(5)-C(6)	120.67(18)	H(20)-C(20)-H(19)	109.50(0)
N(2)-C(6)-C(5)	111.04(16)	C(19)-C(21)-C(22)	122.92(16)
N(2)-C(6)-H(6)	109.40(0)	C(19)-C(21)-H(21)	118.50(0)
C(5)-C(6)-H(6)	109.40(0)	C(22)-C(21)-H(21)	118.50(0)
N(2)-C(6)-H(5)	109.40(0)	C(21)-C(22)-C(23)	117.84(16)
C(5)-C(6)-H(5)	109.40(0)	C(21)-C(22)-C(25)	121.67(15)
H(6)-C(6)-H(5)	108.00(0)	C(23)-C(22)-C(25)	120.46(16)
N(2)-C(7)-C(9)	117.60(15)	O(2)-C(23)-C(17)	118.42(15)
N(2)-C(7)-C(8)	123.52(16)	O(2)-C(23)-C(22)	121.48(15)
C(9)-C(7)-C(8)	118.88(15)	C(17)-C(23)-C(22)	120.10(16)
C(7)-C(8)-H(7)	109.50(0)	C(25)-C(24)-H(22)	109.50(0)
C(7)-C(8)-H(9)	109.50(0)	C(25)-C(24)-H(24)	109.50(0)

H(7)-C(8)-H(9)	109.50(0)	H(22)-C(24)-H(24)	109.50(0)
C(7)-C(8)-H(8)	109.50(0)	C(25)-C(24)-H(23)	109.50(0)
H(7)-C(8)-H(8)	109.50(0)	H(22)-C(24)-H(23)	109.50(0)
H(9)-C(8)-H(8)	109.50(0)	H(24)-C(24)-H(23)	109.50(0)
C(10)-C(9)-C(15)	118.67(16)	N(4)-C(25)-C(22)	117.60(15)
C(10)-C(9)-C(7)	120.91(15)	N(4)-C(25)-C(24)	122.21(17)
C(15)-C(9)-C(7)	120.42(15)	C(22)-C(25)-C(24)	120.18(16)
C(11)-C(10)-C(9)	121.93(16)	N(4)-C(26)-C(27)	109.88(16)
C(11)-C(10)-H(10)	119.00(0)	N(4)-C(26)-H(26)	109.70(0)
C(9)-C(10)-H(10)	119.00(0)	C(27)-C(26)-H(26)	109.70(0)
C(10)-C(11)-C(13)	118.06(16)	N(4)-C(26)-H(25)	109.70(0)
C(10)-C(11)-C(12)	121.14(16)	C(27)-C(26)-H(25)	109.70(0)
C(13)-C(11)-C(12)	120.79(16)	H(26)-C(26)-H(25)	108.20(0)
C(11)-C(12)-H(11)	109.50(0)	N(3)-C(27)-C(28)	121.61(19)
C(11)-C(12)-H(12)	109.50(0)	N(3)-C(27)-C(26)	116.80(2)
H(11)-C(12)-H(12)	109.50(0)	C(28)-C(27)-C(26)	121.50(2)
C(11)-C(12)-H(13)	109.50(0)	C(29)-C(28)-C(27)	120.20(2)
H(11)-C(12)-H(13)	109.50(0)	C(29)-C(28)-H(27)	119.90(0)
H(12)-C(12)-H(13)	109.50(0)	C(27)-C(28)-H(27)	119.90(0)
C(14)-C(13)-C(11)	122.46(16)	C(28)-C(29)-C(30)	119.00(2)
C(14)-C(13)-H(14)	118.80(0)	C(28)-C(29)-H(28)	120.50(0)
C(11)-C(13)-H(14)	118.80(0)	C(30)-C(29)-H(28)	120.50(0)
C(13)-C(14)-C(15)	118.74(16)	C(31)-C(30)-C(29)	118.10(2)
C(13)-C(14)-C(16)	120.87(15)	C(31)-C(30)-H(29)	121.00(0)
C(15)-C(14)-C(16)	120.39(15)	C(29)-C(30)-H(29)	121.00(0)
O(1)-C(15)-C(14)	118.36(15)	N(3)-C(31)-C(30)	124.10(2)
O(1)-C(15)-C(9)	121.50(15)	N(3)-C(31)-H(30)	117.90(0)
C(14)-C(15)-C(9)	120.14(15)	C(30)-C(31)-H(30)	117.90(0)