SUPPLEMENTARY MATERIAL

A highly selective fluorescent sensor for detection of trivalent metal ions based on a simple Schiff-base

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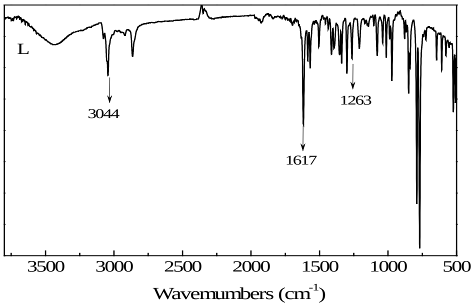

Figure 1S. *FT- IR spectrum of the sensor L*

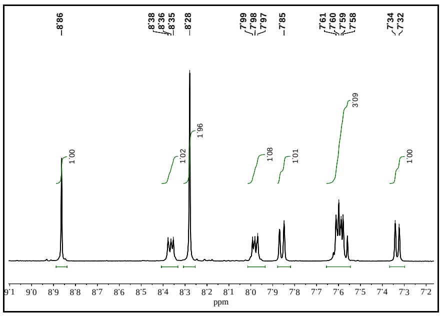

Figure 2S. *^{1}H-NMR spectrum of the sensor L*

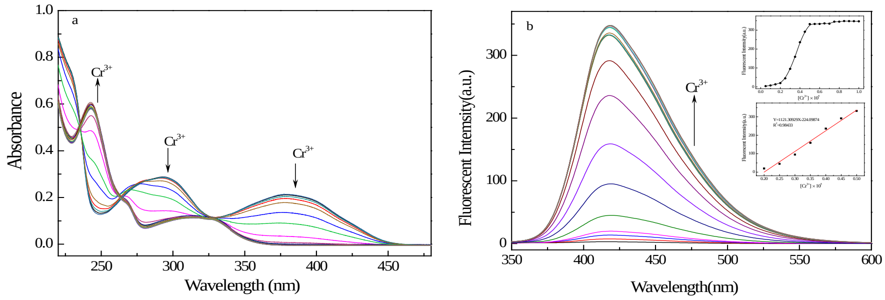

Figure 3S. *(a) UV-vis absorbance spectra and (b) Fluorescence spectra (λ_{ex}=327 nm) of sensor* ***L*** *(10 μmol L^{-1}) with gradual addition of Cr^{3+} in ethanol solution (0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95, 1.0 equiv)*

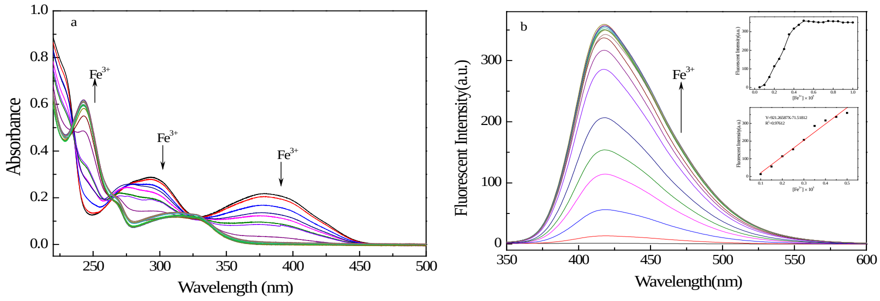

Figure 4S. *(a) UV-vis absorbance spectra and (b) Fluorescence spectra (λ_{ex}=327 nm) of sensor* ***L*** *(10 μM) with gradual addition of Fe^{3+} in ethanol solution (0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95, 1.0 equiv)*

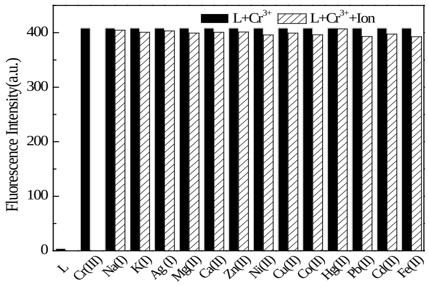

Figure 5S. *The selectivity of sensor* ***L*** *for Cr^{3+} in the presence of other metal ions in ethanol solution (λ_{ex}=327 nm). The response is normalized with respect to background fluorescence of the free sensor* ***L*** *(10 μmol L^{-1}), Cr^{3+} (10 μmol L^{-1}) is added at first, then other metal ions were added (10 μmol L^{-1})*

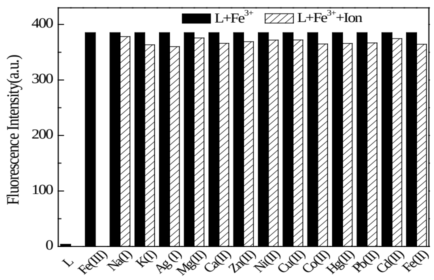

Figure 6S. *The selectivity of sensor* ***L*** *for Fe^{3+} in the presence of other metal ions in ethanol solution (λ_{ex}=327 nm). The response is normalized with respect to background fluorescence of the free sensor* ***L*** *(10 μmol L^{-1}), Fe^{3+} (10 μmol L^{-1}) is added at first, then other metal ions were added (10 μmol L^{-1})*

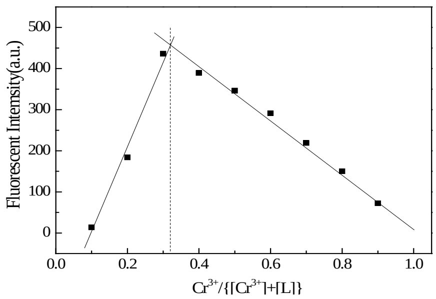

Figure 7S. *Job's plot according to the method for continuous variations, indication the 2:1 stoichiometry for **L**-Cr^{3+} (the total concentration of **L** and Cr^{3+} is 20 μM) (λ_{ex}=327 nm)*

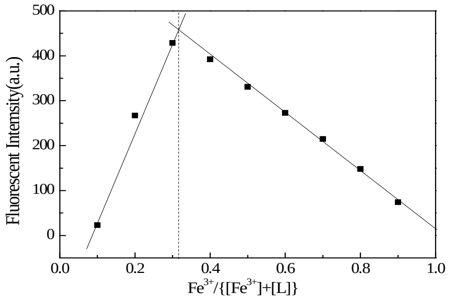

Figure 8S. *Job's plot according to the method for continuous variations, indication the 2:1 stoichiometry for **L**-Fe^{3+} (the total concentration of **L** and Fe^{3+} is 20 μmol L^{-1}) (λ_{ex}=327 nm)*

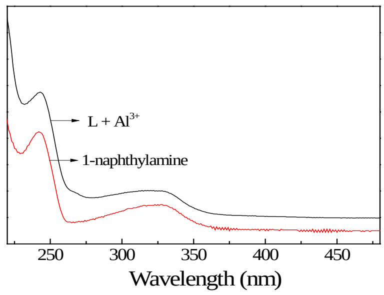

Figure 9S. *UV-vis absorbance spectra of 1-naphthylamine, sensor **L** in the presence of Al^{3+}*

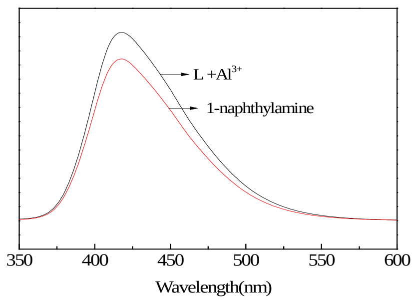

Figure 10S. *Fluorescence spectra (λ_{ex}=327 nm) of 1-naphthylamine, sensor **L** in the presence of Al^{3+}*

Table 1S. Crystallographic data for the sensor **L**

Formula	$C_{28}H_{20}N_2$
M_r	384.46
Crystal system	Monoclinic
Space group	$P2_1/c$
Crystal color	Yellow
a, Å	11.834(5)
b, Å	7.181(3)
c, Å	24.082(9)
α, deg	90
β, deg	98.508(7)
γ, deg	90
V, Å^3	2024.0(14)
Z	4
D_{calcd}, g cm^{-3}	1.262
F(000), e	808.0
Param. refined	272
$R(F)/wR(F^2)^a$ (all refl.)	0.0776/0.1154
μ(MoK_α), cm^{-1}	0.74
GoF $(F^2)^b$	1.019

Table 2S. Crystal data of the sensor **L**

Formula	$C_{28}H_{20}N_2$
Formula Weight	384.46
Crystal System	Monoclinic
Space group	$P2_1/c$ (No. 14)
a, b, c [Angstrom]	11.834(5) 7.181(3) 24.082(9)
alpha, beta, gamma [deg]	90 98.508(7) 90
Z	4
D(calc) [g/cm^3]	1.262
Mu(MoKa) [/mm]	0.074
F(000)	808.0
Crystal Size [mm]	0.37 x 0.37 x 0.30
Temperature (K)	296
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.71, 26.00
Dataset	-14: 12 ; -7: 8 ; -29: 29
Tot., Uniq. Data, R(int)	10679, 3969, 0.0395
Observed Data [I > 2.0 sigma(I)]	2513
Nref, Npar	3969, 272
R, wR_2, S	0.0776, 0.1154, 1.019
$w=1/[\sigma^2(F_o^2)+(0.0495P)^2+0.0795P]$	where $P=(F_o^2+2F_c^2)/3$
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.145, 0.149

Table 3S. Bond distances (Angstrom) of the sensor **L**

Bond Distances (Angstrom)			
N(1)-C(12)	1.272(2)	N(2)-C(6)	1.2754(19)
N(1)-C(4)	1.4149(19)	N(2)-C(10)	1.4201(19)
C(3)-C(23)	1.414(2)	C(6)-C(7)	1.464(2)
C(3)-C(5)	1.419(2)	C(6)-H(6)	0.9300
C(3)-C(4)	1.429(2)	C(7)-C(13)	1.391(2)
C(4)-C(16)	1.369(2)	C(7)-C(8)	1.393(2)
C(5)-C(24)	1.414(2)	C(8)-C(13)#2	1.376(2)
C(5)-C(9)	1.416(2)	C(8)-H(8)	0.9300
C(9)-C(19)	1.352(2)	C(10)-C(21)	1.371(2)
C(9)-H(9)	0.9300	C(10)-C(15)	1.429(2)
C(11)-C(18)	1.376(2)	C(13)-C(8)#2	1.376(2)
C(11)-C(14)	1.392(2)	C(13)-H(13)	0.9300
C(11)-H(11)	0.9300	C(15)-C(27)	1.410(2)
C(12)-C(14)	1.463(2)	C(15)-C(17)	1.421(2)
C(12)-H(12)	0.9300	C(17)-C(25)	1.411(3)
C(14)-C(18)#1	1.391(2)	C(17)-(26)	1.419(3)
C(16)-C(19)	1.400(2)	C(21)-C(28)	1.403(2)
C(16)-H(16)	0.9300	C(21)-H(21)	0.9300
C(18)-C(14)#1	1.391(2)	C(25)-(28)	1.357(3)
C(18)-H(18)	0.9300	C(25)-H(25)	0.9300
C(19)-H(19)	0.9300	C(26)-C(29)	1.355(3)
C(20)-C(24)	1.356(2)	C(26)-H(26)	0.9300
C(20)-C(22)	1.398(2)	C(27)-C(30)	1.363(2)
C(20)-H(20)	0.9300	C(27)-H(27)	0.9300
C(22)-C(23)	1.365(2)	C(28)-H(28)	0.9300
C(22)-H(22)	0.9300	C(29)-(30)	1.398(3)
C(23)-H(23)	0.9300	C(29)-(29)	0.9300
C(24)-H(24)	0.9300	C(30)-(30)	0.9300

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z #2 -x+2,-y+1,-z.

Table 4S. Bond angles (Degrees) of the sensor **L**

Bond Angles (Degrees)			
C(12)-N(1)-C(4)	119.18(14)	C(6)-N(2)-C(10)	118.30(14)
C(23)-C(3)-C(5)	118.65(15)	N(2)-C(6)-C(7)	123.16(15)
C(23)-C(3)-C(4)	122.77(14)	N(2)-C(6)-H(6)	118.4
C(5)-C(3)-C(4)	118.56(14)	C(7)-C(6)-H(6)	118.4
C(16)-C(4)-N(1)	122.53(15)	C(13)-C(7)-C(8)	118.18(14)
C(16)-C(4)-C(3)	119.93(14)	C(13)-C(7)-C(6)	119.66(15)
N(1)-C(4)-C(3)	117.47(13)	C(8)-C(7)-C(6)	122.13(14)
C(24)-C(5)-C(9)	122.51(15)	C(13)#2-C(8)-C(7)	120.61(15)
C(24)-C(5)-C(3)	118.50(15)	C(13)#2-C(8)-H(8)	119.7
C(9)-C(5)-C(3)	118.98(15)	C(7)-C(8)-H(8)	119.7
C(19)-C(9)-C(5)	121.17(15)	C(21)-C(10)-N(2)	121.92(16)
C(19)-C(9)-H(9)	119.4	C(21)-C(10)-C(15)	119.95(15)
C(5)-C(9)-H(9)	119.4	N(2)-C(10)-C(15)	117.87(14)
C(18)-C(11)-C(14)	120.91(16)	C(8)#2-C(13)-C(7)	121.21(15)
C(18)-C(11)-H(11)	119.5	C(8)#2-C(13)-H(13)	119.4
C(14)-C(11)-H(11)	119.5	C(7)-C(13)-H(13)	119.4
N(1)-C(12)-C(14)	122.31(16)	C(27)-C(15)-C(17)	118.89(17)
N(1)-C(12)-H(12)	118.8	C(27)-C(15)-C(10)	122.69(15)
C(14)-C(12)-H(12)	118.8	C(17)-C(15)-C(10)	118.42(16)
C(18)#1-C(14)-C(11)	118.56(15)	C(25)-C(17)-C(26)	122.33(17)
C(18)#1-C(14)-C(12)	121.58(16)	C(25)-C(17)-C(15)	119.39(17)
C(11)-C(14)-C(12)	119.86(15)	C(26)-C(17)-C(15)	118.28(18)
C(4)-C(16)-C(19)	121.05(15)	C(10)-C(21)-C(28)	120.93(18)
C(4)-C(16)-H(16)	119.5	C(10)-C(21)-H(21)	119.5

C(19)-C(16)-H(16)	119.5	C(28)-C(21)-H(21)	119.5
C(11)-C(18)-C(14)#1	120.53(16)	C(28)-C(25)-C(17)	120.88(17)
C(11)-C(18)-H(18)	119.7	C(28)-C(25)-H(25)	119.6
C(14)#1-C(18)-H(18)	119.7	C(17)-C(25)-H(25)	119.6
C(9)-C(19)-C(16)	120.30(16)	C(29)-C(26)-C(17)	121.21(18)
C(9)-C(19)-H(19)	119.9	C(29)-C(26)-H(26)	119.4
C(16)-C(19)-H(19)	119.9	C(17)-C(26)-H(26)	119.4
C(24)-C(20)-C(22)	120.23(16)	C(30)-C(27)-C(15)	120.72(17)
C(24)-C(20)-H(20)	119.9	C(30)-C(27)-H(27)	119.6
C(22)-C(20)-H(20)	119.9	C(15)-C(27)-H(27)	119.6
C(23)-C(22)-C(20)	120.42(17)	C(25)-C(28)-C(21)	120.40(18)
C(23)-C(22)-H(22)	119.8	C(25)-C(28)-H(28)	119.8
C(20)-C(22)-H(22)	119.8	C(21)-C(28)-H(28)	119.8
C(22)-C(23)-C(3)	120.86(16)	C(26)-C(29)-C(30)	120.20(19)
C(22)-C(23)-H(23)	119.6	C(26)-C(29)-H(29)	119.9
C(3)-C(23)-H(23)	119.6	C(30)-C(29)-H(29)	119.9
C(20)-C(24)-C(5)	121.34(16)	C(27)-C(30)-C(29)	120.69(19)
C(20)-C(24)-H(24)	119.3	C(27)-C(30)-H(30)	119.7
C(5)-C(24)-H(24)	119.3	C(29)-C(30)-H(30)	119.7

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z #2 -x+2,-y+1,-z.