Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

Homopropargyl as a novel recognizing moiety of fluorescent probe for detection of palladium in living cells

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1. General

The detection limit

The detection limit was calculated from fluorescence titration. In the absence of Pd^{2+}, the fluorescence emission spectra of probe **1** were measured by five times and the standard deviation of blank measurement was achieved. To gain the slop, the fluorescence intensity at 508 nm was plotted to the concentration of Pd^{2+}. The detection limit was calculated according to equation showing below:

$$\text{Detection limit} = 3\sigma/k$$

Where σ is the standard deviation of blank measurement, k is the slope between the fluorescence intensities versus the concentrations of Pd^{2+}.

MTT assay experiment. MTT experiment was performed in 96-well plate to assess the cytotoxicity of the probe. The MTT assay in A549 cells with the probe concentrations from 1.25 to 20 μM in comparison with the blank and negative control. Cells were plated on cell plates at 4×10^3 cells per well and allowed to incubate for 24 hours. The probe in various concentrations were added to the well and incubated for 24 hours followed by classical MTT treatment and data acquiring.

2. Supplementary Date

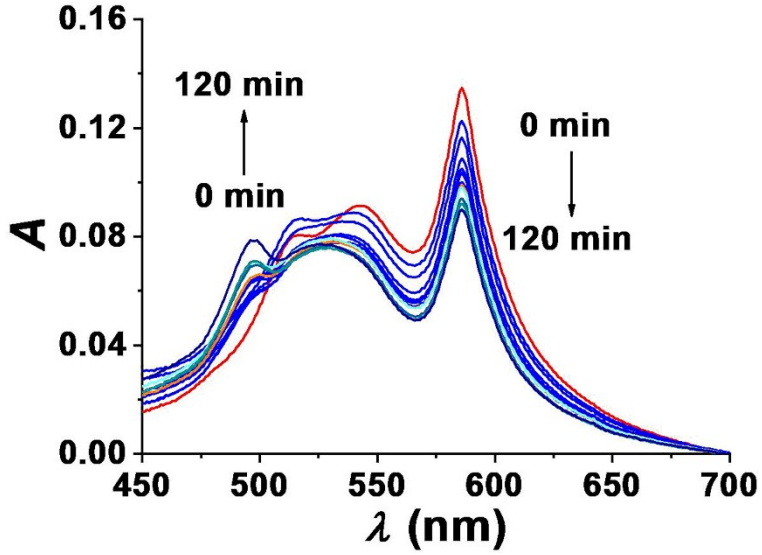


Fig. S1. Time-dependent absorption spectral changes for probe **1** (10 μM) with 10 equiv. of Pd^{2+} in acetonitrile/PBS buffer (1 : 99, v/v, 10 mM, pH 7.4) at 37 °C.

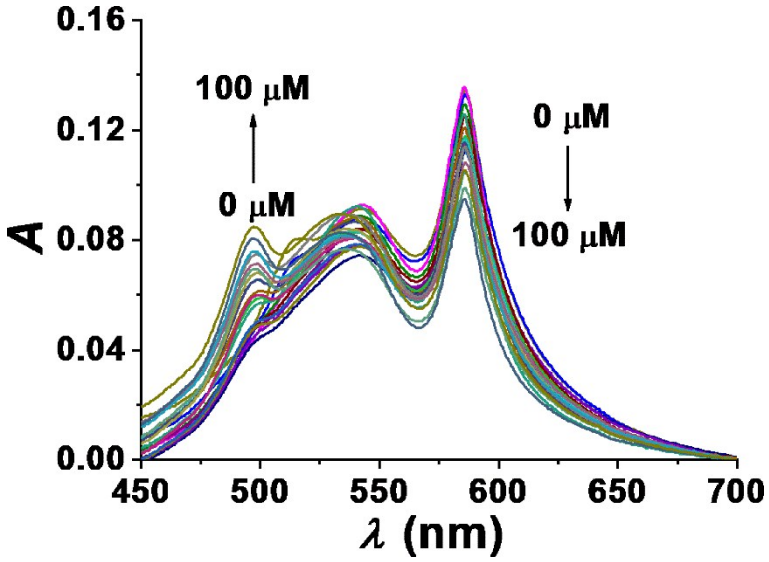


Fig. S2. Absorption spectral changes of probe **1** (10 μM) upon addition of increasing concentrations of Pd^{2+}. Each spectrum was recorded 120 min after addition of Pd^{2+} in acetonitrile/PBS buffer (1 : 99, v/v, 10 mM, pH 7.4) at 37 °C.

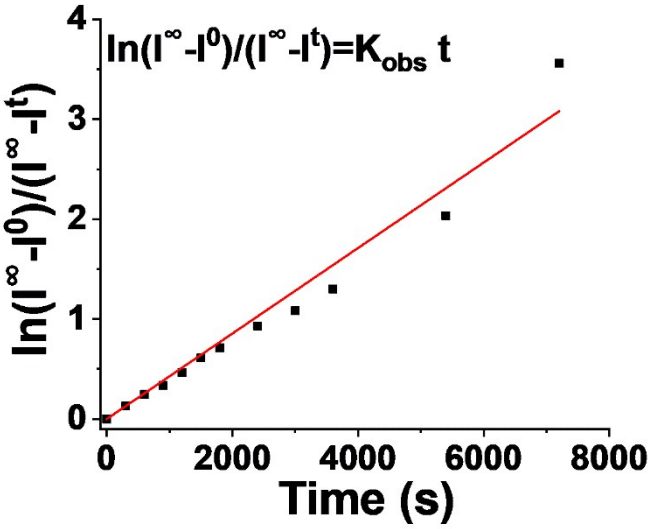


Fig. S3. Fluorescence kinetic adjusted. Experimental conditions: probe **1** (10 μM) with 10 equiv. of Pd^{2+} in acetonitrile/PBS buffer (1 : 99, v/v, 10 mM, pH 7.4) at 37 °C (λ_{ex} = 465 nm).

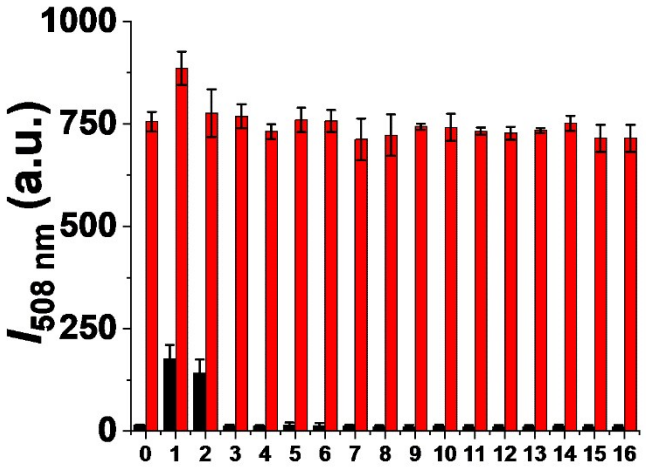


Fig. S4. The fluorescence intensity at 508 nm of probe **1** (10 μM) in the presence of 100 μM of various analytes prior to (black bars) and after (red bars) addition of 100 μM Pd^{2+} to the individual probe/analyte solution. (0) blank; (1) Pd^{0}; (2) Hg^{2+}; (3) Ag^{+}; (4) Co^{2+}; (5) Cu^{2+}; (6) Fe^{3+}; (7) Mg^{2+}; (8) Ni^{2+}; (9) Zn^{2+}; (10) Ca^{2+}; (11) Mn^{2+}; (12) Ba^{2+}; (13) Al^{3+}; (14) Li^{+}; (15) Na^{+} (1 mM); (16) K^{+}(1 mM). Each data point was recorded 120 min after addition of various analytes in acetonitrile/PBS buffer (1 : 99, v/v, 10 mM, pH 7.4) at 37 °C (λ_{ex} = 465 nm).

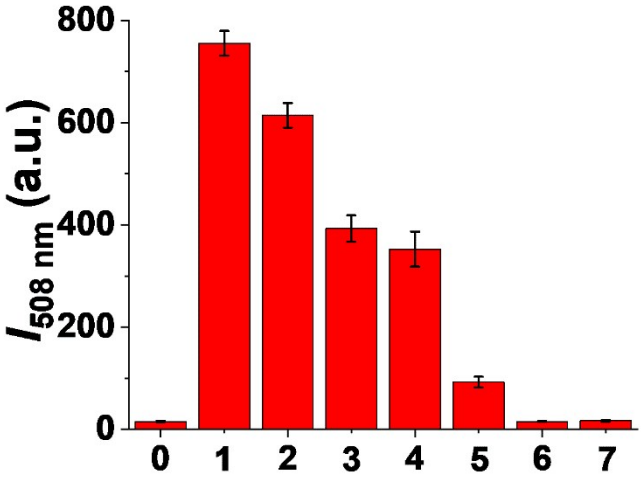


Fig. S5. Comparison of the fluorescence intensity changes on different palladium complexes. (0) probe only; (1) $PdCl_2$; (2) $Pd(CF_3COO)_2$; (3) $Pd(OAc)_2$; (4) K_2PdCl_6; (5) $Pd(PPh_3)_4$; (6) $Pd(PPh_3)_2Cl_2$; (7) $PdCl_2(dppf)_2$. Each data point was recorded 120 min after addition of various analytes in acetonitrile/PBS buffer (1 : 99, v/v, 10 mM, pH 7.4) at 37 °C (λ_{ex} = 465 nm).

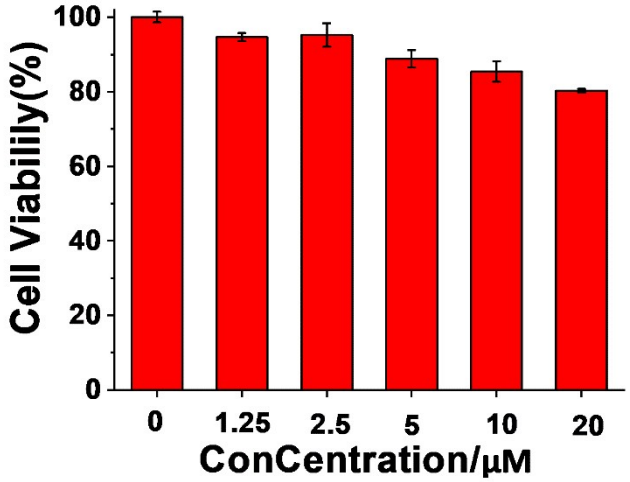


Fig. S6. Cell viability assay of probe **1** in HeLa Cells, all compounds were incubated with the cells for 48 hours, and the cells viability was observed via MTT assays.

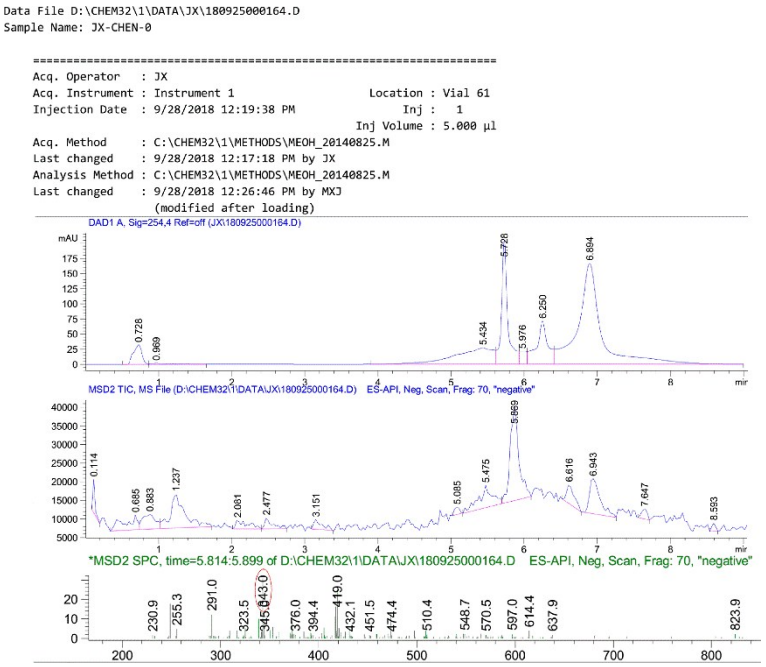


Fig. S7. The ESI-MS of probe **1**.

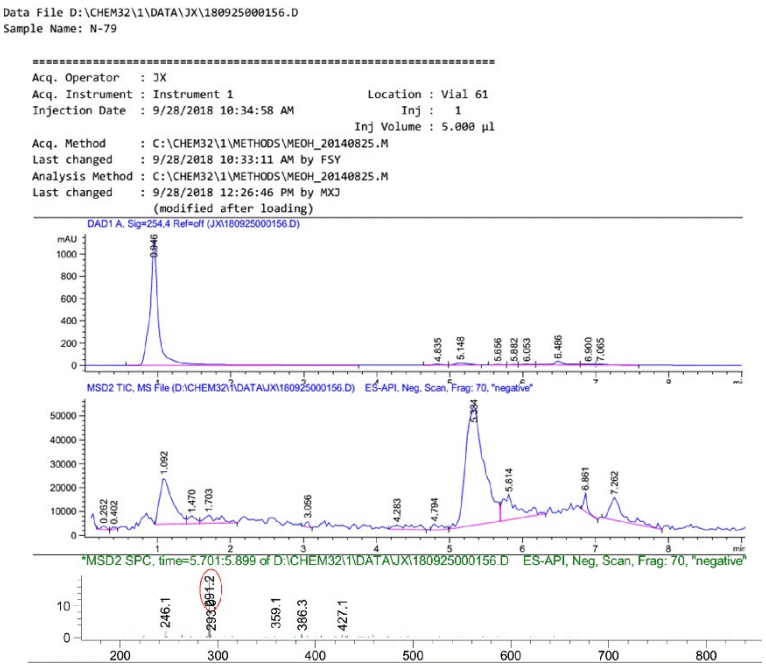
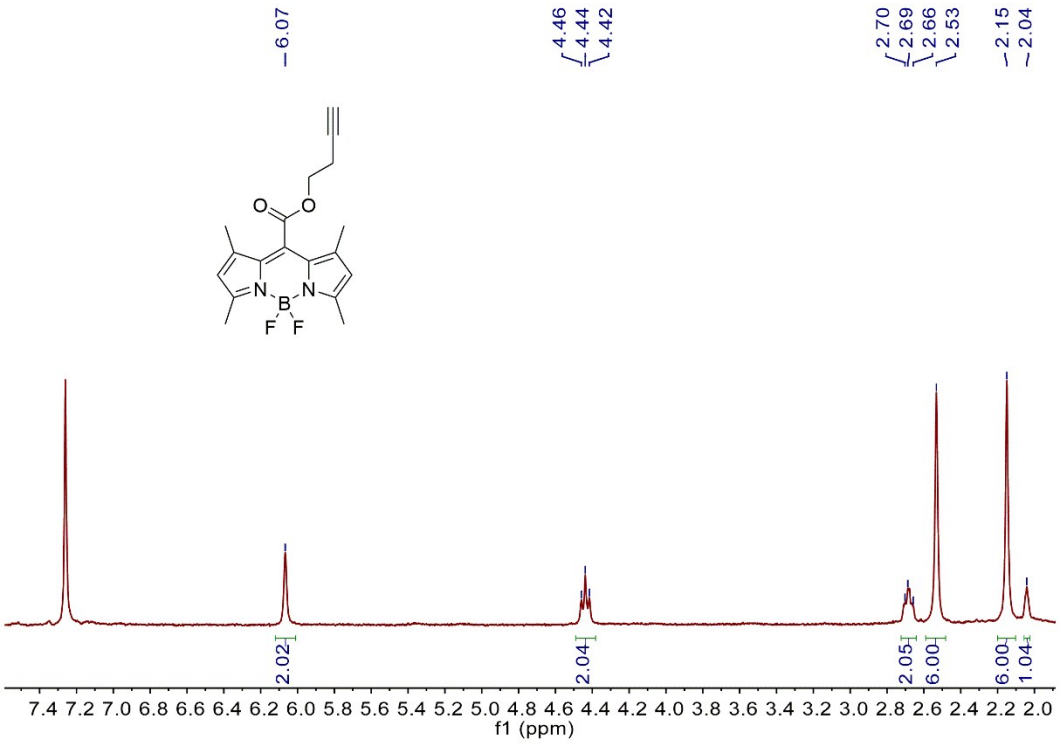


Fig. S8. The ESI-MS of probe **1** upon addition of Pd^{2+}.

3. NMR data

^{1}H NMR of probe **1**



^{13}C NMR of probe **1**