Support Information for:

A triphenylamine-based colorimetric and "turn-on" fluorescent probe for live-cell detection of cyanide anion

Shaodan Wang,[a] Hai Xu,[a] Qingbiao Yang,[*a] Yan Song,[*b] and Yaoxian Li [a]

[a] *Department of Chemistry, Jilin University, Changchun 130021, P. R. China.*

Fax: +86-431-88499576; Tel: +86-431-88499576;

E-mail: yangqb@jlu.edu.cn.

[b] *College of Materials Science and Engineering, Jilin University of Chemical Technology, Jilin 132022, PR China. Fax: +86-432- 63083094;*

E-mail: songyan199809@163.com.

1、**Characterization of the compounds**

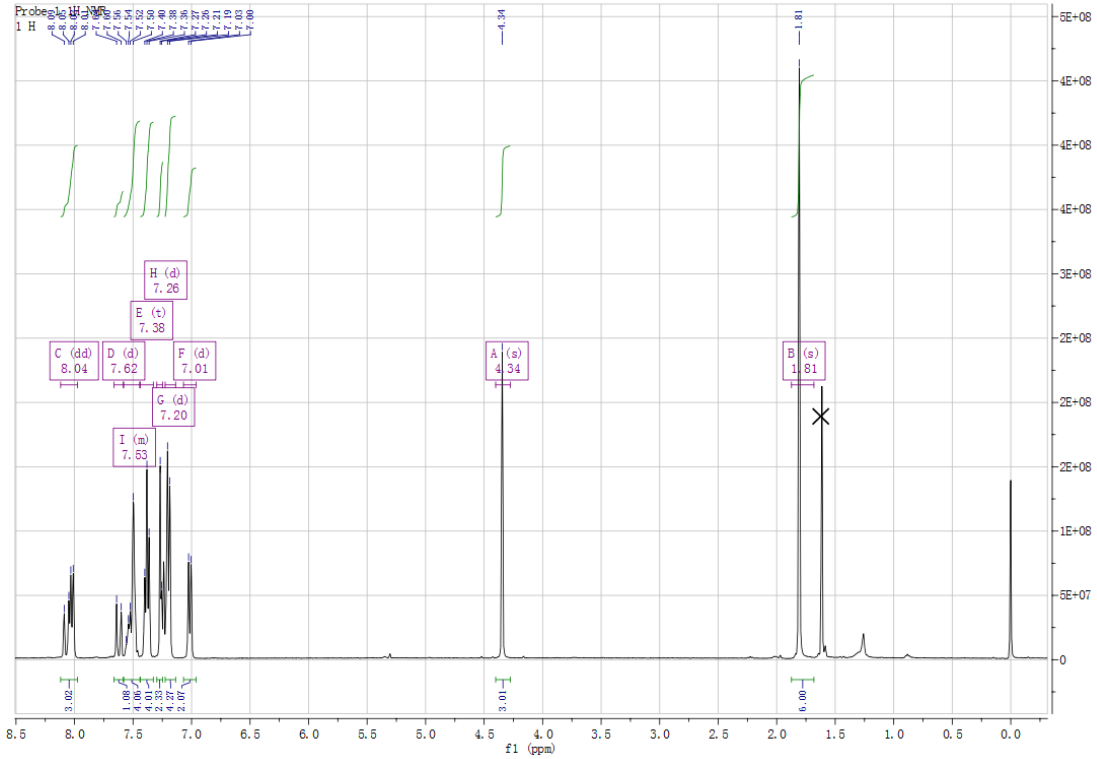

Fig. S1. ^{1}H NMR spectrum of probe **1** in $CDCl_3$.

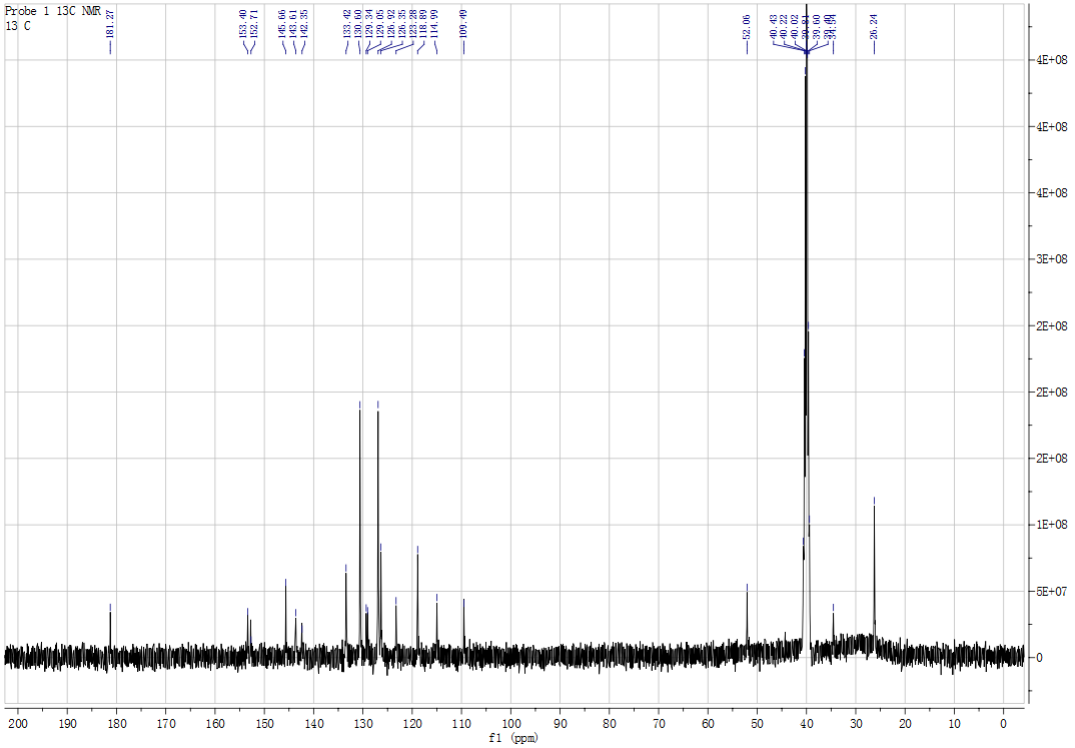

Fig. S2. ^{13}C NMR spectrum of probe **1** in DMSO-d6.

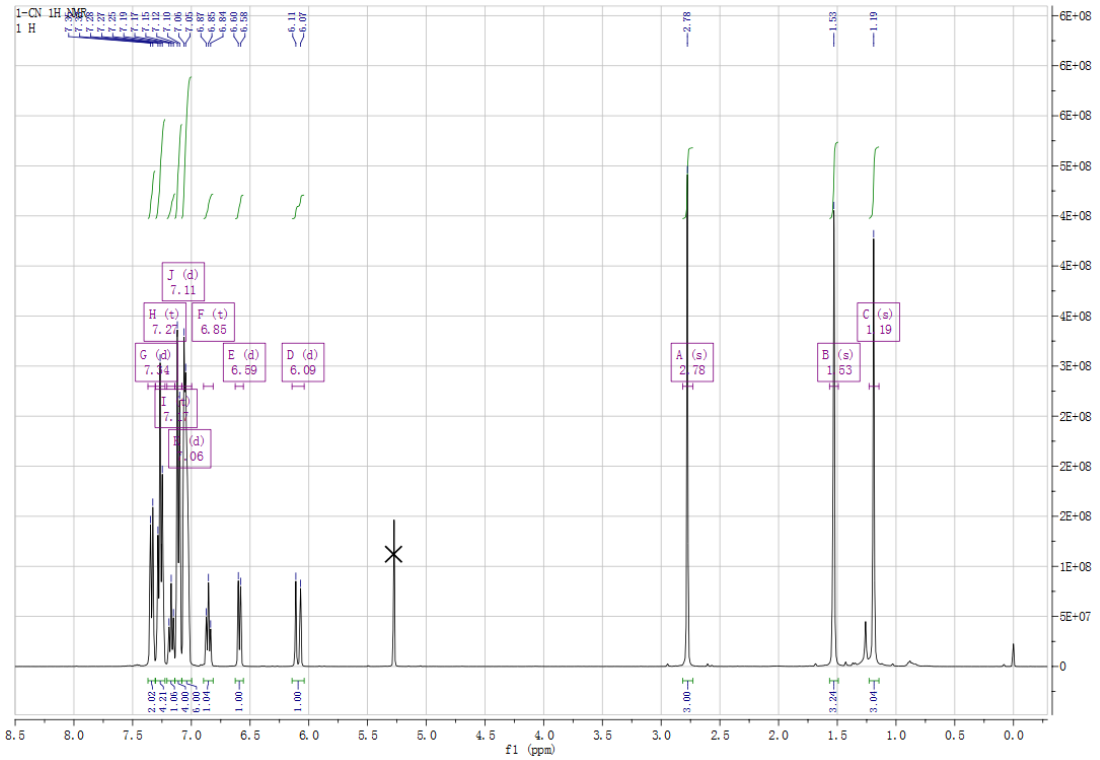

Fig. S3. ^{1}H NMR spectrum of **1-CN** in $CDCl_3$.

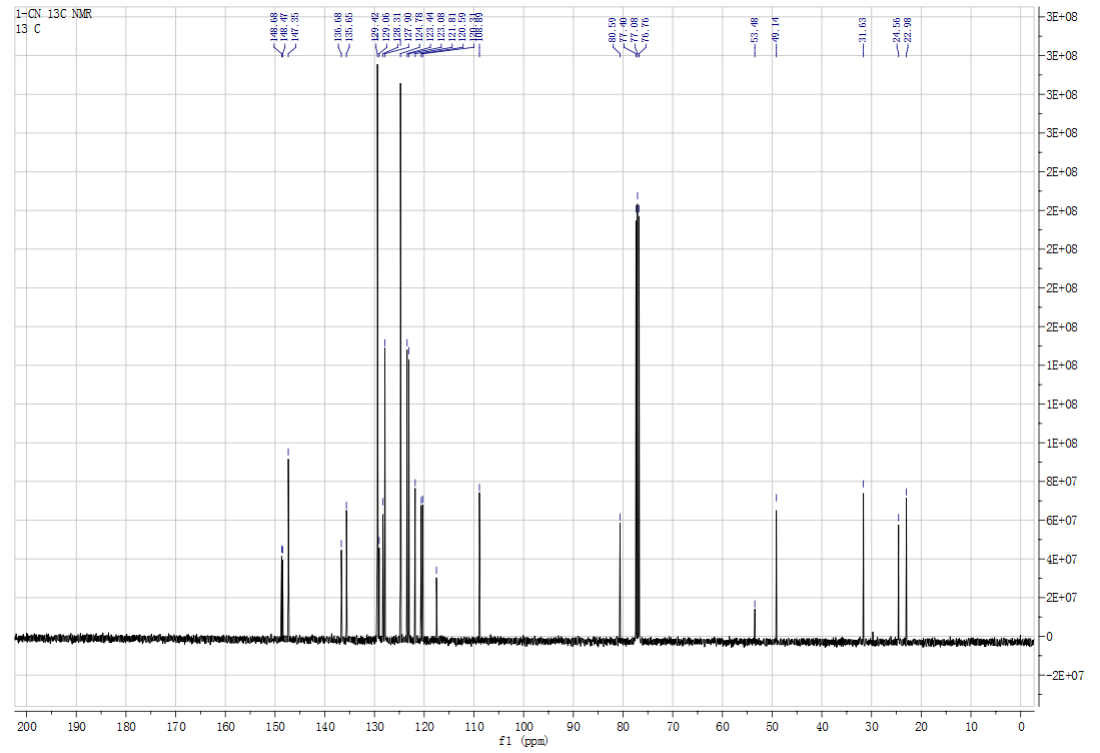

Fig. S4. ^{13}C NMR spectrum of **1-CN** in $CDCl_3$.

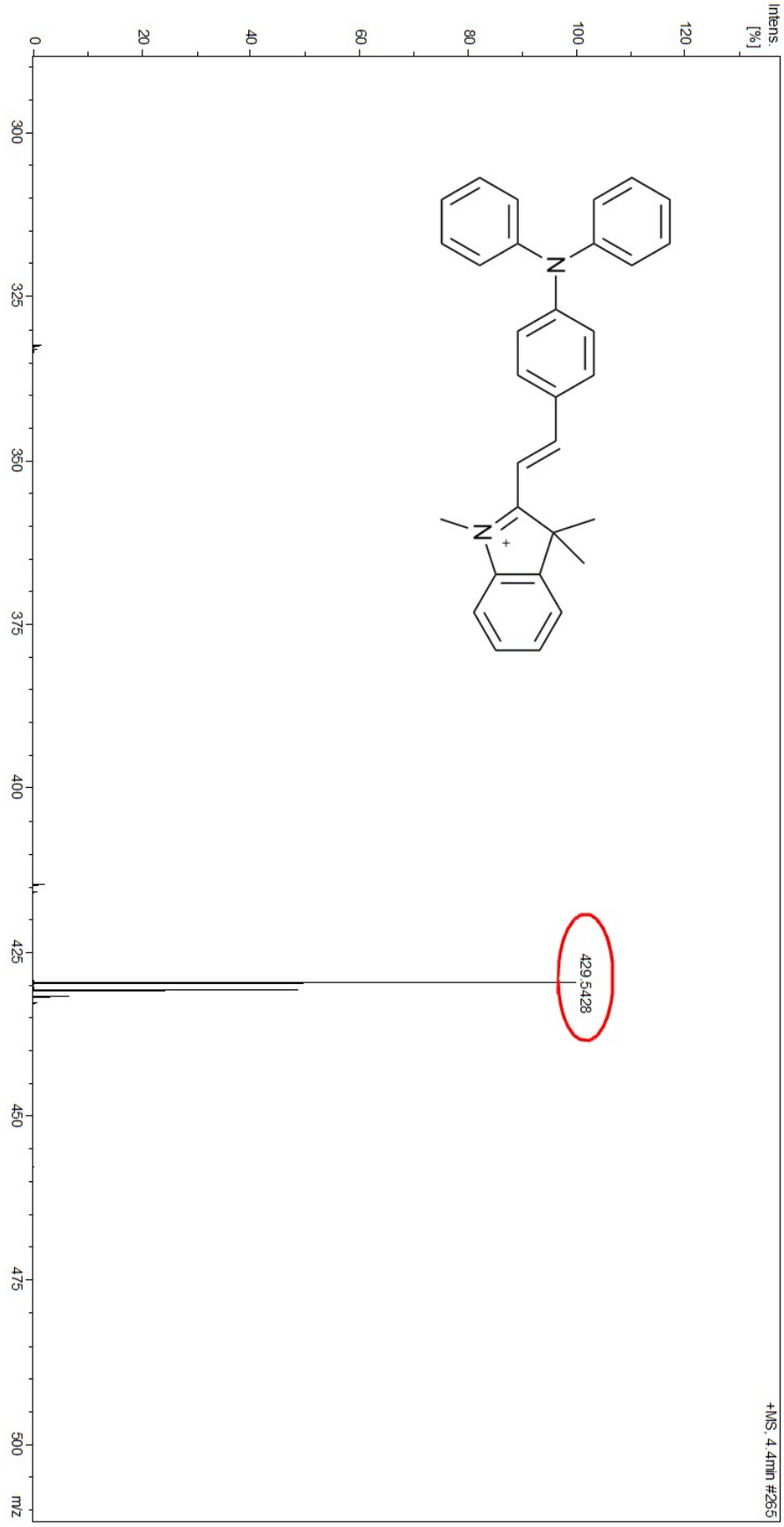

Fig. S5. The HRMS Spectra of probe **1**.

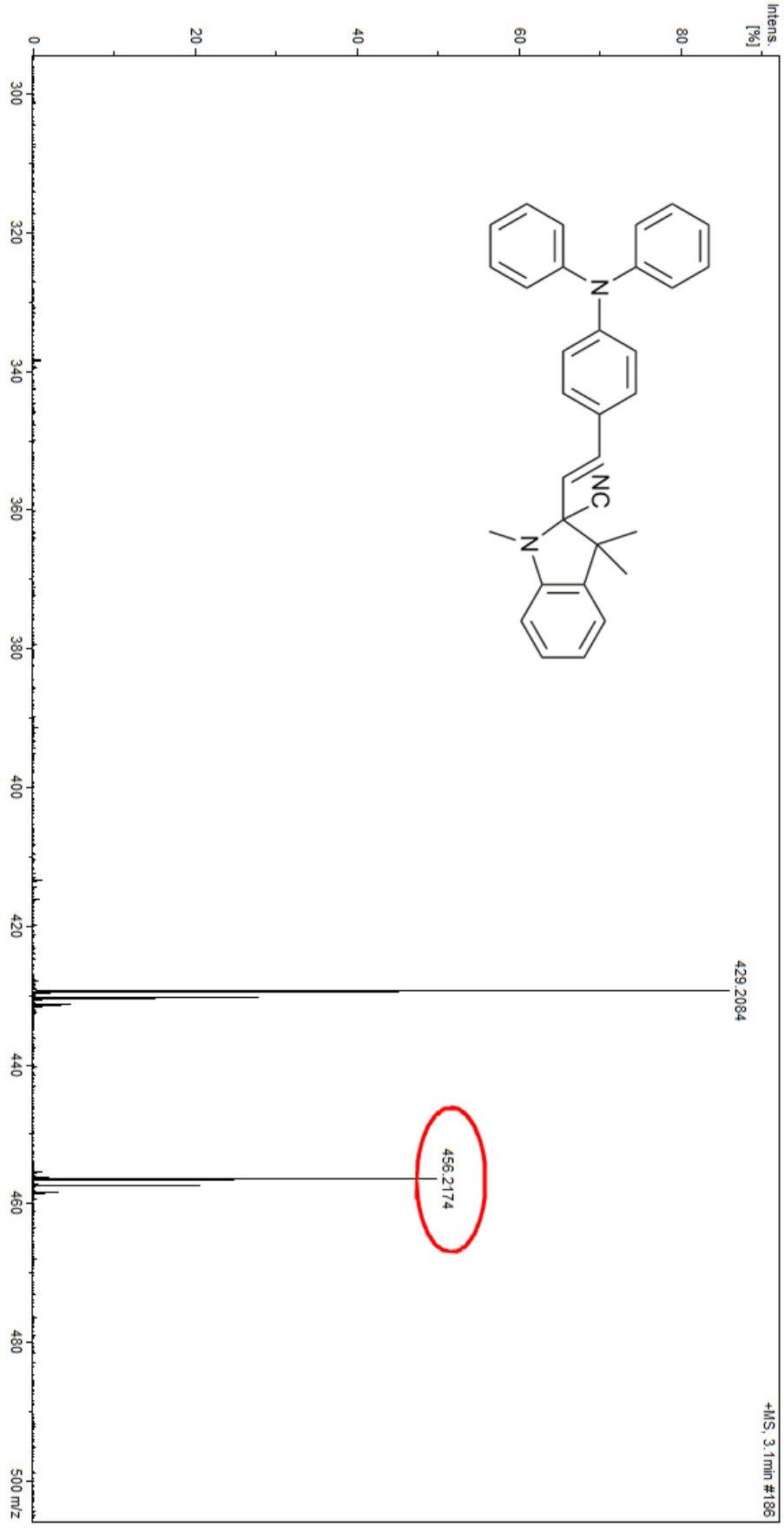

Fig. S6. The HRMS Spectra of **1-CN**.

2、**Supplemental spectra and data**

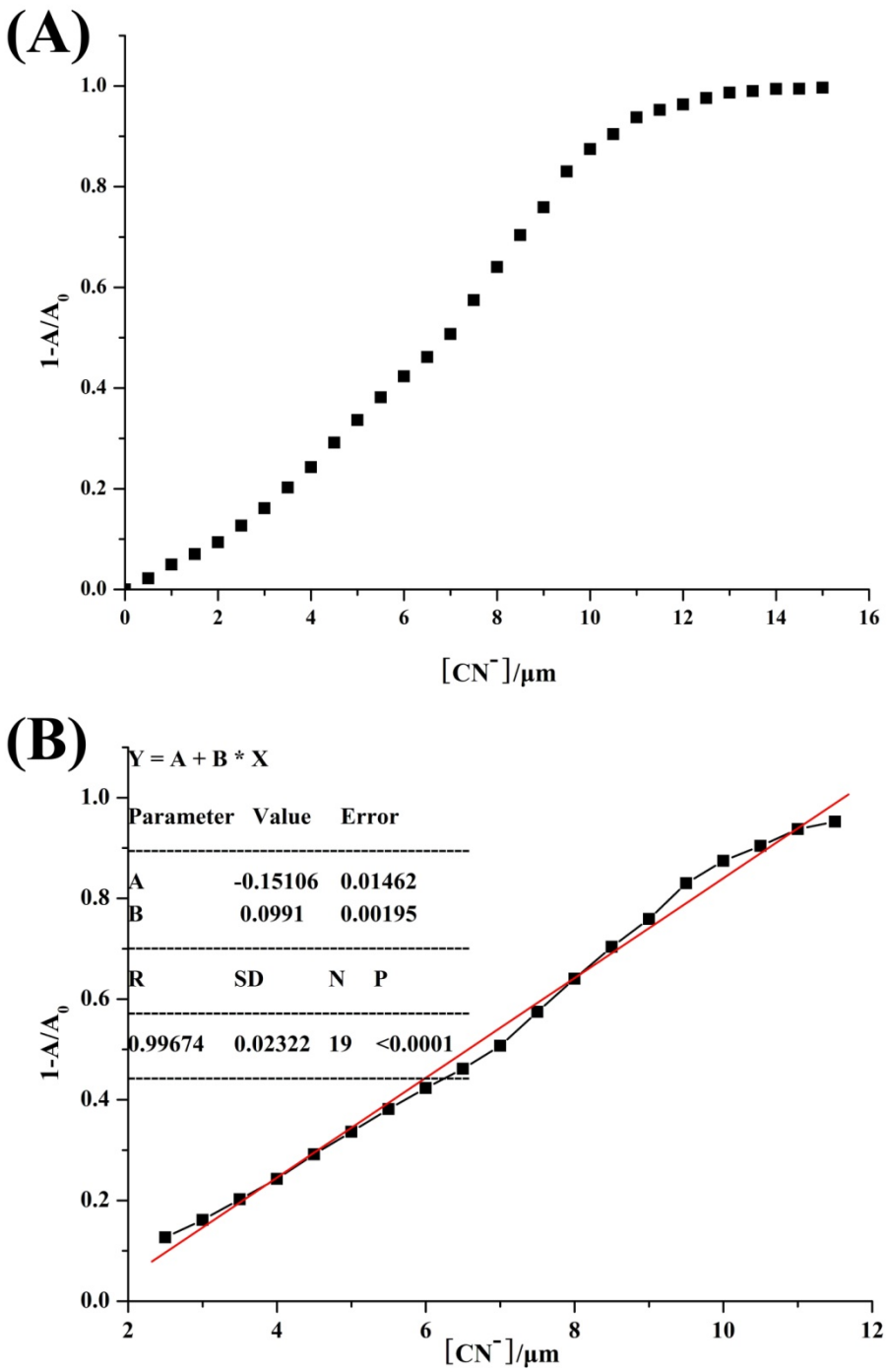

Fig. S7. (A): (1-A/A_0) plots of probe **1** (5.0 μM) at 532 nm vs. the concentration of CN^-; (B) shows the linear relation for concentration of CN^- in the range of 2.5-11.5 μM.

Fig. S8. Color fading (up) and florescence increasing (down) of probe **1** (5.0 μM) with the gradual addition of CN^- (from left to right: 0 μM, 2.0 μM, 4.0 μM, 6.0 μM, 8.0 μM, 10.0 μM, 12.0 μM, 14.0 μM).

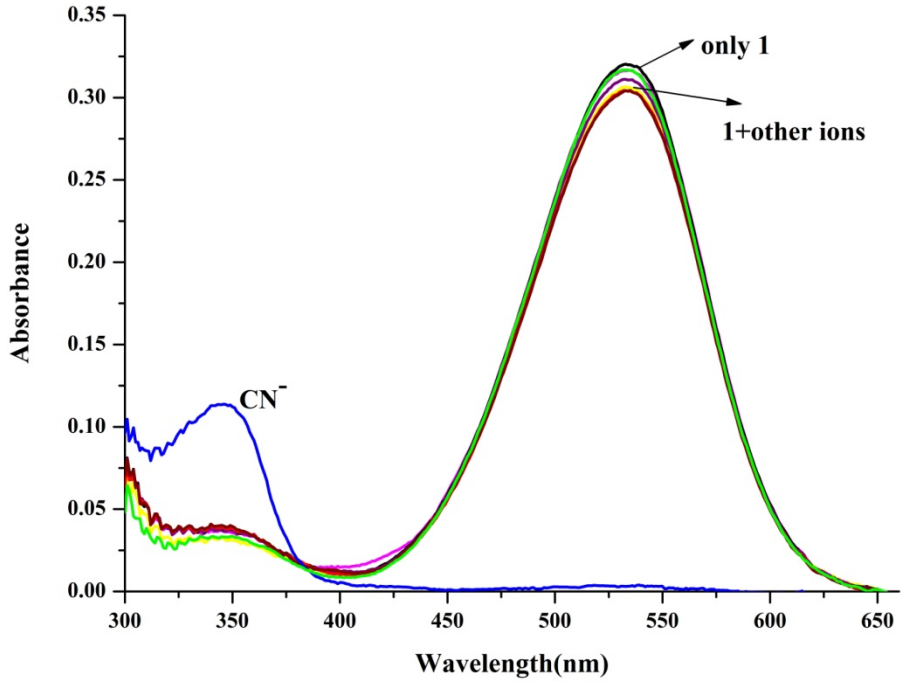

Fig. S9. Absorption spectra spectra of **1** (5.0 μM) with various analytes in EtOH-Tris·HCl buffer (10.0 mM, PH=7.4, 4:6, v/v). λ_{ex}=345 nm, slits: 5 nm/2.5 nm.

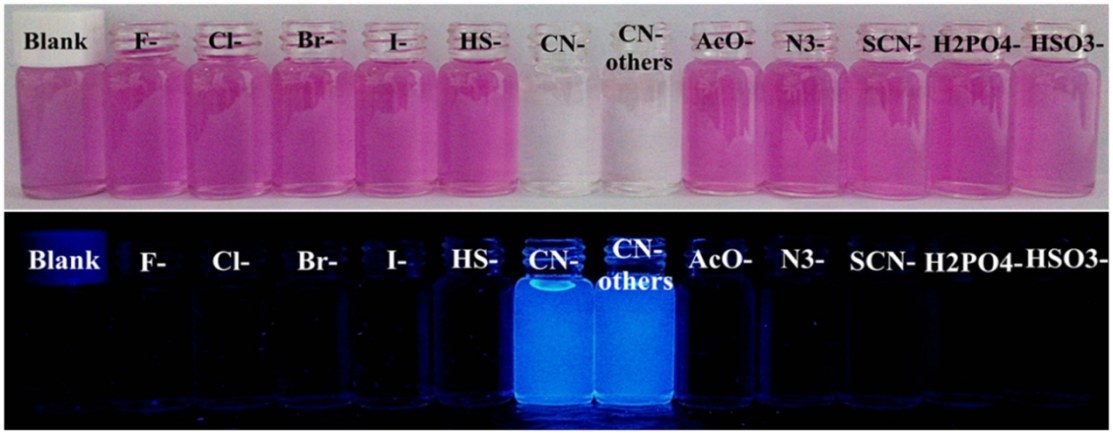

Fig. S10. Colorimetric (up) and fluorescent changes (down) of probe **1** (5.0 μM) in the presence of CN^- (15.0 μM) and 10.0 equiv. of other anions.

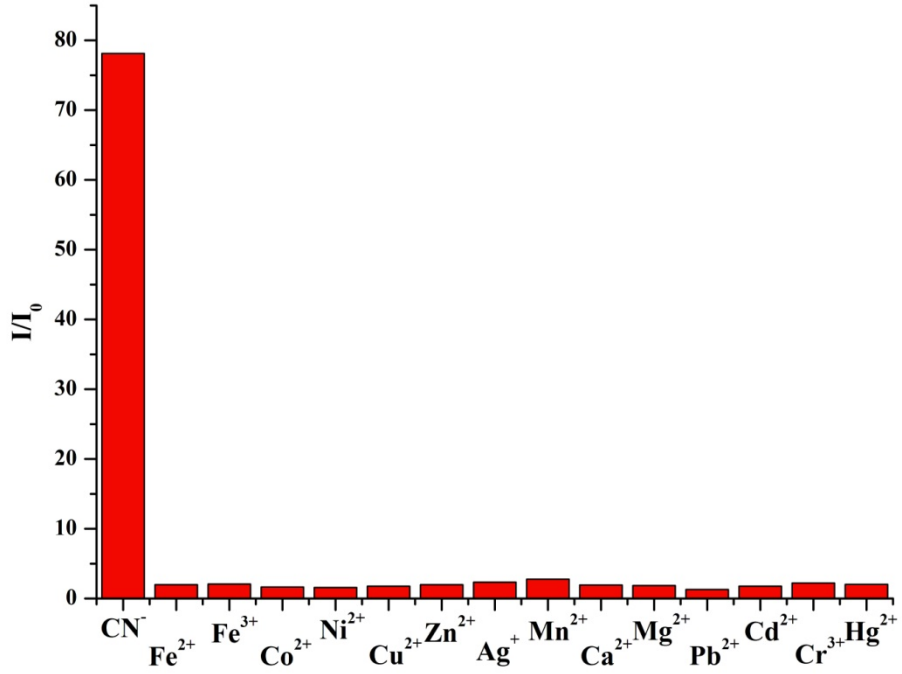

Fig. S11. Variation of the relative fluorescence intensity at 445 nm of **1** (5.0 μM) in the presence of CN^- (15.0 μM) and metal ions (Fe^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Ag^+, Mn^{2+}, Ca^{2+}, Mg^{2+}, Pb^{2+}, Cd^{2+}, Cr^{3+}, Hg^{2+}), respectively; the concentration of each metal ion except CN^- was 150.0 μM; all solutions were prepared in aqueous solution and excitation wavelength was 345 nm.

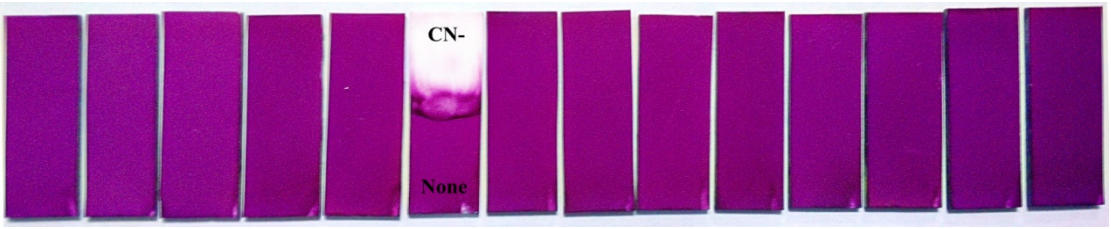

Fig. S12. Photograph of the TLC plates towards carious anions. (from left to right : F^-, Cl^-, Br^-, I^-, NO_3^-,CN^-, SO_4^{2-}, HS^-, AcO^-, N_3^-, SCN^-, $H_2PO_4^-$, HPO_4^{2-}, HSO_3^-).

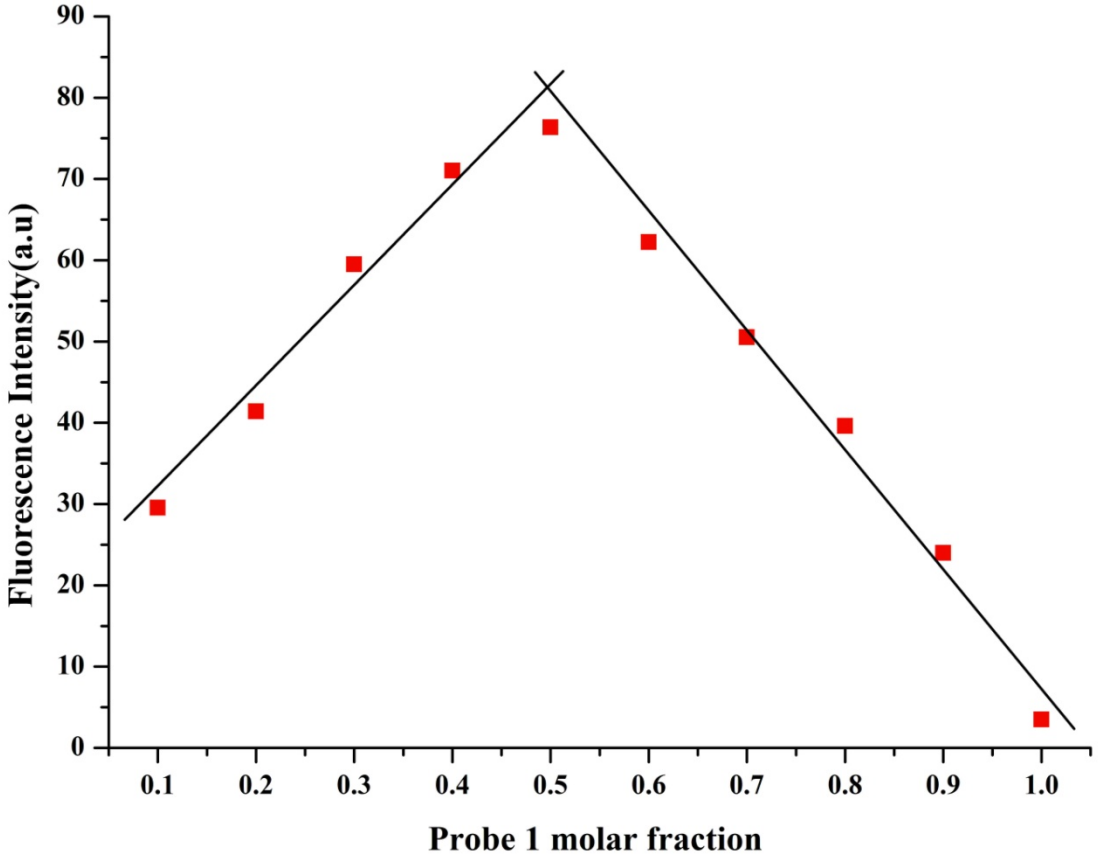

Fig. S13. Job's plot for determining the binding stoichiometry of probe **1** and CN^- in EtOH-Tris·HCl buffer (10 mM, pH = 7.4, 4:6, v/v). The total concentration of probe **1** and CN^- was 10 μM.

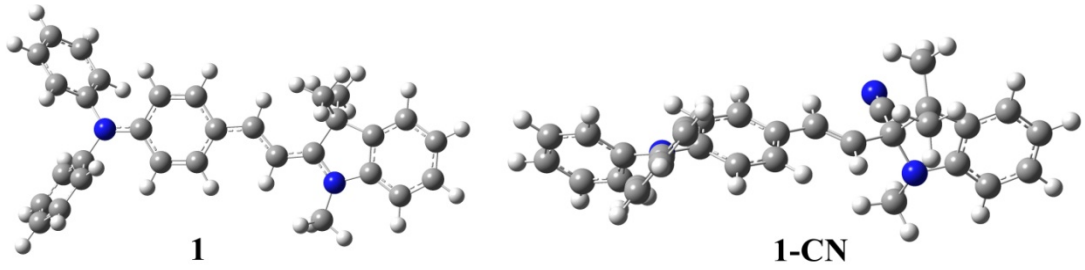

Fig. S14. The optimized structures of **1** and **1-CN**.

Fig. S15. The calculated results of transitions with oscillator strength above 0.1.

Absorption of 1:

```
Excited State   1:      Singlet-A      2.3566 eV  526.12 nm  f=1.3456
     114 ->115         0.70508
Excited State   2:      Singlet-A      3.1100 eV  398.67 nm  f=0.2143
     112 ->115         0.17873
     113 ->115         0.67434
Excited State  12:      Singlet-A      4.5970 eV  269.71 nm  f=0.1241
     114 ->119         0.68715
```

Absorption of 1-CN:

```
Excited State   1:      Singlet-A      3.4697 eV  357.33 nm  f=0.7646
     121 ->122         0.69727
Excited State   4:      Singlet-A      4.0622 eV  305.21 nm  f=0.1859
     121 ->123         0.13536
     121 ->124         0.68326
Excited State  14:      Singlet-A      5.0546 eV  245.29 nm  f=0.2774
     117 ->122        -0.15658
     119 ->122        -0.37022
     120 ->128        -0.33933
     120 ->129        -0.11884
     121 ->129         0.37620
Excited State  23:      Singlet-A      5.5187 eV  224.66 nm  f=0.1001
     114 ->122        -0.27852
     114 ->127         0.10356
     115 ->122        -0.25972
     116 ->124         0.29271
     119 ->123         0.34187
     119 ->124         0.24322
     119 ->126         0.17366
Excited State  30:      Singlet-A      5.8485 eV  211.99 nm  f=0.1084
     115 ->124        -0.15762
     117 ->123         0.57946
     117 ->124         0.15690
     120 ->130         0.15385
```

120 ->131 -0.19057
121 ->132 -0.10079

Emission of 1-CN:

Excited State 1: Singlet-A 2.5499 eV 486.23 nm f=0.0559
121 ->122 0.70349
Excited State 4: Singlet-A 4.2048 eV 294.87 nm f=0.1331
116 ->122 0.17000
121 ->124 0.57719
121 ->126 -0.34333
Excited State 5: Singlet-A 4.2629 eV 290.85 nm f=0.6503
116 ->122 -0.19440
117 ->122 -0.24969
118 ->122 0.19509
119 ->122 0.58081
121 ->126 -0.10523
Excited State 7: Singlet-A 4.3464 eV 285.26 nm f=0.1369
117 ->122 0.15197
118 ->122 0.60850
119 ->122 -0.18268
121 ->124 -0.14161
121 ->126 -0.19659
Excited State 8: Singlet-A 4.3875 eV 282.59 nm f=0.1975
116 ->122 -0.24123
117 ->122 0.49644
119 ->122 0.14783
121 ->124 0.26668
121 ->126 0.26327
Excited State 9: Singlet-A 4.4322 eV 279.73 nm f=0.4104
115 ->122 0.12108
116 ->122 0.48936
117 ->122 0.32264
119 ->122 0.28516
121 ->124 -0.17009
121 ->126 -0.11295