Supporting Information for

Triphenylphosphine-assisted highly sensitive fluorescent chemosensor for ratoimetric detection of palladium in solution and living cells

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1. Comparison of the analytical performance of our two chemosensors

Table 1 The analytical performance of our two chemosensors

	fluorescence imaging	linear range (μM)	Detection Limit (nM)	Pd^{2+} concentration to be incubated with cells (μM)
previous chemosensor	ratiometric	0~7	70	40
chemosensor **1**	ratiometric	0.02~0.25	1	0.3

2. Analysis of the reaction mechanism by HPLC method

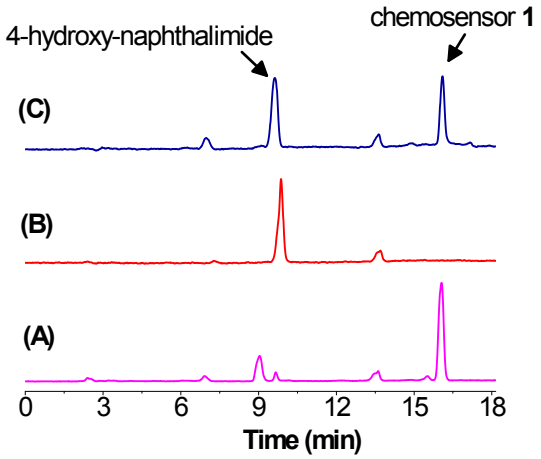

Figure S1. Monitoring the reaction processes by HPLC. **(A)** The spectral of chemosensor **1**-$Pd(PPh_3)_4$ reaction system in THF; **(B)** The spectral of chemosensor **1**-$Pd(PPh_3)_4$-$NaBH_4$ reaction system in THF; **(C)** The spectral of chemosensor **1**-PPh_3-$PdCl_2$ reaction system in PBS solution (pH=7.4). All reaction were performed for 12h and then analyzed by HPLC at 254 nm absorption wavelength. The samples were analyzed by reverse-phase HPLC with a linear gradient [C18-ST: starting eluent 50% CH_3CN/0.1% TFA aq; final eluent 90% CH_3CN/0.1% TFA aq.; gradient duration 10 min; flow rate = 1 mL/min].

3. Time-dependent fluorescence intensity ratio changes of chemosensor 1 during reacting with Pd^{2+}

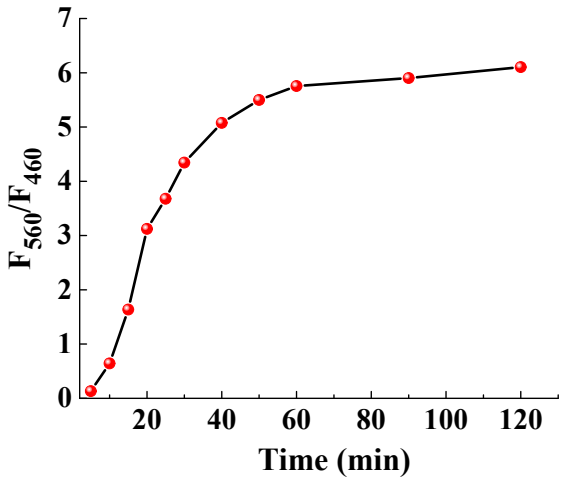

Figure S2. Fluorescence intensity ratios (F_{560nm}/F_{460nm}) in PBS buffer (10 mM, pH 7.4) with reaction time of 5, 10, 15, 20, 25, 30, 40, 50, 60, 90, 120 min. The measurements were performed after reacting chemosensor **1** (5 μM) and PPh_3 (4 μM) with Pd^{2+} (0.5 μM) at room temperature. λ_{ex} = 410 nm.

4. Calculation for detection limit

The detection limit was calculated based on the fluorescence titration. In the absence of Pd^{2+}, the fluorescence emission of chemosensor **1** was measured ten times and the standard deviation of blank measurement was obtained. To gain the slope, the logarithm of the fluorescence intensity ratio at two emission peaks, log (F_{560}/F_{460}), was plotted versus Pd^{2+} concentration. The detection limit was calculated according to the following equation:

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

Where σ is the standard deviation of blank measurements and k is the slope of log ($F_{560\ nm}/F_{460nm}$) versus Pd^{2+} concentration

5. Cytotoxicity assays

RAW264.7 macrophage cells were cultured in culture media (DMEM) in an atmosphere of 5% CO_2 and 95% air at 37 °C. The cells were seeded into 96-well plates at a density of 5×10^3 cells per well in culture media, then 5, 10 and 20 μM chemosensor **1** (containing 4 μM PPh_3) were added respectively. Next, the cells were incubated at 37 °C in an atmosphere of 5% CO_2 and 95% air for 24 h. Finally, 10 μL 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT, 5 mg/mL) was added and were cultured for another 4 h, respectively.

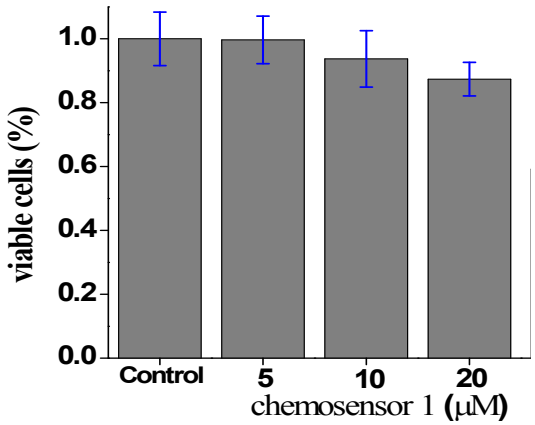

Fig. S3 Cytotoxicity assays of chemosensor **1** (containing 4 μM PPh_3) at different concentrations for RAW264.7 macrophage cells

6. NMR and ESI-MS spectra of chemosensor 1 and its Pd^0-catalyzed deallylation product

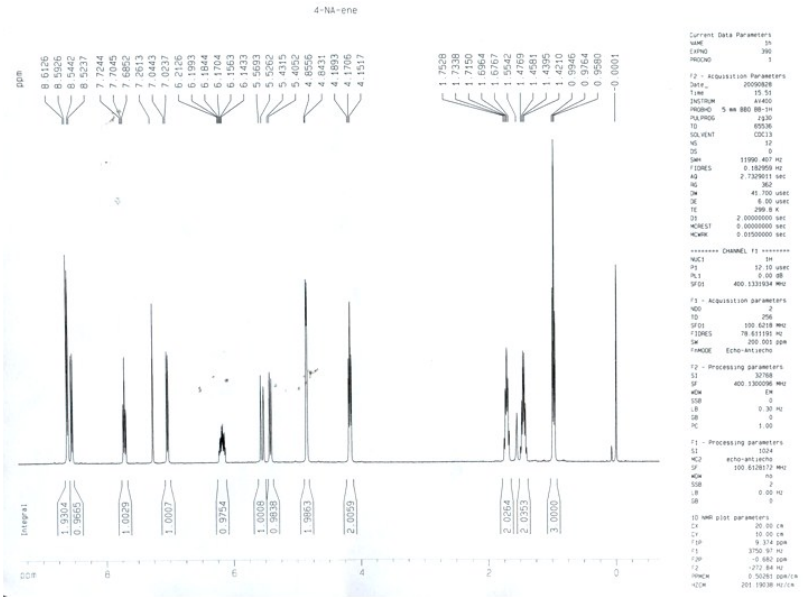

Figure S4. ^{1}H-NMR spectrum of chemosensor 1

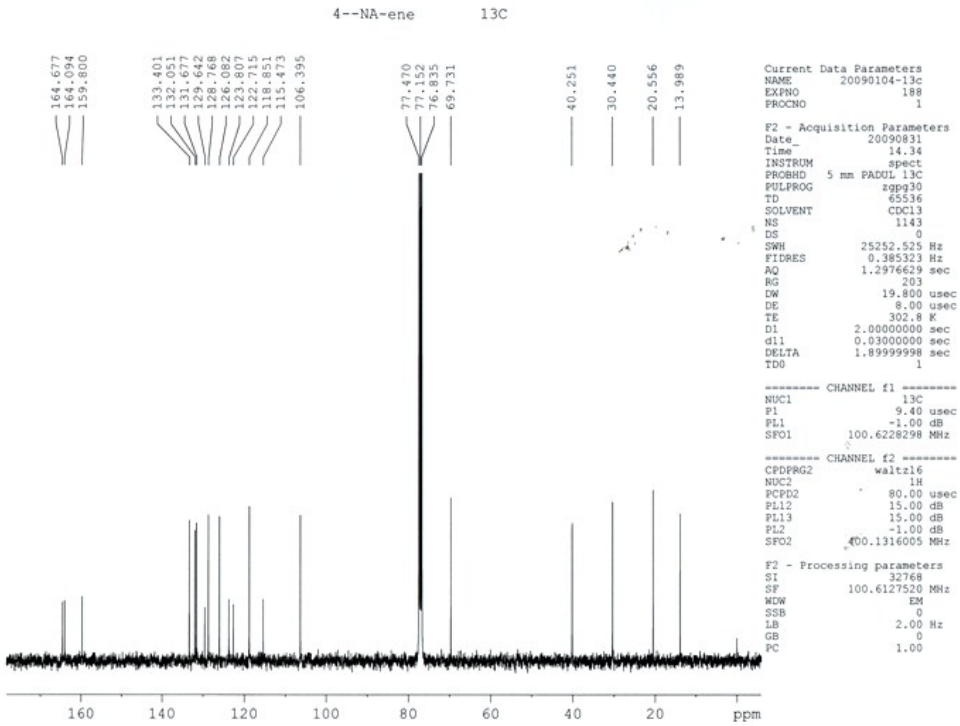

Figure S5. ^{13}C-NMR spectrum of chemosensor 1

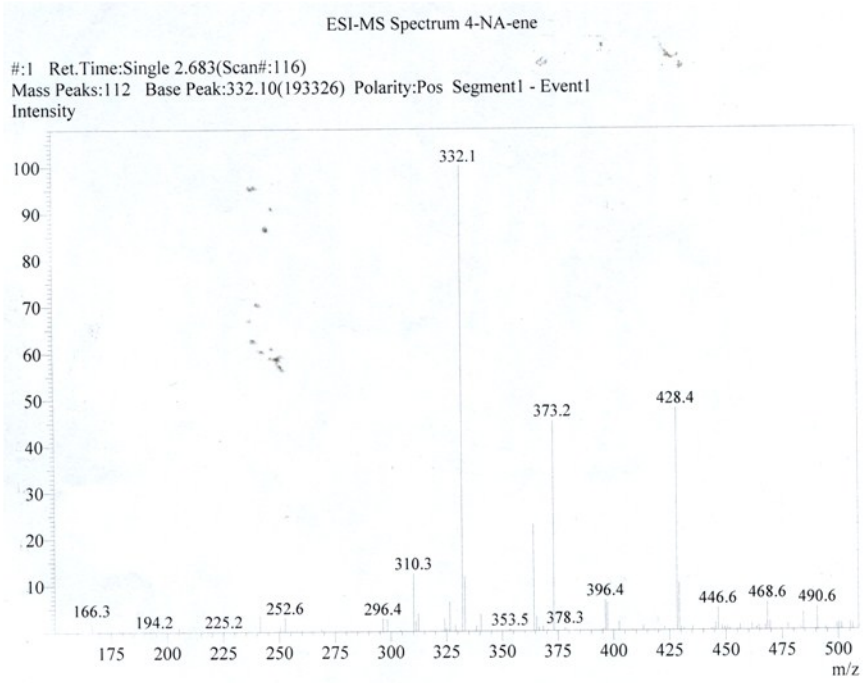

Figure S6. ESI-MS spectrum of chemosensor 1

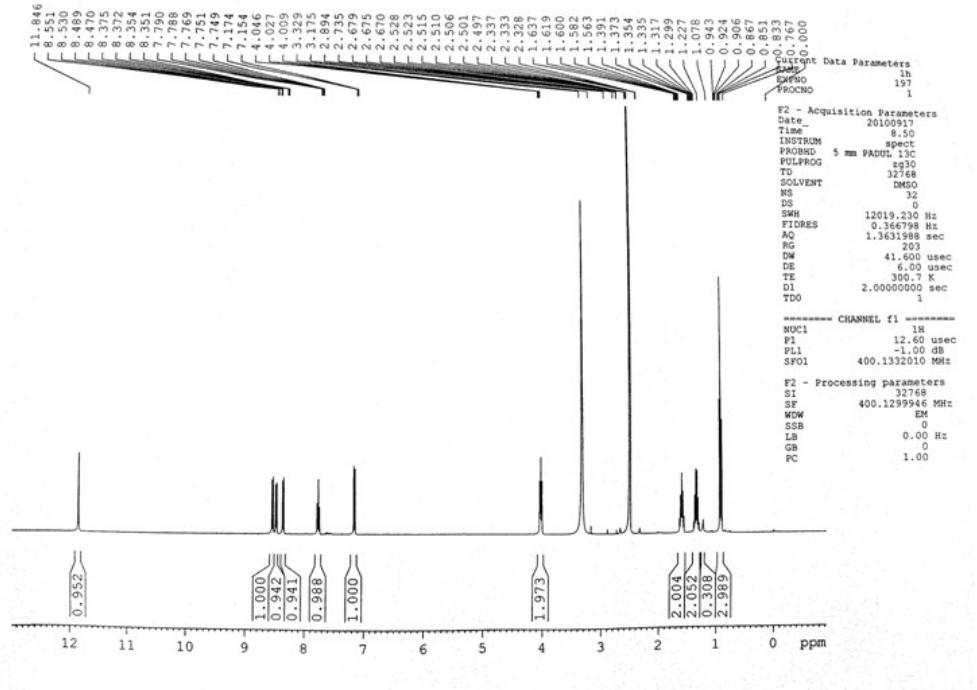

Figure S5. ^{1}H-NMR spectrum of the Pd^{0}-catalyzed deallylation product

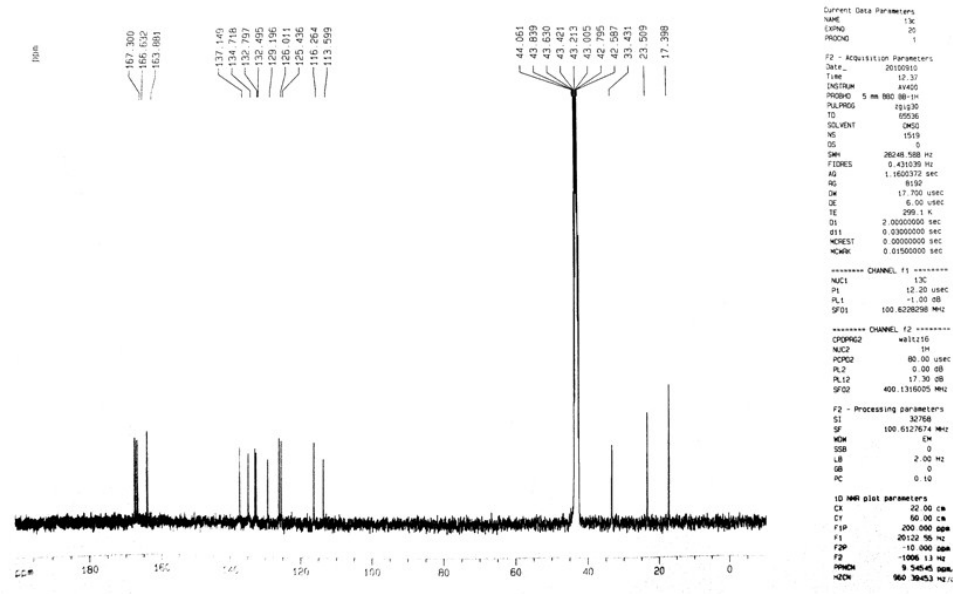

Figure S7. ^{1}C-NMR spectrum of the Pd^{0}-catalyzed deallylation product

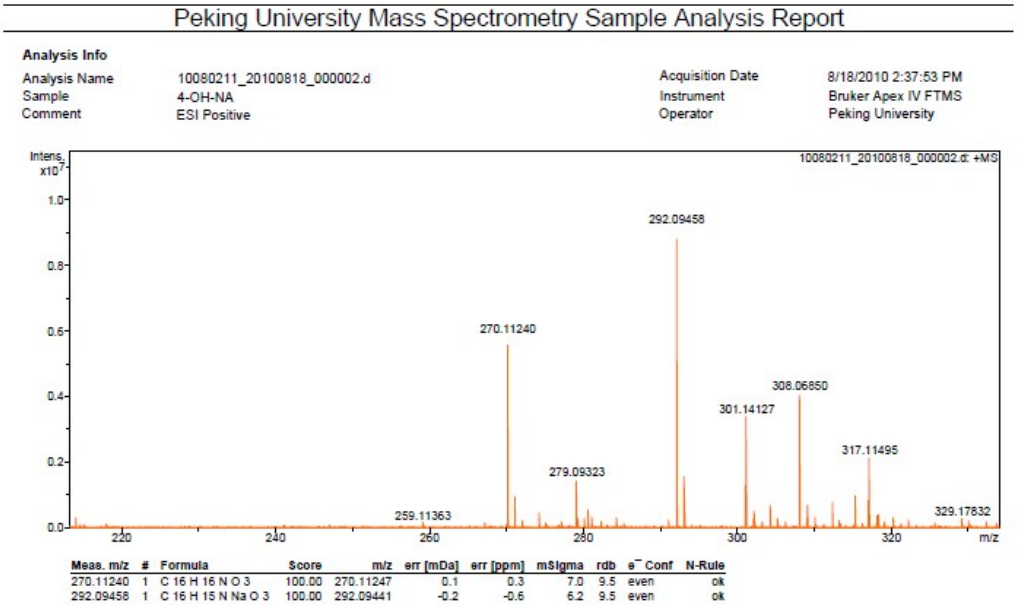

Figure S8. ESI-MS spectrum of the Pd^{0}-catalyzed deallylation product