Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supplementary Information

Selective and sensitive fluorescence-shift probes based on two dansyl groups for mercury(II) ion detection

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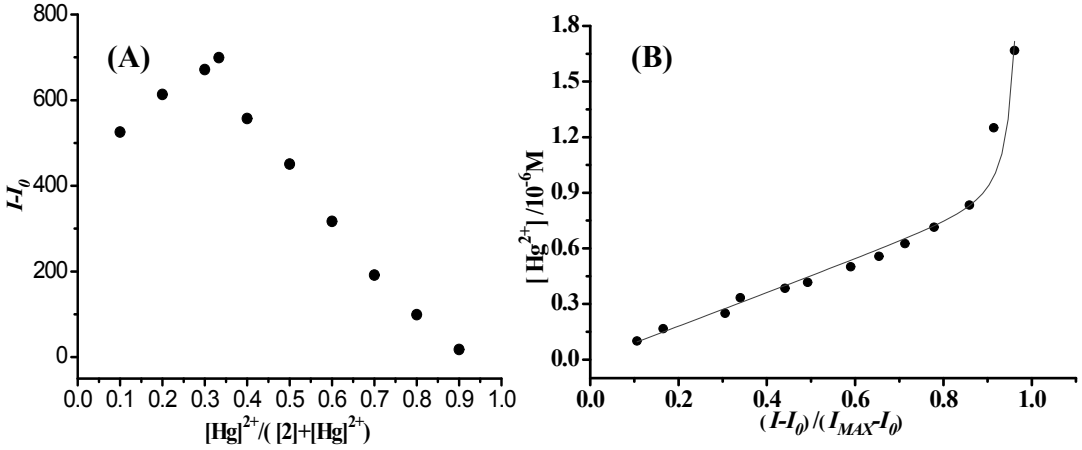

Fig.S1 (A) Fluorescence intensity changes of peak at 498 nm of **2** and Hg^{2+} with a total concentration of 20.0 μM in NaH_2PO_4/Na_2HPO_4 buffered solution (methanol-15%, pH 6.5), indicating a 2:1 stoichiometric ration of **2**: Hg^{2+} (λ_{ex} = 340 nm, λ_{em} = 498 nm). (B) Estimation of binding constant for **2** and Hg^{2+}, the plot was calculated based on the equation and a 2:1 binding model (λ_{ex} = 340 nm, λ_{em} = 498 nm)

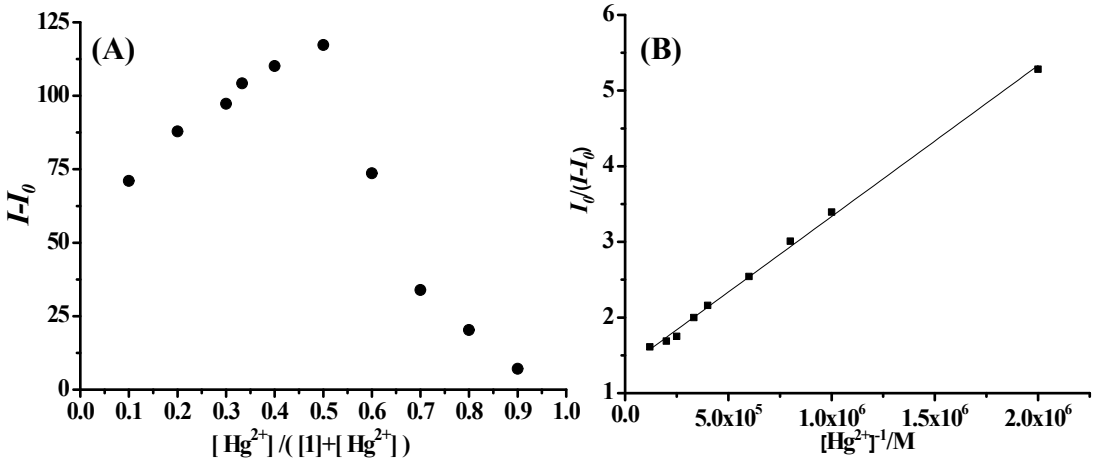

Fig.S2 (A) Fluorescence intensity changes of peak at 498 nm of **1** and Hg^{2+} with a total concentration of 20.0 μM in NaH_2PO_4/Na_2HPO_4 buffered solution (methanol-25%, pH 6.5), indicating a 1:1 stoichiometric ration of **1**: Hg^{2+} (λ_{ex} = 340 nm, λ_{em} = 498 nm). (B) Estimation of binding constant for **1** and Hg^{2+}, the plot was calculated based on the equation and a 2:1 binding model (λ_{ex} = 340 nm, λ_{em} = 498 nm)

The pH influence on the selectivity of compound 1 and 2

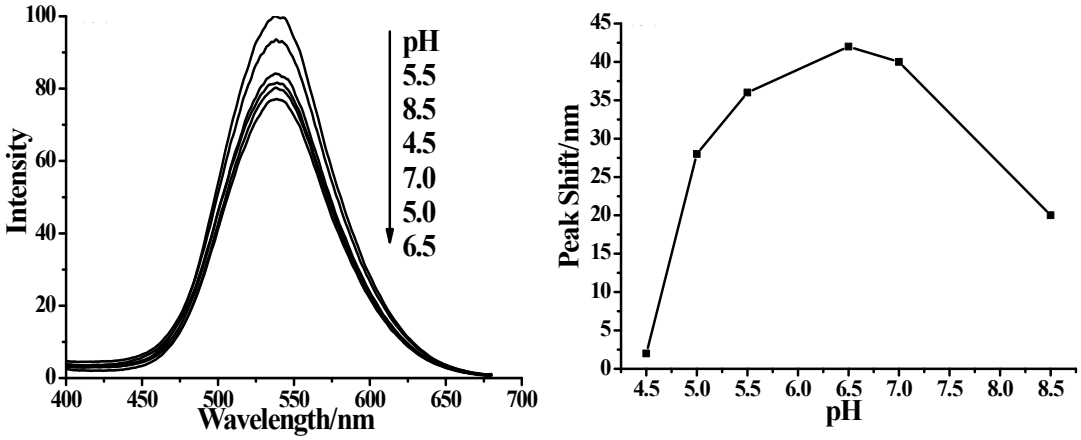

Fig.S3 (a) Fluorescence spectra of **2** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-15 %) under different pH value excited at 340 nm (without the addition of $Hg(NO_3)_2$); (b) Fluorescence spectra of **2** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-15 %) under different pH value excited at 340 nm. The blue-shift of maximum emission peak upon addition of 5.0 μM $Hg(NO_3)_2$.

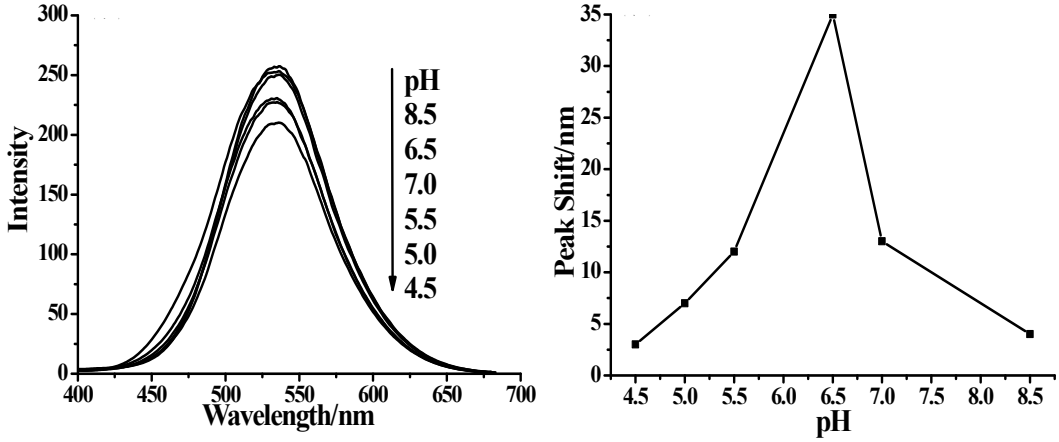

Fig.S4 (a) Fluorescence spectra of **1** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-25 %) under different pH value excited at 340 nm (without the addition of $HgCl_2$); (b) Fluorescence spectra of **2** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-25 %) under different pH value excited at 340 nm. The blue-shift of maximum emission peak upon addition of 5.0 μM $Hg(NO_3)_2$.

Reversibility study of 1 and 2 with EDTA

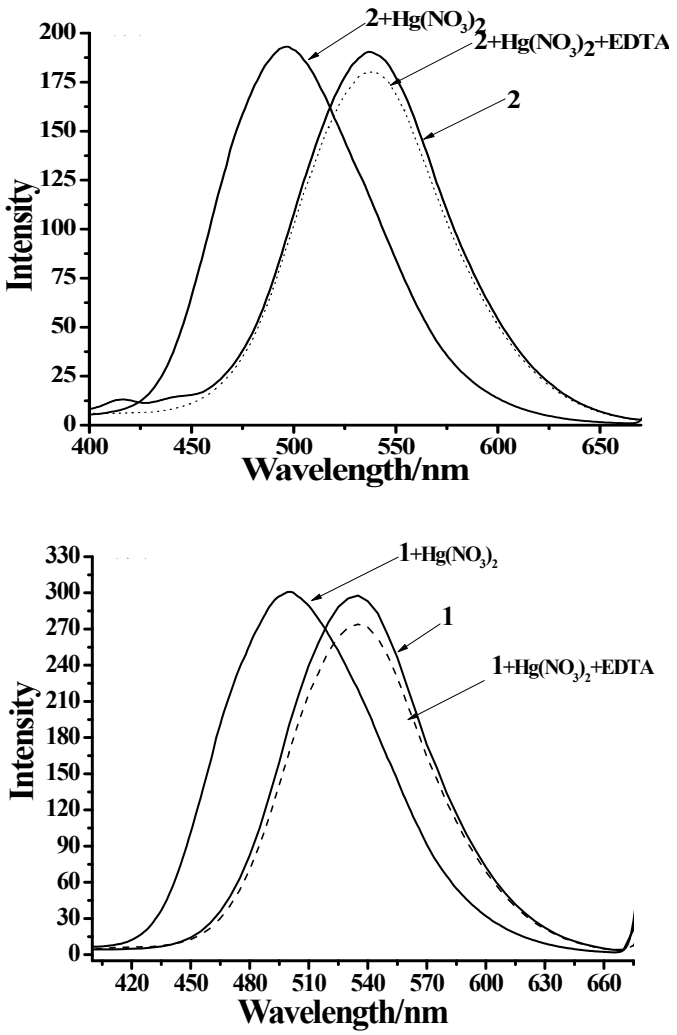

Fig.S5 (a) Fluorescence spectra of **2** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-15 %) upon addition of $Hg(NO_3)_2$ (2.5 μM) and EDTA (25.0 μM) at an excitation of 340 nm; (b) Fluorescence spectra of **1** (5.0 μM) in NaH_2PO_4/Na_2HPO_4 buffered solution (Methanol-25 %) upon addition of $Hg(NO_3)_2$ (2.5 μM) and EDTA (25.0 μM) at an excitation of 340 nm.

NMR date of 1 and 1-Hg^{2+}

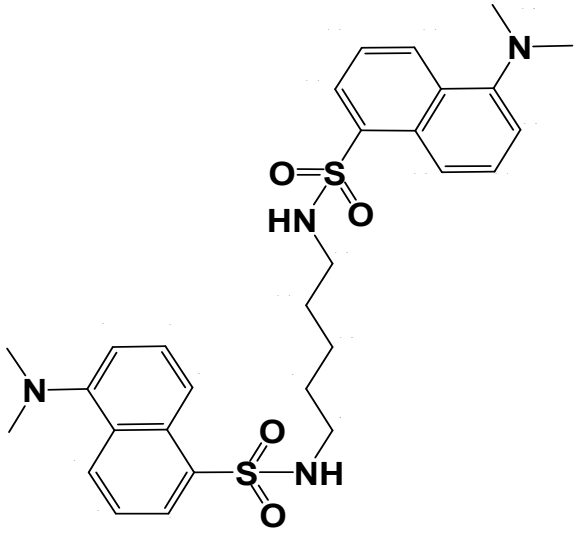

Fig.S6 Atomic numbering of **1**

Table S1 Hydrogen chemical shifts (δ, in ppm) for **2** and its complex with Hg (II); atomic numbering is shown in Fig.S6

	1	**1-Hg^{2+} (2:1,m/m)**	**1-Hg^{2+}(1:1,m/m)**	**Δλ(ppm)**	**Δλ(ppm)**
H3(15)	8.470-8.491	8.482-8.503	8.486-8.502	0.012	0.016-0.011
H1(13)	8.224-8.246	8.441-8.463	8.465-8.482	0.217	0.241-0.236
H6(19)	8.089-8.119	8.177-8.196	8.186-8.204	0.088-0.077	0.097-0.085
H2(14)、H5(17)	7.545-7.586	7.672-7.712	7.691-7.732	0.127-0.126	0.146
H4(16)	7.221-7.239	7.533-7.553	7.576-7.595	0.312-0.314	0.355-0.356
H7(18)	2.809	3.051	3.081	0.242	0.272
H8(12)	2.517-2.551	2.590-2.624	2.594-2.628	0.073	0.077-0.078
H9(11)	0.933	1.017	1.019	0.084	0.085
H10	0.726	0.844	0.855	0.118	0.129

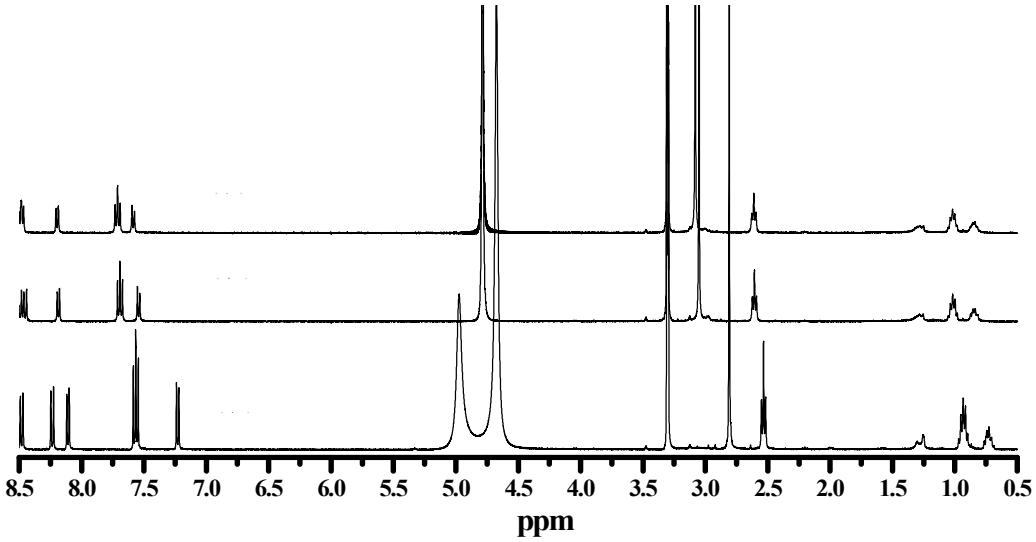

Fig.S7 Selected region of the ^{1}H NMR spectra of (a) **1**, (b)**1**/Hg^{2+}(2:1), (c) **1**/Hg^{2+}(1:1) in MeOH-d_4:D_2O (7:2, V/V).

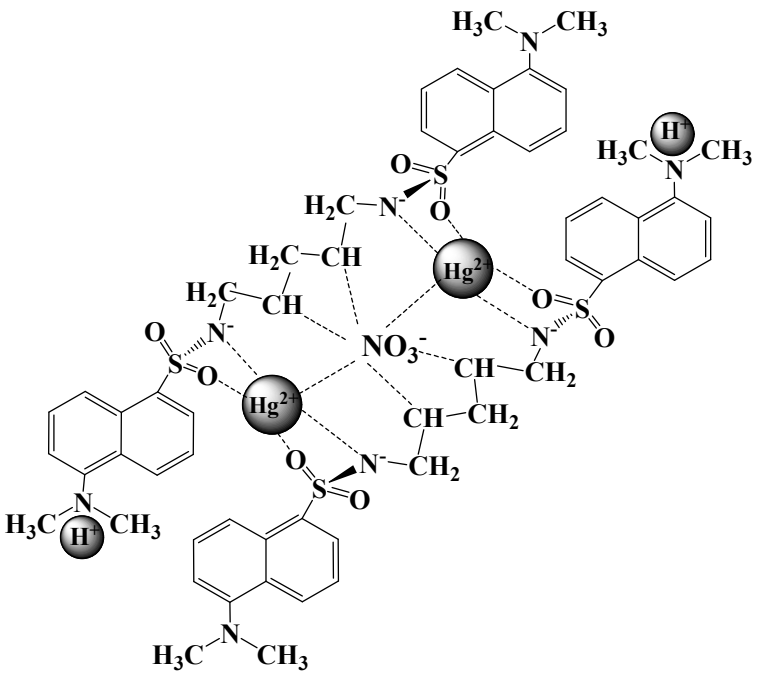

Fig. S8 Proposed coordination model for **1**-Hg^{2+}

The ESI-MS spectra of 2 and 2+$Hg(NO_3)_2$

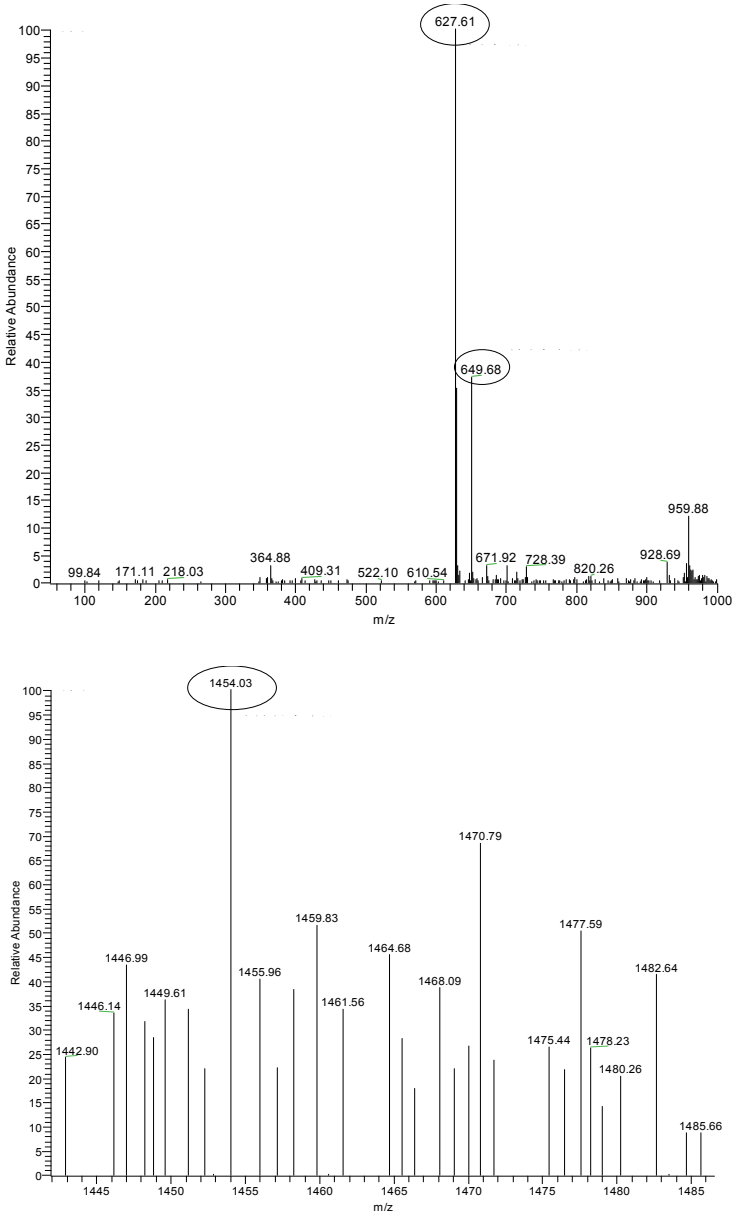

Fig.S9 The ESI-MS spectra of **2** in the absence (a) and presence (b) of $Hg(NO_3)_2$ in CH_3OH.

NMR date of 2 and 2-Hg (II)

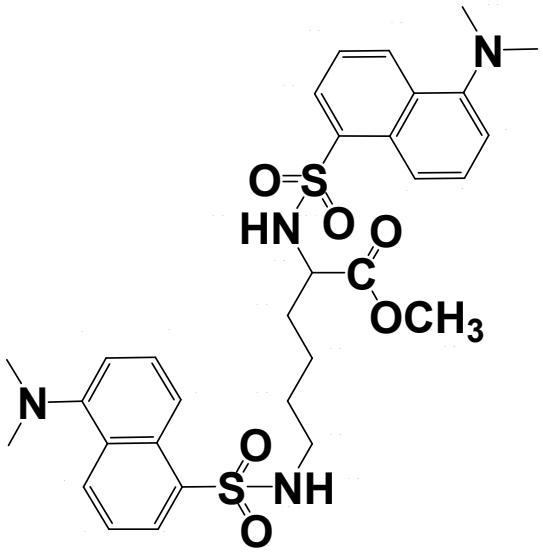

Fig.S10 Atomic numbering of **2**

Table S2 Hydrogen chemical shifts (δ, in ppm) for **2** and its complex with Hg (II); atomic numbering is shown in Fig.S10

	2	**2-Hg^{2+}(5:1,m/m)**	**2-Hg^{2+}(2:1,m/m)**	**$\Delta\delta_1$/ppm**	**$\Delta\delta_2$/ppm**
H12 H7	8.244-8.204	8.450-8.414	8.463-8.437	0.106-0.210	0.119-0.233
H11 H8	7.652-7.601	7.761-7.716	7.779-7.734	0.109-0.115	0.127-0.133
H10	8.549-8.528	8.534-8.511	8.530-8.508	-0.015--0.017	-0.019--0.020
H9	7.339-7.320	7.631-7.610	7.672-7.652	0.292-0.290	0.333-0.332
H20	3.269	3.211	3.209	-0.058	-0.060
H18	3.383	3.448	3.453	0.065	0.070
H17	1.219	1.265	1.274	0.046	0.055
H16	0.678	0.740	0.743	0.062	0.065
H15	0.878	0.937	0.944	0.059	0.066
H14	2.470-2.395	2.517-2.436	3.531-3.439	0.047-0.041	0.061-0.044
H21	2.742	2.988	3.018	0.246	0.276
H3	7.189-7.170	7.506-7.487	7.547-7.528	0.317	0.358
H6 H1	8.120-8.102	8.196-8.177	8.206-8.188	0.076-0.075	0.086-0.086
H4	8.457-8.436	8.484-8.464	8.486-8.473	0.027-0.028	0.029-0.037
H22	2.871	3.097	3.126	0.226	0.255
H2 H5	7.570-7.530	7.687-7.654	7.705-7.693	0.117-0.124	0.235-0.163

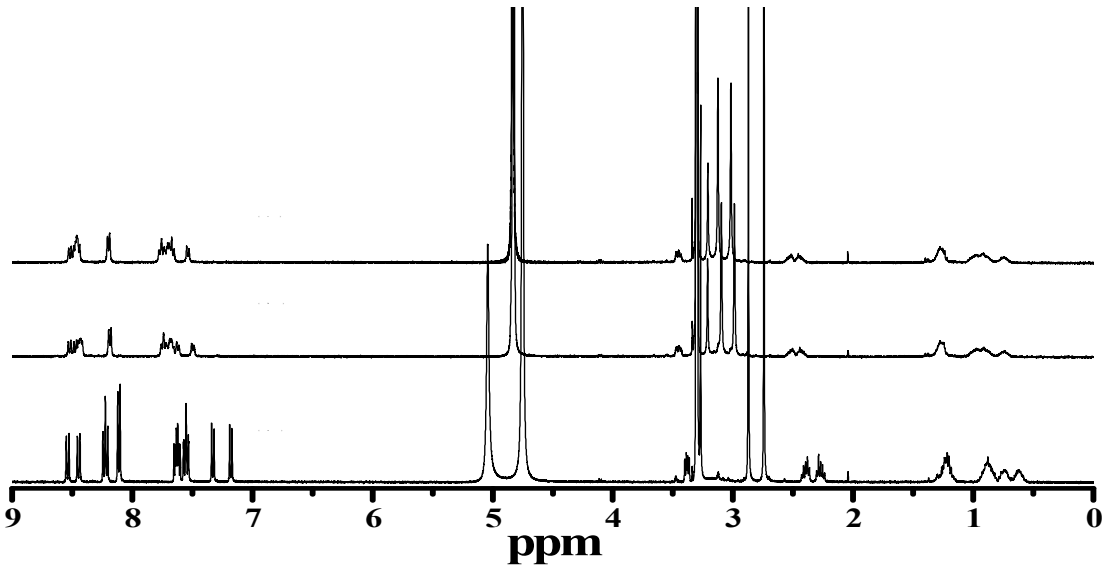

Fig.S11 Selected region of the ^{1}H NMR spectra of (a) **2**, (b) **2**/Hg^{2+}(5:1), (c) **2**/Hg^{2+} (2:1) in MeOH-d_4:D_2O (2:1, V/V).

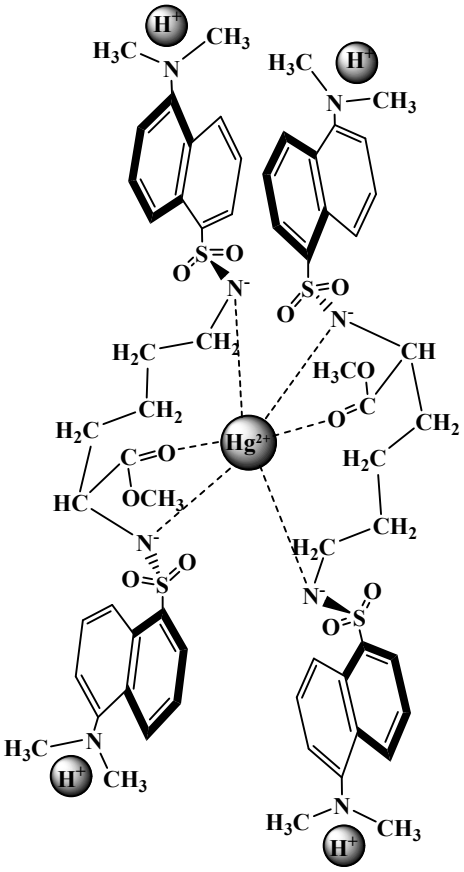

Fig. S12 Proposed coordination model for **2**-Hg^{2+}