Supplementary data for

Highly selective and water-soluble peptidyl chemosensors for copper(II) and mercury(II) ions based on a β-hairpin structure

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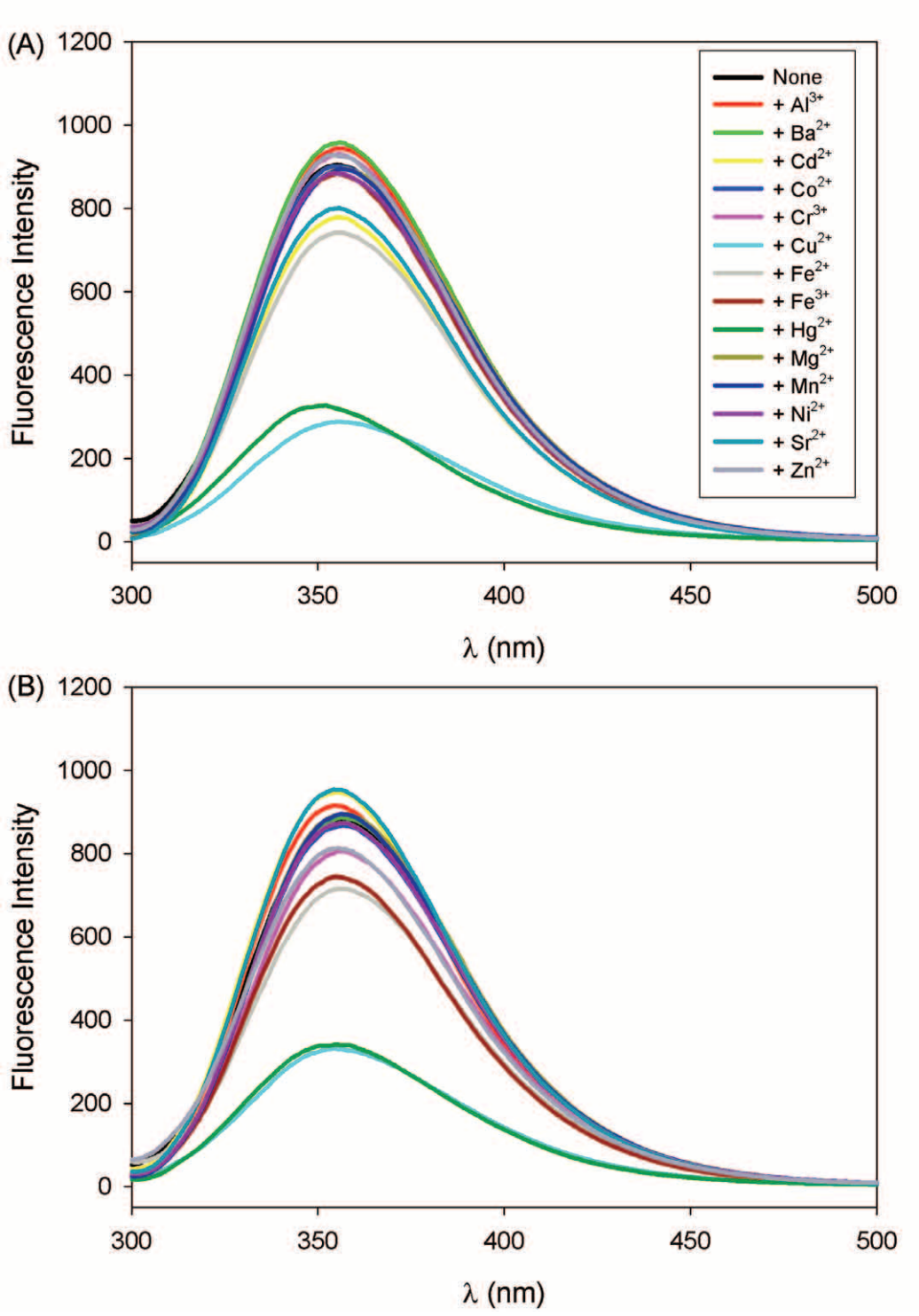


Fig. S1. Emission spectra for (A) **HP7-H2H11** and (B) **HP7-H1H12** in the presence of various metal ions. All measurements were conducted in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C) and the excitation wavelength was 280 nm. The peptide concentration was 10 μM and metal concentration was 20 μM.

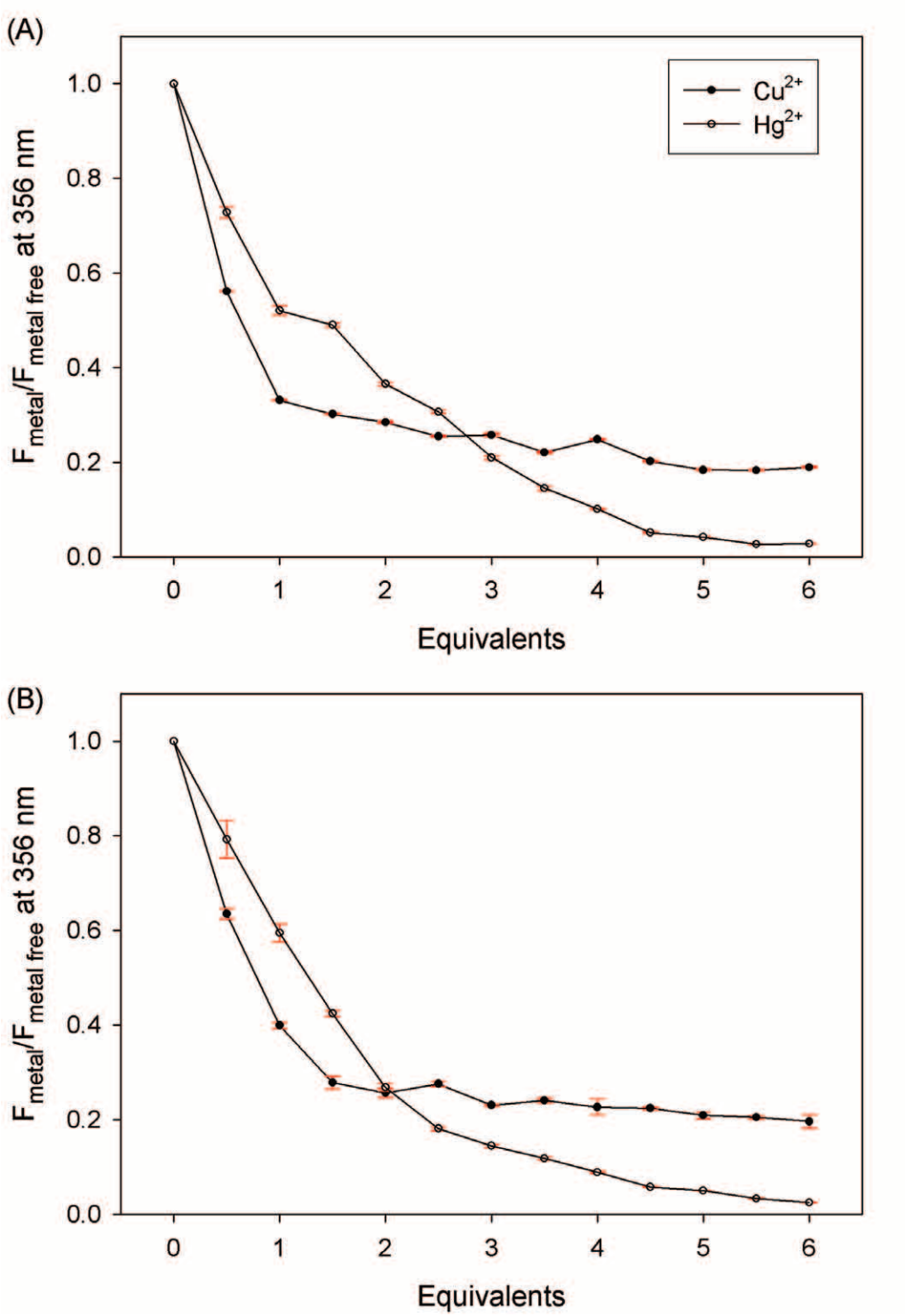


Fig. S2. Relative fluorescence intensity of (A) **HP7-H2H11** and (B) **HP7-H1H12** in the presence of different equivalents of Cu^{2+} or Hg^{2+}. Each data point was obtained by averaging three measurements and the error bars are in red. All measurements were conducted in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C) with a peptide concentration of 30 μM.

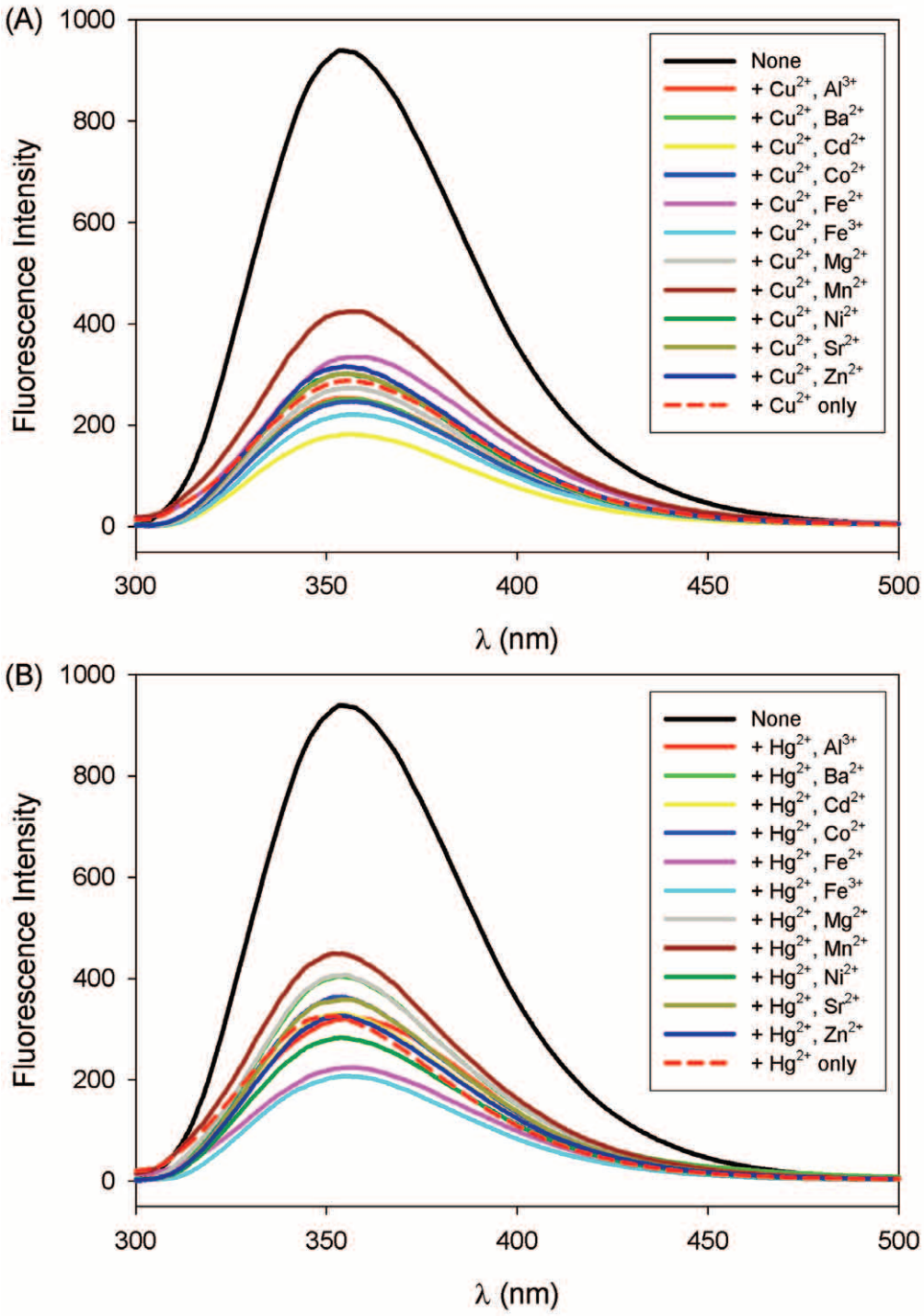


Fig. S3. Emission spectra of **HP7-H2H11** in the presence of (A) Cu^{2+} and other metal ions (B) Hg^{2+} and other metal ions. All measurements were conducted in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C) and the excitation wavelength was 280 nm. The concentrations of peptides and metals were 10 μM and 20 μM respectively.

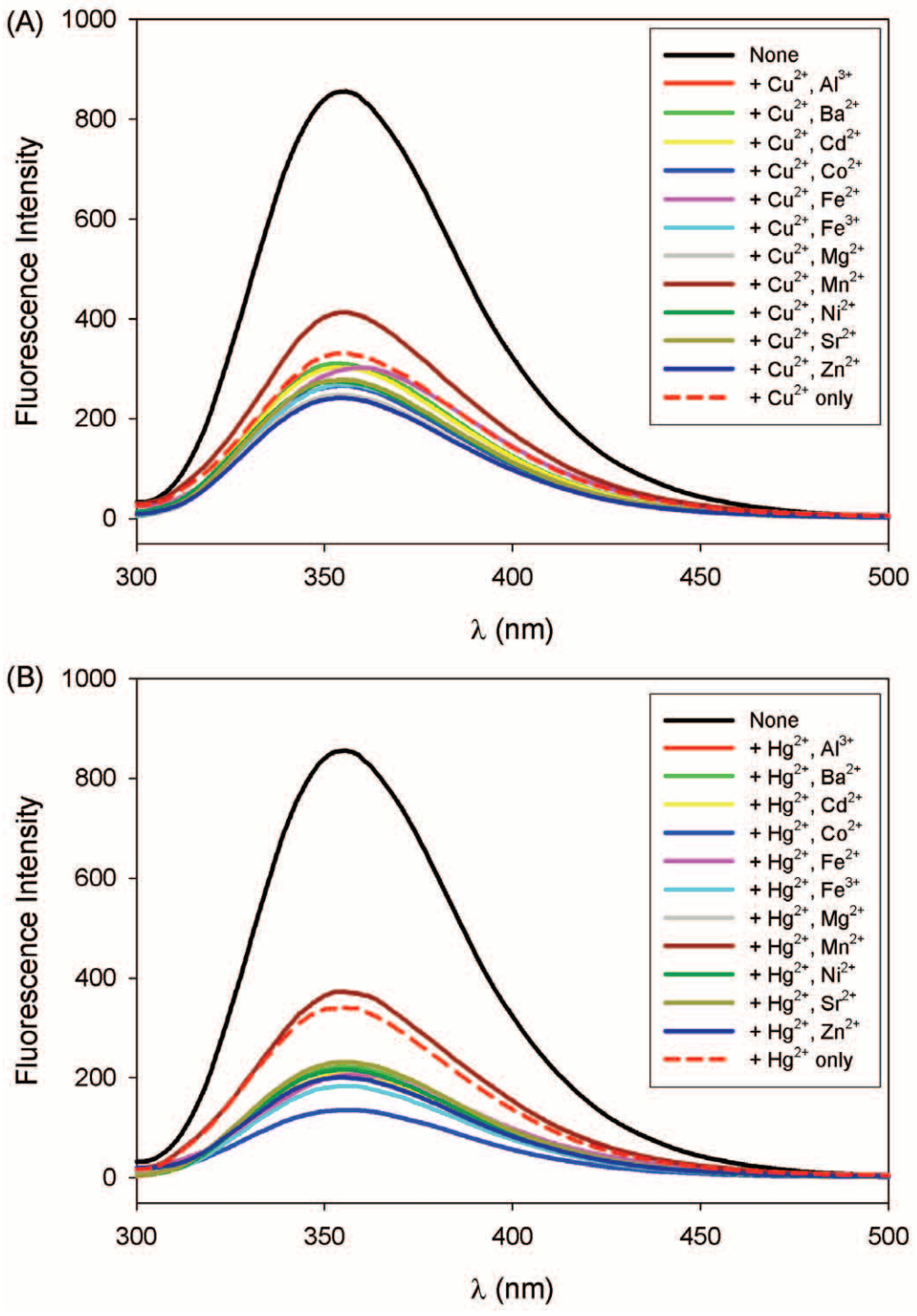


Fig. S4. Emission spectra of **HP7-H1H12** in the presence of (A) Cu^{2+} and other metal ions (B) Hg^{2+} and other metal ions. All measurements were conducted in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C) and the excitation wavelength was 280 nm. The concentrations of peptides and metals were 10 μM and 20 μM respectively.

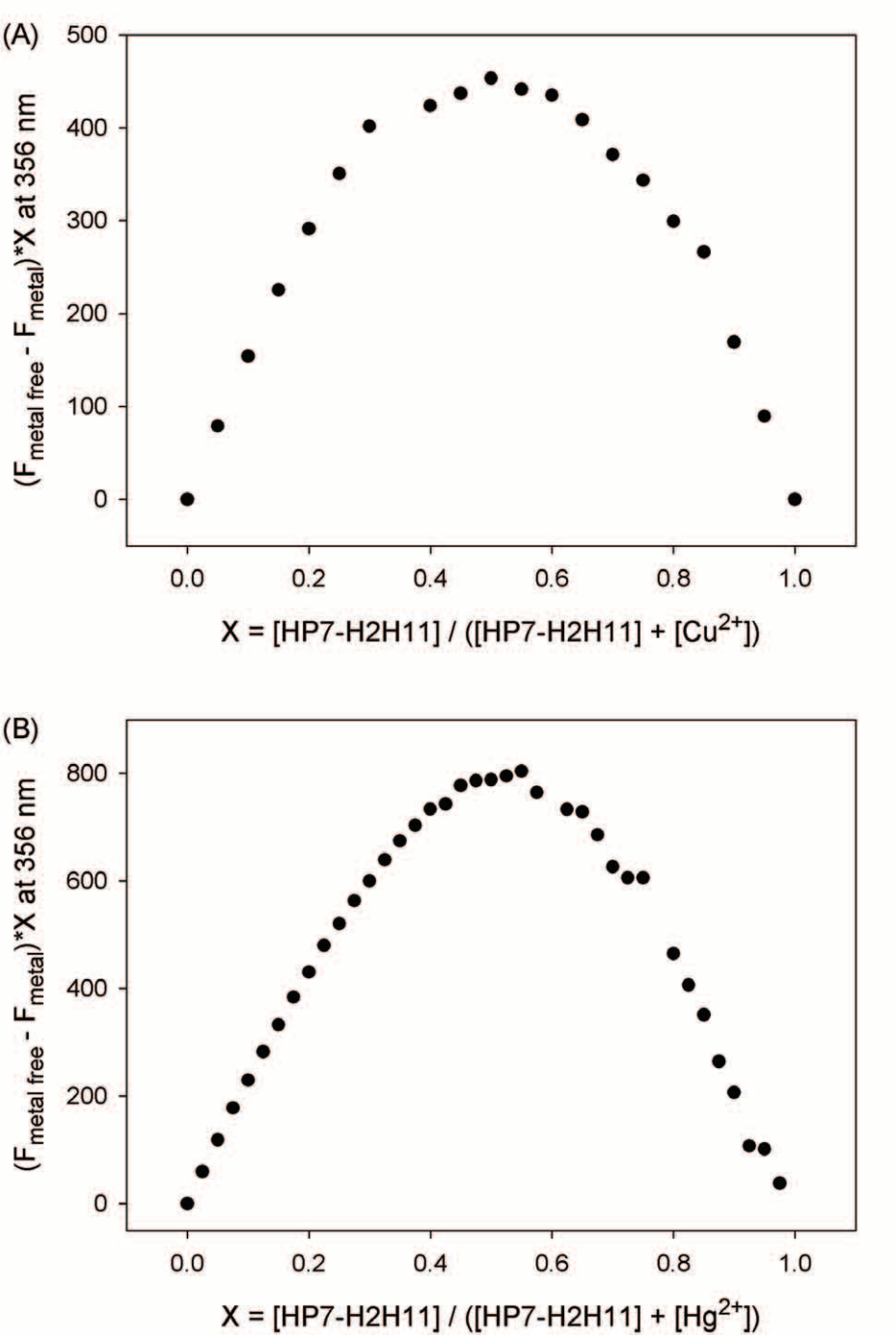


Fig. S5. Job's plots for **HP7-H2H11** with (A) Cu^{2+} and (B) Hg^{2+} in pH 7.5 and 20 mM phosphate buffer solution at ambient temperature (~ 25 °C).

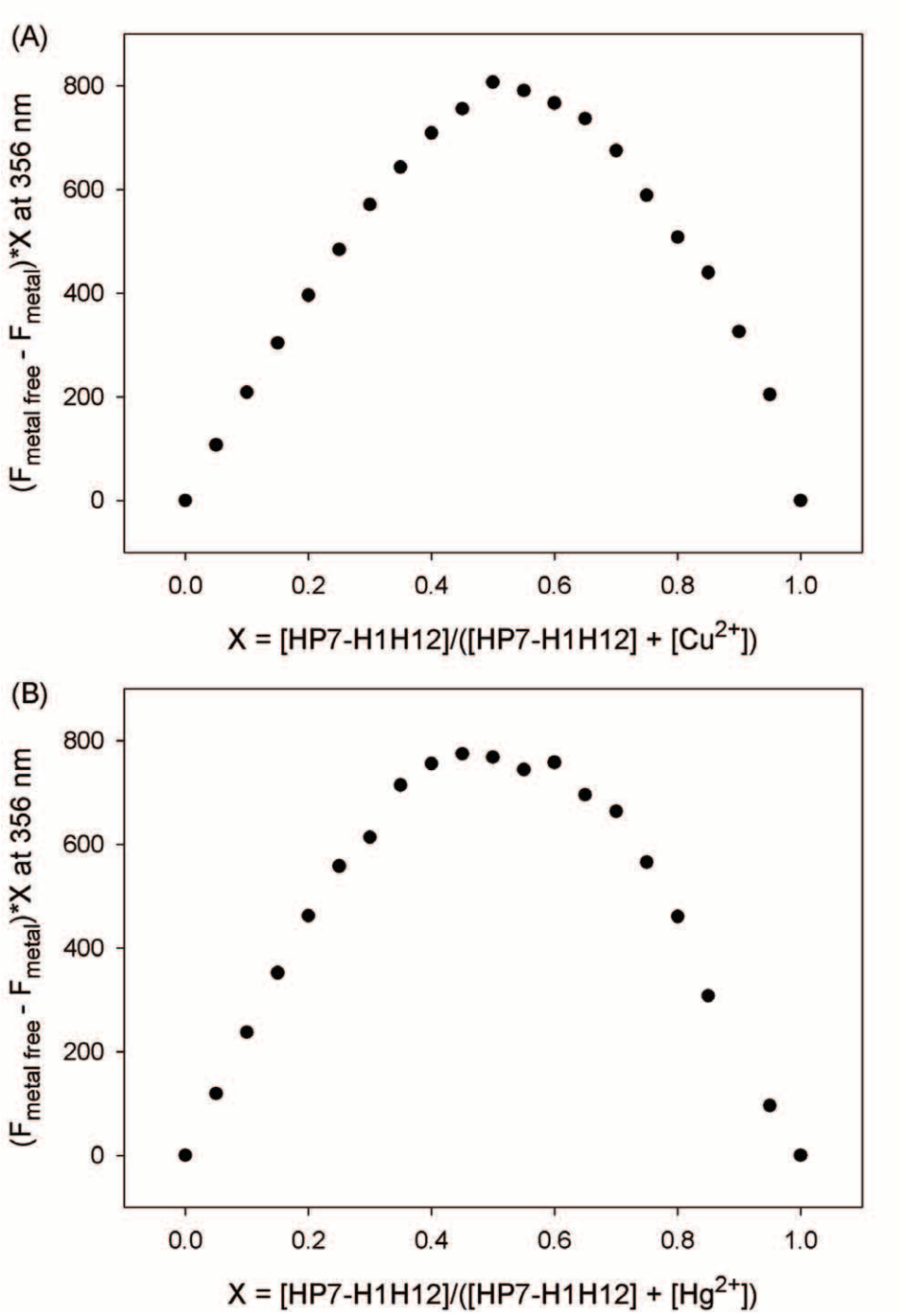
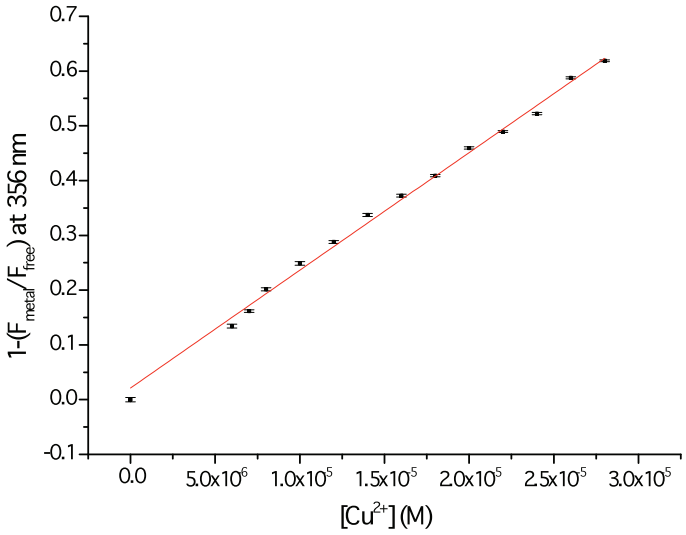


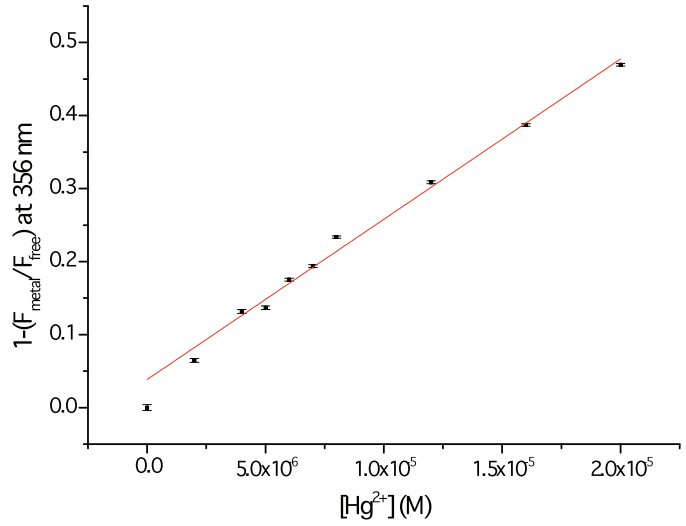
Fig. S6. Job's plots for **HP7-H1H12** with (A) Cu^{2+} and (B) Hg^{2+} in pH 7.5 and 20 mM phosphate buffer solution at ambient temperature (~ 25 °C).

(A)



Linear regression data, $y = a + mx$		
Parameter	Value	Error
a	0.0213	0.0073
m	21499.11	364.98
R^2	0.99627	
Standard deviation of blank measurements (σ)		0.00396

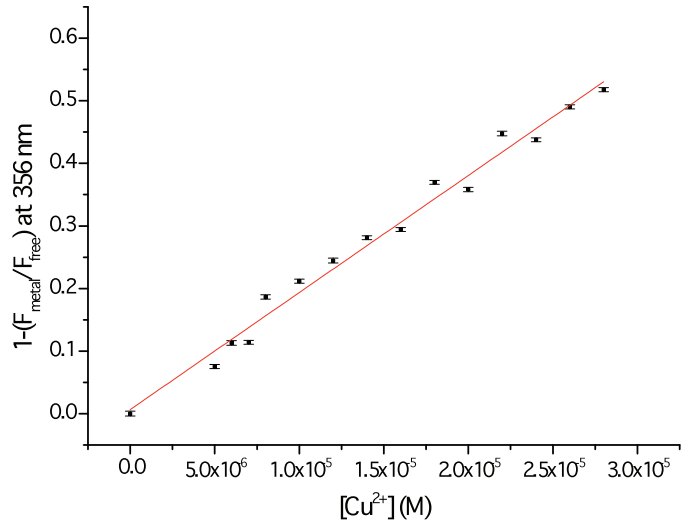
(B)



Linear regression data, $y = a + mx$		
Parameter	Value	Error
a	0.0384	0.0084
m	21946.57	713.73
R^2	0.99056	
Standard deviation of blank measurements (σ)		0.00396

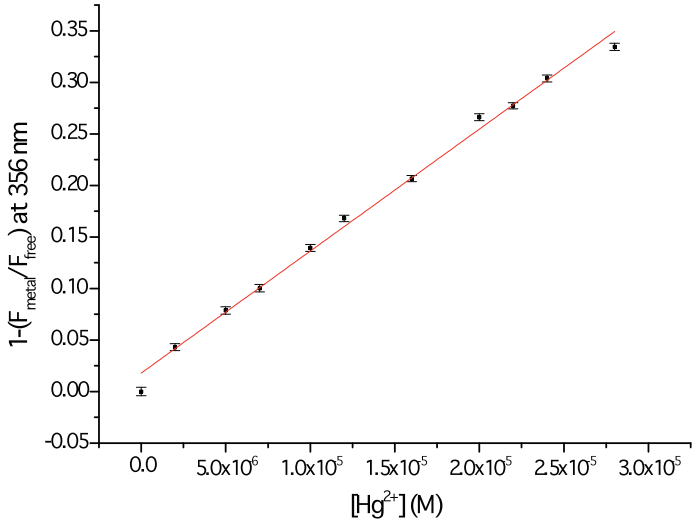
Fig. S7. Calibration curves of **HP7-H2H11** for the detection of (A) Cu^{2+} and (B) Hg^{2+} in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C). The peptide concentration was 30 μM and the excitation wavelength was 280 nm.

(A)



Linear regression data, $y = a + mx$		
Parameter	Value	Error
a	0.0066	0.0112
m	18700.92	667.46
R^2	0.98246	
Standard deviation of blank measurements (σ)		0.00390

(B)



Linear regression data, $y = a + mx$		
Parameter	Value	Error
a	0.0180	0.0049
m	11832.34	297.36
R^2	0.99372	
Standard deviation of blank measurements (σ)		0.00410

Fig. S8. Calibration curves of **HP7-H1H12** for the detection of (A) Cu^{2+} and (B) Hg^{2+} in pH 7.5 and 20 mM phosphate buffer at ambient temperature (~ 25 °C). The peptide concentration was 30 μM and the excitation wavelength was 280 nm.