Electronic supplementary information

Fluorescent probe mimicking multiple logic gates and a molecular keypad lock upon interaction with Hg^{2+} and bovine serum albumin

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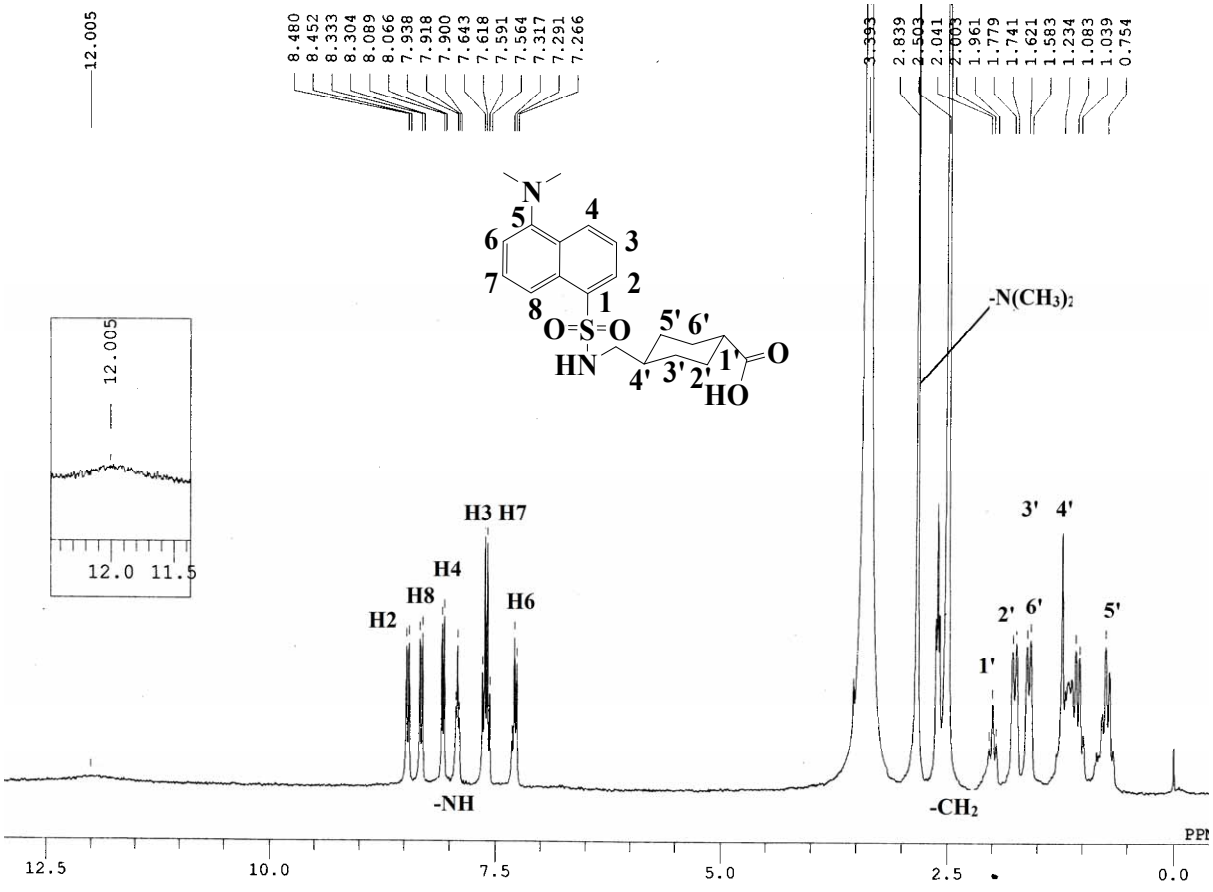

Figure S1: ^{1}H NMR Spectrum of **1** in DMSO-d_6

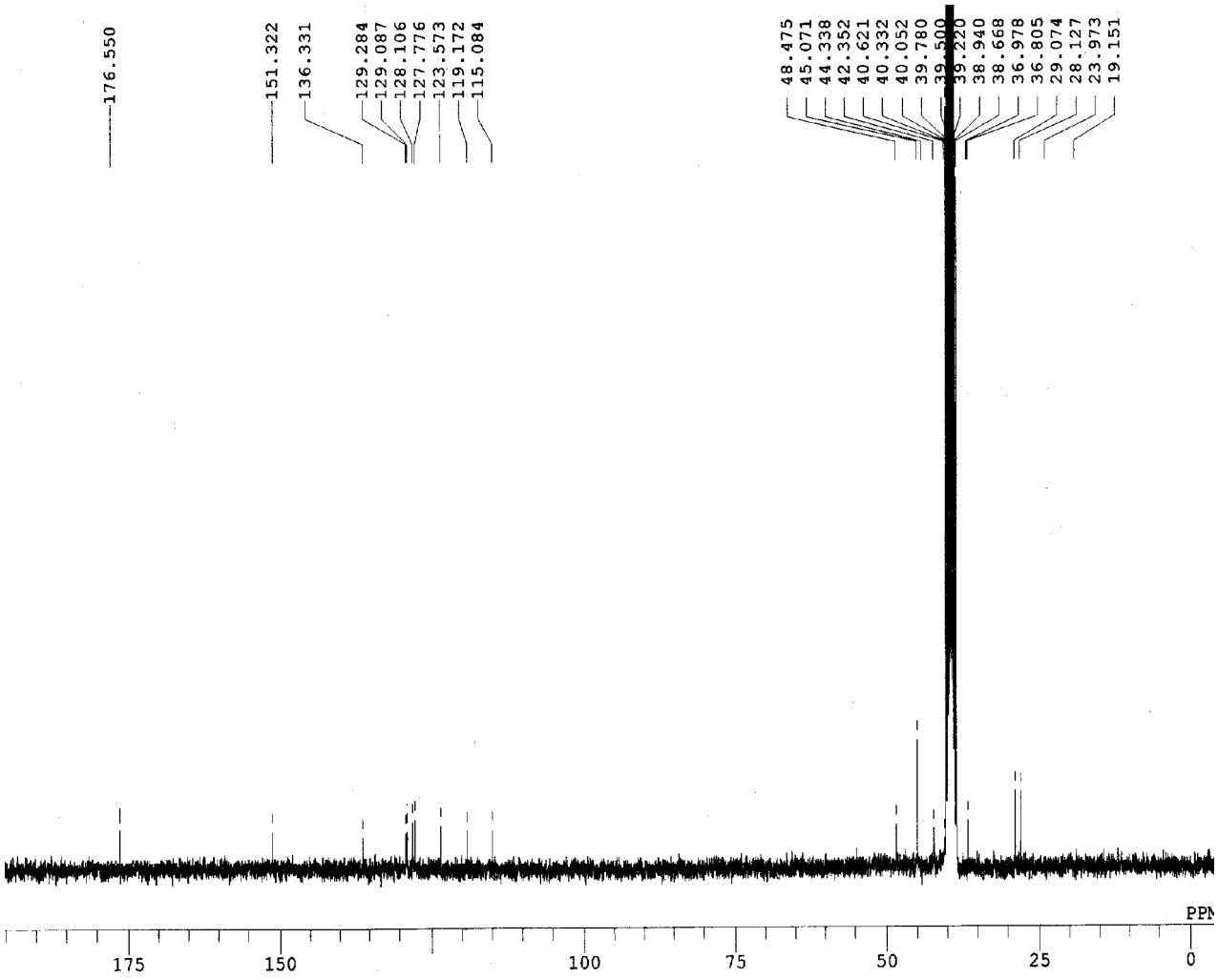

Figure S2: ^{13}C NMR Spectrum of **1**in DMSO-d_6.

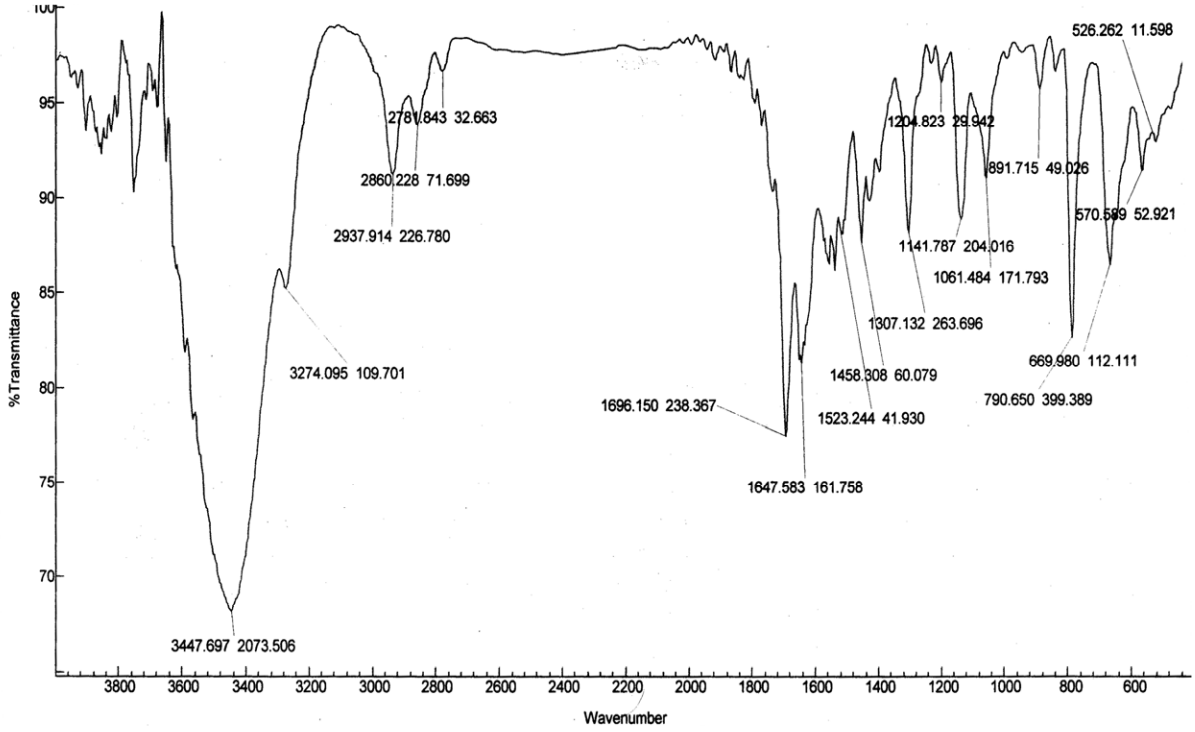

Figure S3: FT-IR spectrum of **1**.

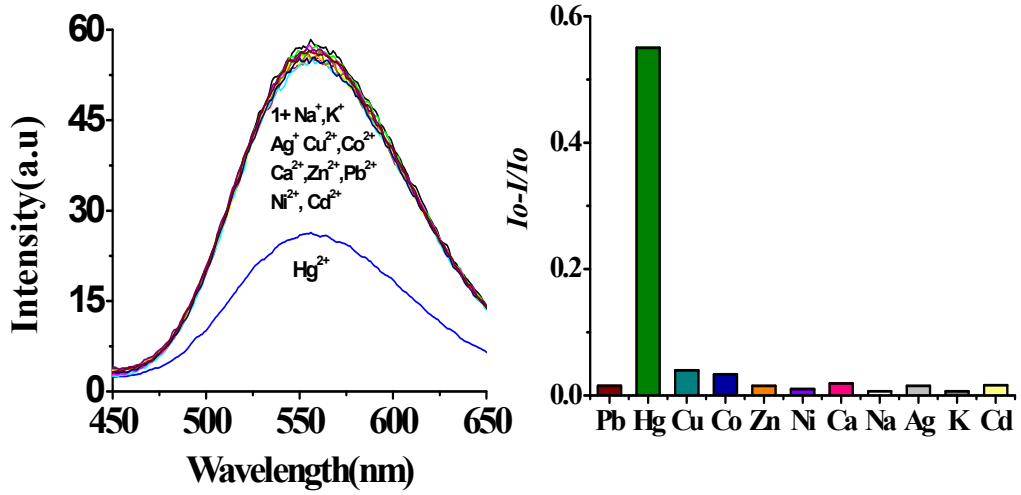

Figure S4. Change in emission spectra and relative fluorescence intensity (Bar diagram) of **1** upon interaction of metal ions (10 equiv) in NaOAc buffer (50 mM; pH = 6.7).

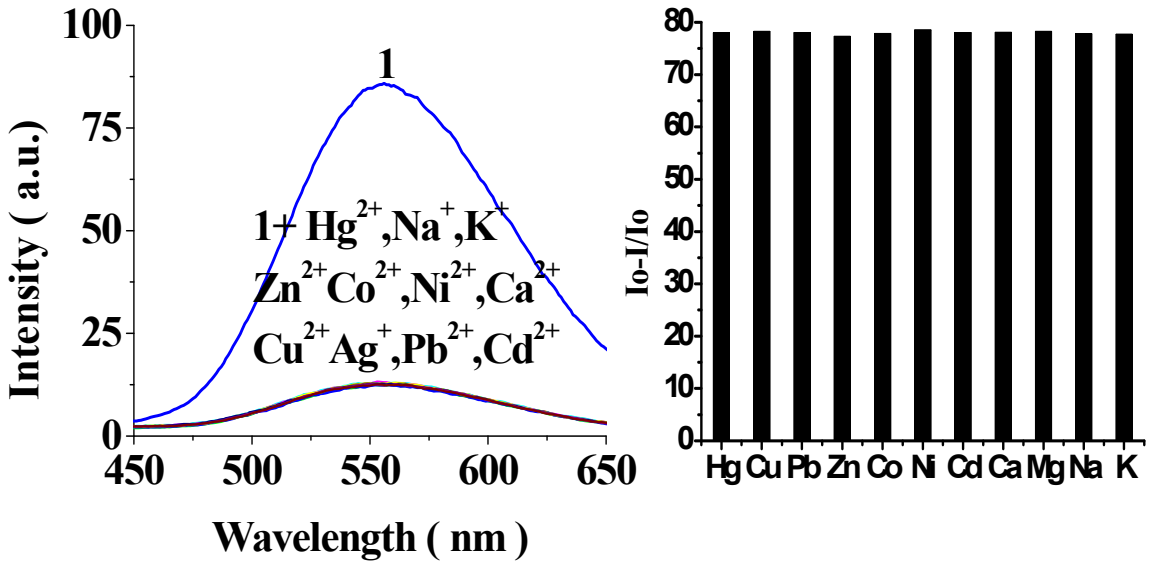

Figure S5: Competitive metal ion study illustrates change in emission spectra and relative fluorescence intensity (Bar diagram) upon addition of tested metal ions (20 equiv) to the solution of **1**+Hg^{2+} in NaOAc buffer (50 mM; pH = 6.7).

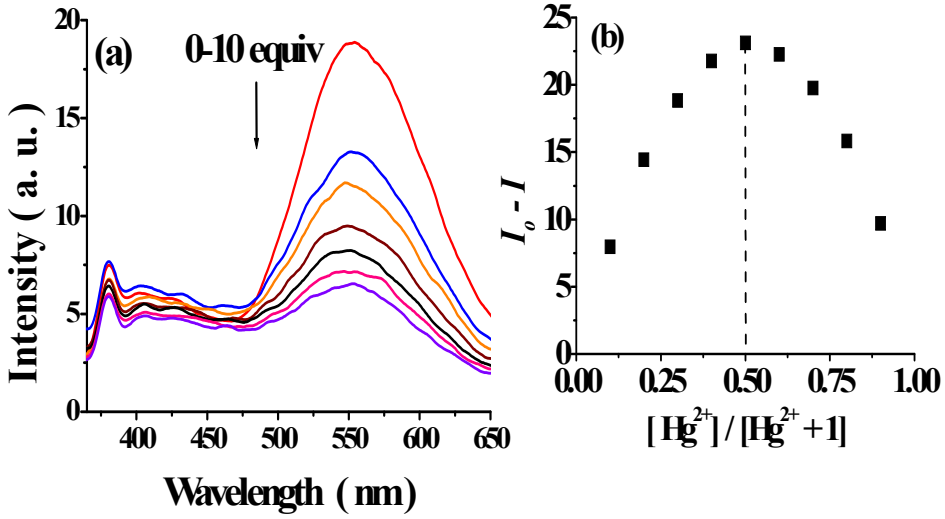

Figure S6: Fluorescence titration spectra of **1** (10 μM) with Hg^{2+} (0-10 equiv) ions in NaOAc buffer (50 mM; pH = 6.7). (b) Job's plot shows a 1:1 stoichiometry between **1** and Hg^{2+} ions.

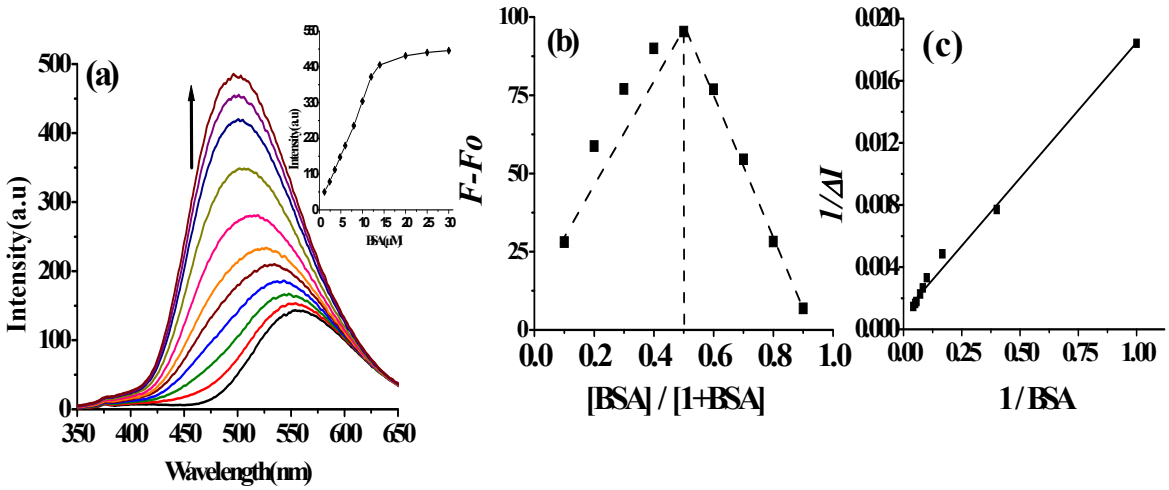

Figure S7: Fluorescence titration spectra of **1** with (a) BSA in NaOAc buffer (50 mM; pH = 6.7). Inset shows the change in fluorescence intensity with respect to concentration of BSA. (b) Job's plot indicating a 1:1 stoichiometry between **1** and BSA. (c) B-H plot of **1** with BSA

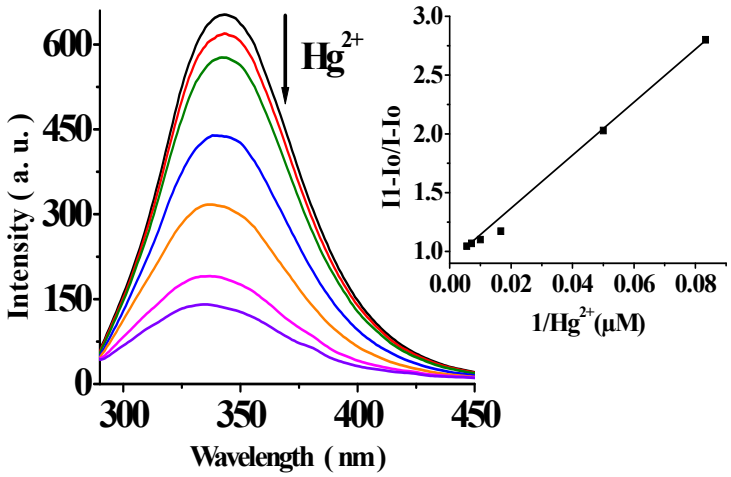

Figure S8: Fluorescence titration spectra of BSA (5 μM) at 278 nm excitation wavelength upon addition of Hg^{2+} (0-44 equiv) ions in NaOAc buffer (50 mM; pH=6.7). Inset: B-H plots show for a 1:1 complexation in the presence of Hg^{2+} ions.

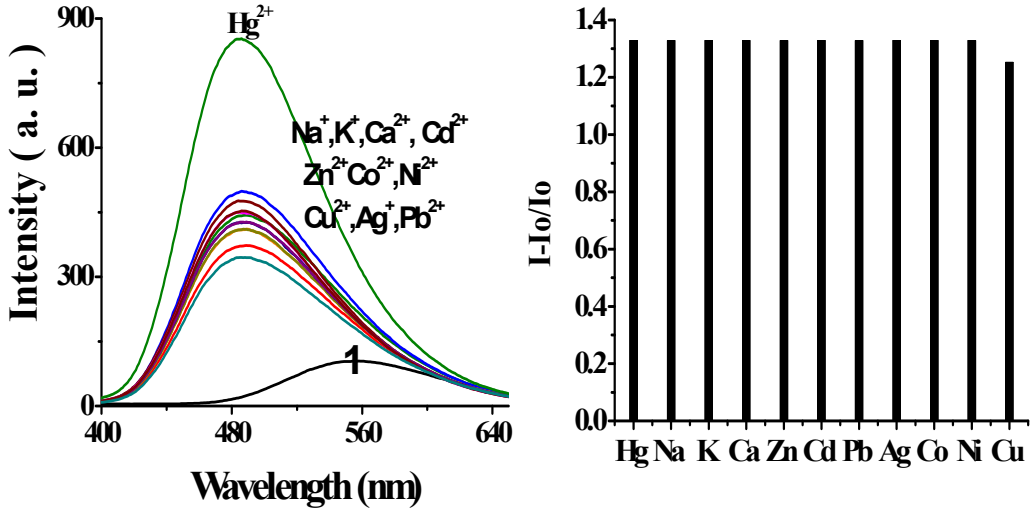

Figure S9: Emission spectra of interaction study of **1**+ BSA in presence of different metal ion (10 equiv). Bar graph indicates change in relative fluorescence intensity of **1**+BSA+ Hg^{2+} upon interference of tested metal ions.

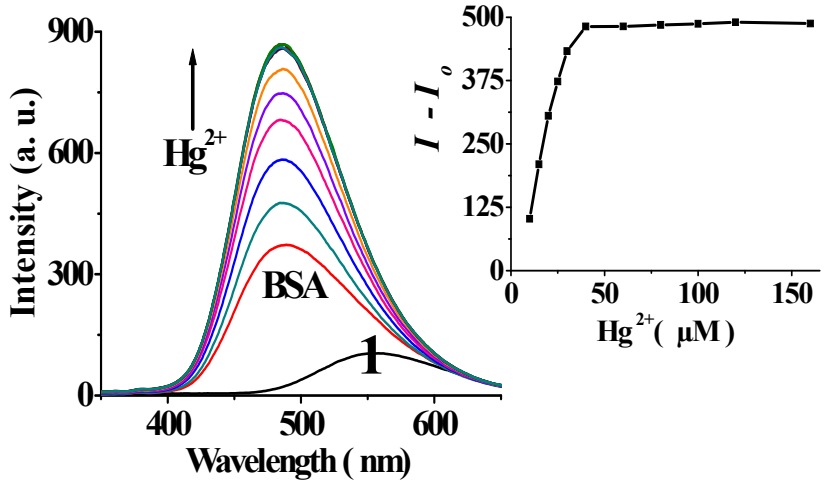

Figure S10: Fluorescence titration spectra of **1**+BSA with Hg^{2+} ions.

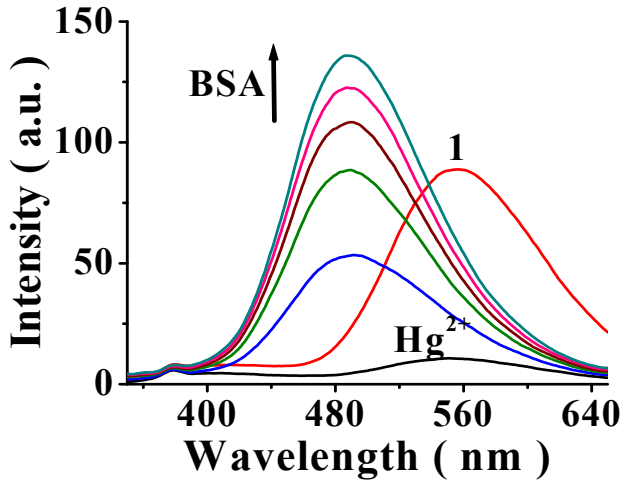

Figure S11: Fluorescence titration spectra of **1**+Hg^{2+} with BSA.

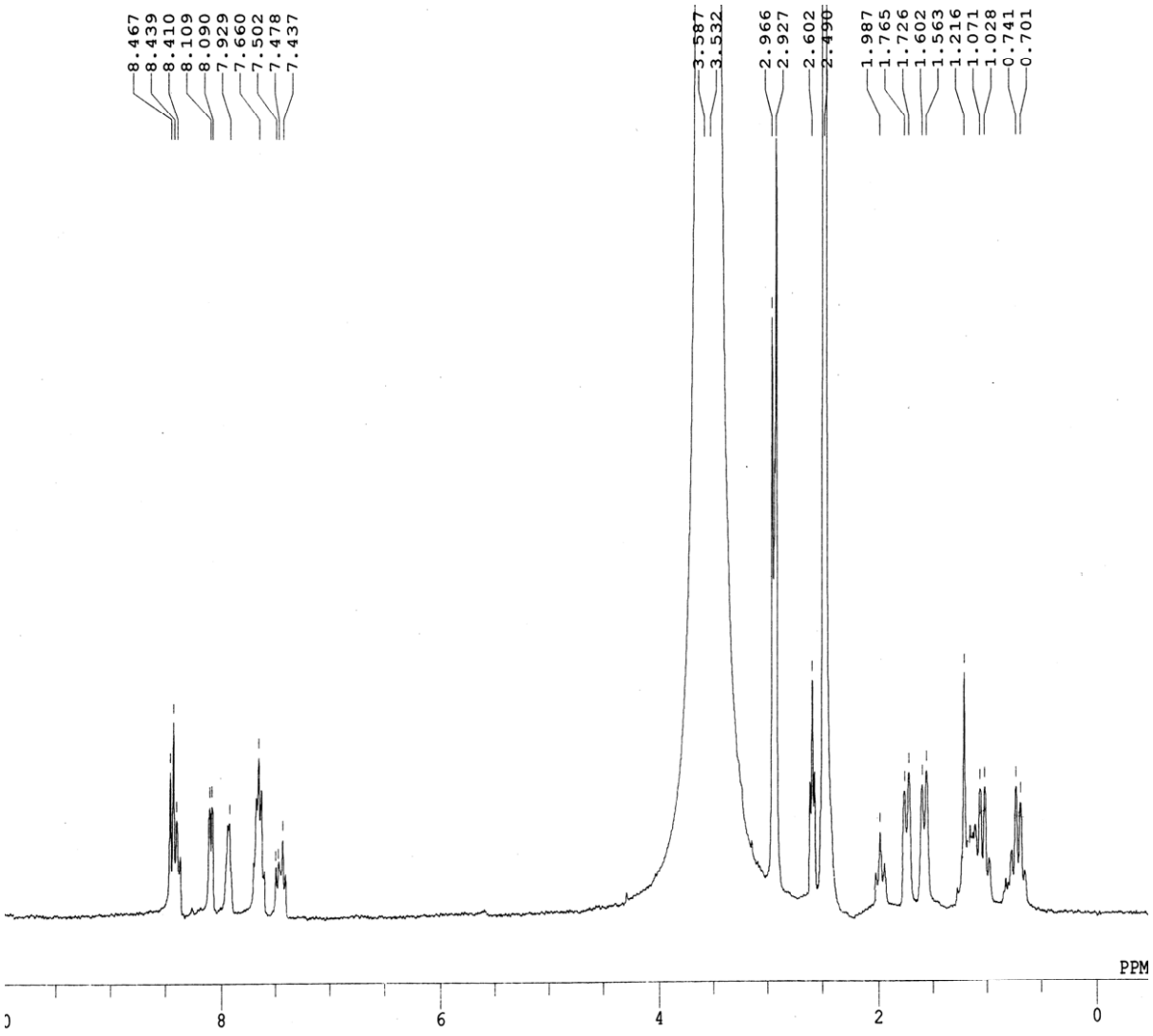

Figure S12: ^{1}H NMR spectrum of **1** upon addition of Hg^{2+} (0.5 equiv) in DMSO-d_6.

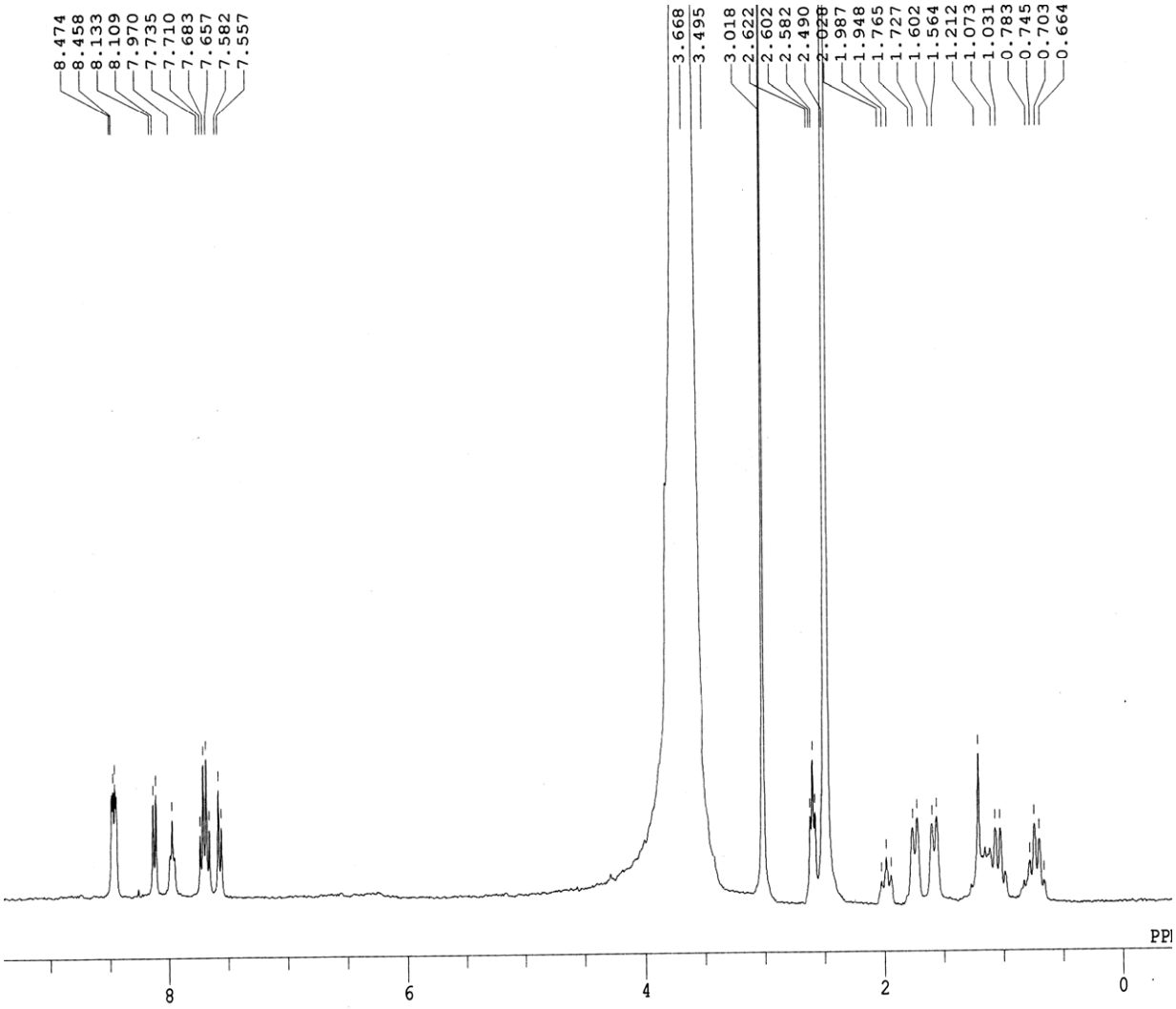

Figure S13: ^{1}H NMR spectrum of **1** upon addition of Hg^{2+} (1 equiv) in DMSO-d_6.

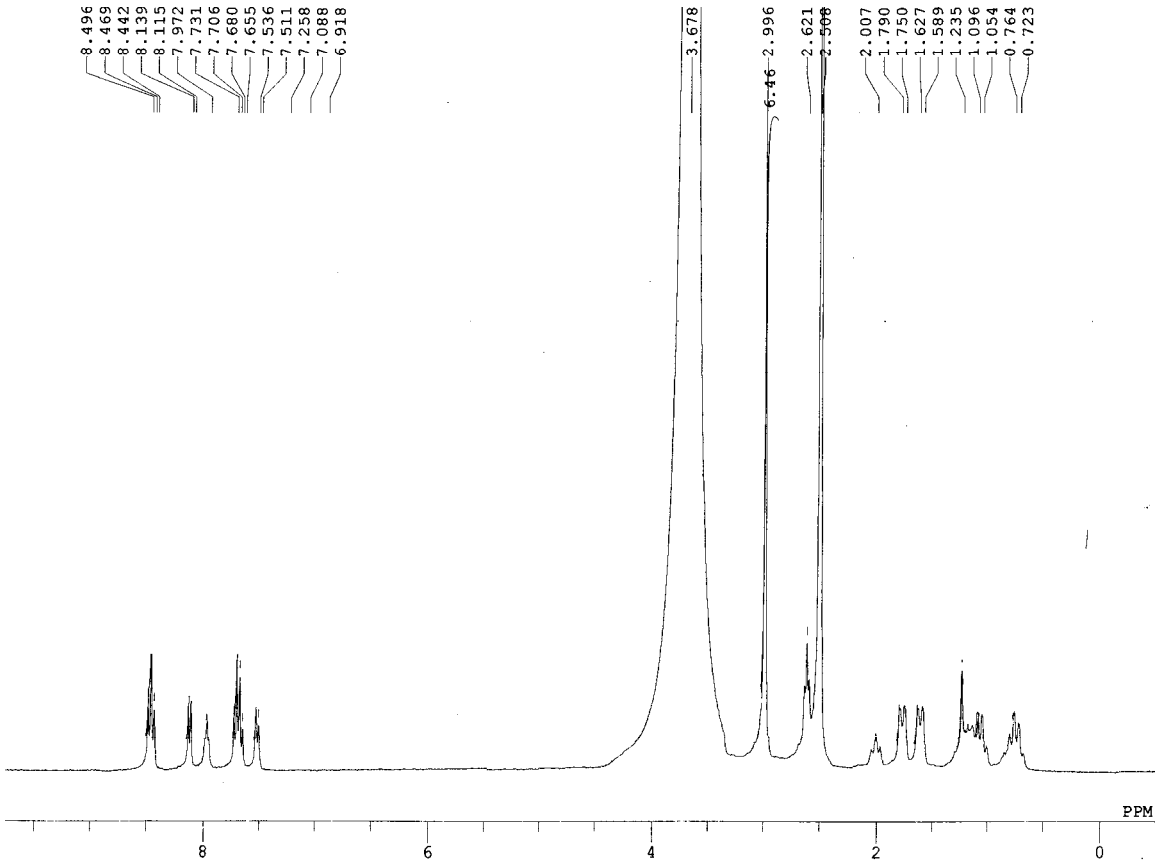

Figure S14: ^{1}H NMR spectrum of **1** upon addition of Hg^{2+} (1.5 equiv) in DMSO-d_6.

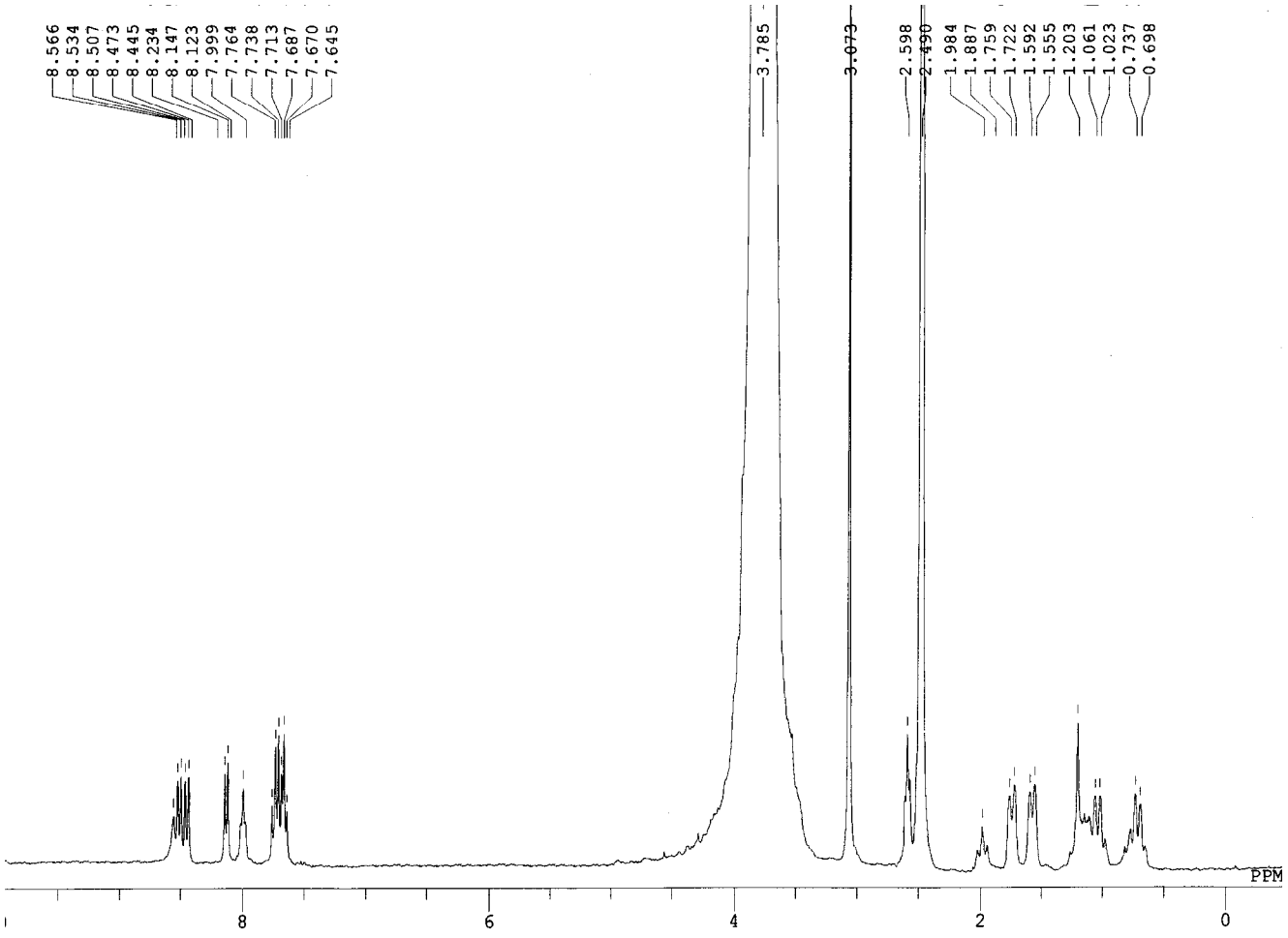

Figure S15: ^{1}H NMR spectrum of **1** upon 2.0 equiv addition of Hg^{2+} in DMSO-d_6.

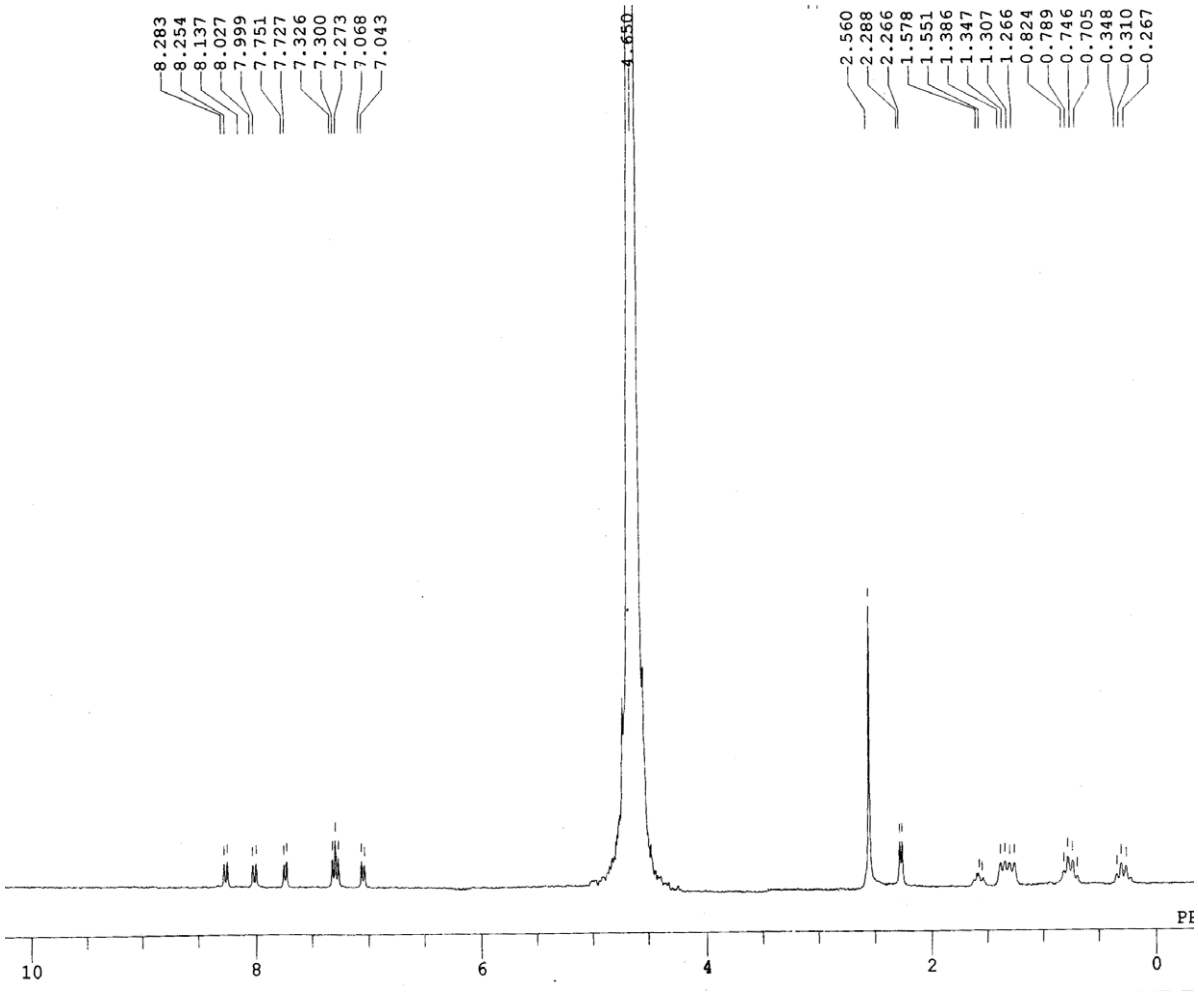

Figure S16. ^{1}H NMR spectrum of **1** in D_2O.

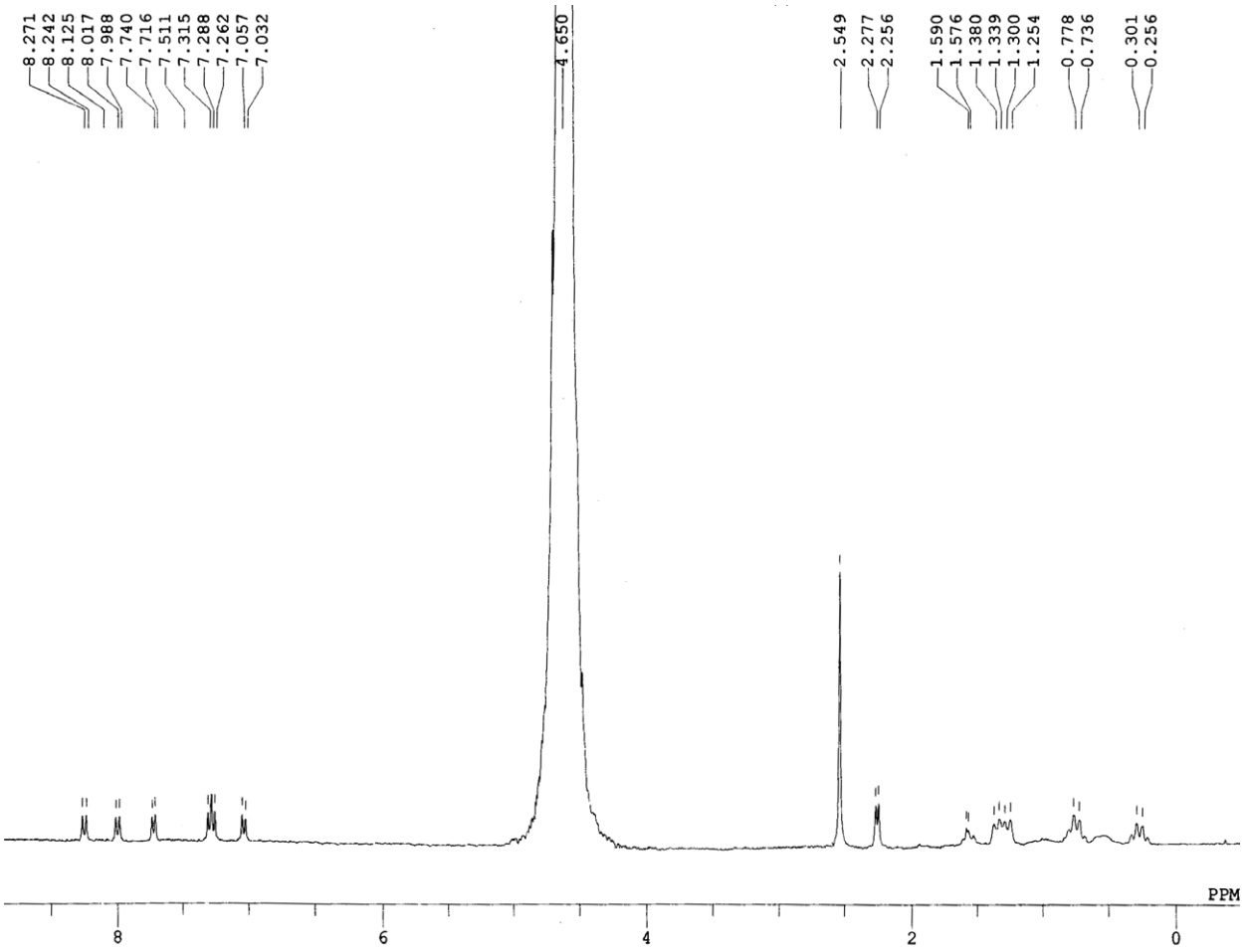

Figure S17. ^{1}H NMR spectrum of **1** after addition of 0.01 equiv of BSA in D_2O.

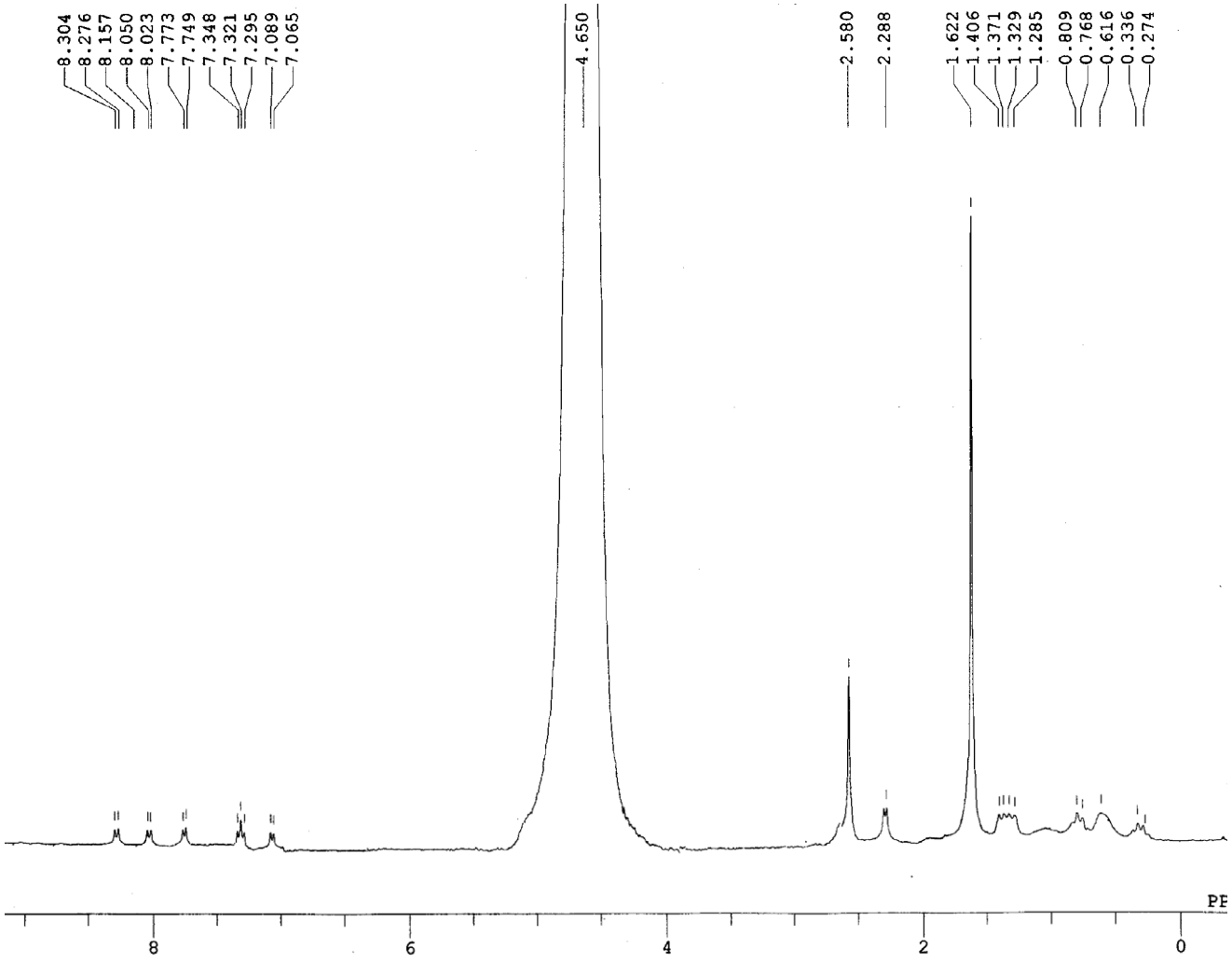

Figure S18. ^{1}H NMR spectrum of **1** having 0.01 equiv of BSA after addition of 1 equiv of Hg^{2+} ion in D_2O.

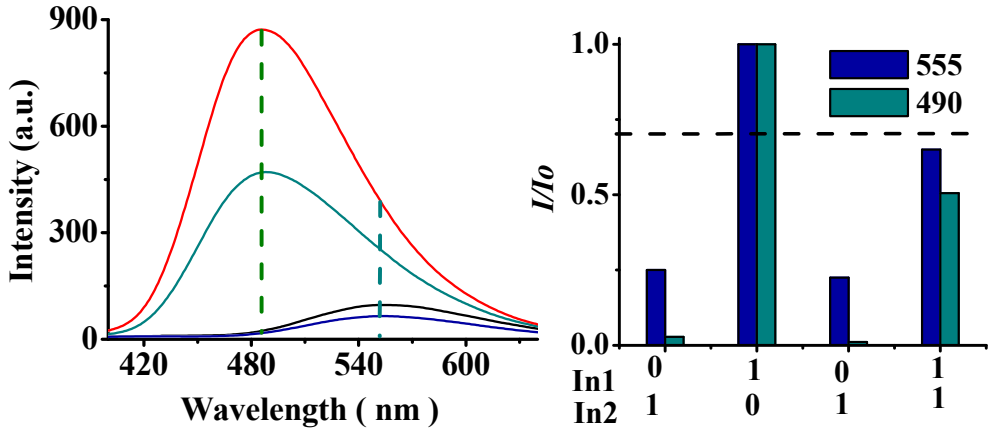

Figure S19. Change in emission spectra and output intensities (bar diagram) of **1** upon chemical inputs of A (output of AND logic BSA / Hg^{2+}) and EDTA.

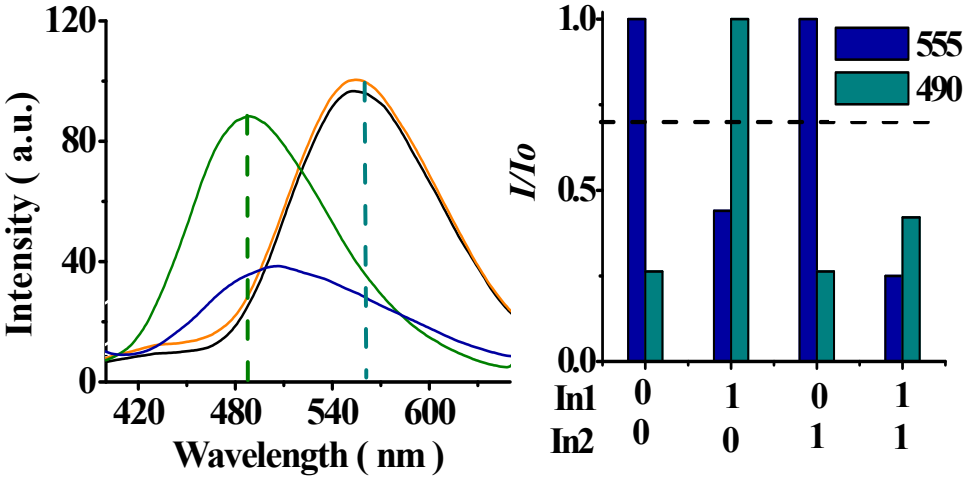

Figure S20. Change in emission spectra and output intensities (bar diagram) of **1** upon chemical inputs of B (output of INHIBIT logic Hg^{2+}/BSA) and Urea.

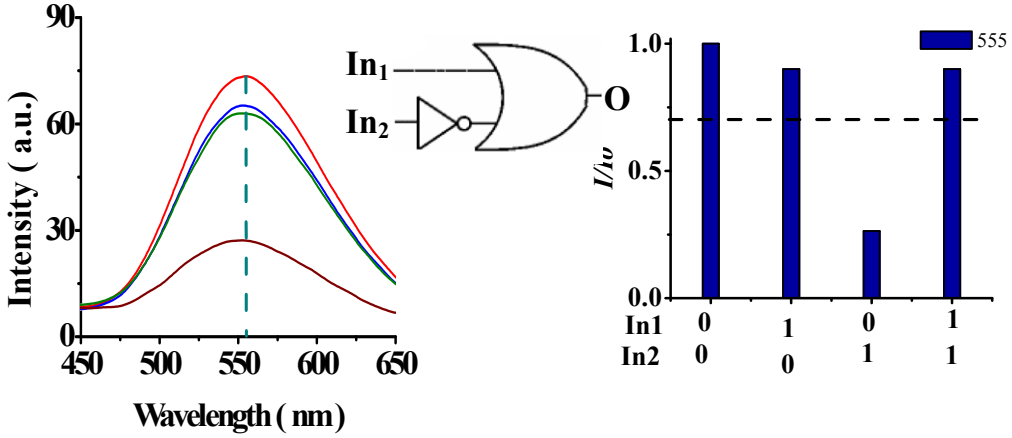

Figure S21. Change in emission spectra and output intensities (bar diagram) of **1** upon chemical inputs of EDTA and Hg^{2+} metal ions.

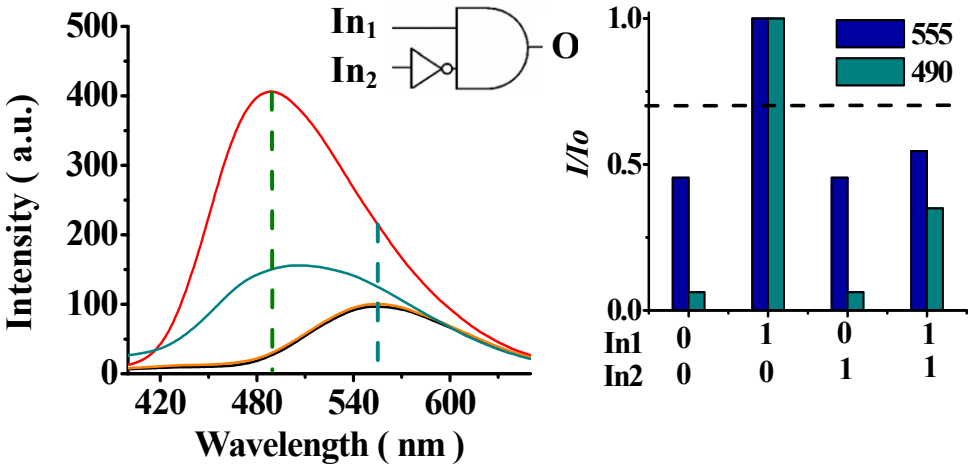

Figure S22. Change in emission spectra and output intensities (bar diagram) of **1** upon chemical inputs of BSA and Urea.

Table S1:- Truth table of INHIBIT (A = output of AND logic and EDTA), INHIBIT, TRANFER (B = output of INHIBIT logic and Urea), IMPLICATION (Hg^{2+} and EDTA) and INHIBIT (BSA and Urea) logic functions.

In1 A	In2 EDTA	Output 555 490 nm
0	0	0
1	0	1
0	1	0
1	1	0

In1 B	In2 UREA	Output 555 490nm F D
0	0	1 0
1	0	0 1
0	1	1 0
1	1	0 0

In1 EDTA	In2 Hg^{2+}	Output 555 490 nm
0	0	1
1	0	1
0	1	0
1	1	1

In1 BSA	In2 UREA	Output 555 490 nm
0	0	0
1	0	1
0	1	0
1	1	0

Table S2:-Truth table of logic circuit of probe with sequential Inputs of BSA, Hg^{2+} (workings as a keypad lock on applying BSA as In_1 and Hg^{2+} as In_2) and reset functions of EDTA and urea (reset keys).

BSA	Hg^{2+}	EDTA	Urea	Output
0	0	0	0	0
1	0	0	0	0
0	1	0	0	0
0	0	1	0	0
0	0	0	1	0
1	1	0	0	1
1	0	1	0	0
1	0	0	1	0
0	1	1	0	0
0	1	0	1	0
0	0	1	1	0
1	1	0	1	0
1	1	1	0	0
0	1	1	1	0
1	0	1	1	0
1	1	1	1	0