## **Supplementary Information For:**

## Electrophilicity Modulated Targeted Luminescence of MOF Coated Cotton Composite for Dual Analyte Detection in Aqueous Medium

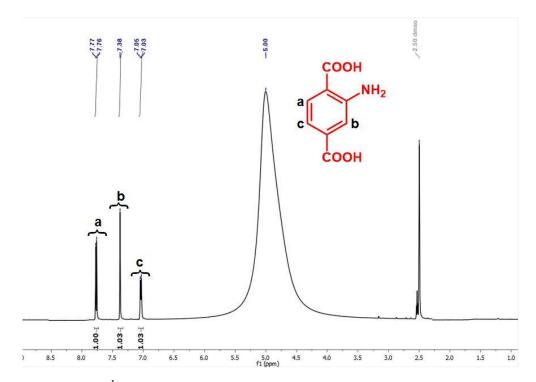
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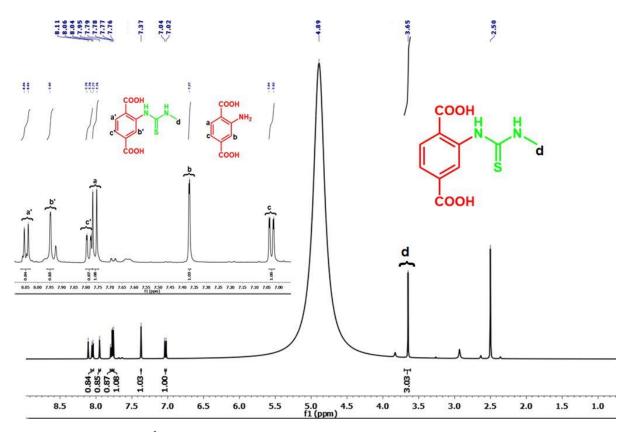
\*To whom correspondence should be addressed. E-mail: sbiswas@iitg.ac.in; Tel: 91-3612583309.

## **Materials and Characterization Methods:**

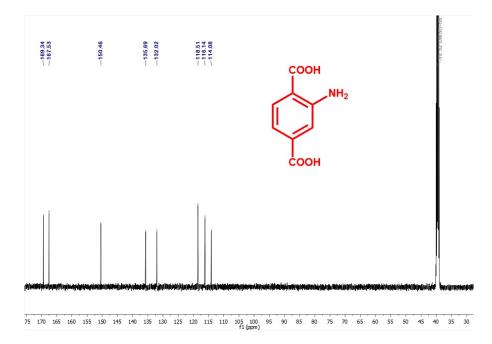
All the chemicals were purchased from commercial sources and used without further purification. A Bruker Avance III 600 NMR spectrometer was utilized for recording <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra at 500 MHz. The mass spectrum (in -ve ESI mode) was measured with a BRUKER AUTOFLEX SPEED high-resolution mass spectrometer. Fourier transform infrared (FT-IR) spectroscopy data were recorded in the region 400-4000 cm<sup>-1</sup> at room temperature with the Perkin Elmer Spectrum Two FT-IR spectrometer. The following indications were used to indicate the corresponding absorption bands: very strong (vs), strong (s), medium (m), weak (w), shoulder (sh) and broad (br). Thermogravimetric analysis (TGA) was carried out with a Perkin Elmer TGA 4000 thermal analyzer in the temperature range of 30-700 °C under N<sub>2</sub> atmosphere at the rate of 4 °C min<sup>-1</sup>. Powder X-ray diffraction (PXRD) data were collected in transmission mode using a Bruker D2 Phaser X-ray diffractometer (30 kV, 10 mA) using Cu-Ka ( $\lambda = 1.5406$  Å) radiation. The specific surface area for N<sub>2</sub> sorption was calculated on a Quantachrome Autosorb iQMP gas sorption analyzer at -196 °C. FE-SEM images were collected with a Zeiss (Sigma 300) scanning electron microscope. The compound was activated at 100 °C for 24 h under a dynamic vacuum. The solid-state UV-Vis spectra were measured using UV-2600 spectrophotometer. Fluorescence emission studies were performed at room temperature using a HORIBA JOBIN YVON Fluoromax-4 spectrofluorometer.



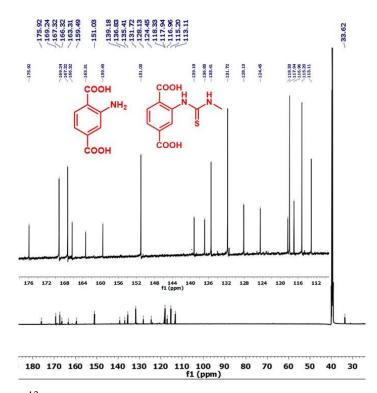
**Figure S1.** Digested <sup>1</sup>H NMR spectrum of **Hf-UiO-66-NH**<sub>2</sub> (digested using 10  $\mu$ L of 40% HF in 500  $\mu$ L of DMSO-D<sub>6</sub> and 20 mg of MOF).



**Figure S2.** Digested <sup>1</sup>H NMR spectrum of **Hf-UiO-66-NHCSNHCH<sub>3</sub>** MOF (digested using 10  $\mu$ L of 40% HF in 500  $\mu$ L of DMSO-D<sub>6</sub> and 20 mg of MOF).



**Figure S3.** Digested <sup>13</sup>C NMR spectrum of **Hf-UiO-66-NH**<sub>2</sub> (digested using 10  $\mu$ L of 40% HF in 500  $\mu$ L of DMSO-D<sub>6</sub> and 20 mg of MOF).



**Figure S4.** Digested <sup>13</sup>C NMR spectrum of **Hf-UiO-66-NHCSNHCH<sub>3</sub>** MOF (digested using 10  $\mu$ L of 40% HF in 500  $\mu$ L of DMSO-D<sub>6</sub> and 20 mg of MOF).

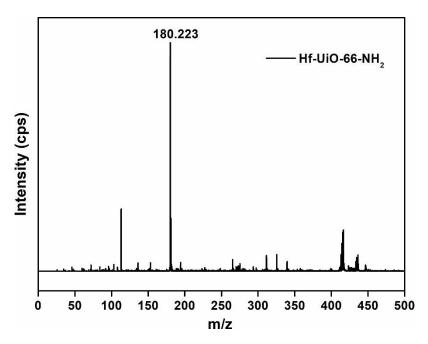


Figure 5. Mass spectrum of  $Hf-UiO-66-NH_2$  after digestion by HF in methanol/water mixture.

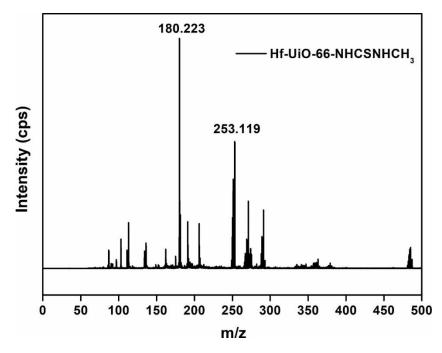


Figure S6. Mass spectrum of Hf-UiO-66-NHCSNHCH<sub>3</sub> after digestion by HF in methanol/water mixture.

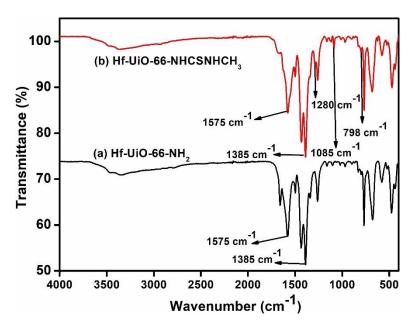


Figure S7. AT-IR spectra of Hf-UiO-66-NH<sub>2</sub> (black) and Hf-UiO-66-NHCSNHCH<sub>3</sub> (red).

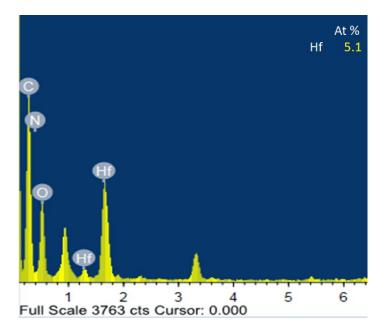


Figure S8. TEM-EDX spectrum of Hf-UiO-66-NH<sub>2</sub>.

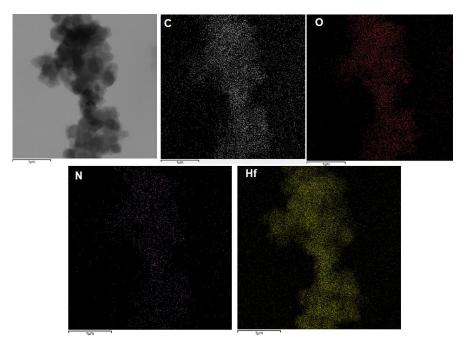


Figure S9. TEM-EDX elemental mapping of Hf-UiO-66-NH<sub>2</sub>.

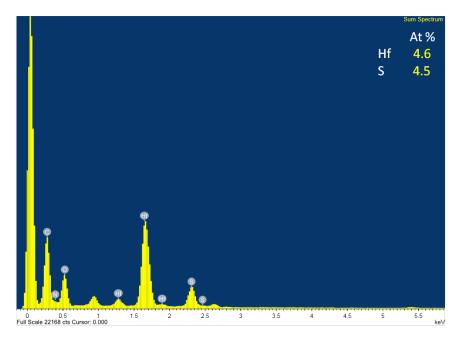


Figure S10. TEM-EDX spectrum of Hf-UiO-66-NHCSNHCH<sub>3</sub>.

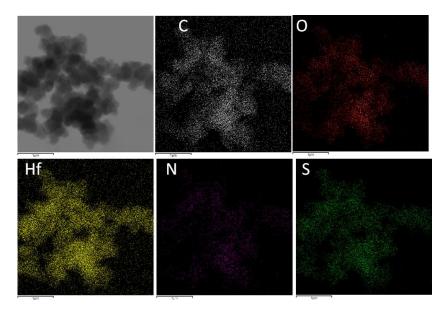


Figure S11. TEM-EDX mapping of Hf-UiO-66-NHCSNHCH<sub>3</sub>.

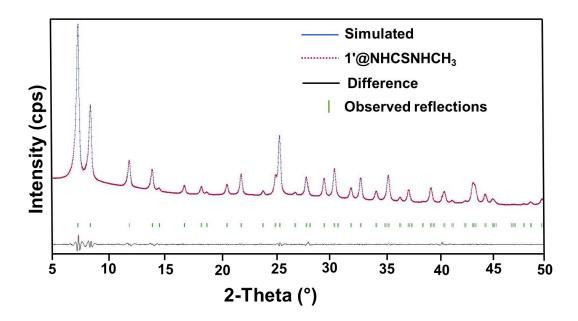
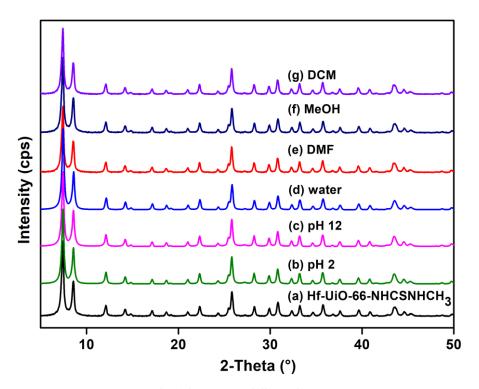


Figure S12. Pawley fit plot for the PXRD pattern of Hf-UiO-66-NHCSNHCH<sub>3</sub> (R<sub>wp</sub> and R<sub>p</sub> are 1.6% and 2.3%, respectively).

<b>Table S1.</b> Indexing parameters of simulated UiO-66 and Hf-UiO-66-NHCSNHCH3.

Compound name	[Hf <sub>6</sub> O <sub>4</sub> (OH) <sub>4</sub> (BDC-	UiO-66 (reported) <sup>1</sup>
	NHCSNHCH <sub>3</sub> ) <sub>6</sub> ]·4H <sub>2</sub> O·5DMF	
	( <b>1</b> ) (this work)	
Crystal System	Cubic	Cubic
$\mathbf{a} = \mathbf{b} = \mathbf{c} \ (\mathbf{A})$	20.743 (5)	20.700 (2)
$\alpha = \beta = \gamma (^{\circ})$	90	90
$V(Å^3)$	8924.6 (35)	8870.3 (2)
Radiation	Cu Kal	Cu Kal



**Figure S13**. PXRD patterns of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> (black) and PXRD pattern of the recovered sample after stirring in (b) pH 2 solution (green), (c) pH 12 solution (pink), (d) water (blue), (e) DMF (red), (f) MeOH (deep blue), (g) DCM (violet).

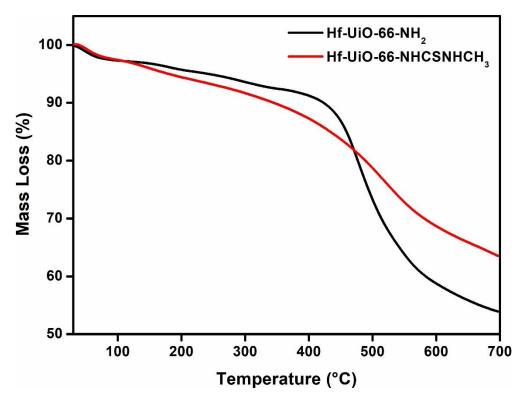


Figure S14. TG curves of Hf-UiO-66-NHCSNHCH3 and Hf-UiO-66-NH<sub>2</sub> measured at - 196  $^{\circ}$ C.

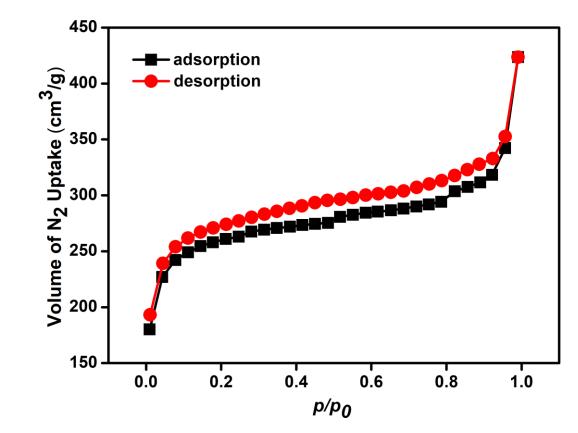


Figure S15. N<sub>2</sub> sorption isotherms of Hf-UiO-66-NH<sub>2</sub> measured at -196 °C.

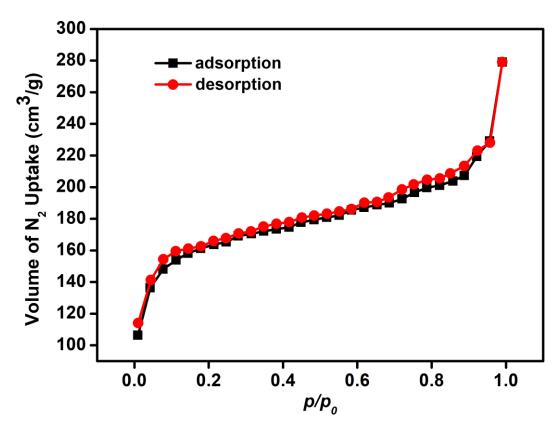


Figure S16. N<sub>2</sub> sorption isotherms of Hf-UiO-66-NHCSNHCH<sub>3</sub> measured at -196 °C.

Volume	Intra-Day	Fluorescence	Emission	Mean ( $\chi$ )	Standard	Relative
of Hg <sup>2+</sup>	-	Intensity (cps)	)		Deviation	Standard
solution					(σ)	Deviation
added						(RSD)
0 µL	461358.6	462046.4	461947.9	461784.3	371.9	0.081
50 µL	214541.7	215282.9	216689.2	215504.6	1090.8	0.506
100 µL	124669.3	125729.4	126317.4	125572.0	835.3	0.665
150 μL	77811.0	77153.8	77527.4	77497.4	329.6	0.425
200 µL	48169.6	48736.6	48896.6	48600.9	382.0	0.786
250 μL	33920.7	33296.7	33558.1	33591.8	313.4	0.933
300 µL	22522.4	22841.6	22217.5	22527.1	312.1	1.385
Volume	Inter-Day	Fluorescence	Emission	Mean ( $\chi$ )	Standard	Relative
of Hg <sup>2+</sup>	-	Intensity (cps)	)		Deviation	Standard
solution					(σ)	Deviation
added						(RSD)
0 µL	461358.6	462579.4	460047.9	461328.6	1266.0	0.274
50 µL	214541.7	220282.9	218689.7	217837.9	2963.8	1.361
100 µL	124669.3	126532.4	125212.4	125471.4	958.2	0.764
150 µL	77811.0	78039.8	76513.3	77454.7	823.2	1.061
200 µL	48169.6	48254.6	49038.6	48487.6	479.1	0.988
250 µL	33920.7	32485.2	34061.1	33489.0	872.1	2.604
300 µL	22522.4	21832.6	23424.5	22593.2	798.3	3.533

**Table S2.** Intra-day and inter-day precession towards detection of  $Hg^{2+}$  towards with standard deviation and relative standard deviation.

**Table S3.** Intra-day and inter-day precession towards detection of NH<sub>2</sub>-NH<sub>2</sub> with standard deviation and relative standard deviation.

Volume of	Intra-Day	Fluorescence	Emission	Mean ( $\chi$ )	Standard	Relative
NH <sub>2</sub> -NH <sub>2</sub>	]	Intensity (cps)	)		Deviation	Standard
Solution					(σ)	Deviation
Added						(RSD)
0 µL	164150.3	163163.2	163084.1	163465.9	594.1	0.363
50 µL	560246.9	562283.7	563234.3	561921.6	1526.2	0.272
100 µL	1406800.8	1402152.4	1408004.7	1405652.1	3090.1	0.220
150 μL	2516240.9	2513823.7	2508612.3	2512891.8	3898.2	0.155
200 µL	3628730.1	3623210.1	3625432.7	3625790.9	2777.3	0.077
250 µL	4351430.3	4356219.3	4359842.8	4355830.7	4219.8	0.097
300 µL	5075660.6	5084791.6	5078214.6	5079555.4	4711.1	0.093
Volume of	Inter-Day	Fluorescence	e Emission	Mean ( $\chi$ )	Standard	Relative
NH <sub>2</sub> -NH <sub>2</sub>	]	Intensity (cps)	)		Deviation	Standard
Solution					(σ)	Deviation
Added						(RSD)
0 µL	164150.3	162578.7	163897.5	163608.8	920.4	0.563
50 µL	560246.9	562237.3	558721.9	560402.04	1762.8	0.315
100 µL	1406800.8	1415758.9	1413975.5	1412178.1	4742.2	0.336

150 μL	2516240.9	2508278.4	2509391.8	2511303.4	4311.3	0.1717
200 µL	3628730.1	3609873.7	3619854.5	3614486.1	5033.2	0.139
250 μL	4351430.3	4360429.6	4349852.3	4353904.0	5706.2	0.1311
300 µL	5075660.6	5100874.7	4997528.2	5058021.0	53884	1.0653

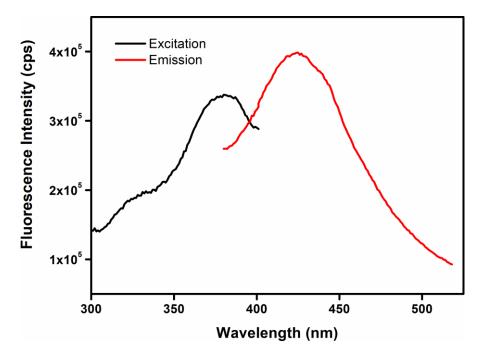
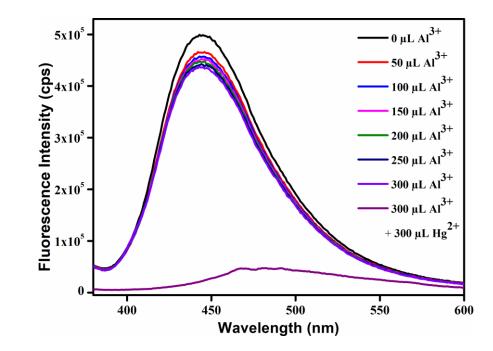
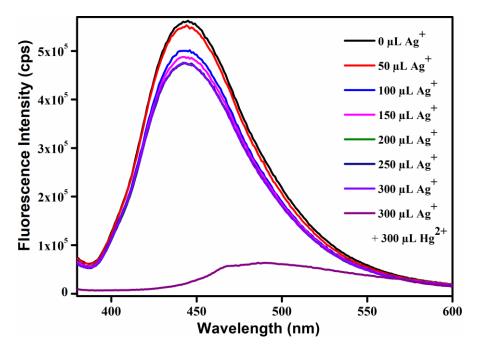


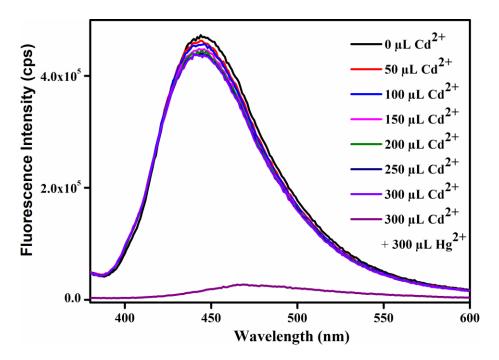
Figure S17. Fluorescence excitation and emission spectra of Hf-UiO-66-NHCSNHCH<sub>3</sub>.



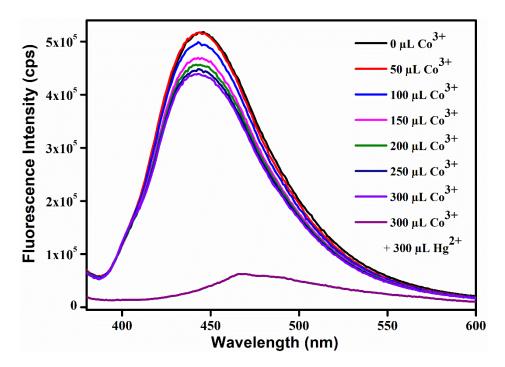
**Figure S18.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Al<sup>3+</sup> solution.



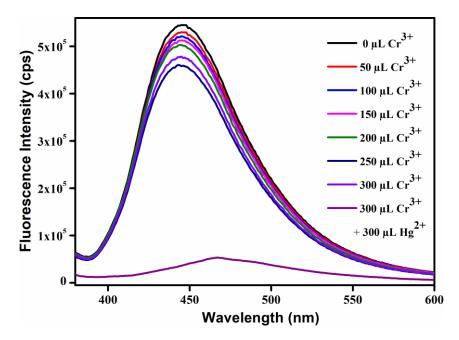
**Figure S19.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH<sub>3</sub>** with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Ag<sup>+</sup> solution.



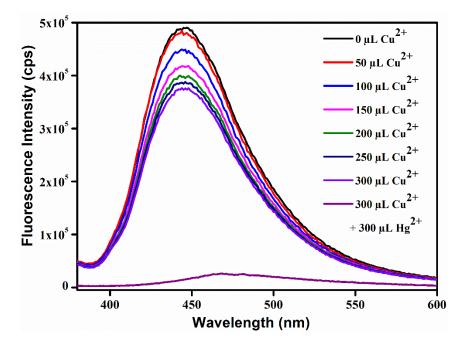
**Figure S20.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Cd<sup>2+</sup> solution.



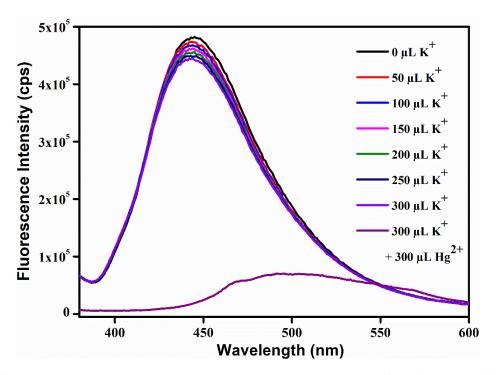
**Figure S21.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Co<sup>3+</sup> solution.



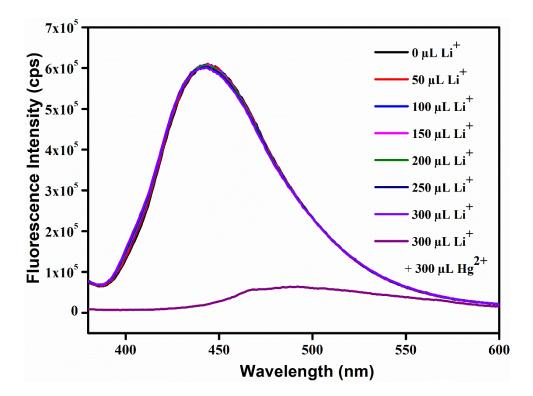
**Figure S22.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Cr<sup>3+</sup> solution.



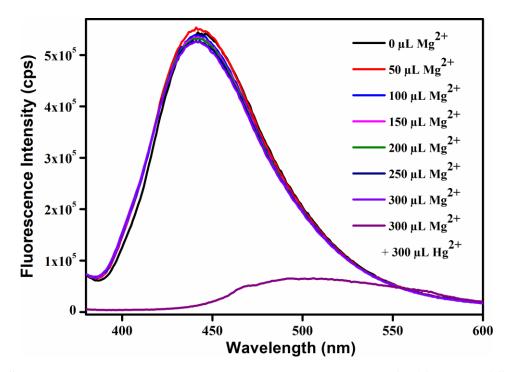
**Figure S23.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH<sub>3</sub>** with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Cu<sup>2+</sup> solution.



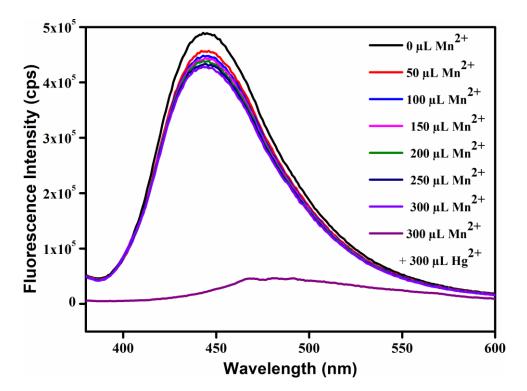
**Figure S24.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous K<sup>+</sup> solution.



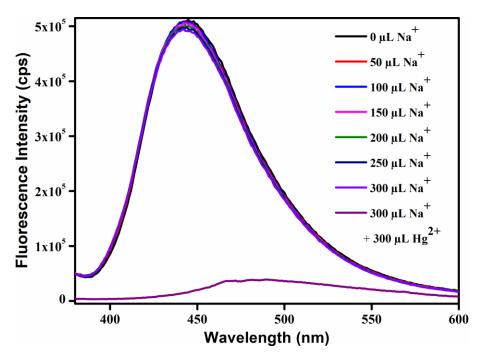
**Figure S25.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Li<sup>+</sup> solution.



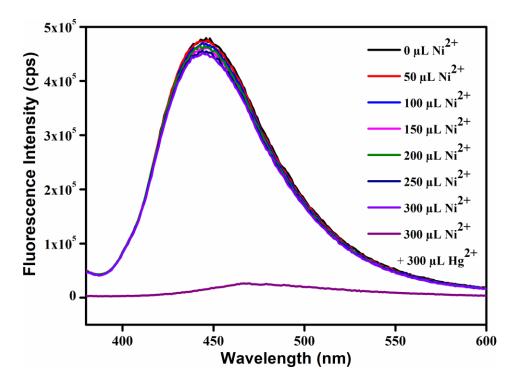
**Figure S26.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Mg<sup>2+</sup> solution.



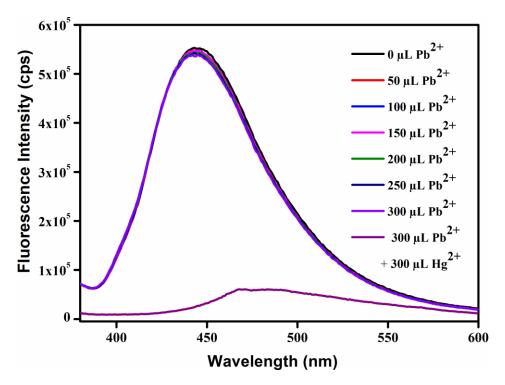
**Figure S27.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Mn<sup>2+</sup> solution.



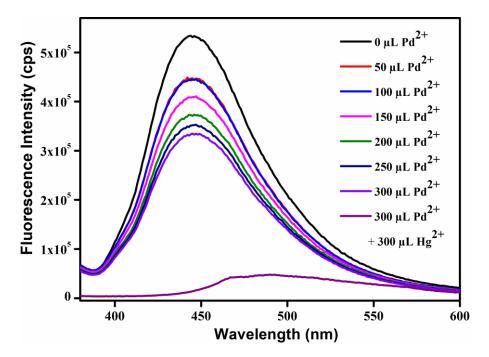
**Figure S28.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Na<sup>+</sup> solution.



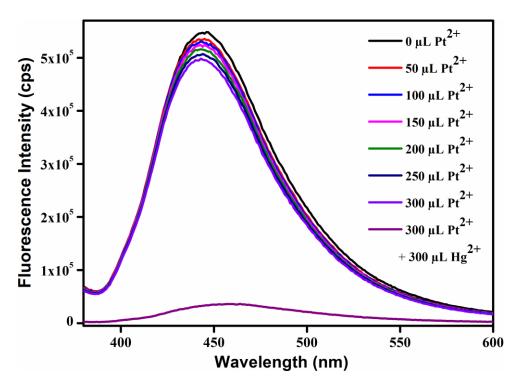
**Figure S29.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Ni<sup>2+</sup> solution.



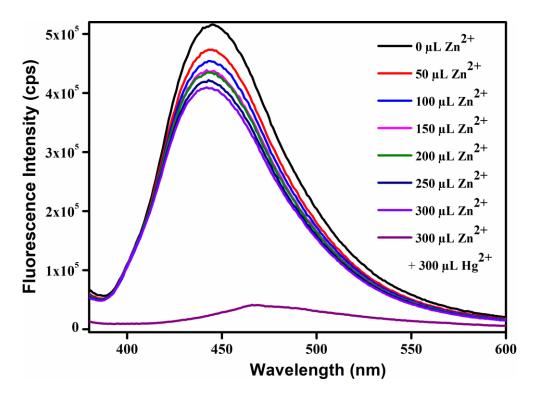
**Figure S30.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH<sub>3</sub>** with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Pb<sup>2+</sup> solution.



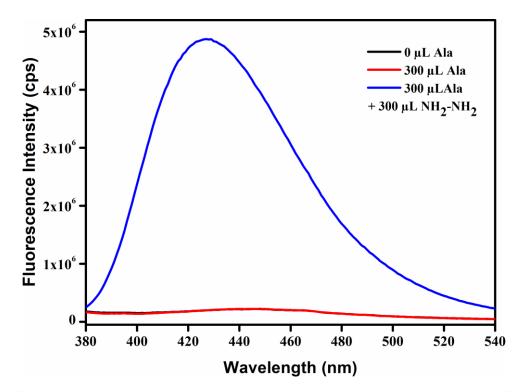
**Figure S31.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Pd<sup>2+</sup> solution.



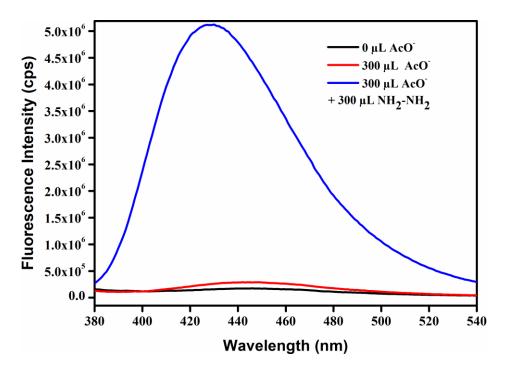
**Figure S32.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH<sub>3</sub>** with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Pt<sup>2+</sup> solution.



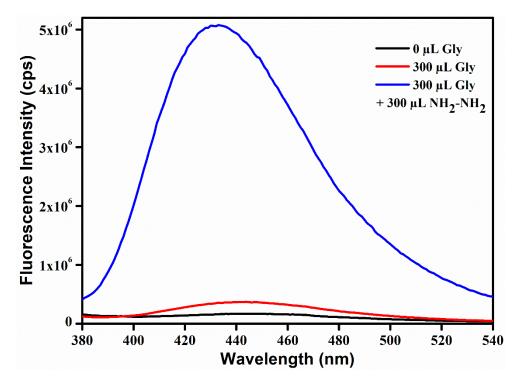
**Figure S33.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous Hg<sup>2+</sup> solution in the presence of 300  $\mu$ L of 10 mM aqueous Zn<sup>2+</sup> solution.



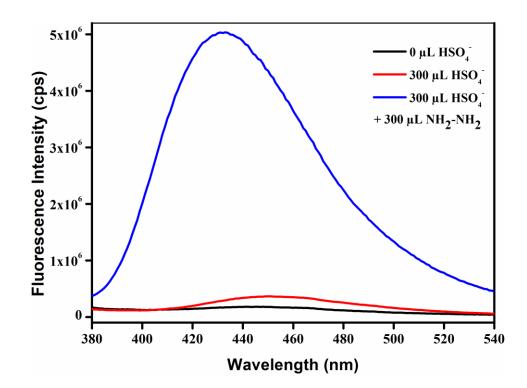
**Figure S34.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous alanine solution.



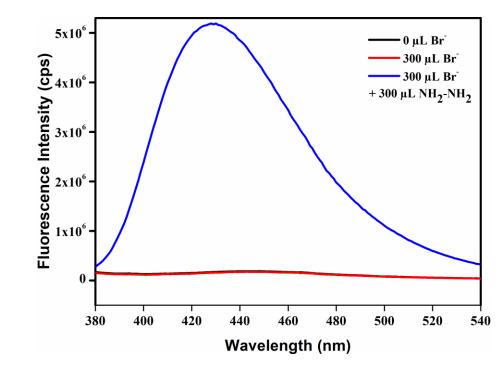
**Figure S35.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous CH<sub>3</sub>COO<sup>-</sup> solution.



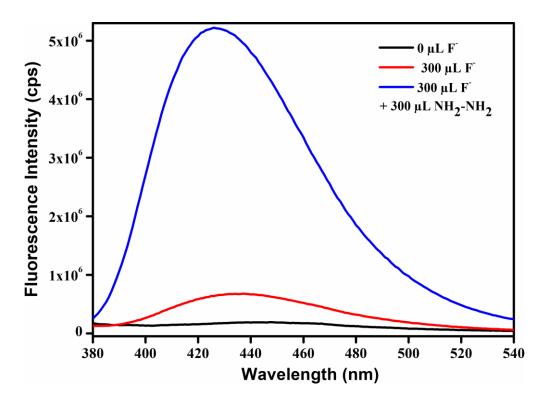
**Figure S36.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous glycine solution.



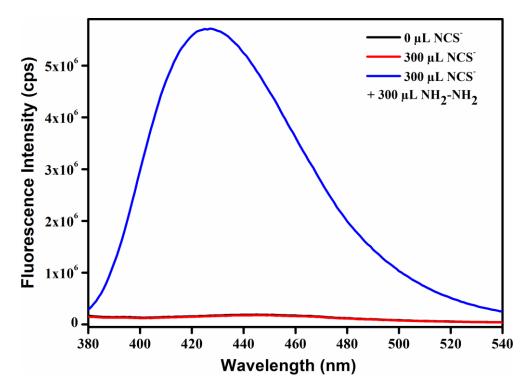
**Figure S37.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous HSO<sub>4</sub><sup>-</sup> solution.



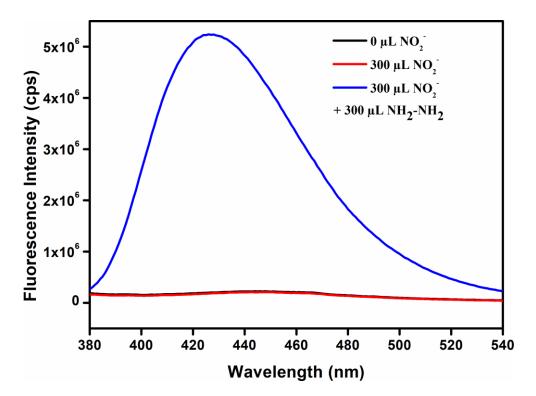
**Figure S38.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous Br<sup>-</sup> solution.



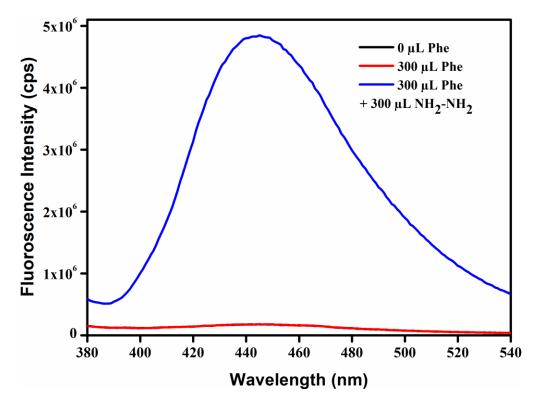
**Figure S39.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous F<sup>-</sup> solution.



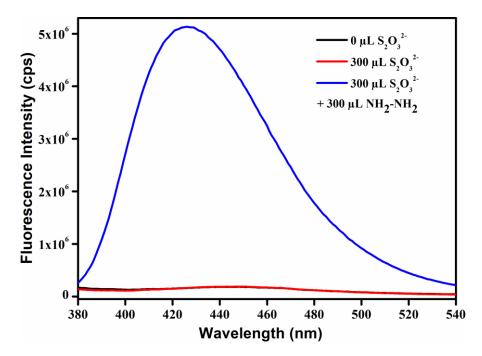
**Figure S40.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous NCS<sup>-</sup> solution.



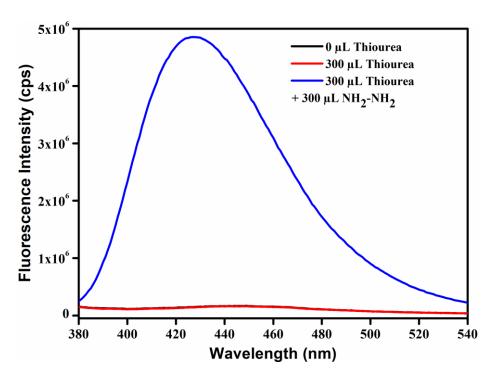
**Figure S41.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous NO<sub>2</sub><sup>-</sup> solution.



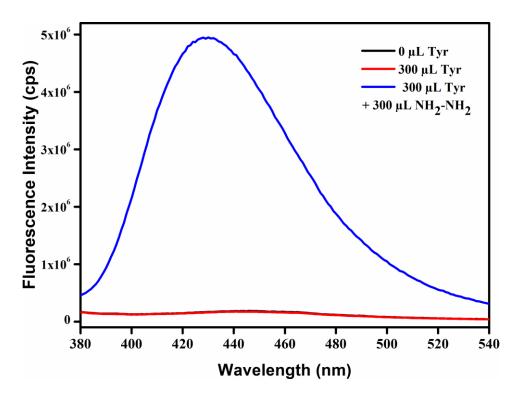
**Figure S42.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sup>3</sup> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous phenyl alanine solution.



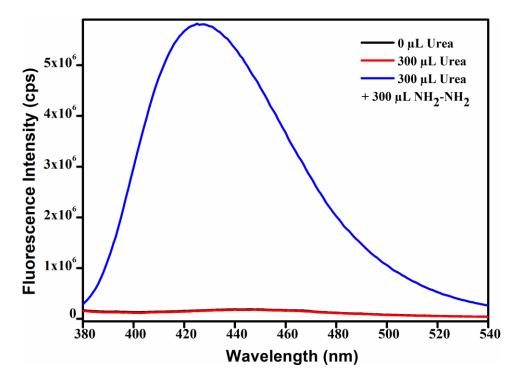
**Figure S43.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous S<sub>2</sub>O<sub>3</sub><sup>2-</sup> solution.



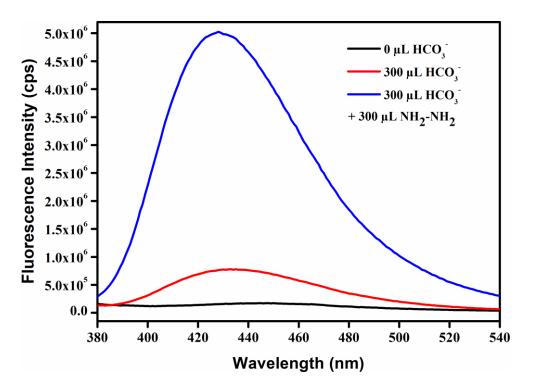
**Figure S44.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous thiourea solution.



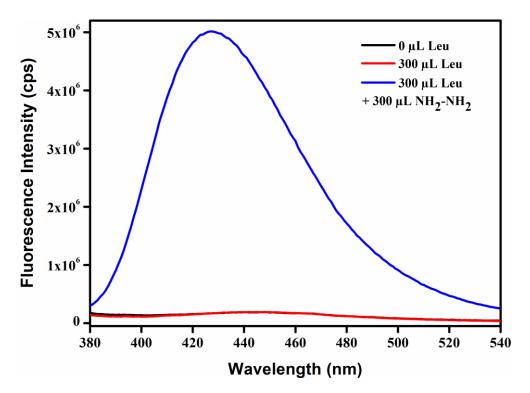
**Figure S45.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous tyrosine solution.



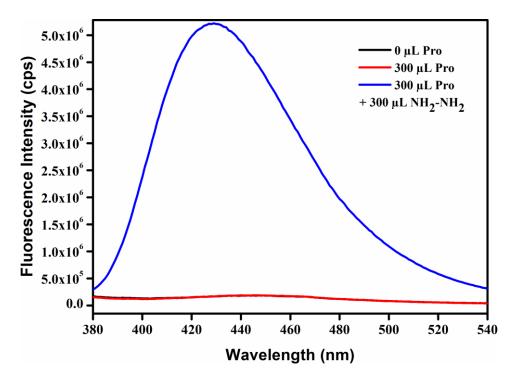
**Figure S46.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous urea solution.



**Figure S47.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous HCO<sub>3</sub><sup>-</sup> solution.



**Figure S48.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous leucine solution.



**Figure S49.** Change in fluorescence emission intensity of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> with the addition of 300  $\mu$ L of 10 mM aqueous hydrazine solution in the presence of 300  $\mu$ L of 10 mM aqueous proline solution.

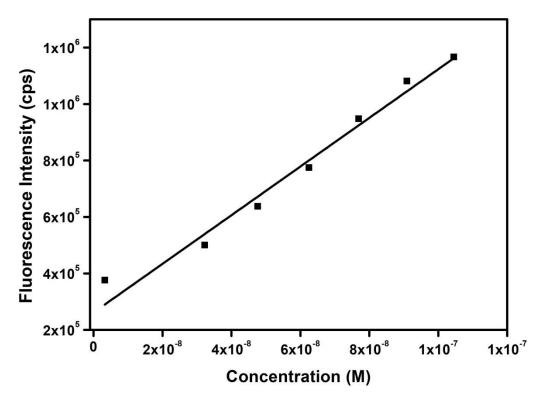


Figure S50. Change in the fluorescence intensity of Hf-UiO-66-NHCSNHCH<sub>3</sub> in water as a function of concentration of  $NH_2$ - $NH_2$  (with error bars).

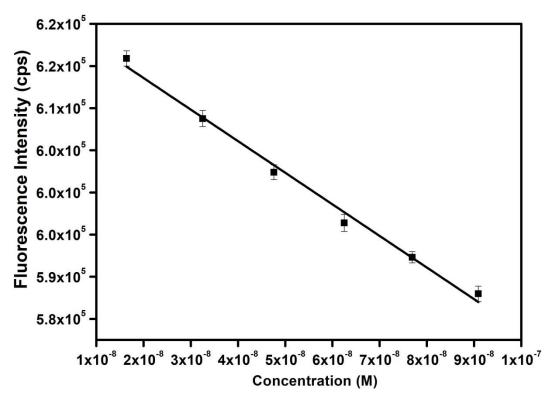


Figure S51. Change in the fluorescence intensity of Hf-UiO-66-NHCSNHCH<sub>3</sub> as a function of concentration of  $Hg^{2+}$  (with error bars).

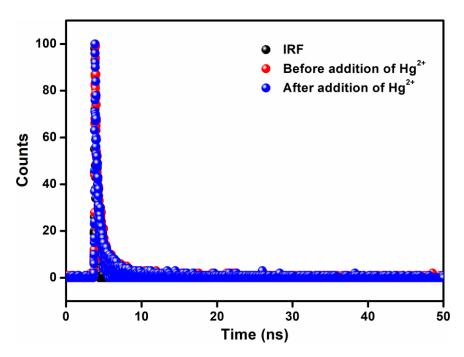
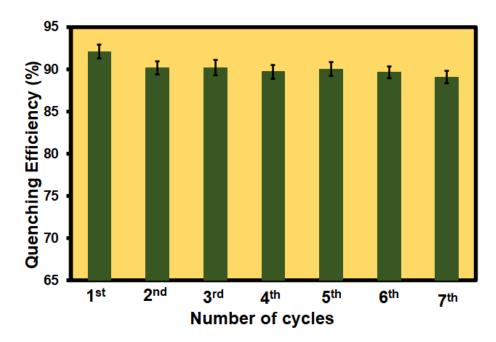


Figure S52. Fluorescence life-time decay curve of probe  $Hf-UiO-66-NHCSNHCH_3$  before and after the addition of  $Hg^{2+}$ .

**Table S4.** Fluorescence life time change (in ns) of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> before and after the addition of 300  $\mu$ L of aqueous Hg<sup>2+</sup> solution.

Volume of Hg <sup>2+</sup> solution added (µL)	B <sub>1</sub>	a <sub>1</sub>	$\tau_1$ (ns)	<τ>* (ns)	$\chi^2$
0	0.0782	1	0.476	0.476	1.054
300	0.0741	1	0.479	0.479	1.001



**Figure S53**. Recyclability of probe **Hf-UiO-66-NHCSNHCH**<sub>3</sub> towards the detection of  $Hg^{2+}$  for 7 cycles with almost equal quenching efficiency up to 7<sup>th</sup> cycle.

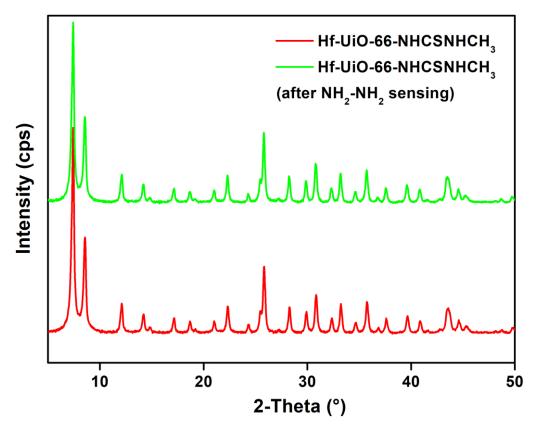
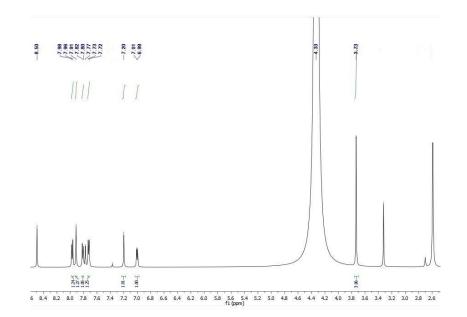
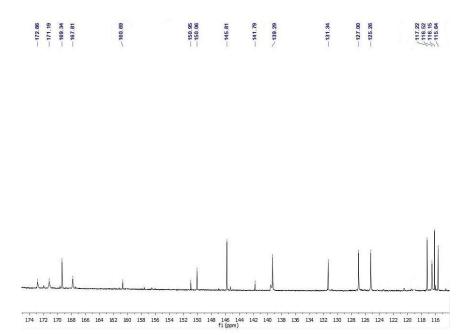


Figure S54. PXRD patterns of Hf-UiO-66-NHCSNHCH<sub>3</sub> before (red) and after (green) sensing of hydrazine.



**Figure S55.** Digested <sup>1</sup>H NMR spectrum of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> after treatment with hydrazine.



**Figure S56.** Digested <sup>13</sup>C NMR spectrum of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> after treatment with hydrazine.

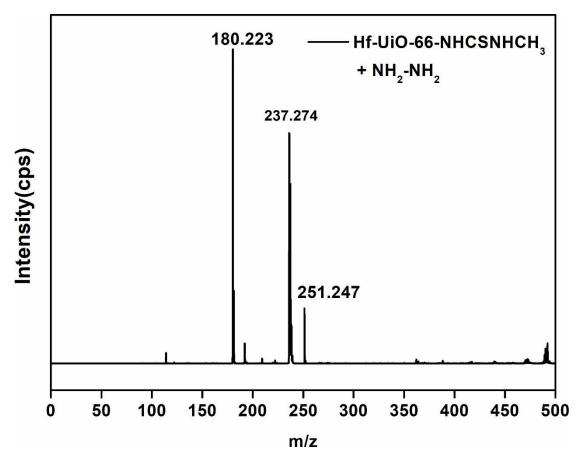


Figure S57. Digested mass spectra spectrum of  $Hf-UiO-66-NHCSNHCH_3$  after treatment with hydrazine in methanol and water mixture.

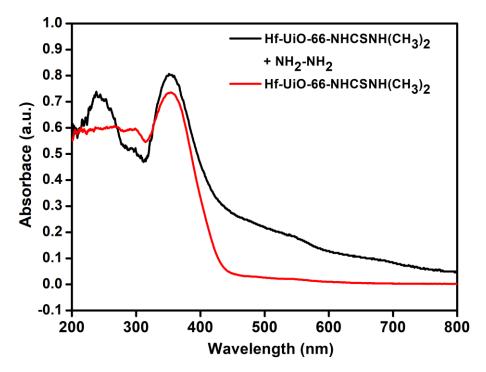


Figure S58. UV-Vis spectrum of  $Hf-UiO-66-NHCSNHCH_3$  before (black) and after (red) sensing of  $NH_2-NH_2$  in solid state.

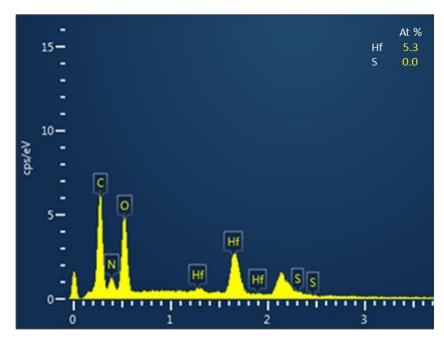


Figure S59. EDX spectrum of recovered  $Hf-UiO-66-NHCSNHCH_3$  after sensing of  $NH_2-NH_2$ .

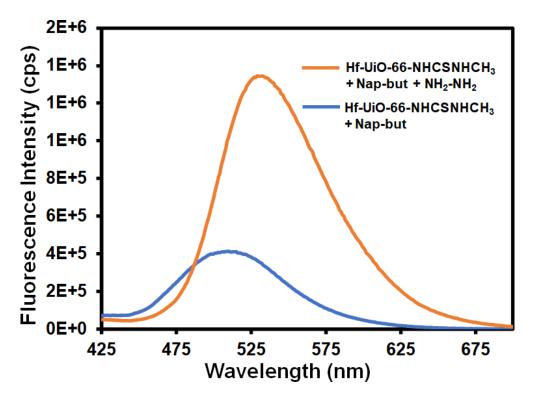


Figure S60. Change in fluorescence emission intensity of Nap-but ( $H_2S$  sensor) in the presence of probe Hf-UiO-66-NHCSNHCH<sub>3</sub> and after addition of NH<sub>2</sub>-NH<sub>2</sub>.



Figure S61. Change in colour of Hf-UiO-66-NHCSNHCH<sub>3</sub> +  $Pb(CH_3COO)_2$  aqueous mixture after the addition of NH<sub>2</sub>-NH<sub>2</sub>.

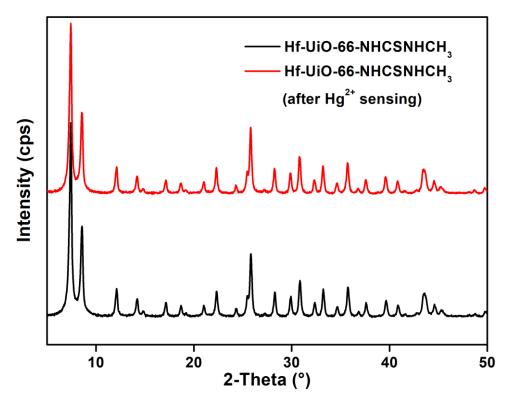
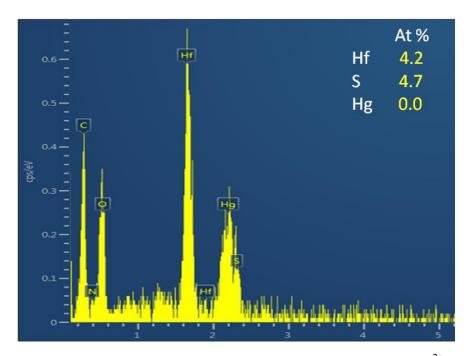
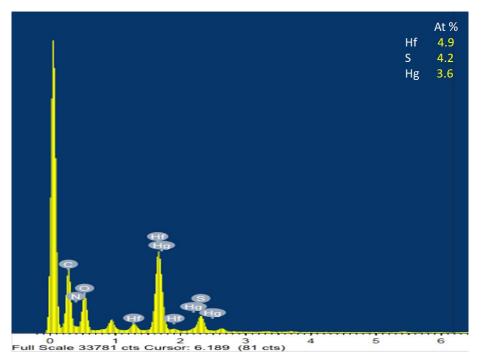


Figure S62. PXRD pattern of Hf-UiO-66-NHCSNHCH<sub>3</sub> before (black) and after (red) the addition of aqueous solution of  $Hg^{2+}$ .



**Figure S63.** TEM-EDX spectrum of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> after  $Hg^{2+}$  sensing after through washing.



**Figure S64.** TEM-EDX spectrum of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> after  $Hg^{2+}$  sensing and without through washing.

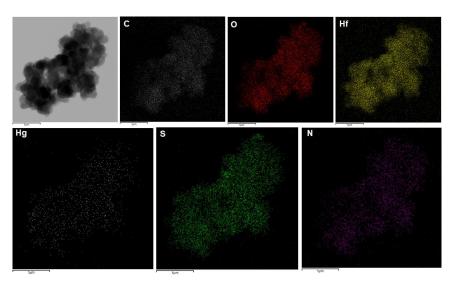
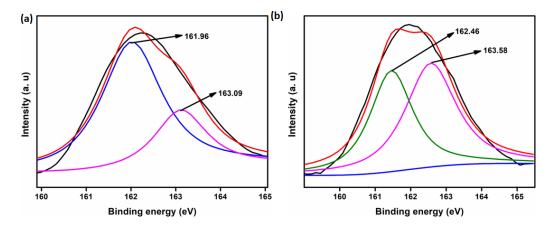
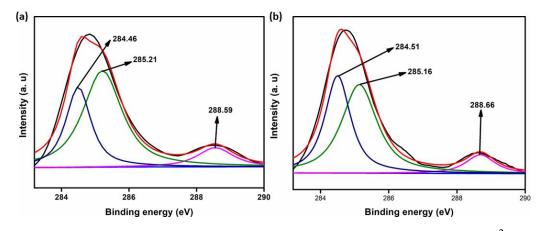


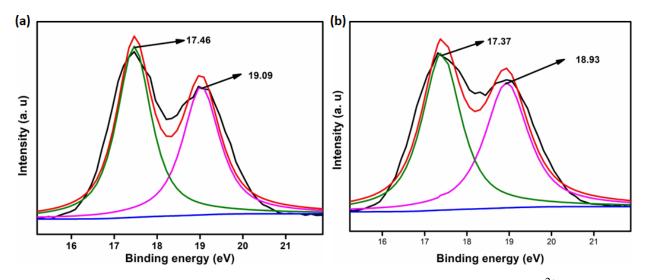
Figure S65. TEM-EDX mapping of Hf-UiO-66-NHCSNHCH<sub>3</sub> after  $Hg^{2+}$  sensing and without washing.



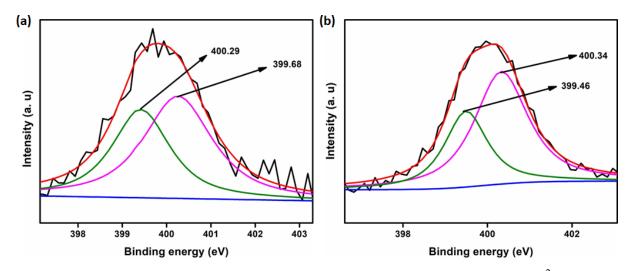
**Figure S66.** Fitted XPS spectra of S (2s) before (a) and after (b) treatment of  $Hg^{2+}$  with **Hf-UiO-66-NHCSNHCH**<sub>3</sub>.



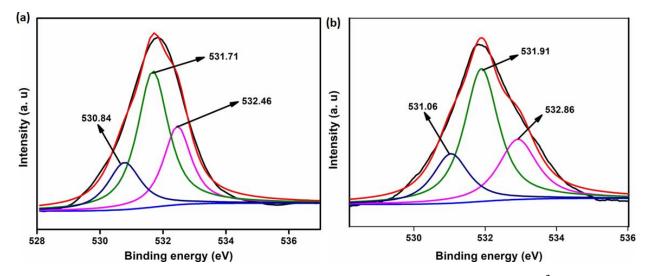
**Figure S67.** Fitted XPS spectra of C (1s) before (a) and after (b) treatment of  $Hg^{2+}$  with **Hf-UiO-66-NHCSNHCH**<sub>3</sub>.



**Figure S68.** Fitted XPS spectra of Hf (4f) before (a) and after (b) treatment of  $Hg^{2+}$  with **Hf-UiO-66-NHCSNHCH**<sub>3</sub>.



**Figure S69.** Fitted XPS spectra of N (1s) before (a) and after (b) treatment of  $Hg^{2+}$  with **Hf**-UiO-66-NHCSNHCH<sub>3</sub>.



**Figure S70.** Fitted XPS spectra of O (1s) before (a) and after (b) treatment of  $Hg^{2+}$  with **Hf-UiO-66-NHCSNHCH**<sub>3</sub>.

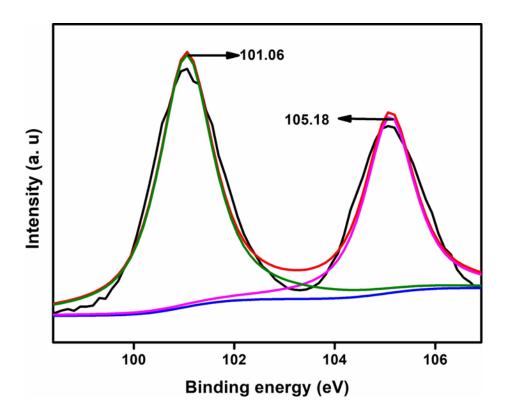


Figure S71. Fitted XPS spectra of Hg (4f) after treatment of  $Hg^{2+}$  with Hf-UiO-66-NHCSNHCH<sub>3</sub>.

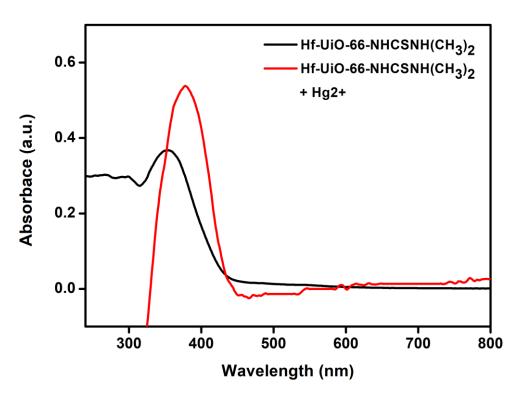
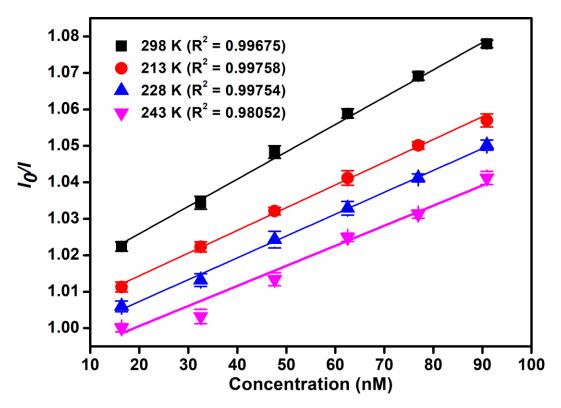
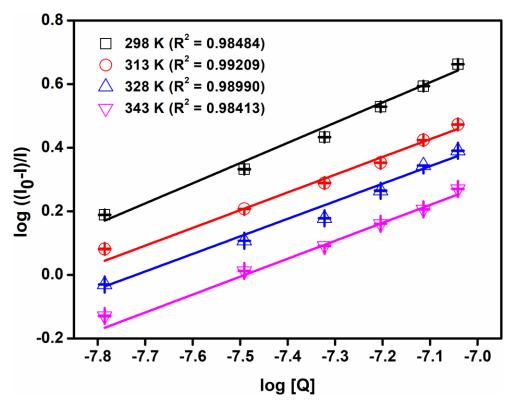


Figure S72. Solid-state UV-Vis spectrum of  $Hf-UiO-66-NHCSNHCH_3$  before (black) and after (red) sensing of  $Hg^{2+}$ .



**Figure S73.** Stern-Volmer plots (with error bars) for fluorescence quenching of **Hf-UiO-66-NHCSNHCH**<sub>3</sub> by  $Hg^{2+}$  at different temperatures.



**Figure S74.** Modified Stern-Volmer plots (with error bars) between  $log((I_0-I)/I)$  and log [Q].

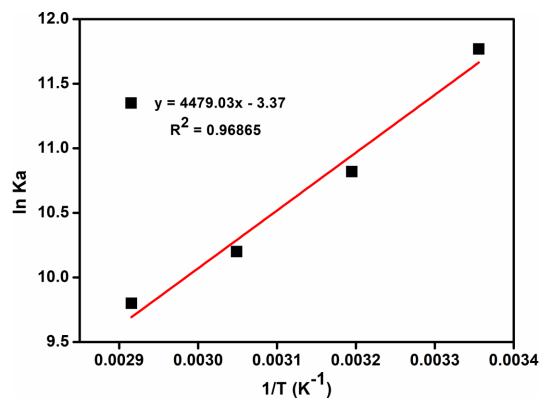


Figure S75. Van't Hoff plot for interaction of  $Hf-UiO-66-NHCSNHCH_3$  with  $Hg^{2+}$ .

Table S5. Comparison of the response time, detection limit and sensing media used for the
reported fluorescent chemosensors of NH <sub>2</sub> -NH <sub>2</sub> in the literature.

Sl. No.	Sensor Material	Type of Material	Sensing Medium	Mode of Detection	Detection Limit	Response Time	Ref.
1	$[Zr_6O_4(OH)_4(BDC\text{-}O\text{-}SO_2\text{-}Ph\text{-}NO_2)_6]\cdot11H_2O\cdot4DMF$	MOF	water	turn-on	52.6 nM	2 min	2
2	Zr-UiO-66-(OCOCH <sub>3</sub> ) <sub>2</sub>	MOF	water	turn-on	78.8 nM	seconds	3
3	UiO-66-phmd	MOF	HEPES buffer	turn-on	0.87 µM	20 min	4
4	BTI	organic- molecule	HEPES buffer	turn-on	2.9 ppb	20 min	5
5	HyP-1	organic- molecule	PBS buffer	turn-on	0.035 ppb	1 h	6
6	P1	organic- molecule	PRS buffer	turn-on	1.79 nM	40 s	7
7	BPB	BODIPY- based organic molecule	HEPES buffer	turn-off	1.87 μ <b>M</b>	-	8

8	Naphsulf-O	Organic- molecule	PBS buffer	turn-on	22 nM	40 min	9
9	BBHC	Organic- molecule	PBS buffer	turn-on	0.43 µM	1 min	10
10	CFAc	Organic- molecule	PBS buffer	ratio-metric	0.0474 μM	-	11
11	BI-E	near-infrared fluorescent probe	PBS buffer	turn-on	0.057 μM	1 min	12
12	NA-N <sub>2</sub> H <sub>4</sub>	naphthalimid e based organic molecule	HEPES buffer	ratio-metric	9.4 nM	15 min	13
13	ТАРНР	organic- molecule	HEPES buffer	ratio-metric	0.3 µM	60 min	14
14	AB-NDI	organic- molecule	DMSO	turn-on	-	-	15
15	TNQ	organic- molecule	PBS buffer	ratio-metric	-	-	16
16	НВТМ	organic- molecule	PBS buffer	turn-on	29 µM	55 min	17
17	NAC	naphthalene based organic molecule	HEPES buffer	turn-on	4.5 μΜ	4 min	18
18	DPA	organic- molecule	DMSO/ PBS buffer solution (4/6, v/v)	turn-on	1.9 nM	8 min	19
19	probe 1 probe 2	pyrene- and anthraceneba sed organic molecule	HEPES buffer	turn-on	0.17 μM 0.24 μM	3 min	20
20	SF-Azo compounds	organic- molecule	$CH_{3}OH/H_{2}$ $O (v/v = 1:1)$	turn-on	2.33 mM	18-42 min	21
21	levulinated hydroxyl- coumarin 1	organic- molecule	acetate buffer	turn-on	2.46 µM	15 min	22
22	Compound 6a	organic- molecule	HEPES/ DMSO (1:1, v/v)	turn-on and ratiometric	0.19 μΜ	-	23
23	NS-N <sub>2</sub> H <sub>4</sub>	organic- molecule	$\frac{PBS}{DMSO} (v/v = 2/1)$	turn-on	-	240 min	24
24	PBF	organic- molecule	CH <sub>3</sub> CN– H <sub>2</sub> O (6: 4, v/v)	turn-on	0.41 μM	1 min	25
25	Hf-UiO-66-NHCSNHCH <sub>3</sub>	MOF	H <sub>2</sub> O	turn-on	1.9 nM	0.8 min	this work

Table S6. Comparison of the response time, detection limit and sensing media used for the
reported chemosensors of $Hg^{2+}$ in the literature using fluorometric method.

Sl. No.	Sensor Material	Type of Material	Sensing Medium	Detection Limit (nM)	Response Time (min)	Ref.
1	Thiosemicarbazone	organic- molecule	0.01 M acetic acid/sodium acetate buffer	770	-	26
2	GT capped AgNPs	nanoparticles	water	0.037	0-60	27
3	Azo Crown ether	organic molecule	methanol	13900	-	28
4	Rhodamine 6 G based	Rh-complex	THF: Water (8:2, v/v, pH = 7)	30.37	-	29
5	Tetraphenyl ethylene based AIE probe	organic molecule	water	63	-	30
6	Squaraine based fluorescent probe	organic molecule	Ethanol: Water (20:80, v/v)	21.9	3	31
7	Rhodamine appended terphenyl	organic molecule	THF	500	30	32
8	Double naphthalene Schiff base	organic compound	DMSO	55.9	80	33
9	2-Hydroxy benzothiazole modified rhodol	organic compound	THF: HEPES (4:6, v/v)	270	-	34
10	Nitrogen-doped carbon quantum dots	quantum dots	water	230	15	35
11	$[Ni(3-bpd)_2(NCS)_2]_n$	MOF	water	-	120	36
12	[PCN-221]	MOF	water	10	1	37
13	[Cu(Dcbb)(Bpe)].Cl	MOF	HEPES buffer	3.2 and 3.3	30	38
14	UiO-66@ Butyne	MOF	water	10.9	3	39

15	Ln(TATAB) (DMF) <sub>4</sub> (H <sub>2</sub> O)(MeOH) <sub>0.5</sub>	MOF	water	4.4	-	40
16	Eu <sup>3+</sup> /CDs@MOF-253	MOF	water	47.88	3	41
17	[Cu(Cdcbp)(H <sub>2</sub> O)2·2H 2O] <sub>n</sub>	MOF	water	2.3	2	42
18	Al-MOF (TAM)	MOF	water	2.94	0.5	43
19	$[Cu(Cbdcp)(Dps) \\ (H_2O)_3] \cdot 6H_2O_n$	MOF	HEPES buffer	2.6	10	44
20	Cd–EDDA	MOF	water	2	0.25	45
21	tetrahydrodibenzo phenanthridine derivatives	organic compound	DMSO : THF = 1 : 1	0.91 0.041	1	46
22	$[Zn(L)(BBI).(H_2O)_2]$ $[Cd(L)(TPOM)0_{.75}] \cdot xS$	MOF	water	-		47
33	IITG-5a	MOF	water	5	1	48
34	Hf-UiO-66-NHCSNHCH <sub>3</sub>	MOF	H <sub>2</sub> O	4	0.16	this work

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