Supplementary information

Fig. S1. ^{1}H NMR spectra (400 MHz) of **1o** measured in DMSO-d_6.

Fig. S2. ^{13}C NMR spectra (100 MHz) of **1o** measured in DMSO-d_6.

Fig. S3. Mass spectra of **1o**.

Fig. S4. Mass spectra of **1o** and CN^-.

Fig. S5. Mass spectra of **1o** and Al^{3+}.

Fig. S6. (A) Job's plot showing the 1:1 complex between CN^- and **1o**, (B) The association constant of **1o** with CN^- was calculated to be 1.8×10^5 L·mol^{-1}, (C) LOD for CN^- was 1.0×10^{-7} mol L^{-1}.

Table S1. Comparative study of analytical performance of **1o** with the recently reported sensors for CN^-.

Fig. S7. Frontier molecular orbital diagrams and energy gaps of **1o** and **1o**+Al^{3+}.

Fig. S8. (A) Job's plot showing the 1:1 complex between Al^{3+} and **1o**. (B) The association constant of **1O** with Al^{3+} was calculated to be 6.7×10^4 L mol^{-1} (C) LOD for Al^{3+} was 3.0×10^{-9} mol L^{-1}.

Table S2. Comparative study of analytical performance of **1o** with the recently reported sensors for Al^{3+}.

Table S3. Truth table for all possible strings of four binary-inputs data and the corresponding output digit of photochromic behavior of **1o**.

Table S4. Detection of Al^{3+} in natural water samples.

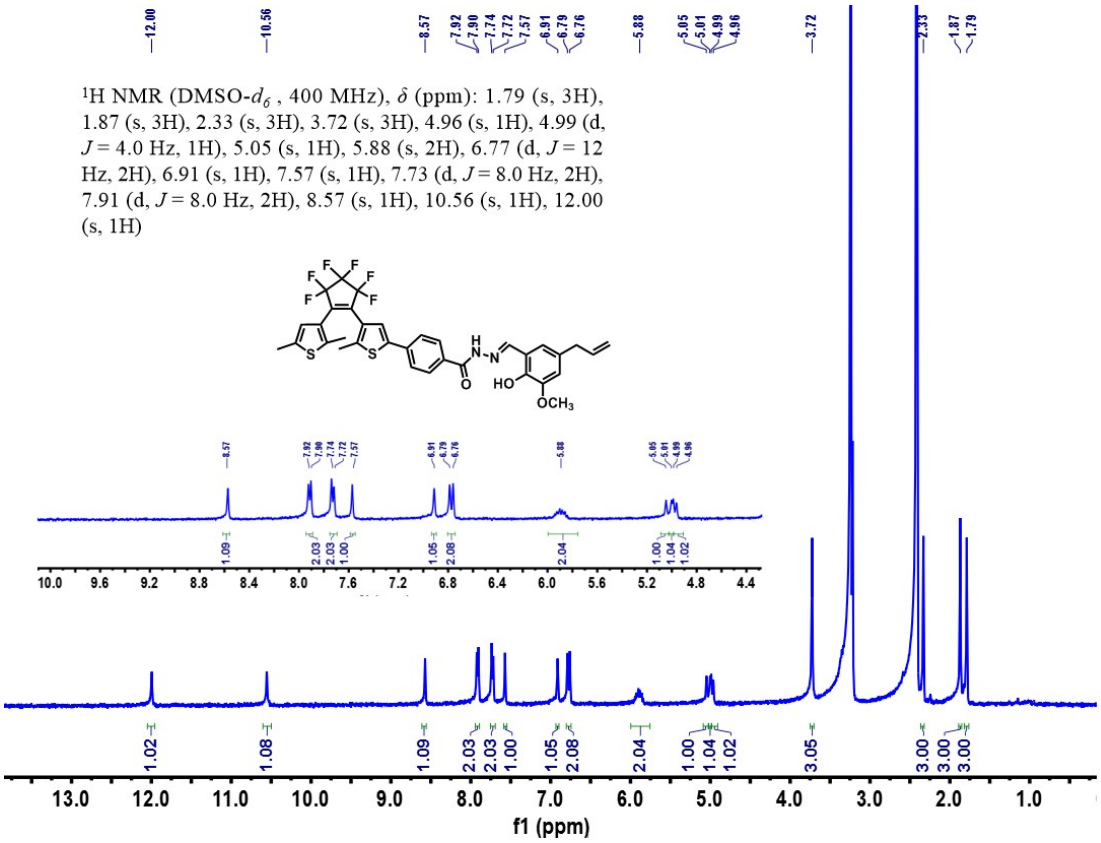

12.00
10.56
8.57
7.92
7.90
7.74
7.72
7.57
6.91
6.79
6.76
5.88
5.05
5.01
4.99
4.96
3.72
2.33
1.87
1.79
1H NMR (DMSO-d_6 , 400 MHz), δ (ppm): 1.79 (s, 3H), 1.87 (s, 3H), 2.33 (s, 3H), 3.72 (s, 3H), 4.96 (s, 1H), 4.99 (d, J = 4.0 Hz, 1H), 5.05 (s, 1H), 5.88 (s, 2H), 6.77 (d, J = 12 Hz, 2H), 6.91 (s, 1H), 7.57 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.91 (d, J = 8.0 Hz, 2H), 8.57 (s, 1H), 10.56 (s, 1H), 12.00 (s, 1H)
F
S
H
N
O
HO
OCH3
1.09
2.03
2.03
1.00
1.05
2.08
2.04
1.00
1.04
1.02
10.0
9.6
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
1.02
1.08
1.09
2.03
2.03
1.00
1.05
2.08
2.04
1.00
1.04
1.02
3.05
3.00
3.00
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)

Fig. S1

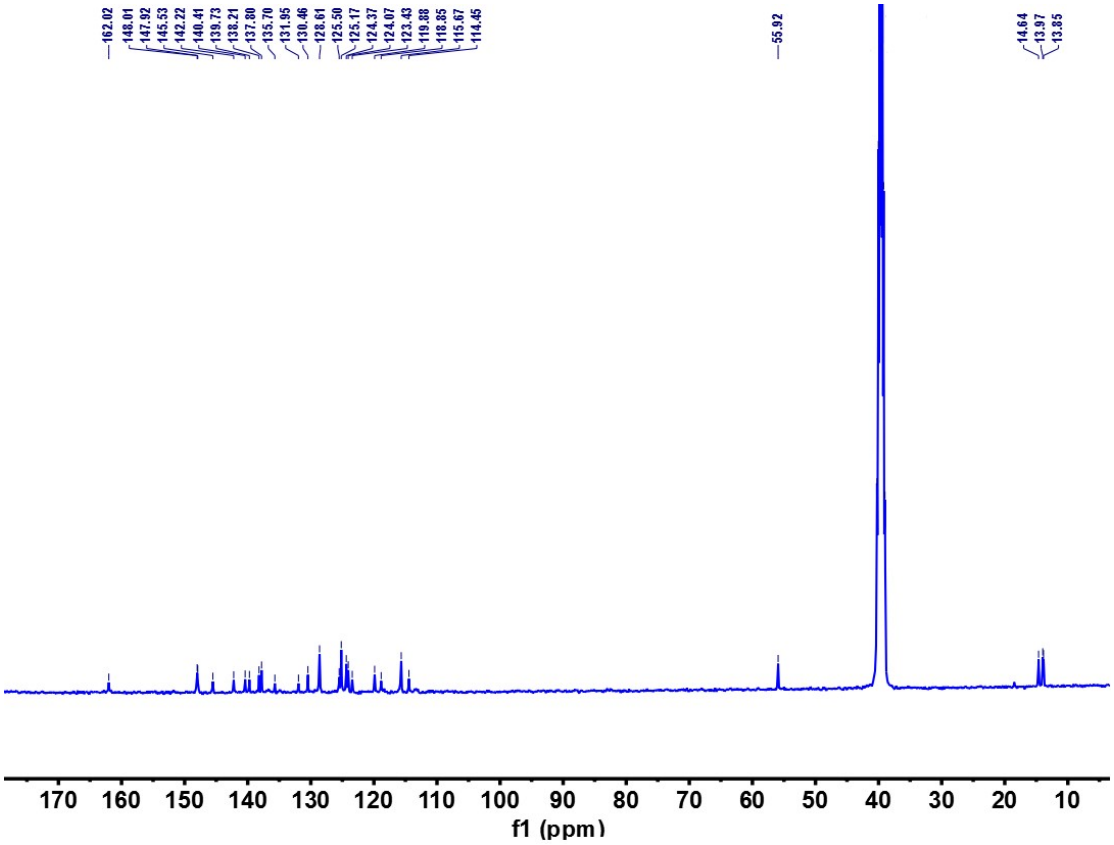

162.02
148.01
147.92
145.53
142.22
140.41
139.73
138.21
137.80
135.70
131.95
130.46
128.61
125.50
125.17
124.37
124.07
123.43
119.88
118.85
115.67
114.45
55.92
14.64
13.97
13.85
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

Fig. S2

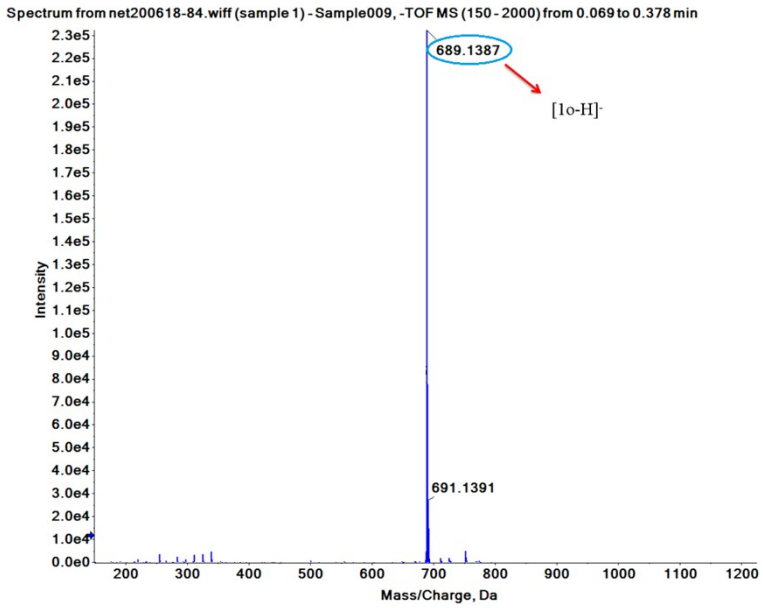

Spectrum from net200618-84.wiff (sample 1) - Sample009, -TOF MS (150 - 2000) from 0.069 to 0.378 min
689.1387
[1o-H]-
691.1391
Intensity
Mass/Charge, Da
2.3e5
2.2e5
2.1e5
2.0e5
1.9e5
1.8e5
1.7e5
1.6e5
1.5e5
1.4e5
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
200
300
400
500
600
700
800
900
1000
1100
1200

Fig. S3

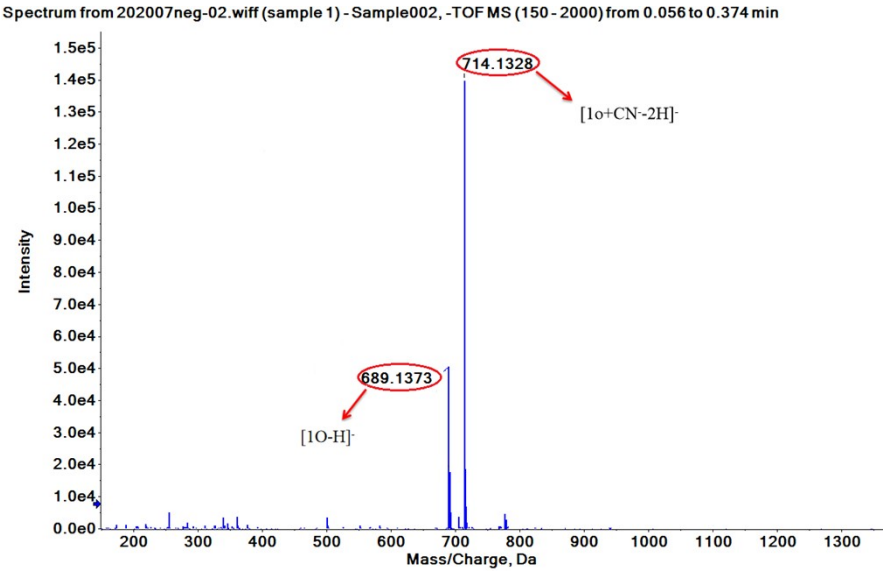

Spectrum from 202007neg-02.wiff (sample 1) - Sample002, -TOF MS (150 - 2000) from 0.056 to 0.374 min
Intensity
1.5e5
1.4e5
1.3e5
1.2e5
1.1e5
1.0e5
9.0e4
8.0e4
7.0e4
6.0e4
5.0e4
4.0e4
3.0e4
2.0e4
1.0e4
0.0e0
714.1328
[1o+CN-2H]-
689.1373
[1O-H]-
200
300
400
500
600
700
800
900
1000
1100
1200
1300
Mass/Charge, Da

Fig. S4

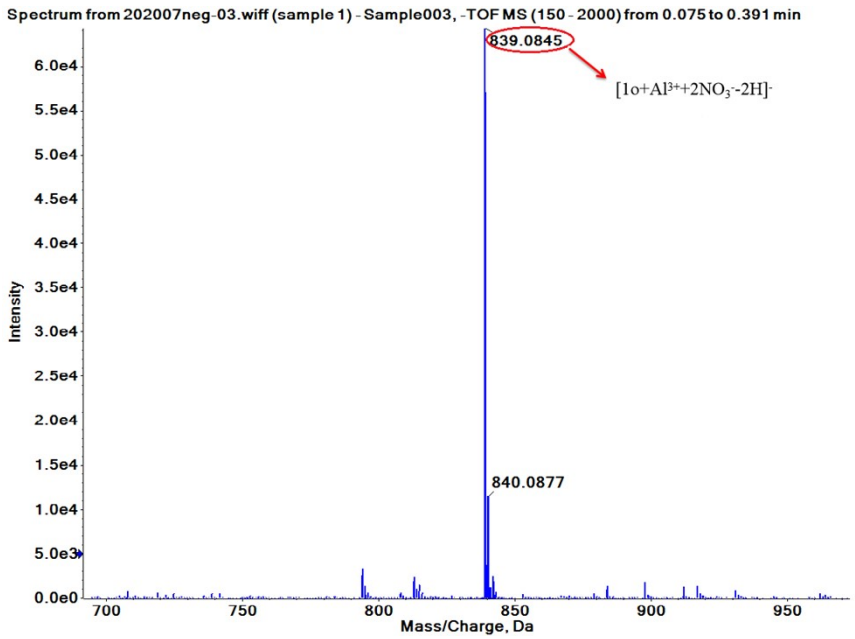

Spectrum from 202007neg-03.wiff (sample 1) - Sample003, -TOF MS (150 - 2000) from 0.075 to 0.391 min
839.0845
[1o+Al3++2NO3--2H]-
840.0877
Intensity
6.0e4
5.5e4
5.0e4
4.5e4
4.0e4
3.5e4
3.0e4
2.5e4
2.0e4
1.5e4
1.0e4
5.0e3
0.0e0
700
750
800
850
900
950
Mass/Charge, Da

Fig. S5

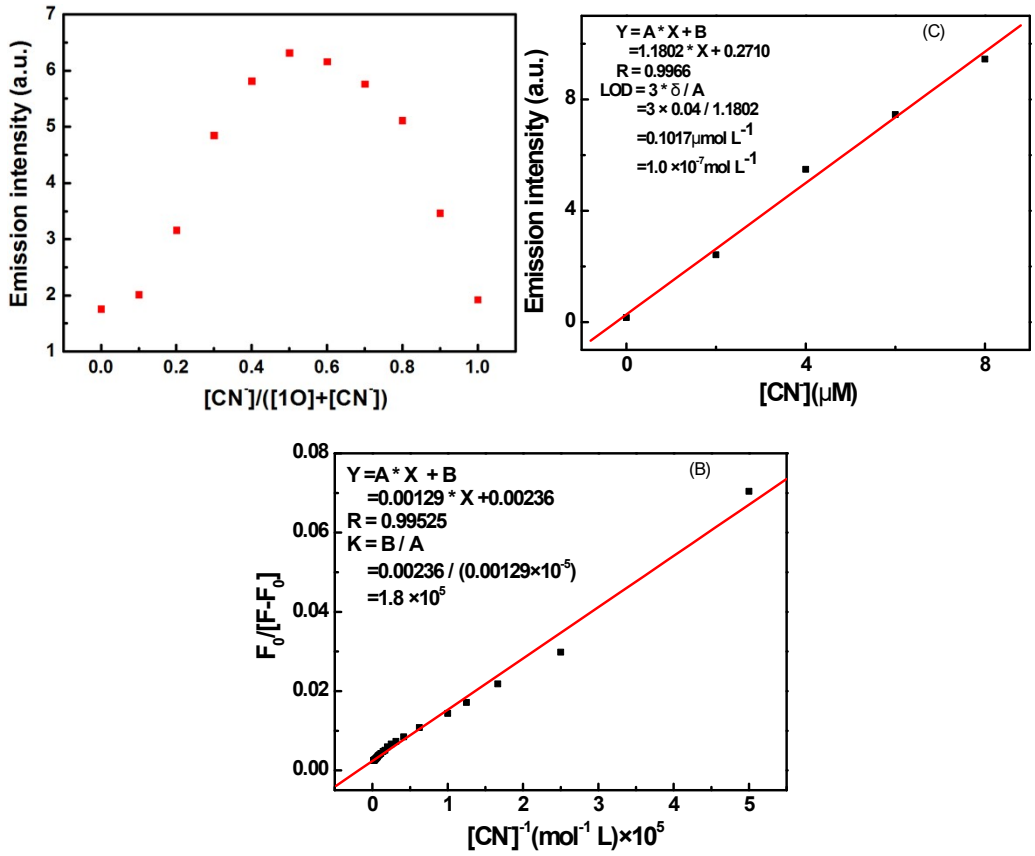

Emission intensity (a.u.)
[CN-]/([1O]+[CN-])
Y = A * X + B
=1.1802 * X + 0.2710
R = 0.9966
LOD = 3 * δ / A
=3 × 0.04 / 1.1802
=0.1017μmol L-1
=1.0 ×10-7mol L-1
(C)
[CN-](μM)
Y =A * X + B
=0.00129 * X +0.00236
R = 0.99525
K = B / A
=0.00236 / (0.00129×10-5)
=1.8 ×105
(B)
F0/[F-F0]
[CN]-1(mol-1 L)×105

Fig. S6

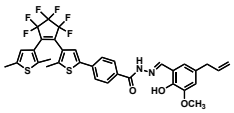
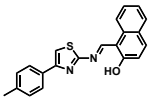
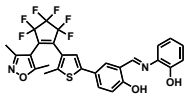
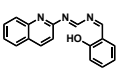
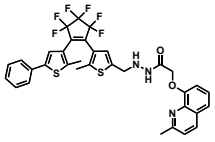
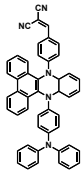
Structure	Media	Detectionlimit (mol L^{-1})	Association constant	Approaches	Ref.
	CH_3CN	1.0×10^{-7}	1.80×10^5	Colorimetric Fluorescent	Present work
	DMSO/bis-tris buffffer (1/1, v/v)	1.94×10^{-5}	NO	Colorimetric	65
	CH_3CN	7.145×10^{-7}	NO	Colorimetric Fluorescent	66
	DMSO/H2O (3/2, v/v)	4.5×10^{-7}	NO	Colorimetric Fluorescent	67
	CH_3CN	1.34×10^{-5}	NO	Colorimetric Fluorescent	68
	DMSO/H_2O (1:99, v/v)	1.12×10^{-6}	NO	Colorimetric Fluorescent	69

Table S1

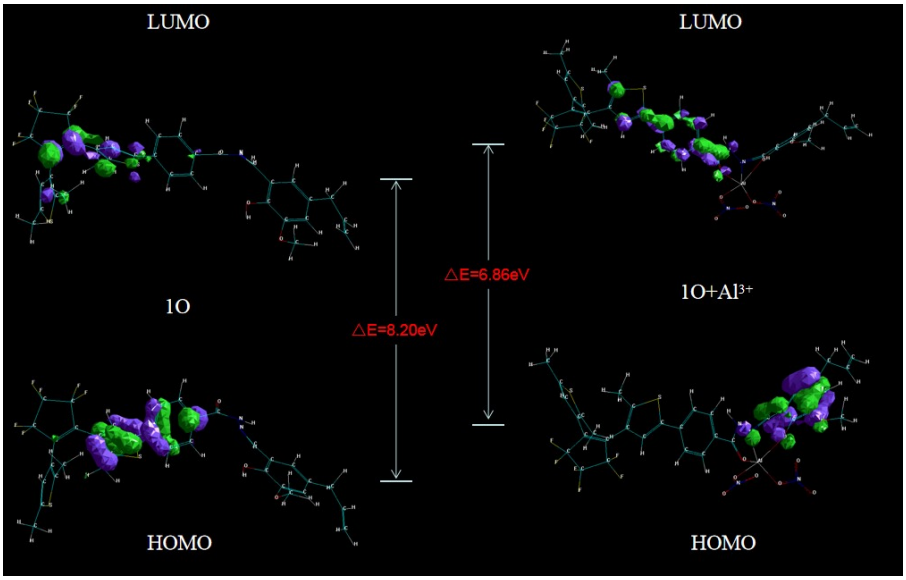


Fig. S7

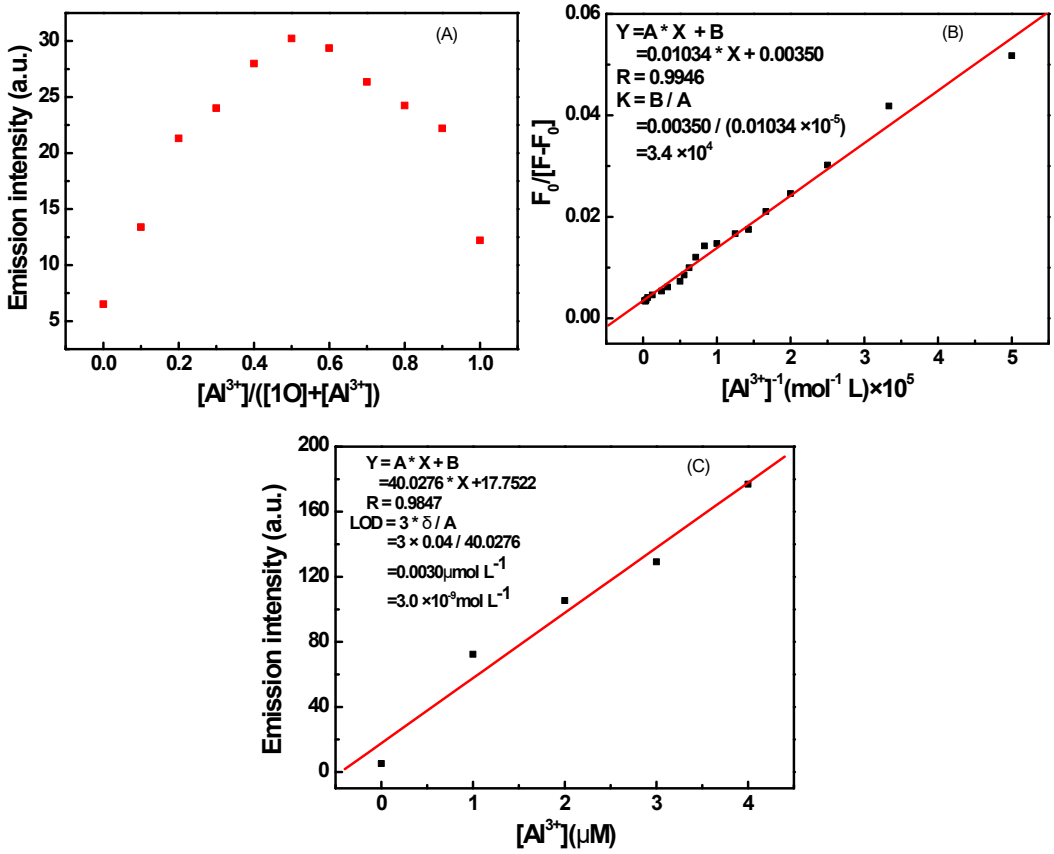

(A)
Emission intensity (a.u.)
[Al3+]/([1O]+[Al3+])
(B)
Y=A*X+B
=0.01034*X+0.00350
R=0.9946
K=B/A
=0.00350/(0.01034×10-5)
=3.4×104
F0/[F-F0]
[Al3+]-1(mol-1 L)×105
(C)
Y=A*X+B
=40.0276*X+17.7522
R=0.9847
LOD=3*δ/A
=3×0.04/40.0276
=0.0030μmol L-1
=3.0×10-9mol L-1
Emission intensity (a.u.)
[Al3+](μM)

Fig. S8

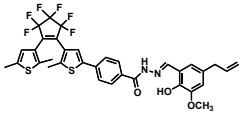
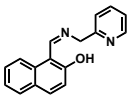
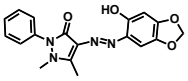
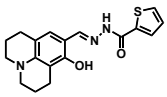
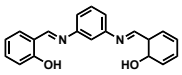
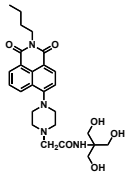
Structure	Media	Detectionlimit (mol L^{-1})	Association constant	Approaches	Ref.
	CH_3CN	3.0×10^{-9}	3.4×10^{4}	Fluorescent	Present work
	CH_3CN : H2O (3/7, v/v)	6.48×10^{-2}	1.0×10^{4}	Colorimetric Fluorescent	73
	MeOH : H_2O (1/1)	3.55×10^{-7}	5.42×10^{5}	Colorimetric Fluorescent	74
	CH_3CN	2.05×10^{-8}	6.35×10^{4}	Colorimetric Fluorescent	41
	MeOH	4.79×10^{-8}	1.41×10^{4}	Fluorescent	75
	MeOH	7.4×10^{-6}	7.60×10^{4}	Colorimetric Fluorescent	76

Table S2

Input				output[a]
In1 (UV)	In2 (Vis)	In3 (CN^-/Zn^{2+})	In4 (HCl/EDTA)	λ_{em} = 585/534 nm
0	0	0	0	0
0	0	0	1	0
0	0	1	0	1
0	1	1	0	1
0	1	1	1	0
1	0	0	0	0
1	1	0	0	0
1	1	1	0	1
1	0	1	0	0
1	0	0	1	0
1	0	1	1	0
1	1	1	1	0
1	1	0	1	0
0	1	0	1	0
0	0	1	1	0
0	1	0	0	0

[a] When the emission intensity at 585/534 nm more than 426-fold/351-fold of the original state, the output signal is defined as '1', otherwise defined as '0'.

Table S3

Sample	Al^{3+} added (uM)	Al^{3+} determined (uM)	Recovery (%)
Tap water	2.00	2.02	101
	4.00	4.12	103
	8.00	8.32	104
Ganjiang river	2.00	1.82	91
	4.00	3.72	93
	8.00	7.44	93

Table S4