Supporting Information

A highly sensitive sensor for colorimetric detection of palladium (II) in lysosome and its application

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Contents

Materials and instruments

All reagents and organic solvents used in this paper were of analytical grade and were purchased from Aladdin Ltd, and were used directly unless otherwise stated. The silica gel (200-400 mesh) packed for the column chromatography was provided by Qingdao Ocean Chemicals. Spectral properties were tested by UV-2550 UV/Vis spectrophotometer (Hitachi Japan) and F-4600 fluorescence spectrophotometer (Hitachi Japan), respectively. The chemical structure characterizations were measured by nuclear magnetic resonance (NMR) spectra (Bruker AVANCE III 400 M/300 M) and high resolution mass spectra (Agilent 6510 Q-TOF LC/MS instrument (Agilent Technologies, Palo Alto, CA)), respectively. The pH was recorded by FE 20/EL 20PH meter (Mettler-Toledo Instruments (Shanghai) CO., Ltd.). Cell imaging was conducted in a laser scanning confocal microscope (Olympus FV 1000-IX81).

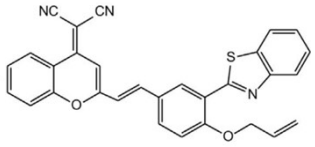
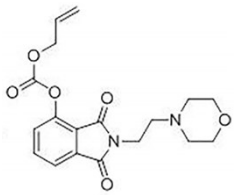
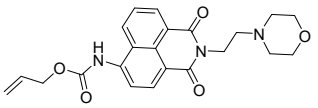
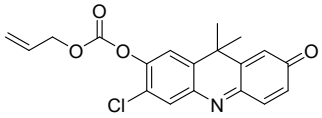
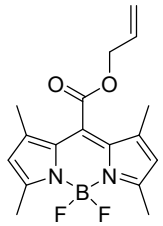
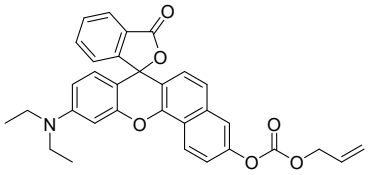
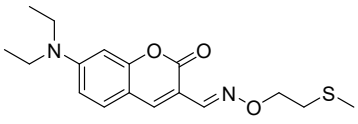
Standard MTT assay

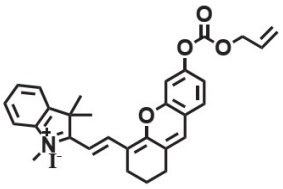
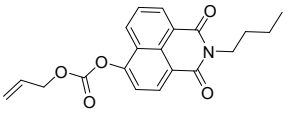
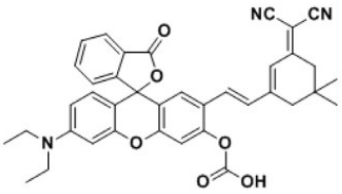
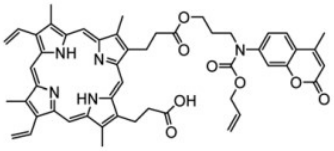
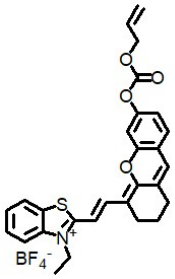
HeLa cells were inoculated into 96-well plates and allowed to adhere for 12 hours. And then, different concentrations of **BHCy-Pd** (0, 0.1, 0.5, 1, 2, and 5 μM) were added to the cells and cultured for another 24 hours. The culture solution was changed and washed three times with PBS, and then 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide was added to each well and cultured for another 4 hours. The culture solution was changed again and washed before adding DMSO, and then the absorbencies were measured at 490 nm after standing for 2 hours.

Configuration method of metal solutions

The stock solutions of metal ions for were prepared from their chloride or nitrate salts in redistilled water. The stock solutions of anions for selective experiments were prepared with metal sodium salts in redistilled water. The solution was shaken well and kept at room temperature.

Table S1. Comparison of **BHCy-Pd** with reported Pd^{2+} probes.

No.	Structures	λ_{em} (nm)	Targeting	LOD (nM)	*Ref.*
1		717	no	48	*Talanta, 183 (2018) 164–171*
2		511	Lysosome	28	*Spectrochim. Acta A Mol. Biomol. Spectrosc., 205 (2018) 66–71*
3		545	Lysosome	9	*Talanta, 231 (2021) 122365*
4		665	no	2.2	*Sens. Actuators Chem. B, 258 (2018) 98–104*
5		513	no	20.3	*Dyes Pigment., 170 (2019) 107656*
6		636	no	1.6	*Dyes Pigment., 152 (2018) 112–117*
7		500	no	41.5	*Dyes Pigment., 148 (2018) 286-291*

8		721	no	22.4	*Dyes Pigment., 137 (2017) 293-298*
9		560	no	16	*Chin. Chem. Lett., 31 (2020) 2913–2916*
10		735	no	140	*Spectrochim. Acta A Mol. Biomol. Spectrosc., 267 (2022) 120500*
11		440	no	382	*Chem. Sci., 12 (2021) 9977–9982*
12		**740**	**Lysosome**	**5.9**	***This work***

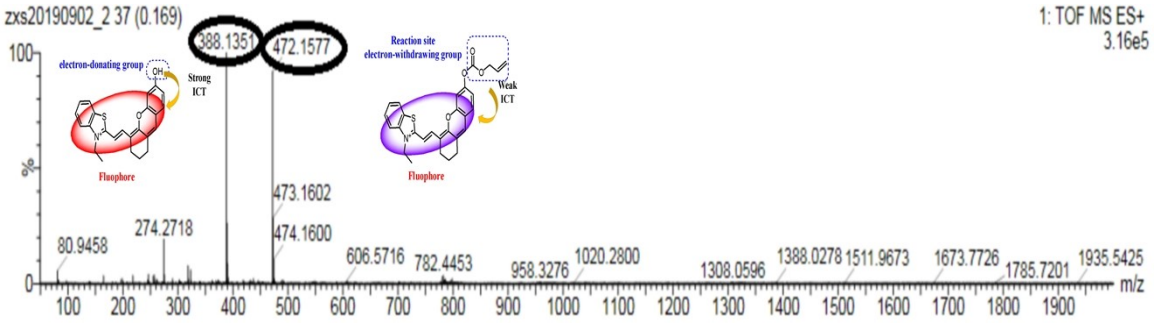


Fig. S1. HRMS spectrum of **BHCy-Pd** recorded after reaction with 0.5 equiv. $PdCl_2$.

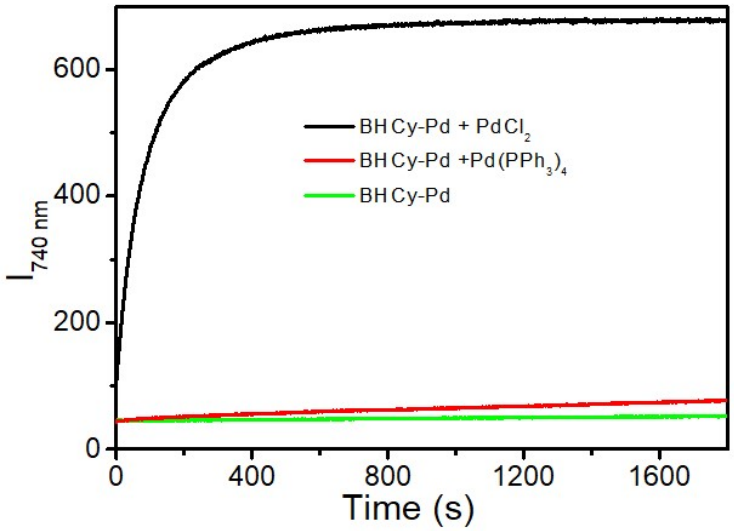


Fig. S2. Time-dependent fluorescence responses of **BHCy-Pd** (10 μM) in the absence/presence of $PdCl_2$ (10 μM) and $Pd(PPh_3)_4$ (10 μM). The conditions: PBS (10 mM, pH 7.4, containing 25% EtOH), λ_{ex} = 680 nm, slit = 5/5 nm.

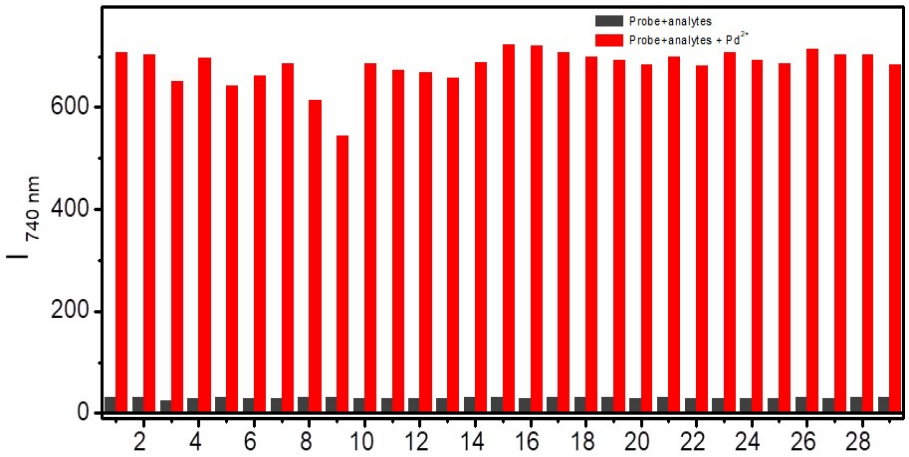


Fig. S3. Fluorescence intensity of **BHCy-Pd** (10 μM) at 740 nm upon addition of different species (10 μM) in the absence/presence of Pd^{2+} (10 μM). 1-29: blank, Li^+, Fe^{3+}, Cu^{2+}, Pb^{2+}, Zn^{2+}, Mg^{2+}, Ag^+, Hg^{2+}, Al^{3+}, Cd^{2+}, Co^{2+}, Cr^{2+}, Ca^{2+}, Na^+, Ni^{2+}, K^+, Mn^{2+}, CO_3^{2-}, I^-, Br^-, AcO^-, HOCl, H_2O_2, NO_2^-, Cys, Hcy, GSH, Vc. The conditions: PBS (10 mM, pH 7.4, containing 25% EtOH), λ_{ex} = 680 nm, slit = 5/5 nm.

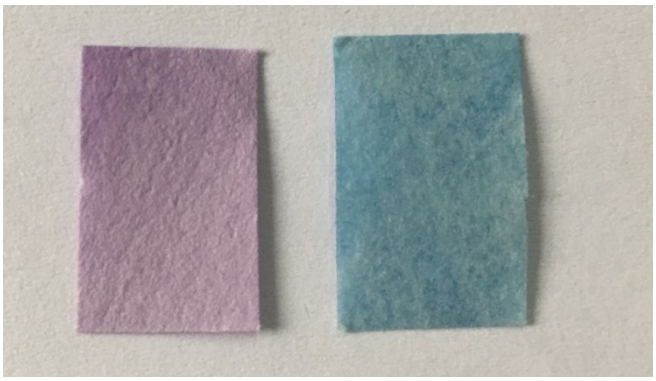


Fig. S4. Color change of test strip before and after treated with Pd^{2+} (1 μM).

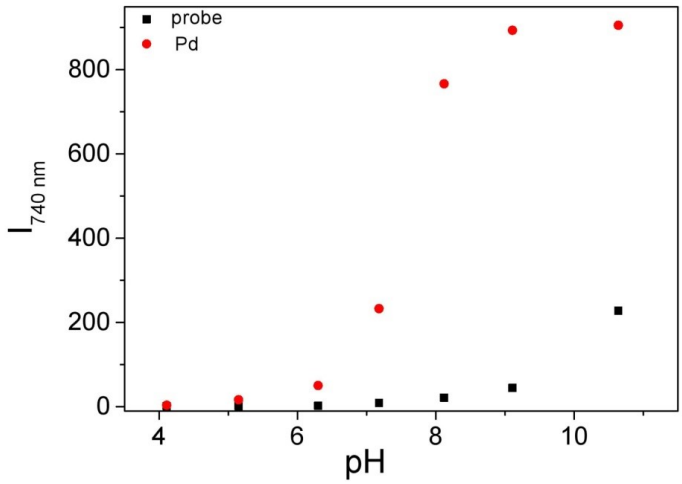


Fig. S5 Fluorescence intensity of **BHCy-Pd** (10 μM) at 740 nm at different pH buffer in the absence/presence of Pd^{2+} (10 μM).

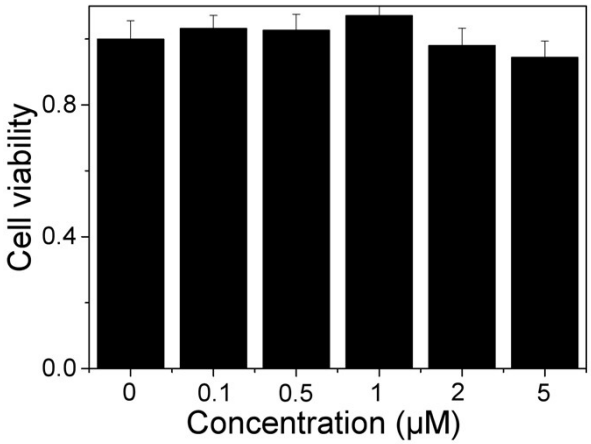


Fig. S6 MTT assay for the survival rate of HeLa cells treated with various concentrations of **BHCy-Pd** for 24 h. Error bars represent the standard deviations of 5 trials.

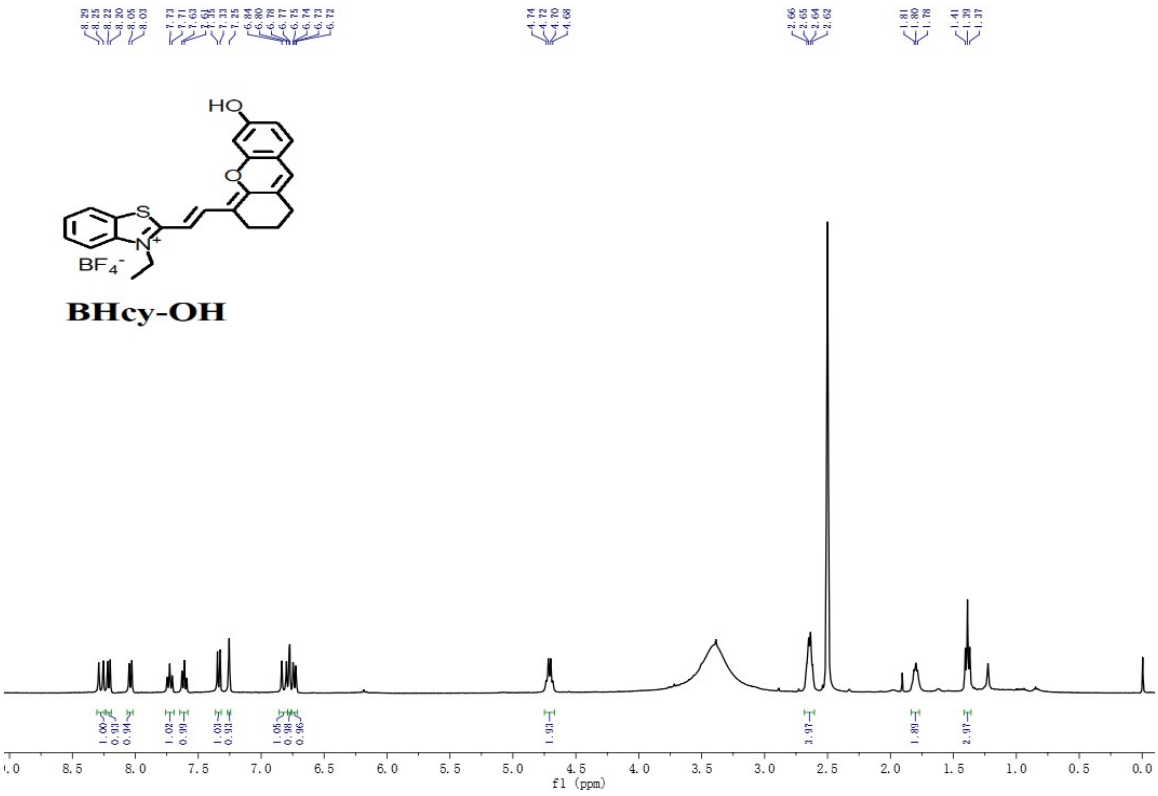


Fig. S7 ^{1}H NMR spectra of compound **BHCy-OH** in DMSO-d_6.

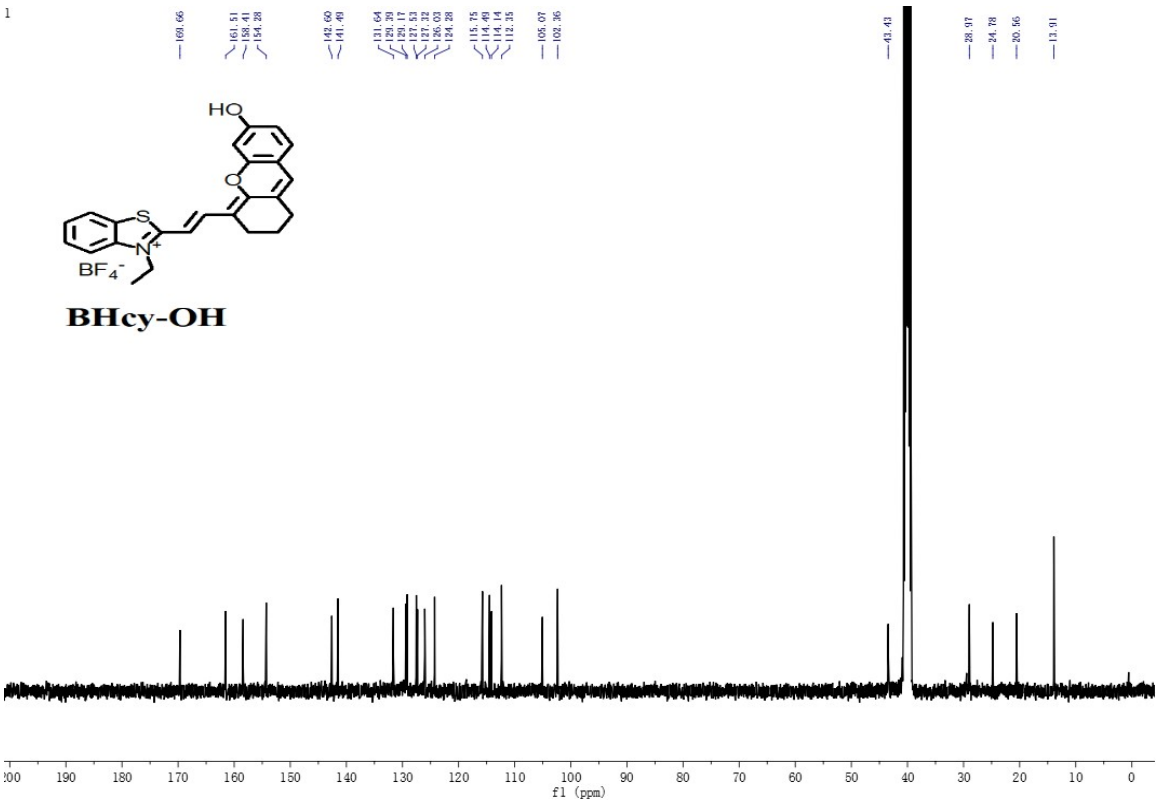


Fig. S8 ^{13}C NMR spectra of compound **BHCy-OH** in DMSO-d_6.

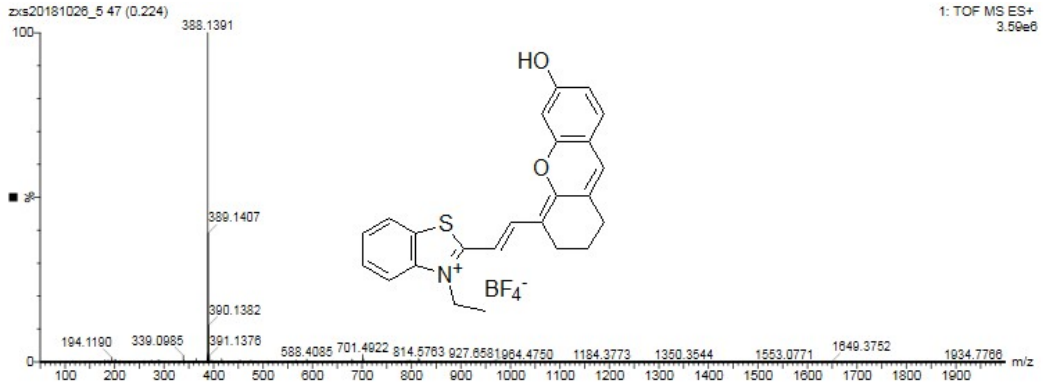


Fig. S9. HRMS spectrum of compound **BHCy-OH**.

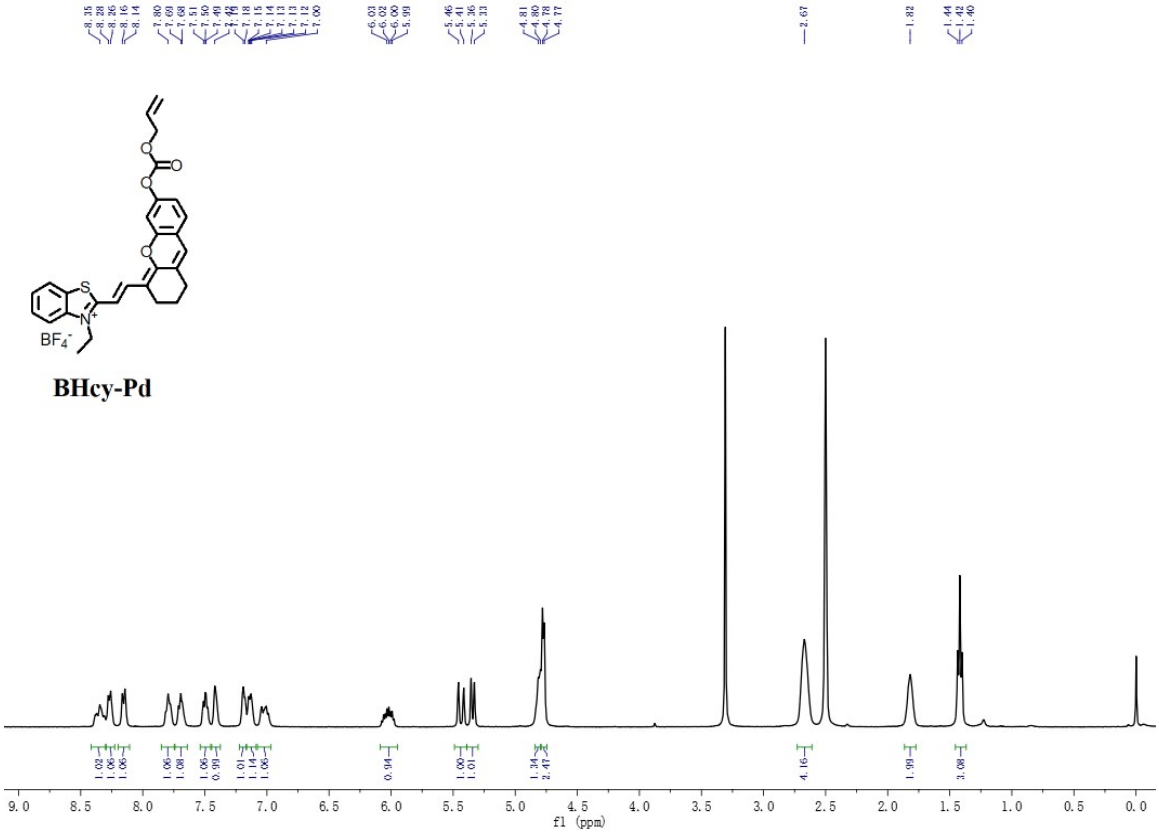


Fig. S10 ^{1}H NMR spectra of compound **BHCy-Pd** in DMSO-d_6.

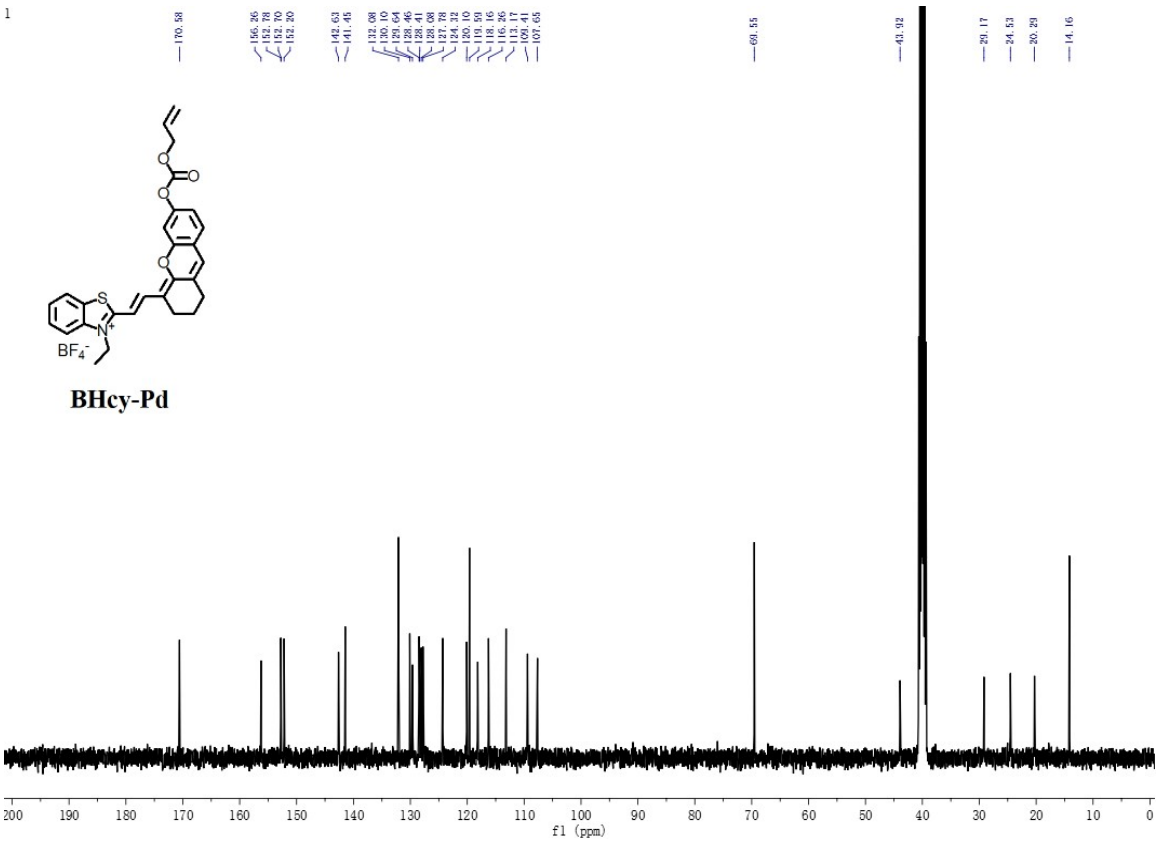


Fig. S11 ^{13}C NMR spectra of compound **BHCy-Pd** in DMSO-d_6.

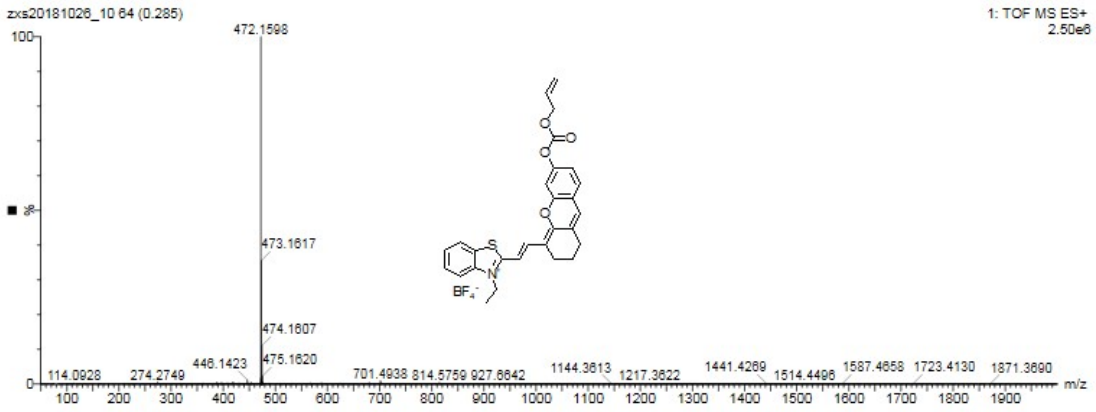


Fig. S12 HRMS spectra of compound **BHCy-Pd**.