

# **Stimuli-Sensitive Pyrenylated Hydrogels as Optical Sensing Platform for Multiple Metal Ions**

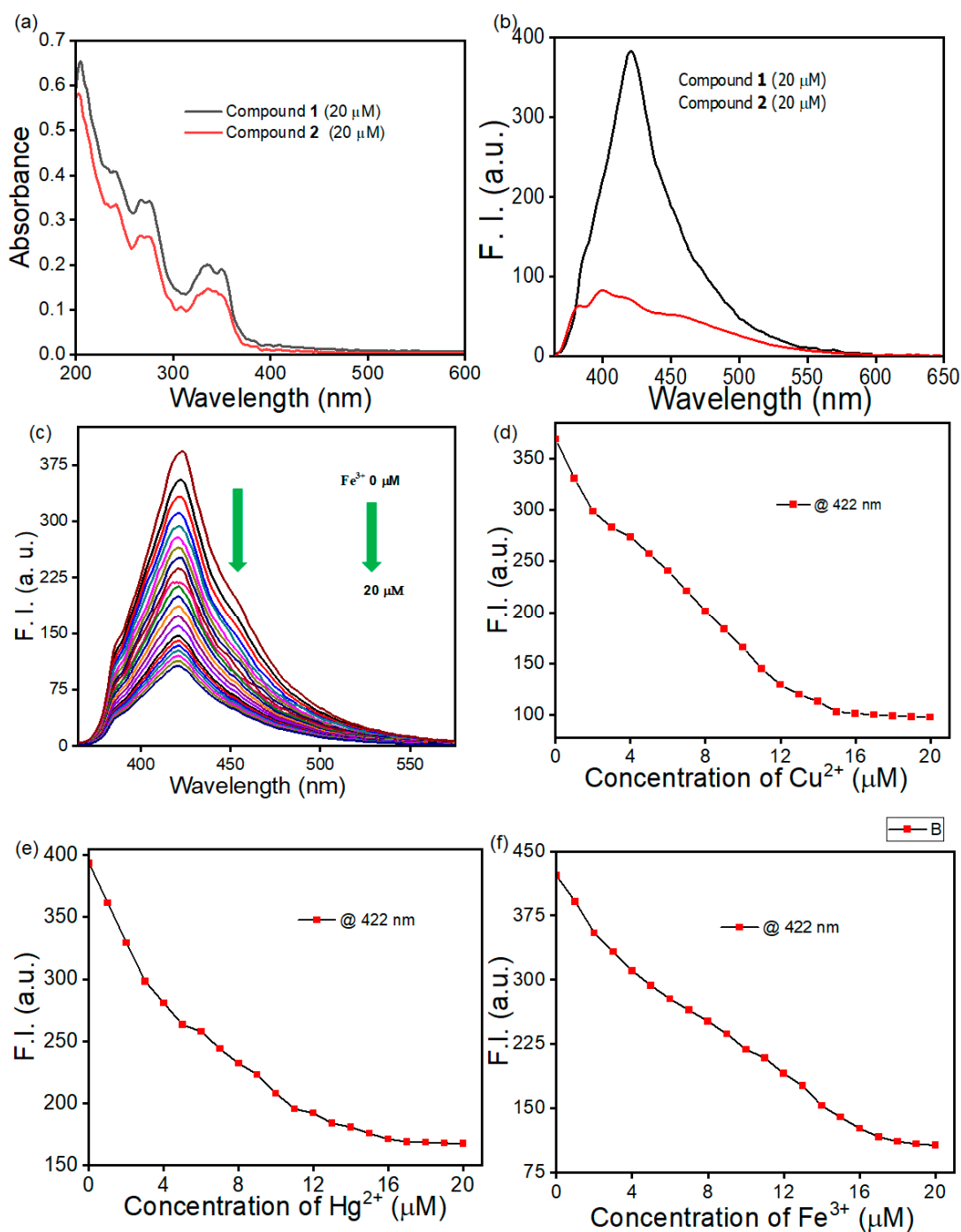
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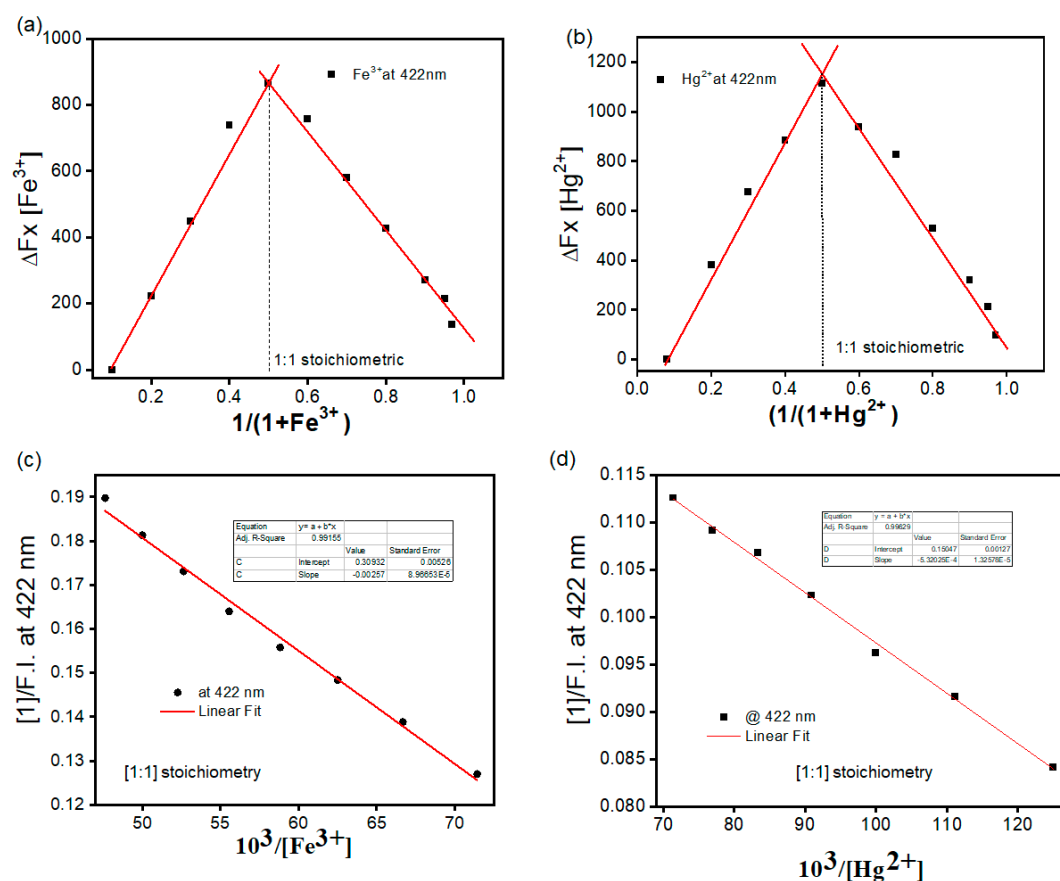
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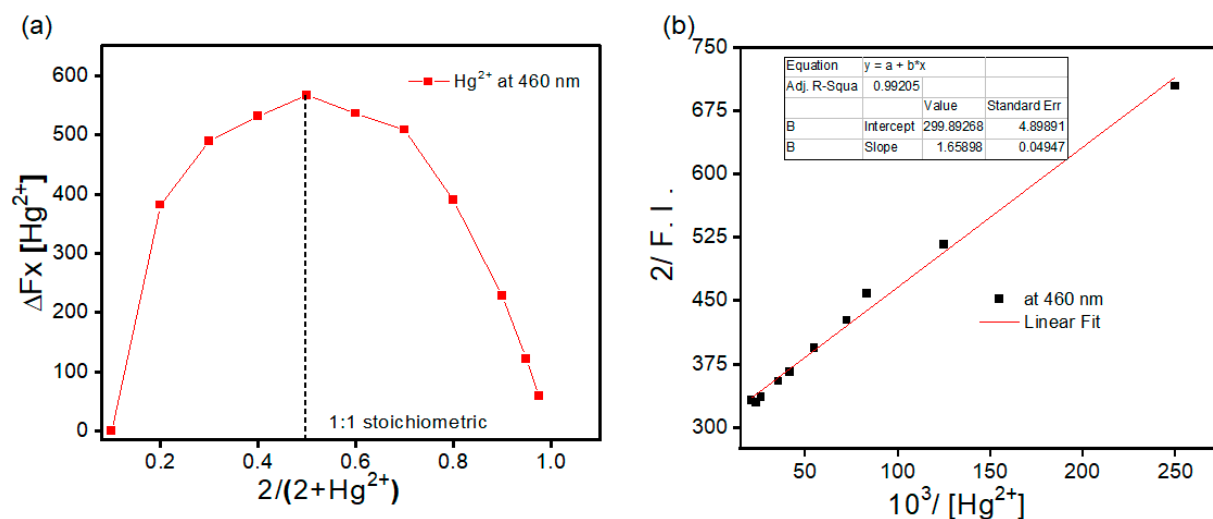
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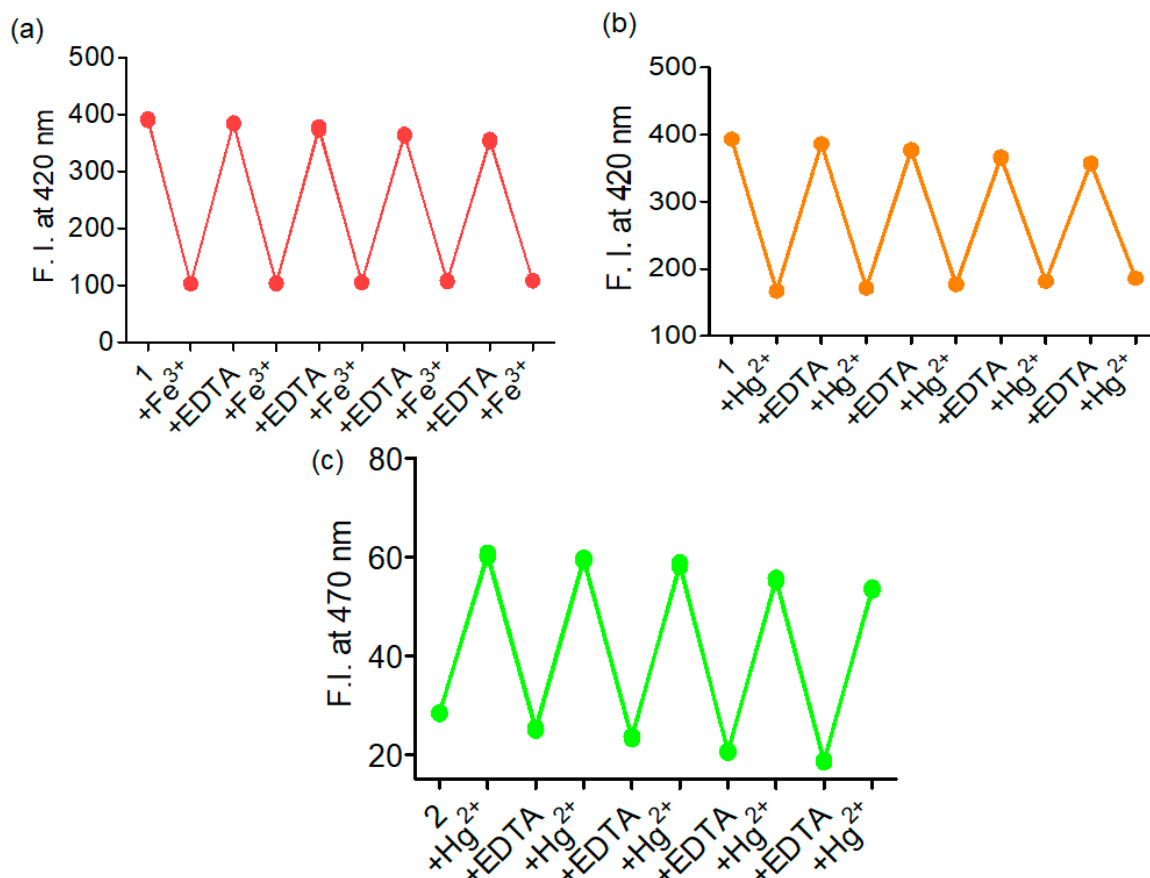
**Figure S1.** (a) Absorbance spectra of the compound **1** (20  $\mu\text{M}$ ) and **2** (20  $\mu\text{M}$ ) in water. (b) Emission spectra of compound **1** (20  $\mu\text{M}$ ,  $\lambda_{\text{ex}} = 345 \text{ nm}$ ) and **2** (20  $\mu\text{M}$ ,  $\lambda_{\text{ex}} = 345 \text{ nm}$ ) in water. (c) Fluorescence titration of compound **1** (20  $\mu\text{M}$ ,  $\lambda_{\text{ex}} = 345 \text{ nm}$ ) with increasing concentration of  $\text{Fe}^{3+}$ . Change in the emission intensity of compound **1** in the presence of increasing concentrations of (d)  $\text{Cu}^{2+}$ , (e)  $\text{Hg}^{2+}$ , and (f)  $\text{Fe}^{3+}$ .



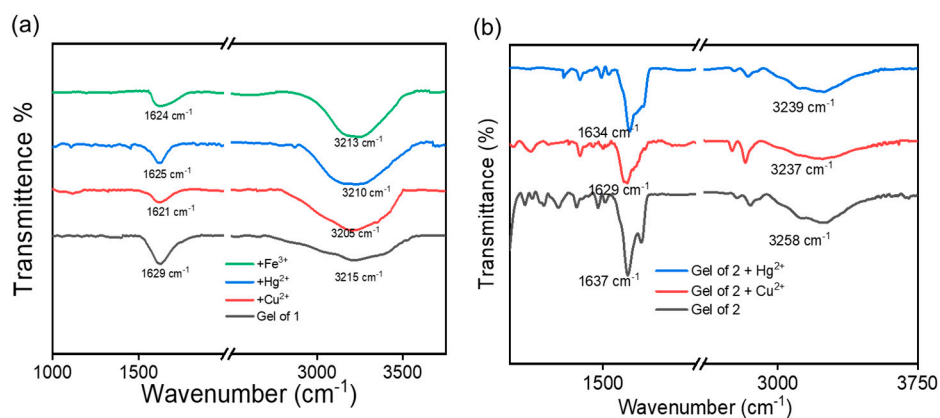
**Figure S2:** Jobs plot for the interaction of compound 1 with (a)  $\text{Fe}^{3+}$ , (b)  $\text{Hg}^{2+}$ . Calculation of binding constant for compound 1 with (c)  $\text{Fe}^{3+}$ , (d)  $\text{Hg}^{2+}$ .



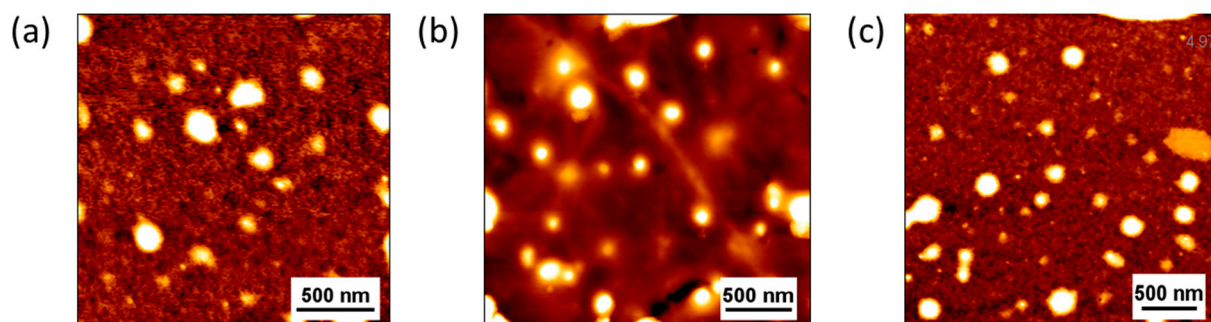
**Figure S3:** (a) Jobs plot for the interaction of compound 2 with  $\text{Hg}^{2+}$ . (b) Calculation of binding constant for the interaction of compound 2 with  $\text{Hg}^{2+}$ .



**Figure S4:** EDTA-mediated recovery plot for the interaction of compound **1** with (a)  $\text{Fe}^{3+}$  and (b)  $\text{Hg}^{2+}$ . (c) EDTA-mediated recovery plot for the interaction of compound **2** with  $\text{Hg}^{2+}$ .



**Figure S5:** FT-IR spectra for the interaction of (a) compound **1** with  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ , and  $\text{Hg}^{2+}$ , and (b) compound **2** with  $\text{Cu}^{2+}$  and  $\text{Hg}^{2+}$ .



**Figure S6:** AFM images for the interaction of compound **1** with  $\text{Cu}^{2+}$ ,  $\text{Fe}^{3+}$ , and  $\text{Hg}^{2+}$ .

**Table S1:** Recovery experiment of (a)  $\text{Cu}^{2+}$ , (b)  $\text{Fe}^{3+}$ , and (c)  $\text{Hg}^{2+}$  using compound **1** (20  $\mu\text{M}$ ) and in a tap water sample.

(a)

$\text{Cu}^{2+}$ added ( $\mu\text{M}$ )	$\text{Cu}^{2+}$ calculated Std plot: $Y = 341.71 - 17.41x$			$\text{Cu}^{2+}$ found	Recovery	RSD (%)
0	0	0	0	0	0	0
2	2.12	2.25	2.05	2.14	107.00	4.74
4	4.06	4.22	4.11	4.13	103.25	1.98
6	6.11	6.02	6.09	6.07	101.1	0.78
8	8.23	8.09	8.15	8.16	102.00	0.86
10	10.14	10.04	10.31	10.16	101.6	1.34

(b)

$\text{Hg}^{2+}$ added ( $\mu\text{M}$ )	$\text{Hg}^{2+}$ calculated Std plot: $Y = 322.02 - 12.72x$			$\text{Hg}^{2+}$ found	Recovery	RSD (%)
0	0	0	0	0	0	0
2	2.20	2.15	2.11	2.15	103.00	2.09
4	4.34	4.12	4.48	4.31	107.83	4.21
6	6.09	6.19	6.37	6.22	103.61	2.28
8	8.09	8.36	8.21	8.22	102.75	1.65
10	10.09	10.39	10.15	10.21	102.10	1.55

(c)

$\text{Fe}^{3+}$ added ( $\mu\text{M}$ )	$\text{Fe}^{3+}$ calculated Std plot: $Y = 351.27 - 14.40x$			$\text{Fe}^{3+}$ found	Recovery	RSD (%)
0	0	0	0	0	0	0
2	2.18	2.05	2.12	2.12	102.56	3.07
4	4.46	4.15	4.28	4.30	107.50	3.62
6	6.19	6.03	6.43	6.22	103.67	3.24
8	8.15	8.35	8.07	8.19	102.37	1.76
10	10.11	10.35	10.06	10.17	101.70	1.52

**Table S2:** Recovery experiment of (a)  $\text{Cu}^{2+}$  and (b)  $\text{Hg}^{2+}$  using compound **2** (20  $\mu\text{M}$ ) in a tap water sample.

(a)

$\text{Cu}^{2+}$ added ( $\mu\text{M}$ )	$\text{Cu}^{2+}$ calculated Std plot: $Y = 48.56 - 1.14x$			$\text{Cu}^{2+}$ found	Recovery	RSD (%)
0	0	0	0	0	0	0
2	2.22	2.16	2.30	2.23	103.67	3.15
4	4.16	4.32	4.01	4.16	104.08	3.72
6	6.18	6.09	6.29	6.19	103.11	1.62
8	8.12	8.02	8.25	8.13	101.63	1.42
10	10.04	10.19	10.28	10.17	101.70	1.19

(b)

$\text{Hg}^{2+}$ added ( $\mu\text{M}$ )	$\text{Hg}^{2+}$ calculated Std plot: $Y = 0.935x + 31.64$			$\text{Hg}^{2+}$ found	Recovery	RSD (%)
0	0	0	0	0	0	0
2	2.30	2.15	2.22	2.21	102.50	3.38
4	4.16	4.02	4.35	4.18	104.41	3.97
6	6.23	6.05	6.33	6.20	103.39	2.29
8	8.01	8.22	8.39	8.21	102.58	2.32
10	10.25	10.11	10.35	10.24	102.36	1.18