Supporting Information

A new multifunctional Schiff base as fluorescence sensor for Al^{3+} and colorimetric sensor for CN^- in aqueous media: application to bioimaging

Seul Ah Lee,[a] Ga Rim You,[a] Ye Won Choi,[a] Hyun Yong Jo,[a] Ah Ram Kim,[b] Insup Noh,[b] Sung-Jin Kim,[c] Youngmee Kim,[c] Cheal Kim[a]*

[a]*Department of Fine Chemistry and Department of Interdisciplinary Bio IT Materials, Seoul National University of Science and Technology, Seoul 139-743, Korea. Fax: +82-2-973-9149; Tel: +82-2-970-6693; E-mail: cheалkim@seoultech.ac.kr*

[b]*Department of Chemical Engineering, Seoul National University of Science & Technology, Seoul 139-743, Korea.*

[c]*Department of Chemistry and Nano Science, Ewha Womans University, Seoul 120-750, Korea.*

Table S1. Bond lengths [Å] and angles [°] for **1**.

C(1)-C(2)	1.384(4)
C(1)-C(6)	1.394(4)
C(1)-C(7)	1.492(4)
C(2)-C(3)	1.382(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.364(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.384(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.392(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.240(3)
C(7)-N(1)	1.342(4)
C(8)-N(2)	1.295(4)
C(8)-C(9)	1.433(4)
C(8)-H(8)	0.9500
C(9)-C(19)	1.403(4)
C(9)-C(10)	1.405(4)
C(10)-O(2)	1.368(3)
C(10)-C(11)	1.390(4)
C(11)-C(20)	1.414(4)
C(11)-C(12)	1.500(4)
C(12)-C(13)	1.5388(19)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.502(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-N(3)	1.456(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-N(3)	1.453(4)

C(15)-C(16)	1.500(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.5368(19)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.501(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.377(4)
C(18)-C(20)	1.421(4)
C(19)-H(19)	0.9500
C(20)-N(3)	1.384(4)
N(1)-N(2)	1.395(3)
N(1)-H(1N)	0.94(3)
O(2)-H(2A)	0.8400

C(2)-C(1)-C(6)	118.4(3)
C(2)-C(1)-C(7)	117.9(3)
C(6)-C(1)-C(7)	123.6(3)
C(3)-C(2)-C(1)	120.7(4)
C(3)-C(2)-H(2)	119.6
C(1)-C(2)-H(2)	119.6
C(4)-C(3)-C(2)	121.0(4)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	119.5(3)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	120.0(4)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.4(3)
C(5)-C(6)-H(6)	119.8
C(1)-C(6)-H(6)	119.8

O(1)-C(7)-N(1)	121.4(3)
O(1)-C(7)-C(1)	121.6(3)
N(1)-C(7)-C(1)	116.9(3)
N(2)-C(8)-C(9)	122.2(3)
N(2)-C(8)-H(8)	118.9
C(9)-C(8)-H(8)	118.9
C(19)-C(9)-C(10)	117.0(3)
C(19)-C(9)-C(8)	119.6(3)
C(10)-C(9)-C(8)	123.2(3)
O(2)-C(10)-C(11)	117.1(3)
O(2)-C(10)-C(9)	120.4(3)
C(11)-C(10)-C(9)	122.5(3)
C(10)-C(11)-C(20)	118.3(3)
C(10)-C(11)-C(12)	119.7(3)
C(20)-C(11)-C(12)	121.9(3)
C(11)-C(12)-C(13)	111.2(3)
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12B)	109.4
C(13)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0
C(14)-C(13)-C(12)	109.8(3)
C(14)-C(13)-H(13A)	109.7
C(12)-C(13)-H(13A)	109.7
C(14)-C(13)-H(13B)	109.7
C(12)-C(13)-H(13B)	109.7
H(13A)-C(13)-H(13B)	108.2
N(3)-C(14)-C(13)	111.4(3)
N(3)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14A)	109.3
N(3)-C(14)-H(14B)	109.3
C(13)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
N(3)-C(15)-C(16)	111.3(3)
N(3)-C(15)-H(15A)	109.4

C(16)-C(15)-H(15A)	109.4
N(3)-C(15)-H(15B)	109.4
C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(15)-C(16)-C(17)	109.3(3)
C(15)-C(16)-H(16A)	109.8
C(17)-C(16)-H(16A)	109.8
C(15)-C(16)-H(16B)	109.8
C(17)-C(16)-H(16B)	109.8
H(16A)-C(16)-H(16B)	108.3
C(18)-C(17)-C(16)	109.7(3)
C(18)-C(17)-H(17A)	109.7
C(16)-C(17)-H(17A)	109.7
C(18)-C(17)-H(17B)	109.7
C(16)-C(17)-H(17B)	109.7
H(17A)-C(17)-H(17B)	108.2
C(19)-C(18)-C(20)	118.0(3)
C(19)-C(18)-C(17)	121.4(3)
C(20)-C(18)-C(17)	120.6(3)
C(18)-C(19)-C(9)	123.3(3)
C(18)-C(19)-H(19)	118.3
C(9)-C(19)-H(19)	118.3
N(3)-C(20)-C(11)	119.7(3)
N(3)-C(20)-C(18)	119.5(3)
C(11)-C(20)-C(18)	120.8(3)
C(7)-N(1)-N(2)	119.2(3)
C(7)-N(1)-H(1N)	123(2)
N(2)-N(1)-H(1N)	118(2)
C(8)-N(2)-N(1)	115.0(3)
C(20)-N(3)-C(15)	121.7(3)
C(20)-N(3)-C(14)	120.1(3)
C(15)-N(3)-C(14)	116.3(3)
C(10)-O(2)-H(2A)	109.5

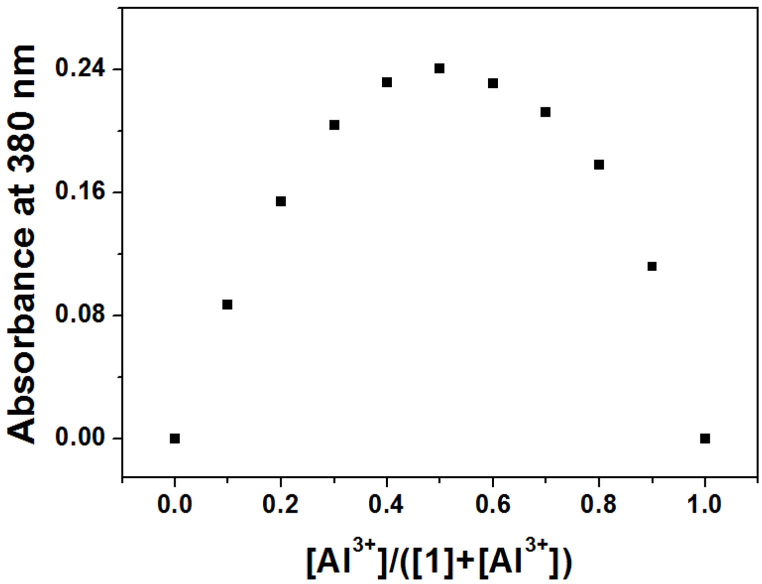

Fig. S1 Job plot for the binding of **1** with Al^{3+}. Absorbance at 380 nm was plotted as a function of the molar ratio $[Al^{3+}]/([\mathbf{1}] + [Al^{3+}])$. The total concentration of aluminum ions with receptor **1** was 1.0×10^{-5} M

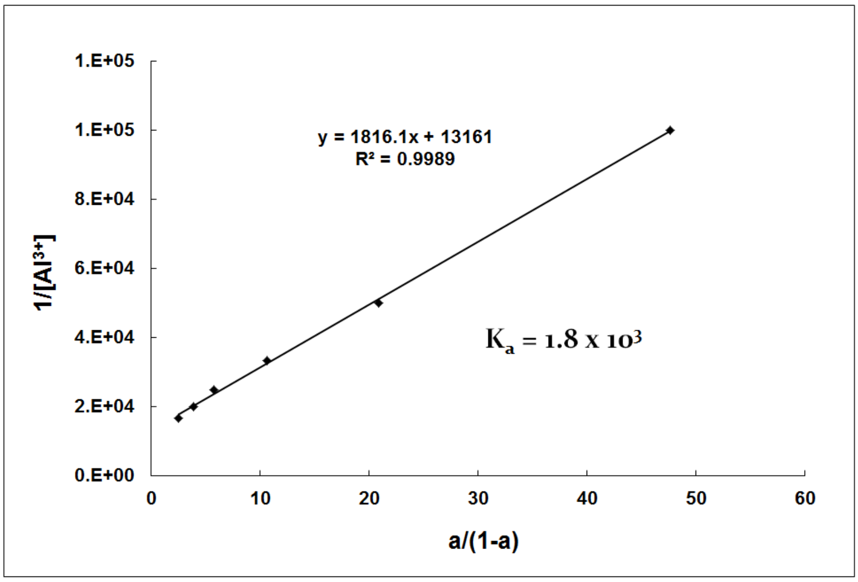

Fig. S2 Li plot (fluorescence intensity at 488 nm) of **1**, assuming a 1:1 stoichiometry for asso ciation between **1** and Al^{3+}.

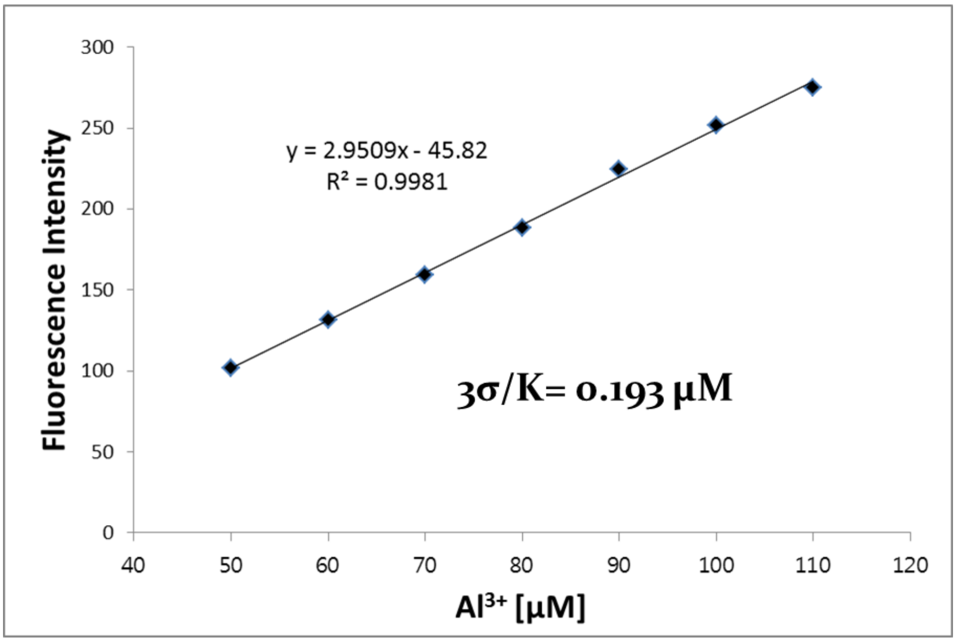

Fig. S3 Determination of the detection limit based on change in the ratio (fluorescence intensi ty at 488 nm) of **1** (10 μM) with Al^{3+}.

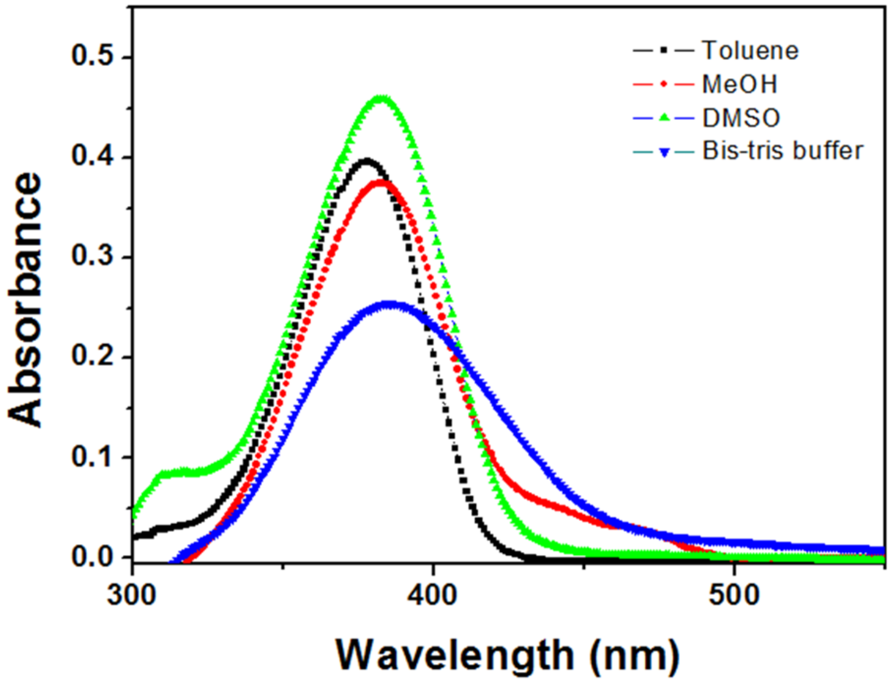

Fig. S4 Absorption spectra of **1** (30 μM) in various solvents.

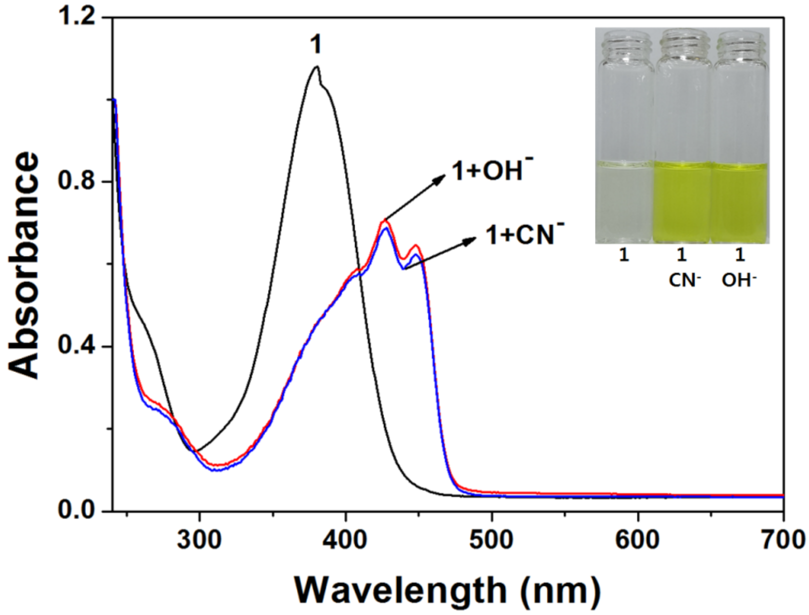

Fig. S5 Changes in the UV-vis spectra of receptor **1** (30 μM) upon addition of CN^- (200 equiv) and OH^- (tetrabutylammonium, 200 equiv), respectively, in bis-tris buffer/methanol (7/3, v/v).

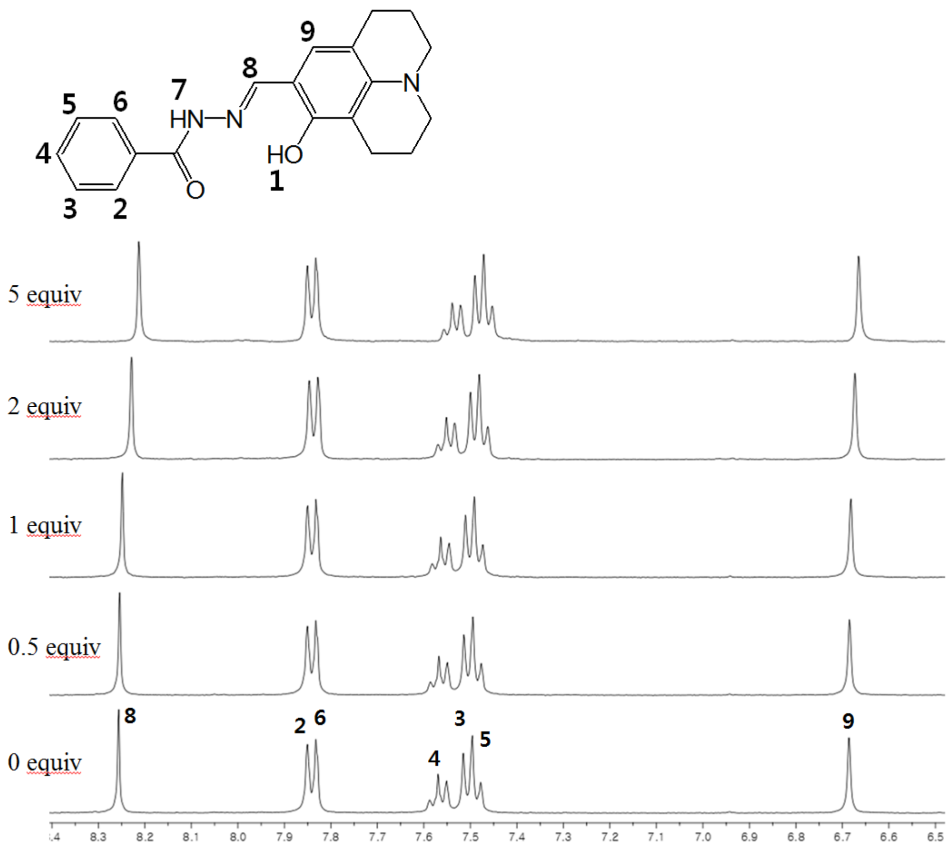

Fig. S6 [1]H NMR titration of **1** with CN^- in a mixture of DMSO-d_6 / D_2O (9:1, v/v)