Electronic Supplementary Information (ESI) for New Journal of Chemistry

# Electronic Supplementary Information

# A Sensitive Colorimetric and Ratiometric Fluorescent Chemodosimeter for $Hg^{2+}$ and Its Application for Bioimaging

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## Contents

## 1. Fluorescence spectra

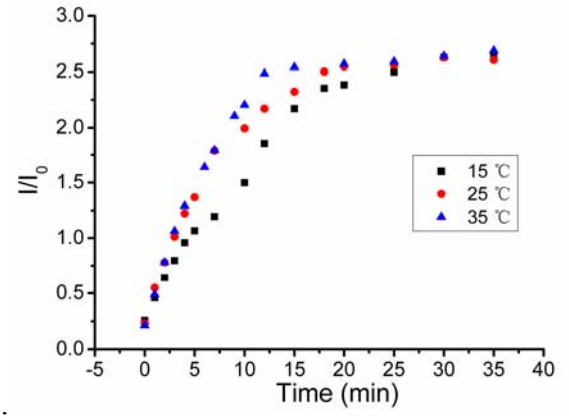


**Fig. S1**. The time-dependent fluorescence intensity change acquired for a mixture of 5 μM **1** and 5 μM $HgCl_2$ at 15 °C, 25 °C and 35 °C in PBS buffer solutions (containing 1% $CH_3CN$). Ex = 408 nm. Slit: 10.0 nm/10.0 nm.

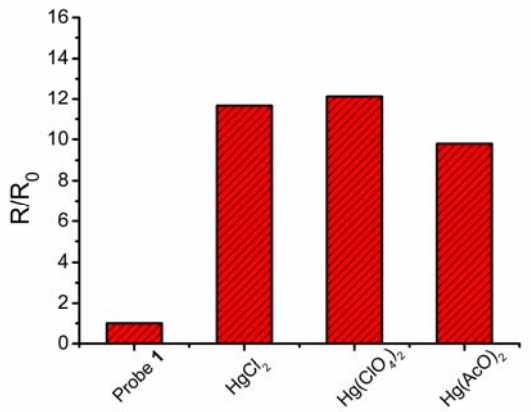


**Fig. S2.** Fluorescence responses of **1** (5 μM) to mercury metal sources: $HgCl_2$ (5 μM), $Hg(ClO_4)_2$ (5 $\mu$M) and $Hg(OAc)_2$ (5 μM), in PBS buffer solutions (pH = 7.4, containing 1% $CH_3CN$). Bars represent the ratio of the fluorescence intensity ratio in the presence (R) and absence ($R_0$) of mercury metal sources. $R = I_{550\ nm}/I_{506\ nm}$, Ex = 408 nm. Slit: 10.0 nm/10.0 nm. Each spectrum was acquired 30 min after mercury metal sources addition.

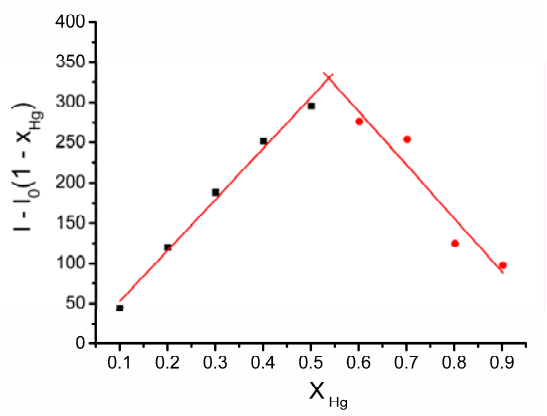


**Fig. S3.** Job's plot for determining the stoichiometry of **1** and $Hg^{2+}$ in PBS buffer solutions (pH = 7.4, containing 1% $CH_3CN$,); The total concentration of **1** and $Hg^{2+}$ was 5 μM; $X_{Hg} = [Hg^{2+}]/([Hg^{2+}]+ [\mathbf{1}]$; Ex = 408 nm. Slit: 10.0 nm/10.0 nm.

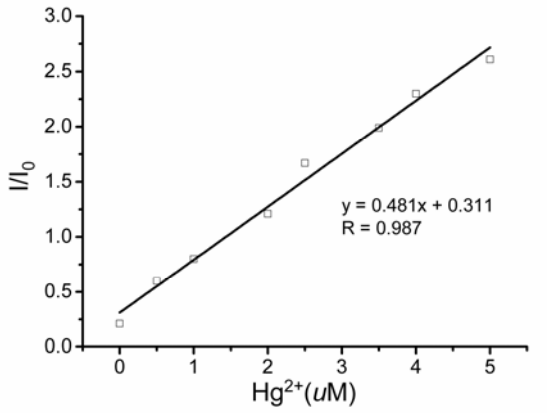


**Fig. S4.** Fluorescence spectra of **1** in the presence of increasing concentrations of $HgCl_2$ (0, 0.5, 1, 2, 2.5, 3.5, 4, 5 μM) in PBS buffer solutions (containing 1% $CH_3CN$). Ex = 408 nm. Slit: 10.0 nm/10.0 nm. Each spectrum was acquired 15 min after $HgCl_2$ addition at 25 °C.

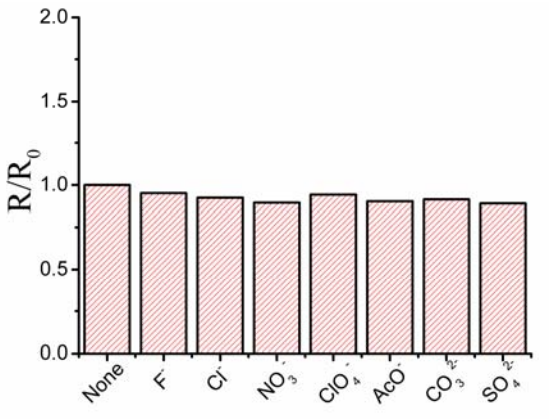


**Fig. S5.** Fluorescence spectra of **1** (5 μM) in the absence and presence of different anions (5 equiv): $F^-$, $Cl^-$, $NO_3^-$, $ClO_4^-$, $AcO^-$, $CO_3^{2-}$ and $SO_4^{2-}$ (as their $Na^+$ or $K^+$ salts) in PBS buffer solutions (pH = 7.4, containing 1% $CH_3CN$). Bars represent the ratio of the fluorescence intensity ratio in the presence (R) and absence ($R_0$) of various anions. R = $I_{550\ nm}/I_{506\ nm}$, Ex = 408 nm. Slit: 10.0 nm/10.0 nm. Each spectrum was acquired 30 min after anions addition at 25 °C.

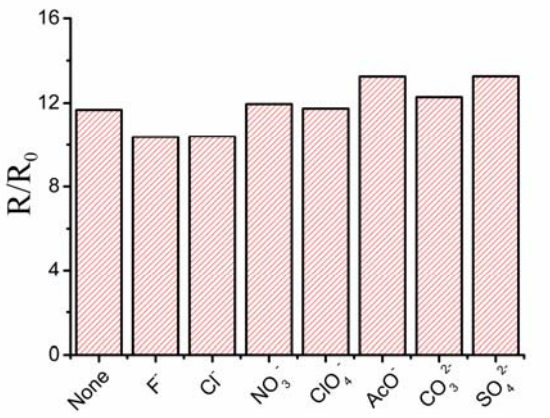


**Fig. S6.** Fluorescence spectra of **1**-$Hg^{2+}$ system (5 μM) in the absence and presence of different anions (5 equiv): $F^-$, $Cl^-$, $NO_3^-$, $ClO_4^-$, $AcO^-$, $CO_3^{2-}$ and $SO_4^{2-}$ (as their $Na^+$ or $K^+$ salts) in PBS buffer solutions (pH = 7.4, containing 1% $CH_3CN$). Bars represent the ratio of the fluorescence intensity ratio in the presence (R) and absence ($R_0$) of various anions. R = $I_{550\ nm}/I_{506\ nm}$, Ex = 408 nm. Slit: 10.0 nm/10.0 nm. Each spectrum was acquired 30 min after anions addition at 25 °C.

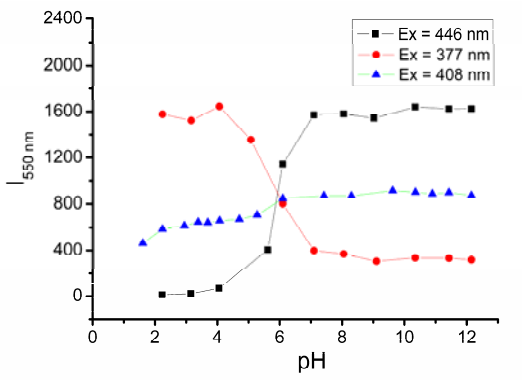


**Fig. S7** The fluorescence intensity of **2**(5 μM) as a function of pH in aqueous solutions(containing 1% $CH_3CN$).

## 2. Determination of the detection limit

The detection limit was calculated based on the fluorescence titration. The fluorescence emission spectrum of **1** was measured by ten times and the standard deviation of blank measurement was achieved. To gain the slope, the ratio of the fluorescence intensity at 550 nm to the fluorescence intensity at 506 nm ($I_{550\ nm}/I_{506\ nm}$) was plotted as a concentration of $Hg^{2+}$. So the detection limit was calculated with the following equation:

Detection limit = $3\sigma/k$

Where σ is the standard deviation of blank measurement, $k$ is the slope between the fluorescence intensity ratios versus $Hg^{2+}$.

The detection limits for $Hg^{2+}$ concentration were deduced to be 3.6 nM.

## 3. NMR Data

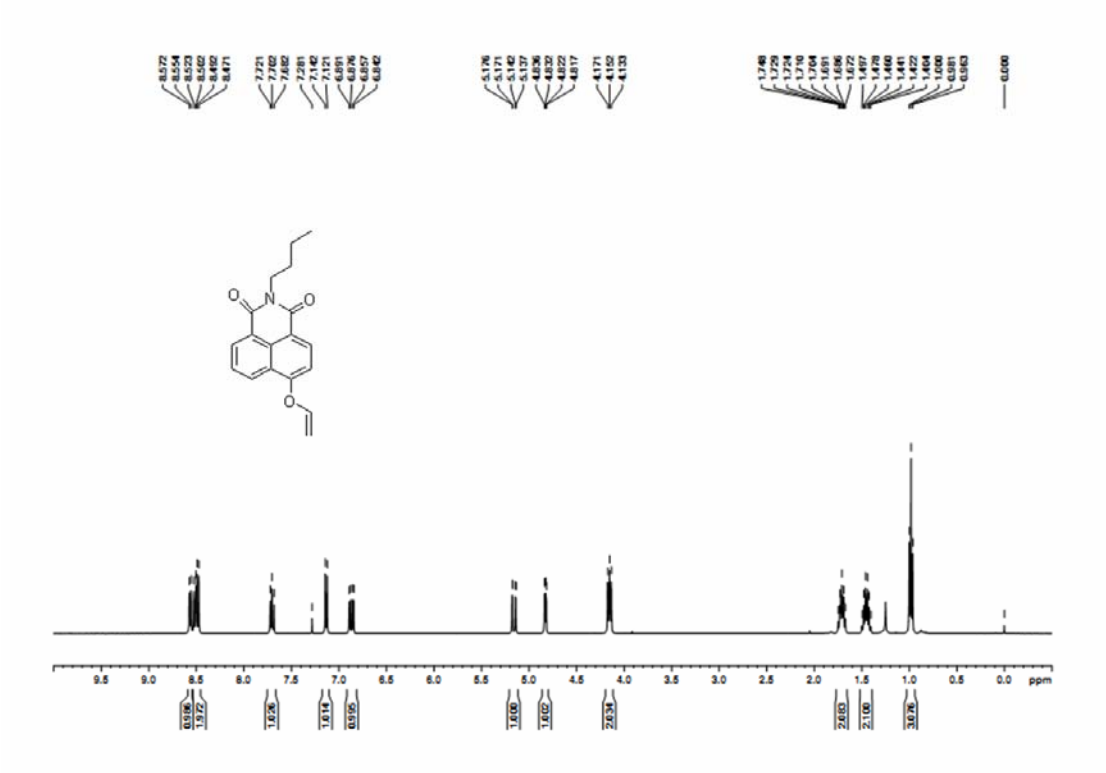

**Fig. S8** $^{1}$H NMR spectrum of chemodosimeter **1** ($CDCl_3$)

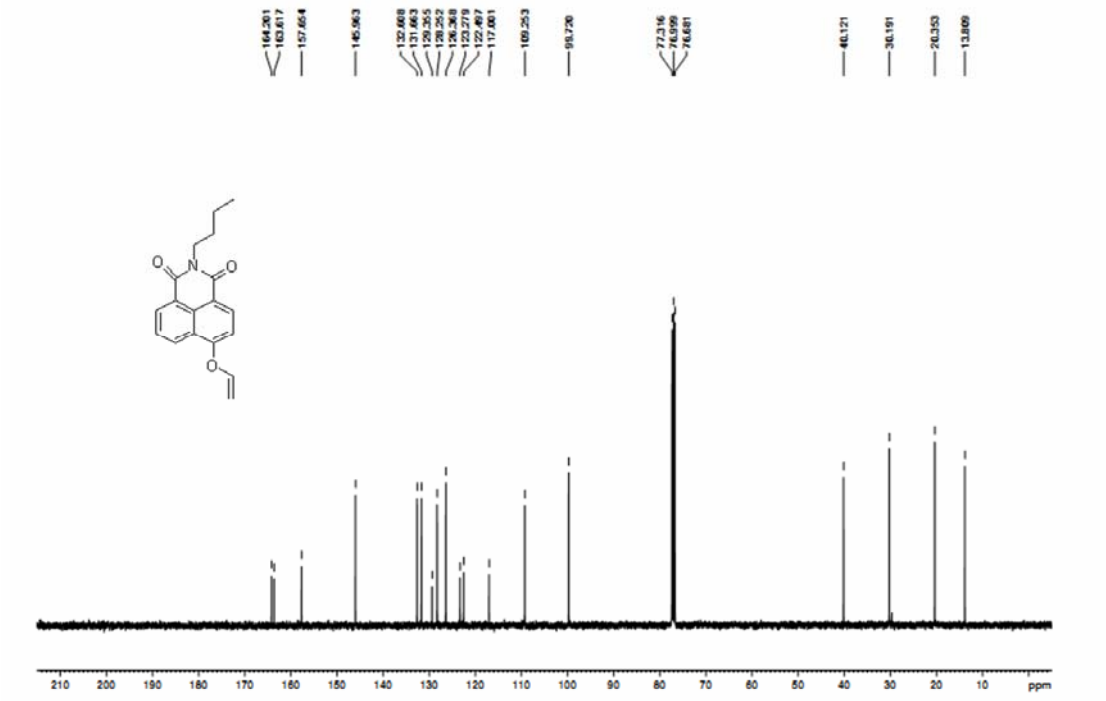

**Fig. S9** $^{13}$C NMR spectrum of chemodosimeter **1** ($CDCl_3$)

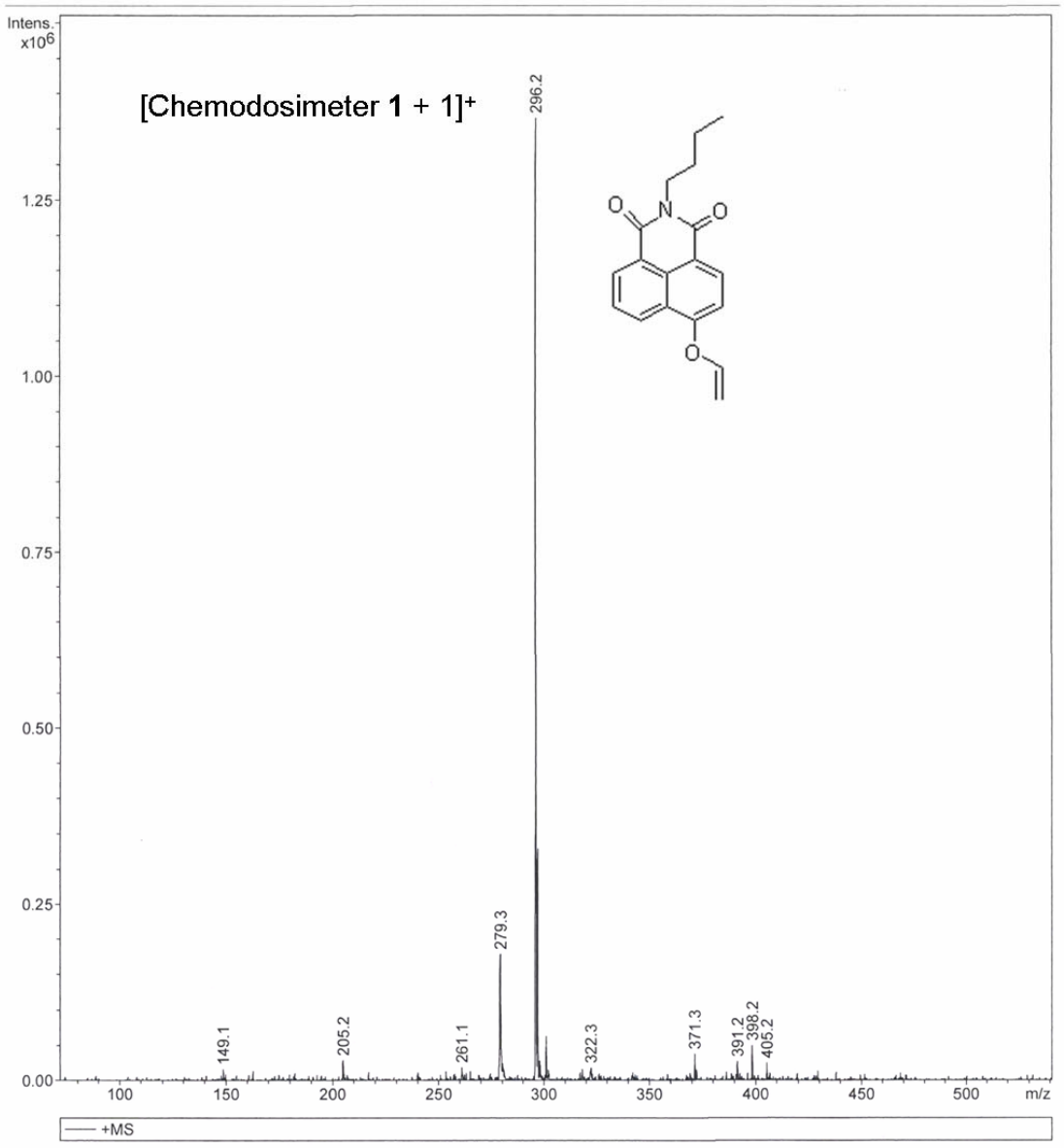


**Fig. S10** ESI-mass spectrum of chemodosimeter **1**

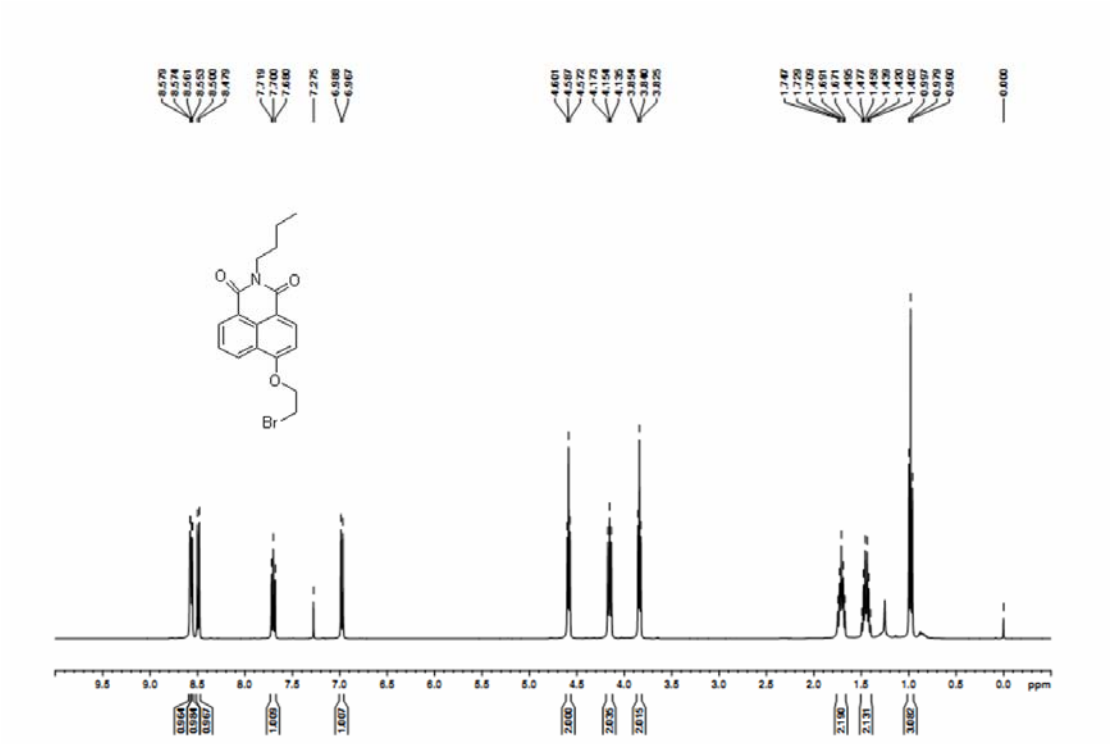


**Fig. S11** $^{1}$H NMR spectrum of compound **3** ($CDCl_3$)

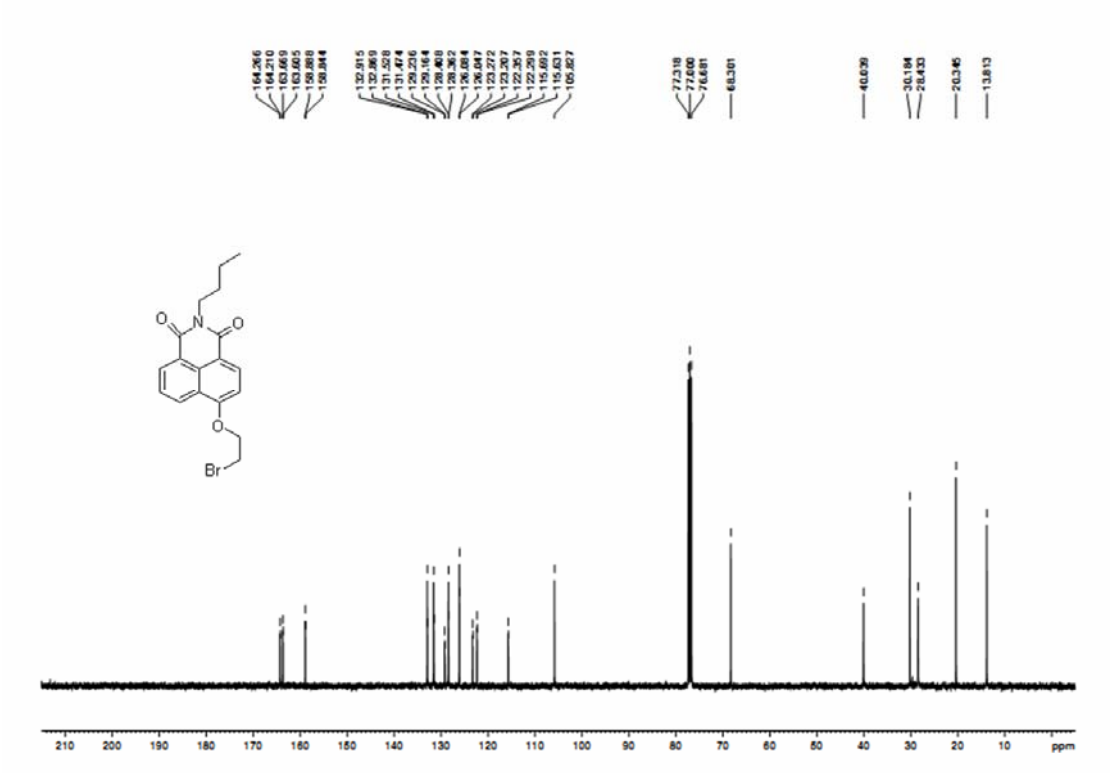


**Fig. S12** $^{13}$C NMR spectrum of compound **3** ($CDCl_3$)

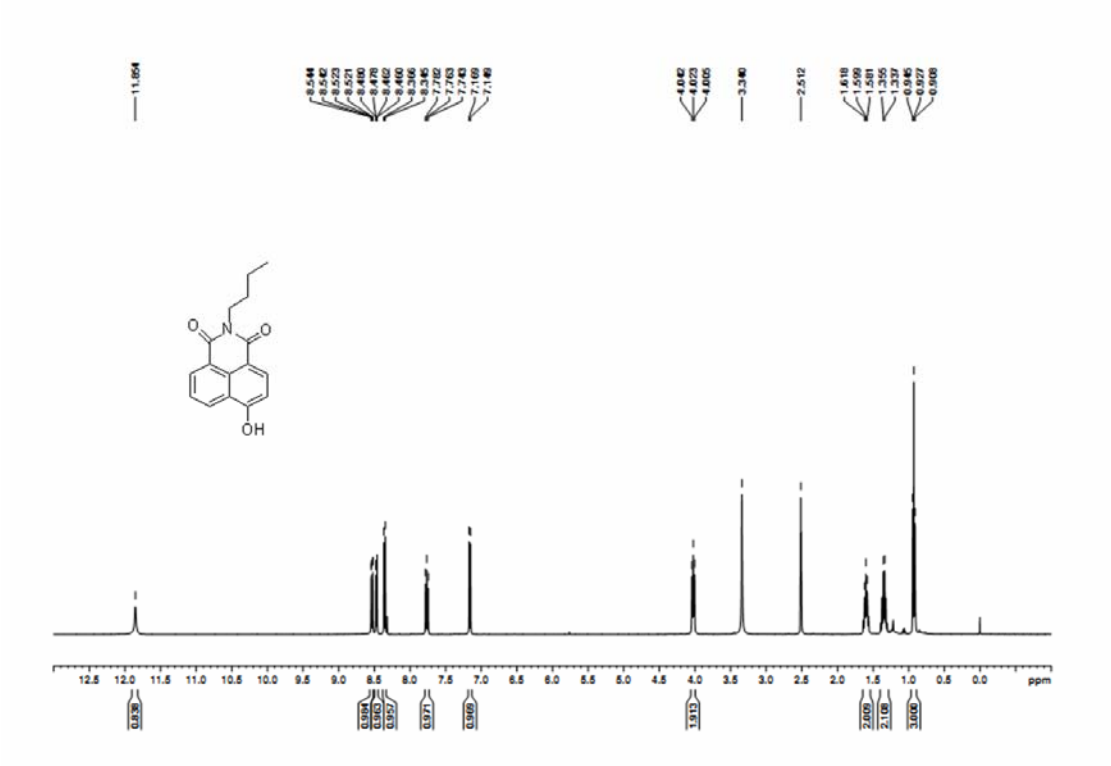


**Fig. S13** $^{1}$H NMR spectrum of compound **2** ($d_6$-DMSO)

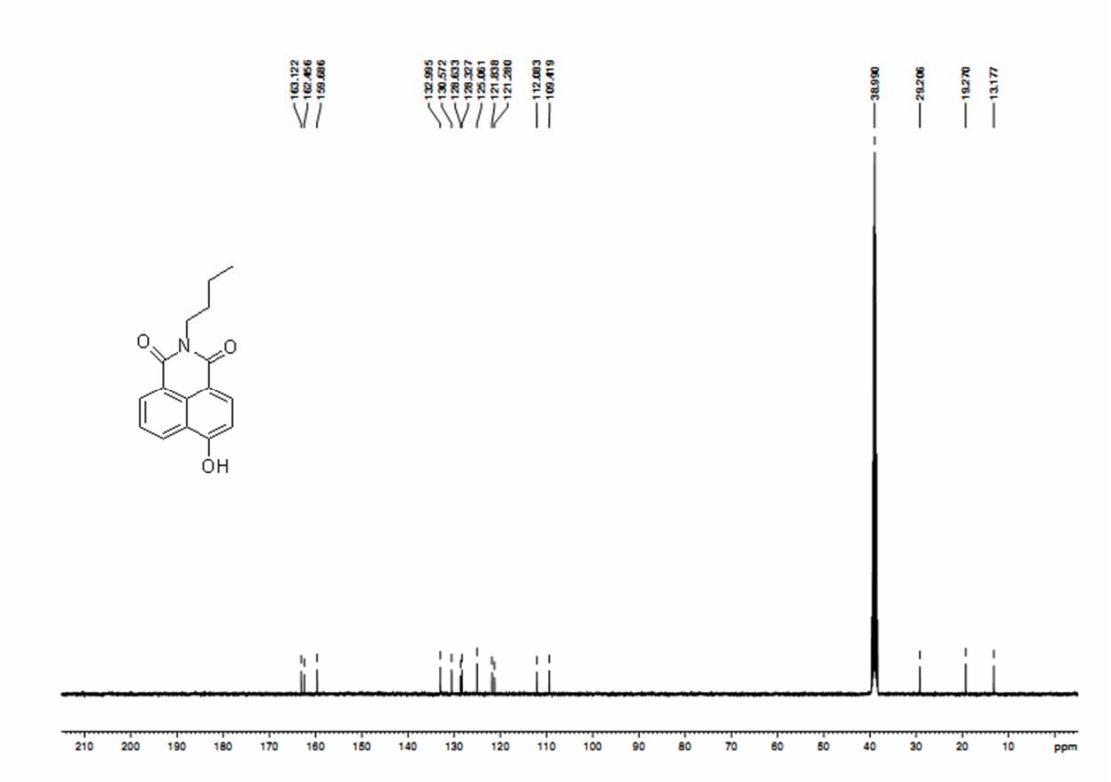


**Fig. S14** $^{13}$C NMR spectrum of compound **2** ($d_6$-DMSO)

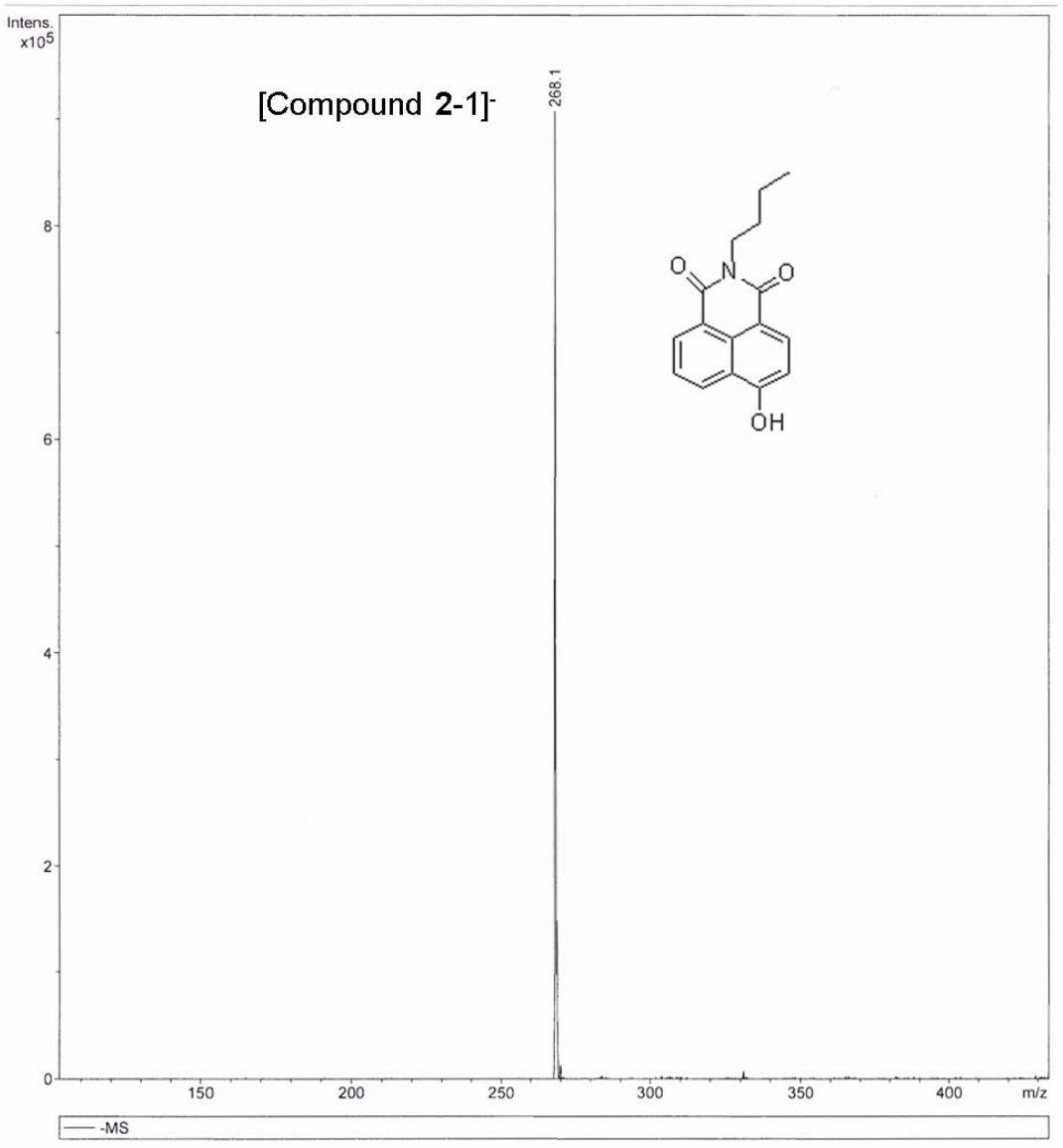


**Fig. S15** ESI-mass spectrum of compound **2**