A highly selective fluorescent sensor for Al^{3+} and use of the resultant complex as a secondary sensor for PPi in aqueous media: its applicability in live cell imaging

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(Electronic Supplementary Information)

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Fig. S9 Absorption spectra of **L**-Al^{3+} ensemble upon addition of increasing amounts of PPi (0-5 equiv.) in HEPES buffer (20 mM, 10% EtOH, pH = 7.04). The arrows indicate the changes in the absorbance with the increased PPi ions.

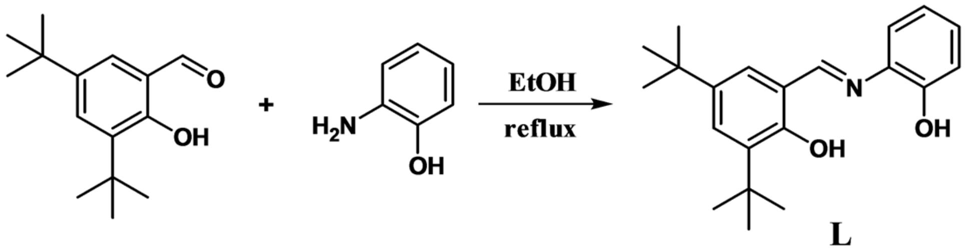
Fig. S10 ESI-MS spectrum of PPi added **L**-Al^{3+}complex in EtOH-H_2O (v/v = 1/1).

Fig. S11 Fluorescence changes at 497 nm of **L** (10 μM) and **L**-Al^{3+} (10 equiv.) in aqueous solution at different pH scale.

Table S1 Crystal data and structure refinement for **L**.

Table S2 Bond lengths [Å] and angles [deg] for **L.**

Scheme S1 The synthesis of sensor **L**.



L

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

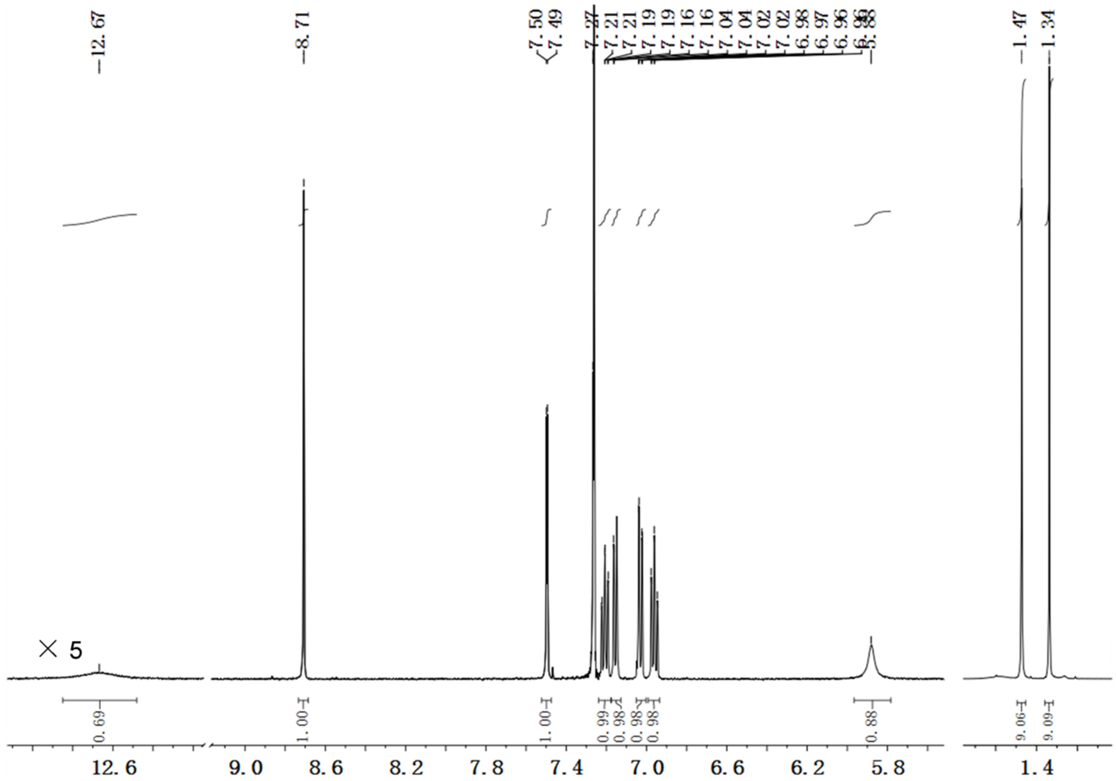


Fig. S2 ^{13}C NMR spectrum of **L** in $CDCl_3$.

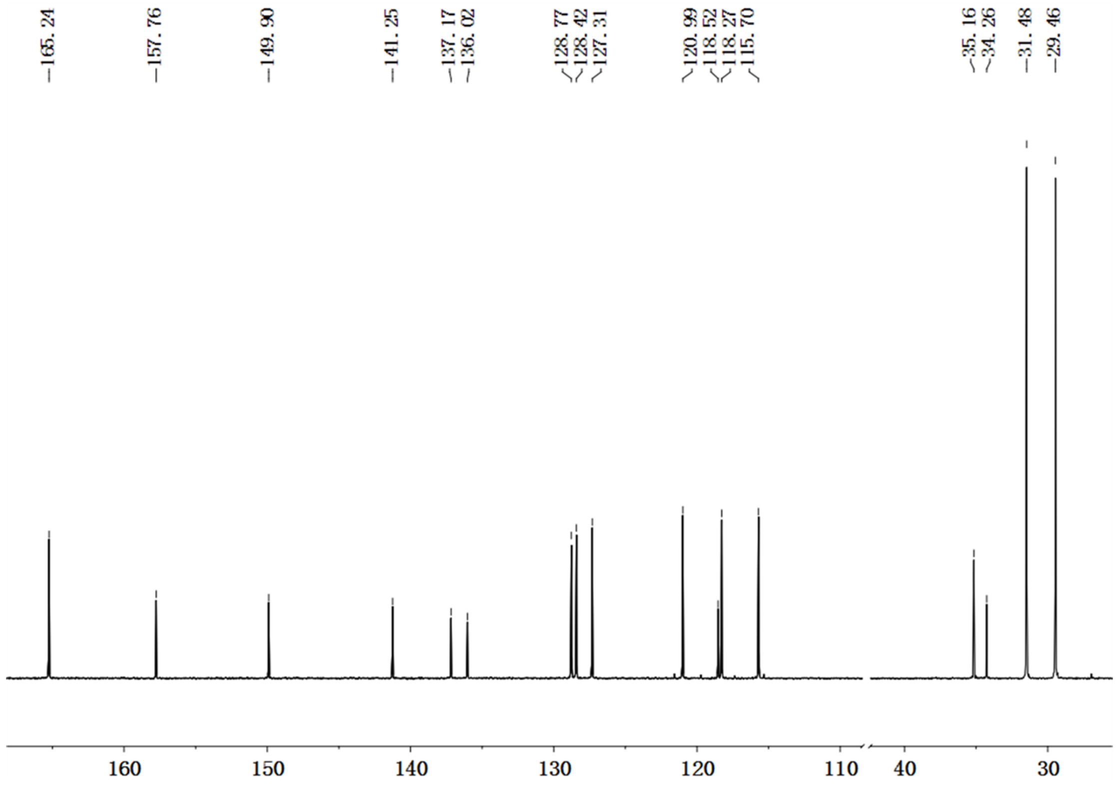


Fig. S3 FT-IR spectrum of **L**.

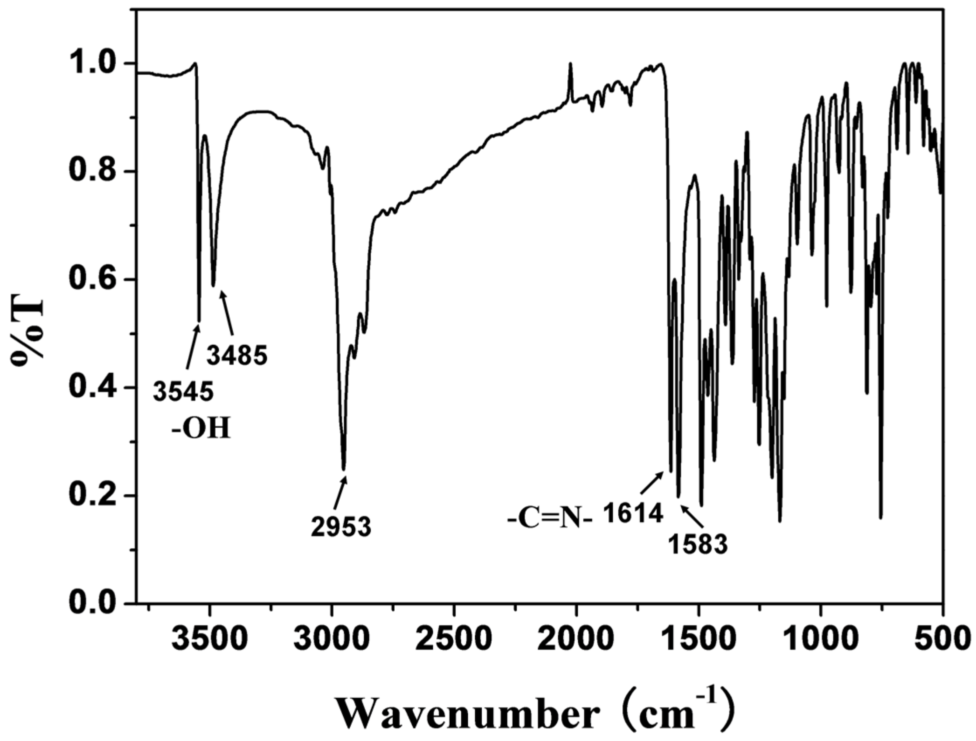


Fig. S4 ESI-MS spectrum of **L** in EtOH.

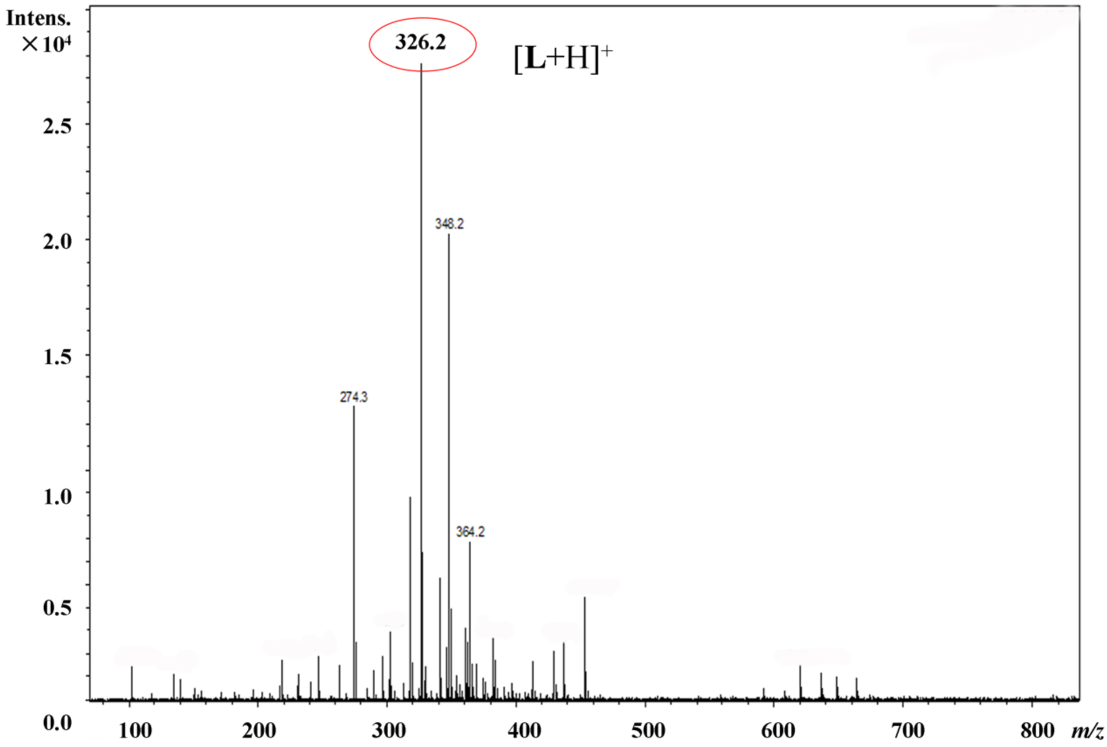


Fig. S5 Absorption spectra of **L** (40 μM) upon addition of increasing amounts of Al^{3+} ion (0-11 equiv.) in HEPES buffer (20 mM, 10% EtOH, pH = 7.04). The arrows indicate the changes in the absorbance with the increased Al^{3+} ions.

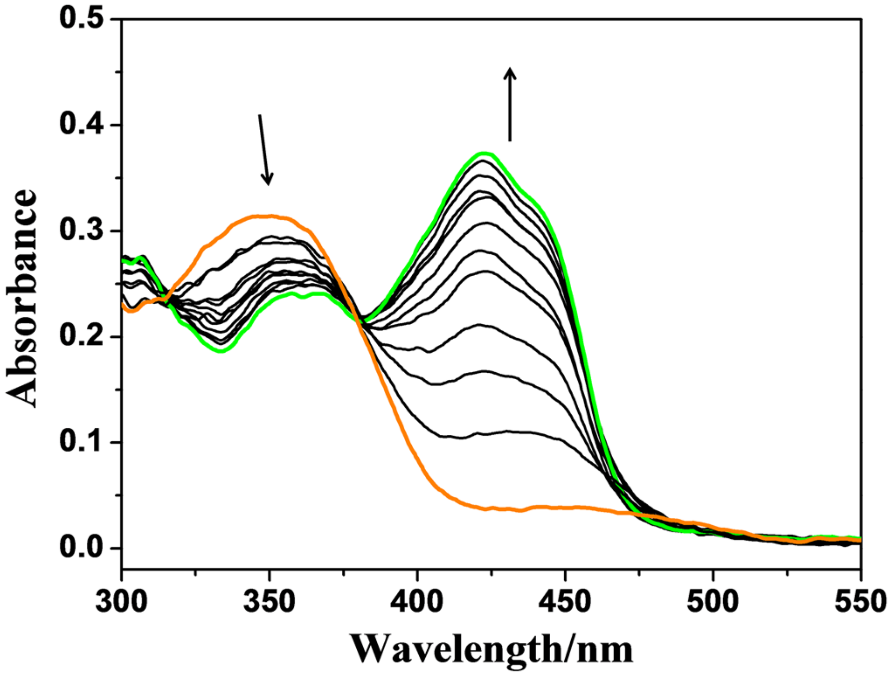


Fig. S6 Relative fluorescence of **L** and its complexation with Al^{3+} in the presence of various metal ions in HEPES buffer (20 mM, 1% EtOH, pH = 7.04). Response of **L** was included as controls. Conditions: **L**, 10 μM; Al^{3+}, 10 equiv.; other metal ions, 10 equiv. (λ_{ex} = 420 nm).

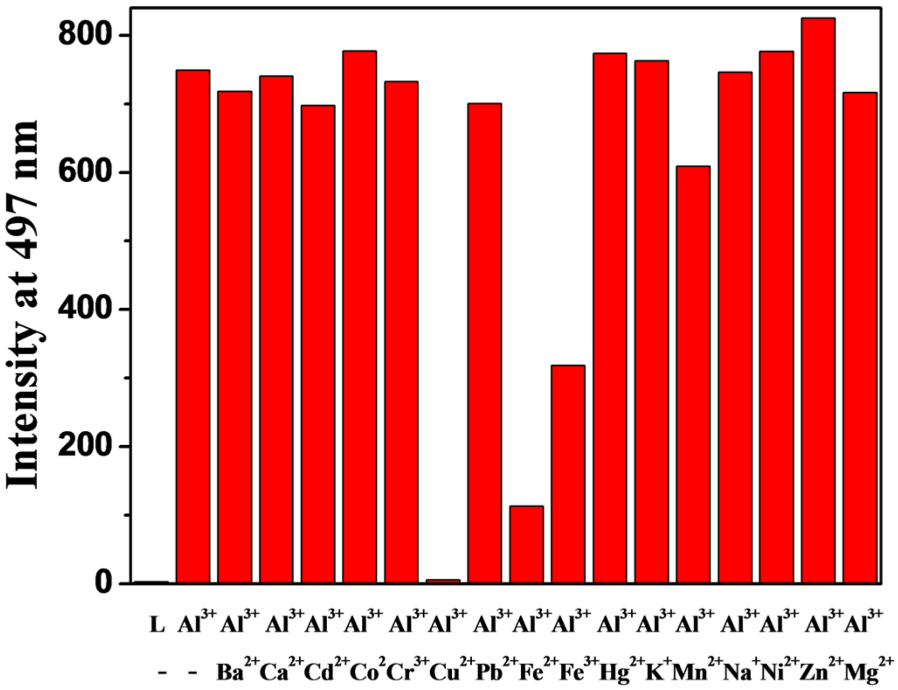


Fig. S7 Job's plot for the binding of **L** with Al^{3+}. The total concentration of **L** and Al^{3+} was 20 μM.

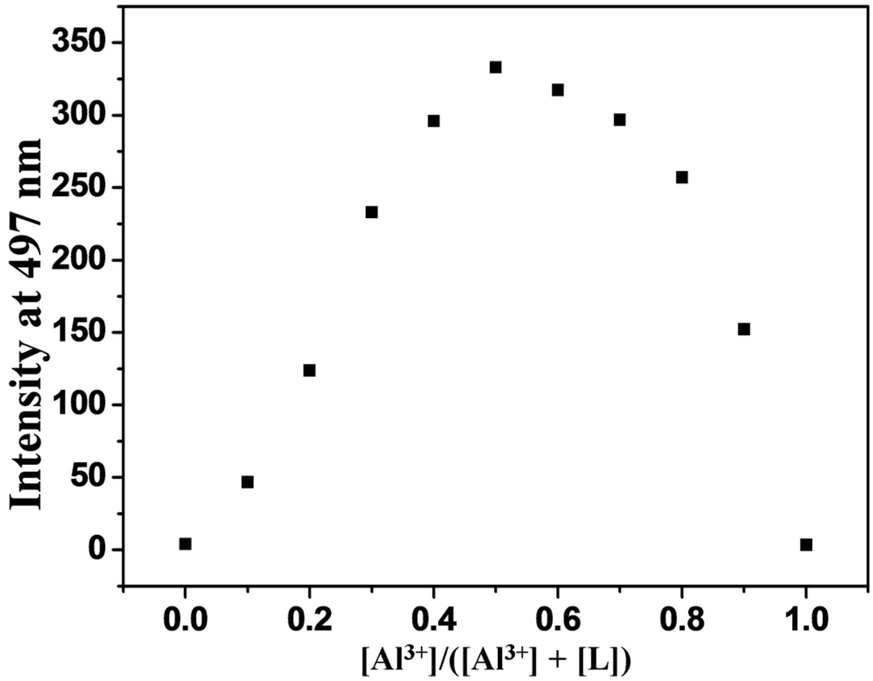


Fig. S8 Benesi-Hildebrand analysis of the emission changes for the complexation between **L** and Al^{3+}.

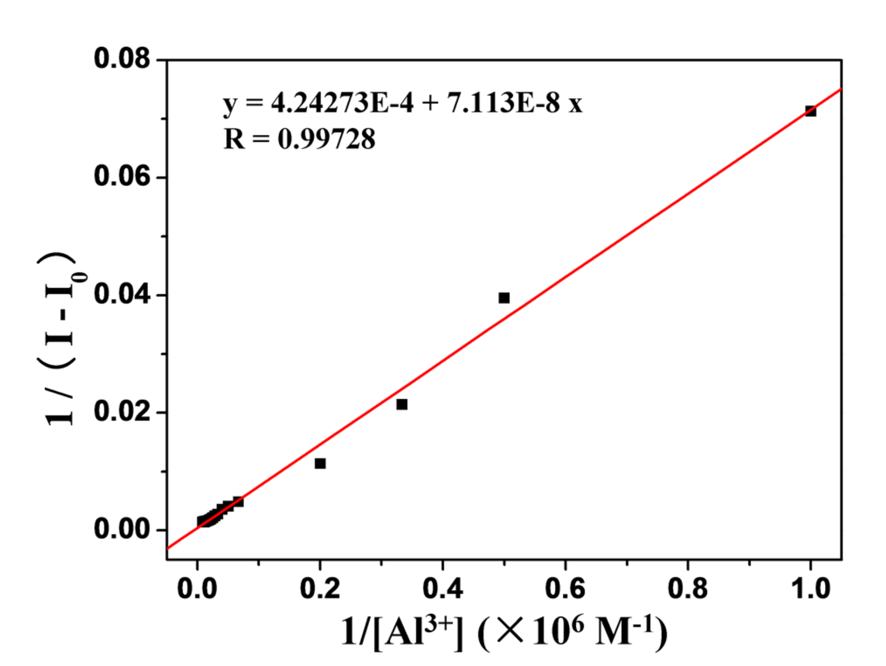


Fig. S9 Absorption spectra of **L**-Al^{3+} ensemble upon addition of increasing amounts of PPi (0-5 equiv.) in HEPES buffer (20 mM, 10% EtOH, pH = 7.04). The arrows indicate the changes in the absorbance with the increased PPi ions.

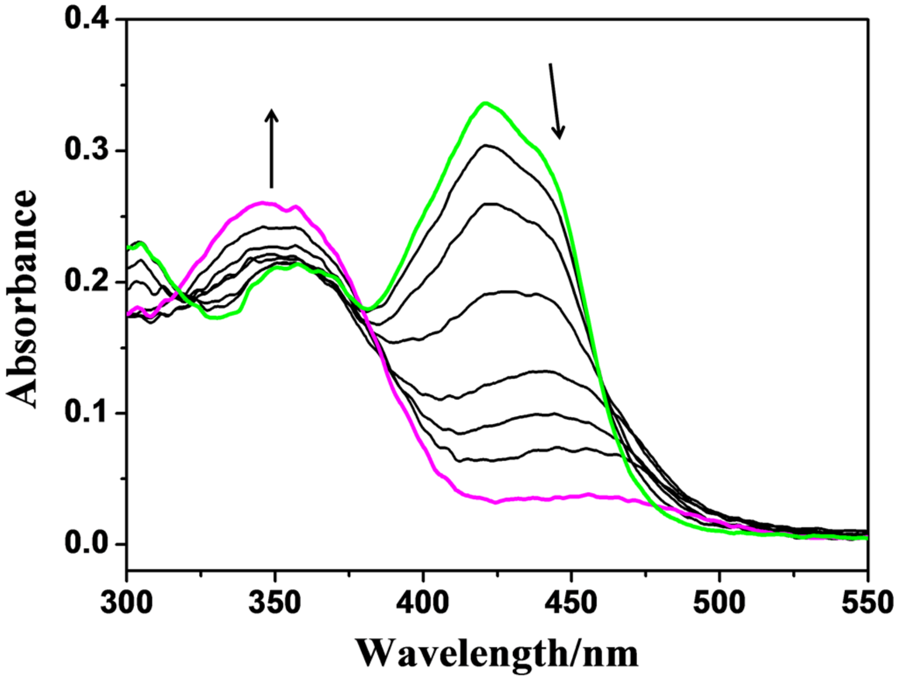


Fig. S10 ESI-MS spectrum of PPi added **L**-Al^{3+}complex in EtOH-H_2O (v/v = 1/1).

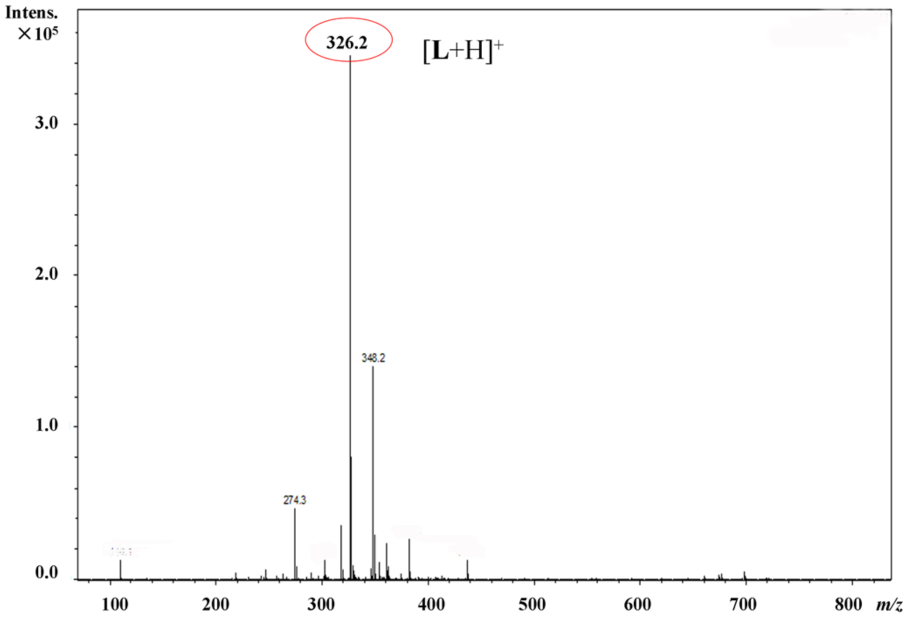


Fig. S11 Fluorescence changes at 497 nm of **L** (10 μM) and **L**-Al^{3+} (10 equiv.) in aqueous solution at different pH scale.

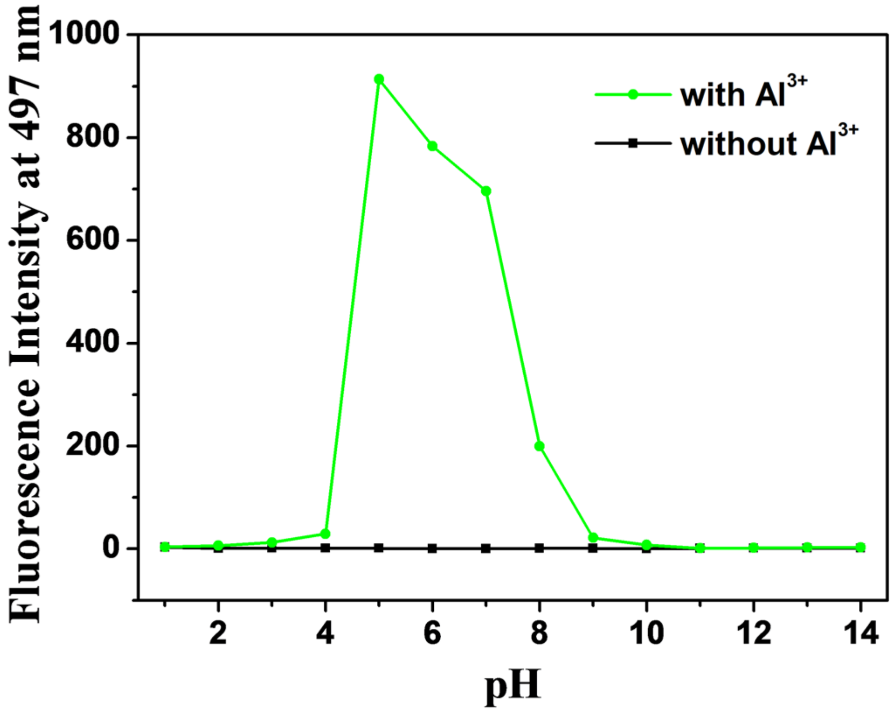


Table S1 Crystal data and structure refinement for **L**.

Empirical formula	$C_{21}H_{27}NO_2$
Formula weight	325.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a= 9.781(2) Å α=101.66(3)°
	b=10.651(2) Å β=90.36(3)°
	c= 20.744(4) Å γ=114.08(3)°
Volume	1922.8(7) $Å^3$
Z	4
Density (calculated)	1.124 g cm^{-1}
Absorption coefficient	0.071 mm^{-1}
Crystal size	0.13 × 0.12 × 0.11 mm^3
Reflections collected	10917
Independent reflected	6731 [R(int) = 0.0885]
Data/restrains/parameters	6731 / 0 / 445
Goodness-of-fit on F^2	0.981
final *R* indices [$I>2(I)$]	R_1= 0.0605, wR_2=0.0925
R indices (all data)	R_1= 0.2117, wR_2=0.1188
Largest diff. peak and hole	0.258 and -0.215 e $Å^{-3}$

Table S2 Bond lengths [Å] and angles [deg] for **L.**

C(1)-O(1)	**1.345(4)**
C(1)-C(6)	**1.415(5)**
C(1)-C(2)	**1.417(5)**
C(2)-C(3)	**1.368(5)**
C(2)-C(14)	**1.548(5)**
C(3)-C(4)	**1.410(5)**
C(4)-C(5)	**1.380(5)**
C(4)-C(18)	**1.515(6)**
C(5)-C(6)	**1.361(5)**
C(6)-C(7)	**1.440(5)**
C(7)-N(1)	**1.263(5)**
C(8)-C(13)	**1.358(5)**
C(8)-C(9)	**1.396(5)**
C(8)-N(1)	**1.427(5)**
C(9)-C(10)	**1.389(6)**
C(10)-C(11)	**1.360(6)**
C(11)-C(12)	**1.408(6)**
C(12)-C(13)	**1.379(5)**
C(13)-O(2)	**1.390(5)**
C(14)-C(17)	**1.524(5)**
C(14)-C(15)	**1.526(6)**
C(14)-C(16)	**1.528(5)**
C(18)-C(20)	**1.461(6)**
C(18)-C(19)	**1.519(6)**
C(18)-C(21)	**1.563(7)**
C(22)-O(3)	**1.369(4)**
C(22)-C(23)	**1.374(5)**
C(22)-C(27)	**1.398(5)**
C(23)-C(24)	**1.426(5)**
C(23)-C(28)	**1.430(5)**
C(24)-C(25)	**1.354(5)**
C(25)-C(26)	**1.392(5)**
C(25)-C(35)	**1.573(5)**
C(26)-C(27)	**1.408(5)**
C(27)-C(39)	**1.532(5)**
C(28)-N(2)	**1.289(4)**
C(29)-C(34)	**1.357(5)**
C(29)-N(2)	**1.409(4)**
C(29)-C(30)	**1.410(5)**
C(30)-C(31)	**1.357(5)**
C(30)-O(4)	**1.372(4)**
C(31)-C(32)	**1.358(5)**

C(32)-C(33)	**1.393(5)**
C(33)-C(34)	**1.373(5)**
C(35)-C(37)	**1.529(5)**
C(35)-C(38)	**1.529(5)**
C(35)-C(36)	**1.544(5)**
C(39)-C(41)	**1.536(5)**
C(39)-C(40)	**1.541(5)**
C(39)-C(42)	**1.550(5)**
O(1)-C(1)-C(6)	**120.7(4)**
O(1)-C(1)-C(2)	**117.9(4)**
C(6)-C(1)-C(2)	**121.4(4)**
C(3)-C(2)-C(1)	**114.8(4)**
C(3)-C(2)-C(14)	**122.8(4)**
C(1)-C(2)-C(14)	**122.3(4)**
C(2)-C(3)-C(4)	**125.7(4)**
C(5)-C(4)-C(3)	**116.6(4)**
C(5)-C(4)-C(18)	**121.2(4)**
C(3)-C(4)-C(18)	**122.2(4)**
C(6)-C(5)-C(4)	**121.7(4)**
C(5)-C(6)-C(1)	**119.8(4)**
C(5)-C(6)-C(7)	**118.0(4)**
C(1)-C(6)-C(7)	**122.2(4)**
N(1)-C(7)-C(6)	**123.5(4)**
C(13)-C(8)-C(9)	**119.6(4)**
C(13)-C(8)-N(1)	**118.2(4)**
C(9)-C(8)-N(1)	**122.2(4)**
C(10)-C(9)-C(8)	**119.7(5)**
C(11)-C(10)-C(9)	**120.8(5)**
C(10)-C(11)-C(12)	**119.1(5)**
C(13)-C(12)-C(11)	**119.8(5)**
C(8)-C(13)-C(12)	**120.9(5)**
C(8)-C(13)-O(2)	**122.0(4)**
C(12)-C(13)-O(2)	**117.0(5)**
C(17)-C(14)-C(15)	**106.5(4)**
C(17)-C(14)-C(16)	**106.5(4)**
C(15)-C(14)-C(16)	**111.2(4)**
C(17)-C(14)-C(2)	**112.6(4)**
C(15)-C(14)-C(2)	**109.6(4)**
C(16)-C(14)-C(2)	**110.3(4)**
C(20)-C(18)-C(4)	**112.6(4)**
C(20)-C(18)-C(19)	**111.8(5)**
C(4)-C(18)-C(19)	**112.6(4)**
C(20)-C(18)-C(21)	**108.7(5)**

C(4)-C(18)-C(21)	**107.1(5)**
C(19)-C(18)-C(21)	**103.4(5)**
O(3)-C(22)-C(23)	**119.3(4)**
O(3)-C(22)-C(27)	**120.0(4)**
C(23)-C(22)-C(27)	**120.7(4)**
C(22)-C(23)-C(24)	**119.0(4)**
C(22)-C(23)-C(28)	**120.9(4)**
C(24)-C(23)-C(28)	**119.4(4)**
C(25)-C(24)-C(23)	**123.0(4)**
C(24)-C(25)-C(26)	**115.8(4)**
C(24)-C(25)-C(35)	**123.8(4)**
C(26)-C(25)-C(35)	**120.0(4)**
C(25)-C(26)-C(27)	**124.5(4)**
C(22)-C(27)-C(26)	**116.9(4)**
C(22)-C(27)-C(39)	**121.1(4)**
C(26)-C(27)-C(39)	**122.0(4)**
N(2)-C(28)-C(23)	**125.9(4)**
C(34)-C(29)-N(2)	**122.4(4)**
C(34)-C(29)-C(30)	**119.0(4)**
N(2)-C(29)-C(30)	**118.6(4)**
C(31)-C(30)-O(4)	**117.1(4)**
C(31)-C(30)-C(29)	**121.2(4)**
O(4)-C(30)-C(29)	**121.8(4)**
C(30)-C(31)-C(32)	**119.8(5)**
C(31)-C(32)-C(33)	**119.4(4)**
C(34)-C(33)-C(32)	**121.2(4)**
C(29)-C(34)-C(33)	**119.4(4)**
C(37)-C(35)-C(38)	**110.7(4)**
C(37)-C(35)-C(36)	**106.6(4)**
C(38)-C(35)-C(36)	**109.7(4)**
C(37)-C(35)-C(25)	**111.3(3)**
C(38)-C(35)-C(25)	**108.3(3)**
C(36)-C(35)-C(25)	**110.3(4)**
C(27)-C(39)-C(41)	**109.4(4)**
C(27)-C(39)-C(40)	**109.9(3)**
C(41)-C(39)-C(40)	**111.0(3)**
C(27)-C(39)-C(42)	**111.2(3)**
C(41)-C(39)-C(42)	**108.5(3)**
C(40)-C(39)-C(42)	**106.8(4)**
C(7)-N(1)-C(8)	**119.5(4)**
C(28)-N(2)-C(29)	**119.1(3)**