Electronic Supplementary Information

A selective fluorescent probe for detection of gold(III) ions and its application to bioimaging

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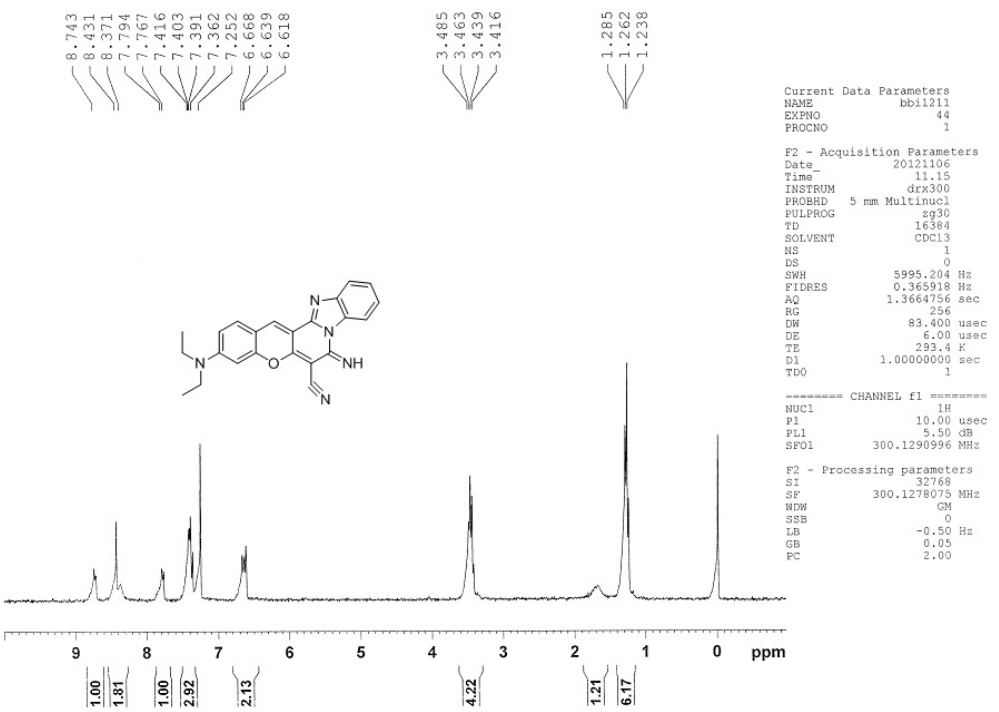
Materials and Methods

All chemicals and solvents were of analytic grade and bought from Sigma-Aldrich or Beiing City wihout further purification. The deionized water was used to prepare all aqueous solutions. The solutions of anions were prepared from their sodium salts and the solutions of metal ions were prepared from their chloride or nitrate salts. All spectroscopic measurements were performed in CH_3CN-HEPES buffer (10 mmol/L, pH 7.4, v:v=1:1). HEPES buffer solutions were obtained by adding NaOH 5 M or 6 M HCl solution into 10 mM aqueous HEPES using a Mettler pH meter. The probe Fluorescent Red GK was dissolved into absolute CH_3CN to prepare the stock solutions with a concentration of 2.0 mmoL. The UV/Visible spectra were recorded on a Cary 50 Bio UV-Vis spectrophotometer in a in a 4.5 ml (1 cm in diameter) cuvette with 2 ml solution. Fluorescence spectra were measured on Cary Eclipse fluorescence spectrophotometer. All data were treated with the Origin 8.0 program. Absorption maxima, λ_{max}. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 300 and Bruker 75 spectrometer. ESI was measured with an LTQ-MS (Thermo) instrument. Chemical shifts are given in parts per million downfield from tetramethylsilane (0.0 ppm) for spectra.

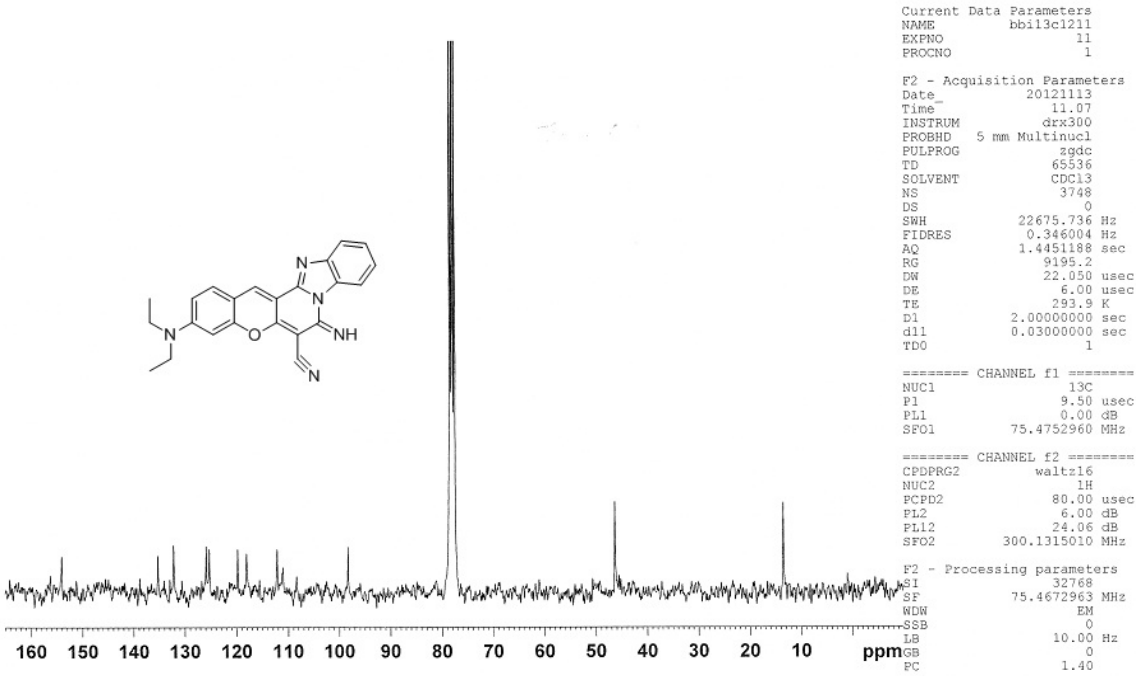
Measurement procedure

The procedures were shown as followings: in 10 mmoL, pH 7.4 HEPES buffer solution containing 2 μmoL the probe and Au^{3+} sample was gradually titrated into the solution. All Fluorescence spectra data were recorded at 30 s after the Au^{3+} addition. All UV-Vis spectra data were recorded at 30 s after the Au^{3+} addition.

Figure S1: ^{1}H NMR, ^{13}C NMR, ESI-MS spectra of the probe



(a)



(b)

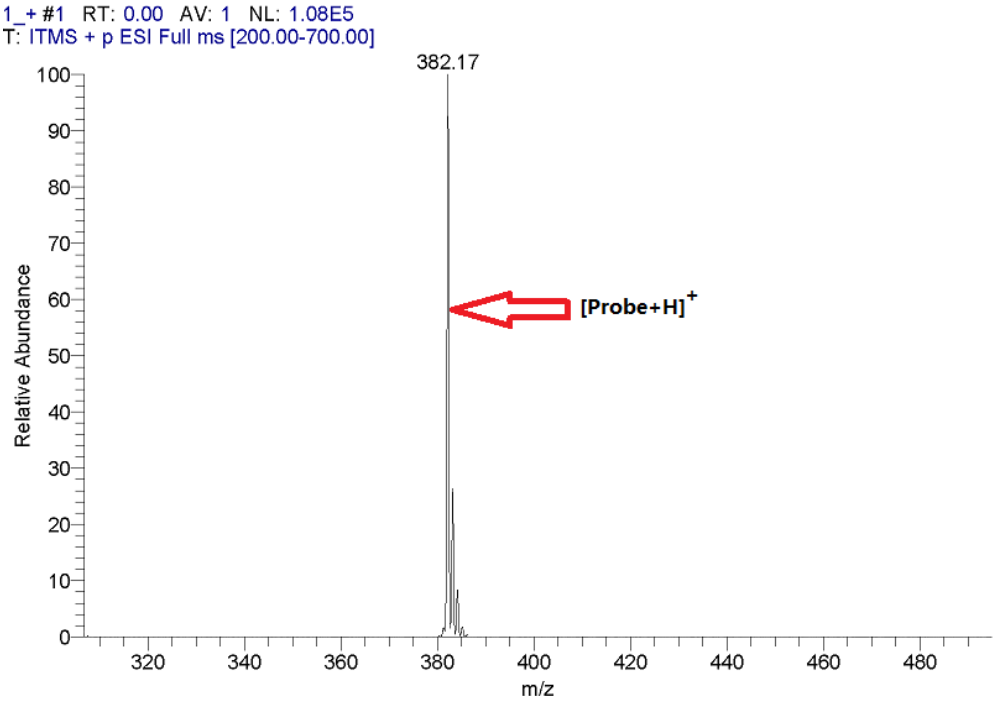


Figure S1: ^{1}H NMR (300 MHz, 25 °C, $CDCl_3$): δ 8.74 (d, 1H), 8.40 (t, 2H), 7.78 (d, 1H), 7.39 (m, 3H), 6.64 (t, 2H), 3.45 (m, 4H), 1.26 (t, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ156.8, 154.1, 139.6, 135.3, 132.2, 131.9, 125.9, 125.3, 119.8, 118.1, 116.6, 112.3, 111.0, 108.6, 98.4, 46.4, 13.6; ESI-MS m/z: $[probe+ H]^+$ Calcd for $C_{23}H_{20}N_5O$ 382.17, Found 382.17; Elemental analysis (calcd. %) for $C_{23}H_{19}N_5O$: C, 72.42; H, 5.02; N, 18.36; Found: C, 72.38; H, 5.06, N, 18.40.

Figure S2: Absorption spectra of the probe upon addition all kinds of analytes

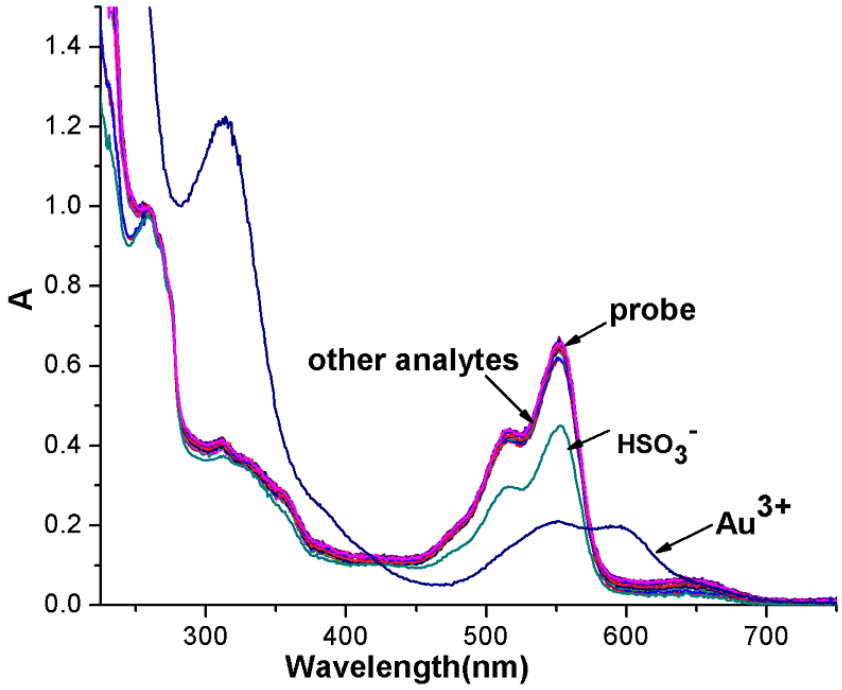


Figure S2: The selectivity of FRGK for Au^{3+}, HSO_3^-, Cu^{2+}, Ca^{2+}, Fe^{2+}, Zn^{2+}, Ni^{2+}, Bi^{3+}, Co^{2+}, VO^{2+}, Mn^{2+}, Ru^{3+}, Cd^{2+}, Pb^{2+}, Ag^+, La^{3+}, Ce^{4+}, Yb^{3+}, Cr^{2+}, Er^{3+}, Sn^{2+}, Au^+, Zr^{4+}, Pd^{2+}, Fe^{3+}, Eu^{3+} and Hg^{2+}.

Figure S3: The emission spectra with all the investigated analytes.

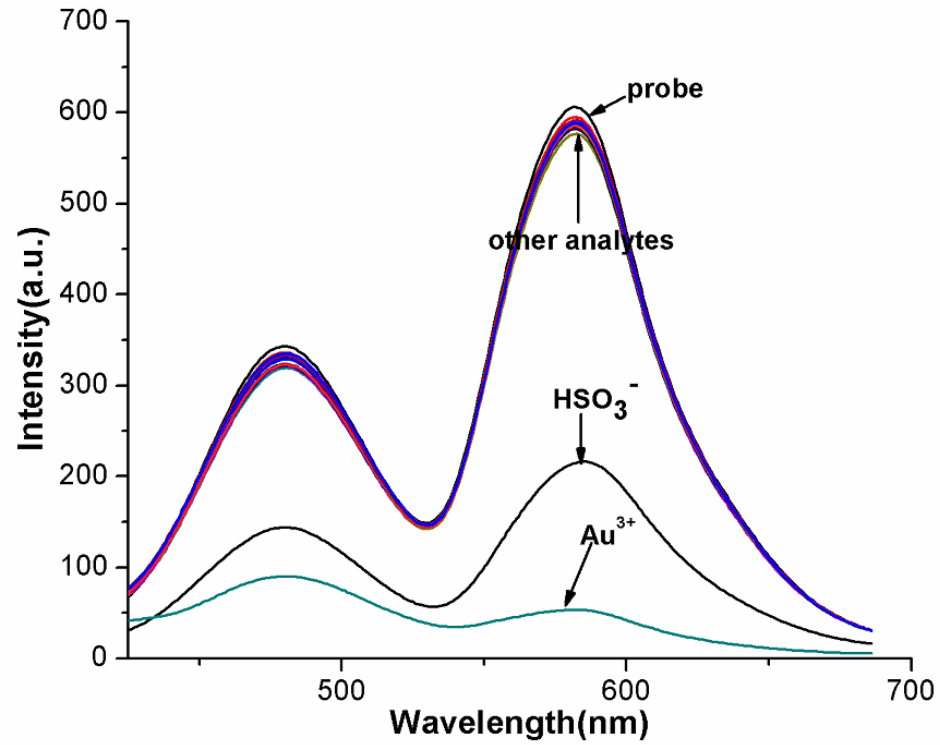


Figure S3: The selectivity of FRGK for Au^{3+}, HSO_3^-, Cu^{2+}, Ca^{2+}, Fe^{2+}, Zn^{2+}, Ni^{2+}, Bi^{3+}, Co^{2+}, VO^{2+}, Mn^{2+}, Ru^{3+}, Cd^{2+}, Pb^{2+}, Ag^{+}, La^{3+}, Ce^{4+}, Yb^{3+}, Cr^{2+}, Er^{3+}, Sn^{2+}, Au^{+}, Zr^{4+}, Pd^{2+}, Fe^{3+}, Eu^{3+} and Hg^{2+}.

Figure S4: The disturbance from other anlaytes

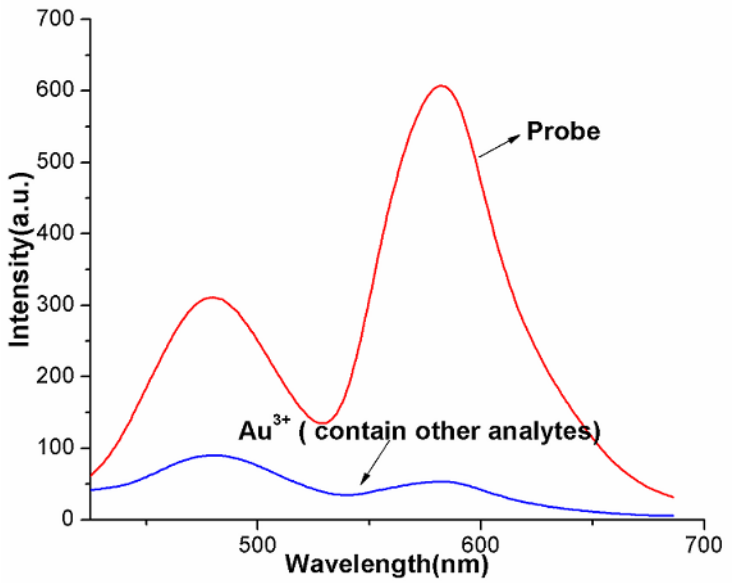
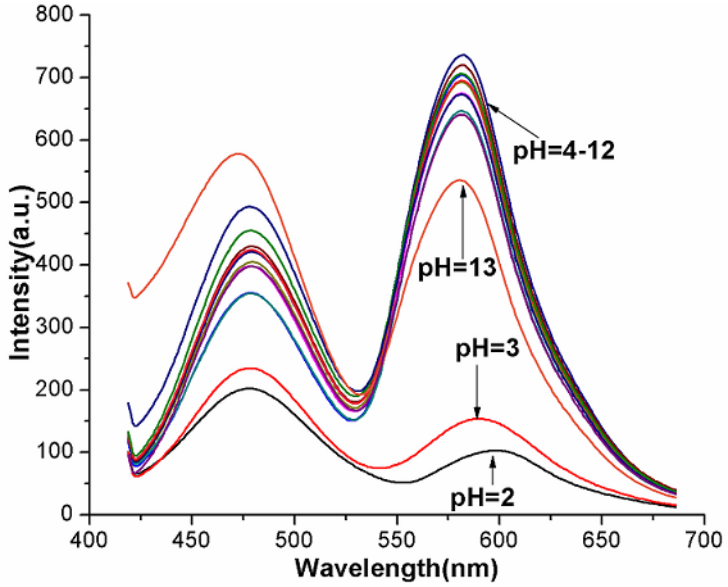
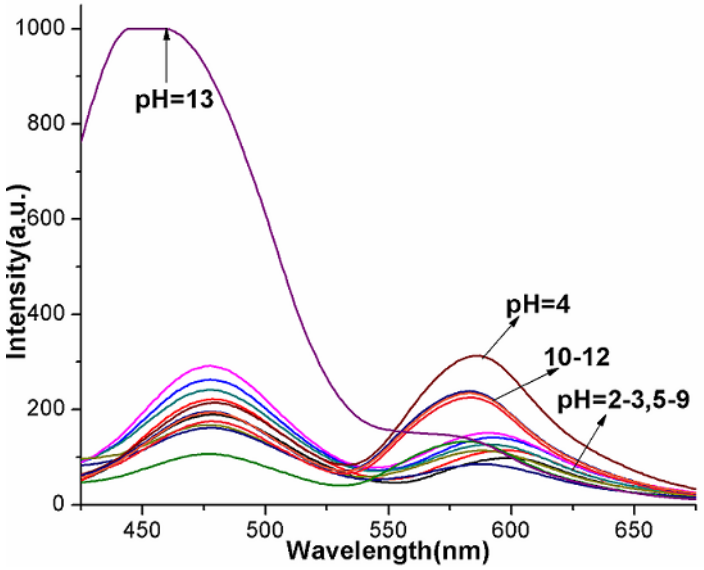


Figure S4: The fluorescence spectra of probe (2 μmoL) in the presence of various analytes in CH_3CN-HEPES (1:1, v/v, pH 7.4) solution: containing Cu^{2+}, Ca^{2+}, Fe^{2+}, Zn^{2+}, Ni^{2+}, Bi^{3+}, Co^{2+}, VO^{2+}, Mn^{2+}, Ru^{3+}, Cd^{2+}, Pb^{2+}, Ag^{+}, La^{3+}, Ce^{4+}, Yb^{3+}, Cr^{2+}, Er^{3+}, Sn^{2+}, Au^{+}, Zr^{4+}, Pd^{2+}, Fe^{3+}, Eu^{3+} and Hg^{2+}.

Figure S5: Choice of pH-range for the Measurement



(a)



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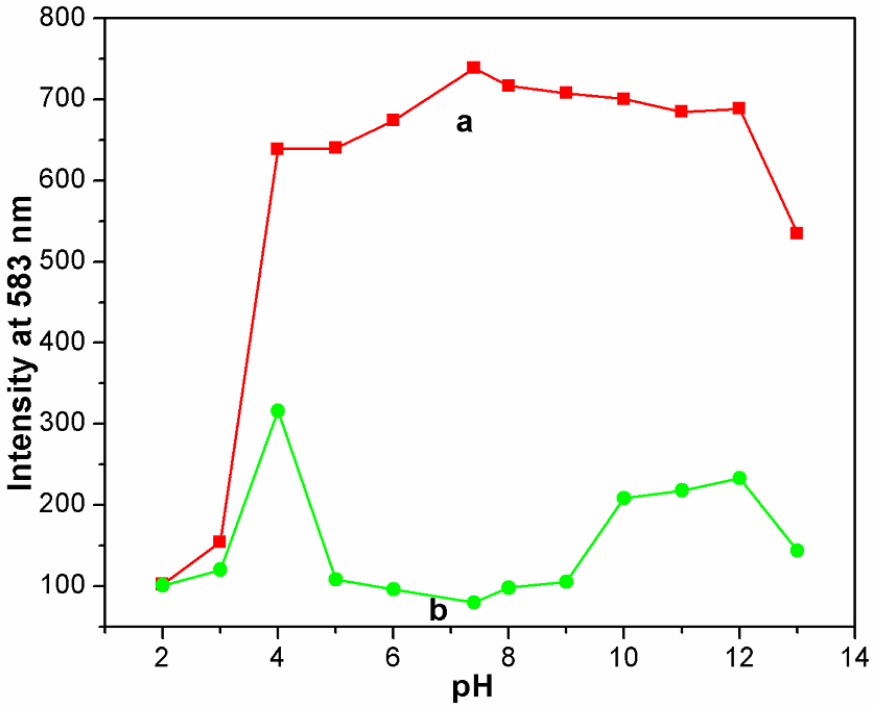

(c)

Figure S5: Fluorescence spectral responses of free probe (a) and probe-Au^{3+} (b) for pH.

Figure S6: Detection limit for Au^{3+}

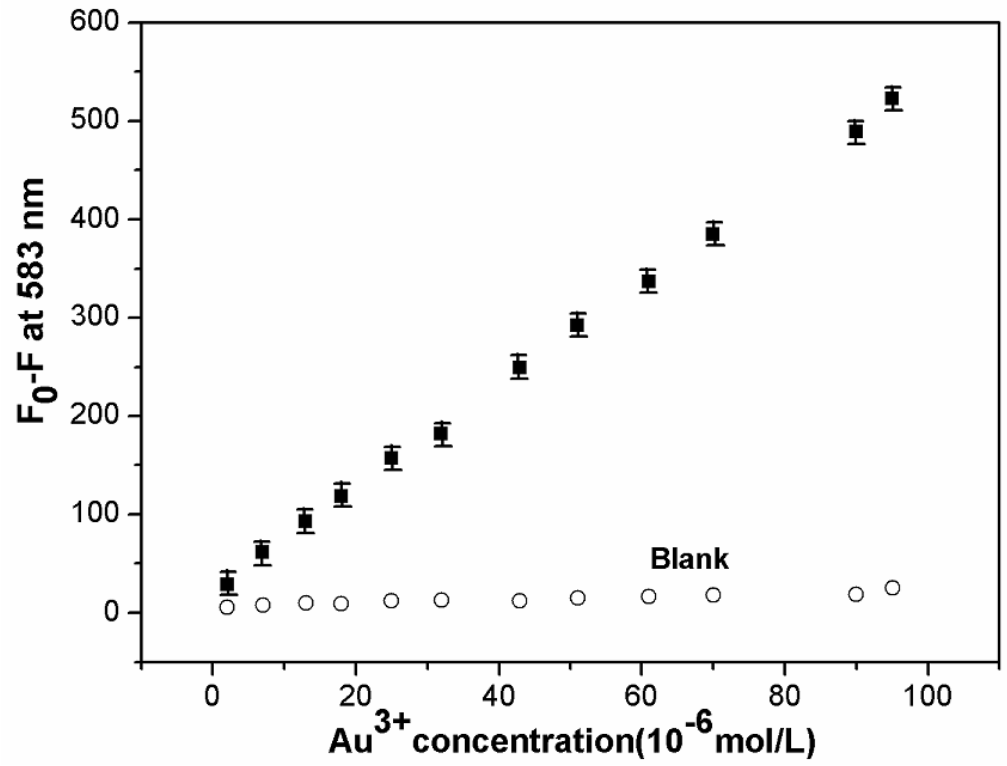

Figure S6: Detection limits for Au^{3+} as low as 1.23 μmol/L.

Figure S7: ESI-MS spectra of the probe-Au^{3+} complex

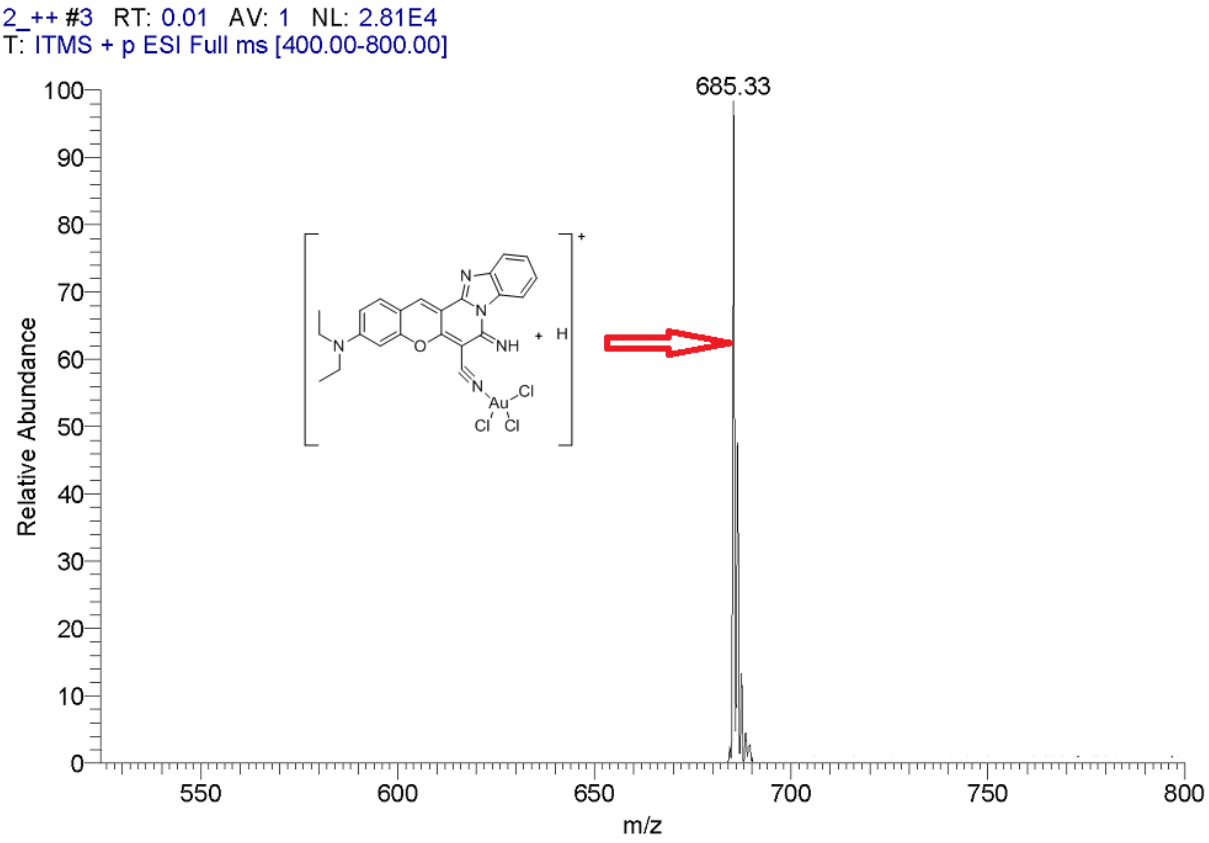

Figure S7: The ESI-MS of product obtained by mixing probe $AuCl_3$, m/z: $[Probe\text{-}Au^{3+} + H]^+$ Calcd for $C_{23}H_{19}AuCl_3N_5O$ 685.76, Found 685.33.