

**Fig. S1** Fluorescence spectra of DP-4 (20  $\mu\text{M}$ ) excited at 295 nm in the presence of various ions in 10 mM HEPES buffer at pH 7.1. The molar ratio of metal/D-P4 is 1:1.

**Fig. S2** Fluorescence emission spectra of D-P4 (20.0  $\mu\text{M}$ ) excited at 295 nm with addition of increasing concentrations of  $\text{Cu}^{2+}$  (0-25.0  $\mu\text{M}$ ) (a) and  $\text{Hg}^{2+}$  (0-7.0  $\mu\text{M}$ ) (b) in 10 mM HEPES buffer at pH 7.1.

**Fig. S3** Benesi-Hildebrand plots for the determination of the binding constants of D-P5 (100.0  $\mu\text{M}$ ) with  $\text{Cu}^{2+}$  (a) and  $\text{Hg}^{2+}$  (b).

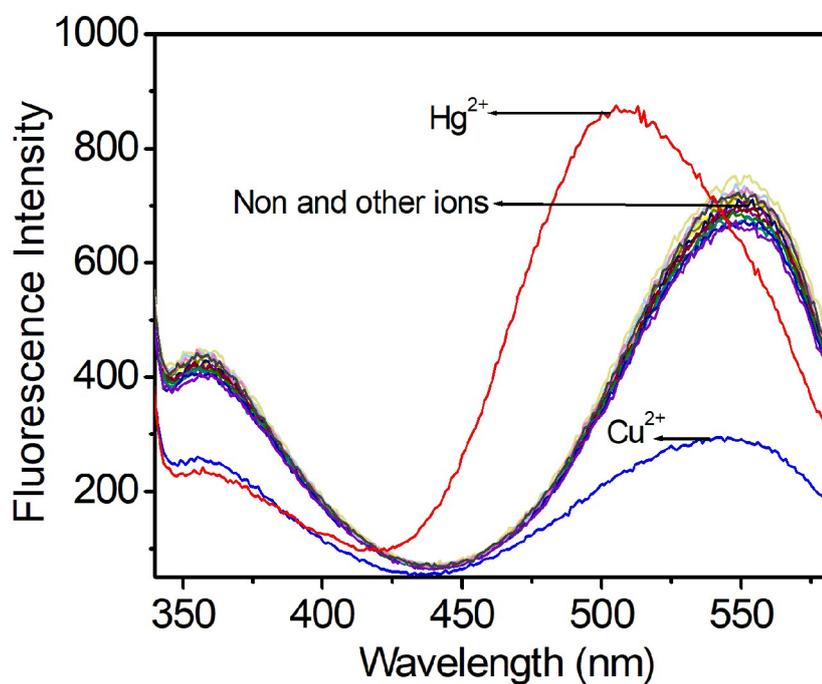
**Fig. S4** Absorption spectra of D-P4 (20.0  $\mu\text{M}$ ) in the absence and presence of  $\text{Cu}^{2+}$  (0.5 equiv.) and  $\text{Hg}^{2+}$  (0.5 equiv.) in 10 mM HEPES buffer solution at pH 7.1.

**Fig. S5** Fluorescence spectra of regeneration of D-P4-Hg (20.0  $\mu\text{M}$ ) system by Cys in 10 mM HEPES buffer solution.  $\text{Hg}^{2+}$  (1/3 equiv.) and Cys (1/3 equiv.).

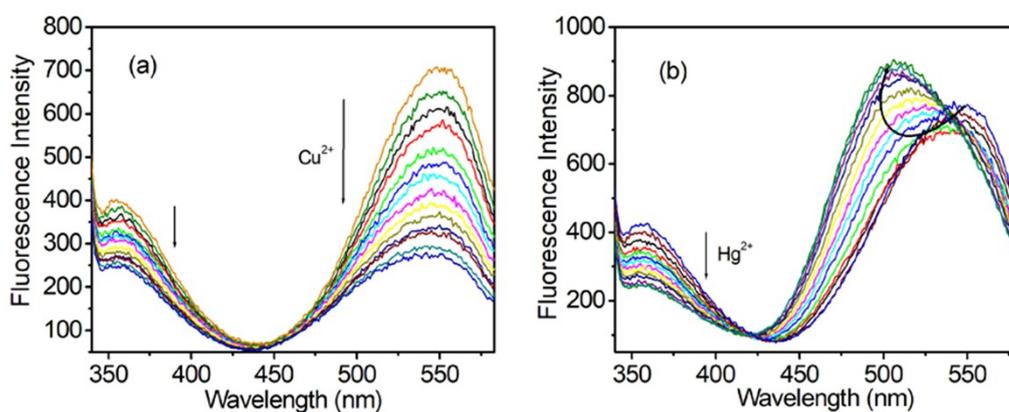
**Fig. S6** Absorption spectra of D-P4 (20.0  $\mu\text{M}$ ), D-P4-Hg (1/3 equiv.) and D-P4-Hg in the presence of Cys (1/3 equiv.)

**Fig. S7** Absorption spectra of D-P4 (20.0  $\mu\text{M}$ ), D-P4-Hg (1/3 equiv.) and D-P4-Hg in the presence of Cys (1/3 equiv.)

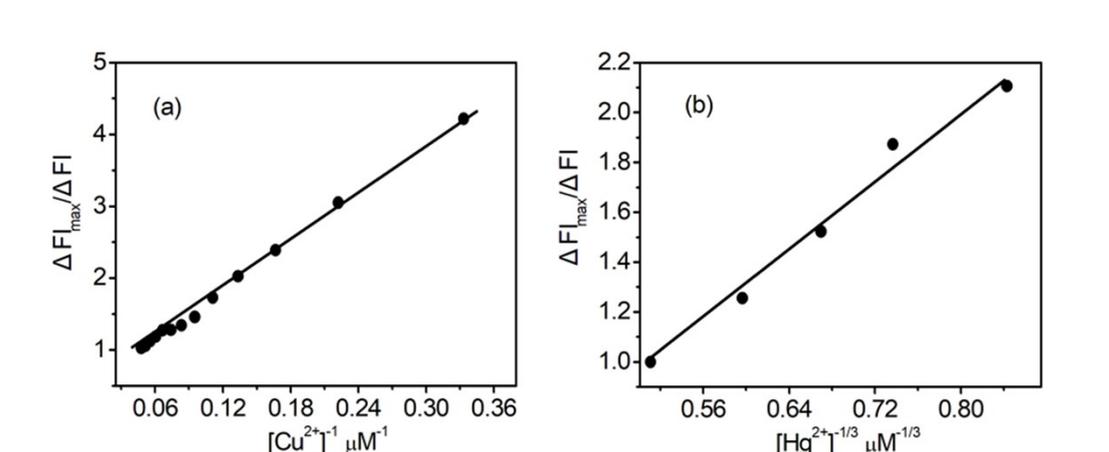
**Fig. S8** Linear relationship of emission intensity at 505 nm with the concentrations of Cys in 10 mM HEPES buffer solution at pH 7.1.



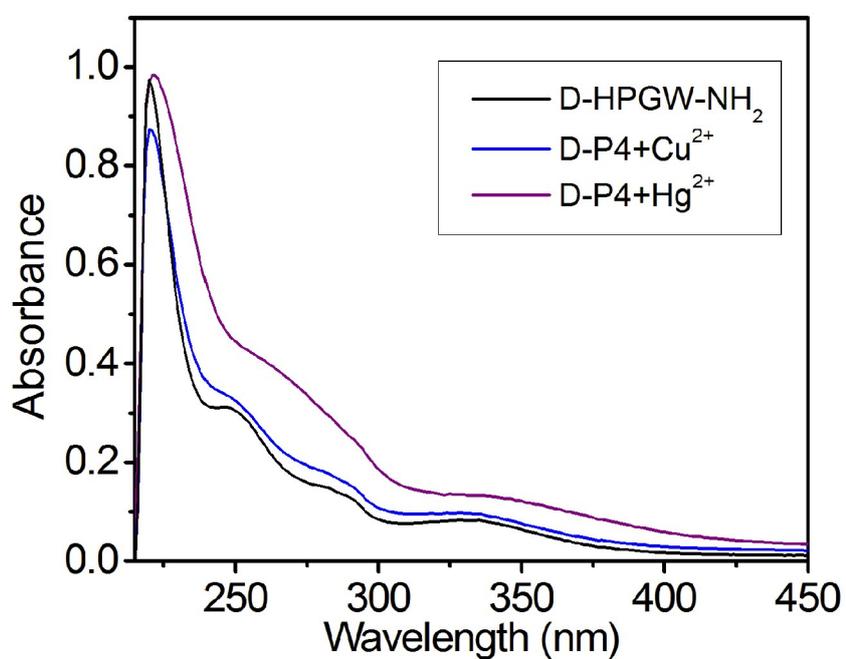
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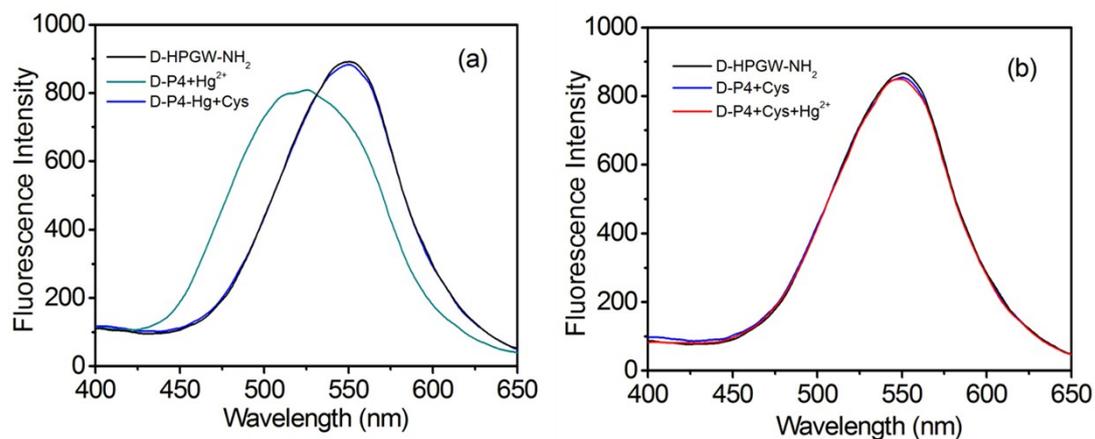
**Fig. S2** Fluorescence emission spectra of D-P4 (20.0  $\mu\text{M}$ ) excited at 295 nm with addition of increasing concentrations of  $\text{Cu}^{2+}$  (0-25.0  $\mu\text{M}$ ) (a) and  $\text{Hg}^{2+}$  (0-7.0  $\mu\text{M}$ ) (b) in 10 mM HEPES buffer at pH 7.1.



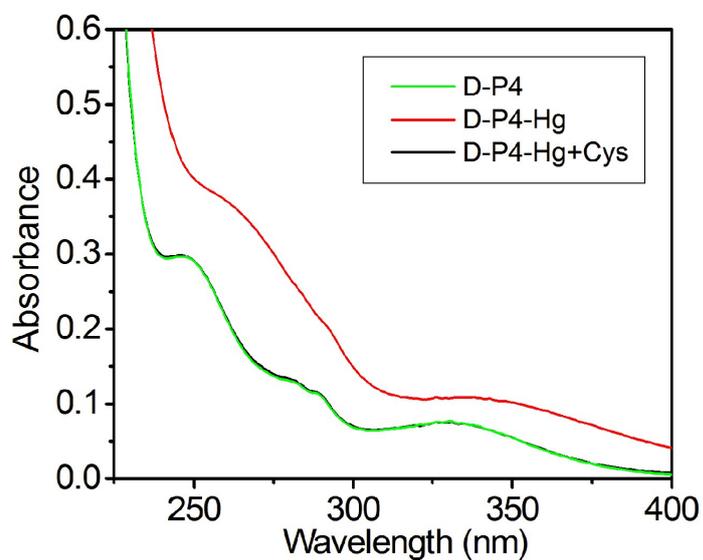
**Fig. S3** Benesi-Hildebrand plots for the determination of the binding constants of D-P5 (100.0  $\mu M$ ) with  $Cu^{2+}$  (a) and  $Hg^{2+}$  (b).



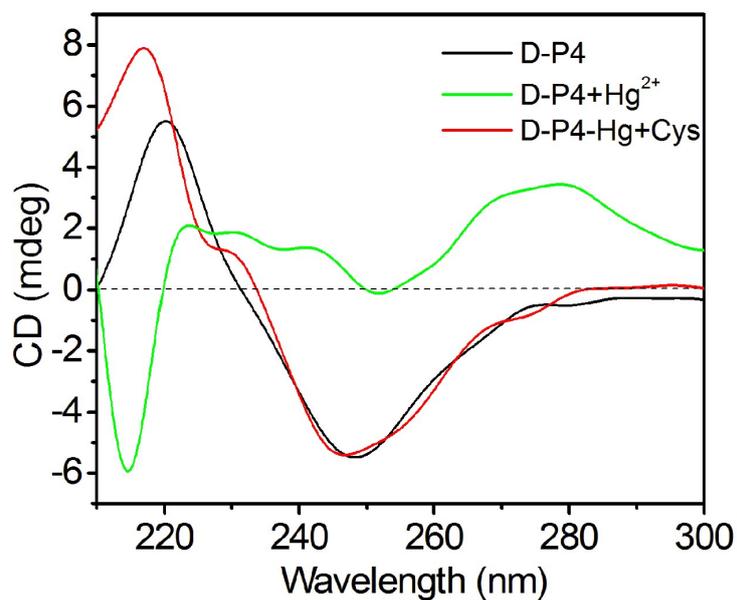
**Fig. S4** Absorption spectra of D-P4 (20.0  $\mu M$ ) in the absence and presence of  $Cu^{2+}$  (0.5 equiv.) and  $Hg^{2+}$  (0.5 equiv.) in 10 mM HEPES buffer solution at pH 7.1.



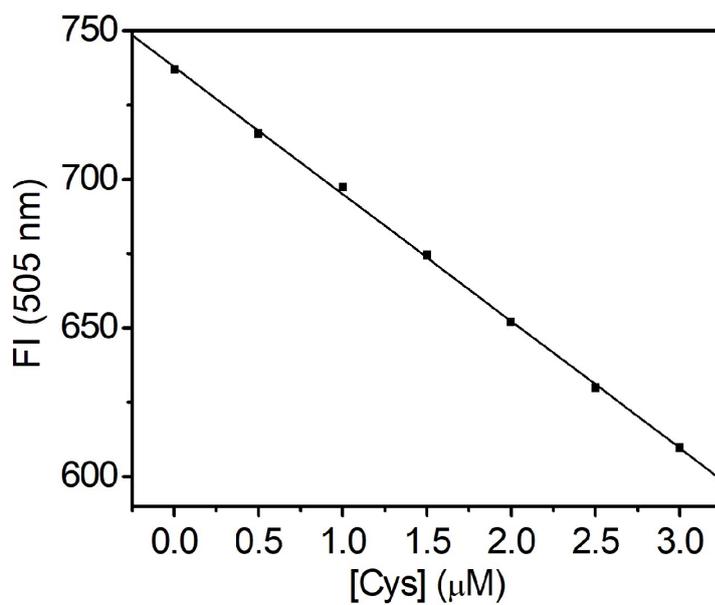
**Fig. S5** Fluorescence spectra of regeneration of D-P4-Hg (20.0  $\mu\text{M}$ ) system by Cys in 10 mM HEPES buffer solution. Hg<sup>2+</sup> (1/3 equiv.) and Cys (1/3 equiv.).



**Fig. S6** Absorption spectra of D-P4 (20.0  $\mu\text{M}$ ), D-P4-Hg (1/3 equiv.) and D-P4-Hg in the presence of Cys (1/3 equiv.)



**Fig. S6** CD spectra of D-P4 (20.0  $\mu\text{M}$ ), D-P4-Hg (1/3 equiv.) and D-P4-Hg in the presence of Cys (1/3 equiv.)



**Fig. S8** Linear relationship of emission intensity at 505 nm with the concentrations of Cys in 10 mM HEPES buffer solution at pH 7.1.