Mercury$^{(II)}$-mediated formation of imide-Hg-imide complexes

Can-liang Fang, [a, b] Jin Zhou, [a, b] Xiang-jun Liu, [a] Ze-hui Cao, [a] and Di-hua Shangguan*

Beijing National Laboratory for Molecular Sciences, Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China; E-mail: sgdh@iccas.ac.cn
[b] *Graduate School of the Chinese Academy of Sciences, Beijing 100039, China*

Electronic Supporting Information

MS spectra of imide-Hg-imide:

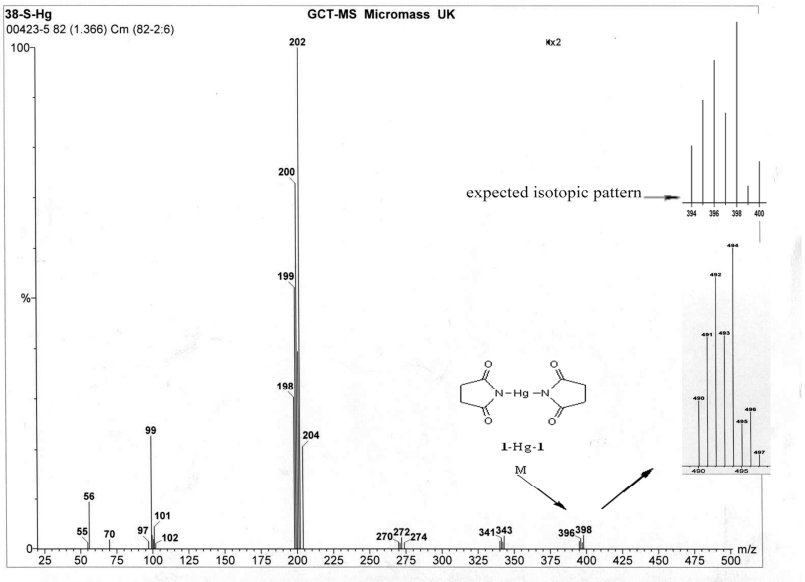


Fig. S1a EI-MS of complex **1**-Hg-**1**

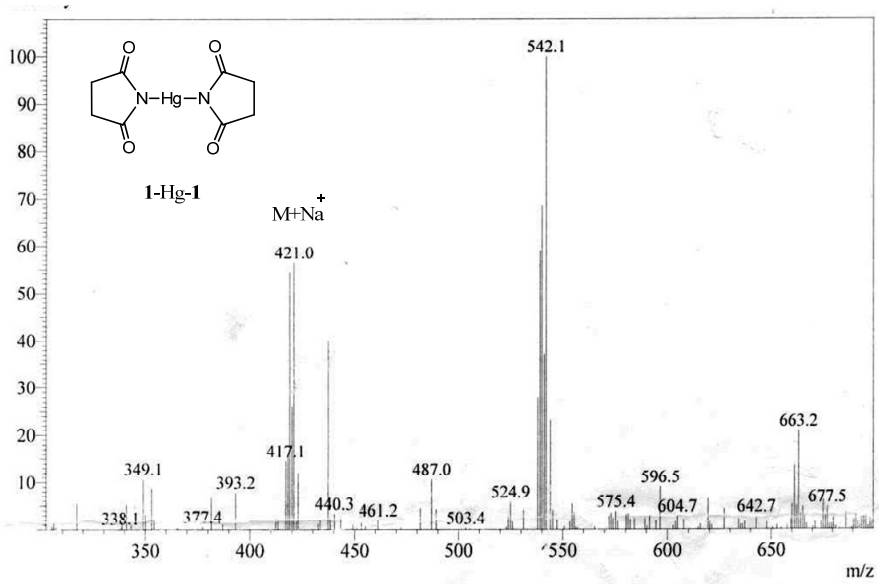


Fig. S1b ESI-MS of complex **1**-Hg-**1**

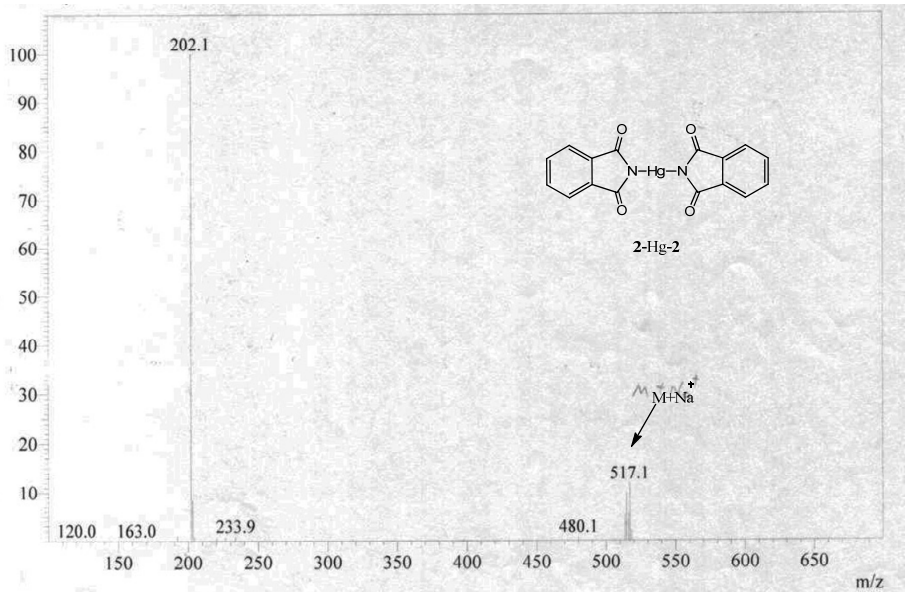


Fig. S1c ESI-MS of complex **2**-Hg-**2**

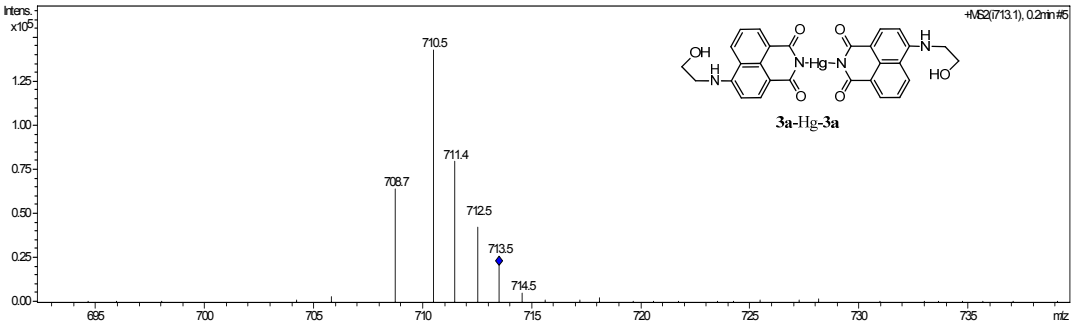


Fig. S1d ESI-MS of complex **3a**-Hg-**3a**

^{1}H NMR of 1, 1-Hg-1

All ^{1}H NMR spectra were measured in DMSO-*d6* or CD_3OH on a Bruker AVANCE-400 NMR spectrometer (400 MHz) with TMS as an internal reference

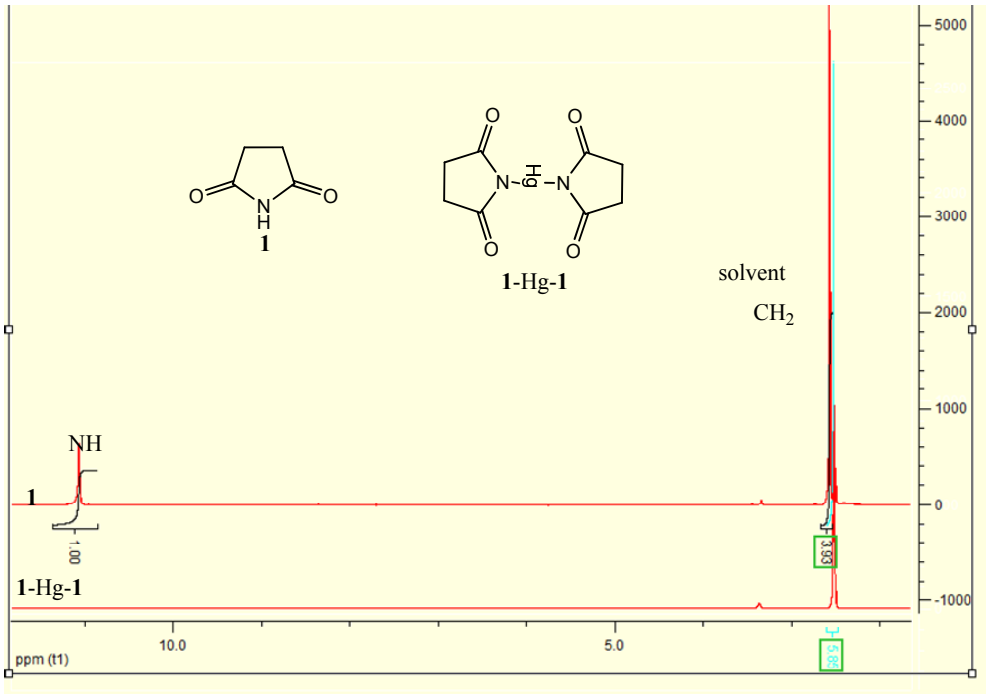


Fig. S2a ^{1}H NMR spectra of ligand **1** and **1**-Hg-**1** (400 MHz, DMSO-*d6*). **T**his figure clearly shows the complete disappearance of imido proton peak**.** However the methylene protons peak and DMSO solvent residual peak partly overlapped. Therefore ^{1}H NMR spectra (Fig. S2b) were also measured in CD_3OD to see the methylene protons peak shift.

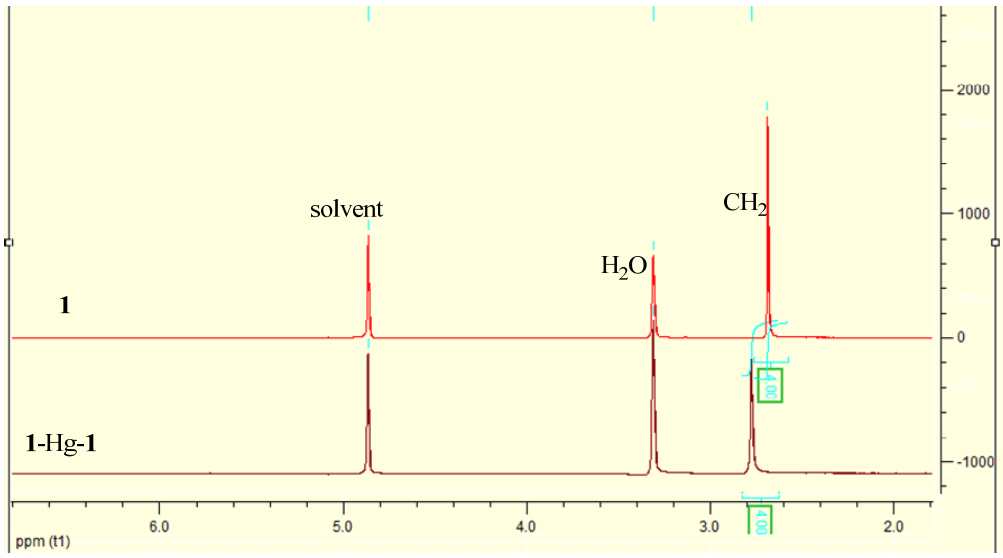


Fig. S2b ^{1}H NMR spectra of ligand **1** and **1**-Hg-**1** complex (400 MHz, CD_3OD). This figure clearly shows the downfield shift of methylene protons peak.

X-ray photoelectron spectra of 2, 2-Hg-2

X-ray photoelectron spectroscopy data were obtained with an ESCALab220i-XL electron spectrometer from VG Scientific using 300W AlKα radiation. The base pressure was about 3×10^{-9} mbar. The binding energies were referenced to the C1s line at 284.8 eV from adventitious carbon.

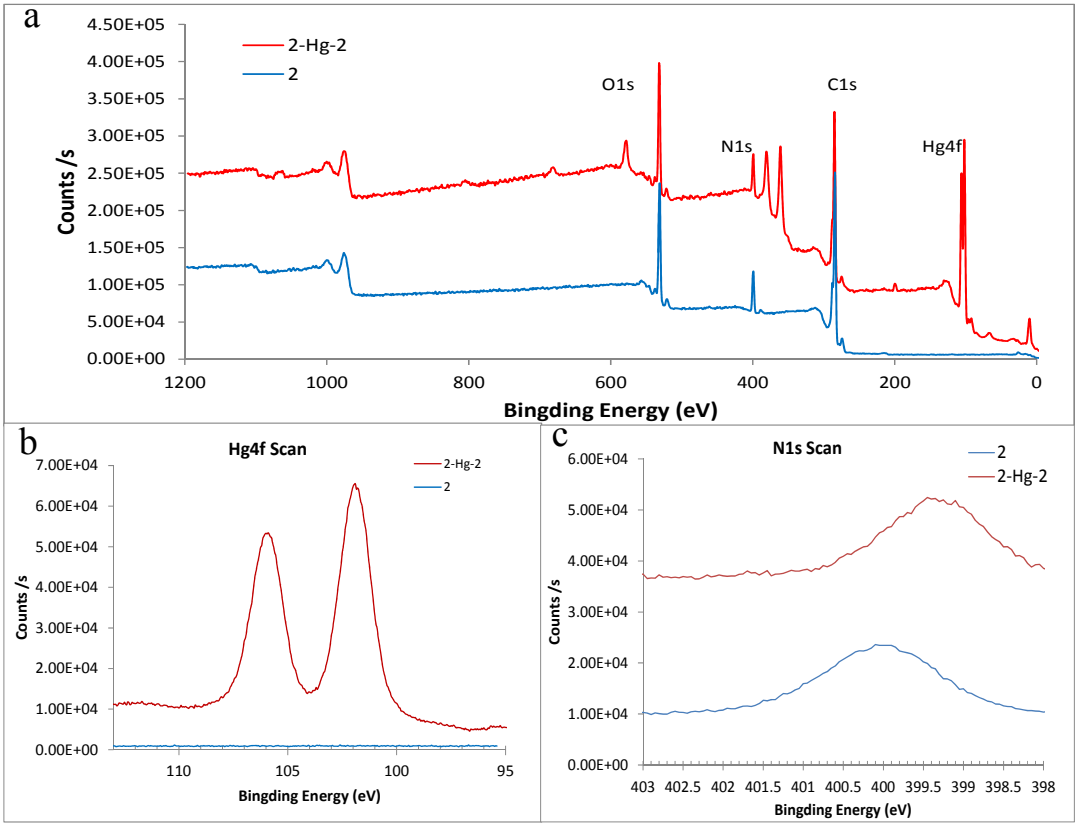


Fig. S3 XPS spectrum of **2** and **2**-Hg-**2** (a: survey spectrum; b: high-resolution Hg 4f spectrum; c: high-resolution N 1s spectrum.)

Table S1 Atom Ratio of complex **3a**-Hg-**3a**

Name	Area (P) CPS.eV	SF	Atom. %	Atom Ratio	Theoretical Ratio
C1s, 284.8eV	30060	1	72.54	28.00	28
O1s, 532.5eV	18163	2.93	14.96	5.77	6
N1s, 399.3eV	7522	1.8	10.08	3.89	4
Hg4f, 101.5eV	18893.6	18.89	2.41	0.93	1

Table S2 Atom Ratio of complex **2**-Hg-**2**

Name	Area (P) CPS.eV	SF	At. %	Atom Ratio	Theoretical Ratio
C1s, 284.8eV	130291	1	68.31	15.73	16
N1s, 399.3eV	26527.3	1.8	8.21	1.89	2
O1s, 531.6eV	84561.2	2.93	17.37	4.00	4
Hg4f, 101.8eV	196098	18.89	5	1.15	1

IR spectra of 2, 3a and complexes

FTIR spectra were measured with a Bruker Tensor27 spectrometer with KBr discs

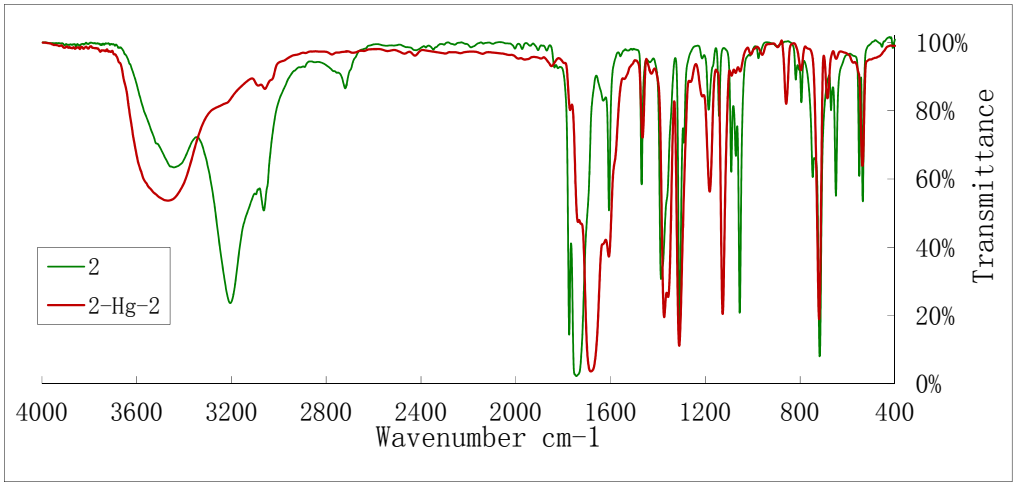


Fig. S4a IR spectrum of **2** (green) and **2**-Hg-**2**(red).

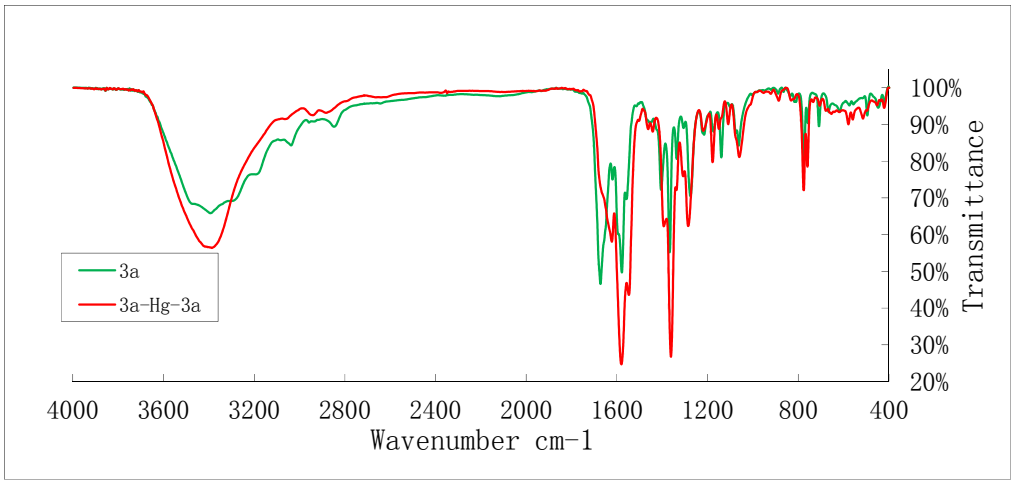


Fig. S4b IR spectrum of **3** (green) and **3a**-Hg-**3a** (red)**.**

Fluorescence detection

Appropriate amount of various Naphthalimides was dissolved in DMSO/EtOH as stock solutions. Then 1μl of Naphthalimides solution was added into 200μl water or phosphate buffer (20 mM pH 7.50). All the fluorescence measurements were taken on a SpectraMax M5 (Molecular Devices Corporation, USA)

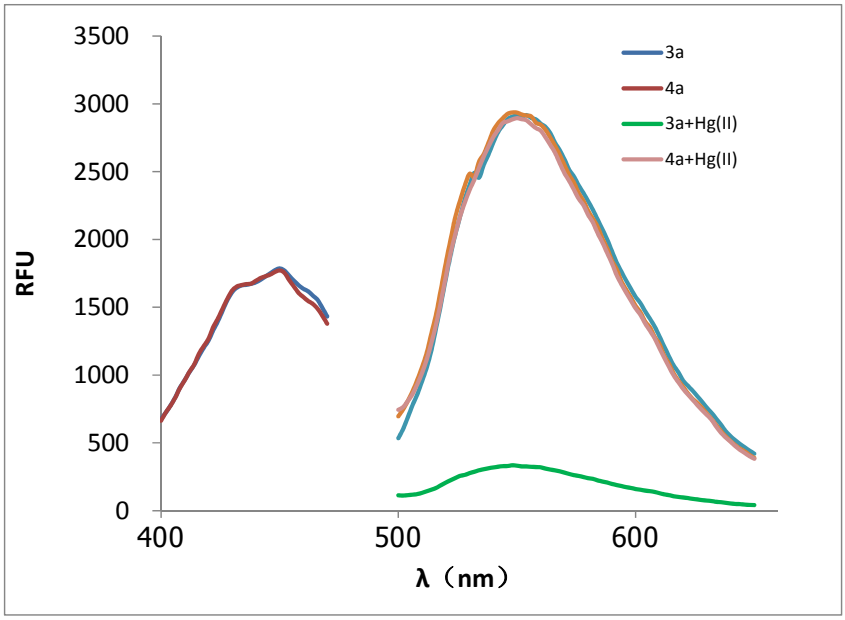


Fig. S5 Excitation and emission spectra of **3a** and **4a** in phosphate buffer at pH 7.50. (left, excitation spectra, fixed emission at 550 nm; right, emission spectra, fixed excitation at 440 nm.).

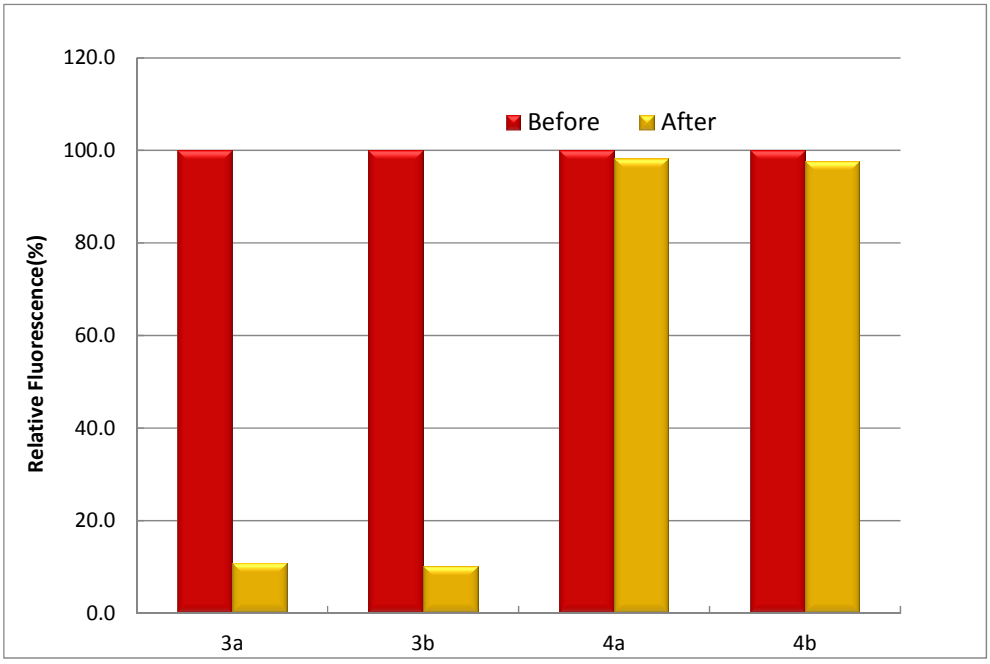


Fig. S6 The fluorescence change of **3a, 3b**, **4a and 4b** before and after adding 50 μM Hg(II) ions

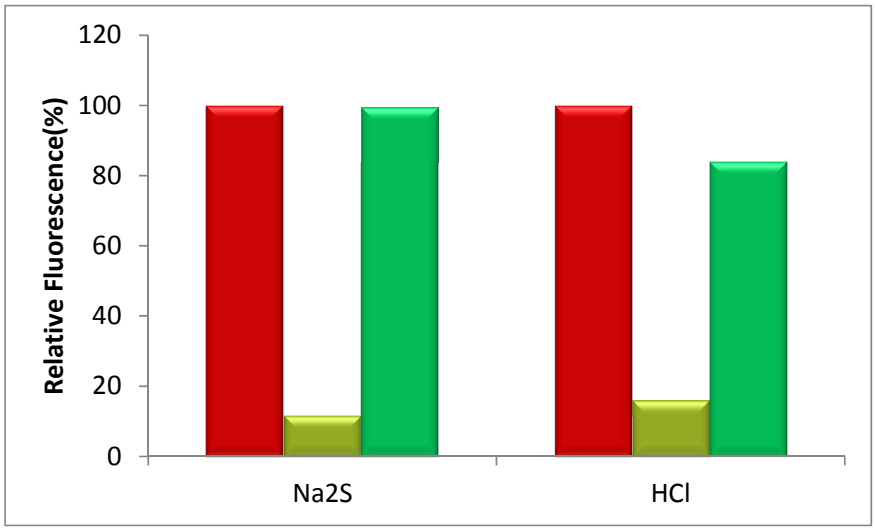


Fig. S7 The fluorescence restoration of **3a** (column red, 5 μM **3a**; yellow, adding 25 μM Hg(II); green, adding 25 μM Hg(II) and 0.5 mM Na_2S or 1 mM HCl)

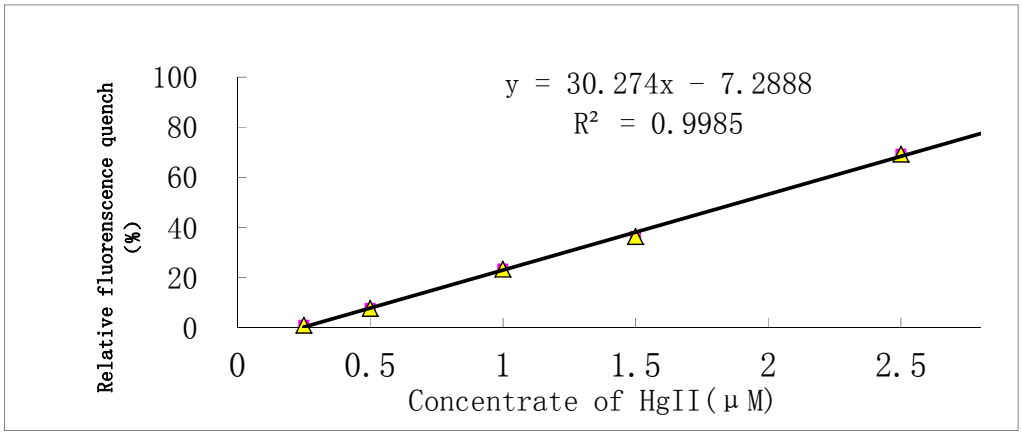


Fig. S8 The linearity of the relative fluorescence change with the concentrate of Hg(II) ions

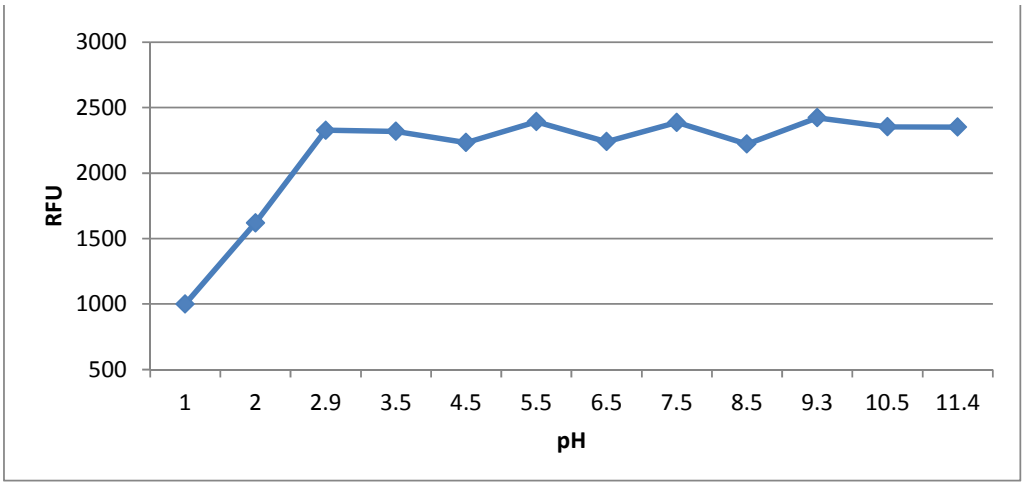
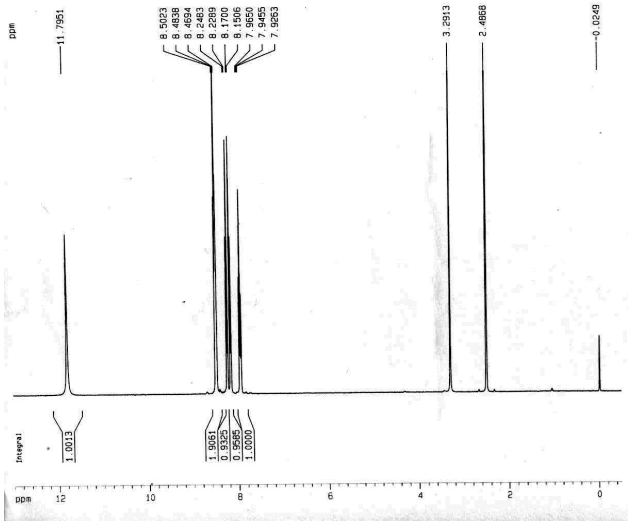
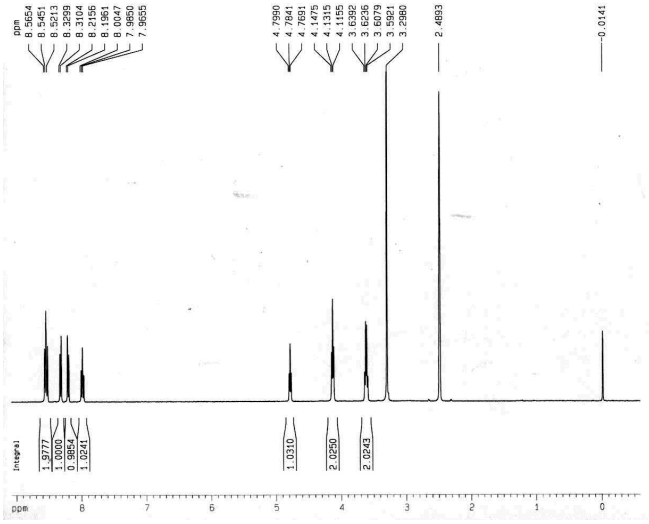


Fig. S9 Fluorescence intensities of **3a** at different pH (phosphate buffer 20 mM) (**3a**, 5 μM)

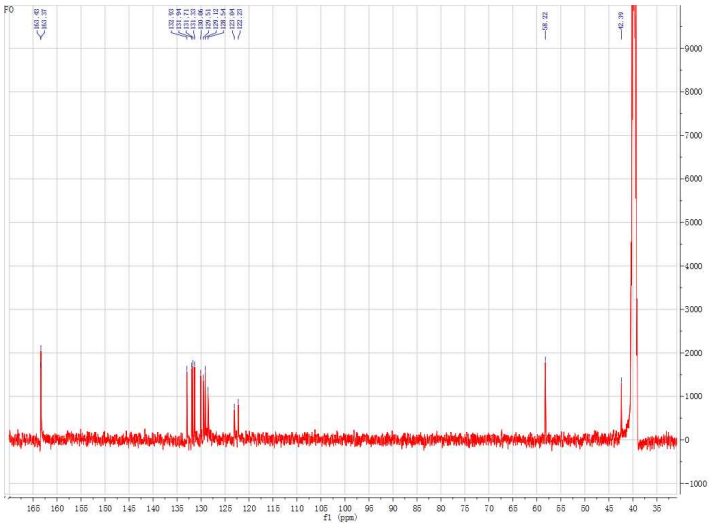
^{1}H NMR spectra for products:



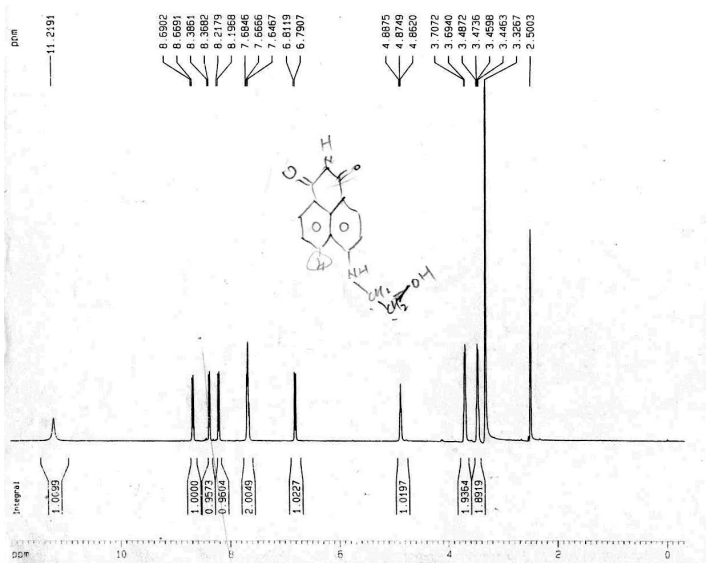
4-Bromo-1,8-naphthalimide



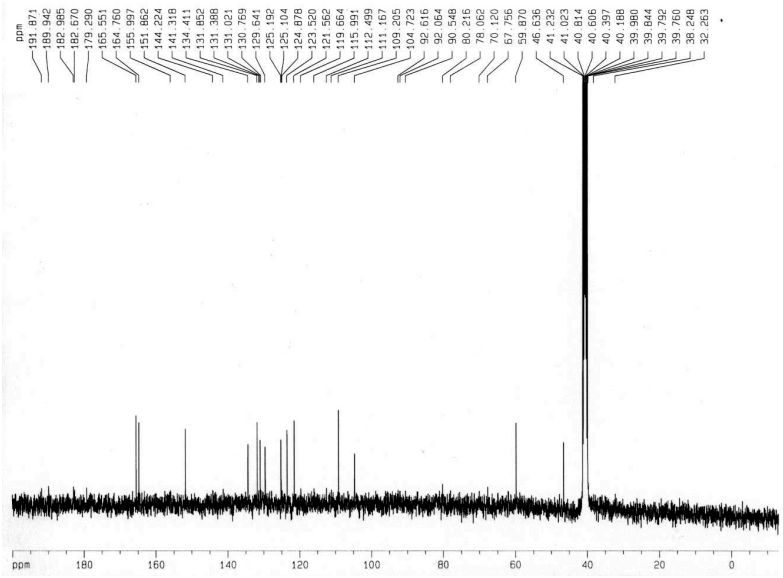
4-Bromo-N-(2-hydroxyethyl)-1, 8-naphthalimide



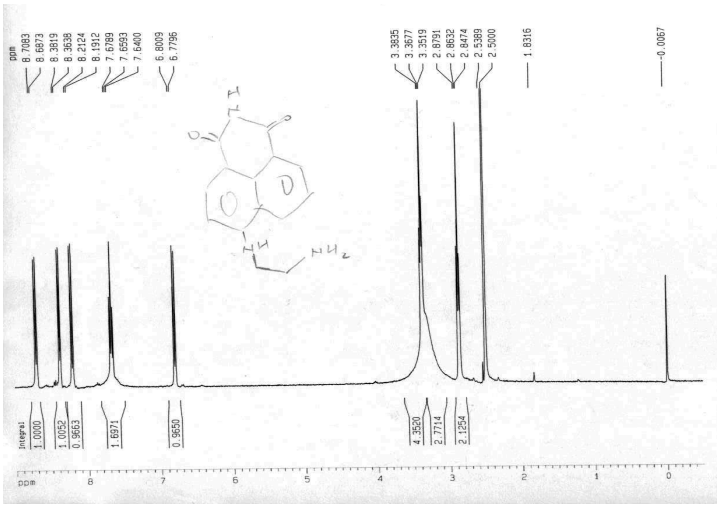
4-Bromo-N-(2-hydroxyethyl)-1, 8-naphthalimide



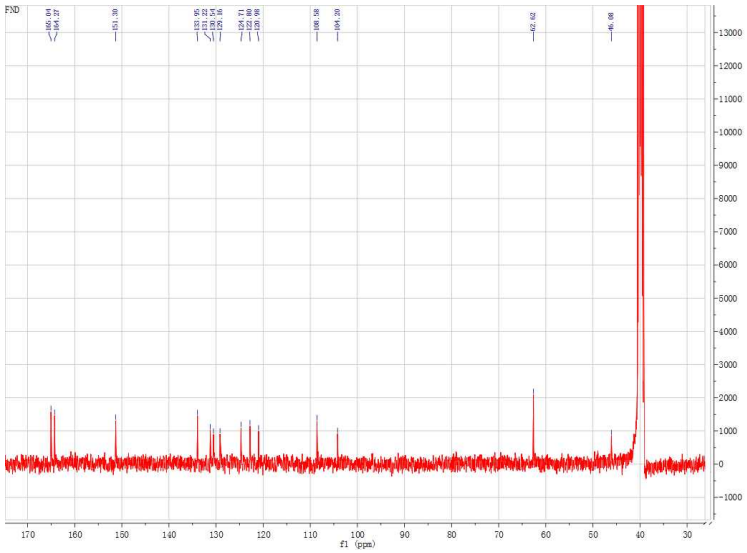
3a



3a



3b



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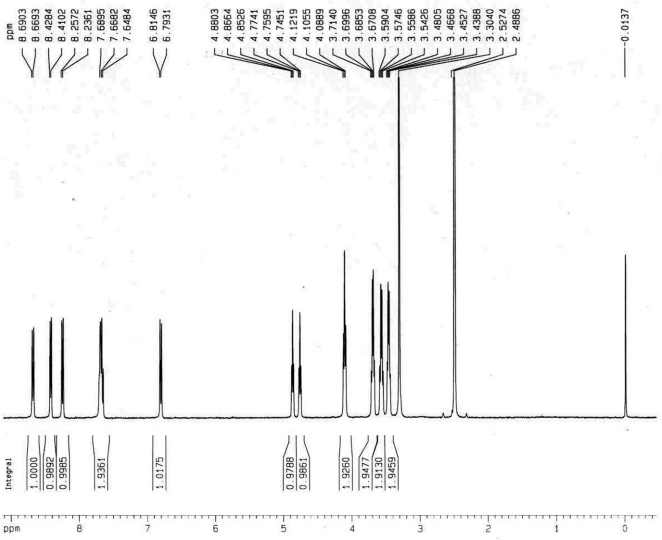
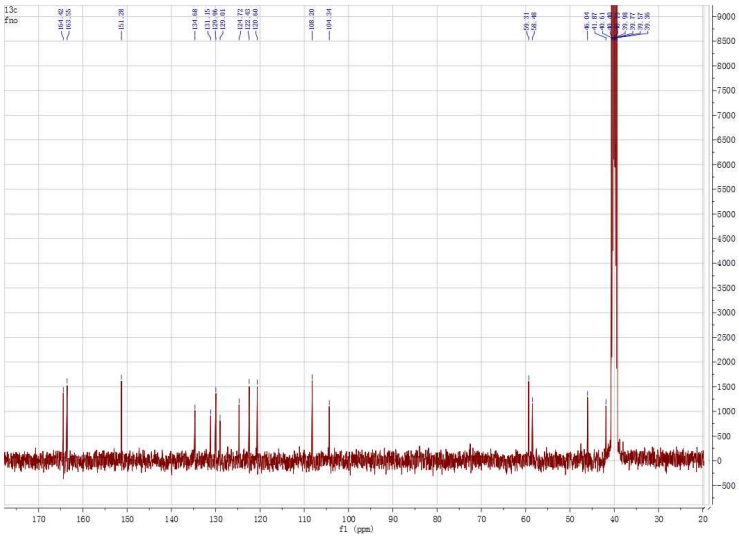
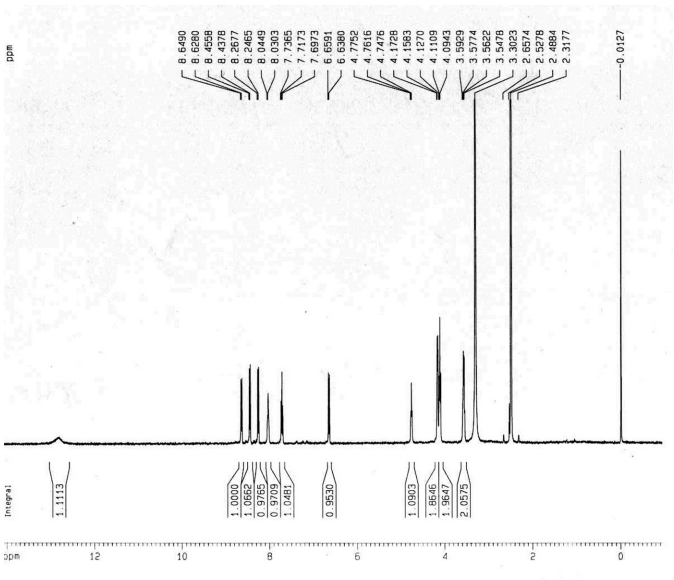


4a



4a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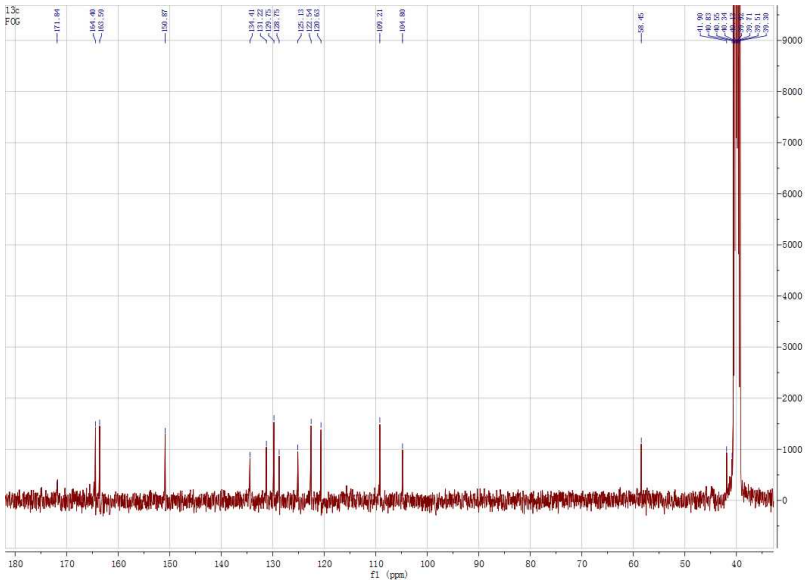
4b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f1 (ppm)

4b