

Sequential Ag^+ /Bi thiol and Synchronous Ag^+ / Hg^{2+} Biosensing with Zwitterionic Cu^{2+} -Based Metal–Organic Frameworks

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Table S1. Summary of Crystallographic Data for MOFs **1** and **2**

	1	2
Formula	C ₂₅ H ₃₅ CuN ₃ O ₁₅ S	C ₉₆ H ₆₈ Cu ₄ N ₁₂ O ₁₈ S ₂
FW	713.16	1995.90
Crystal system	triclinic	triclinic
Space group	<i>P</i> −1	<i>P</i> −1
<i>a</i> (Å)	11.944(4)	11.3364(11)
<i>b</i> (Å)	12.209(5)	22.492(2)
<i>c</i> (Å)	12.690(5)	24.752(2)
α (°)	108.719(8)	66.251(2)
β (°)	99.862(8)	88.427(2)
γ (°)	107.399(8)	82.262(2)
<i>V</i> (Å ³)	1597.7(10)	5721.8(10)
<i>Z</i>	2	2
ρ_{calc} , g cm ^{−3}	1.482	1.158
μ , mm ^{−1}	0.822	0.830
<i>F</i> (000)	742	2040
Total reflns.	21010	79117
Uniq. reflns.	7025	23033
Reflns. (<i>I</i> ≥ 2σ(<i>I</i>))	4970	12961
<i>R</i> _{int}	0.0704	0.0839
Parameters	409	1011
<i>R</i> ₁ ^{<i>a</i>}	0.0825	0.1198
<i>wR</i> ₂ ^{<i>b</i>}	0.2375	0.3433
<i>GOF</i> ^{<i>c</i>}	1.042	1.103
$\rho_{\text{max}}/\rho_{\text{min}}$, e Å ^{−3}	1.393/−0.912	0.981/−4.890

^{*a*} $R_I = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$, $GOF = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where *n* is the number of reflections and *p* is total number of parameters refined.

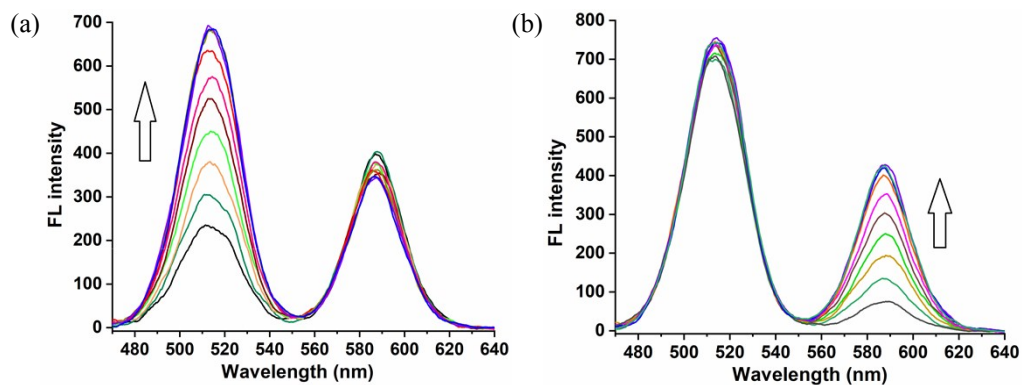


Figure S1. Fluorescence recovery of the P-DNAs@2 (50 nM/50 nM/5 μM) sensing system (a) at different concentrations of Hg^{2+} with the saturated concentration of Ag^+ and (b) at different concentrations of Ag^+ with the saturated concentration of Hg^{2+} .